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On the Total Number of Matchings of Trees with Prescribed Diameter

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Abstract: Let $G = (V(G), E(G))$ be a graph. An $m-$matchings of G is a set of edges of size m in which any two edges are mutually independent. Denote by $z(G, m)$ the number of $m-$matchings of G. Let $z(G)$ be the total number of matchings in G, namely $z(G) = \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} z(G, m)$. It's well-known that $z(G)$ are also named as Hosoya index. Let $\mathcal{T}_{n,d}$ be the set of trees of on n vertices with diameter d. In this paper, the trees with minimal Hosoya index are uniquely determined among all trees in $\mathcal{T}_{n,d}$.

Key words: Hosoya index; Trees; Diameter; Matching

1 Introduction

Let $G = (V(G), E(G))$ denote a graph whose set of vertices and set of edges are $V(G)$ and $E(G)$ respectively. For any $v \in V(G)$, we denote the neighbors of v as $N_G(v)$. By $n(G)$, we denote the number of vertices of G.

Two edges in G are said to be mutually independent if there are not incident in G. An m-matching of G is a set of edges of size m in which any two edges are mutually independent. By $z(G, m)$, we denote the number of m-matchings of G. For any graph G, we set $z(G, 0) = 1$. By $z(G)$, we denote total number of matchings in G. Then $z(G) = \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} z(G, m)$. It's well known that $z(G)$ is also called to be Hosaya index.

The Hosoya index $z(G)$ was introduced by Hosoya in [2] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures [3]. Many researchers have devoted to investigating the Hosoya index $z(G)$ for a given graph G. To determine the graph with extremal (maximal or minimal) Hosoya index $z(G)$ is of much interest in Combinatorial chemistry. Gutman in [4] proved that the linear hexagonal chain is the unique chain with minimal Hosoya index among all hexagonal chains. Zhang [5] showed that zig-zag hexagonal chain is the unique chain with maximal Hosoya index among all hexagonal chains. Later, Zhang et al [6] gave a new proof of the results in [4] and [5]. In [7], Zhang determined the unique graph with minimal and second minimal Hosoya indices among all catacondensed systems. In [8], The path and star have been shown to have the maximal and minimal Hosoya indices resp. among all trees on n vertices. Hou in [9] characterized the trees having minimal and second minimal Hosoya indices among all trees with a given size of matching. [10], Yu et al investigated the graphs having minimal Hosoya index among all graphs with given edge-independence number and cyclomatic number. In [11], Yu et al investigated the trees having minimal Hosoya index among all trees with k-pendent vertices.

All graphs considered here are both finite and simple. We denote, respectively, by S_n and P_n the star and path with n vertices. By $T - u$ and $T - uv$, we denote respectively the graphs that arises from T by

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deleting the vertex $u \in V(T)$ and the edge $uv \in E(T)$. Likewise, $T + uv$ denotes the graph that arises from T by adding an edge $uv \notin E(T)$. Let $\mathcal{T}_{n,d}$ denote the set of trees of n vertices and diameter at d. A caterpillar is a tree if deleting all its pendent vertices will reduce it to a path.

Let (G_1, v_1) and (G_2, v_2) be two graphs rooted at v_1 and v_2 respectively, then $G = (G_1, v_1) \bowtie (G_1, v_2)$ denote the graph obtained by identifying v_1 with v_2 as one common vertex.

Let F_n denote the $n - th$ Fibonacci number, we have $F_n + F_{n+1} = F_{n+2}$ with initial conditions $F_0 = F_1 = 1$.

Other notations and terminology not defined here will conform to those in Ref.[1].

In this paper, we investigate the Hosoya index for trees in $\mathcal{T}_{n,d}$. We determined the unique trees with minimal Hosoya index among all trees in $\mathcal{T}_{n,d}$.

2 Main result and its proof

We begin with several important lemmas which will be helpful to the proofs of our main results .

Lemma 1 . ([8])*Let G be a graph and v any vertex in $V(G)$, then*

$$z(G) \quad = \quad z(G - v) + \sum_{u} z(G - \{u,\ v\})$$

where the summation extends over all vertices u adjacent to v.

