Extremal trees for the modified first Zagreb connection index with fixed number of segments or vertices of degree 2

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1. Introduction

Throughout the paper, we are concerned with only simple and finite graphs. For a vertex \( v \in V(G) \), the degree of \( v \) is denoted by \( d_v \) and is defined as the number of vertices adjacent to \( v \). By an \( n \)-vertex graph, we mean a graph with \( n \) vertices. Denote by \( N(v) \) the set of all vertices adjacent to a vertex \( v \in V(G) \). If \( V(G) = \{v_1, v_2, \ldots, v_n\} \) is the vertex set of a graph \( G \), the sequence \( (d_{v_1}, d_{v_2}, \ldots, d_{v_n}) \) is called degree sequence of \( G \). Undefined terminologies and notations of (chemical) graph theory can be found in [1–3].

A topological index is a numerical value associated with a graph in such a way that it remains unchanged under graph isomorphism. Many topological indices have been extensively used in mathematical chemistry to predict the certain properties of chemical compounds. The first Zagreb index \( M_1 \) (appeared in [4]) and the second Zagreb index \( M_2 \) (devised in [5]) are among the oldest and the most studied degree-based topological indices. For a graph \( G \), these indices are defined as:

\[
M_1(G) = \sum_{v \in V(G)} (d_v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_ud_v,
\]

where \( E(G) \) represents the edge set of \( G \). Till now, many papers have been devoted to these Zagreb indices, for example see the surveys [6–8], particularly the recent ones [9–12], the papers [13–24], and the related references cited therein.

The following topological index \( ZC_1^1 \) is known as the modified first Zagreb connection index [14] and is defined as

\[
ZC_1^1(G) = \sum_{v \in V(G)} d_v \tau_v
\]

where \( \tau_v \) is the connection number of the vertex \( v \) (i.e. the number of vertices having distance 2 from \( v \), see in [25]). Actually, the topological index \( ZC_1^1 \) was initially appeared within a formula of the total electron energy of alternant hydrocarbons, derived by Gutman and Trinajstić [4] in 1972. It needs to be mentioned here that the index \( ZC_1^1 \) was referred as the third leap Zagreb index in [26]. After appearance of the papers [14, 26], mathematical properties of the modified first Zagreb connection index \( ZC_1^1 \) have been studied in a considerable number of papers [26–38].

A vertex of degree at least 3 is called a branching vertex. Let \( P : u_0u_1u_2 \cdots u_r \) be a path of length \( r \geq 2 \) in a graph. The vertices \( u_0 \) and \( u_r \) are called terminal vertices of \( P \). If \( r \geq 3 \), the vertices \( u_1, u_2, \ldots, u_{r-1} \) are called non-terminal vertices of \( P \). An internal path in a graph is a path in which both the terminal vertices are branching and all the non-terminal vertices (if exist) have degree 2. A segment of a tree \( T \) is a non-trivial path \( P' \) in \( T \) with the property that neither of the terminal vertices of \( P' \) has degree 2 and that all the non-terminal vertices (if exist) of \( P' \) have degree 2.
Denote by $T'_{n,k}$ the class of all $n$-vertex trees with exactly $k$ segments. In this paper, our aim is to provide a solution of the following problem.

**Problem 1.1:** Characterize all the graphs with the maximal/minimal modified first Zagreb connection index $ZC_1^*$ from the class $T'_{n,k}$.

It can easily be observed that the $n$-vertex path graph, $P_n$, is the unique element of $T'_{n,1}$, whereas the class $T'_{n,2}$ is empty. Thus, Problem 1.1 is well-defined for $3 \leq k \leq n - 1$. Also, Ducoffe et al. [30] proved that the star graph $S_n$ has the maximal $ZC_1^*$ value among all the $n$-vertex trees, which implies that $S_n$ has the maximal $ZC_1^*$ value among all the members of $T'_{n,n-1}$ as well. Consequently, while solving Problem 1.1 concerning maximal $ZC_1^*$ value, we will consider the constrain $3 \leq k \leq n - 2$, and while solving the remaining part of Problem 1.1 we will assume $3 \leq k \leq n - 1$.

