ON MAXIMAL ENERGY AND HOSOYA INDEX OF TREES
WITHOUT PERFECT MATCHING

HONGBO HUA

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Abstract

Let $G$ be a simple undirected graph. The energy $E(G)$ of $G$ is the sum of the absolute values of the eigenvalues of the adjacent matrix of $G$, and the Hosoya index $Z(G)$ of $G$ is the total number of matchings in $G$. A tree is called a nonconjugated tree if it contains no perfect matching. Recently, Ou [‘Maximal Hosoya index and extremal acyclic molecular graphs without perfect matching’, Appl. Math. Lett. 19 (2006), 652–656] determined the unique element which is maximal with respect to $Z(G)$ among the family of nonconjugated $n$-vertex trees in the case of even $n$. In this paper, we provide a counterexample to Ou’s results. Then we determine the unique maximal element with respect to $E(G)$ as well as $Z(G)$ among the family of nonconjugated $n$-vertex trees for the case when $n$ is even. As corollaries, we determine the maximal element with respect to $E(G)$ as well as $Z(G)$ among the family of nonconjugated chemical trees on $n$ vertices, when $n$ is even.

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1. Introduction

Let $G$ be a simple graph with $n$ vertices and let $A(G)$ be its adjacency matrix. The characteristic polynomial $P_G(\lambda)$ of $A(G)$ is defined as

$$P_G(\lambda) = \det(\lambda I - A(G)) = \sum_{i=0}^{n} a_i \lambda^{n-i},$$

where $I$ is the unit matrix of order $n$.

The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of the equation $P_G(\lambda) = 0$ are called the eigenvalues of $G$. It is evident that each $\lambda_i$ ($i = 1, 2, \ldots, n$) is real since $A(G)$ is symmetric.

For a graph $G$, the energy $E(G)$ of $G$ is defined to be the sum of the absolute values of the eigenvalues of the adjacent matrix of $G$.

In chemistry, the (experimentally determined) heats of formation of conjugated hydrocarbons are closely related to total $\pi$-electron energy. Within the framework
of the so-called HMO model the total $\pi$-electron energy is calculated from the

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$  

It is well known [2] that if $G$ is a bipartite graph on $n$ vertices, then $P_G(x)$ can be expressed as

$$P_G(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} a_{2k}(G)x^{n-2k} = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b_{2k}(G)x^{n-2k},$$

where $b_{2k}(G) \geq 0$ for $k = 0, 1, \ldots, \lfloor n/2 \rfloor$. In particular, $b_0(G) = 1$ and $b_2(G)$ equals the number of edges of $G$.

Suppose that $G_1$ and $G_2$ are bipartite graphs. If $b_{2k}(G_1) \geq b_{2k}(G_2)$ holds for all $k \geq 0$, then we write $G_1 \succeq G_2$ or $G_2 \preceq G_1$. If $G_1 \succeq G_2$ and there exists some $k_0$ such that $b_{2k_0}(G_1) > b_{2k_0}(G_2)$, then we write $G_1 > G_2$ or $G_2 < G_1$. Also, we write $G_1 \sim G_2$ if $G_1 \succeq G_2$ and $G_2 \preceq G_1$.

It is known [8] that for a bipartite graph $G$ of order $n$, its energy $E(G)$ can be expressed as the Coulson integral formula

$$E(G) = \frac{2}{\pi} \int_0^{\infty} \frac{1}{x^2} \ln\left(\sum_{k=0}^{\lfloor n/2 \rfloor} b_{2k}(G)x^{2k}\right) dx. \quad (1.1)$$

From (1.1),

$$G_1 > G_2 \Rightarrow E(G_1) > E(G_2),$$

$$G_1 \succeq G_2 \Rightarrow E(G_1) \geq E(G_2).$$

The Hosoya index of $G$ is the total number of matchings in $G$, namely

$$Z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G; k),$$

where $n$ is the number of vertices in $G$, and $m(G; k)$ is the number of $k$-matchings in $G$. A $k$-matching of $G$ is a $k$-element subset of its edge set, in which any two edges are mutually independent.

