MINIMAL ESTRADA INDICES OF THE TREES WITH A PERFECT MATCHING∗

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Abstract. Let \(H_n\) be the set of the trees having a perfect matching with \(n\) vertices. The ordering of the trees in \(H_n\) according to their minimal Estrada indices is investigated. The trees with the smallest and the second smallest Estrada indices among \(H_n\), with \(n \geq 6\), are obtained.

Key words. Estrada indices, Perfect matching, Trees.

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1. Introduction. Let \(G\) be a simple graph with a vertex set \(V(G)\), where \(|V(G)| = n\). Let \(\Phi(G, \lambda) = \text{det}[\lambda I - A(G)]\) be the characteristic polynomial of \(G\), where \(A(G)\) is the adjacency matrix of \(G\) and \(I\) the unit matrix of order \(n\) [4]. Denote by \(\lambda_1 \geq \cdots \geq \lambda_n\) the \(n\) roots of \(\Phi(G, \lambda) = 0\). Obviously, \(\lambda_1, \ldots, \lambda_n\) are all real numbers since \(A(G)\) is a real symmetric matrix. The Estrada index (EI) of \(G\), a newly proposed graph-spectrum-based invariant, is defined by [12]

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

(1.1)

Recall that 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 \(u, v \in V(G)\), let \(W_k(G; u, v)\) be the set of the \((u, v)\)-walks of length \(k\) in \(G\), and \(M_k(G; u, v)\) be the number of the elements in \(W_k(G; u, v)\). Similarly, let \(W_k(G; v)\) be the set of the \((v, v)\)-walks of length \(k\) in \(G\), and \(M_k(G; v)\) be the number of the elements in \(W_k(G; v)\). Let \(M_{2k}(G, u, [v])\) be the number of the close \((u, u)\)-walks of length \(2k\) starting at \(u\) and passing \(v\) in \(G\). 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

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k in $G$. From the Taylor expansion of $e^{\lambda_i}$, $EE(G)$ in (1.1) can be rewritten as

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

(1.2)

In particular, if $G$ is a bipartite graph, then $M_{2k+1}(G) = 0$ for $k \geq 0$. Hence, we have

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

(1.3)

Let $G_1$ and $G_2$ be two bipartite graphs of order $n$. If $M_{2k}(G_1) \geq M_{2k}(G_2)$ holds for any positive integer $k$, then $EE(G_1) \geq EE(G_2)$ and we denote $G_1 \succeq G_2$. 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 denote $G_1 \succ G_2$.

The EI has found numerical applications in biology, complex networks and chemistry. It was used to quantify the degree of folding of long-chain molecules, especially proteins. It was also shown that the EI provides a measure of the centrality of complex network. In addition, a connection between the EI and the concept of extended atomic branching was pointed out by Estrada et al. For some mathematical properties of EI, including the lower and upper bounds for it, one can refer to [2, 15, 17].

In addition to the ordinary Estrada index, defined in terms of the eigenvalues of the adjacency matrix, Eq. (1.1), several analogous graph invariants have recently been considered. Of these worth mentioning are the Laplacian and signless Laplacian Estrada indices, based on the eigenvalues of the Laplacian and signless Laplacian matrix, the resolvent Estrada index, based on the resolvent of the adjacency matrix, and the skew Estrada index of oriented graphs.

The characterization of graphs having the extremal Estrada indices (EIs) is an interesting problem and has been obtained successfully. For the characterization of the unicyclic graphs, the bicyclic graphs and the tricyclic graphs, etc., one can refer to [8, 23, 24, 25, 27]. 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, and the trees with a given number of pendant vertices, etc., one can refer to [7, 5, 6, 10, 21, 26]. Recently, Wang obtained the trees with the largest and the second largest Estrada indices among the set of trees with a perfect matching. From the references, one can find that many results are related to the graphs with the maximal EIs. However, until now, only a few results about the graphs having the minimal EIs have been obtained.

Recall that molecules with the Kekulé structures are molecular graphs with perfect matchings. Let $H_n$ be the set of trees with a perfect matching having $n$ vertices.
Obviously, $n$ is an even. In this paper, we will study the ordering of the trees in $\mathcal{H}_n$ in terms of their minimal EIs. Thus, we characterize the acyclic Kekuléan $\pi$-electron systems with the smallest and the second smallest EIs.

