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THE DISTANCE SPECTRAL RADIUS OF GRAPHS WITH GIVEN NUMBER OF ODD VERTICES

HONGYING LIN† AND BO ZHOU†

Abstract. The graphs with smallest, respectively largest, distance spectral radius among the connected graphs, respectively trees with a given number of odd vertices, are determined. Also, the graphs with the largest distance spectral radius among the trees with a given number of vertices of degree 3, respectively given number of vertices of degree at least 3, are determined. Finally, the graphs with the second and third largest distance spectral radius among the trees with all odd vertices are determined.

Key words. Distance spectral radius, Distance matrix, Distance Perron vector, Odd vertex, Maximum degree, Graph, Tree.

AMS subject classifications. 05C50, 15A18.

1. Introduction. Throughout this paper, we consider simple graphs. Let $G$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The distance between vertices $u, v \in V(G)$, denoted by $d_G(u, v)$, is the length of a shortest path between them. The distance matrix of $G$, denoted by $D(G)$, is the matrix $D(G) = (d_G(u, v))_{u,v \in V(G)}$. Since $D(G)$ is real and symmetric, its eigenvalues are real. The distance spectral radius of $G$, denoted by $\rho(G)$, is the largest eigenvalue of $D(G)$. Since $D(G)$ is irreducible, we have by the Perron-Frobenius theorem that $\rho(G)$ is simple, and there is a unique positive unit eigenvector $x(G)$ of $D(G)$ corresponding to $\rho(G)$, which is called the distance Perron vector of $G$.

The study of eigenvalues of the distance matrix of a connected graph dates back to the classical work of Graham and Pollack [5], Graham and Lovász [4], and Edelberg et al. [2]. For more details on spectra of distance matrices and especially on distance spectral radius, one may refer to the recent survey of Aouchiche and Hansen [1].

A vertex is an odd vertex (respectively, even vertex) if its degree is odd (respectively, even). It is well known that the number of odd vertices in a graph is always even. A vertex in a tree with degree at least 3 is known as a branch vertex. The
number of branch vertices may be used to analyze graph structures, see, e.g. [3, 7]. In this paper, we determine the graphs with smallest, respectively largest, distance spectral radius among the connected graphs, respectively trees with a given number of odd vertices. Also, we determine the graphs with the largest distance spectral radius among the trees with a given number of vertices of degree 3, respectively given number of vertices of degree at least 3. Finally, we determine the graphs with the second and third largest distance spectral radius among the trees with all odd vertices.

2. Preliminaries. Let $G$ be a connected graph with $V(G) = \{v_1, \ldots, v_n\}$. A column vector $x = (x_{v_1}, \ldots, x_{v_n})^\top \in \mathbb{R}^n$ (whether it is the distance Perron vector of $G$ or not) can be considered as a function defined on $V(G)$ which maps vertex $v_i$ to $x_{v_i}$, i.e., $x(v_i) = x_{v_i}$ for $i = 1, \ldots, n$. Then

$$x^\top D(G)x = \sum_{\{u, v\} \subseteq V(G)} 2d_G(u, v)x ux_v,$$

and $\lambda$ is an eigenvalue of $D(G)$ with corresponding eigenvector $x$ if and only if $x \neq 0$ and for each $u \in V(G)$,

$$\lambda x_u = \sum_{v \in V(G)} d_G(u, v)x_v.$$

We call (2.1) the $(\lambda, x)$-eigenequation for $G$ at $u$. For a unit column vector $x \in \mathbb{R}^n$ with at least one nonnegative entry, by Rayleigh’s principle, we have

$$\rho(G) \geq x^\top D(G)x$$

with equality if and only if $x$ is the distance Perron vector of $G$.

For a connected graph $G$ with $v \in V(G)$, let $\delta_G(v)$ be the degree of $v$ in $G$, and let $N_G(v)$ be the set of neighbors of $v$ in $G$.

Let $P_n$, $C_n$, $S_n$ and $K_n$ be respectively the path, the cycle, the star and the complete graph on $n$ vertices.

A caterpillar is a tree such that the deletion of all pendant vertices yields a path. Obviously, $S_n$ and $P_n$ are caterpillars.

Let $G$ be a connected graph. For $V_1 \subseteq V(G)$, $G - V_1$ denotes the graph obtained from $G$ by deleting all vertices of $V_1$ (and the incident edges). If $V_1 = \{u\}$, then we write $G - u$ for $G - \{u\}$. For $E_1 \subseteq E(G)$, $G - E_1$ denotes the graph obtained from $G$ by deleting all edges of $E_1$. If $E_1 = \{uv\}$, then we write $G - uv$ for $G - \{uv\}$. If $E'$ is a subset of edges of the complement of $G$, then $G + E'$ denotes the graph obtained from $G$ by inserting all edges of $E'$. If $E' = \{uv\}$, then we write $G + uv$ for $G + \{uv\}$.
For a subgraph $H$ of a connected graph $G$, let $\sigma_G(H)$ be the sum of the entries of the distance Perron vector of $G$ corresponding to the vertices in $V(H)$.

**Lemma 2.1.** [9] Let $G$ be a connected graph with $u, v \in V(G)$. If $uv \notin E(G)$, then $\rho(G) > \rho(G + uv)$.

**Lemma 2.2.** [10] Let $G$ be a connected graph on $n$ vertices with $u, v \in V(G)$, and let $u'$ and $v'$ be pendant neighbors of $u$ and $v$, respectively. Let $x = x(G)$. Then $x_{u'} = x_{v'} = \frac{\rho(G)}{\rho(G)^2} (x_u - x_v)$.

**Lemma 2.3.** [11][12] Let $G$ be a connected graph and $u$ a cut vertex of $G$. Suppose that $G - u$ consists of vertex disjoint subgraphs $G_1, G_2$ and $G_3$. Let $G'_3$ be the subgraph of $G$ induced by $V(G_3) \cup \{u\}$. For $v \in V(G_2)$, let $G' = G - \{uw : w \in N_{G'_3}(u)\} + \{uw : w \in N_{G'_3}(u)\}$.

If $\sigma_G(G_1) \geq \sigma_G(G_2)$, then $\rho(G') > \rho(G)$.

**Lemma 2.4.** [10] Let $G$ be a connected graph and $uv$ a non-pendant cut edge of $G$. Let $G'$ be the graph obtained from $G$ by contracting $uv$ to a vertex $u$ and attaching a pendant vertex $v$ to $u$. Then $\rho(G') < \rho(G)$.

3. Distance spectral radius of graphs with given number of odd vertices.

For integers $n$ and $k$ with $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$, let $\mathcal{G}(n,k)$ be the set of connected graphs with $n$ vertices and $2k$ odd vertices, and let $K_n(k)$ be the graph obtained from $K_n$ by deleting $k$ pairwise disjoint edges. In particular, $K_n(0) = K_n$.

**Theorem 3.1.** Let $G \in \mathcal{G}(n,k)$, where $n \geq 3$ and $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

(i) If $n$ is odd, then $\rho(G) \geq \rho(K_n(k))$ with equality if and only if $G \cong K_n(k)$.

(ii) If $n$ is even, then $\rho(G) \geq \rho(K_n\left(\frac{n}{2} - k\right))$ with equality if and only if $G \cong K_n\left(\frac{n}{2} - k\right)$.

**Proof.** Let $G$ be the graph in $\mathcal{G}(n,k)$ with minimum distance spectral radius.

If $n$ is odd and $k = 0$, or $n$ is even and $k = \frac{n}{2}$, then by Lemma 2.1 $G \cong K_n(0)$. If $n$ is even and $k = 0$, then since $G$ is a spanning subgraph of $K_n\left(\frac{n}{2}\right)$, we have by Lemma 2.1 that $G \cong K_n\left(\frac{n}{2}\right)$.

Suppose $1 \leq k < \frac{n}{2}$. For $z \in V(G)$, let $N_z = V(G) \setminus (N_{G}(z) \cup \{z\})$. Obviously, $|N_z| = n - 1 - \delta_G(z)$.

Let $V_1$ (respectively, $V_2$) be the set of odd (respectively, even) vertices of $G$. Suppose that there are vertices $u \in V_1$ and $v \in V_2$ such that $uv \notin E(G)$. Let $G' = G + uv$. Note that $\delta_G'(u) = \delta_G(u) + 1$ is even and $\delta_G'(v) = \delta_G(v) + 1$ is odd. We have $G' \in \mathcal{G}(n,k)$. By Lemma 2.4, $\rho(G') < \rho(G)$, a contradiction. Thus, each
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vertex of $V_1$ is adjacent to each vertex of $V_2$.