Another formula (see [6]) for the Hosoya index of a graph $G$ is

$$\ln Z(G) = \sum_{+} \ln(1 + \lambda_j^2),$$

where the summation is over all positive eigenvalues of $G$. It is convenient to set $m(G; 0) = 1$, $m(G; 1) = |E(G)|$ and $m(G; k) = 0$ (for $k > n/2$), where $|E(G)|$ is the number of edges in $G$. According to Sach’s theorem [2], if $G$ is a tree, then $b_{2k}(G) = m(G; k)$. Thus,

$$G_1 > G_2 \Rightarrow Z(G_1) > Z(G_2),$$

$$G_1 \succeq G_2 \Rightarrow Z(G_1) \geq Z(G_2).$$
There are numerous recent results on these two subjects: see [1, 4, 5, 7, 10, 12, 13, 15, 16, 21–24, 26] for graph energy, and [6, 9, 11, 14, 17, 19, 20, 23, 25] for the Hosoya index.

It is well known that among all $n$-vertex trees, the path $P_n$ is the unique maximal element with respect to $E(G)$ as well as $Z(G)$. A tree is called a nonconjugated tree if it contains no perfect matching. When $n$ is odd, the path $P_n$ is still the unique element which is maximal with respect to $E(G)$ as well as $Z(G)$ among all nonconjugated $n$-vertex trees. So it is of interest to find the maximal element with respect to $E(G)$ as well as $Z(G)$ among all nonconjugated $n$-vertex trees for the case when $n$ is even. Ou [18] investigated the above problem and determined the unique element which is maximal with respect to $Z(G)$. Unfortunately, Ou’s results have been found to be incorrect.

In this paper, we reconsider this question and determine the unique maximal element with respect to $E(G)$ as well as $Z(G)$ among all nonconjugated $n$-vertex trees for the case when $n$ is even. As corollaries, we also determine the maximal element with respect to $E(G)$ as well as $Z(G)$ among the family of nonconjugated chemical trees on $n$ vertices when $n$ is even.

2. Revisiting Ou’s results

Let $T_{r_1,r_2,r_3}$ be the star-like tree as shown in Figure 1.

If a graph $G$ contains a perfect matching, we say that $G$ has $\mathcal{PM}$. Let $\mathcal{NT}_n$ denote the set of trees of $n$ vertices, which possess no $\mathcal{PM}$. Recently, Ou [18] claimed the following results.

**Lemma A.** [18, Lemma 4] Let $T$ be a $4m$-vertex tree and $k$ be a nonnegative integer. If $T \in \mathcal{NT}_{4m}$, then $m(T; k) \leq m(T_{1,2m−1,2m−1}; k)$ with equality holding if and only if $T \cong T_{1,2m−1,2m−1}$.

**Lemma B.** [18, Lemma 5] Let $T$ be a $4m+2$-vertex tree and $k$ be a nonnegative integer. If $T \in \mathcal{NT}_{4m+2}$, then $m(T; k) \leq m(T_{1,2m+1,2m−1}; k)$ with equality holding if and only if $T \cong T_{1,2m+1,2m−1}$.

Let $F_n$ denote the $n$th Fibonacci number.
**Theorem C.** [18, Theorem 1] Let $T$ be a $4m$-vertex tree and $k$ be a nonnegative integer. If $T \in \mathcal{N}T_{4m}$, then $Z(T) \geq 2F_{2m}F_{2m+1}$ with equality holding if and only if $T \cong T_{1,2m-1,2m-1}$.

**Theorem D.** [18, Theorem 2] Let $T$ be a $4m + 2$-vertex tree and $k$ be a nonnegative integer. If $T \in \mathcal{N}T_{4m+2}$, then $Z(T) \leq F_{2m+2}^2 + F_{2m}F_{2m+1}$ with equality holding if and only if $T \cong T_{1,2m+1,2m-1}$.

Lemmas A and B are evidently false, which can easily be seen from the following counterexample to Lemma A.

**Example 2.1.** Let $n = 12$ and consider $T_{3,3,5}$ and $T_{1,5,5}$.

From Lemma 3.1 below,
\[
m(T_{1,5,5}; k) = m(P_5 \cup P_7; k) + m(P_4 \cup P_5 \cup P_1; k-1),
\]
\[
m(T_{3,3,5}; k) = m(P_5 \cup P_7; k) + m(P_4 \cup P_3 \cup P_3; k-1).
\]

Note that $m(P_3 \cup P_3; 2) = 4 > 3 = m(P_5 \cup P_1; 2)$. So, $m(T_{1,5,5}; 3) < m(T_{3,3,5}; 3)$, a contradiction to $T_{3,3,5} \preceq T_{1,5,5}$, as claimed by Lemma A. Thus, Lemma A is incorrect. Similarly, Lemma B is also incorrect, and thus Theorems C and D turn out to be incorrect.

