

TREES WITH GIVEN MAXIMUM DEGREE MINIMIZING THE SPECTRAL RADIUS*

XUE DU[†] AND LINGSHENG SHI[‡]

Abstract. The spectral radius of a graph is the largest eigenvalue of the adjacency matrix of the graph. Let $T^*(n, \Delta, l)$ be the tree which minimizes the spectral radius of all trees of order n with exactly l vertices of maximum degree Δ . In this paper, $T^*(n, \Delta, l)$ is determined for $\Delta = 3$, and for $l \leq 3$ and n large enough. It is proven that for sufficiently large n , $T^*(n, 3, l)$ is a caterpillar with (almost) uniformly distributed legs, $T^*(n, \Delta, 2)$ is a dumbbell, and $T^*(n, \Delta, 3)$ is a tree consisting of three distinct stars of order Δ connected by three disjoint paths of (almost) equal length from their centers to a common vertex. The unique tree with the largest spectral radius among all such trees is also determined. These extend earlier results of Lovász and Pelikán, Simić and Tošić, Wu, Yuan and Xiao, and Xu, Lin and Shu.

Key words. Maximum degree, Optimizing, Spectral radius, Tree.

AMS subject classifications. 05C05, 05C35, 05C50.

1. Introduction. Throughout graphs are simple. For a graph $G = (V, E)$ and a vertex $v \in V$, we denote the degree of v , that is the number of edges incident with v , by $d(v)$. We denote by $\Delta(G)$ the maximum degree of G . The adjacency matrix of graph G is denoted by $A(G)$, and its characteristic polynomial is denoted by $\phi_G(\lambda)$, or ϕ_G for short. The *spectral radius* of G , denoted by $\rho(G)$, is defined as the largest root of ϕ_G .

As proposed by Brualdi and Solheid [2], an interesting problem in the spectra of graphs is to determine the extremal graphs in some class with respect to the spectral radius. In 1973, Lovász and Pelikán [11] found that of all trees the star has the largest spectral radius and the path has the smallest, respectively. In 2005, Simić and Tošić [14] determined the tree whose spectral radius has the largest value among all trees of order n with a given maximum degree. This result together with [6]

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confirms a conjecture of Fischermann et al [5]. Meanwhile it is easy to show that the broom has the smallest spectral radius, see [18]. In 2004, Wu et al. [17] determined the extremal trees among all trees with at most three vertices of maximum degree three. In 2008, Bıykoğlu and Leydold [1] described the structure of graphs with the largest spectral radius among all connected graphs with a given degree sequence. A sequence $\pi := (d_0, d_1, \dots, d_{n-1})$ of nonnegative integers is called *degree sequence* if there exists a graph of order n for which $d_0, d_1, \dots, d_{n-1}$ are the degrees of its vertices, (and the degrees are enumerated in non-increasing order). As in [1], *majorization* defines a partial ordering on degree sequences. More precisely, for two sequences $\pi = (d_0, d_1, \dots, d_{n-1})$ and $\pi' = (d'_0, d'_1, \dots, d'_{n-1})$, $\pi \neq \pi'$, we write $\pi \triangleleft \pi'$ if and only if $\sum_{i=0}^j d_i \leq \sum_{i=0}^j d'_i$ for all $j = 0, 1, \dots, n-1$ (recall that the degree sequences are non-increasing). Let $G = (V, E)$ be a connected graph with a root v_0 . Then a well-ordering $\prec$ of the vertices is called *breadth-first search ordering* with decreasing degrees (*BFD-ordering* for short) if the following holds for all vertices $u, v, u_i, v_i \in V$:

- if $u_1 \prec u_2$, then $v_1 \prec v_2$ for all children v_1 of u_1 and v_2 of u_2 , respectively;
- if $v \prec u$, then $d(v) \geq d(u)$.

A connected graph that has a BFD-ordering of its vertices is called a *BFD-graph*.