**Case 1.** $n$ is odd.

Suppose that there is a vertex $u \in V_2$ with $\delta_G(u) < n - 1$. Then $\delta_G(u) \leq n - 3$. Let $t = \frac{n - \delta_G(u)}{2}$. Then $t$ is a positive integer, and $|N_u| = n - 1 - \delta_G(u) = 2t$. Let $N_u = \{u_1, \ldots, u_{2t}\}$. Suppose that $u_1$ is not adjacent to $v_{2t}$. Let $G'' = G + \{uu_1, u_{2t}, u_1u_{2t}\}$. Obviously, $G'' \in G(n, k)$. By Lemma 2.1, $\rho(G'') < \rho(G)$, a contradiction. Thus, $u_1u_{2t} \in E(G)$.

Let $G'' = G - u_1u_{2t} + \{uu_1, u_{2t}\}$. Obviously, $G'' \in G(n, k)$. Let $H_1$ and $H_2$ be the subgraphs of $G''$ induced by $V_1$ and $V_2 \backslash (N_u \cup \{u_1\})$, respectively. Let $x' = x(G'')$. From [2.1] for $G''$ at $u$ and $u_1$, we have

$$\rho(G'')x''_u = \sigma_G^+(H_1) + \sigma_G^+(H_2) + x''_{u_1} + 2x''_{u_2} + \cdots + 2x''_{u_{2t-1}} + x''_{u_{2t}},$$

$$\rho(G'')x''_{u_1} \leq \sigma_G^+(H_1) + 2\sigma_G^+(H_2) + 2x''_{u_2} + \cdots + 2x''_{u_{2t-1}} + 2x''_{u_{2t}} + x''_{u_1}.$$

Thus,

$$(\rho(G'') + 1) \left(2x''_{u} - x''_{u_1}\right) \geq \sigma_G^+(H_1) + x''_{u_1} + 2x''_{u_2} + \cdots + 2x''_{u_{2t-1}} + x''_{u_2} > 0,$$

which implies that $2x''_{u} - x''_{u_1} > 0$. Similarly, $2x''_{u} - x''_{u_{2t}} > 0$.

As we pass from $G$ to $G''$, the distance between $u_1$ and $u_{2t}$ is increased by 1, the distance between $u$ and $u_1$ is decreased by 1, the distance between $u$ and $u_{2t}$ is decreased by 1, and the distance between any other vertex pair remains unchanged. Therefore,

$$\frac{1}{2}(\rho(G) - \rho(G'')) \geq \frac{1}{2} x^T (D(G) - D(G'')) x$$

$$= x''_u (x''_{u_1} + x''_{u_{2t}}) - x''_{u_1} x''_{u_{2t}}$$

$$= \frac{1}{2} \left( (2x''_{u} - x''_{u_1}) x''_{u_1} + (2x''_{u} - x''_{u_{2t}}) x''_{u_{2t}} \right) > 0.$$ 

This leads to the contradiction that $\rho(G) > \rho(G'')$. Thus, the degree of each vertex in $V_2$ is $n - 1$.

Suppose that there is a vertex $u \in V_1$ with $\delta_G(u) < n - 2$. Then $\delta_G(u) \leq n - 4$. Let $t = \frac{n - \delta_G(u)}{2}$. Then $t$ is a positive integer, and $|N_u| = 2t + 1$. Let $N_u = \{u_1, \ldots, u_{2t+1}\}$. Arguing as above we see $u_1u_{2t+1} \in E(G)$. Let $G''' = G - u_1u_{2t+1} + \{u_1, u_{2t+1}\}$. Obviously, $G''' \in G(n, k)$. As above, we have $\rho(G) > \rho(G''')$, a contradiction. Thus, the degree of each vertex in $V_1$ is $n - 2$.

Since each even degree is $n - 1$ and each odd degree is $n - 2$, we have $G \cong K_n(k)$. 

Case 2. \( n \) is even.

Similarly to the proof in Case 1, we have that each odd degree is \( n - 1 \) and each even degree is \( n - 2 \). Thus, \( G \cong K_n \left( \frac{n}{2} - k \right) \).

**Lemma 3.2.** Let \( T \) be a tree with \( u \in V(T) \), and let \( N_T(u) = \{u_1, \ldots, u_k\} \), where \( k \geq 3 \). Let \( T_i \) be the component of \( T - u \) containing \( u_i \) for \( 1 \leq i \leq k \). Let \( T' = T - \{uw_i: 2 \leq i \leq l\} + \{uw_i: 2 \leq i \leq l\} \), where \( 2 \leq t \leq k - 1 \) and \( w \in V(T_k) \). If \( \sigma_T(T_i) \geq \sigma_T(T_k) \), then \( \rho(T') > \rho(T) \).

**Proof.** Let \( x = x(T) \). As we pass from \( T \) to \( T' \), the distance between a vertex of \( V(T_2) \cup \cdots \cup V(T_t) \) and a vertex of \( V(T_1) \cup \{w\} \) is increased by \( d_T(u, w) \), the distance between a vertex of \( V(T_2) \cup \cdots \cup V(T_t) \) and a vertex of \( V(T_k) \) is decreased by at most \( d_T(u, w) \), and the distance between any other vertex pair is increased or remains unchanged. Thus,

\[
\frac{1}{2} (\rho(T') - \rho(T)) \geq \frac{1}{2} x^T (D(T') - D(T)) x
\]

\[
\geq d_T(u, w) \sum_{i=2}^{t} \sigma_T(T_i) (\sigma_T(T_i) - \sigma_T(T_k) + x_u)
\]

\[
> 0.
\]

Therefore, \( \rho(T') > \rho(T) \).

Let \( G_1(s, t) \) be the graph shown in Fig. 1, where \( G_1 \) is a nontrivial connected graph, and \( s, t \geq 1 \).

![Graph G1(s, t)](image)

**Fig. 1.** Graph \( G_1(s, t) \).

**Lemma 3.3.** Let \( G_1 \) be a nontrivial connected graph. For \( s \geq t \geq 2 \), we have

\[
\rho(G_1(s + 1, t - 1)) > \rho(G_1(s, t)).
\]

**Proof.** Let \( G = G_1(s, t) \). Let \( G_2 \) and \( G_3 \) be the components of \( G - u_{s+1} \) containing \( u_1 \) and \( u_{s+t+1} \), respectively. Let

\[
G' = G - \{u_{s+2}u_{s+2}, u_{s+1}v_{s+1}\} + \{u_{s+2}u_{s+1}, u_{s+1}v_{s+2}\}.
\]
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Obviously, \( G_1(s + 1, t - 1) \cong G' \). Let \( x = x(G) \).

Claim 1. \( \sigma_G(G_1) - x_{v_{s+2}} > 0 \).

Choose \( z \in V(G_1) \) such that \( d_G(z, v_{s+1}) = \max_{v \in V(G_1)} d_G(v, v_{s+1}). \) Let \( d = d_G(z, v_{s+1}). \) Since \( |V(G_1)| \geq 2, d \geq 1, \) and \( z \neq v_{s+1}. \) From (2.1) for \( G \) at \( v_{s+1}, z \) and \( v_{s+2}, \) we have

\[
\begin{align*}
\rho(G)x_{v_{s+1}} &= dx + 3x_{v_{s+2}} + \sum_{w \in V(G_1) \setminus \{z, v_{s+1}\}} d_G(v_{s+1}, w)x_w \\
&\quad + \sum_{w \in V(G) \setminus (V(G_1) \cup \{v_{s+2}\})} d_G(v_{s+1}, w)x_w,
\end{align*}
\]

\[
\begin{align*}
\rho(G)x_z &= dx_{v_{s+1}} + (d + 3)x_{v_{s+2}} + \sum_{w \in V(G_1) \setminus \{z, v_{s+1}\}} d_G(z, w)x_w \\
&\quad + \sum_{w \in V(G) \setminus (V(G_1) \cup \{v_{s+2}\})} d_G(z, w)x_w,
\end{align*}
\]

\[
\begin{align*}
\rho(G)x_{v_{s+2}} &= 3x_{v_{s+1}} + (d + 3)x_z + \sum_{w \in V(G_1) \setminus \{z, v_{s+1}\}} (d_G(v_{s+1}, w) + 3)x_w \\
&\quad + \sum_{w \in V(G) \setminus (V(G_1) \cup \{v_{s+2}\})} d_G(v_{s+2}, w)x_w.
\end{align*}
\]