2. Transformations for studying the Estrada indices. To deduce the main results of this paper, Lemmas 2.1–2.4 are simply quoted here.

Let $v \in V(G)$, and $d_G(v)$ be the degree of $v$ of $G$. A pendant path at $v$ of $G$ is a path in $G$ connecting vertex $v$ and a pendant vertex such that all internal vertices (if exist) in this path have degree two and $d_G(v) \geq 3$.

**Lemma 2.1.** [21] Let $w$ be a vertex of the nontrivial connected graph $G$. For nonnegative integers $p$ and $q$, let $G(p, q)$ denote the graph obtained from $G$ by attaching at $w$ pendant paths $P = wv_1v_2 \cdots v_p$ and $Q = wu_1u_2 \cdots u_q$ 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 $H$.

**Lemma 2.2.** [9] Let $G$ and $H$ be two vertex-disjoint graphs with $u, v \in V(G)$ and $z \in V(H)$, where $|V(H)| \geq 2$. For each positive integer $k$, if $M_k(G; u) \geq M_k(G; v)$ and there exists at least one $k$ such that $M_k(G; u) > M_k(G; v)$ holds, then $EE(G(u) \cdot H(z)) > EE(G(v) \cdot H(z))$.

**Lemma 2.3.** [8, 22] Let $A$, $B$ and $C$ be three connected graphs, and each of which has at least two vertices. Let $u$ and $v$ be two different vertices of $C$, $u' \in V(A)$ and $v' \in V(B)$. Let $H = A(u') \cdot C(u), G = H(v') \cdot B(v')$ and $G' = H(u) \cdot B(v')$. Suppose that there exists an automorphism $\theta$ of $C$ such that $\theta(u) = v$, then

(i) $M_k(H, u) \geq M_k(H, v)$ for all positive integer $k$ and it is strict for some positive integer $k_0$;

(ii) $M_k(G') \geq M_k(G)$ for all positive integer $k$ and it is strict for some positive integer $k_0$.

**Lemma 2.4.** [7] Let $u$ be a non-isolated vertex of a simple graph $H$. If $H_1$ and $H_2$ are the graphs obtained from $H$ by identifying an end vertex $v_1$ and an internal vertex $v_2$ of the path $P_{n+b+1}$ with $u$, respectively (see Figs. 2.1(a) and 2.1(b)), then $M_{2k}(H_2) > M_{2k}(H_1)$ for $n \geq 3$ and $k \geq 2$.

3. The smallest and the second smallest trees with the minimal Estrada indices in $\mathcal{H}_n$. In this section, we study the ordering of the trees in $\mathcal{H}_n$ according to their minimal EIs. Some definitions are introduced first.

We classify $\mathcal{H}_n$ into three subsets $\mathcal{H}_n^1$, $\mathcal{H}_n^2$ and $\mathcal{H}_n^3$, where $\mathcal{H}_n^1$ is the subset of
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\( H \) in which there exists at most one vertex having degree 3 and all other vertices having degrees 2 or 1; \( H_n^2 \) is the subset of \( H_n \) in which there exists at least one vertex having degree greater than 3; and \( H_n^3 \) is the subset of \( H_n \) in which there exist at least two vertices having degrees 3 and all other vertices having degrees 2 or 1. Obviously, \( H_n = H_n^1 \cup H_n^2 \cup H_n^3 \).

Let \( lT_r^b \) be the tree obtained by attaching three pendant paths of length \( l \), \( r \) and \( b \) at a common vertex \( u \), where \( l + r + b + 1 = n \), \( l \) and \( r \) are even with \( l, r \geq 0 \) and \( b \) is odd with \( b \geq 1 \). Specially, if at least one of \( l \) and \( r \) is 0, then \( lT_r^b \) is the path \( P_n \).

Obviously, \( lT_r^b \) has a perfect matching. By the definition of \( H_n^1 \), if \( T \in H_n^1 \), then \( T \) is \( lT_r^b \). For example, \( lT_r^b \) is shown in Fig. 3.1.