LEMMA 1.1. [1] Let $\mathcal{T}_\pi$ denote the set of all trees with given degree sequence π . Then a tree T with degree sequence π has the largest spectral radius in $\mathcal{T}_\pi$ if and only if it is a BFD-tree. T is then uniquely determined up to isomorphism. Moreover, if T' is the tree with the largest spectral radius in $\mathcal{T}_{\pi'}$ with $\pi \triangleleft \pi'$, then $\rho(T) < \rho(T')$.

As a consequence of Lemma 1.1, the following result is immediate.

THEOREM 1.2. The unique BFD-tree with the maximal (with respect to the majorization ordering) degree sequence maximizes the spectral radius of all trees with given number of vertices of maximum degree.

In this paper, we continue the study of trees with the smallest spectral radius of all trees with given number of vertices of maximum degree. Let $T^*(n, \Delta, l)$ be the tree which minimizes the spectral radius of all trees of order n with exactly l vertices of maximum degree Δ . We determine $T^*(n, \Delta, l)$ for sufficiently large n and $\Delta = 3$ or $l \leq 3$. Let $T(k_1, k_2, \dots, k_r)$ (r is a nonnegative integer) denote the tree with maximum degree three shown in Fig. 1.1, where k_i denotes the number of vertices of degree two between the i -th vertex and the $i+1$ -th vertex of degree three ordered from the left to the right.

THEOREM 1.3. For $l \geq 3$ and n large enough, $T^*(n, 3, l) \cong T(k_1, k_2, \dots, k_{l-1})$ satisfying

$$1. \ 2 \lfloor \frac{s+1}{2} \rfloor - 1 \leq k_i \leq \lceil s \rceil + 1 \text{ for } 2 \leq i \leq l-2 \text{ and } \lfloor \frac{s-3}{2} \rfloor \leq k_j < \frac{s-1.88}{2} \text{ for}$$

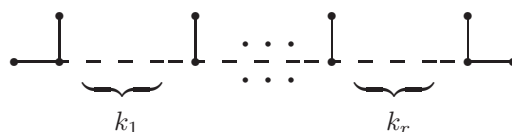


FIG. 1.1. The graph $T(k_1, k_2, \dots, k_r)$.

1. $j = 1, l - 1$, where $s = \frac{n-3}{l-2} - 2$;
2. $1 \leq k_i - 2k_j \leq 5$ for $2 \leq i \leq l - 2$ and $j = 1, l - 1$;
3. $|k_i - k_j| \leq 1$, for $2 \leq i, j \leq l - 2$.

In particular, if $n - 5l + 7$ is divisible by $2(l - 2)$, then

$$T^*(n, 3, l) \cong T\left(\frac{s-3}{2}, s, s, \dots, s, \frac{s-3}{2}\right);$$

and if $n = 2(k + 2)(l - 2) + 2$, $k \in \mathbb{N}$ and $3 \leq l \leq 10$, then

$$T^*(n, 3, l) \cong T(k - 1, 2k + 2, \dots, 2k + 2, k - 1).$$

Moreover, $\rho(T^*(n, 3, l)) \rightarrow \sqrt{2 + \sqrt{5}}$ as $n \rightarrow \infty$.

COROLLARY 1.4. For n large enough, the following hold:

$$\begin{aligned}
 T^*(n, 3, 3) &\cong T(\lfloor n/2 \rfloor - 4, \lceil n/2 \rceil - 4); \\
 T^*(n, 3, 4) &\cong \begin{cases} T(k - 1, 2k + 2, k - 1) & \text{for } n = 4k + 10, \\ T(k - 1, 2k + 3, k - 1), T(k - 1, 2k + 2, k) & \\ \text{or } T(k, 2k + 1, k) & \text{for } n = 4k + 11, \\ T(k, 2k + 2, k) & \text{for } n = 4k + 12, \\ T(k, 2k + 3, k) & \text{for } n = 4k + 13; \end{cases} \\
 T^*(n, 3, 5) &\cong \begin{cases} T(k - 1, 2k + 1, 2k + 1, k - 1) & \text{for } n = 6k + 12, \\ T(k - 1, 2k + 1, 2k + 2, k - 1) & \text{for } n = 6k + 13, \\ T(k - 1, 2k + 2, 2k + 2, k - 1) & \text{for } n = 6k + 14, \\ T \in \{T(k - 1, 2k + 2, 2k + 3, k - 1), \\ T(k - 1, 2k + 2, 2k + 2, k), T(k, 2k + 1, 2k + 2, k)\} & \text{for } n = 6k + 15, \\ T(k, 2k + 2, 2k + 2, k) & \text{for } n = 6k + 16, \\ T(k, 2k + 2, 2k + 3, k) & \text{for } n = 6k + 17. \end{cases}
 \end{aligned}$$