Note that for \( w \in V(G) \setminus (V(G_1) \cup \{v_{s+2}\}), d_G(v_{s+1}, w) + d_G(z, w) - d_G(v_{s+2}, w) \geq 0. \) Thus,

\[
\begin{align*}
\rho(G) \left(x_{v_{s+1}} + x_z - x_{v_{s+2}}\right) &\geq (d - 3)x_{v_{s+1}} - 3x_z + (d + 6)x_{v_{s+2}} \\
&\quad + \sum_{w \in V(G_1) \setminus \{z, v_{s+1}\}} (d_G(z, w) - 3)x_w,
\end{align*}
\]

and

\[
\begin{align*}
(\rho(G) + 3) \left(\sigma_G(G_1) - x_{v_{s+2}}\right) &\geq \rho(G) \left(x_{v_{s+1}} + x_z - x_{v_{s+2}}\right) + 3 \left(\sigma_G(G_1) - x_{v_{s+2}}\right) \\
&\geq (d - 3)x_{v_{s+1}} - 3x_z + (d + 6)x_{v_{s+2}} \\
&\quad + \sum_{w \in V(G_1) \setminus \{z, v_{s+1}\}} (d_G(z, w) - 3)x_w \\
&\quad + 3 \left(x_{v_{s+1}} + x_z + \sum_{w \in V(G_1) \setminus \{z, v_{s+1}\}} x_w - x_{v_{s+2}}\right) \\
&= dx_{v_{s+1}} + (d + 3)x_{v_{s+2}}
\end{align*}
\]
Therefore, Claim 1 follows.

**Claim 2.** \( \sigma_G(G_2) \geq \sigma_G(G_3) \).

Let \( y_k = x_{u_k} + x_{v_k} \) for \( 2 \leq k \leq s + t \), \( y_1 = x_{u_1} \), and \( y_{s+t+1} = x_{u_{s+t+1}} \). Suppose

\[
\sum_{i=1}^{s} y_i < \sum_{i=1}^{t} y_{s+i+1}.
\]

From (2.1) for \( G \) at \( u_k \) with \( 1 \leq k \leq s + t + 1 \), we have

\[
\rho(G) (x_{u_{s+2}} - x_{u_i}) = 2 \left( \sum_{j=1}^{s} y_j - \sum_{j=1}^{t} y_{s+i+1} \right)
\]

and

\[
\rho(G) (x_{u_{s+i+1}} - x_{u_{s+i-1}}) = \rho(G) (x_{u_{s+2}} - x_{u_{s+i}})
\]

\[
= 2 \left( \sum_{j=1}^{s} y_{s+1-j} - \sum_{j=1}^{t} y_{s+i+1+j} \right)
\]

for \( 2 \leq i \leq t - 1 \). We now prove that \( x_{u_{s+i+1}} - x_{u_{s+i-1}} < 0 \) for \( 1 \leq i \leq t \) by induction on \( i \). If \( i = 1 \), then from (3.1) and (3.2), we have \( x_{u_{s+2}} - x_{u_s} < 0 \), and by Lemma 2.2, \( y_{s+2} = x_{u_{s+2}} + x_{v_{s+2}} < x_{u_s} + x_{v_s} = y_s \). Suppose \( 2 \leq i \leq t - 1 \) and \( x_{u_{s+i+1}} - x_{u_{s+i-1}} < 0 \) for \( 1 \leq j \leq i-1 \). In particular, \( x_{u_{s+i}} - x_{u_{s+i-1}} < 0 \). By Lemma 2.2, \( y_{s+i+1+j} = x_{u_{s+i}+j} \) and \( x_{v_{s+i+j}} < x_{u_{s+i}+j} + x_{v_{s+i+j}} = y_{s+i+1+j} \). Thus, \( \sum_{j=1}^{i-1} y_{s+1+j} = \sum_{j=1}^{i-1} y_{s+1+j} < 0 \). Now from (3.1) and (3.3), we have \( x_{u_{s+1+i}} - x_{u_{s+1-i}} < x_{u_{s+i}} - x_{u_{s+2+i}} < 0 \) for \( 2 \leq i \leq t \). It follows that \( x_{u_{s+i+1}} - x_{u_{s+i}} > 0 \) for \( 1 \leq i \leq t \). Thus,

\[
\sum_{i=1}^{s} y_i - \sum_{i=1}^{t} y_{s+i+1} \geq \sum_{i=1}^{t} y_i - \sum_{i=1}^{t} y_{s+i+1} > 0,
\]

which leads to the contradiction that \( \sum_{i=1}^{s} y_i \geq \sum_{i=1}^{t} y_{s+i+1} \). Hence, \( \sum_{i=1}^{s} y_i - \sum_{i=1}^{t} y_{s+i+1} \geq 0 \), from which Claim 2 follows.

As we pass from \( G \) to \( G' \), the distance between a vertex of \( V(G_1) \) and a vertex of \( V(G_2) \cup \{u_{s+1}\} \) is increased by \( 1 \), the distance between a vertex of \( V(G_1) \) and a
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vertex of $V(G_3 \setminus \{v_{s+2}\})$ is decreased by 1, the distance between $v_{s+2}$ and a vertex of $V(G_3 \setminus \{v_{s+2}\})$ is increased by 1, the distance between $v_{s+2}$ and a vertex of $V(G_2) \cup \{u_{s+1}\}$ is decreased by 1, and the distance between any other vertex pair remains unchanged. Thus,

$$\frac{1}{2} (\rho(G') - \rho(G)) \geq \frac{1}{2} x^T (D(G') - D(G)) x$$

$$= \sigma_G(G_1) \left( \sigma_G(G_2) + x_{u_{s+1}} \right) - \sigma_G(G_1) \left( \sigma_G(G_3) - x_{v_{s+2}} \right)$$

$$+ x_{v_{s+2}} \left( \sigma_G(G_3) - x_{v_{s+2}} \right) - x_{v_{s+2}} \left( \sigma_G(G_2) + x_{u_{s+1}} \right)$$

$$= (\sigma_G(G_2) - \sigma_G(G_3) + x_{v_{s+2}} + x_{u_{s+1}}) \sigma_G(G_1) - x_{v_{s+2}},$$

which, together with Claims 1, 2, implies that $\rho(G') > \rho(G)$. \[\Box\]

For $b \geq a \geq 0$ with $2(a + b) \leq n$, let $C(n, a, b)$ be the tree obtained from the path $P_{n-a-b}$ with consecutive vertices $u_0, u_1, \ldots, u_{n-a-b-1}$ by attaching a pendant vertex $v_i$ to vertex $u_i$ for $i \in \{1, \ldots, a\} \cup \{n-a-2b-1, \ldots, n-a-b-2\}$. In particular, $C(n, 0, 0)$ is just the path $P_n$.

**Lemma 3.4.** \[\Box\] Let $T$ be a tree with $n \geq 4$ vertices. If $T \neq P_n$ and $C(n, 0, 1)$, then $\rho(T) < \rho(C(n, 0, 1)) < \rho(P_n)$.

**Lemma 3.5.** If $a \geq 0$, $b \geq a + 2$, and $2(a + b) + 2 < n$, then

$$\rho(C(n, a + 1, b - 1)) > \rho(C(n, a, b)).$$

**Proof.** Let $T = C(n, a, b)$, $p = \lceil \frac{n-a-b-2}{2} \rceil$, and $q = \lceil \frac{n-a-b-2}{2} \rceil$. Let $x = x(T)$. For $0 \leq i \leq n - a - b - 1$, let $s_i = x_{u_i}$ if $u_i$ has no pendant vertex, and $s_i = x_{u_i} + x_{v_i}$ otherwise.

