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THE DIRICHLET SPECTRAL RADIUS OF TREES*

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Abstract. In this paper, the trees with the largest Dirichlet spectral radius among all trees with a given degree sequence are characterized. Moreover, the extremal graphs having the largest Dirichlet spectral radius are obtained in the set of all trees of order n with a given number of pendant vertices.

Key words. Dirichlet spectral radius, Degree sequence, Tree.

AMS subject classifications. 05C50.

1. Introduction. In this paper, we only consider simple connected graphs. Let $G = (V(G), E(G))$ be a graph of order n with vertex set $V(G) = \{v_0, v_1, \ldots, v_{n-1}\}$ and edge set $E(G)$. Let $d(v)$ denote the degree of a vertex v. Then $\pi(G) = (d(v_0), d(v_1), \ldots, d(v_{n-1}))$ is called the *degree sequence* of G. A sequence of positive integers $\pi = (d_0, d_1, \ldots, d_{n-1})$ is said to be a *tree degree sequence* if there exists at least one tree whose degree sequence is π. The Laplacian matrix of G is defined as $L(G) = D(G) - A(G)$, where $D(G)$ and $A(G)$ denote the diagonal matrix of vertex degrees and the adjacency matrix of G, respectively. Let $\mathcal{T}_\pi$ be the set of all the trees with a given degree sequence π, where $\pi = (d_0, d_1, \ldots, d_{n-1})$ satisfies $d_0 \geq d_1 \geq \cdots \geq d_{n-1}$. The adjacency eigenvalues and Laplacian eigenvalues of graphs have been intensively investigated during the last decades. Bıyıkoğlu et al. [1] and Zhang [12] determined all graphs with the maximal spectral radius and Laplacian spectral radius among all trees with a given degree sequence, respectively. Tan [10] determined the trees with the largest Laplacian spectral radius among all weighted trees with a given degree sequence and positive weight set. A graph $G = (V_0 \cup \partial V, E_0 \cup \partial E)$ with boundary consists of a set of interior vertices V_0, boundary vertices ∂V, interior edges E_0 that connect interior vertices, and boundary edges ∂E that join interior vertices with boundary vertices (see [7]). A real number λ is called a *Dirichlet eigenvalue* of G if there exists a function $f \neq 0$ such that they satisfy the Dirichlet eigenvalue

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problem:

$$\begin{cases} L(G)f(u) = \lambda f(u), & u \in V_0, \\ f(u) = 0, & u \in \partial V. \end{cases}$$

The function f is called a *Dirichlet eigenfunction* corresponding to λ (see [7]). The largest Dirichlet eigenvalue of G is called *Dirichlet spectral radius*, denoted by $\lambda(G)$. Recently, there is an increasing interest in the Dirichlet eigenvalues of graphs (see [2], [3] and [7]), since it can be regarded to be analogous to the Dirichlet eigenvalues of Laplacian operator on a manifold. The related eigenvalue problems have been occasionally occurred in fields like game theory [4], network analysis [5], and Pattern Recognition [8]. In this paper, we regard pendant vertices as boundary vertices and assume that both the set V_0 and the set ∂V are not empty. Motivated by the above results, we will study the Dirichlet spectral radius of graphs in $\mathcal{T}_\pi$. The main result of this paper is as follows:

THEOREM 1.1. *For a given tree degree sequence π, T^*_π (see in Section 3) is the unique tree with the largest Dirichlet spectral radius in $\mathcal{T}_\pi$.*

The rest of the paper is organized as follows. In Section 2, some notations and results are presented. In Section 3, we present the proof of Theorem 1.1 and some corollaries.

2. Preliminaries. Let $R_G(f)$ be the Rayleigh quotient of Laplace operator L on real-valued function f on $V(G)$, where

$$R_G(f) = \frac{< Lf, f >}{< f, f >} = \frac{\sum_{uv\in E} (f(u) - f(v))^2}{\sum_{v\in V} f^2(v)}.$$

Let $\mathcal{F}$ denote the set of all real-valued functions f on $V(G)$ with $f(u) = 0$ for any boundary vertex u. The following proposition states a well-known fact about the Rayleigh quotients.