Corollary 1.4 shows that the bounds on k_i 's in Theorem 1.3 are best possible, although the number 1.88 in the upper bound can slightly be improved to $2 - \frac{\ln(\lambda_0/2)}{\ln x_2}$,

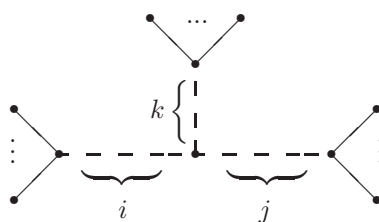


FIG. 1.2. The graph $Y(\Delta; i, j, k)$.

where $\lambda_0 = \sqrt{2 + \sqrt{5}}$ and $x_2 = (\lambda_0 + \sqrt{\lambda_0^2 - 4})/2$. Let $Y(\Delta; i, j, k)$ denote the tree of order $3\Delta + i + j + k + 1$ with maximum degree Δ , consisting of three distinct stars of order Δ connected by three disjoint paths of length $i + 1, j + 1, k + 1$ respectively from their centers to a common vertex as depicted in Fig. 1.2.

THEOREM 1.5. *For $l \leq 3$, $T^*(n, \Delta, l)$ is uniquely determined up to isomorphism as follows:*

1. $T^*(n, \Delta, 2)$ consists of two stars linked by a path.
2. For $\Delta \geq 4$ and n large enough, $T^*(n, \Delta, 3) \cong Y(\Delta; i, j, k)$ where i, j, k differ by at most one.

Moreover, $\rho(T^*(n, \Delta, l)) \rightarrow \frac{\Delta-1}{\sqrt{\Delta-2}}$ as $n \rightarrow \infty$ except for $\Delta = l = 3$.

The rest of the paper is organized as follows. In Section 2, we list some known results which will be used later on. In Section 3, we use the technique of diagonalization to evaluate the characteristic polynomial of trees and then prove Theorem 1.3 and Corollary 1.4. In Section 4, we use the limit point theory of Hoffman [7] to prove Theorem 1.5. At last, we finish with some final remarks in Section 5.

2. Lemmas. In this section, we collect some known results which will be used later on.

LEMMA 2.1. [4, 10] *The following hold for graphs G_1 and G_2 .*

1. If G_1 is connected and G_2 is a proper subgraph of G_1 , then $\rho(G_2) < \rho(G_1)$.
 Moreover, if $V(G_1) = V(G_2)$, then $\phi_{G_2}(\lambda) > \phi_{G_1}(\lambda)$ for $\lambda \geq \rho(G_1)$.
2. If $\phi_{G_1}(\rho(G_2)) < 0$, then $\rho(G_1) > \rho(G_2)$.

LEMMA 2.2. [12] *The following hold for a connected graph G .*

1. If $e = uv$ is a bridge of G , then $\phi_G = \phi_{G-e} - \phi_{G-u-v}$;
2. If v is not in any cycle of G , then $\phi_G = \lambda \phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v}$.

An *internal path* of a graph G is a sequence of vertices $v_1, v_2, \dots, v_k$ with $k \geq 2$ such that

- the vertices in the sequence are distinct (except possibly $v_1 = v_k$);
- v_i is adjacent to v_{i+1} ($i = 1, 2, \dots, k-1$);
- the vertex degrees satisfy $d(v_1) \geq 3$, $d(v_2) = \dots = d(v_{k-1}) = 2$ (unless $k = 2$) and $d(v_k) \geq 3$.