A natural problem arising from this is the following. Among all graphs in $\mathcal{N}T_n$ with $n$ even, which graph is the maximum element with respect to $E(G)$ as well as $Z(G)$? Our theorems below will provide a satisfactory answer to this question.

### 3. Determining the nonconjugated tree with maximal energy and Hosoya index

We first recall some previously established results, which will be helpful in proving our main results.

**Lemma 3.1.** [8] Let $G$ be a graph with $n \geq 2$ vertices and let $uv$ be an edge in $G$. Then for all $k \geq 0$,
\[
m(G; k) = m(G - uv; k) + m(G - \{u, v\}; k-1).
\]
In particular, if $uv$ is an edge such that $v$ is a pendant vertex, then
\[
m(G; k) = m(G - v; k) + m(G - \{u, v\}; k-1)
\]
for all $k \geq 0$.

**Lemma 3.2.** [9] Let $P_n$ be a path on $n = 4s + t$, $0 \leq t \leq 3$ vertices. Then
\[
P_n \preceq P_{2s} \cup P_{n-2} \preceq P_4 \cup P_{n-4} \preceq \cdots \preceq P_{2s} \cup P_{2s+t}
\]
\[
\preceq P_{2s+1} \cup P_{2s+t-1} \preceq P_{2s-1} \cup P_{2s+t+1} \preceq \cdots \preceq P_3 \cup P_{n-3} \preceq P_1 \cup P_{n-1}.
\]

**Lemma 3.3.**

(i) For $s \geq 2$, $3 \leq k \leq 2s - 1$ and $k$ odd, $P_{2s+1} \cup P_{2s-1} > P_{2s+k} \cup P_{2s-k}$.
(ii) For $s \geq 1$, $3 \leq k \leq 2s + 1$ and $k$ odd, $P_{2s+1} \cup P_{2s+1} > P_{2s+k} \cup P_{2s+2-k}$.
PROOF. We only consider the proof of (i) here. The proof of (ii) can be derived in the same way. By Lemma 3.2, it suffices to prove that

$$m(P_{2s+1} \cup P_{2s-1}; 3) > m(P_{2s+3} \cup P_{2s-3}; 3).$$

It is well known [3] that

$$m(P_n; k) = \binom{n - k}{k}$$

and therefore

$$m(P_{2s+1} \cup P_{2s-1}; 3) = m(P_{2s+1}; 3) + m(P_{2s+1}; 2)m(P_{2s-1}; 1) + m(P_{2s+1}; 1)m(P_{2s-1}; 2) + m(P_{2s-1}; 3)$$

$$= \binom{2s - 2}{3} + \binom{2s - 1}{2}(2s - 2) \binom{3}{1}$$

$$\binom{2s}{1} \binom{2s - 3}{2} + (2s - 4) \binom{3}{1}$$

$$= \frac{1}{3}(8s^3 - 48s^2 + 100s - 72) + 8s^3 - 18s^2 + 20s - 2,$$

$$m(P_{2s+3} \cup P_{2s-3}; 3) = m(P_{2s+3}; 3) + m(P_{2s+3}; 2)m(P_{2s-3}; 1) + m(P_{2s+3}; 1)m(P_{2s-3}; 2) + m(P_{2s-3}; 3)$$

$$= \binom{2s}{3} + \binom{2s + 1}{2}(2s - 4) \binom{3}{1}$$

$$\binom{2s + 2}{1}(2s - 5) + (2s - 6) \binom{3}{1}$$

$$= \frac{1}{3}(8s^3 - 48s^2 + 148s - 168) + 8s^3 - 24s^2 + 4s + 30.$$

It follows that

$$m(P_{2s+1} \cup P_{2s-1}; 3) - m(P_{2s+3} \cup P_{2s-3}; 3) = 6s^2 > 0,$$

which completes the proof. □

PROPOSITION 3.4. Let s (≥ 3) be an odd number. There exist three odd numbers s₁, s₂ and s₃ such that s₁ + s₂ + s₃ = s and |sᵢ - sⱼ| ≤ 2 for 1 ≤ i < j ≤ 3.