PROPOSITION 2.1. *For a graph $G = (V_0 \cup \partial V, E_0 \cup \partial E)$ with boundary, we have*

$$\lambda(G) = \max_{f\in\mathcal{F}} R_G(f) = \max_{f\in\mathcal{F}} \frac{< Lf, f >}{< f, f >}.$$

Moreover, if $R_G(f) = \lambda(G)$ for a function $f \in \mathcal{F}$, then f is a Dirichlet eigenfunction of $\lambda(G)$.

Let $Q(G) = D(G) + A(G)$ be the signless Laplacian matrix of G and its Rayleigh

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quotient is denoted by

$$\Delta_G(f) = \frac{< Qf, f >}{< f, f >} = \frac{\sum\limits_{uv \in E} (f(u) + f(v))^2}{\sum\limits_{v \in V} f^2(v)}.$$

A real number μ is called a *signless Dirichlet eigenvalue* of G if there exists a function $f \neq 0$ on $V(G)$ such that for $u \in V(G)$,

$$\begin{cases} Q(G)f(u) = \mu f(u), & u \in V_0, \\ f(u) = 0, & u \in \partial V. \end{cases}$$

The largest signless Dirichlet eigenvalue of $Q(G)$, denoted by $\mu(G)$, is called the *signless Dirichlet spectral radius*. The function f is called a *signless Dirichlet eigenfunction* of $\mu(G)$. Then we have the following

PROPOSITION 2.2. *For a graph $G = (V_0 \cup \partial V, E_0 \cup \partial E)$ with boundary we have*

$$\mu(G) = \max_{f \in \mathcal{F}} \Delta_G(f) = \max_{f \in \mathcal{F}} \frac{< Qf, f >}{< f, f >}.$$

Moreover, if $\Delta_G(f) = \mu(G)$ for a function $f \in \mathcal{F}$, then f is a signless Dirichlet eigenfunction of $\mu(G)$.

A *discrete signless Dirichlet operator* $Q_0(G)$ of a graph G is the signless Laplacian matrix $Q(G)$ restricted to interior vertices, i.e., $L_0(G) = D_0(G)+A_0(G)$, where $A_0(G)$ is the adjacency matrix of the graph $G(V_0, E_0)$ induced by the interior vertices and $D_0(G)$ is the degree diagonal matrix $D(G)$ restricted to the interior vertices $V_0(G)$. Note that $Q_0(G)$ is a irreducible nonnegative symmetric matrix. By the Perron-Frobenius Theorem, we have the following lemma.

LEMMA 2.3. *Let G be a tree. Then the signless Dirichlet spectral radius $\mu(G)$ of G is positive. Moreover, if f is a signless Dirichlet eigenfunction of $\mu(G)$, then $f(v) > 0$ for all $v \in V_0(G)$ or $f(v) < 0$ for all $v \in V_0(G)$.*

Let f be a unit eigenvector of $\mu(G)$. We call f a *Dirichlet Perron vector* of G if $f(v) > 0$ for any $v \in V_0(G)$.

LEMMA 2.4. *Let G be a tree. Then $\lambda(G) = \mu(G)$.*

Proof. Without loss of generality, assume that $G = (V_1, V_2, E(G))$ is a tree with bipartition V_1 and V_2. Let f be Dirichlet Perron vector of G. Define $f_1(x) = sign(x)f(x)$, where $sign(x) = 1$ if $x \in V_1$ and $sign(x) = -1$ if $x \in V_2$. Then we have

$$\mu(G) = \Delta_G(f) = \sum_{uv \in E} (f(u) + f(v))^2 = \sum_{uv \in E} (f_1(u) - f_1(v))^2 = R_G(f_1) \leq \lambda(G).$$

The condition $\lambda(G) \leq \mu(G)$ follows analogously. □

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3. The trees with the largest Dirichlet spectral radius in $\mathcal{T}_\pi$. In this section, we will characterize the trees with the largest Dirichlet spectral radius in $\mathcal{T}_\pi$. Let $G+uv$ (resp. $G-uv$) denote the graph obtained from G by adding (resp. deleting) an edge uv in G. The following lemmas will be used in our proof.