LEMMA 2.3. [8] Let uv be an edge of a connected graph G of order n , and denote by $G_{u,v}$ the graph obtained from G by subdividing the edge uv (that is, by inserting a new vertex w and edges wu, wv in $G - uv$). Then the following hold:

1. If uv does not belong to an internal path of G and $G \neq C_n$, then $\rho(G_{u,v}) > \rho(G)$.
2. If uv belongs to an internal path of G and $G \neq T^*(n, 3, 2)$, then $\rho(G_{u,v}) < \rho(G)$.

LEMMA 2.4. [7] Let A_{-1} be a principal submatrix of order $n-1$ of a symmetric matrix A_0 of order n with non-negative entries. Define A_i recursively by $A_i = \begin{pmatrix} A_{i-1} & e_{i-1} \\ e_{i-1}^T & 0 \end{pmatrix}$ where $e_{i-1} = (0, 0, \dots, 0, 1)^T$. Assume further that $\lim_{i \rightarrow \infty} \rho(A_i) > 2$. Then $\lim_{i \rightarrow \infty} \rho(A_i)$ is the largest positive root of $\frac{1}{2}(\lambda + \sqrt{\lambda^2 - 4})\phi(A_0) - \phi(A_{-1})$, where $\phi(A_0)$ and $\phi(A_{-1})$ are the characteristic polynomial of A_0 and A_{-1} , respectively.

LEMMA 2.5. [7] Let G_1 and G_2 be disjoint connected graphs, v_1 be a vertex of degree at least 2 in G_1 , v_2 be a vertex of degree at least 2 in G_2 , and (G_i, v_i, n) ($i = 1, 2$) be the graph obtained from G_i by appending a path of order n to v_i in G_i and (G_1, v_1, n, v_2, G_2) the graph obtained from G_1 and G_2 by joining them by a path of order n connecting v_1 and v_2 . Define $\rho(G_i, v_i) = \lim_{n \rightarrow \infty} \rho(G_i, v_i, n)$ for $i = 1, 2$ and $\rho(G_1, v_1, G_2) = \lim_{n \rightarrow \infty} \rho(G_1, v_1, n, v_2, G_2)$. Then

$$\rho(G_1, v_1, G_2) = \max\{\rho(G_1, v_1), \rho(G_2, v_2)\}.$$

LEMMA 2.6. [15] Let G_1 and G_2 be connected graphs with $a \in V(G_1)$ and $b \in V(G_2)$, and let H_1 and H_2 be the two graphs shown in Fig. 2.1, then $\rho(H_1) = \rho(H_2)$.

Woo and Neumaier [16] examined the structure of graphs with spectral radius at most $3/\sqrt{2}$. The resulting families of graphs resemble the knotted strings used by the Incas for information storage. They therefore use their term *quipus* for these graphs. An *open quipu* is a tree of maximum degree three such that all vertices of degree three lie on a path. A *closed quipu* is a connected unicyclic graph of maximum degree three such that all vertices of degree three lie on a cycle. A *dagger* is a path with a 3-claw

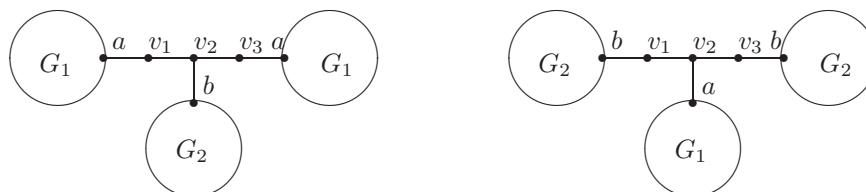


FIG. 2.1. The graphs H_1 and H_2 .

attached to an end vertex.

LEMMA 2.7. [16] *A graph whose spectral radius in $(2, 3/\sqrt{2}]$ is either an open quipu, a closed quipu, or a dagger.*

According to Cioabă et al. [3], a *Laundry graph* is obtained from $T(0, 0, \dots, 0)$ and four additional distinct vertices by inserting a matching between the four vertices and the four (left and right most) leaves of $T(0, 0, \dots, 0)$, respectively.