Let \( G \) in Lemma 2.1 be \( P_{b+1} \). Repeatedly using Lemma 2.1, we can obtain Corollary 3.1.

**Corollary 3.1.** \( lT_r^b > lT_r^{b+1} > \ldots > lT_{n-l-3} > lT_{n-l-2} \sim P_n \), where \( r \geq l \geq 2 \) and \( b \geq 1 \).

Let \( G \) in Lemma 2.1 be \( P_{l+1} \). Repeatedly using Lemma 2.1 we get Corollaries 3.2 and 3.3.

**Corollary 3.2.** \( lT_r^b > lT_{r+1}^{b+1} > \ldots > lT_{n-l-3} > lT_{n-l-2} > lT_{n-l-1} \sim P_n \), where \( b > r \geq 2 \).

**Corollary 3.3.** \( lT_r^b > lT_{r+1}^{b+1} > \ldots > lT_{n-l-3} > lT_{n-l-2} > lT_{n-l-1} \sim P_n \), where \( r > b \geq 1 \).
3.6 is thus proved.

Let \( H_n \) be the complete ordering of the trees in \( H_n \) in terms of their minimal EIs.

**Theorem 3.5.** For \( t T'_n \in H_n \) with \( n \geq 8 \), we have the ordering as follows.

(i) As \( n = 4h \) with \( h \geq 2 \), \( T_4^2 \succ T_4^3 \succ T_4^4 \succ \cdots \succ T_4^n \geq T_4^{n-3} \geq T_4^{n-4} \geq T_4^{n-5} \simeq P_n \).

(ii) As \( n = 4h + 2 \) with \( h \geq 2 \), \( T_4^2 \succ T_4^3 \succ T_4^4 \succ \cdots \succ T_4^n \geq T_4^{n-3} \geq T_4^{n-4} \geq T_4^{n-5} \simeq P_n \).

**Proof.** As \( n \geq 8 \), by Corollary 3.3, we get \( T_4^n \geq T_4^{n-3} \simeq P_n \). In Corollary 3.1 let \( b = 1 \). Using Corollary 3.1 repeatedly, we obtain Theorem 3.5.

From Corollaries 3.1 and 3.2 we obtain the first four trees in \( H_n \) with the minimal EIs in Theorem 3.6.

**Theorem 3.6.** Let \( T \in H_n \setminus \{ P_n, T_2, T_3^6 \} \) and \( n \geq 8 \). We have

\[
T \geq T_2 \geq T_3^6 \geq T_2 \geq T_3^6 \geq T_2 \geq T_3^6 \geq T_2 \simeq P_n,
\]

where \( EE(T_2^n) = EE(T_2^n) \) if and only if \( n = 8 \).

**Proof.** As \( n \geq 8 \), it follows directly from Corollary 3.3 (let \( l = 2 \)) that \( T_2^n \geq T_2 \geq T_2 \geq T_2 \geq T_2 \geq T_2 \simeq P_n \), where \( EE(T_2^n) = EE(T_2^n) \) if and only if \( n = 8 \).

Next, let \( T_2^n \in H_n \) and \( n \geq 8 \). As \( b \geq 3 \) and \( n \geq 8 \), we will prove

\[
T_2^n \geq T_2^n \geq T_2^n \geq T_2^n \geq T_2^n \geq T_2^n \geq T_2^n \geq T_2^n \simeq P_n.
\]

In \( T_2^n \), we have \( l, r \geq 2 \) since \( T_2^n \not\simeq P_n \). We assume \( r \geq l \geq 2 \). As \( l = 2 \), we have \( r \geq 4 \) since \( T_2^n \not\simeq T_2^n \). Thus, as \( r \geq 4 \) and \( b \geq 3 \), \( 3.1 \) follows from Corollary 3.3 directly. As \( l \geq 4 \), we have \( r \geq l \geq 4 \). It follows from Corollary 3.3 that \( T_2^n \geq T_2^n \geq T_2^n \geq T_2^n \geq T_2^n \simeq P_n \). Since \( l + r - 2 \geq 6 \) and \( b \geq 3 \), by Corollary 3.3 we get \( T_2^n \geq T_2^n \geq T_2^n \simeq P_n \). Therefore, we have \( T_2^n \geq T_2^n \geq T_2^n \). Namely, \( 3.1 \) holds. Theorem 3.6 is thus proved.

