Electronic Journal of Linear Algebra

Volume 31 *Volume 31: (2016)* Article 21

2016

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Recommended Citation
Lin, Hongying and Zhou, Bo. (2016), "The distance spectral radius of graphs with given number of odd vertices", *Electronic Journal of Linear Algebra*, Volume 31, pp. 286-305.
DOI: https://doi.org/10.13001/1081-3810.2877

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 286-305, May 2016

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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

*Received by the editors on January 19, 2015. Accepted for publication on April 7, 2016. Handling Editor: Bryan L. Shader.

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Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 286-305, May 2016

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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 $V(G) = \{v_1, \dots, v_n\}$. A column vector $x = (x_{v_1}, \dots, x_{v_n})^\top \in \mathbb{R}^n$ (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 $i = 1, \dots, n$. Then

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

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

$$\lambda x_u = \sum_{v\in V(G)} d_G(u,v)x_v. \tag{2.1}$$

We call (2.1) the (λ, 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 $V_1 \subset V(G)$, $G - V_1$ 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 $G + \{uv\}$.

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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*

$$G' = G - \left\{uw : w \in N_{G'_3}(u)\right\} + \left\{vw : w \in N_{G'_3}(u)\right\}.$$

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 $\mathbb{G}(n, k)$ 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 $G \in \mathbb{G}(n, k)$, 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 $\rho(G) \geq \rho\left(K_n\left(\frac{n}{2} - k\right)\right)$ with equality if and only if $G \cong K_n\left(\frac{n}{2} - k\right)$.

Proof. Let G be the graph in $\mathbb{G}(n, k)$ 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 $G' \in \mathbb{G}(n, k)$. By Lemma 2.1, $\rho(G') < \rho(G)$, a contradiction. Thus, each

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
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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 $t = \frac{n-1-\delta_G(u)}{2}$. 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 u_{2t}. Let $G' = G + \{uu_1, uu_{2t}, u_1u_{2t}\}$. Obviously, $G' \in \mathbb{G}(n,k)$. By Lemma 2.1, $\rho(G') < \rho(G)$, a contradiction. Thus, $u_1u_{2t} \in E(G)$.

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

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

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

Thus,

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

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,

$$\begin{aligned}\frac{1}{2}(\rho(G) - \rho(G'')) &\geq \frac{1}{2}x^\top(D(G) - D(G''))x \\ &= x'_u\left(x'_{u_1} + x'_{u_{2t}}\right) - x'_{u_1}x'_{u_{2t}} \\ &= \frac{1}{2}\left(\left(2x'_u - x'_{u_{2t}}\right)x'_{u_1} + \left(2x'_u - x'_{u_1}\right)x'_{u_{2t}}\right) \\ &> 0.\end{aligned}$$

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 $t = \frac{n-2-\delta_G(u)}{2}$. 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 $G'' = G - u_1u_{2t+1} + \{uu_1, uu_{2t+1}\}$. Obviously, $G'' \in \mathbb{G}(n,k)$. 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 $G \cong K_n(k)$.

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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 $T' = T - \{uu_i : 2 \leq i \leq t\} + \{wu_i : 2 \leq i \leq t\}$, where $2 \leq t \leq k-1$ and $w \in V(T_k)$. If $\sigma_T(T_1) \geq \sigma_T(T_k)$, 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 $V(T_1) \cup \{u\}$ 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,

$$\begin{aligned}\frac{1}{2}(\rho(T') - \rho(T)) &\geq \frac{1}{2}x^\top(D(T') - D(T))x \\ &\geq d_T(u,w)\sum_{i=2}^{t}\sigma_T(T_i)\left(\sigma_T(T_1) - \sigma_T(T_k) + x_u\right) \\ &> 0.\end{aligned}$$

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 $s,t \geq 1$.

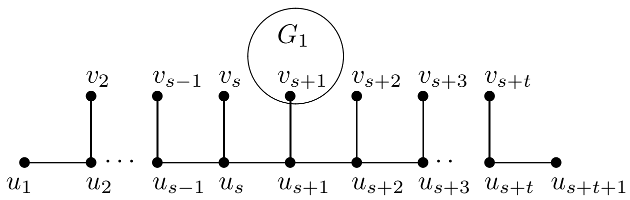

Fig. 1. Graph $G_1(s,t)$.