It is well-known fact that the number of segments in a tree can be determined from the number of vertices of degree 2 (and vice versa), see [39] for details. Thus, graphs with the extremum $ZC_1^*$ values in the class of all $n$-vertex trees having fixed number of vertices of degree 2, follows directly from the solution of Problem 1.1.

### 2. On the minimum modified first Zagreb connection index of trees with given number of segments

Let $ST_{min}' \in T'_{n,k}$ be the tree with the minimal modified first Zagreb connection index among all the members of $T'_{n,k}$, where $3 \leq k \leq n - 1$ and $n > 5$ because for $n = 4$ and $n = 5$, we have trivial results. In order to prove the main result of this section, we firstly prove some lemmas concerning the structure of the tree $ST_{min}'$. Throughout this section, whenever we consider a tree $T$ with the property $V(T) = V(ST_{min}')$, then by $dv_r$ and $N(v)$ we always mean the degree of the vertex $v$ in $ST_{min}'$ and the set of vertices adjacent to $v$ in $ST_{min}'$, respectively.

**Lemma 2.1:** The tree $ST_{min}' \in T'_{n,k}$ has the maximum degree at most 4.

**Proof:** Contrarily, we assume that $ST_{min}'$ contains a vertex $v$ of degree greater than 4. Let $P : v_0v_1 \cdots v_{k-1}v_k(= v) v_1v_2 \cdots v_{i-1}v_{i+1}$ be a longest path in a tree $ST_{min}' \in T'_{n,k}$ containing $v$. It is obvious that $dv_k = dv_{i+1} = 1$. Suppose that the vertices $u_1$ and $u_2$ are those neighbors of $v$, that do not lie on the path $P$. If $T' = ST_{min}' - \{u_1v, u_2v\} + \{u_1v_{i+1}, u_2v_{i+1}\}$, then $T' \in T'_{n,k}$. We consider two cases.

**Case 1:** $i = r$ or $i = 1$.

We only consider the possibility $i = r$ because for $i = 1$, the proof is analogous. We note that all the neighbors of the vertex $v$, except $v_{i-1}$ are pendant vertices.

Because of the fact $dv_r \geq 2$, we have

$$ZC_1^*(ST_{min}') - ZC_1^*(T') = (dv_r - 1)(dv_r - dv_r - 1) + 2dv_r dv_{i-1} - dv_r - dv_{i-1}$$

which is a contradiction to the choice of $ST_{min}'$.

**Case 2:** $2 \leq i \leq r - 1$.

The inequalities $dv_r \geq 5$, and $dv_i \leq 4$ implies that

$$\sum_{z \in N(v), z \neq u_1, u_2} (4dv_r - 2) \geq (4dv_r - 2).$$

Thus, we have

$$ZC_1^*(ST_{min}') - ZC_1^*(T') = (2dv_r - dv_r - dv_r - dv_r) + (2dv_r dv_r - dv_r - dv_r) + (2dv_r - dv_r - dv_r) + (2dv_r - dv_r - dv_r - 1) - (2dv_r - dv_r - dv_r - 2) - (2dv_r - dv_r - dv_r - 2) + (2dv_r - dv_r - dv_r - dv_r - 2) + (2dv_r - dv_r - dv_r - dv_r - 2) > 0,$$

which is again a contradiction to minimality of $ST_{min}'$.