**Lemma 3.7.** If \( H_1 \) (see Fig. 2.1(a)) in Lemma 2.4 has a perfect matching, then \( H_1 \) (see Fig. 2.1(b)) has a perfect matching too.
Proof. If $H_2$ has a perfect matching, then the vertex $u$ of $H_2$ (as shown in Fig. 2.1(a)) must be matched with another vertex (denoted by $w$) of $H_2$. If $w \in V(H) \setminus \{u\}$, then $a$ and $b$ are even. If $w \not\in V(H)$, then one of $a$ and $b$ is odd and the another is even. We can easily check that $H_1$ has a perfect matching too.

By Lemmas 3.4 and 3.7, we obtain Corollary 3.8 as follows.

**Corollary 3.8.** Let $T \in \mathcal{H}_n$ with $n \geq 6$. In $T$, if there exists an vertex (denoted by $u$) satisfying that $d_T(u) \geq 3$ and there are two pendant paths attaching at $u$ of $T$, then we have another tree $T' \in \mathcal{H}_n$ satisfying $d_{T'}(u) = d_T(u) - 1$ and $EE(T) > EE(T')$.

From Corollary 3.8, we deduce Lemmas 3.9 and 3.10 as follows.

**Lemma 3.9.** If $T \in \mathcal{H}_n^2$, then there exists a tree $T_1 \in \mathcal{H}_n^2$ (see Fig. 3.2(a)) such that $EE(T) \geq EE(T_1)$, with the equality if and only if $T \cong T_1$.

**Proof.** Let $T \in \mathcal{H}_n^2$. By the definition of $\mathcal{H}_n^2$, we get that $T$ has at least one vertex having degree greater than 3.

Case (i): Only one vertex of $T$ (denoted by $u$) has degree greater than 3.

Subcase (i.i): All the degrees of the vertices in $V(T) \setminus \{u\}$ are 2 or 1.

Obviously, $u$ of $T$ is attached by $d_T(u)$ pendant paths of $T$. Using Corollary 3.8 ($d_T(u) - 4$) times on $u$ of $T$, we get Lemma 3.9.

Subcase (i.ii): There exist $k \geq 1$ vertices in $V(T) \setminus \{u\}$ having degree 3.

We can choose one vertex (denoted by $s$) of $T$ such that $d_T(s) = 3$ and $s$ is attached by two pendant paths of $T$. By Corollary 3.8, we get $EE(T) > EE(T')$, where $T' \in \mathcal{H}_n^2$, $d_T(s) = 2$, and $T'$ has $k - 1$ vertices having degree 3. Repeatedly using the same procedure, we obtain $EE(T') \geq EE(T'''')$, where $T''' \in \mathcal{H}_n^2$, $T'''$ has only one vertex $u$ having degree greater than 3 and all other vertices of $T'''$ having degrees 2 or 1. Furthermore, by the proof of Subcase (i.ii), we can get that there exists a tree $T_1 \in \mathcal{H}_n^2$ with $EE(T'''') \geq EE(T_1)$. Thus, we obtain $EE(T) > EE(T_1)$.

Case (ii): There exist $k \geq 2$ vertices of $T$ having degrees greater than 3.

In this case, we can choose one vertex (denoted by $w$) of $T$ such that $d_T(w) \geq 3$ and $w$ is attached by ($d_T(w) - 1$) pendant paths. Repeatedly using Corollary 3.8 ($d_T(w) - 2$) times on $w$ of $T$, we get a new tree $T' \in \mathcal{H}_n^2$ satisfying $d_{T'}(w) = 2$ and $EE(T) > EE(T')$. Repeatedly using the same procedure, we can obtain a tree $T''' \in \mathcal{H}_n^2$ such that $EE(T') \geq EE(T'''')$, where $T'''$ has only one vertex having degree greater than 3 and all other vertices of $T'''$ having degrees 2 or 1. Furthermore, by the proof of Subcase (i.ii), we can get that there exists a tree $T_1 \in \mathcal{H}_n^2$ with
$EE(T^n) \geq EE(T_1)$. Thus, we obtain $EE(T) > EE(T_1)$. \qed

![Diagram](image)

**Fig. 3.2.** (a) $T_1: \sum_{i=1}^{4} a_i = n - 1$ with $a_i \geq 1$. (b) $T_2: \sum_{i=1}^{5} a_i = n - 1$ with $a_i \geq 1$.