Lemma 2. ([8])*Let G be a graph and uv any edge in $E(G)$, then*

$$z(G) = z(G - uv) + z(G - \{u,\ v\}).$$

Lemma 3. ([8])*Let G be a graph with m components $G_1,\ G_2,\ \cdots G_m$. Then $z(G) = \prod_{i=1}^{m} z(G_i)$.*

Lemma 4. ([12])*Let T be a tree. Then $n + 1 \le z(T) \le F_n$ and $z(T) = F_n$ if and only if $T \cong P_n$ and $z(T) = n + 1$ if and only if $T \cong S_n$.*

Lemma 5. *Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$ be two graphs. If $V(G_1) = V(G_2)$ and $E(G_1) \subset E(G_2)$, then $z(G_1) < z(G_2)$.*

Proof. Let $V(G_1) = V(G_2)$ and $E(G_2) = E(G_1) \bigcup \{e_1,\ e_2,\ \cdots e_k\}$, where $e_i = u_i v_i (i = 1, 2 \cdots k)$ are edges in $E(G_2)$.

Suppose $V(G_2^{(1)}) = V(G_2)$ and $E(G_2) = E(G_2^{(1)}) \bigcup \{e_1\}$. It follows from lemma 2 that $z(G_2) = z(G_2 - u_1 v_1) + z(G_2 - \{u_1,\ v_1\}) > z(G_2 - u_1 v_1) = z(G_2^{(1)})$. Let $V(G_2^{(1)}) = V(G_2^{(2)})$ and $E(G_2^{(1)}) = E(G_2^{(2)}) \bigcup \{e_2\}$, then by lemma 2 once again, we have $z(G_2^{(1)}) = z(G_2^{(1)} - u_2 v_2) + z(G_2^{(1)} - \{u_2,\ v_2\}) > z(G_2^{(1)} - u_2 v_2) = z(G_2^{(2)})$.
Similarly, we have $z(G_2) > z(G_2^{(1)}) > z(G_2^{(2)}) > \cdots > z(G_2^{(k)}) > z(G_1)$. This completes the proof. □

In the following, we shall investigate the smallest value of Hosoya index for trees in $\mathcal{T}_{n,d}$. Before we introduce our main results, we need to state and prove the following lemma.

Lemma 6. *For a given graph $G = (G', v_i) \bowtie (T, v_i)$, we have $z(G) \ge z((G', v_i) \bowtie (S_{n(T)}, v_i))$ with equality holding if and only if $T \cong S_{n(T)}$. Moreover, v_i is the center of $S_{n(T)}$.*

Proof. It follows from lemma 1 that

$$\begin{aligned} z(G) &= z(G-v_i)+\sum_{u\in N_G(v_i)} z(G-\{u,v_i\}) \\ &= z[(G^{'}-v_i)\bigcup(T-v_i)]+\sum_{u\in N_{G^{'}}(v_i)} z(G-\{u,v_i\})+\sum_{u\in N_T(v_i)} z(G-\{u,v_i\}) \\ &= z[(G^{'}-v_i)\bigcup(T-v_i)]+\sum_{u\in N_{G^{'}}(v_i)} z[(G^{'}-\{u,v_i\})\bigcup(T-v_i)] \\ &+ \sum_{u\in N_T(v_i)} z[(G^{'}-v_i)\bigcup(T-\{u,v_i\})]. \end{aligned}$$

Let $N_T(v_i)=\{v_{i1},\ \cdots v_{is}\}$ ($s\geq 1$) and $G_1=G^{'}-v_i$. By T_{ij}, we denote the subtree containing v_{ij} of $T-v_i$ for $j=1,\ 2,\ \cdots s$, then $T-v_i=\bigcup\limits_{j=1}^{s} T_{ij}$. By lemma 3, we have

$$\begin{aligned} z(G) &= z(G_1)z(\bigcup_{j=1}^{s} T_{ij})+\sum_{u\in N_{G^{'}}(v_i)} z(G_1-u)z(\bigcup_{j=1}^{s} T_{ij})+\sum_{u\in N_T(v_i)} z(G_1)z(\bigcup_{j=1}^{s} T_{ij}-u) \\ &= [z(G_1)+\sum_{u\in N_{G^{'}}(v_i)} z(G_1-u)]z(\bigcup_{j=1}^{s} T_{ij})+z(G_1)\sum_{k=1}^{s} z[(\bigcup_{j=1,j\neq k}^{s} T_{ij})\bigcup(T_{ik}-v_{ik})] \\ &= [z(G_1)+\sum_{u\in N_{G^{'}}(v_i)} z(G_1-u)]z(\bigcup_{j=1}^{s} T_{ij})+z(G_1)\sum_{k=1}^{s}\prod_{j=1,j\neq k}^{s} z(T_{ij})z(T_{ik}-v_{ik}). \end{aligned}$$

Let $x=z(G_1)+\sum\limits_{u\in N_{G^{'}}(v_i)} z(G_1-u)$ and $y=z(G_1)$. Then $x>y\geq 1$.