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

$$G' = G - \{u_{s+2}v_{s+2}, u_{s+1}v_{s+1}\} + \{u_{s+2}v_{s+1}, u_{s+1}v_{s+2}\}.$$

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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

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

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,

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

and

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

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A publication of the International Linear Algebra Society
Volume 31, pp. 286-305, May 2016

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$$+ \sum_{w \in V(G_1)\setminus\{z, v_{s+1}\}} d_G(z,w)x_w$$
$$> 0.$$

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

$$\sum_{i=1}^{s} y_i < \sum_{i=1}^{t} y_{s+1+i}. \tag{3.1}$$

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

$$\rho(G)\left(x_{u_{s+2}} - x_{u_s}\right) = 2\left(\sum_{j=1}^{s} y_j - \sum_{j=1}^{t} y_{s+1+j}\right) \tag{3.2}$$

and

$$\begin{aligned}
&\rho(G)\left(x_{u_{s+1+i}} - x_{u_{s+1-i}}\right) - \rho(G)\left(x_{u_{s+i}} - x_{u_{s+2-i}}\right)\\
&= 2\left(\sum_{j=i}^{s} y_{s+1-j} - \sum_{j=i}^{t} y_{s+1+j}\right)\\
&= 2\left(\sum_{j=1}^{s} y_j - \sum_{j=1}^{t} y_{s+1+j}\right) - 2\left(\sum_{j=1}^{i-1} y_{s+1-j} - \sum_{j=1}^{i-1} y_{s+1+j}\right)
\end{aligned} \tag{3.3}$$

for $2 \leq i \leq t-1$. We now prove that $x_{u_{s+1+i}} - x_{u_{s+1-i}} < 0$ 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 $x_{u_{s+1+j}} - x_{u_{s+1-j}} < 0$ for $1 \leq j \leq i-1$. In particular, $x_{u_{s+i}} - x_{u_{s+2-i}} < 0$. By Lemma 2.2, $y_{s+1+j} = x_{u_{s+1+j}} + x_{v_{s+1+j}} < x_{u_{s+1-j}} + x_{v_{s+1-j}} = y_{s+1-j}$. 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 $x_{u_{s+1-i}} - x_{u_{s+1+i}} > 0$ for $1 \leq i \leq t$. Thus,

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

which leads to the contradiction that $\sum_{i=1}^{s} y_i \geq \sum_{i=1}^{t} y_{s+1+i}$. Hence, $\sum_{i=1}^{s} y_i - \sum_{i=1}^{t} y_{s+1+i} \geq 0$, 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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A publication of the International Linear Algebra Society
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vertex of $V(G_3)\backslash\{v_{s+2}\}$ is decreased by 1, the distance between v_{s+2} and a vertex of $V(G_3)\backslash\{v_{s+2}\}$ 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,

$$\begin{aligned}\frac{1}{2}(\rho(G')-\rho(G)) \geq \frac{1}{2}x^\top(D(G')-D(G))x\\ &= \sigma_G(G_1)\left(\sigma_G(G_2)+x_{u_{s+1}}\right)-\sigma_G(G_1)\left(\sigma_G(G_3)-x_{v_{s+2}}\right)\\ &\quad +x_{v_{s+2}}\left(\sigma_G(G_3)-x_{v_{s+2}}\right)-x_{v_{s+2}}\left(\sigma_G(G_2)+x_{u_{s+1}}\right)\\ &= \left(\sigma_G(G_2)-\sigma_G(G_3)+x_{v_{s+2}}+x_{u_{s+1}}\right)\left(\sigma_G(G_1)-x_{v_{s+2}}\right),\end{aligned}$$

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

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. [10] *Let T be a tree with $n\geq 4$ vertices. If $T\ncong P_n$ 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 $T=C(n,a,b)$, $p=\lfloor\frac{n-a-b-2}{2}\rfloor$, 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 $\sum_{i=0}^{p}s_i\geq\sum_{i=q+1}^{n-a-b-1}s_i$. 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

$$\rho(T)\left(x_{u_p}-x_{u_{q+1}}\right)=(q+1-p)\left(\sum_{i=q+1}^{n-a-b-1}s_i-\sum_{i=0}^{p}s_i\right), \tag{3.4}$$

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, $x_{v_{p-j}}\leq x_{v_{q+1+j}}$, 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,

$$\rho(T)\left(x_{u_{p-i}}-x_{u_{q+1+i}}\right)-\rho(T)\left(x_{u_{p+1-i}}-x_{u_{q+i}}\right)$$