PROOF. Let s (≥ 3) be an odd number. If s = 3t, we must have t ≡ 1 (mod 2), and thus we let sᵢ = t for 1 ≤ i ≤ 3. If s = 3t + 1, we must have t ≡ 0 (mod 2), and thus we let s₁ = s₂ = t + 1, s₃ = t - 1. If s = 3t + 2, we must have t ≡ 1 (mod 2), and thus, we let s₁ = s₂ = t + 2, s₃ = t.

Denote by $T_{r_1,r_2,r_3}$ the set of all star-like trees of the form $T_{r_1,r_2,r_3}$ with $r_1 + r_2 + r_3 + 1 = 4m$ or $4m + 2$, and $r_i ≡ 1$ (mod 2) for each 1 ≤ i ≤ 3. Further, we let $T^*_{r_1,r_2,r_3}$ be the tree in $T_{r_1,r_2,r_3}$ with an additional condition that |rᵢ - rⱼ| ≤ 2 for 1 ≤ i < j ≤ 3. By Proposition 3.4, $T^*_{r_1,r_2,r_3}$ is well defined. Also, such a tree is unique by Proposition 3.4.
LEMMA 3.5. Let $T$ be any graph in $T_{r_1,r_2,r_3}$ with $n = 4m$ or $4m + 2$, and $m \geq 1$. Then $T \preceq T_{r_1,r_2,r_3}$. Moreover, $T \sim T_{r_1,r_2,r_3}^*$ if and only if $T \cong T_{r_1,r_2,r_3}^*$.

PROOF. If $n = 4m$ and $m = 1$, $T$ is isomorphic to $T_{1,1,1}$. If $n = 4m$ and $m = 2$, $T$ is isomorphic to $T_{1,3,3}$. If $n = 4m + 2$ and $m = 1$, $T$ is isomorphic to $T_{1,1,3}$. The lemma is evidently true for these three cases. Suppose now that $T_0 = T_{r_1,r_2,r_3}$ is a tree in $T_{r_1,r_2,r_3}$ such that $T_0 \succeq T$ for any $T \in T_{r_1,r_2,r_3}$, but $T_0 \not\cong T_{r_1,r_2,r_3}$ both for $n = 4m$, $m \geq 3$ and for $n = 4m + 2$, $m \geq 2$. Then there must exist $r_1$ and $r_2$, such that $r_2 - r_1 \geq 4$ (or $r_1 - r_2 \geq 4$). Assume that $r_1 + r_2 = 2t$. Then by Lemmas 3.1, 3.2 and 3.3, $T_0 \prec T_{x,y,r_3} \in T_{r_1,r_2,r_3}$, where $x$ and $y$ are numbers chosen by the following rules: if $t \equiv 0 \pmod{2}$, we let $x = t - 1$ and $y = t + 1$, or $x = t + 1$ and $y = t - 1$; if $t \equiv 1 \pmod{2}$, we let $x = y = t$. In fact, by Lemma 3.1,

\[ m(T_0; k) = (m(P_{r_1+r_2+1} \cup P_{r_3}) + m(P_{r_3-1} \cup P_{r_1} \cup P_{r_2}) - k), \]

\[ m(T_{x,y,r_3}; k) = (m(P_{r_1+r_2+1} \cup P_{r_3}) + m(P_{r_3-1} \cup P_{x} \cup P_{r_3}) - k). \]

This contradicts our choice of $T_0$, which completes the proof.

We mention here a well-known result, as it will play an important role in proving our main result.

LEMMA 3.6. [8] Let $T$ be a tree with $n$ vertices. Then $T \preceq P_n$. Moreover, $T \sim P_n$ if and only if $T \cong P_n$.

In the rest of this paper, we will always denote the number of elements in a vertex subset $A$ by $|A|$. Before presenting our main results, it is necessary to state and prove the following lemma.

LEMMA 3.7. Let $T$ be a tree in $\mathcal{NT}_n$ with $n = 4m$ or $n = 4m + 2$, and $m \geq 1$. Then $T \preceq T_{r_1,r_2,r_3}^*$. Moreover, $T \sim T_{r_1,r_2,r_3}^*$ if and only if $T \cong T_{r_1,r_2,r_3}^*$.