Let $A=z(\bigcup\limits_{j=1}^{s} T_{ij})$ and $B=\sum\limits_{k=1}^{s}\prod\limits_{j=1,j\neq k}^{s} z(T_{ij})z(T_{ik}-v_{ik})$. It's easy to see that $A=z(\bigcup\limits_{j=1}^{s} T_{ij})=\prod\limits_{j=1}^{s} z(T_{ij})\geq 1\times 1\times\cdots\times 1=1$. The above equality holds if and only if $T_{ij}\cong P_1$ for $j=1,\cdots s$, that is

$$T\cong S_{n(T)}. \tag{1}$$

Note that $B=\sum\limits_{k=1}^{s}\prod\limits_{j=1,j\neq k}^{s} z(T_{ij})z(T_{ik}-v_{ik})=\prod\limits_{j=1}^{s} z(T_{ij})\sum\limits_{k=1}^{s}\frac{z(T_{ik}-v_{ik})}{z(T_{ik})}$.

If $s=1$, then $B=z(T_{i1}-v_{i1})\geq 1$, where the equality holds if and only if $T_{i1}-v_{i1}\cong P_1$ or $T_{i1}-v_{i1}=\emptyset$.

If $s\geq 2$, without loss of generality, we may assume that $\frac{z(T_{i1}-v_{i1})}{z(T_{i1})}=min\{\frac{z(T_{ik}-v_{ik})}{z(T_{ik})},k=1,\cdots s\}$. Then $B\geq s\prod\limits_{j=1}^{s} z(T_{ij})\frac{z(T_{i1}-v_{i1})}{z(T_{i1})}=sz(T_{i1}-v_{i1})z(T_{i2})\cdots z(T_{is})\geq s\times 1\times 1\times\cdots\times 1=s$. Thus $B\geq s$ with equality holding if and only if the following three equations hold together:

$$\frac{z(T_{i1}-v_{i1})}{z(T_{i1})}=\frac{z(T_{ik}-v_{ik})}{z(T_{ik})}\quad for\quad k=1,\cdots,s; \tag{2}$$

$$T_{ij}\cong P_1\qquad for\quad j=2,\cdots s; \tag{3}$$

and

$$T_{i1}-v_{i1}\cong P_1\quad or\quad T_{i1}-v_{i1}=\emptyset. \tag{4}$$

If $T_{i1}-v_{i1}\cong P_1$, then $T_{i1}\cong P_2$. But then $\frac{z(T_{i1}-v_{i1})}{z(T_{i1})}=\frac{1}{2}\neq 1=\frac{z(T_{ik}-v_{ik})}{z(T_{ik})}\quad for\quad k=2,\cdots s$, a contradiction to (2). So $T_{i1}-v_{i1}=\emptyset$, that is $T_{i1}\cong P_1$. Combining this fact with Eq.(3), we have $B\geq s$ with equality holds if and only if $T_{ij}\cong P_1$ for $j=1,2,\cdots s$, i.e., $T\cong S_{n(T)}$.

When $s = 1$, we have $z(G) = Ax + By \geq 1.x + 1.y = z(G_1) + \sum_{u\in N_{G'}(v_i)} z(G_1 - u) + z(G_1) = z((G', v_i) \bowtie (S_2, v_i))$. The above equality holds if and only if $A = 1$ and $B = 1$. One can easily see that $T_{i1} - v_{i1} \not\cong P_1$, for otherwise $T_{i1} \cong P_2$. Then $A > 1$ and $z(G) > z((G', v_i) \bowtie (S_2, v_i))$. So $T_{i1} - v_{i1} = \emptyset$, i.e., $T_{i1} \cong P_1$. Thus $z(G) \geq z((G', v_i) \bowtie (S_2, v_i))$ with equality holding if and only if $T \cong S_2$.

