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ON MAXIMAL ENERGY AND HOSOYA INDEX OF TREES WITHOUT PERFECT MATCHING

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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 λ_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 π-electron energy. Within the framework of the so-called HMO model the total π-electron energy is calculated from the eigenvalues of a pertinently constructed molecular graph G by the equation $E(G) = \sum_{i=1}^{n} |\lambda_i|$.

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 $G_1 \succ G_2$ or $G_2 \prec G_1$. 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

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

From (1.1),

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2),$$
$$G_1 \succeq G_2 \Rightarrow E(G_1) \geq E(G_2).$$

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 $m(G; 0) = 1$, $m(G; 1) = |\mathcal{E}(G)|$ and $m(G; k) = 0$ (for $k > n/2$), where $|\mathcal{E}(G)|$ 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,

$$G_1 \succ G_2 \Rightarrow Z(G_1) > Z(G_2),$$
$$G_1 \succeq G_2 \Rightarrow Z(G_1) \geq Z(G_2).$$

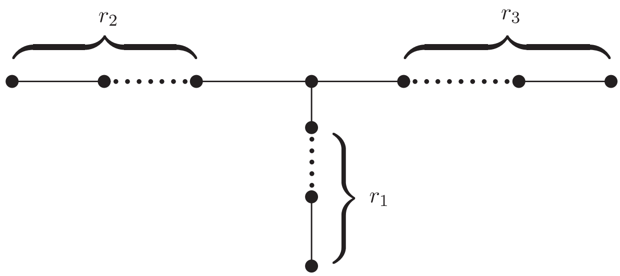

FIGURE 1. The graph T_{r_1,r_2,r_3}.

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 nth Fibonacci number.

THEOREM C. [18, Theorem 1] *Let T be a $4m$-vertex tree and k be a nonnegative integer. If $T \in \mathcal{NT}_{4m}$, then $Z(T) \le 2F_{2m}F_{2m+1}$ 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 $T \in \mathcal{NT}_{4m+2}$, then $Z(T) \le F_{2m+2}^2 + F_{2m}F_{2m+1}$ 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,

$$\begin{aligned} m(T_{1,5,5}; k) &= m(P_5 \cup P_7; k) + m(P_4 \cup P_5 \cup P_1; k-1), \\ m(T_{3,3,5}; k) &= m(P_5 \cup P_7; k) + m(P_4 \cup P_3 \cup P_3; k-1). \end{aligned}$$

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 $\mathcal{NT}_n$ 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 $n \ge 2$ vertices and let uv be an edge in G. Then for all $k \ge 0$,*

$$m(G; k) = m(G - uv; k) + m(G - \{u, v\}; k-1).$$

In particular, if uv is an edge such that v is a pendent vertex, then

$$m(G; k) = m(G - v; k) + m(G - \{u, v\}; k-1)$$

for all $k \ge 0$.

LEMMA 3.2. [9] *Let P_n be a path on $n = 4s + t$, $0 \le t \le 3$ vertices. Then*

$$\begin{aligned} P_n &\succeq P_2 \cup P_{n-2} \succeq P_4 \cup P_{n-4} \succeq \cdots \succeq P_{2s} \cup P_{2s+t} \\ &\succeq P_{2s+1} \cup P_{2s+t-1} \succeq P_{2s-1} \cup P_{2s+t+1} \succeq \cdots \succeq P_3 \cup P_{n-3} \succeq P_1 \cup P_{n-1}. \end{aligned}$$

LEMMA 3.3.

(i) *For $s \ge 2$, $3 \le k \le 2s-1$ and k odd, $P_{2s+1} \cup P_{2s-1} \succ P_{2s+k} \cup P_{2s-k}$.*

(ii) *For $s \ge 1$, $3 \le k \le 2s+1$ and k odd, $P_{2s+1} \cup P_{2s+1} \succ P_{2s+k} \cup P_{2s+2-k}$.*