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A publication of the International Linear Algebra Society
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$$
\begin{aligned}
&= 2\left(\sum_{j=q+1+i}^{n-a-b-1} s_j - \sum_{j=0}^{p-i} s_j\right)\\
&= 2\left(\sum_{j=q+1}^{n-a-b-1} s_j - \sum_{j=0}^{p} s_j\right) - 2\sum_{j=0}^{i-1}(s_{q+1+j} - s_{p-j})\\
&\le 0,
\end{aligned}
$$

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

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

$$
\begin{aligned}
&\rho(T)\left(x_{u_i} - x_{u_{n-a-b-1-i}}\right) - \rho(T)\left(x_{u_{i-1}} - x_{u_{n-a-b-i}}\right)\\
&= 2\sum_{j=0}^{i-1}(s_j - s_{n-a-b-1-j})\\
&\le 0.
\end{aligned}
$$

Hence, $x_{u_i} - x_{u_{n-a-b-1-i}} \le x_{u_{i-1}} - x_{u_{n-a-b-i}} \le 0$. Thus, $x_{u_i} \le x_{u_{n-a-b-1-i}}$ for $0 \le i \le p$. In particular, $x_{u_p} \le x_{u_{q+1}}$, 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 $0 \le i \le a$.

Claim 2. $x_{v_{n-a-2b-1}} < x_{u_{n-a-2b}} + x_{v_{n-a-2b}}$.

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

$$
d_T(u_{n-a-2b}, u) + d_T(v_{n-a-2b}, u) - d_T(v_{n-a-2b-1}, u) \ge 0,
$$

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

$$
\begin{aligned}
\rho(T)\left(x_{u_{n-a-2b}} + x_{v_{n-a-2b}} - x_{v_{n-a-2b-1}}\right) &= -x_{u_{n-a-2b}} - 2x_{v_{n-a-2b}} + 5x_{v_{n-a-2b-1}}\\
&\quad + \sum_{u\in V'}\left(d_T(u_{n-a-2b}, u) + d_T(v_{n-a-2b}, u)\right.\\
&\quad \left.- d_T(v_{n-a-2b-1}, u)\right)x_u\\
&\ge -x_{u_{n-a-2b}} - 2x_{v_{n-a-2b}} + 5x_{v_{n-a-2b-1}}.
\end{aligned}
$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 286-305, May 2016

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Thus,

$$(\rho(T)+2)\left(x_{u_{n-a-2b}}+x_{v_{n-a-2b}}-x_{v_{n-a-2b-1}}\right)\geq x_{u_{n-a-2b}}+3x_{v_{n-a-2b-1}}>0,$$

from which Claim 2 follows.

Claim 3. $x_{u_{a+1+i}}-x_{u_{n-a-2b-1-i}}>x_{u_{a+2+i}}-x_{u_{n-a-2b-2-i}}>0$ for $0\leq i\leq\lfloor\frac{n-1}{2}\rfloor-b-a-1$.

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 $a+1\leq i\leq\lfloor\frac{n-1}{2}\rfloor-b$. Let $t=\lfloor\frac{n-1}{2}\rfloor$ and $t_1=\lceil\frac{n-1}{2}\rceil$. By the proof of Claim 1, $\sum_{j=0}^{t-b}s_j<\sum_{j=q+1}^{n-a-b-1}s_j$. Since $t-b\leq q-1$, we have

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

We prove that $x_{u_i}>x_{u_{n-2b-i}}$ for $a+1\leq i\leq t-b$ by induction on i. For $i=t-b$, we have

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

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

$$\begin{aligned}&\rho(T)\left(x_{u_i}-x_{u_{n-2b-i}}\right)-\rho(T)\left(x_{u_{i+1}}-x_{u_{n-2b-1-i}}\right)\\&=2\left(\sum_{j=n-2b-i}^{n-a-b-1}s_j-\sum_{j=0}^{i}s_j\right)\\&=2\left(\sum_{j=n-b-t}^{n-a-b-1}s_j-\sum_{j=0}^{t-b}s_j\right)-2\sum_{j=i+1}^{t-b}\left(s_{n-2b-j}-s_j\right)\\&>0,\end{aligned}$$

and thus, $x_{u_i}-x_{u_{n-2b-i}}>x_{u_{i+1}}-x_{u_{n-2b-1-i}}>0$. This proves Claim 3.

Claim 4. $x_{u_{n-a-2b-1}}<x_{u_{n-2a-b-2}}$.