LEMMA 3.1. (See also [12]) *Let $T \in \mathcal{T}_\pi$ and $uv, xy \in E(T)$ such that v and y are not in the path from u to x. Let f be the Dirichlet Perron vector of T and $T' = T - uv - xy + uy + xv$. Then $T' \in \mathcal{T}_\pi$ and $\lambda(T') \geq \lambda(T)$ if $f(u) \geq f(x)$ and $f(y) \geq f(v)$. Moreover, $\lambda(T') > \lambda(T)$ if one of the two inequalities is strict.*

Proof. Let f be the Dirichlet Perron vector of T. Clearly, $T' \in \mathcal{T}_\pi$. Then we have

$$\begin{aligned}\lambda(T') - \lambda(T) &\geq \Delta_{T'}(f) - \Delta_T(f)\\ &= (f(u)+f(y))^2 + (f(x)+f(v))^2 - (f(u)+f(v))^2 - (f(x)+f(y))^2\\ &= 2(f(u)-f(x))(f(y)-f(v))\\ &\geq 0.\end{aligned}$$

If $\lambda(T') = \lambda(T)$, then f also must be a signless Dirichlet eigenfunction of $\lambda(T')$. By

$$\begin{aligned}\lambda(T)f(u) &= \sum_{z, zu \in E(T)\setminus\{uv\}} (f(u)+f(z)) + (f(u)+f(v))\\ &= \lambda(T')f(u)\\ &= \sum_{z, zu \in E(T)\setminus\{uv\}} (f(u)+f(z)) + (f(u)+f(y)),\end{aligned}$$

we have $f(y) = f(v)$. Similarly, we have $f(u) = f(x)$. So, the assertion holds. □

Let $dist(v)$ denote the distance between v and v_0, where v_0 is the root of G. We call y a *child* of x and x the *parent* of y, if $xy \in E(G)$ with $dist(y) = dist(x)+1$.

LEMMA 3.2. *Let $T = (V_0 \cup \partial V, E_0 \cup \partial E)$ be a tree with the largest Dirichlet spectral radius in $\mathcal{T}_\pi$ and f be the Dirichlet Perron vector of T. Then the vertices of T can be relabelled $\{v_0, v_1, \ldots, v_{n-1}\}$ such that the following hold:*

(1) $f(v_0) \geq f(v_1) \geq \cdots \geq f(v_{n-1})$;

(2) *Let v_0 be the root of T, then $dist(v_0) \leq dist(v_1) \leq \cdots \leq dist(v_{n-1})$;*

(3) *If $v_i, v_s \in V(T)$ with $i < s$, then for any child v_j of v_i and any child v_t of v_s, there must be $j < t$.*

Proof. Let $V(T) = \{v_0, v_1, \ldots, v_{n-1}\}$ such that $f(v_0) \geq f(v_1) \geq \cdots \geq f(v_{n-1})$. We start with the vertex v_0. If $v_0v_1 \in V(T)$, there is nothing to do. Otherwise, there exists a child x_0 of v_0 with $f(v_1) \geq f(x_0)$. If $f(v_1) = f(x_0)$, we exchange the labelling of v_1 and x_0. In the following, we assume $f(v_1) > f(x_0)$. Then v_1 is not a pendant

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vertex. Since T is connected, there exist a path $P_{0,1}$ from v_0 to v_1 and a parent u_1 of v_1 which is in $P_{0,1}$ and can not be v_0. Since v_1 is an interior vertex, there is also some child w_1 of v_1 which is not in $P_{0,1}$. If $x_0 \in P_{0,1}$, let $T_1 = T - v_0x_0 - v_1w_1 + v_0v_1 + x_0w_1$. Otherwise, let $T_1 = T - v_0x_0 - v_1u_1 + v_0v_1 + x_0u_1$. Since $f(v_0) \geq f(w_1)$, $f(v_1) > f(x_0)$ and $f(v_0) \geq f(u_1)$, we have $\lambda(T_1) > \lambda(T)$ by Lemma 3.1. It is a contradiction to our assumption that T has the largest Dirichlet spectral radius in $\mathcal{T}_\pi$. Let $s_0 = d(v_0)$. By the same way, we can prove that v_0 is also adjacent to $v_2, v_3, \ldots, v_{s_0}$.