**Claim 1.** $x_{u_{i+1}} - x_{u_{n-a-b-2-i}} > x_{u_i} - x_{u_{n-a-b-1-i}} > 0$ for $0 \leq i \leq a$.

First we prove that $x_{u_p} > x_{u_{q+1}}$. Suppose $\sum_{i=0}^{p} s_i \geq \sum_{i=q+1}^{p} s_i$. We prove that $x_{u_{p-i}} \leq x_{u_{q+1+i}}$ for $0 \leq i \leq p$ by induction on $i$. For $i = 0$, we have

$$\rho(T) (x_{u_p} - x_{u_{q+1}}) = (q + 1 - p) \left( \sum_{i=q+1}^{p} s_i - \sum_{i=0}^{p} s_i \right),$$

and thus, $x_{u_p} \leq x_{u_{q+1}}$. Suppose $i \geq 1$ and $x_{u_{p-j}} \leq x_{u_{q+1+j}}$ for $0 \leq j \leq i - 1$. If $\delta_T(u_p-j) = 2$, then $s_{p-j} = x_{u_{p-j}} \leq x_{u_{q+1+j}} \leq s_{q+1+j}$. If $\delta_T(u_p-j) = 3$, then by Lemma 2.2, $x_{u_{p-j}} \leq x_{v_{q+1+j}}$, and thus, $s_{p-j} = x_{u_{p-j}} + x_{v_{p-j}} \leq x_{u_{q+1+j}} + x_{v_{q+1+j}} = s_{q+1+j}$. In either case, $s_{p-j} \leq s_{q+1+j}$. Hence,

$$\rho(T) (x_{u_{p-i}} - x_{u_{q+1+i}}) - \rho(T) (x_{u_{p+1-i}} - x_{u_{q+i}}).$$
we have from (2.1) for \(H\). Hence,

\[
\sum_{j=q+1}^{p-1} s_j - \sum_{j=0}^{p-1} s_j \leq x
\]

and thus, \(x_{u_{p-i}} - x_{u_{q+1+i}} \leq x_{u_{p-i}} - x_{u_{q+i}}. \) It follows that \(x_{u_{p-i}} \leq x_{u_{q+1+i}}\) for \(0 \leq i \leq p\), and thus, \(s_{p-i} \leq s_{q+1} + 1\) for \(0 \leq i \leq p\). Since \(b \geq a + 2\), there exists an \(i\) with \(0 \leq i \leq p\) such that \(\delta T(u_{p-i}) = 2\) and \(\delta T(u_{q+1+i}) = 3\), and thus, \(s_{p-i} = x_{u_{p-i}} \leq x_{u_{q+1+i}} \leq s_{q+1} + 1\). This leads to the contradiction that \(\sum_{i=0}^{p} s_i < \sum_{i=q+1}^{n-a-b-1} s_i\), by (3.4), we have \(x_{u_p} > x_{u_{q+1}}\).

Suppose \(x_{u_0} \leq x_{u_{n-a-b-1}}. \) We prove that \(x_{u_i} \leq x_{u_{n-a-b-1}}\), for \(0 \leq i \leq p\) by induction on \(i\). Suppose \(i \geq 1\) and \(x_{u_j} \leq x_{u_{n-a-b-1}}\), for \(0 \leq j \leq i-1\). As above, we have by Lemma 2.2 that \(s_j \leq s_{n-a-b-1-j}\). It follows that

\[
\rho(T) \left(x_{u_i} - x_{u_{n-a-b-1-i}}\right) - \rho(T) \left(x_{u_{i-1}} - x_{u_{n-a-b-1}}\right)
= 2 \sum_{j=0}^{i-1} \left(s_j - s_{n-a-b-1-j}\right)
\leq 0.
\]

Hence, \(x_{u_i} - x_{u_{n-a-b-1-i}} \leq x_{u_{i-1}} - x_{u_{n-a-b-1}} \leq 0\). Thus, \(x_{u_i} \leq x_{u_{n-a-b-1-i}}\) for \(0 \leq i \leq p\). In particular, \(x_{u_p} \leq x_{u_{q+1}}\), which is a contradiction. It follows that \(x_{u_0} > x_{u_{n-a-b-1}}\), and as above, we have by induction that \(x_{u_{i+1}} - x_{u_{n-a-b-2-i}} > x_{u_{i}} - x_{u_{n-a-b-1-i}}\) for \(0 \leq i \leq a\).

Claim 2. \(x_{v_{n-a-2b-1}} < x_{v_{n-a-2b}} + x_{v_{n-a-2b}}. \)

Let \(V' = V(T)\setminus\{v_{n-a-2b-1}, u_{n-a-2b}, v_{n-a-2b}\}\). Since for \(u \in V'\),

\[
d_T(u_{n-a-2b}, u) + d_T(v_{n-a-2b}, u) - d_T(v_{n-a-2b-1}, u) \geq 0,
\]

we have from [2.1] for \(T\) at \(u_{n-a-2b}, v_{n-a-2b}\) and \(v_{n-a-2b-1}\) that

\[
\rho(T) \left(x_{u_{n-a-2b}} + x_{v_{n-a-2b}} - x_{v_{n-a-2b-1}}\right) = -x_{u_{n-a-2b}} - 2x_{v_{n-a-2b}} + 5x_{v_{n-a-2b-1}}
\]

\[
+ \sum_{u \in V'} \left(d_T(u_{n-a-2b}, u) + d_T(v_{n-a-2b}, u) - d_T(v_{n-a-2b-1}, u)\right) x_u
\]

\[
\geq -x_{u_{n-a-2b}} - 2x_{v_{n-a-2b}} + 5x_{v_{n-a-2b-1}}.
\]
Thus,

\[(\rho(T) + 2) \left( x_{u_{n-a-2b}} + x_{v_{n-a-2b}} - x_{v_{n-a-2b-1}} \right) \geq x_{u_{n-a-2b}} + 3x_{v_{n-a-2b-1}}, \]

from which Claim 2 follows.

Claim 3. \( x_{u_{a+i+1}} - x_{u_{n-a-2b-1-i}} > x_{u_{a+i+1}} - x_{u_{n-a-2b-2-i}}, 0 \leq i \leq \left\lfloor \frac{n-1}{2} \right\rfloor - b - a - 1. \)

It is sufficient to prove that \( x_{u_i} - x_{u_{n-2b-i}} > x_{u_{i+1}} - x_{u_{n-2b-1-i}} > 0 \) for \( a + 1 \leq i \leq n - 2b - 1 \). Let \( t = \left\lfloor \frac{n-1}{2} \right\rfloor \) and \( t_1 = \left\lfloor \frac{n-1}{2} \right\rfloor. \) By the proof of Claim 1, \( \sum_{j=0}^{t-b} s_j < \sum_{j=q+1}^{t-b} s_j \). Since \( t - b \leq q - 1 \), we have

\[
\sum_{j=0}^{t-b} s_j < \sum_{j=q+1}^{t-b} s_j \leq \sum_{j=t-b+2}^{n-a-b-1} s_j.
\]

We prove that \( x_{u_{i+1}} = x_{u_{n-2b-1-i}} \) for \( a + 1 \leq i \leq t - b \). For \( i = t - b \), we have

\[
\rho(T) \left( x_{u_{i+1}} - x_{u_{n-2b-1}} \right) = (t_1 + 1 - t) \left( \sum_{j=0}^{t-b} s_j - \sum_{j=0}^{t-b} s_j \right) > 0.
\]

Hence, \( x_{u_{i+1}} > x_{u_{n-2b-1}} \). Suppose \( a + 1 \leq i \leq t - b - 1 \) and \( x_{u_{i}} > x_{u_{n-2b-j}} \) for \( i + 1 \leq j \leq t - b \). Then

\[
\rho(T) \left( x_{u_{i}} - x_{u_{n-2b-j}} \right) - \rho(T) \left( x_{u_{i+1}} - x_{u_{n-2b-1-i}} \right)
= 2 \left( \sum_{j=n-2b-1}^{n-a-b-1} s_j - \sum_{j=0}^{t-b} s_j \right)
= 2 \left( \sum_{j=n-2b}^{n-a-b-1} s_j - \sum_{j=0}^{t-b} s_j \right) - 2 \sum_{j=i+1}^{t-b} (s_{n-2b-j} - s_j)
> 0,
\]

and thus, \( x_{u_{i}} - x_{u_{n-2b-j}} > x_{u_{i+1}} - x_{u_{n-2b-1-i}} \geq 0 \). This proves Claim 3.

Claim 4. \( x_{u_{n-a-2b-1}} > x_{u_{n-2a-b-1}} \).

By Claim 1, \( x_{u_{i}} > x_{u_{n-a-2b-1-i}} \) for \( 0 \leq i \leq a \). As above, we have by Lemma 2 that \( s_1 > s_{n-a-b-1-i} \). Thus, \( \sum_{i=0}^{a} s_i > \sum_{i=0}^{a} s_{n-a-b-1-i} \). Let \( m = \left\lfloor \frac{a}{2} \right\rfloor \) and \( m_1 = \left\lfloor \frac{b}{2} \right\rfloor \).