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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

$$\begin{aligned}
m(P_{2s+1} \cup P_{2s-1};\, 3) &= m(P_{2s+1};\, 3) + m(P_{2s+1};\, 2)m(P_{2s-1};\, 1) \\
&\quad + m(P_{2s+1};\, 1)m(P_{2s-1};\, 2) + m(P_{2s-1};\, 3) \\
&= \binom{2s-2}{3} + \binom{2s-1}{2}\binom{2s-2}{1} \\
&\quad + \binom{2s}{1}\binom{2s-3}{2} + \binom{2s-4}{3} \\
&= \frac{1}{3}(8s^3 - 48s^2 + 100s - 72) + 8s^3 - 18s^2 + 20s - 2,
\end{aligned}$$

$$\begin{aligned}
m(P_{2s+3} \cup P_{2s-3};\, 3) &= m(P_{2s+3};\, 3) + m(P_{2s+3};\, 2)m(P_{2s-3};\, 1) \\
&\quad + m(P_{2s+3};\, 1)m(P_{2s-3};\, 2) + m(P_{2s-3};\, 3) \\
&= \binom{2s}{3} + \binom{2s+1}{2}\binom{2s-4}{1} \\
&\quad + \binom{2s+2}{1}\binom{2s-5}{2} + \binom{2s-6}{3} \\
&= \frac{1}{3}(8s^3 - 48s^2 + 148s - 168) + 8s^3 - 24s^2 + 4s + 30.
\end{aligned}$$

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 s_1, s_2 and s_3 such that $s_1 + s_2 + s_3 = s$ and $|s_i - s_j| \leq 2$ for $1 \leq i < j \leq 3$.*

PROOF. Let s (≥ 3) be an odd number. If $s = 3t$, we must have $t \equiv 1 \pmod 2$, and thus we let $s_i = t$ for $1 \leq i \leq 3$. If $s = 3t + 1$, we must have $t \equiv 0 \pmod 2$, and thus we let $s_1 = s_2 = t + 1$, $s_3 = t - 1$. If $s = 3t + 2$, we must have $t \equiv 1 \pmod 2$, and thus, we let $s_1 = s_2 = t + 2$, $s_3 = t$.

Denote by $\mathcal{T}_{r_1,r_2,r_3}$ 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 $r_i \equiv 1 \pmod 2$ for each $1 \leq i \leq 3$. Further, we let $T^*_{r_1,r_2,r_3}$ be the tree in $\mathcal{T}_{r_1,r_2,r_3}$ with an additional condition that $|r_i - r_j| \leq 2$ for $1 \leq i < j \leq 3$. By Proposition 3.4, $T^*_{r_1,r_2,r_3}$ is well defined. Also, such a tree is unique by Proposition 3.4.

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LEMMA 3.5. *Let T be any graph in $\mathcal{T}_{r_1,r_2,r_3}$ 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 $\mathcal{T}_{r_1,r_2,r_3}$ such that $T_0 \succeq T$ for any $T \in \mathcal{T}_{r_1,r_2,r_3}$, but $T_0 \ncong T^*_{r_1,r_2,r_3}$ 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, $T_0 \prec T_{x,y,r_3} \in \mathcal{T}_{r_1,r_2,r_3}$, 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,

$$m(T_0; k) = m(P_{r_1+r_2+1} \cup P_{r_3}; k) + m(P_{r_3-1} \cup P_{r_1} \cup P_{r_2}; k - 1),$$
$$m(T_{x,y,r_3}; k) = m(P_{r_1+r_2+1} \cup P_{r_3}; k) + m(P_{r_3-1} \cup P_x \cup P_y; k - 1).$$

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 $\mathcal{A}$ by $|\mathcal{A}|$. 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 $T \ncong P_{4m}$. 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

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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

$$m(T;k)=m(P_{r_1}\cup T';k)+m(P_{r_1-1}\cup P_{r_2}\cup\cdots\cup P_{\Delta_T(G)};k-1),$$
$$m(T_{r_1,x,y};k)=m(P_{r_1}\cup P_{4m-r_1};k)+m(P_{r_1-1}\cup P_x\cup P_y;k-1),$$

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 that T' is a tree of $4m-r_1$ vertices not isomorphic to P_{4m-r_1}. Then $T'\prec P_{4m-r_1}$ by Lemma 3.6.

Note also that

$$P_{r_2}\cup\cdots\cup P_{\Delta_T(G)}\prec P_{r_2}\cup P_{4m-r_1-1-r_2},$$

and that $4m-r_1-1-r_2$ is an odd number. So

$$P_{r_2}\cup\cdots\cup P_{\Delta_T(G)}\prec P_{r_2}\cup P_{4m-r_1-1-r_2}\preceq P_x\cup P_y$$

by Lemma 3.3. Thus, $T\prec T_{r_1,x,y}\preceq T^*_{r_1,r_2,r_3}$ 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 $V_p(T)=\{v\in V(T)\mid d(v)=1\}$. For any vertex $w\in V_\Delta(T)$, let

$$P_w(T)=\{u\in V_p(T)\mid d(u,w)<d(u,x)\text{ for any }x\in V_\Delta(T)\}.$$

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 $z\in V_p(T)$, 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 betweenw_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 $\mathcal{PM}$.