**Lemma 2.2:** The tree $ST_{min}' \in T'_{n,k}$ contains at most one vertex of degree 4.

**Proof:** Contrarily, assume that $v_i$ and $v_j$, with $i < j$, are two vertices of degree 4 in $ST_{min}'$. Let $P : v_0v_1 \cdots v_{i-1}v_i v_{i+1} \cdots v_{j-1}v_j v_{j+1}$ be a longest path in $ST_{min}' \in T'_{n,k}$ containing $v_i$ and $v_j$ such that $dv_k \leq 3$ for $j + 1 \leq k \leq r$ whenever $j < r$. Certainly, $dv_0 = dv_{i+1} = 1$. Suppose that $u_1, u_2$ are those neighbors of $v_i, v_j$, respectively, that do not lie on the path $P$. If $T' = ST_{min}' - \{u_1v_i, u_2v_j\} + \{u_1v_{i+1}, u_2v_{j+1}\}$, then it is obvious that $T' \in T'_{n,k}$.

**Case 1:** $j = r$ and $j \neq i + 1$. 


We note that all the neighbors of \( v_i \) except \( v_{i-1} \) are pendant. Bearing in mind the facts \( d_{v_{i-1}} \geq 2 \) and
\[
\sum_{x \in N(v_j), x \neq u_1} (2d_x - 1) \geq 5,
\]
we get
\[
Z^*_c(ST'_\text{min}) - Z^*_c(T') = (2(4)d_{u_1} - 4 - d_{u_1}) + \sum_{x \in N(v_j), x \neq u_1} (2(4)d_x - 4 - d_x)
+ 3(2(4)(1) - 4 - 1) + (2(4)(d_{v_{i-1}}) - 4 - d_{v_{i-1}})
- \sum_{x \in N(v_j), x \neq u_1} (2(3)d_x - 3 - d_x)
- (2(3)(d_{v_{i-1}}) - 3 - d_{v_{i-1}})
- (2(3)(1) - 1 - 3) - (2(3)(3) - 3 - 3)
- (2(3)d_{u_1} - 3 - d_{u_1})
- (2(3) - 3 - 1)
= 2d_{u_1} + 2d_{v_{i-1}} - 9 + \sum_{x \in N(v_j), x \neq u_1} (2d_x - 1) > 0,
\]
which is a contradiction to the choice of \( ST'_\text{min} \).

Case II. \( j \neq r, j \neq i + 1 \).

From the inequalities
\[
\sum_{x \in N(v_j), x \neq u_1} (2d_x - 1) \geq 5,
\]
\[
\sum_{y \in N(v_j), y \neq u_2} (2d_y - 1) \geq 7,
\]
and \( d_{v_j} \leq 3 \), it follows that
\[
Z^*_c(ST'_\text{min}) - Z^*_c(T') = \sum_{x \in N(v_j), x \neq u_1} (2d_x - 1) + \sum_{y \in N(v_j), y \neq u_2} (2d_y - 1)
+ 2d_{u_1} + 2d_{v_{i-1}} - 4d_{v_j} > 0,
\]
which is again a contradiction to the minimality of \( Z^*_c(ST'_\text{min}) \).

Case III. \( j = i + 1, j \neq r \).

In this case, we have
\[
Z^*_c(ST'_\text{min}) - Z^*_c(T') = \sum_{x \in N(v_j), x \neq u_1, v_j} (2d_x - 1) + \sum_{y \in N(v_j), y \neq u_2, v_j} (2d_y - 1)
+ 2d_{u_1} + 2d_{u_2} - 4d_{v_j} + 12 > 0,
\]
again a contradiction.

Case IV. \( j = r \) and \( r = i + 1 \).

It is clear that, in this case, \( v_j \) has three pendant neighbors. If \( x \) is a neighbor of \( v_j \) different from the vertices \( u_1, v_{i-1}, v_j \), then it holds that
\[
Z^*_c(ST'_\text{min}) - Z^*_c(T') = 2d_{u_1} + 2d_{v_{i-1}} + 2d_x + 2 > 0,
\]
which is again a contradiction.

In each of the four possible cases, we arrive at a contradiction and hence we conclude that the tree \( ST'_\text{min} \) cannot have more than one vertex of degree 4.

Denote by \( |V_i(G)| \) (or simply, by \( |V_i| \)) the number of vertices of degree \( i \) in a graph \( G \). From Lemmas 2.1 and 2.2, it follows that \( |V_i(ST'_\text{min})| = 0 \) for \( i \geq 5 \) and \( |V_4(ST'_\text{min})| = 0 \) or 1.