**Lemma 3.10.** If $T \in \mathcal{H}_n^3$, then there exists a tree $T_2 \in \mathcal{H}_n^3$ (see Fig. 3.2(b)) such that $EE(T) \geq EE(T_2)$, with the equality if and only if $T \cong T_2$.

**Proof.** Let $T \in \mathcal{H}_n^3$. We get that $T$ has at least two vertices having degree 3 and all other vertices of $T$ having degrees 2 or 1. If $T$ has two vertices (denoted by $u$ and $v$) having degree 3, then $T \cong T_2$. If $T$ has at least three vertices having degree 3, then by the methods similar to those for Subcase (i.ii) in Lemma 3.9, we get Lemma 3.10.\qed

In $T_2$, if $a_1 = a_2 = a_3 = a_4 = 2$, then we denote $T_2$ by $I_n$.

**Theorem 3.11.** Let $T \in \mathcal{H}_n^2$ and $n \geq 10$, we have $T \succ T_{3}^{n-6}$ or $T \succ I_n$.

**Proof.** Let $T \in \mathcal{H}_n^2$ and $n \geq 10$. By Lemma 3.9, there exists a tree $T_1$ such that $T_1 \in \mathcal{H}_n^2$ and $T \cong T_1$. Since $T_1$ has a perfect matching, in $T_1$, only one of $a_i$ ($1 \leq i \leq 4$) is odd. We assume that $a_1$ is odd. Therefore, $a_2, a_3$, and $a_4$ are even. We let $a_1 \geq a_3 \geq a_2 \geq 2$. Two cases are considered as follows.

**Case (i):** At least one of $a_2, a_3$ and $a_4$ is not less than 4.

Without loss of generality, we let $a_4 \geq 4$. Since $a_4 \geq a_3 \geq 2$, by Corollaries 3.8 and 3.1, $T_1 \succ T_{a_4} \succ T_{a_3} \geq T_{a_1} \succ T_{a_2}$. Since $a_1 + a_2 \geq 3$ and $a_3 + a_4 - 2 \geq 4$, $2^{a_1 + a_2} \geq T_{a_3} \succ I_n$ follows from Corollary 3.3. In conclusion, we get $T \geq T_1 \succ T_{3}^{n-6}$.

**Case (ii):** $a_2 = a_3 = a_4 = 2$.

Let $C$ in Lemma 2.3 be $P_{n-4} = v_1v_2v_3v_{n-4}$, $u$ in Lemma 2.3 be $v_3$ of $P_{n-4}$, and $v$ in Lemma 2.3 be $v_{n-6}$ of $P_{n-4}$. In $C$, we can check that there exists an automorphism $\theta$ such that $\theta(u) = v$. Let $H = P_{n-4}(v_3) \cdot P_3(v_0)$, where $P_3 = v_0v_1v_2$. Since $T_1 \cong H(u) \cdot P_3(v_0)$ and $I_n \cong H(v) \cdot P_3(v_0)$, by Lemma 2.3, we obtain $T_1 \succ I_n$ as $n \geq 10$. Therefore, $T \geq T_1 \succ I_n$ as $n \geq 10$. \qed
To obtain the tree with the minimal EI in $H_n^4$, we introduce Lemmas 3.12 and 3.13 first. Two trees $J_n$ and $K_n$ are introduced. In $T_2$, if $a_1 = a_2 = a_3 = 2$ and $a_4 = 4$, then we denote $T_2$ by $J_n$. In $T_2$, if $a_2 = a_3 = 2$ and $a_1 = a_4 = 4$, then we denote $T_2$ by $K_n$.

Fig. 3.3. (a) $2T^2_{n-7}$. (b) $2T^4_{n-9}$.