By Claim 1, $x_{u_i}>x_{u_{n-a-b-1-i}}$ for $0\leq i\leq a$. As above, we have by Lemma 2.2 that $s_i>s_{n-a-b-1-i}$. Thus, $\sum_{i=0}^{a}s_i>\sum_{i=0}^{a}s_{n-a-b-1-i}=\sum_{i=n-2a-b-1}^{n-a-b-1}s_i$. Let $m=\lfloor\frac{b-a}{2}\rfloor$ and $m_1=\lceil\frac{b-a}{2}\rceil$.

Suppose $\sum_{i=0}^{n-a-2b-2+m}s_i\leq\sum_{i=n-2a-b-1-m}^{n-a-b-1}s_i$. We prove that $x_{u_{n-a-2b-2+i}}\geq x_{u_{n-2a-b-1-i}}$ for $1\leq i\leq m$ by induction on i. For $i=m$, we have

$$\rho(T)\left(x_{u_{n-a-2b-2+m}}-x_{u_{n-2a-b-1-m}}\right)$$

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A publication of the International Linear Algebra Society
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$$
\begin{aligned}
&= (m_1+1-m)\left(\sum_{i=n-2a-b-1-m}^{n-a-b-1} s_i - \sum_{i=0}^{n-a-2b-2+m} s_i\right)\\
&\geq 0.
\end{aligned}
$$

Hence, $x_{u_{n-a-2b-2+m}} \geq x_{u_{n-2a-b-1-m}}$. Suppose $1 \leq i \leq m-1$ and $x_{u_{n-a-2b-2+j}} \geq x_{u_{n-2a-b-1-j}}$ for $i+1 \leq j \leq m$. By Lemma 2.2, $s_{n-a-2b-2+j} \geq s_{n-2a-b-1-j}$ for $i+1 \leq j \leq m$. Hence,

$$
\begin{aligned}
&\rho(T)\left(x_{u_{n-a-2b-2+i}} - x_{u_{n-2a-b-1-i}}\right) - \rho(T)\left(x_{u_{n-a-2b-1+i}} - x_{u_{n-2a-b-2-i}}\right)\\
&= 2\left(\sum_{j=n-2a-b-1-i}^{n-a-b-1} s_j - \sum_{j=0}^{n-a-2b-2+i} s_j\right)\\
&= 2\left(\sum_{j=n-2a-b-1-m}^{n-a-b-1} s_j - \sum_{j=0}^{n-a-2b-2+m} s_j\right) - 2\sum_{j=i+1}^{m}\left(s_{n-2a-b-1-j} - s_{n-a-2b-2+j}\right)\\
&\geq 0,
\end{aligned}
$$

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

$$
\begin{aligned}
\sum_{i=0}^{n-a-2b-2+m} s_i &\geq \sum_{i=0}^{a} s_i + \sum_{i=1}^{m} s_{n-a-2b-2+i}\\
&> \sum_{i=n-2a-b-1}^{n-a-b-1} s_i + \sum_{i=n-2a-b-1-m}^{n-2a-b-2} s_i\\
&= \sum_{i=n-2a-b-1-m}^{n-a-b-1} s_i,
\end{aligned}
$$

a contradiction. Thus, $\sum_{i=0}^{n-a-2b-2+m} s_i > \sum_{i=n-2a-b-1-m}^{n-a-b-1} s_i$. This proves Claim 4.

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

$$
\frac{1}{2}(\rho(T') - \rho(T)) \geq \frac{1}{2}x^{\top}(D(T') - D(T))x = x_{v_{n-a-2b-1}} W, \tag{3.5}
$$

where

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 286-305, May 2016

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$$W = r\sum_{i=0}^{a}(s_{n-a-b-1-i} - s_i) + r\sum_{i=1}^{b-a-1} s_{n-a-2b-1+i} + \sum_{i=0}^{\lceil \frac{r}{2}\rceil -1} (r-2i)\left(x_{u_{n-a-2b-1-i}} - x_{u_{a+1+i}}\right),$$

and $r = n-2a-2b-2$.

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

$$\begin{aligned}
\rho(T)\left(x_{u_{a+1}} - x_{u_{n-a-2b-1}}\right) &= W + r x_{v_{n-a-2b-1}} \\
&< W + r\left(x_{u_{n-a-2b}} + x_{v_{n-a-2b}}\right) \\
&= 2W + \sum_{i=0}^{\lceil \frac{r}{2}\rceil -1} (r-2i)\left(x_{u_{a+1+i}} - x_{u_{n-a-2b-1-i}}\right) \\
&\quad + r\sum_{i=0}^{a}(s_i - s_{n-a-b-1-i}) - F \\
&< 2W + \sum_{i=0}^{\lceil \frac{r}{2}\rceil -1} (r-2i)\left(x_{u_{a+1}} - x_{u_{n-a-2b-1}}\right) \\
&\quad + r(2a+1)\left(x_{u_{a+1}} - x_{u_{n-2a-b-2}}\right) \\
&< 2W \\
&\quad + \left(\sum_{i=0}^{\lceil \frac{r}{2}\rceil -1} (r-2i) + (2a+1)r\right)\left(x_{u_{a+1}} - x_{u_{n-a-2b-1}}\right).
\end{aligned}$$