**Lemma 2.3:** For the tree \( ST'_\text{min} \in T'_n,k \) with \( 3 \leq k \leq n - 1 \), the following result hold.

(a) \( |V_4| = 0 \) if and only if \( k \equiv 1(\operatorname{mod} 2) \), \( |V_3| = \frac{k+1}{2} \) and
\( |V_3| = \frac{k-1}{2} \).

(b) \( |V_4| = 1 \) if and only if \( k \equiv 0(\operatorname{mod} 2) \), \( |V_1| = \frac{k+4}{2} \) and
\( |V_3| = \frac{k-4}{2} \).

**Proof:** By Lemmas 2.1, the tree \( ST'_\text{min} \) has maximum degree at most 4. Thus, it holds that
\[
n = |V_1| + |V_2| + |V_3| + |V_4| (1)
\]
and
\[
|V_1| + 2|V_2| + 3|V_3| + 4|V_4| = 2(n - 1).
\]
From Equations (1) and (2), it follows that
\[
|V_1| = |V_3| + 2|V_4| + 2. \quad (3)
\]
By using (3) in the equation \( k = (|V_1| + |V_3| + |V_4|) - 1 \), we get
\[
k \equiv |V_4| + 1 \quad (\text{mod} 2). \quad (4)
\]
Now, by using the identity \( |V_2| = n - k - 1 \) (see [39] for details) in (2), we have
\[
|V_1| + 4|V_4| = 2k - 3|V_3|. \quad (5)
\]
By solving (3) and (5) for the unknowns \( |V_1| \) and \( |V_3| \), we get
\[
|V_1| = \frac{k + |V_4| + 3}{2} \quad (6)
\]
and
\[
|V_3| = \frac{k - 3|V_4| - 1}{2}. \quad (7)
\]
From (4), (6) and (7), the desired results follow.

Now, in order to obtain the exact structure of the tree \( ST'_\text{min} \), we need to place the vertices of degree 2 on the appropriate place and for this purpose, we prove the following lemmas.

**Lemma 2.4:** If the tree \( ST'_\text{min} \in T'_n,k \) contains at least two branching vertices (that is, if \( k \geq 5 \)), then it does not contain any pendant vertex adjacent to a vertex of degree 2.
Proof: Contrarily, we assume that there is a path $P: u_0 u_1 u_2 \cdots u_{t-1} u_t$ in $ST_{\min}^*$ where $d_i \geq 3$, $d_{u_0} = 1$, $d_{u_t} = \cdots = d_{u_{t-1}} = 2$ and $t \geq 1$. Let $w$ be a neighbor of $v$ lying on some internal path (the existence of $w$ is confirmed because of the assumption that the number of branching vertices is greater than one). If $T' = ST_{\min}^* - \{u_0 u_1, u_1 v, vw\} + \{u_0 v, uv_0, u_0 w\}$ then $T' \in T_{n,k}'$. Now, we have

$$ZC_1^*(ST_{\min}^*) - ZC_1^*(T') = 2d_v - 2d_v - 4d_w + 4,$$

which is positive because the function $f$ defined by $f(x,y) = 2x - 2y + 4$, with $x \geq 3$ and $y \geq 2$, is increasing in both variables $x$ and $y$, hence we have $ZC_1^*(T') < ZC_1^*(ST_{\min}^*)$, a contradiction to the definition of $ST_{\min}^*$. ■

Lemma 2.5: If the tree $ST_{\min}^* \in T_{n,k}'$ contains any pair of adjacent branching vertices, then it does not contain any internal path of length greater than 2.