When $s \geq 2$, we have

$$\begin{aligned} z(G) &= Ax + By \\ &\geq 1.x + s.y \\ &= z(G_1) + \sum_{u\in N_{G'}(v_i)} z(G_1 - u) + sz(G_1) \\ &= z((G', v_i) \bowtie (S_{n(T)}, v_i)). \end{aligned}$$

Thus, we have $z(G) \geq z((G', v_i) \bowtie (S_{n(T)}, v_i))$ with equality holding if and only if $A = 1$ and $B = s$. Combining this fact with Eq.(1), the above equality holds if and only if $T \cong S_{n(T)}$. This completes the proof. □

When $d = n - 1$ or $d = 2$, T is a path or star. We can easily determine its Hosoya index, so we will assume that $3 \leq d \leq n - 2$ in the following.

Lemma 7. *For $3 \leq d \leq n - 2$, let T be a tree in $\mathcal{T}_{n,d}$ such that $z(T)$ is as small as possible, then T is a caterpillar.*

Proof. Suppose T is a tree in $\mathcal{T}_{n,d}$ such that $z(T)$ is as small as possible and T isn't a caterpillar.

Let $P_{d+1} = v_0v_1 \cdots v_d$ be a diametrical path in T. Since $d \leq n - 2$, there exist at least one vertex v_i in P_{d+1} such that $d(v_i) \geq 3$ where $1 \leq i \leq d - 1$. Let $T(v_i)$ denote the subtree containing v_i of $T - \{v_{i-1}v_i, v_iv_{i+1}\}$. Since T is not a caterpillar , then there exist at least one vertex , say v_j in P_{d+1}, such that $d(v_j) \geq 3$ and $T(v_j)$ isn't a star. Let $N(v_j) - \{v_{j-1}, v_{j+1}\} = \{v_{j1}, \cdots, v_{jt}\}(t \geq 1)$ and $T'(v_j)$ denote the subtree containing v_j of $T - \{v_jv_{j1}, \cdots, v_jv_{jt}\}$.

Then $T = (T'(v_j), v_j) \bowtie (T(v_j), v_j)$. Since $d \geq 3$, then $T'(v_j)$ is not a star. Also, $T(v_j)$ is not a caterpillar by hypothesis. Then by lemma 6, we have $z(T) > z((T'(v_j), v_j) \bowtie (S_{n(T(v_j))}, v_j))$, where the graph $(T'(v_j), v_j) \bowtie (S_{n(T(v_j))}, v_j)$ is obtained by replacing $T(v_j)$ in T by the star $S_{n(T(v_j))}$. It's a contradiction to the minimality of T.

Therefore, the proof is completed. □

By $T(n, d; n_1, n_2, \cdots, n_{d-1})$, we denote a caterpillar in $\mathcal{T}_{n,d}$, where n_i $(i = 1, 2, \cdots d-1)$ is the number of pendent vertices adjacent to v_i $(i = 1, 2, \cdots d - 1)$.

Let $T_{n,d,1} = T(n, d; n-d-1, 0, \cdots, 0)$; $T_{n,d,2} = T(n, d; 0, n-d-1, \cdots, 0)$; ... $T(n, d; 0, 0, \cdots, n-d-1, \cdots, 0) = T_{n,d,i}$, ... $T(n, d; 0, 0, \cdots 0, n - d - 1) = T_{n,d,d-1}$.

Lemma 8. *Let T be a tree in $\mathcal{T}_{n,d}$ such that $z(T)$ is as small as possible, then $T \cong T_{n,d,i}$, where $3 \leq d \leq n - 4$ and $1 \leq i \leq d - 1$.*

Proof. Let T be a tree in $\mathcal{T}_{n,d}$ such that $z(T)$ is as small as possible. From lemma 7, we know that T is a caterpillar.

Let $P_{d+1} = v_0v_1 \cdots v_d$ be a diametrical path in T. Since $d \leq n - 4$, then there're at least three pendent vertices lying outside the path P_{d+1}.

We distinguish between the following two cases.

Case 1 There exists some v_i $(1 \leq i \leq d - 1)$ such that $d(v_i) \geq 4$.

If $d(v_j) = 2$ for $1 \leq j \leq d - 1, j \neq i$, then the result holds. Suppose that there exist some v_j in the path P_{d+1} such that $d(v_j) \geq 3$.

Let $N(v_i) - \{v_{i-1}, v_{i+1}\} = \{v_{i1}, \cdots, v_{im}\}$ and $N(v_j) - \{v_{j-1}, v_{j+1}\} = \{v_{j1}, \cdots, v_{jk}\}$. Without loss of generality, we may assume that $1 \leq i < j \leq d - 1$.