**Lemma 3.12.** As $n \geq 12$, we have $J_n > I_n$.

**Proof.** For simplicity, let $H$ be $2T^2_{n-7}$ (see Fig. 3.3(a)), where $n \geq 12$. In $2T^2_{n-7}$, let $u, v, w$, and $w'$ with $1 \leq i \leq 5$ be the eight vertices, as shown in Fig. 3.3(a). Next, we prove

$$M_k(H; u) \geq M_k(H; v)$$

holds for all $k \geq 0$ and there exists a $k_0 \geq 0$ such that $M_{k_0}(H; u) > M_{k_0}(H; v)$.

Let $H_1$ be one of the two components of $H - \{uw\}$ which contains the vertex $v$ of $H$, namely, $H_1$ is the path $P_4 = wvw_2w_1$. Similarly, let $H_2$ be one of the two components of $H - \{uv\}$ which contains the vertex $u$ of $H$. We can easily check that $H_1$ is isomorphic to a subgraph (denoted by $H'_2$) of $H_2$, where $H'_2$ is the path $P_4 = w_4w_3wv$. Obviously, for all $k \geq 0$, $M_k(H'_2; u) = M_k(H_2; v)$. Thus, for all $k \geq 0$, we have

$$M_k(H_2; u) = M_k(H'_2; u) + M_k(H_2; u, [w])$$

$$
\geq M_k(H_1; v)
$$

(3.3)

$$M_k(H; u) = M_k(H; u, [v]) + M_k(H_2; u)$$

since $M_k(H_2; u, [w]) \geq 0$. As $k = 6$, we can check that $M_k(H_2; u, [w]) = 1 > 0$. Therefore, $M_k(H_2; u) > M_k(H_1; v)$. Namely, there exist a $k_0$ such $M_{k_0}(H_2; u) > M_{k_0}(H_1; v)$. By the methods similar to those for (3.3), we can prove $M_k(H_2; u, w) \geq M_k(H_1; v, w)$ for all $k \geq 0$.

As $k \geq 0$, we obtain

$$M_k(H; v) = M_k(H; v, [u]) + M_k(H_1; v),$$

(3.4)

$$M_k(H; u) = M_k(H; u, [v]) + M_k(H_2; u).$$

(3.5)
From (3.3) and (3.5), to obtain (3.2), we only need to prove
\[ M_k(H; u, [v]) \geq M_k(H; v, [u]) \]
since (5.33) holds.

For an arbitrary \( W \in \mathcal{W}_k(H; v, [u]) \), we decompose \( W \) into \( W_1W_2 \), where \( W_1 \) is the shortest \((v, u)-\)section of \( W \) (consisting of a \((v, w)\)-walk in \( H_1 \) and a single edge \( wu \)), and \( W_2 \) is the remaining \((u, v)\)-section of \( W \). Thus, we get

\[ M_k(H; v, [u]) = \sum_{k_1 + k_2 = k} M_{k_1-1}(H_1; v, w)M_{k_2}(H; u, v). \]

Similarly,

\[ M_k(H; u, [v]) = \sum_{k_1 + k_2 = k} M_{k_1-1}(H_2; u, w)M_{k_2}(H; v, u). \]

For all even \( k_2 \geq 0 \), obviously \( M_{k_2}(H; u, v) = M_{k_2}(H; v, u) \). Since for all \( k_1 \geq 0 \), \( M_{k_1-1}(H_2; u, w) \geq M_{k_1-1}(H_1; v, w) \), it follows from (3.6) and (3.7) that
\[ M_k(H; u, [v]) \geq M_k(H; v, [u]). \]

Furthermore, by (3.3), (3.4), and (3.5), we get (3.2).

Obviously, \( J_n \cong H(u) \cdot P_3(v_0) \) and \( I_n \cong H(v) \cdot P_3(v_0) \), where \( P_3 = v_0v_1v_2 \). Thus, by Lemma 2.2, we obtain Lemma 3.13.

**Lemma 3.13.** As \( n \geq 14 \), we have \( K_n \gg J_n \gg I_n \).

**Proof.** For simplicity, let \( Q \) be \( 2T_{n-9}^4 \) (see Fig. 3.3(b)), where \( n \geq 14 \). In \( 2T_{n-9}^4 \), let \( u, v, w \), and \( w_i \) with \( 1 \leq i \leq 5 \) be the eight vertices, as shown in Fig. 3.3(b). By the methods similar to those for (3.3) in Lemma 3.12, we can prove \( M_k(Q; u) \geq M_k(Q; v) \) for all \( k \geq 0 \) and there exists a \( k_0 = 6 \) such that \( M_{k_0}(Q; u) > M_{k_0}(Q; v) \).