Hence,

$$(3.6) \qquad 2W > \left(\rho(T) - \left(\sum_{i=0}^{\lceil \frac{r}{2}\rceil -1} (r-2i) + (2a+1)r\right)\right)\left(x_{u_{a+1}} - x_{u_{n-a-2b-1}}\right).$$

Claim 5. The minimum row sum of $D(T)$ is larger than $\sum_{i=0}^{\lceil \frac{r}{2}\rceil -1}(r-2i)+(2a+1)r$.

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A publication of the International Linear Algebra Society
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For $0 \le j \le a$,

$$\begin{aligned}\sum_{u\in V(T)} d_T(u_j,u) &> \sum_{i=a+1}^{n-a-2b-2} d_T(u_a,u_i) + d_T(u_a,u_{n-a-b-1})\\ &\quad + \sum_{i=n-2a-b-1}^{n-a-b-2} (d_T(u_a,u_i)+d_T(u_a,v_i))\\ &> \sum_{i=1}^{n-2a-2b-2} i + r + \sum_{i=n-2a-b-1}^{n-a-b-2} 2r\\ &> \sum_{i=0}^{\lceil \frac{r}{2}\rceil -1} (r-2i) + (2a+1)r.\end{aligned}$$

If $a \ge 1$, then for $1 \le j \le a$,

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

For $a+1 \le j \le n-a-2b-2$,

$$\begin{aligned}\sum_{u\in V(T)} d_T(u_j,u) &> \sum_{i=a+1}^{n-a-2b-2} d_T(u_j,u_i) + d_T(u_j,u_0)\\ &\quad + \sum_{i=1}^{a} (d_T(u_j,u_i)+d_T(u_j,v_i)+d_T(u_j,u_{n-a-b-1-i})\\ &\quad + d_T(u_j,v_{n-a-b-1-i})) + d_T(u_j,u_{n-a-b-1})\\ &> \sum_{i=a+1}^{n-a-2b-2} d_T\left(u_{a+\lceil \frac{r+1}{2}\rceil}, u_i\right) + (2a+1)r\\ &= \sum_{i=0}^{\lceil \frac{r}{2}\rceil -1} (r-2i) + (2a+1)r.\end{aligned}$$

For $n-a-2b-1 \le j \le n-a-b-1$,

$$\begin{aligned}\sum_{u\in V(T)} d_T(u_j,u) &> \sum_{i=a+1}^{n-a-2b-2} d_T(u_{n-a-2b-1},u_i) + d_T(u_{n-a-2b-1},u_0)\\ &\quad + \sum_{i=1}^{a}(d_T(u_{n-a-2b-1},u_i) + d_T(u_{n-a-2b-1},v_i))\end{aligned}$$

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$$> \sum_{i=1}^{n-2a-2b-2} i + (2a+1)r$$

$$> \sum_{i=0}^{\lceil \frac{r}{2} \rceil -1} (r-2i) + (2a+1)r.$$

For $n-a-2b-1 \le j \le n-a-b-2$,

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

Thus, Claim 5 follows.

Since $\rho(T)$ is bounded below by the minimum row sum of $D(T)$ [6, p. 24], we have by Claim 5 that $\rho(T) > \sum_{i=0}^{\lceil \frac{r}{2} \rceil -1} (r-2i) + (2a+1)r$. Now by (3.6) and Claim 3, $W > 0$, and thus by (3.5), $\rho(T') - \rho(T) > 0$. ☐

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 $k \ge 3$. If $\Delta(T) = 3$, then $\rho(T) \le \rho\left(C\left(n, \lfloor \frac{k-2}{2} \rfloor, \lceil \frac{k-2}{2} \rceil\right)\right)$ with equality if and only if $T \cong C\left(n, \lfloor \frac{k-2}{2} \rfloor, \lceil \frac{k-2}{2} \rceil\right)$.*

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 $4 \le k \le \frac{n}{2}$. 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., $U \ne \emptyset$.