Suppose \( \sum_{i=0}^{n-2a-b-1} s_i \leq \sum_{i=n-2a-b-1-m}^{a} s_{i}. \) We prove that \( x_{u_{n-a-2b-1-i}} \geq x_{n-a-2b-1-i} \) for \( 1 \leq i \leq m \). We have

\[
\rho(T) \left( x_{u_{n-a-2b-1-i}} - x_{n-a-2b-1-i} \right)
= 2 \left( \sum_{j=n-2b-1}^{n-a-b-1} s_j - \sum_{j=0}^{t-b} s_j \right)
= 2 \left( \sum_{j=n-2b}^{n-a-b-1} s_j - \sum_{j=0}^{t-b} s_j \right) - 2 \sum_{j=i+1}^{t-b} (s_{n-2b-j} - s_j)
> 0,
\]

and thus, \( x_{u_{i}} - x_{u_{n-2b-j}} > x_{u_{i+1}} - x_{u_{n-2b-1-i}} \geq 0 \). This proves Claim 4.
a contradiction. Thus, \( x_{u_{n-a-2b-1-j}} \geq x_{u_{n-a-2b-1-m}} \). Suppose \( 1 \leq i \leq m - 1 \) and \( x_{u_{n-a-2b-2+j}} \geq x_{u_{n-a-2b-1-j}} \) for \( i + 1 \leq j \leq m \). By Lemma 2.2, \( s_{n-a-2b-2+j} \geq s_{n-a-2b-1-j} \) for \( i + 1 \leq j \leq m \). Hence,

\[
\rho(T) \left( x_{u_{n-a-2b-2+i} - x_{u_{n-a-2b-1-i}}} \right) - \rho(T) \left( x_{u_{n-a-2b-1+i} - x_{u_{n-a-2b-1-i}}} \right)
\]

\[
= 2 \left( \sum_{j=n-2a-b-1-i}^{n-a-b-1} s_j - \sum_{j=0}^{n-a-2b-2+i} s_j \right)
\]

\[
= 2 \left( \sum_{j=n-2a-b-1-i}^{n-a-b-1} s_j - \sum_{j=0}^{n-a-2b-2+m} s_j \right) - 2 \sum_{j=i+1}^{m} (s_{n-a-2b-1-j} - s_{n-a-2b-2+j})
\]

\[\geq 0,\]

and thus, \( x_{u_{n-a-2b-2+i}} - x_{u_{n-a-2b-1-i}} \geq x_{u_{n-a-2b-1+i}} - x_{u_{n-a-2b-2-i}} \geq 0 \). It follows that for \( 1 \leq i \leq m \), \( x_{u_{n-a-2b-2+i}} \geq x_{u_{n-a-2b-1-i}} \). As above, \( s_{n-a-2b-2+i} \geq s_{n-a-2b-1-i} \). Thus, \( \sum_{i=1}^{m} s_{n-a-2b-2+i} \geq \sum_{i=1}^{m} s_{n-a-2b-1-i} = \sum_{i=n-2a-b-1}^{n-a-b-1} s_i, \) and

\[
\sum_{i=0}^{n-a-2b-2+m} s_i \geq \sum_{i=0}^{n-a-b-1} s_i + \sum_{i=1}^{m} s_{n-a-2b-2+i}
\]

\[
> \sum_{i=n-2a-b-1}^{n-a-b-1} s_i + \sum_{i=n-2a-b-1-m}^{n-2a-b-2} s_i
\]

\[
= \sum_{i=n-2a-b-1-m}^{n-a-b-1} s_i,
\]

a contradiction. Thus, \( \sum_{i=1}^{n-a-2b-2+m} s_i > \sum_{i=n-2a-b-1-m}^{n-a-b-1} s_i \). This proves Claim 4.

Let \( T' = C(n, a + 1, b - 1) \). It is easily seen that

\[
\frac{1}{2} (\rho(T') - \rho(T)) \geq \frac{1}{2} x^\top (D(T') - D(T)) x = x_{u_{n-a-2b-1}} W,
\]

where
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\[ W = r \sum_{i=0}^{n} (s_{n-a-b-1-i} - s_i) + r \sum_{i=1}^{b-a-1} s_{n-a-2b-1+i} \]

\[ + \sum_{i=0}^{[\frac{x}{2}]-1} (r - 2i) (x_{u_{n-a-2b-1-i}} - x_{u_{a+1+i}}), \]

and \( r = n - 2a - 2b - 2. \)

From Claim 1, \( s_0 - s_{n-a-b-1} = x_{u_0} - x_{n-a-b-1} < x_{u_{a+1}} - x_{u_{n-a-b-2}}. \) By Lemma 2.2 and Claim 1, \( s_i - s_{n-a-b-1-i} \leq \left(1 + \frac{a}{\rho(T)^2}\right) (x_{u_{a+1}} - x_{u_{n-a-b-2}}) < 2 \left(x_{u_{a+1}} - x_{u_{n-a-b-2}}\right) \) for \( 1 \leq i \leq a. \)

Let

\[ F = \begin{cases} 0 & \text{if } b = a + 2, \\ r \sum_{i=2}^{b-a-1} s_{n-a-2b+1+i} & \text{if } b > a + 2. \end{cases} \]

By Claims 2, 3 and 4,

\[ \rho(T) \left(x_{u_{a+1}} - x_{u_{n-a-2b-1}}\right) = W + rx_{v_{n-a-2b-1}} \]

\[ < W + r \left(x_{u_{n-a-2b}} - x_{v_{n-a-2b}}\right) \]

\[ = 2W + \sum_{i=0}^{[\frac{x}{2}]-1} (r - 2i) (x_{u_{a+1+i}} - x_{u_{n-a-2b-1-i}}) \]

\[ + r \sum_{i=0}^{a} (s_i - s_{n-a-b-1-i}) - F \]

\[ < 2W + \sum_{i=0}^{[\frac{x}{2}]-1} (r - 2i) (x_{u_{a+1}} - x_{u_{n-a-2b-1}}) \]

\[ + r(2a + 1) (x_{u_{a+1}} - x_{u_{n-a-b-2}}) \]

\[ < 2W \]

\[ + \left(\sum_{i=0}^{[\frac{x}{2}]-1} (r - 2i) + (2a + 1)r\right) (x_{u_{a+1}} - x_{u_{n-a-2b-1}}). \]

Hence,

\[ 2W > \left(\rho(T) - \sum_{i=0}^{[\frac{x}{2}]-1} (r - 2i) + (2a + 1)r\right) (x_{u_{a+1}} - x_{u_{n-a-2b-1}}). \]

Claim 5. The minimum row sum of \( D(T) \) is larger than \( \sum_{i=0}^{[\frac{x}{2}]-1} (r - 2i) + (2a + 1)r. \)
For $0 \leq j \leq a$,
\[
\sum_{u \in V(T)} d_T(u, j) > \sum_{i=a+1}^{n-a-2b-2} d_T(u_i, u) + d_T(u_n-a-b-1, u)
\]
\[
+ \sum_{i=n-2a-b-1}^{n-a-b-2} (d_T(u_i, u) + d_T(u_i, v_i))
\]
\[
> \sum_{i=1}^{n-2a-2b-2} i + \sum_{i=n-2a-b-1}^{n-a-b-2} 2r
\]
\[
> \sum_{i=0}^{\lceil \frac{r}{2} \rceil - 1} (r - 2i) + (2a + 1)r.
\]

If $a \geq 1$, then for $1 \leq j \leq a$,
\[
\sum_{u \in V(T)} d_T(v_j, u) > \sum_{u \in V(T)} d_T(u_j, u) > \sum_{i=0}^{\lceil \frac{r}{2} \rceil - 1} (r - 2i) + (2a + 1)r.
\]

For $a+1 \leq j \leq n-a-2b-2$,
\[
\sum_{u \in V(T)} d_T(u_j, u) > \sum_{i=a+1}^{n-a-2b-2} d_T(u_j, u_i) + d_T(u_j, u_0)
\]
\[
+ \sum_{i=1}^{a} (d_T(u_j, u_i) + d_T(u_j, v_i) + d_T(u_j, u_{n-a-b-1-i})
\]
\[
+ d_T(u_j, v_{n-a-b-1-i}) + d_T(u_j, u_{n-a-b-1})
\]
\[
> \sum_{i=a+1}^{n-a-2b-2} d_T(u_{a+\lceil \frac{r}{2} + 1 \rceil}, u_i) + (2a + 1)r
\]
\[
= \sum_{i=0}^{\lceil \frac{r}{2} \rceil - 1} (r - 2i) + (2a + 1)r.
\]

For $n-a-2b-1 \leq j \leq n-a-b-1$,
\[
\sum_{u \in V(T)} d_T(u_j, u) > \sum_{i=a+1}^{n-a-2b-2} d_T(u_{n-a-2b-1}, u_i) + d_T(u_{n-a-2b-1}, u_0)
\]
\[
+ \sum_{i=1}^{a} (d_T(u_{n-a-2b-1}, u_i) + d_T(u_{n-a-2b-1}, v_i))
\]
For \( n - a - 2b - 1 \leq j \leq n - a - b - 2 \),

\[
\sum_{u \in V(T)} d_T(v_j, u) > \sum_{u \in V(T)} d_T(u_j, u) > \sum_{i=0}^{[\frac{\delta}{2}] - 1} (r - 2i) + (2a + 1)r.
\]

Thus, Claim 5 follows.