Let T' be obtained as follows.

$$T^{'} = T - v_jv_{j1} - \cdots - v_jv_{jk} + v_iv_{j1} + \cdots + v_iv_{jk}.$$

We will show that $z(T) > z(T^{'})$ by induction on the order of T. Assume that the result holds for trees T in $\mathcal{T}_{n-1,d}$.

From lemma 1, we have

$$z(T^{'}) = z(T^{'} - v_{i1}) + z(T^{'} - \{v_{i1}, v_i\}),$$

and

$$z(T) = z(T - v_{i1}) + z(T - \{v_{i1}, v_i\}).$$

Since $T - v_{i1} \in \mathcal{T}_{n-1,d}$, then we have $z(T - v_{i1}) > z(T^{'} - v_{i1})$ by induction hypothesis.

Also, $z(T^{'} - \{v_{i1}, v_i\}) = z(T_1)z(T_2)z[(m+k-1)P_1] = z(T_1)z(T_2 \bigcup kP_1)z[(m-1)P_1]$ and $z(T - \{v_{i1}, v_i\}) = z(T_3)z(T_4)z[(m-1)P_1]$, where T_1 and T_2 denote resp. the subtrees containing v_{i-1} and $v_{i+1}$of $T^{'} - v_i$, while T_3 and T_4 denote resp. the subtrees containing v_{i-1} and $v_{i+1}$of $T - v_i$. Obviously $T_1 \cong T_3$.

Note that $V(T_2 \bigcup kP_1) = V(T_4)$ and $E(T_2 \bigcup kP_1) \subset E(T_4)$. So $z(T_2 \bigcup kP_1) < z(T_4)$ by lemma 5. Thus $z(T - \{v_{i1}, v_i\}) > z(T^{'} - \{v_{i1}, v_i\})$ and then $z(T) > z(T^{'})$, a contradiction to the choice of T.

Case 2 For each $1 \leq i \leq d-1$, $d(v_i) = 2$ or 3.

Since $d \leq n-4$, there exist at least three pendent vertices lying outside the path P_{d+1}. Let v_i be a vertex with $d(v_i) = 3$. we obtain $T^{'}$ by deleting all the pendent edges of T incident with each v_j ($1 \leq j \leq d-1$ and $j \neq i$) and attaching all the deleted edges to the vertex v_i.

We will prove that $z(T) > z(T^{'})$ by induction on the order of T. Assume that the result holds for trees T in $\mathcal{T}_{n-1,\,d}$.

Let u be the pendent vertex adjacent to v_i in T. From lemma 1, we have

$$z(T^{'}) = z(T^{'} - u) + z(T^{'} - \{u, v_i\}),$$

and

$$z(T) = z(T - u) + z(T - \{u, v_i\}).$$

Since $T - u \in \mathcal{T}_{n-1,\,d}$, we have $z(T - u) > z(T^{'} - u)$ by induction hypothesis.

By T_1 and T_2, we denote resp . the subtrees containing v_{i-1} and $v_{i+1}$of $T - v_i$. Then $z(T - \{u, v_i\}) = z(T_1 \bigcup T_2)$ and $z(T^{'} - \{u, v_i\}) = z[P_i \bigcup P_{d-i} \bigcup (n-d-2)P_1]$.

One can easily see that $V(T_1 \bigcup T_2) = V(P_i \bigcup P_{d-i} \bigcup (n-d-2)P_1)$ and $E(P_i \bigcup P_{d-i} \bigcup (n-d-2)P_1) \subset E(T_1 \bigcup T_2)$. So $z(T - \{u, v_i\}) > z(T^{'} - \{u, v_i\})$ by lemma 5. Thus $z(T) > z(T^{'})$, a contradiction to the choice of T once again.

Therefore, the desired result follows from the proofs of cases 1 and 2. □

Lemma 9. *For* $2 \leq i \leq \lfloor \frac{n}{2} \rfloor$, *we have* $z(P_i \bigcup P_{n-i}) > z(P_1 \bigcup P_{n-1})$.