Obviously, the diameter of T is $n-(k-2)-1 = n-k+1$. Let $u_0u_1 \dots u_{n-k+1}$ be a diametrical path of T. Assume without loss of generality that $\delta_T(u_1) \le \delta_T(u_{n-k})$. Then $2 \le \delta_T(u_1) \le \delta_T(u_{n-k}) \le 3$.

Suppose $\delta_T(u_{n-k}) = 2$. Then $\delta_T(u_1) = 2$ and there is u_j with $2 \le j \le n-k-1$ 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 $\sigma_T(T_1) \ge \sigma_T(T_2)$. 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 3.5, $\rho(T) = \rho(C(n,0,k-2)) < \rho\left(C\left(n, \lfloor \frac{k-2}{2} \rfloor, \lceil \frac{k-2}{2} \rceil\right)\right)$, a contradiction. If $T-U$ has at least two nontrivial components, then there are vertices

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A publication of the International Linear Algebra Society
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u_i and u_j with $2 \le i < j \le n-k-1$ such that $\delta_T(u_i) = 3$ and $\delta_T(u_j) = 2$. Let v_i 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 $\sigma_T(T_1) \ge \sigma_T(T_2)$. Let $T'' = T - u_iv_i + u_jv_i$. 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, $\delta_T(u_1) = 3$, 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 $2 \le i < j < l \le n-k-1$ in T such that $\delta_T(u_j) = 3$ and $\{u_i, u_l\} \subseteq U$. 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 $\sigma_T(T_1) \ge \sigma_T(T_2)$. Let $T' = T - u_jv_j + u_lv_j$. By Lemma 2.3, $\rho(T) < \rho(T')$, a contradiction. Thus, $T - U$ contains exactly two nontrivial components, implying that $T \cong C(n, a, b)$, where $a + b = k - 2$, and $a, b \ge 1$. By Lemma 3.5, $T \cong C\left(n, \lfloor\frac{k-2}{2}\rfloor, \lceil\frac{k-2}{2}\rceil\right)$. ◻

For integers n and k with $1 \le k \le \lfloor\frac{n}{2}\rfloor$, let $\mathbb{T}(n,k)$ be the set of trees with n vertices and $2k$ odd vertices.

THEOREM 3.7. *Let $T \in \mathbb{T}(n,k)$, where $1 \le k \le \lfloor\frac{n}{2}\rfloor$. Then*

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

with equality if and only if $T \cong C\left(n, \lfloor\frac{k-1}{2}\rfloor, \lceil\frac{k-1}{2}\rceil\right)$.

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

Suppose $k \ge 3$. Let T be a tree in $\mathbb{T}(n,k)$ with maximum distance spectral radius.

Suppose that the maximum odd degree is larger than 3. Then $\delta_T(u) = 2t + 1$ for some $u \in V(T)$ and $t \ge 2$. Let $N_T(u) = \{u_1, \dots, u_{2t+1}\}$. Let T_i be the component of $T - u$ containing u_i, where $1 \le i \le 2t + 1$. Assume without loss of generality that $\sigma_T(T_1) \ge \sigma_T(T_{2t+1})$. Let w be a pendant vertex of T in $V(T_{2t+1})$. Let $T' = T - \{uu_i : 3 \le i \le 2t\} + \{wu_i : 3 \le i \le 2t\}$. Note that the degrees of u and w remain odd in T'. Then $T' \in \mathbb{T}(n,k)$. By Lemma 3.2, $\rho(T') > \rho(T)$, a contradiction. Thus, the maximum odd degree is 3.

If n is even, and $k = \frac{n}{2}$, then by Lemma 3.3, $T \cong C\left(n, \lfloor\frac{k-1}{2}\rfloor, \lceil\frac{k-1}{2}\rceil\right)$.

Suppose $k < \frac{n}{2}$. Let U be the set of even vertices of T. Then $|U| \ge 1$. Suppose that the maximum even degree is larger than 2. Then $\delta_T(u) = 2t$ for some $u \in V(T)$ and $t \ge 2$. Let $N_T(u) = \{u_1, \dots, u_{2t}\}$. Let T_i be the component of $T - u$ containing u_i, where $1 \le i \le 2t$. Assume without loss of generality that $\sigma_T(T_1) \ge \sigma_T(T_{2t})$. Let w be a pendant vertex of T in $V(T_{2t})$. Let $T' = T - uu_2 + wu_2$. Note that the degree of u is odd and the degree of w is even in T'. Then $T' \in \mathbb{T}(n,k)$. By Lemma 2.3,