PROOF. We only consider here the case when $n = 4m$. The case when $n = 4m + 2$ can be dealt with in a fully analogous manner. If $m = 1$, then $T_{1,1,1}$ is the unique element in $\mathcal{NT}_n$, and the result is evidently true. So we may suppose that $m \geq 2$. Since $T \in \mathcal{NT}_n$, then $T \not\cong P_{4m}$. That is to say, $T$ has at least one vertex of degree greater than or equal to 3. Let $\Delta(T)$ be the maximum vertex-degree in $T$. Also, we use $V_{\Delta}(T)$ to denote the set $\{v \in V(T) \mid d(v) = \Delta(T)\}$. For any $T$ in $\mathcal{NT}_n$, we clearly have $|V_{\Delta}(T)| \geq 1$. We shall prove the lemma by induction on $|V_{\Delta}(T)|$. When $|V_{\Delta}(T)| = 1$, the lemma follows from Lemma 3.3 for the case $\Delta(T) = 3$. So we may suppose that $\Delta(T) \geq 4$. In this case, $T$ must be isomorphic to a star-like tree with maximum vertex-degree $\Delta(T) \geq 4$. Let $d(v) = \Delta(T)$ and $T - \{v\} = P_{r_1} \cup P_{r_2} \cup \cdots \cup P_{r_{\Delta(T)}}$. It can be seen that among all the $r_i$, there are at least three odd positive numbers. Assume without loss of generality that $r_i$, $i = 1, 2, 3$, are odd positive numbers. Let $Q = \{r_1, r_2, r_3, \ldots\}$ be the set of all odd positive numbers among $r_1, r_2, r_3, \ldots, r_{\Delta(T)}$. If there exists some $r_i \in Q$ such that $r_i = 1$, then one can easily prove that $T \prec T_{1,(2m-1),(2m-1)}$. It follows from Lemma 3.5 that $T \prec T_{1,(2m-1),(2m-1)} \prec T_{r_1,r_2,r_3}^*$. Suppose now that $r_i \geq 3$ for any $r_i \in Q$. Let $u$ be the vertex in $P_{r_1}$ (if there is more
than one $P_{r_1}$ in $T - \{v\}$, we may take any one of them) such that $u$ is adjacent to $v$ in $T$. Write $T - uv = P_{r_1} \cup T'$. By Lemma 3.1, we obtain
\begin{align*}
m(T; k) &= m(P_{r_1} \cup T'; k) + m(P_{r_1-1} \cup P_{r_2} \cup \cdots \cup P_{\Delta T(G)}; k - 1), \\
m(T_{r_1,x,y}; k) &= m(P_{r_1} \cup P_{4m-r_1}; k) + m(P_{r_1-1} \cup P_x \cup P_y; k - 1),
\end{align*}
where $x$ and $y$ are odd numbers with the condition that $x + y = 4m - r_1 - 1$. Also, if $4m - r_1 - 1 = 4t + 2$, then $x = y = 2t + 1$; if $4m - r_1 - 1 = 4t$, then $x = 2t + 1$ and $y = 2t - 1$, or $x = 2t + 1$ and $y = 2t - 1$.

Note also that
\[ P_{r_2} \cup \cdots \cup P_{\Delta T(G)} < P_{r_2} \cup P_{4m-r_1-1-r_2}, \]
and that $4m - r_1 - 1 - r_2$ is an odd number. So
\[ P_{r_2} \cup \cdots \cup P_{\Delta T(G)} < P_{r_2} \cup P_{4m-r_1-1-r_2} \leq P_x \cup P_y \]
by Lemma 3.3. Thus, $T < T_{r_1,x,y} \leq T_{r_1,r_2,r_3}^*$ by Lemma 3.5.