Next we proceed in an analogous way with all children of v_1 and prove that the vertices $v_{d(v_0)+1}, v_{d(v_0)+2}, \ldots, v_{s_1}$ are adjacent to v_1, where $s_1 = d(v_0) + d(v_1) - 1$. Let $s_{r-1} = d(v_0) + d(v_1) + \cdots + d(v_{r-1}) - r + 1$. Now assume that v_{r-1} has already been adjacent to the respective vertices $v_{s_{r-2}+1}, v_{s_{r-2}+2}, \ldots, v_{s_{r-2}+d(v_{r-1})-1}$. In the following, we observe the vertex v_r. If v_r is adjacent to $v_{s_{r-1}+1}$, there is nothing to do. Otherwise, there exist a child x_r of v_r with $f(v_{s_{r-1}+1}) \geq f(x_r)$ and a path $P_{r,s_{r-1}+1}$ from v_r to $v_{s_{r-1}+1}$. Without loss of generality, assume $f(v_{s_{r-1}+1}) > f(x_r)$. Then there exist a parent u_r of $v_{s_{r-1}+1}$ in $P_{r,s_{r-1}+1}$ and some child w_r which is not in $P_{r,s_{r-1}+1}$. Let $T_r = T - v_rx_r - v_{s_{r-1}+1}w_r + v_rv_{s_{r-1}+1} + x_rw_r$(if $x_r \in P_{r,s_{r-1}+1}$) or $T_r = T - v_rx_r - v_{s_{r-1}+1}u_r + x_ru_r + v_rv_{s_{r-1}+1}$ (if $x_r \notin P_{r,s_{r-1}+1}$). Since $f(v_r) \geq f(u_r), f(v_r) \geq f(w_r)$ and $f(v_{s_{r-1}+1}) > f(x_r)$, we have $\lambda(T_r) > \lambda(T)$ by Lemma 3.1. It is a contradiction to our assumption that T has the largest Dirichlet spectral radius in $\mathcal{T}_\pi$. By the same procedure, we can prove that v_r is adjacent to the respective vertices $v_{s_{r-1}+2}, v_{s_{r-1}+3}, \ldots, v_{s_{r-1}+d(v_r)-1}$. By the induction, the assertion holds. □

LEMMA 3.3. *Let $G = (V_0 \cup \partial V, E_0 \cup \partial E)$ be a graph with boundary and P be a path from an interior vertex v_1 to another interior vertex v_2. Suppose that $v_1u_i \in E(G)$, $v_2u_i \notin E(G)$ and u_i is not on the path P for $i = 1, 2, \ldots, t$ with $t \leq d(v_1) - 2$. By deleting the t edges $v_1u_1, v_1u_2, \ldots, v_1u_t$ and adding the t edges $v_2u_1, v_2u_2, \ldots, v_2u_t$ we get a new tree G'. Let f be the Dirichlet Perron vector of G. Then if $f(v_1) \leq f(v_2)$, we have*

$$\lambda(G') > \lambda(G).$$

Proof. By

$$\begin{aligned}\lambda(G') - \lambda(G) &\geq \Delta_{G'}(f) - \Delta_G(f) \\ &= \sum_{i=1}^{t}(f(v_2) + f(u_i))^2 - \sum_{i=1}^{t}(f(v_1) + f(u_i))^2 \\ &\geq 0,\end{aligned}$$

we have $\lambda(G') \geq \lambda(G)$. If $\lambda(G') = \lambda(G)$, then f also must be a signless Dirichlet

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eigenfunction of $\lambda(G')$. By

$$\begin{aligned}\lambda(G')f(v_1) &= \sum_{x,v_1x\in G'}(f(v_1)+f(x))\\ &= \lambda(G)f(v_1)\\ &= \sum_{x,v_1x\in G'}(f(v_1)+f(x))+\sum_{i=1}^{t}(f(v_1)+f(u_i)),\end{aligned}$$

we have $\sum_{i=1}^{t}(f(v_1)+f(u_i))=0$. This is a contradiction with $f(v_1)>0$ and $f(u_i)\geq 0$. So, the assertion holds. The proof is completed. ☐