Since \( \rho(T) \) is bounded below by the minimum row sum of \( D(T) \) [\( \rho \) p. 24], we have by Claim 5 that \( \rho(T) > \sum_{i=0}^{[\frac{\delta}{2}] - 1} (r - 2i) + (2a + 1)r \). Now by (3.6) and Claim 3, \( W > 0 \), and thus by (3.6), \( \rho(T') - \rho(T) > 0 \). \( \Box \)

Let \( \Delta(G) \) be the maximum degree of a graph \( G \).

**Lemma 3.6.** Let \( T \) be a caterpillar with \( n \) vertices and \( k \) pendant vertices, where \( k \geq 3 \). If \( \Delta(T) = 3 \), then \( \rho(T) \leq \rho(C(n, \lfloor \frac{k-2}{2} \rfloor, \lceil \frac{k-2}{2} \rceil)) \) with equality if and only if \( T \cong C(n, \lfloor \frac{k-2}{2} \rfloor, \lceil \frac{k-2}{2} \rceil) \).

**Proof.** If \( n \) is even and \( k = \frac{n}{2} + 1 \), then the result is trivial. If \( k = 3 \), then the result follows from Lemma 3.4.

Suppose \( 4 \leq k \leq \frac{n}{2} \). Let \( T \) be a caterpillar with maximum distance spectral radius satisfying the hypothesis in the lemma.

Let \( U \) be the set of vertices of degree 2 in \( T \). Then \( k + 2|U| + 3(n-k-|U|) = 2(n-1) \), and thus, \( |U| = n - 2k + 2 > 0 \), i.e., \( U \neq \emptyset \).

Obviously, the diameter of \( T \) is \( n - (k-2) - 1 = n - k + 1 \). Let \( u_0u_1 \ldots u_{n-k+1} \) be a diametrical path of \( T \). Assume without loss of generality that \( \delta_T(u_1) \leq \delta_T(u_{n-k}) \).

Then \( 2 \leq \delta_T(u_1) \leq \delta_T(u_{n-k}) \leq 3 \).

Suppose \( \delta_T(u_{n-k}) = 2 \). Then \( \delta_T(u_1) = 2 \) and there is \( u_j \) with \( 2 \leq j \leq n - k - 1 \) such that \( \delta_T(u_j) = 3 \). Let \( v_j \) be the pendant neighbor of \( u_j \). Let \( T_1 \) and \( T_2 \) be the nontrivial components of \( T - u_j \) containing \( u_0 \) and \( u_{n-k+1} \), respectively. Assume without loss of generality that \( \sigma_T(T_1) \geq \sigma_T(T_2) \). Let \( T' = T - u_jv_j + u_{n-k}v_j \). Obviously, \( T' \) is a caterpillar with \( n \) vertices and \( k \) pendant vertices, and \( \Delta(T') = 3 \). By Lemma 2.3, \( \rho(T) < \rho(T') \), a contradiction. Thus, \( \delta_T(u_{n-k}) = 3 \).

Suppose \( \delta_T(u_1) = 2 \). If \( T - U \) has exactly one nontrivial component, then \( T \cong C(n, 0, k - 2) \), and by Lemma 2.3, \( \rho(T) = \rho(C(n, 0, k - 2)) < \rho(C(n, \lfloor \frac{k-2}{2} \rfloor, \lceil \frac{k-2}{2} \rceil)) \), a contradiction. If \( T - U \) has at least two nontrivial components, then there are vertices
u_i and u_j with 2 ≤ i < j ≤ n − k − 1 such that δ_T(u_i) = 3 and δ_T(u_j) = 2. Let v be the pendant neighbor of u_i. Let T_1 and T_2 be the components of T − u_i containing u_0 and u_{n−k+1}, respectively. Assume without loss of generality that σ_T(T_1) ≥ σ_T(T_2).

Let T'' = T − u_iv_i + u_jv_j. Obviously, T'' is a caterpillar with n vertices and k pendant vertices, and Δ(T'') = 3. By Lemma 2.3, ρ(T) < ρ(T''), a contradiction. Thus, δ_T(u_1) = 3, and T − U has at least two nontrivial components.

Suppose that T − U has at least three nontrivial components. There are three vertices u_i, u_j, u_l with 2 ≤ i < j < l ≤ n − k − 1 in T such that δ_T(u_j) = 3 and {u_i, u_l} ⊆ U. Let T_1 and T_2 be the nontrivial components of T − u_j containing u_i and u_l, respectively. Let v_j be the pendant neighbor of u_j. Assume without loss of generality that σ_T(T_1) ≥ σ_T(T_2). Let T' = T − u_jv_j + u_lv_j. By Lemma 2.3, ρ(T) < ρ(T'), a contradiction. Thus, T − U contains exactly two nontrivial components, implying that T ≅ C(n, a, b), where a + b = k − 2, and a, b ≥ 1. By Lemma 3.5, T ≅ C(n, ⌊k−2−1−2⌋, ⌊k−2−1−2⌋).

For integers n and k with 1 ≤ k ≤ ⌊n−2−4⌋, let T(n, k) be the set of trees with n vertices and 2k odd vertices.

**Theorem 3.7.** Let T ∈ T(n, k), where 1 ≤ k ≤ ⌊n−2−4⌋. Then

$$\rho(T) ≤ \rho(C\left(n, \left\lfloor \frac{k−1−1−2}{2} \right\rfloor, \left\lceil \frac{k−1−1−2}{2} \right\rceil\right))$$

with equality if and only if T ≅ C(n, ⌊k−2−1−2⌋, ⌊k−2−1−2⌋).

**Proof.** If k = 1, 2, then the result follows from Lemma 3.4.

Suppose k ≥ 3. Let T be a tree in T(n, k) with maximum distance spectral radius.

Suppose that the maximum odd degree is larger than 3. Then δ_T(u) = 2t + 1 for some u ∈ V(T) and t ≥ 2. Let N_T(u) = {u_1, ..., u_{2t+1}}. Let T_i be the component of T − u containing u_i, where 1 ≤ i ≤ 2t + 1. Assume without loss of generality that σ_T(T_1) ≥ σ_T(T_{2t+1}). Let w be a pendant vertex of T in V(T_{2t+1}). Let T' = T − {wu_i : 3 ≤ i ≤ 2t} + {wu_i : 3 ≤ i ≤ 2t}. Note that the degrees of u and w remain odd in T'. Then T' ∈ T(n, k). By Lemma 3.2, ρ(T') > ρ(T), a contradiction. Thus, the maximum odd degree is 3.

If n is even, and k = ⌊n−2−4⌋, then by Lemma 3.3, T ≅ C(n, ⌊k−2−1−2⌋, ⌊k−2−1−2⌋).

Suppose k < ⌊n−2−4⌋. Let U be the set of even vertices of T. Then |U| ≥ 1. Suppose that the maximum even degree is larger than 2. Then δ_T(u) = 2t for some u ∈ V(T) and t ≥ 2. Let N_T(u) = {u_1, ..., u_{2t}}. Let T_i be the component of T − u containing u_i, where 1 ≤ i ≤ 2t. Assume without loss of generality that σ_T(T_1) ≥ σ_T(T_{2t}). Let w be a pendant vertex of T in V(T_{2t}). Let T' = T − uw_2 + uw_2. Note that the degree of u is odd and the degree of w is even in T'. Then T' ∈ T(n, k). By Lemma 2.3.
\( \rho(T') > \rho(T) \), a contradiction. Thus, the maximum even degree is 2, and each vertex in \( U \) is of degree 2 in \( T \).

Suppose that \( T \) is not a caterpillar. Since \( \Delta(T) = 3 \), there is a vertex \( u \) of degree 3 in the graph obtained from \( T \) by deleting all pendant vertices. Let \( N_T(u) = \{u_1, u_2, u_3\} \). Obviously, \( \delta_T(u_i) \geq 2 \) for \( i = 1, 2, 3 \). Let \( T_i \) be the component of \( T - u \) containing \( u_i \), where \( 1 \leq i \leq 3 \).