Proof. It follows from lemmas 3 and 4 that $z(P_i \bigcup P_{n-i}) - z(P_{i-1} \bigcup P_{n-i+1}) = z(P_i)z(P_{n-i}) - z(P_{i-1})z(P_{n-i+1}) = F_iF_{n-i} - F_{i-1}F_{n-i+1}$. Note that

$$\begin{aligned} F_iF_{n-i} - F_{i-1}F_{n-i+1} &= (F_{i-1} + F_{i-2})(F_{n-i+1} - F_{n-i-1}) - F_{i-1}F_{n-i+1} \\ &= -(F_{i-1}F_{n-i-1} - F_{i-2}F_{n-i}) \\ &= \cdots \\ &= (-1)^{i-1}(F_1F_{n-2i+1} - F_0F_{n-2i+2}) \\ &= (-1)^iF_{n-2i}. \end{aligned}$$

So, for $2 \leq i \leq \lfloor \frac{n}{2} \rfloor$, we have $F_iF_{n-i} - F_1F_{n-1} = (F_{n-4} - F_{n-6}) + (F_{n-8} - F_{n-10}) + \cdots > 0$, that is $F_iF_{n-i} > F_1F_{n-1}$. This completes the proof. □

In the following, we will determine the unique trees in $\mathcal{T}_{n,d}$ having the smallest Hosoya index.

Theorem 10. *Let T be a tree in $\mathcal{T}_{n,d}$ with $3 \leq d \leq n-2$, then $z(T) \geq z(T_{n,d,1})$ with equality holds if and only if $T \cong T_{n,d,1}$.*

Proof. Suppose that T is a tree in $\mathcal{T}_{n,d}$ with $z(T)$ taking the smallest value.

We distinguish among the following three cases.

Case 1. $3 \leq d \leq n-4$.

By lemma 8, we have $T \cong T_{n,d,i}$ in this case. In the following, we'll show that $z(T_{n,d,i}) \geq z(T_{n,d,1})$ and the equality holds if and only if $i = 1$, i.e., $T_{n,d,i} \cong T_{n,d,1}$.

We proceed by induction on the order of T. Suppose that the result holds for all trees in $\mathcal{T}_{n-1,\ d}$ with $3 \leq d \leq n-4$. For $1 \leq i \leq d-1$, let u_i be one pendent vertex adjacent to v_i (in fact, the maximum-degree vertex in $T_{n,d,i}$).

From lemma 1, we have

$$\begin{aligned} z(T_{n,\ d,\ i}) &= z(T_{n,\ d,\ i} - u_i) + z(T_{n,\ d,\ i} - \{u_i,\ v_i\}) \\ &= z(T_{n-1,\ d,\ i}) + z[(n-d-2)P_1 \bigcup P_i \bigcup P_{d-i}]. \end{aligned}$$

Since $T_{n,\ d,\ i} - u_i \in \mathcal{T}_{n-1,\ d}$, then by induction hypothesis, we have $z(T_{n-1,\ d,\ i}) \geq z(T_{n-1,\ d,\ 1})$ with equality holds if and only if $T_{n-1,\ d,\ i} \cong T_{n-1,\ d,\ 1}$.

Moreover, it follows from lemma 9 that $z[(n-d-2)P_1 \bigcup P_i \bigcup P_{d-i}] = z(P_i \bigcup P_{d-i}) \geq z(P_1 \bigcup P_{d-1}) = z[(n-d-2)P_1]z(P_1 \bigcup P_{d-1}) = z[(n-d-1)P_1 \bigcup P_{d-1}]$ with equality holds if and only if $i = 1$. Thus, $z(T_{n,\ d,\ i}) \geq z(T_{n,\ d,\ 1})$ with equality holds if and only if $i = 1$, that is $T_{n,\ d,\ i} \cong T_{n,\ d,\ 1}$.

Case 2. $d = n-2$.

Then there exists exactly one pendent vertex, say u in T, lying outside the diametrical path P_{d+1}.

Let v_i be the unique neighbor of u in T. Then $z(T) = z(T-u) + z(T - \{u,\ v_i\}) = z(P_{d+1}) + z(P_i \bigcup P_{d-i}) \geq z(P_{d+1}) + z(P_1 \bigcup P_{d-1}) = z(T_{n,\ n-2,\ 1})$ with equality holds if and only if $i = 1$, that is $T \cong T_{n,\ n-2,\ 1}$.

Case 3. $d = n-3$.

By lemma 7, T is a caterpillar. Then there are exactly two pendent vertices lying outside the diametrical path P_{d+1}.

The following two subcases should be considered.

Subcase 3.1. $T \cong T_{n,\ n-3,\ i}$ for some positive integer $i \in [1,\ d-1]$.