In the following, we use the method of [12] to define a special tree T_π^* with a given nonincreasing tree degree sequence $\pi=(d_0,d_1,\ldots,d_{n-1})$as follows. Select a vertex $v_{0,1}$ as the root of T_π^*. and begin with $v_{0,1}$ of the zero-th layer. Let $s_1=d_0$ and select s_1 vertices $v_{1,1},v_{1,2},\ldots,v_{1,s_1}$ of the first layer as the children of $v_{0,1}$. Next we construct the second layer as follows. Let $s_2=\sum_{i=1}^{s_1}d_i-s_1$ and select s_2 vertices $v_{2,1},v_{2,2},\ldots,v_{2,s_2}$ such that $v_{2,1},\ldots,v_{2,d_1-1}$ are the children of $v_{1,1}$, and $v_{2,d_1},\ldots,v_{2,d_1+d_2-2}$ are the children of $v_{1,2}$, …, and $v_{2,d_1+\cdots+d_{s_1-1}-s_1+2},\ldots,v_{2,d_1+\cdots+d_{s_1}-s_1}$ are the children of v_{1,s_1}. Assume that all vertices of the t-st layer have been constructed and are denoted by $v_{t,1},v_{t,2},\ldots,v_{t,s_t}$. We construct all the vertices of the$(t+1)$-st layer by the induction hypothesis. Let $s_{t+1}=d_{s_1+\cdots+s_{t-1}+1}+\cdots+d_{s_1+\cdots+s_t}-s_t$ and select s_{t+1} vertices $v_{t+1,1},v_{t+1,2},\ldots,v_{t+1,s_{t+1}}$ of the$(t+1)$st layer such that $v_{t+1,1},\ldots,v_{t+1,d_{s_1+\cdots+s_{t-1}+1}-1}$ are the children of v_{t1} , …, and $v_{t+1,s_{t+1}-d_{s_1+\cdots+s_t}+2},\ldots,v_{t+1,s_{t+1}}$ are the children of v_{t,s_t}. In this way, we obtain only one tree T_π^* with degree sequence π such that $v_{0,1}$ has the maximum degree in all interior vertices (see Fig. 3.1 for an example).

EXAMPLE 3.4. Let $\pi=(4,3,3,3,2,2,2,2,2,2,1,1,1,1,1,1,1)$. Then T_π^* is as follows:

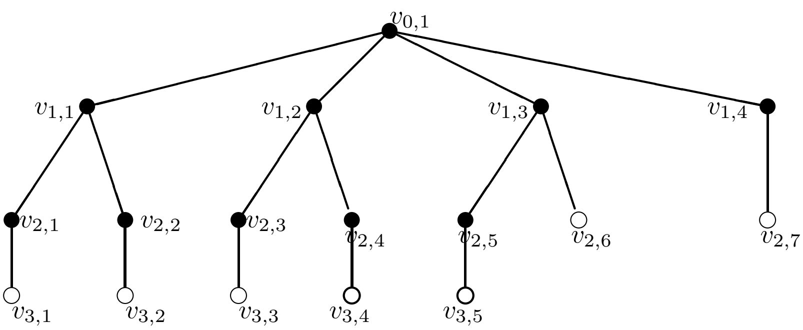

FIG. 3.1. *T_π^* with degree sequence π($\circ\cdots$ boundary vertices).*

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Proof of Theorem 1.1. Let T be a tree with the largest Dirichlet spectral radius in $\mathcal{T}_\pi$. Suppose $V(T) = \{v_0, v_1, \ldots, v_{n-1}\}$ such that they satisfy the three assertions in Lemma 3.2. Let f be the Dirichlet Perron vector of T.

In the following, we will prove that $d(v_0) \geq d(v_1) \geq \cdots \geq d(v_{n-1})$. If the assertion does not hold, there exists the smallest integer $t \in \{0, 1, \ldots, n-1\}$ such that $d(v_t) < d(v_{t+1})$. Since $f(v_t) \geq f(v_{t+1})$, v_t and v_{t+1} are interior vertices. Let $u_1, u_2, \ldots, u_{d(v_{t+1})-1}$ be all the children of v_{t+1}. Then we have $f(v_t) \geq f(v_{t+1}) \geq f(u_i)$ for $1 \leq i \leq d(v_{t+1})-1$ by Lemma 3.2. Let $T_1 = T - v_{t+1}u_1 - v_{t+1}u_2 - \cdots - v_{t+1}u_s + v_t u_1 + v_t u_2 + \cdots + v_t u_s$, where $s = d(v_{t+1}) - d(v_t)$. Then $T_1 \in \mathcal{T}_\pi$ and $\lambda(T_1) > \lambda(T)$ by Lemma 3.3. This is a contradiction to our assumption that T has the largest Dirichlet spectral radius in $\mathcal{T}_\pi$. So, we have $d(v_i) = d_i$ for $0 \leq i \leq n-1$. Clearly, T is isomorphic to T_π^*. The proof is completed. ☐

Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ and $\pi' = (d'_0, d'_1, \ldots, d'_{n-1})$ be two nonincreasing positive sequences. If $\sum\limits_{i=0}^{t} d_i \leq \sum\limits_{i=0}^{t} d'_i$ for $t = 0, 1, \ldots, n-2$ and $\sum\limits_{i=0}^{n-1} d_i = \sum\limits_{i=0}^{n-1} d'_i$, then π' is said to *majorize* π, and is denoted by $\pi \trianglelefteq \pi'$ (see [12]).