We now let $|V_\Delta(T)| = q \geq 2$ and suppose that the theorem is true for small values of $q$. We write $V_{\rho}(T) = \{v \in V(T) | d(v) = 1\}$. For any vertex $w \in V_\Delta(T)$, let
\[ P_w(T) = \{u \in V_{\rho}(T) | d(u, w) < d(u, x) \text{ for any } x \in V_\Delta(T)\}. \]
It can be seen that for $|V_\Delta(T)| \geq 2$, there exist at least two vertices, say $x$ and $y$, in $V_\Delta(T)$ such that $P_x(T) \neq \emptyset$ and $P_y(T) \neq \emptyset$. Moreover, for any $z \in V_{\rho}(T)$, there exists a unique $w \in V_\Delta(T)$ such that $z \in P_w(T)$. Furthermore, for $|V_\Delta(T)| \geq 2$, there exist at least two vertices $x$ and $y$ in $V_\Delta(T)$ such that $|P_x(T)| \geq 2$ and $|P_y(T)| \geq 2$. Let $w$ be a vertex in $V_\Delta(T)$ such that $P_w(T) = \{w_1, w_2, \ldots, w_{\ell}\}$ for $(\ell \geq 2)$. Denote by $S_w$ the set of vertices (other than $w_i$ and $w$) lying on the path between $w_i$ and $w$ for all $i = 1, \ldots, \ell$. We call the induced subtree $G[w, w_1, \ldots, w_{\ell}, S_w]$ of $T$ the pendent subtree of $T$ with respect to $w$, which is denoted by $PS_w(T)$. By our definition of pendent subtree and the above arguments, we know that:

- if $PS_w(T)$ is one pendent subtree of $T$, then $PS_w(T)$ contains no vertex other than $w$ of degree greater than or equal to 3;
- if $T$ is a tree with $|V_\Delta(T)| \geq 2$, then $T$ has at least two pendent subtrees.

We proceed by considering the following two cases.

**Case 1.** $T$ has a pendent subtree, say $PS_w(T)$, which has $PM$.

In this case, $T$ can be viewed as the graph shown in Figure 2(a). By employing Operation I (see Figure 2) on $T$, we obtained a new graph $T^1$, which is obviously a graph in $\mathcal{N}T_n$. Also, one can easily prove that $T < T^1$ by using Lemmas 3.1 and 3.6. Note that
\[ |V_\Delta(T^1)| = |V_\Delta(T)| - 1 = q - 1. \]
Thus $T^1 \leq T_{r_1,r_2,r_3}^*$ by the induction assumption and then $T < T_{r_1,r_2,r_3}^*$.
CASE 2. Any pendent subtree $PS_w(T)$ of $T$ has no $PM$.

By our discussion above, if $|V_\Delta(T)| \geq 2$, then $T$ has at least two pendent subtrees. Suppose that the pendent subtrees of $T$ are $PS_{w_1}$, $PS_{w_2}$, ..., $PS_{w_\ell}$ ($\ell \geq 2$). We can always find two vertices, say $w_1$ and $w_2$, among all the $w_i$, such that

$$d(w_1, w_2) = \max\{d(w_i, w_j) \mid 1 \leq i < j \leq \ell\}.$$

In this case, $T$ can be viewed as the graph shown in Figure 3(a).

**Subcase 2.1.** $|PS_{w_1}(T)| \equiv 1 \pmod{2}$ or $|PS_{w_2}(T)| \equiv 1 \pmod{2}$.

Assume without loss of generality that $|PS_{w_1}(T)| \equiv 1 \pmod{2}$.

**Subcase 2.1.1.** $|PS_{w_1}(T)| \equiv 1 \pmod{2}$ and $G[V(T_0') \cup V(PS_{w_2}(T)) \cup \{w_1\}]$ has no $PM$, where $G[\bullet] = G_T[\bullet]$ denotes the subgraph of $T$ induced by $\bullet$.

By employing Operation II (see Figure 3) on $T$, we obtain a new graph $T^2$, which is obviously a graph in $NT_n$. Also, one can easily prove that $T \prec T^2$ by using Lemmas 3.1 and 3.6. Note that $|V_\Delta(T^2)| = |V_\Delta(T)| - 1 = q - 1$. Thus $T^2 \leq T_{r_1, r_2, r_3}^*$ by the induction assumption and then $T \prec T_{r_1, r_2, r_3}^*$ by using Lemma 3.5.

**Subcase 2.1.2.** $|PS_{w_1}(T)| \equiv 1 \pmod{2}$ and $G[V(T_0') \cup V(PS_{w_2}(T)) \cup \{w_1\}]$ has $PM$. 

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By employing Operation III (see Figure 3) on $T$, we obtain a new graph $T^3$, which is obviously a graph in $\mathcal{N}T_n$. Also, one can easily prove that $T < T^3$. Note that $|V_\Delta(T^3)| = 1$. Thus $T^3 \leq T_{r_1,r_2,r_3}$ by Lemma 3.5 and then $T < T_{r_1,r_2,r_3}$.