LEMMA 2.8. [3, Corollary 3.10(c)] *Let $\{G_i\}_{i \geq 1}$ be a sequence of graphs such that G_i is the subgraph of a Laundry graph, let t_i and l_i be the number of vertices of degree three and the minimal length of a maximal internal paths in G_i , respectively. If $t_i \geq 2$ for all i and $\lim_{i \rightarrow \infty} t_i/l_i = 0$, then $\lim_{i \rightarrow \infty} \rho(G_i) = \sqrt{2 + \sqrt{5}}$.*

LEMMA 2.9. [9] *Suppose G_1 and G_2 are two connected graphs satisfying $G_1 - v_1 \cong G_2 - v_2$ for some vertices $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$. If $\phi_{G_2}(\rho(G_1)) > 0$, then $\rho(G_1) > \rho(G_2)$.*

3. Minimal trees $T^*(n, 3, l)$. It is hard to directly evaluate the characteristic polynomial of graphs. We use the diagonalization introduced in [9]. The idea is the following. Since only concerned with trees and every edge of a tree is a bridge, we can view the expansion of the characteristic polynomial in Lemma 2.2 (1) with a pendent edge $e = uv$ or (2) with a leaf v as a linear recurrence of second order for trees. To simplify the computation, we write it in a matrix (also of second order) form and it then becomes a linear recurrence of first order for tree vectors:

$$\begin{pmatrix} \phi_G \\ \phi_{G-v} \end{pmatrix} = \begin{pmatrix} \lambda & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \phi_{G-v} \\ \phi_{G-v-u} \end{pmatrix}.$$

To do the iteration, we simply diagonalize the coefficient matrix to get its similar normal form $\text{diag}(x_1, x_2)$, and meanwhile the tree vector (ϕ_G, ϕ_{G-v}) is naturally transformed to a new function vector, say $(p_{(G,v)}, q_{(G,v)})$, see Eq. (3.1). Then the characteristic polynomial becomes a simple form in terms of the parameters x_i for $i = 1, 2$, which makes it fairly easy to estimate its spectral radius, see Lemma 3.7.

We repeat the essential steps in [9] to make the diagonalization clear. Let P_n



FIG. 3.1. The graphs G_1 and G_2 .

denote a path of order n . A *rooted graph* (G, v) is a graph G together with a designated vertex v as a root. For $i = 1, 2$ and a given rooted graph (H, v') , we define a new rooted graph (G_i, v) by attaching a path P_i to v' and changing the root from v' to v , see Fig. 3.1.

Let $\lambda_0 = \sqrt{2 + \sqrt{5}}$, and in this section, all λ is considered only in the range $\lambda \geq \lambda_0$. Let x_1 and x_2 be the two roots of the equation $x^2 - \lambda x + 1 = 0$, and let $x_1 \leq x_2$. So we have

$$x_1 = \frac{\lambda - \sqrt{\lambda^2 - 4}}{2}, \quad x_2 = \frac{\lambda + \sqrt{\lambda^2 - 4}}{2},$$

and

$$x_1 + x_2 = \lambda, \quad x_1 x_2 = 1.$$

For any vertex $v \in V(G)$, as in [9] we define two functions of λ : $p_{(G,v)}, q_{(G,v)}$ satisfying the following two conditions:

$$\begin{aligned} \phi_G &= p_{(G,v)} + q_{(G,v)}, \\ \phi_{G-v} &= x_2 p_{(G,v)} + x_1 q_{(G,v)}, \end{aligned}$$

which is equivalent to the following matrix form.

$$\begin{pmatrix} \phi_G \\ \phi_{G-v} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix} \begin{pmatrix} p_{(G,v)} \\ q_{(G,v)} \end{pmatrix}. \quad (3.1)$$

Then we have

$$\begin{pmatrix} p_{(G,v)} \\ q_{(G,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1 & 1 \\ x_2 & -1 \end{pmatrix} \begin{pmatrix} \phi_G \\ \phi_{G-v} \end{pmatrix}.$$

We also define two parameters d_1 and d_2 such that

$$d_1 = \lambda - x_1^3, \quad d_2 = x_2^3 - \lambda,$$

and two matrices A, B such that

$$A = \begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix}, \quad B = \frac{1}{x_2 - x_1} \begin{pmatrix} d_1 & x_1 \\ -x_2 & d_2 \end{pmatrix}.$$