Lemma 3.5. ([12]) *Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ and $\pi' = (d'_0, d'_1, \ldots, d'_{n-1})$ be two nonincreasing graphic degree sequences. If $\pi \trianglelefteq \pi'$, then there exist a series of graphic degree sequences $\pi_1, \pi_2, \ldots, \pi_k$ such that $\pi \trianglelefteq \pi_1 \trianglelefteq \pi_2 \trianglelefteq \cdots \trianglelefteq \pi_k \trianglelefteq \pi'$, and only two components of π_i and π_{i+1} are different by* 1.

Theorem 3.6. *Let π and π' be two tree degree sequences such that they have same frequency of the number 1. If $\pi \trianglelefteq \pi'$, then $\lambda(T_\pi^*) \leq \lambda(T_{\pi'}^*)$ with equality holds if and only if $\pi = \pi'$.*

Proof. Let f be the Dirichlet Perron vector of T_π^* and $v_0, v_1, \ldots, v_{n-1} \in V(T_\pi^*)$ such that they satisfy the three assertions in Lemma 3.2. Then $f(v_0) \geq f(v_1) \geq \cdots \geq f(v_{n-1})$ and $d(v_t) = d_t$ for $0 \leq t \leq n-1$. By Lemma 3.5, without loss of generality, assume $\pi = (d_0, d_1, \ldots, d_{n-1})$ and $\pi' = (d'_0, d'_1, \ldots, d'_{n-1})$ such that $d_i = d'_i - 1$, $d_j = d'_j + 1$ with $0 \leq i < j \leq n-1$, and $d_k = d'_k$ for $k \neq i, j$. Since π and π' have the same frequency of the number 1, we have $d'_j \geq 2$ and $d_j = d'_j + 1 \geq 3$. So, there exists a vertex v_p with $p > j$ such that $v_j v_p \in E(T_\pi^*)$, $v_i v_p \notin E(T_\pi^*)$ and v_p is not in the path from v_i to v_j. Let $T_1 = T_\pi^* - v_j v_p + v_i v_p$. Note $f(v_i) \geq f(v_j)$. We have $T_1 \in \mathcal{T}_{\pi'}$ and $\lambda(T_\pi^*) < \lambda(T_1) \leq \lambda(T_{\pi'}^*)$ by Lemma 3.3. The proof is completed. ☐

Corollary 3.7. *Let $\omega = \{k, 2, \ldots, 2, 1, \ldots, 1\}$ such that the frequency of* 1 *is* k. *Then T_ω^* is the unique tree with the largest Dirichlet spectral radius among all the trees with k pendant vertices.*

Proof. Let T be a tree with k pendant vertices and degree sequence $\pi = (d_0, d_1, \ldots, d_{n-1})$. Then $d_{n-k} = d_{n-k+1} = \cdots = d_{n-1} = 1$ and $d_{n-k-1} \geq 2$. Clearly,

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$\pi \trianglelefteq \omega$. By Theorem 3.6, the assertion holds. □

COROLLARY 3.8. *Let T be a tree of order n with k pendant vertices. If $n \leq 2k+1$, then $\lambda(T) \leq \frac{2+k+\sqrt{k^2-8k+4n}}{2}$ with equality if and only if T is T^*_ω.*

Proof. Let f be the Dirichlet Perron vector of T^*_ω and $u \in V(T^*_\omega)$ with $d(u) = k$. Since $n \leq 2k+1$, the vertex u is adjacent to any vertex v with $d(v) = 2$. By $\lambda(T^*_\omega)f(u) = kf(u)+(n-k-1)f(v)$ and $\lambda(T^*_\omega)f(v) = 2f(v)+f(u)$, we have $\lambda(T^*_\omega) = \frac{2+k+\sqrt{k^2-8k+4n}}{2}$. The assertion holds by Corollary 3.7. □

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