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A publication of the International Linear Algebra Society
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$\rho(T') > \rho(T)$, 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 $\delta_T(v_1) = \delta_T(v_3) = 2$ with $v_1 \in V(T_1)$ and $v_3 \in V(T_3)$, and that $\sigma_T(T_1) \geq \sigma_T(T_3)$. Let $T' = T - uu_2 + v_3u_2$. Obviously, $\delta_{T'}(u)$ is even and $\delta_{T'}(v_3)$ is odd. Thus, $T' \in \mathbb{T}(n, k)$. 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, $G_1(s+1, t-1) \in \mathbb{T}(n, k)$. 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 $T \cong C\left(n, \lfloor \frac{k-1}{2} \rfloor, \lceil \frac{k-1}{2} \rceil\right)$. ◻

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 at least 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 $\rho(T) \leq \rho\left(C\left(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil\right)\right)$ with equality if and only if $T \cong C\left(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil\right)$.*

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 $\sigma_T(T_1) \geq \sigma_T(T_\Delta)$. Let w be a pendant vertex of T in $V(T_\Delta)$. Let $T' = T - \{uu_i : 2 \leq i \leq \Delta - 1\} + \{wu_i : 2 \leq i \leq \Delta - 1\}$. 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 $\sigma_T(T_1) \geq \sigma_T(T_4)$. Let v be a pendant vertex of T in $V(T_4)$, and $T' = T - uu_2 +$

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A publication of the International Linear Algebra Society
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vu_2. 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 $T'' = T' - uu_3 + wu_3$. 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, $T \in \mathbb{T}(n, k + 1)$. By Theorem 3.7, we have $T \cong C\left(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil\right)$. □

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 $\rho(T) \leq \rho\left(C\left(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil\right)\right)$ with equality if and only if $T \cong C\left(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil\right)$.*

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 $T' = T - uu_2 + wu_2$. Obviously, T' is a tree with n vertices and k vertices of degree at least 3. By Lemma 3.2, $\rho(T') > \rho(T)$, a contradiction. Hence, $\Delta \leq 3$, implying that T is a tree with k vertices of degree 3. By Theorem 4.1, $T \cong C\left(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil\right)$. □

5. Distance spectral radius of trees with all odd vertices. For $n \geq 2$, let $\mathbb{T}(2n)$ 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 3.7, we have

Theorem 5.1. *Let $T \in \mathbb{T}(2n)$. 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_{a+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 $T \in \mathbb{T}(2n)$ and $T \ncong S_{2n}$, 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 $\mathbb{T}(2n) \setminus \{S_{2n}\}$. Let t be the diameter of T. Obviously, $t \geq 3$. Let $u_1 \ldots u_{t+1}$ be a diametrical path of

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A publication of the International Linear Algebra Society
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T. Suppose $t \geq 4$. Let $T' = T - \{vu_4 : v \in N_T(u_4)\backslash\{u_3\}\} + \{vu_3 : v \in N_T(u_4)\backslash\{u_3\}\}$. Obviously, $T' \in \mathbb{T}(2n) \setminus \{S_{2n}\}$. By Lemma 2.4, $\rho(T) > \rho(T')$, a contradiction. Thus, $t = 3$, i.e., T is a double star. By Lemma 5.2, $T \cong D_{2n,2}$. ☐

For $n \geq 3$ and $2 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$, 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 $3 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$, 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 $2 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$, $\rho(F(2n, i+1)) > \rho(B(2n, i))$.*

Proof. Let $G = B(2n, i)$ and $G' = B(2n, i) - \{u_i w_2, u_i w_3\} + \{v_{i+1} w_2, v_{i+1} w_3\}$. 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,

$$\begin{aligned}\frac{1}{2}(\rho(G') - \rho(G)) &\geq \frac{1}{2} x^\top (D(G') - D(G))x \\ &= 2\left(x_{w_2} + x_{w_3}\right)\left(x_{u_i} + x_{w_1} - x_{v_{i+1}}\right).\end{aligned}$$