The property $d_1x_2 - d_2x_1 = 2$ follows easily from our definition. The following examples claim the definition. Let v be the center of P_{2k+1} . Then

$$\begin{pmatrix} p_{(P_1,v)} \\ q_{(P_1,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1^2 \\ x_2^2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} p_{(P_3,v)} \\ q_{(P_3,v)} \end{pmatrix} = \lambda \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}.$$

REMARK 3.1. As in [9, Remark 1], it is easily seen that the following are equivalent:

1. $d_2 = \frac{2x_1^{2k+3}}{1-x_1^{2k+4}};$
2. $d_2x_2^{2k+3} - d_1x_1^{2k+3} = 2;$
3. $d_2 = d_1x_1^{2k+2};$
4. $d_2x_2^{k+1} = d_1x_1^{k+1};$
5. $d_2 = 2x_1^{2k+3} + d_1x_1^{2(2k+3)}.$

If “=” in Remark 3.1 is replaced by “ $\geq$ ” everywhere, then they are still equivalent.

LEMMA 3.2. [9] *Let G_1 and G_2 be the graphs shown in Fig. 3.1. Then*

$$\begin{pmatrix} p_{(G_1,v)} \\ q_{(G_1,v)} \end{pmatrix} = A \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} p_{(G_2,v)} \\ q_{(G_2,v)} \end{pmatrix} = B \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}.$$

LEMMA 3.3. [9] *For any tree G and any vertex v ,*

$$\lim_{\lambda \rightarrow +\infty} q_{(G,v)}(\lambda) = +\infty.$$

Given two rooted graphs (H_1, v_1) and (H_2, v_2) , we denote by $(H_1, v_1) \cdot P_1 \cdot (H_2, v_2)$ the graph consisting of graphs H_1, H_2 and another vertex linking to v_1 and v_2 , respectively (as shown in Fig. 3.2).

LEMMA 3.4. [9] *The following equality holds:*

$$\phi_{(H_1,v_1) \cdot P_1 \cdot (H_2,v_2)} = (x_2 - x_1) (q_{(H_1,v_1)}q_{(H_2,v_2)} - p_{(H_1,v_1)}p_{(H_2,v_2)}).$$

LEMMA 3.5. [9] *Let $G_{i,j}$ be the graph shown in Fig. 3.3 where i and j are the numbers of included vertices, respectively. Then*

$$\phi_{G_{i,j}} - \phi_{G_{i+1,j-1}} = (x_1 - x_2) (p_{(H_1,v_1)}q_{(H_2,v_2)}x_2^{j-i-1} - q_{(H_1,v_1)}p_{(H_2,v_2)}x_1^{j-i-1}).$$



FIG. 3.2. The graph $(H_1, v_1) \cdot P_1 \cdot (H_2, v_2)$.

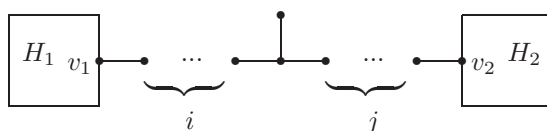


FIG. 3.3. The graph $G_{i,j}$.

LEMMA 3.6. Let $r > 1$ be an integer and ρ the spectral radius of $T(k_1, k_2, \dots, k_r)$. Then $\rho \rightarrow \lambda_0$ and $d_2(\rho) \rightarrow 0$, $d_1 \rightarrow 2x_1$ as $\min\{k_i \mid i = 1, 2, \dots, r\} \rightarrow \infty$.