Obviously, \( K_n \cong Q(u) \cdot P_3(v_0) \) and \( J_n \cong Q(v) \cdot P_3(v_0) \), where \( P_3 = v_0v_1v_2 \). By Lemma 2.2, we get \( K_n > J_n \) as \( n \geq 14 \). Furthermore, by Lemma 3.12, we obtain Lemma 3.13.

Let \( H_{n_1}^{3,1} = \{ T \in H_{n_1}^3 \mid \exists T_2 \text{ such that } T \supseteq T_2 \text{ and } T_2 \text{ has } a_1 = a_3 = 1 \text{ and } a_2, a_4 \geq 2 \} \) and \( H_{n_1}^{3,2} = H_{n_1}^3 \setminus H_{n_1}^{3,1} \). By Lemmas 3.10, 3.13, we get Theorem 3.14 as follows.
Theorem 3.14. Let $T \in H_n^3$ and $n \geq 14$.

(i) If $T \in H_n^{3,1}$, then $T \succ T_1^{n-4}$.

(ii) If $T \in H_n^{3,2}$, then $T \succ T_{n-5}^2$ or $T \succeq I_n$.

Proof. (i) $T \in H_n^{3,1}$ with $n \geq 14$.

If $T \in H_n^{3,1}$, then by Lemma 3.10, there exists a tree $T_2$ such that $T_2 \in H_n^3$ and $T \succeq T_2$. Furthermore, by the definition of $H_n^{3,1}$, $T_2$ (see Fig. 3.2(b)) has $a_1 = a_3 = 1$. Since $T_2$ has a perfect matching, $a_2$ and $a_4$ of $T_2$ must be even with $a_2, a_4 \geq 2$. As $a_3 + a_4 + a_5 \geq 4$, by Corollaries 3.8 and 3.1, we obtain $T_2 \succ a_2^2 I_1^4 \succeq T_1^{n-4}$. Thus, Theorem 3.14(i) holds.

(ii) $T \in H_n^{3,2}$ with $n \geq 14$.

If $T \in H_n^{3,2}$, then by Lemma 3.10, there exists a tree $T_2$ such that $T_2 \in H_n^3$ and $T \succeq T_2$. Since $T_2$ has a perfect matching, all $a_i$ $(1 \leq i \leq 4)$ of $T_2$ are even or at most two of $a_i$ $(1 \leq i \leq 4)$ are odd. Two cases are considered as follows.

Case (i): All $a_i$ of $T_2$ are even with $a_i \geq 2$, where $1 \leq i \leq 4$.

Subcase (i.i): At least one of $a_1 + a_2$ and $a_3 + a_4$ is not less than 8.

We assume $a_1 + a_2 \geq 8$. Since $a_1 + a_2 - 2 \geq 6$ and $a_3 + a_4 + a_5 \geq 5$, by Corollaries 3.8 and 3.1, we obtain $T_2 \succ a_1^2 I_2^4 \succeq T_2^2 \succeq T_1^2$. Thus, we have $T \succ T_2 \succ T_3^6 \succeq T_{n-5}^2$ (by Corollary 3.3).

Subcase (i.ii): $a_1 + a_2$ and $a_3 + a_4$ are less than 8.

If $a_1 + a_2 = 4$ and $a_3 + a_4 = 4$, then $T_2 \succeq I_n$, namely $T \succeq T_2 \succeq I_n$. If $a_1 + a_2 = 4$ and $a_3 + a_4 = 6$ or $a_1 + a_2 = 6$ and $a_3 + a_4 = 4$, then $T_2 \succeq J_n$. By Lemma 3.12, we have $J_n \succeq I_n$. Thus, $T \succeq T_2 \succeq J_n \succeq I_n$. If $a_1 + a_2 = a_3 + a_4 = 6$, then $T_2 \succeq K_n$. From Lemma 3.13, we get $T \succeq T_2 \succeq K_n \succeq I_n$.