Proof: Contrarily, we assume that there is an internal path $u_1 u_2 \cdots u_t$ of length at least 3 in $ST_{\min}^*$ and that there exists a pair of adjacent branching vertices $u$ and $v$ in $ST_{\min}^*$. Let $T' = ST_{\min}^* - \{u_1 u_2, u_2 u_3, uv\} + \{u_1 u_3, u_2 u_2, u_2 v\}$, then $T' \in T_{n,k}'$ and

$$ZC_1^*(ST_{\min}^*) - ZC_1^*(T') = 2d_v - 4d_u - 4d_v + 8,$$

which is positive because the function $f$ defined by $f(x,y) = 2x - 2y + 4$, with $3 \leq x, y \leq 4$, is an increasing function in both variables $x$ and $y$. Hence, we have $ZC_1^*(T') < ZC_1^*(ST_{\min}^*)$, a contradiction. ■

Lemma 2.6: If the tree $ST_{\min}^* \in T_{n,k}'$ contains an edge connecting a vertex of degree 3 and the vertex $u$ of degree 4, then $ST_{\min}^*$ does not contain a vertex of degree 2 with neighbors different from $u$.

Proof: Assume contrarily, that $y, z, v, w$ be the vertices of the tree $ST_{\min}^* \in T_{n,k}'$ such as $uy, zv, vw \in E(ST_{\min}^*)$, $d_y = d_z = 3, d_w = 2$ and $d_v = 2$ (y may coincide with z). If $T' = ST_{\min}^* - \{yz, zv, vw\} + \{uy, vy, zv\}$, $T' \in T_{n,k}'$ and it can be easily seen that the difference $ZC_1^*(ST_{\min}^*) - ZC_1^*(T')$ is equal to 2 or 4 if $d_w = 3$ or 2, respectively. Hence $ZC_1^*(T') < ZC_1^*(ST_{\min}^*)$, a contradiction to the choice of $ST_{\min}^*$. ■

Lemma 2.7: In the tree $ST_{\min}^* \in T_{n,k}'$, the vertex of degree 4 (if exists) contains at most one non-pendant neighbor.

Proof: We assume contrarily that the vertex $u$ of degree 4 in $ST_{\min}^*$ contains at least two non-pendant neighbors (say) $v$ and $w$. Then Lemmas 2.1 and 2.2 ensure that every branching vertex other than $u$ has degree 3. Let $P = v_0 v_1 \cdots v_{i-1} = (v_i v_{i+1} = u) v_{i+1} (w) \cdots v_{i+1}$ be the longest path containing $u, v$ and $w$, where $w$ may coincide with $v$. Keeping in mind Lemma 2.4, one can conclude that $d_v = d_v = 3, 2 \leq d_{v_{i+1}} \leq 3$ and $d_{v_0} = d_{v_{i+1}} = 1$. Let $T' = ST_{\min}^* - \{v_0 v_1, v_{i+1} v_{i+1}, v_{i+1} + 1\}$ and $T' \in T_{n,k}'$, and we have

$$ZC_1^*(ST_{\min}^*) - ZC_1^*(T') = 2(d_v - 1) > 0,$$

which is a contradiction to the choice of $ST_{\min}^*$. ■

Denote by $x_{ij}(G)$ (or simply by $x_{ij}$) the number of edges in a graph $G$ connecting the vertices of degrees $i$ and $j$, then the following system of equations holds for any tree $T$ with maximum degree at most 4:

$$\sum_{1 \leq i \leq 4} x_{ij} + 2x_{ij} = j \cdot n_j$$

where $j = 1, 2, 3, 4$. Denote by $ST_{1}'(n,k)$, for $k \equiv 1(\mod 2)$, the set of all $n$-vertex trees with the degree sequence given as $(3, \ldots, 3, 2, \ldots, 2, 1, \ldots, 1)$ satisfying the following conditions:

- $x_{1,2} = 0$ and $x_{1,3} = \frac{k+3}{2}$,
- $x_{3,3} \neq 0$ implies that $x_{2,2} = 0$,
- $x_{3,3} = 0$ implies that $x_{2,2} \geq 0$. Similarly, we denote by $ST_2'(n,k)$, for $k \equiv 0(\mod 2)$, the set of all $n$-vertex trees with the degree sequence given as $(4, \ldots, 4, 3, \ldots, 3, 2, \ldots, 2, 1, \ldots, 1)$ satisfying the following conditions:

$$\sum_{1 \leq i \leq 4} x_{ij} + 2x_{ij} = j \cdot n_j$$

where $j = 1, 2, 3, 4$ implies that $x_{2,2} = 0$,
- $x_{3,4} = 1$ implies that $x_{3,4} = 0$, for $j = 2, 3$,
- $x_{3,4} = 0$ for $j = 3, 4$ implies that $x_{2,2} \geq 0$.

Now we can state the following theorem.

Theorem 2.1: Let $T \in T_{n,k}'$ where $3 \leq k \leq n - 1$, then

$$ZC_1^*(T) \geq \begin{cases} 2n + 5k - 17 & \text{if } n < \frac{3k-1}{2} \text{ and } k \equiv 1(\mod 2), \\ 4n + 2k - 16 & \text{if } n \geq \frac{3k-1}{2} \text{ and } k \equiv 1(\mod 2), \\ 7k - 23 & \text{if } n = k + 1 \text{ and } k \equiv 0(\mod 2), \\ 2n + 5k - 16 & \text{if } n < \frac{3k-2}{2} \text{ and } k \equiv 0(\mod 2), \\ 4n + 2k - 14 & \text{if } n \geq \frac{3k-2}{2} \text{ and } k \equiv 0(\mod 2). \end{cases}$$

The equality holds if and only if $T \in ST_1'(n,k)$, for $k \equiv 1(\mod 2)$, or $T \in ST_2'(n,k)$, for $k \equiv 0(\mod 2)$.

Proof: By Lemmas 2.1–2.5, one can conclude that the tree $ST_{\min}^* \in ST_1'(n,k)$, for $k \equiv 1(\mod 2)$. Now, if $|V_2(ST_{\min}^*)| < |V_1(ST_{\min}^*)| - 1$, that is $n < \frac{3k-1}{2}$, by using (8) and Lemmas 2.3 and 2.5, we get $x_{2,2} = 0, x_{2,3} = $...
2n - 2k - 2 and \( x_{3,3} = \frac{3k - 2n - 1}{2} \). Also, if \( |V_2(ST'_{\text{min}})| \geq |V_3(ST'_{\text{min}})| - 1 \), that is \( n \geq \frac{3k - 2}{2} \), then Lemmas 2.3-2.5 along with (8) imply that \( x_{3,3} = 0, x_{2,3} = k - 3, x_{2,2} = \frac{2n - 3k + 1}{2} \). Hence,

\[
ZC^*_1(ST'_{\text{min}}) = 2n + 5k - 17 \quad \text{if } n < \frac{3k - 1}{2} \quad \text{and} \quad k \equiv 1 \pmod{2},
\]

and

\[
ZC^*_1(ST'_{\text{min}}) = 4n + 2k - 16 \quad \text{if } n \geq \frac{3k - 1}{2} \quad \text{and} \quad k \equiv 1 \pmod{2}.
\]

Similarly, by Lemmas 2.1-2.7, one can conclude that the tree \( ST' \in ST_2(n, k) \), for \( k \equiv 0 \pmod{2} \). As if \( k = n - 1 \) or \( n = k + 1 \), \( |V_2(ST'_{\text{min}})| = 0 \) which yields \( x_{3,3} = 1, x_{3,3} = \frac{n - 6}{2} \). Hence,

\[
ZC^*_1(ST'_{\text{min}}) = 7k - 23 \quad \text{if } n = k + 1 \quad \text{and} \quad k \equiv 0 \pmod{2}.
\]