**Subcase 2.2.** $|PS_{w_1}(T)| \equiv 0 \pmod{2}$ and $|PS_{w_2}(T)| \equiv 0 \pmod{2}$.

It is obvious that $G[V(T_0') \cup V(PS_{w_2}(T))]$ has no $\mathcal{P}\mathcal{M}$, since $PS_{w_2}(T)$ has no $\mathcal{P}\mathcal{M}$. Thus, Operation III can be employed on $T$ once again, and we obtain the graph $T^3$ (see Figure 3). As in Subcase 2.1.2, we can prove our desired result.

Combining all cases completes the proof. 

**Remark 3.8.** According to our proof of Lemma 3.7, $PS_{w_1}(T)$ and $PS_{w_2}(T)$ are pendent subtrees chosen such that 

$$d(w_1, w_2) = \max\{d(w_i, w_j) \mid 1 \leq i < j \leq l\},$$

among all pendent subtrees $PS_{w_i}(T)$ of $T$ for $1 \leq i \leq l$. In fact, one finds that the reasoning used in case 2 of the proof of Lemma 3.7 remains valid even when $d(w_1, w_2) = 1$; that is, $T_0'$ is an empty set. Moreover, Lemma 3.7 still follows, using the same technique, even when $u = v$ (see Figure 3).

From Lemma 3.7 we immediately obtain the following two theorems.

**Theorem 3.9.** Let $T$ be a tree in $\mathcal{N}T_n$ with $n = 4m$ or $n = 4m + 2$, and $m \geq 1$. Then $Z(T) \leq Z(T_{r_1,r_2,r_3}^*)$. Moreover, $Z(T) = Z(T_{r_1,r_2,r_3}^*)$ if and only if $T \cong T_{r_1,r_2,r_3}^*$.

**Theorem 3.10.** Let $T$ be a tree in $\mathcal{N}T_n$ with $n = 4m$ or $n = 4m + 2$, and $m \geq 1$. Then $E(T) \leq E(T_{r_1,r_2,r_3}^*)$. Moreover, $E(T) = E(T_{r_1,r_2,r_3}^*)$ if and only if $T \cong T_{r_1,r_2,r_3}^*$.

**Remark 3.11.** Let $F_n$ denote the $n$th Fibonacci number. Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = F_1 = 1$. Note that $Z(P_0) = 1$, $Z(P_1) = 1$ and $Z(P_n) = Z(P_{n-1}) + Z(P_{n-2})$. Thus,

$$Z(P_n) = \frac{\sqrt{5}}{5} \left[ \left( \frac{1 + \sqrt{5}}{2} \right)^{n+1} - \left( \frac{1 - \sqrt{5}}{2} \right)^{n+1} \right].$$

So, for a specified value of $n$ in Theorem 3.9, we can compute the exact value of $Z(T_{r_1,r_2,r_3}^*)$.

A chemical tree is a tree in which no vertex has degree greater than 4. If we denote by $\mathcal{N}\mathcal{C}T_n$ the set of nonconjugated chemical trees on $n$ vertices, then by Theorems 3.9 and 3.10 we immediately have the following.

**Corollary 3.12.** Let $T$ be a tree in $\mathcal{N}\mathcal{C}T_n$ with $n = 4m$ or $n = 4m + 2$, and $m \geq 1$. Then $Z(T) \leq Z(T_{r_1,r_2,r_3}^*)$. Moreover, $Z(T) = Z(T_{r_1,r_2,r_3}^*)$ if and only if $T \cong T_{r_1,r_2,r_3}^*$.

**Corollary 3.13.** Let $T$ be a tree in $\mathcal{N}\mathcal{C}T_n$ with $n = 4m$ or $n = 4m + 2$, and $m \geq 1$. Then $E(T) \leq E(T_{r_1,r_2,r_3}^*)$. Moreover, $E(T) = E(T_{r_1,r_2,r_3}^*)$ if and only if $T \cong T_{r_1,r_2,r_3}^*$. 

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HONGBO HUA, Department of Computing Science, Huaiyin Institute of Technology, Huaian, Jiangsu 223003, PR China
e-mail: hongbo.hua@gmail.com