Case (ii): At most two of $a_i$ $(1 \leq i \leq 4)$ of $T_2$ are odd.

Subcase (ii.i): One of $a_i$ $(1 \leq i \leq 4)$ of $T_2$ is odd.

We assume that $a_1$ is odd. Obviously, $a_2, a_3, a_4$ are all even and not less than 2. As $a_1 \geq 1$, from Corollary 3.8 Corollary 3.4 and Theorem 3.5, we obtain $T_2 \succ a_3^2 I_2^4 \succeq T_2^2 \succeq T_3^2$ since $a_3 \geq 2$ and $a_1 + a_2 + a_5 \geq 4$. Thus, $T \succeq T_2 \succeq T_{n-5}^2$.

Subcase (ii.ii): Two of $a_i$ $(1 \leq i \leq 4)$ of $T_2$ are odd.

Let $a_1$ and $a_3$ be odd. Obviously, $a_2$ and $a_4$ are even and not less than 2. Since $T \not\in H_n^{3,1}$, one of $a_1$ and $a_3$ is not less than 3. Let $a_3 \geq 3$. From Corollaries 3.5
3.14(i), we get Theorem 3.15(i). As $n \sim T$ 3.3 and $I$ we get Theorem 3.15(ii).

From Theorems 3.3 and 3.4, we get 

**Theorem 3.15.** Let $T \in H_n$ and $n \geq 14$.

(i) If $T \in H_{n}^{1,1} \cup H_{n}^{3,1}$, then $EE(T) > EE(T_{1}^{n-4}) > EE(P_{n})$, where $T \not\sim P_{n}$, $2T_{1}^{n-4}$.

(ii) If $T \in H_{n}^{1,2} \cup H_{n}^{3,2}$, then $EE(T) > EE(T_{2}^{n-3}) > EE(2T_{1}^{n-4}) > EE(P_{n})$, where $T \not\sim P_{n}$, $2T_{1}^{n-4}, 2T_{2}^{n-5}$.

**Proof.** Let $T \in H_n$ with $n \geq 14$ and $T \not\sim P_n$, $2T_{1}^{n-4}$. From Theorems 3.3 and 3.14(i), we get Theorem 3.15(i). As $n \geq 14$, $2T_{3}^{n-6} \not\sim 2T_{2}^{n-5}$ follows from Corollary 3.3 and $I_n \not\sim T_{2}^{n-5}$ follows from Corollary 3.3. By Theorems 3.6, 3.11, and 3.14(ii), we get Theorem 3.15(ii).

Let $T \in H_n$. We can check that $T \cong P_2$ as $n = 2$, $T \cong P_4$ as $n = 4$, and $T \cong P_6, 2T_2^6$ as $n = 6$. By Lemma 2.3, we have $EE(2T_{1}^{n-4}) > EE(P_{n})$ as $n = 6$. Next, for $n = 8, 10, 12$, we have Theorem 3.16 as follows.

**Theorem 3.16.** Let $T \in H_n$ and $n = 8, 10, 12$. We have

$$EE(T) > EE(2T_{1}^{n-4}) > EE(P_{n}),$$

where $T \not\sim P_{n}$, $2T_{1}^{n-4}$.

**Proof.** Let $T \in H_n$ with $n = 8, 10, 12$ and $T \not\sim P_n$, $2T_{1}^{n-4}$. If $T \in H_{n}^{1,1}$, then by Theorems 3.5 and 3.6, we get Theorem 3.16. If $T \in H_{n}^{2} \cup H_{n}^{3}$, then by Lemma 3.9, Lemma 3.10, and Corollary 3.3, there exits a tree $T_{b}^{r} \in H_{n}^{2}$ such that $EE(T) > EE(T_{b}^{r})$, where $T_{b}^{r} \not\sim P_{n}$. Furthermore, by Theorems 3.3 and 3.6, we have $EE(T_{b}^{r}) > EE(2T_{1}^{n-4})$, where $T_{b}^{r} \not\sim P_{n}$. Thus, we get Theorem 3.16 as $T \in H_{n}^{2} \cup H_{n}^{3}$.

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