**Claim.** \( U \subseteq V(T_i) \) for some \( i \) with \( i = 1, 2, 3 \).

Otherwise, there are two vertices of degree 2 in \( T \), one in \( V(T_i) \) and the other in \( V(T_j) \), where \( 1 \leq i < j \leq 3 \). Assume without loss of generality that \( \delta_T(v_1) = \delta_T(v_2) = 2 \) with \( v_1 \in V(T_i) \) and \( v_2 \in V(T_j) \), and that \( \sigma_T(T_i) \geq \sigma_T(T_j) \). Let \( T' = T - uv_2 + v_3u_2 \). Obviously, \( \delta_T(T') \) is even and \( \delta_T(v_3) \) is odd. Thus, \( T' \in \mathcal{T}(n, k) \).

By Lemma 2.3, \( \rho(T') > \rho(T) \), a contradiction. This proves the Claim.

Since \( \Delta(T) = 3 \), we have by the Claim that \( T \cong G_1(s, t) \) for some \( s \) and \( t \) with \( s \geq t \geq 2 \). Obviously, \( G_1(s + 1, t - 1) \in \mathcal{T}(n, k) \). By Lemma 3.3, \( \rho(G_1(s + 1, t - 1)) > \rho(T) \), a contradiction. Thus, \( T \) is a caterpillar with \( \Delta(T) = 3 \). By Lemma 3.6 we have \( T \cong C(n, \lceil \frac{n}{2} \rceil, \lceil \frac{n}{2} \rceil) \). \( \square \)

### 4. Distance spectral radius of trees with given number of vertices of degree 3 or of degree at least 3

Let \( T \) be a tree with \( n \) vertices, in which \( k \) vertices of degree 3. Let \( r \) be the number of pendant vertices in \( T \). Then \( r + 2(n - r - k) + 3k \leq 2(n - 1) \), i.e., \( r \geq k + 2 \). This implies that \( 2k + 2 \leq k + r \leq n \), and thus, \( k \leq \frac{n}{2} - 1 \). As an application of Theorem 3.7, we have

**Theorem 4.1.** Let \( T \) be a tree on \( n \) vertices with \( k \) vertices of degree 3, where \( n \geq 2 \), and \( 0 \leq k \leq \lfloor \frac{n}{2} \rfloor - 1 \). Then \( \rho(T) \leq \rho(C(n, \lfloor \frac{n}{2} \rfloor, \lfloor \frac{n}{2} \rfloor)) \) with equality if and only if \( T \cong C(n, \lfloor \frac{n}{2} \rfloor, \lfloor \frac{n}{2} \rfloor) \).

**Proof.** If \( k = 0, 1 \), then the result follows from Lemma 3.4.

Suppose \( k \geq 2 \). Let \( T \) be a tree with maximum distance spectral radius on \( n \) vertices with \( k \) vertices of degree 3. Let \( \Delta = \Delta(T) \).

**Case 1.** \( \Delta \geq 5 \). Let \( u \in V(T) \) and \( N_T(u) = \{u_1, \ldots, u_\Delta\} \). Let \( T_i \) be the component of \( T - u \) containing \( u_i \), where \( 1 \leq i \leq \Delta \). Assume without loss of generality that \( \sigma_T(T_i) \geq \sigma_T(T_\Delta) \). Let \( w \) be a pendant vertex of \( T \) in \( V(T_\Delta) \). Let \( T' = T - \{wu_i : 2 \leq i \leq \Delta - 1\} + \{wu_i : 2 \leq i \leq \Delta - 1\} \). Note that the number of vertices of degree 3 in \( T' \) remains \( k \). By Lemma 3.2, \( \rho(T') > \rho(T) \), a contradiction.

**Case 2.** \( \Delta = 4 \). Let \( u \in V(T) \) and \( N_T(u) = \{u_1, u_2, u_3, u_4\} \). Let \( T_i \) be the component of \( T - u \) containing \( u_i \), where \( 1 \leq i \leq 4 \). Assume without loss of generality that \( \sigma_T(T_1) \geq \sigma_T(T_3) \). Let \( v \) be a pendant vertex of \( T \) in \( V(T_4) \), and \( T' = T - uu_2 + uu_3 \).
Let $T'_4$ be the component of $T' - u$ containing $u_4$. Note that $\delta_{T'}(u) = 3$ and $u$ is a cut vertex. Assume without loss of generality that $\sigma_{T'}(T_1) \geq \sigma_{T'}(T'_4)$. Let $w$ be a pendant vertex of $T'$ in $V(T'_4)$ and $T'' = T' - uw_3 + uw_4$. Note that the number of vertices of degree 3 in $T''$ remains $k$. By Lemma 2.3, $\rho(T'') > \rho(T') > \rho(T)$, a contradiction.

Now we have proven that $\Delta = 3$. Let $r$ be the number of pendant vertices in $T$. Since $r + 2(n - k + r) + 3k = 2(n - 1)$, we have $r = k + 2$, and thus, $T \in \mathcal{T}(n, k + 1)$. By Theorem 3.7, we have $T \cong C\left(n, \lceil \frac{k}{2} \rceil, \lfloor \frac{k}{2} \rfloor \right)$. $\blacksquare$

**Theorem 4.2.** Let $T$ be a tree with $n$ vertices and $k$ vertices of degree at least 3, where $0 \leq k \leq \lfloor \frac{n}{2} \rfloor - 1$. Then $\rho(T) \leq \rho(C\left(n, \lceil \frac{k}{2} \rceil, \lfloor \frac{k}{2} \rfloor \right))$ with equality if and only if $T \cong C\left(n, \lceil \frac{k}{2} \rceil, \lfloor \frac{k}{2} \rfloor \right)$.

**Proof.** If $k = 0$, then the result follows from Lemma 3.4.

Suppose $k \geq 1$. Let $T$ be a tree with maximum distance spectral radius among trees with $n$ vertices and $k$ vertices of degree at least 3. Let $\Delta = \Delta(T)$.

Suppose $\Delta \geq 4$. Let $u \in V(T)$ and $N_T(u) = \{u_1, \ldots, u_\Delta\}$. Let $T_i$ be the component of $T - u$ containing $u_i$, where $1 \leq i \leq \Delta$. Assume without loss of generality that $\sigma_T(T_1) \geq \sigma_T(T_\Delta)$. Let $w$ be a pendant vertex of $T$ in $V(T_\Delta)$. Let $T' = T - uw_3 + uw_2$. Obviously, $T'$ is a tree with $n$ vertices and $k$ vertices of degree at least 3. By Lemma 2.3, $\rho(T') > \rho(T)$, a contradiction. Hence, $\Delta \leq 3$, implying that $T$ is a tree with $k$ vertices of degree 3. By Theorem 4.1, $T \cong C\left(n, \lceil \frac{k}{2} \rceil, \lfloor \frac{k}{2} \rfloor \right)$. $\blacksquare$

**5. Distance spectral radius of trees with all odd vertices.** For $n \geq 2$, let $\mathcal{T}(2n)$ be the set of all trees with $2n$ vertices, which are all odd. Let $E_{2n} = C(2n, 0, n - 1)$.

Let $T$ be a tree with $n$ vertices. Then $\rho(T) \geq \rho(S_n)$ with equality if and only if $T \cong S_n$, see [9]. By this result and Theorem 3.4, we have

**Theorem 5.1.** Let $T \in \mathcal{T}(2n)$. Then $\rho(S_{2n}) \leq \rho(T) \leq \rho(E_{2n})$ with left equality if and only if $T \cong S_{2n}$ and right equality if and only if $T \cong E_{2n}$.

For integers $n$ and $a$ with $1 \leq a \leq \lfloor \frac{n-2}{2} \rfloor$, let $D_{n,a}$ be the double star obtained by adding an edge between the center $u$ of $S_{n+1}$ and the center $v$ of $S_{n-a-1}$.

**Lemma 5.2.** [8] For $a \geq 2$, $\rho(D_{n,a}) > \rho(D_{n,a-1})$.

**Theorem 5.3.** Let $T \in \mathcal{T}(2n)$ and $T \not\cong S_{2n}$, where $n \geq 3$. Then $\rho(T) \geq \rho(D_{2n,2})$ with equality if and only if $T \cong D_{2n,2}$.

**Proof.** Let $T$ be the tree with minimum distance spectral radius in $\mathcal{T}(2n) \setminus \{S_{2n}\}$. Let $t$ be the diameter of $T$. Obviously, $t \geq 3$. Let $u_1 \ldots u_{t+1}$ be a diametrical path of
Obviously, \( G \{ \) by 2, the distance between a vertex of \( G \{ \) between a vertex pair remains unchanged. Hence, \( P \) is a double star. By Lemma 5.2, \( T' \cong D_{2n,2} \).