Now, using (8) and Lemmas 2.3-2.7, we can observe that if \( 0 < |V_2(ST'_{\text{min}})| < |V_3(ST'_{\text{min}})| \), that is \( n < \frac{3k - 2}{2} \), \( x_{2,2} = 0, x_{2,3} = 1, x_{2,3} = 2n - 2k - 3, x_{3,3} = \frac{3k - 2n - 2}{2} \) and \( x_{3,3} = 0 \). Also, if \( |V_2(ST'_{\text{min}})| \geq |V_3(ST'_{\text{min}})| \), that is \( n \geq \frac{3k - 2}{2} \), \( x_{2,2} = \frac{2n - 3k + 2}{2}, x_{2,3} = k - 5, x_{2,4} = 1, x_{3,3} = x_{3,4} = 0 \). Hence,

\[
ZC^*_1(ST'_{\text{min}}) = 2n + 5k - 16 \quad \text{if } n < \frac{3k - 2}{2} \quad \text{and} \quad k \equiv 0 \pmod{2},
\]

and

\[
ZC^*_1(ST'_{\text{min}}) = 4n + 2k - 14 \quad \text{if } n \geq \frac{3k - 2}{2} \quad \text{and} \quad k \equiv 0 \pmod{2}.
\]

The required result can be found from Equations (9) to (13) which complete the proof.

3. On the maximum modified first Zagreb connection index of trees with given number of segments

Denote by \( ST'_{\text{max}} \) the tree which maximizes \( ZC^*_1 \) among all the members of the class \( T'_{n,k} \) for \( 3 \leq k \leq n - 2 \).

Lemma 3.1: The tree \( ST'_{\text{max}} \) contains exactly one vertex of degree greater than 2.

Proof: Let \( u \) be a vertex with maximum degree in \( ST'_{\text{max}} \). Clearly, it holds that \( d_u \geq 3 \) as \( k \geq 3 \). Contrarily, suppose \( w \in V(ST'_{\text{max}}) \) is another vertex with degree greater than 2. It holds that \( 3 \leq d_w \leq d_u \). Let \( P = u v_1 \cdots v_k w \) be a path in \( ST'_{\text{max}} \) connecting the vertices \( w \) and \( u \) such that every internal vertex(if exists) of the path \( P \) has degree 2. Let \( N(w) = \{w_1, \ldots, w_{d(w)-1}, v_1\} \) and \( N(u) = \{u_1, \ldots, u_{d(u)-1}, v_1\} \). If \( T' = ST'_{\text{max}} - \{ww|1 \leq i \leq d(w) - 1\} + \{wu|1 \leq i \leq d(w) - 1\} \), then \( T' \in T'_{n,k} \).

We consider the following cases:

Case I: The vertices \( u \) and \( w \) are non-adjacent.

In this case \( d_u = d'_u = 2 \), and we have

\[
ZC^*_1(T') - ZC^*_1(ST'_{\text{max}}) = \sum_{j=1}^{d_u-1} (2du_i + d_{w} - 1) - du_i - du - d_{w} + 1
\]

\[
= \sum_{j=1}^{d_w-1} (2d_{w} + d_{u} - 1) - d_{w} - du - d_{w} + 1
\]

\[
= (4d_{u} + d_{w} - 1) - 2 - du - d_{w} + 1 + (4 - 2 - 1)
\]

\[
= (2du_i - d_{w} - du - d_{w})
\]

\[
= (d_{w} - 1) \sum_{j=1}^{d_{w}-1} (2du_i - 1) + (d_{u} - 1) \sum_{j=1}^{d_{w}-1} (2d_{w} - 1)
\]

\[
> 0,
\]

which is a contradiction to the choice of \( ST'_{\text{max}} \).

Case II: The vertices \( u \) and \( w \) are adjacent.