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 $\mathcal{NT}_n$. Also, one can easily prove that $T\prec T^1$ by using Lemmas 3.1 and 3.6. Note that

$$|V_\Delta(T^1)|=|V_\Delta(T)|-1=q-1.$$

Thus $T^1\preceq T^*_{r_1,r_2,r_3}$ by the induction assumption and then $T\prec T^*_{r_1,r_2,r_3}$.

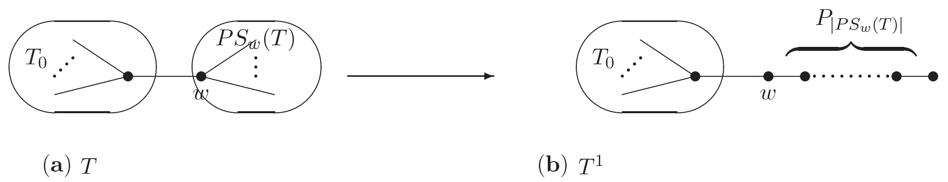

FIGURE 2. (a) ⇒ (b) by Operation I.

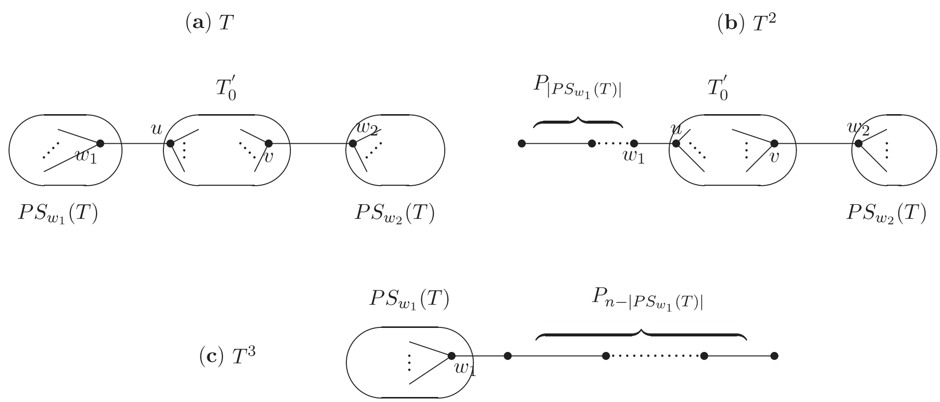

FIGURE 3. (a) ⇒ (b) by Operation II; (a) ⇒ (c) by Operation III.

CASE 2. Any pendent subtree $PS_w(T)$ of T has no $\mathcal{PM}$.

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

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

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 $\mathcal{PM}$, 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 $\mathcal{NT}_n$. Also, one can easily prove that $T \prec T^2$ by using Lemmas 3.1 and 3.6. Note that $|V_\triangle(T^2)| = |V_\triangle(T)| - 1 = q - 1$. Thus $T^2 \preceq T^*_{r_1,r_2,r_3}$ 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 $\mathcal{PM}$.

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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 $\mathcal{NT}_n$. Also, one can easily prove that $T \prec T^3$. Note that $|V_\triangle(T^3)| = 1$. Thus $T^3 \preceq T^*_{r_1,r_2,r_3}$ by Lemma 3.5 and then $T \prec T^*_{r_1,r_2,r_3}$.

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 $\mathcal{PM}$, since $PS_{w_2}(T)$ has no $\mathcal{PM}$. 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

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

among all pendent subtrees $PS_{w_i}(T)$ of T for $1 \le i \le l$. 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 $\mathcal{NT}_n$ with $n = 4m$ or $n = 4m + 2$, and $m \ge 1$. Then $Z(T) \le Z(T^*_{r_1,r_2,r_3})$. 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 $\mathcal{NT}_n$ with $n = 4m$ or $n = 4m + 2$, and $m \ge 1$. Then $E(T) \le E(T^*_{r_1,r_2,r_3})$. 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 nth 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,

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

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 $\mathcal{NCT}_n$ 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 $\mathcal{NCT}_n$ with $n = 4m$ or $n = 4m + 2$, and $m \ge 1$. Then $Z(T) \le Z(T^*_{r_1,r_2,r_3})$. 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 $\mathcal{NCT}_n$ with $n = 4m$ or $n = 4m + 2$, and $m \ge 1$. Then $E(T) \le E(T^*_{r_1,r_2,r_3})$. 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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