For \( n \geq 3 \) and \( 2 \leq i \leq \left\lfloor \frac{n+1}{2} \right\rfloor \), let \( B(2n, i) \) be the caterpillar obtained from the path \( P_n \) with consecutive vertices \( u_1, \ldots, u_n \) by attaching a pendant vertex \( v_j \) to \( u_j \) for \( 2 \leq j \leq n-1 \) with \( j \neq i \) and attaching three pendant vertices \( w_1, w_2, w_3 \) to \( u_i \).

For \( n \geq 5 \) and \( 3 \leq i \leq \left\lfloor \frac{n+1}{2} \right\rfloor \), let \( F(2n, i) \) be the caterpillar obtained from the path \( P_n \) with consecutive vertices \( u_1, \ldots, u_n \) by attaching a pendant vertex \( v_j \) to \( u_j \) for \( 2 \leq j \leq n-1 \) with \( j \neq i \) and adding an edge between \( u_i \) and the center of \( S_3 \).

**Lemma 5.4.** For \( n \geq 5 \), and \( 2 \leq i \leq \left\lfloor \frac{n+1}{2} \right\rfloor \), \( \rho(F(2n, i + 1)) > \rho(B(2n, i)) \).

**Proof.** Let \( G = B(2n, i) \) and \( G' = B(2n, i) - \{u_i, w_2, w_3\} + \{v_{i+1}w_2, v_{i+1}w_3\} \). Obviously, \( G' \cong F(2n, i + 1) \). Let \( x = x(G) \). As we pass from \( G \) to \( G' \), the distance between a vertex of \( \{w_2, w_3\} \) and a vertex of \( \{u_1, \ldots, u_i, v_2, \ldots, v_{i-1}, w_1\} \) is increased by 2, the distance between a vertex of \( \{w_2, w_3\} \) and \( v_{i+1} \) is decreased by 2, and the distance between any other vertex pair remains unchanged. Hence,

\[
\frac{1}{2}(\rho(G') - \rho(G)) \geq \frac{1}{2} x^T (D(G') - D(G)) x = 2(x_{w_2} + x_{w_3})(x_{u_i} + x_{w_1} - x_{v_{i+1}}).
\]

From (2.1) for \( G \) at \( u_i \), \( w_1 \) and \( v_{i+1} \), we have

\[
\rho(G)x_{u_i} = x_{w_1} + x_{w_2} + x_{w_3} + 2x_{v_{i+1}} + \sum_{k=1}^{i-1} d_G(u_i, u_k)x_{u_k} + \sum_{k=2}^{i-1} d_G(u_i, v_k)x_{v_k} + \sum_{k=i+1}^{n} (d_G(u_{i+1}, u_k) + 1)x_{u_k} + \sum_{k=i+2}^{n-1} (d_G(u_{i+1}, v_k) + 1)x_{v_k},
\]

\[
\rho(G)x_{w_1} = x_{u_i} + 2x_{w_2} + 2x_{w_3} + 3x_{v_{i+1}} + \sum_{k=1}^{i-1} (d_G(u_i, u_k) + 1)x_{u_k} + \sum_{k=2}^{i-1} (d_G(u_i, v_k) + 1)x_{v_k} + \sum_{k=i+1}^{n} (d_G(u_{i+1}, u_k) + 2)x_{u_k} + \sum_{k=i+2}^{n-1} (d_G(u_{i+1}, v_k) + 2)x_{v_k},
\]

\[
\rho(G)x_{v_{i+1}} = 2x_{u_i} + 3x_{w_1} + 3x_{w_2} + 3x_{w_3} + \sum_{k=1}^{i-1} (d_G(u_i, u_k) + 2)x_{u_k} + \sum_{k=2}^{i-1} (d_G(u_i, v_k) + 3)x_{v_k} + \sum_{k=i+1}^{n} (d_G(u_{i+1}, u_k) + 3)x_{u_k} + \sum_{k=i+2}^{n-1} (d_G(u_{i+1}, v_k) + 3)x_{v_k}.
\]
We claim that $\Delta \leq 5$. Let $\rho$ denote the spectral radius of $T$ from Theorem 5.1. Therefore, $\rho(G') > \rho(G)$, i.e., $\rho(F(2n, i + 1)) > \rho(B(2n, i))$. 

**Theorem 5.5.** Let $T \in T(2n)$ and $T \neq E_{2n}$, where $n \geq 3$.

(i) For $n = 3, 4$, $\rho(T) \leq \rho(B(2n, 2))$ with equality if and only if $T \cong B(2n, 2)$;

(ii) For $n \geq 5$, $\rho(T) \leq \rho(F(2n, 3))$ with equality if and only if $T \cong F(2n, 3)$.

**Proof.** For $n = 3, 4$, we have $T(2n) = \{E_{2n}, B(2n, 2)\}$, and thus, the result follows from Theorem 5.1.

Suppose $n \geq 5$. Let $T$ be a tree with maximum distance spectral radius in $T(2n)\{E_{2n}\}$. Let $\Delta = \Delta(T)$.

Suppose $\Delta \geq 7$. Let $u \in V(T)$ and $N_T(u) = \{u_1, \ldots, u_\Delta\}$. Let $T_i$ be the component of $T - u$ containing $u_i$, where $1 \leq i \leq \Delta$. Assume without loss of generality that $\sigma_T(T_i) \geq \sigma_T(T_\Delta)$. Let $w$ be a pendant vertex of $T$ in $V(T_\Delta)$. Let $T' = T - \{uw_2, uw_3\} + \{wu_2, uw_3\}$. Then $T' \in T(2n)$ and $T' \neq E_{2n}$. By Lemma 5.2, $\rho(T') > \rho(T)$, a contradiction. Thus, $\Delta = 3$ or 5.

Suppose $\Delta = 5$. By similar argument as above, there is exactly one vertex of degree 5. Let $u_1 \cdots u_{t+1}$ be a longest path passing the vertex of degree 5, say $u_i$, where $2 \leq i \leq t$. Let $v_1, v_2, v_3$ be the other three neighbors of $u_i$ outside the above path. We claim that $v_1, v_2, v_3$ are pendant vertices. Otherwise, suppose that $v_1$ is not
a pendant vertex. Let $T_1$ and $T_2$ be the components of $T-u_i$ containing $u_{i-1}$ and $u_{i+1}$, respectively. Assume without loss of generality that $\sigma_T(T_1) \geq \sigma_T(T_2)$. Let $T' = T - \{u_1v_2, u_2v_3\} + \{u_{i+1}v_2, u_{i+1}v_3\}$. Obviously, $T' \in T(2n)$ and $T' \not\equiv E_{2n}$. By Lemma 3.2, $\rho(T') > \rho(T)$, a contradiction. Since each vertex different from $u_i$ is of degree 1 or 3 in $T$, we have by Lemma 5.3 that $T \cong B(2n, i)$ with $2 \leq i \leq \left\lfloor \frac{n}{2} \right\rfloor$. Suppose $3 \leq i \leq \left\lfloor \frac{n}{2} \right\rfloor$. Let $T' = B(2n, i) - \{u_1v_2, u_2v_3\} + \{u_{i+1}v_2, u_{i+1}v_3\}$ if $\sigma_T(T_1) \leq \sigma_T(T_2)$, and $T' = B(2n, i) - \{u_1v_2, u_2v_3\} + \{u_{i-1}v_2, u_{i-1}v_3\}$ if $\sigma_T(T_1) > \sigma_T(T_2)$. It is easily seen that $T' \cong B(2n, 2)$. By Lemma 5.4 $\rho(T) = \rho(B(2n, i)) < \rho(T') = \rho(B(2n, 2))$, a contradiction. Then $i = 2$, and thus, $T \cong B(2n, 2)$.

Suppose $\Delta = 3$. By Lemma 5.3 $T \cong F(2n, i)$ with $3 \leq i \leq \left\lfloor \frac{n}{2} \right\rfloor$. By Lemma 3.3 $\rho(F(2n, 3)) > \rho(F(2n, 4)) > \cdots > \rho\left(F\left(2n, \left\lfloor \frac{2n}{2} \right\rfloor\right)\right)$. Thus, $T \cong F(2n, 3)$.

By Lemma 5.4 $\rho(B(2n, 2)) < \rho(F(2n, 3))$. Thus, $T \cong F(2n, 3)$. □

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