Let v_i be the vertex of degree 4 (in fact, the maximum-degree vertex) in $T_{n,\ n-3,\ i}$ and u be one pendent vertex adjacent to v_i.

Let u' be one pendent vertex adjacent to v_1 in $T_{n,\ n-3,\ 1}$. From lemma 1, we have

$$\begin{aligned} z(T_{n,\ n-3,\ i}) &= z(T_{n,\ n-3,\ i} - u) + z(T_{n,\ n-3,\ i} - \{u,\ v_i\}) \\ &= z(T_{n-1,\ n-3,\ i} - u) + z(P_1 \bigcup P_i \bigcup P_{d-i}), \end{aligned}$$

and

$$\begin{aligned} z(T_{n,\ n-3,\ 1}) &= z(T_{n,\ n-3,\ 1} - u') + z(T_{n,\ n-3,\ 1} - \{u',\ v_1\}) \\ &= z(T_{n-1,\ n-3,\ 1} - u) + z(2P_1 \bigcup P_{d-1}). \end{aligned}$$

From the proof of case 2, we have $z(T_{n-1,\ n-3,\ i}) \geq z(T_{n-1,\ n-3,\ 1})$. Also, $z(P_1 \bigcup P_i \bigcup P_{d-i}) = z(P_1)z(P_i \bigcup P_{d-i}) = z(P_i \bigcup P_{d-i}) \geq z(P_1 \bigcup P_{d-1}) = z(P_1)z(P_1 \bigcup P_{d-1}) = z(2P_1 \bigcup P_{d-1})$ by lemma 9. The above equality holds if and only if $i = 1$. Hence $z(T_{n,\ n-3,\ i}) \geq z(T_{n,\ n-3,\ 1})$ with equality holds if and only if $i = 1$, i.e., $T_{n,\ n-3,\ i} \cong T_{n,\ n-3,\ 1}$.

Subcase 3.2. $T \ncong T_{n,\ n-3,\ i}$ for any positive integer $i \in [1,\ d-1]$.

There are exactly two pendent vertices lying outside the diametrical path P_{d+1}. Let u be one of such pendent vertices and v_i its unique neighbor. Let u' be one pendent vertex of $T_{n,\ n-3,\ 1}$ adjacent to v_1. we shall show that $z(T) > z(T_{n,\ n-3,\ 1})$.

By lemma 1, we have

$$\begin{aligned} z(T_{n,\ n-3,\ 1}) &= z(T_{n,\ n-3,\ 1} - u^{'}) + z(T_{n,\ n-3,\ 1} - \{u^{'},\ v_1\}) \\ &= z(T_{n-1,\ n-3,\ 1}) + z(2P_1 \bigcup P_{d-1}), \end{aligned}$$

and

$$\begin{aligned} z(T) &= z(T-u) + z(T - \{u,\ v_i\}) \\ &= z(T-u) + z(P_i \bigcup T_0). \end{aligned}$$

where $T-u \in \mathcal{T}_{n-1,\ n-3}$ and $T_0 \cong P_{d-i+1}$ or $T_0 \in \mathcal{T}_{d-i+1,\ d-i-1}$.

Since $T-u \in \mathcal{T}_{n-1,\ n-3}$, then by the proof case 2, we have $z(T-u) \geq z(T_{n,\ n-3,\ 1})$.

If $T_0 \cong P_{d-i+1}$, then $z(P_i \bigcup T_0) = z(P_i \bigcup P_{d-i+1} \geq z(P_1 \bigcup P_d) = z(P_d) > z(P_1 \bigcup P_{d-1}) = z(P_1)z(P_1 \bigcup P_{d-1}) = z(2P_1 \bigcup P_{d-1})$ by lemmas 3 and 5. Thus $z(T) > z(T_{n,\ n-3,\ 1})$, contradicting to the minimality of $z(T)$.

If $T_0 \in \mathcal{T}_{d-i+1,\ d-i-1}$, then $z(T_0) > z(P_{d-i})$. So $z(P_i \bigcup T_0) = z(P_i)z(T_0) > z(P_i)z(P_{d-i}) \geq z(P_1)z(P_{d-1}) = z(P_1 \bigcup P_{d-1}) = z(P_1)z(P_1 \bigcup P_{d-1}) = z(2P_1 \bigcup P_{d-1})$. Thus $z(T) > z(T_{n,\ n-3,\ 1})$, a contradiction to the minimality of $z(T)$ once again.

This completes the proof. □

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