Because of the fact \( 3 \leq k \leq n - 2 \), either

\[
\sum_{j=1}^{d_u-1} (2du_i - 1) > (d_{w} - 1)
\]

or

\[
\sum_{j=1}^{d_w-1} (2d_{w} - 1) > (d_{w} - 1)
\]

and we have

\[
ZC^*_1(T') - ZC^*_1(ST'_{\text{max}}) = \sum_{i=1}^{d_u-1} (2du_i + d_{w} - 1) - du_i - du - d_{w} + 1
\]

\[
= \sum_{j=1}^{d_w-1} (2d_{w} + d_{u} - 1) - d_{w} - du - d_{w} + 1
\]

\[
= (2d_{u} + d_{w} - 1) - 1 - du - d_{w} + 1
\]

\[
= (2du_i - d_{w} - du - d_{w})
\]

\[
= (d_{w} - 1) \sum_{j=1}^{d_{w}-1} (2du_i - 1) + (d_{u} - 1) \sum_{j=1}^{d_{w}-1} (2d_{w} - 1)
\]

\[
> 0,
\]

which is a contradiction to the choice of \( ST'_{\text{max}} \).
If using Lemma 3.1 we assume that $w$ and we obtain

$$\left( \sum_{i=1}^{d_u-1} (2d_{u_i} - 1) - (d_u - 1) \right)$$

which is again a contradiction to the maximality of $ST'_{\max}$.

**Lemma 3.2:** If the tree $ST'_{\max} \in T'_{n,k}$ contains a pendant vertex adjacent to its branching vertex, then $ST'_{\max}$ does not contain a vertex of degree 2 with both non-pendent neighbors.

**Proof:** Let $u$ be a pendant vertex of $ST'_{\max}$ adjacent to a branching vertex $v$. Suppose, on the contrary, that $ST'_{\max}$ has a vertex $w$ of degree 2 such that $N(w) = \{w_1, w_2\}$ and both $w_1$ and $w_2$ are non-pendent vertices ($v$ may coincide with either of the vertices $w_1$ or $w_2$), by using Lemma 3.1 we assume that $d_{w_1} \geq 2$ then $d_{w_2} = 2$. If $T' = ST'_{\max} - \{ww_1, w_2u, u\} + \{w, wu, w_1w_2\}$ then $T' \in T'_{n,k}$ and

$$ZC_1^*(ST'_{\max}) - ZC_1^*(T')$$

and we obtain $ZC_1^*(ST'_{\max}) - ZC_1^*(T') < 0$, a contradiction to the definition of $ST'_{\max}$.

Denote by $S'(n,k)$ the set of all $n$-vertex trees with degree sequence $(k, 2, 2, \ldots, 2, 1, 1, \ldots, 1)$ satisfying the following conditions:

- $x_{1,k} = 2k + 1 - n$ and $x_{2,2i} = 0$ for $n < 2k + 1$,
- $x_{1,k} = k$ and $x_{2,2i} \geq 0$ for $n \geq 2k + 1$. We can state the following result.

**Theorem 3.1:** Let $T \in T'_{n,k}$, where $3 \leq k \leq n - 2$, then

$$ZC_1^*(T) \leq \begin{cases} 2nk - k^2 - 3k & \text{if } n < 2k + 1, \\ 4n + 3k^2 - 9k - 4 & \text{if } n \geq 2k + 1, \end{cases}$$

with equality if and only if $T \in S'(n,k)$.

**Proof:** Keeping in mind Lemmas 3.1 and 3.2, one can conclude that $ST'_{\max} \in S'(n,k)$. Now, if $|V_2(ST'_{\max})| < k$, that is $n < 2k + 1$, by using (8) and Lemmas 3.1 and 3.2, we get $x_{1,2} = x_{2,k} = n - k - 1, x_{2,2} = 0$ and $x_{1,k} = 2k - n + 1$. Also, if $|V_2(ST'_{\max})| \geq k$, that is $n \geq 2k + 1$, Lemmas 3.1 and 3.2 along with (8) imply that $x_{1,k} = 0, x_{1,2} = x_{2,k} = k, x_{2,2} = n - 2k - 1$. Hence,

$$ZC_1^*(ST'_{\max}) = 2nk - k^2 - 3k \quad \text{if } n < 2k + 1,$$

and

$$ZC_1^*(ST'_{\max}) = 4n + 3k^2 - 9k - 4 \quad \text{if } n \geq 2k + 1.$$
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