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

$$\begin{aligned}\rho(G)x_{u_i} &= x_{w_1} + x_{w_2} + x_{w_3} + 2x_{v_{i+1}} + \sum_{k=1}^{i-1} d_G(u_i, u_k)x_{u_k} \\ &\quad + \sum_{k=2}^{i-1} d_G(u_i, v_k)x_{v_k} + \sum_{k=i+1}^{n} (d_G(u_{i+1}, u_k) + 1)x_{u_k} \\ &\quad + \sum_{k=i+2}^{n-1} (d_G(u_{i+1}, v_k) + 1)x_{v_k}, \\ \rho(G)x_{w_1} &= x_{u_i} + 2x_{w_2} + 2x_{w_3} + 3x_{v_{i+1}} + \sum_{k=1}^{i-1}(d_G(u_i, u_k) + 1)x_{u_k} \\ &\quad + \sum_{k=2}^{i-1}(d_G(u_i, v_k) + 1)x_{v_k} + \sum_{k=i+1}^{n} (d_G(u_{i+1}, u_k) + 2)x_{u_k} \\ &\quad + \sum_{k=i+2}^{n-1} (d_G(u_{i+1}, v_k) + 2)x_{v_k}, \\ \rho(G)x_{v_{i+1}} &= 2x_{u_i} + 3x_{w_1} + 3x_{w_2} + 3x_{w_3} + \sum_{k=1}^{i-1}(d_G(u_i, u_k) + 2)x_{u_k}\end{aligned}$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 286-305, May 2016

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$$+\sum_{k=2}^{i-1}(d_G(u_i,v_k)+2)x_{v_k}+\sum_{k=i+1}^{n}(d_G(u_{i+1},u_k)+1)x_{u_k}$$
$$+\sum_{k=i+2}^{n-1}(d_G(u_{i+1},v_k)+1)x_{v_k},$$

and thus,

$$\begin{aligned}(\rho(G)+2)\left(x_{u_i}+x_{w_1}-x_{v_{i+1}}\right) &= x_{u_i}+3x_{v_{i+1}}+\sum_{k=1}^{i-1}(d_G(u_i,u_k)-1)x_{u_k}\\ &\quad+\sum_{k=2}^{i-1}(d_G(u_i,v_k)-1)x_{v_k}\\ &\quad+\sum_{k=i+1}^{n}(d_G(u_{i+1},u_k)+2)x_{u_k}\\ &\quad+\sum_{k=i+2}^{n-1}(d_G(u_{i+1},v_k)+2)x_{v_k}\\ &> 0,\end{aligned}$$

implying that $x_{u_i}+x_{w_1}-x_{v_{i+1}}>0$. Therefore, $\rho(G')>\rho(G)$, i.e., $\rho(F(2n,i+1))>\rho(B(2n,i))$. ☐

THEOREM 5.5. *Let $T\in\mathbb{T}(2n)$ and $T\ncong E_{2n}$, 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 $\mathbb{T}(2n)=\{E_{2n},B(2n,2)\}$, and thus, the result follows from Theorem 5.1.

Suppose $n\geq 5$. Let T be a tree with maximum distance spectral radius in $\mathbb{T}(2n)\backslash\{E_{2n}\}$. 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 $\sigma_T(T_1)\geq\sigma_T(T_\Delta)$. Let w be a pendant vertex of T in $V(T_\Delta)$. Let $T'=T-\{uu_2,uu_3\}+\{wu_2,wu_3\}$. Then $T'\in\mathbb{T}(2n)$ and $T'\ncong E_{2n}$. By Lemma 3.2, $\rho(T')>\rho(T)$, 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

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
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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 $T' = T - \{u_iv_2, u_iv_3\} + \{u_{t+1}v_2, u_{t+1}v_3\}$. Obviously, $T' \in \mathbb{T}(2n)$ and $T' \ncong E_{2n}$. 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 3.3 that $T \cong B(2n, i)$ with $2 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$. Suppose $3 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$. Let $T' = B(2n, i) - \{u_iv_2, u_iv_3\} + \{u_2v_2, u_2v_3\}$ if $\sigma_T(T_1) \leq \sigma_T(T_2)$, and $T' = B(2n, i) - \{u_iv_2, u_iv_3\} + \{u_{n-1}v_2, u_{n-1}v_3\}$ if $\sigma_T(T_1) > \sigma_T(T_2)$. It is easily seen that $T' \cong B(2n, 2)$. By Lemma 3.2, $\rho(T) = \rho(B(2n, i)) < \rho(T') = \rho(B(2n, 2))$, a contradiction. Then $i = 2$, and thus, $T \cong B(2n, 2)$.

Suppose $\Delta = 3$. By Lemma 3.3, $T \cong F(2n, i)$ with $3 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$. By Lemma 3.3, $\rho(F(2n, 3)) > \rho(F(2n, 4)) > \cdots > \rho\left(F\left(2n, \lfloor \frac{n+1}{2} \rfloor\right)\right)$. Thus, $T \cong F(2n, 3)$.

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

Acknowledgment. The authors thank the referee for careful review and helpful comments.

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