Proof. Let $k = \min\{k_i \mid i = 1, 2, \dots, r\}$. By Lemma 2.8, we have that $\rho \rightarrow \lambda_0 = \sqrt{2 + \sqrt{5}}$ as $k \rightarrow \infty$. Since $\lambda_0 = \sqrt{2 + \sqrt{5}}$, we have $\lambda_0^4 - 4\lambda_0^2 - 1 = 0$. Then

$$\begin{aligned} d_2(\lambda_0) &= x_2^3 - \lambda_0 = \frac{1}{8} \left(\lambda_0 + \sqrt{\lambda_0^2 - 4} \right)^3 - \lambda_0 \\ &= \frac{1}{8\lambda_0^3} \left(\lambda_0^2 + \lambda_0 \sqrt{\lambda_0^2 - 4} \right)^3 - \lambda_0 \\ &= \frac{1}{8\lambda_0^3} (\lambda_0^2 + 1)^3 - \lambda_0 \\ &= \frac{1}{8\lambda_0^3} (\lambda_0^2 - 1) (\lambda_0^4 - 4\lambda_0^2 - 1) = 0. \end{aligned}$$

Since d_2 is a continuous function of λ , we have that $d_2(\rho) \rightarrow d_2(\lambda_0) = 0$ as $k \rightarrow \infty$, and since $d_1 x_2 - d_2 x_1 = 2$, we have that $d_1 \rightarrow 2x_1$ as $k \rightarrow \infty$. $\square$

The tree $T(k, 2k + 3, 2k + 3, \dots, 2k + 3, k)$ plays an important role in the proof of Theorem 1.3. The following lemma shows that its spectral radius satisfies a simple equation.

LEMMA 3.7. Let $k \in \mathbb{N}$. Then the spectral radius of the tree $T(k, 2k + 3, \dots, 2k + 3, k)$ is the unique root ρ_{2k+3} of the equation

$$d_2 = \frac{2x_1^{2k+3}}{1 - x_1^{2k+4}}$$

in the interval $(\sqrt{2 + \sqrt{5}}, \infty)$.

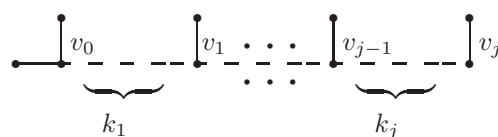


FIG. 3.4. The graph $H(k_1, k_2, \dots, k_j)$.

Proof. Let $G = T(k, 2k+3, \dots, 2k+3, k)$ and v be the leftmost vertex. Let r be one less than the number of vertices of degree three in G . Note that G can be built up from a single vertex with a series of two operations as specified in Lemma 3.2. By Eq. (3.1) and Lemma 3.2, We have

$$\begin{aligned} \phi_G &= (1, 1) \begin{pmatrix} p_{(G,v)} \\ q_{(G,v)} \end{pmatrix} = (1, 1) ABA^k BA^{2k+3} \dots A^{2k+3} BA^k \lambda \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix} \\ &= \lambda(1, 1) ABA^{-1} A^{k+1} BA^{k+2} A^{k+1} \dots A^{k+1} BA^{k+2} (A^{-1})^2 \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix} \\ &= \frac{\lambda}{x_2 - x_1} (d_1 - x_2^3, d_2 + x_1^3) (A^{k+1} BA^{k+2})^{r-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ &= \frac{\lambda}{(x_2 - x_1)^r} (d_1 - x_2^3, d_2 + x_1^3) \begin{pmatrix} d_1 x_1^{2k+3} & 1 \\ -1 & d_2 x_2^{2k+3} \end{pmatrix}^{r-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \end{aligned}$$

By the definition of d_i for $i = 1, 2$, we have $x_2^3 - d_1 = d_2 + x_1^3 = \lambda(x_2 - x_1)^2$, and thus,

$$\phi_G = \frac{\lambda^2}{(x_2 - x_1)^{r-2}} (-1, 1) \begin{pmatrix} d_1 x_1^{2k+3} & 1 \\ -1 & d_2 x_2^{2k+3} \end{pmatrix}^{r-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

We first prove that ρ_{2k+3} is a root of ϕ_G . At $\lambda = \rho_{2k+3}$, by Remark 3.1, we have that $d_2 = \frac{2x_1^{2k+3}}{1-x_1^{2k+4}}$ and $d_2 x_2^{2k+3} - 1 = d_1 x_1^{2k+3} + 1$ are equivalent. Thus,

$$\phi_G(\rho_{2k+3}) = \frac{\rho_{2k+3}^2}{(x_2 - x_1)^{r-2}} (d_1 x_1^{2k+3} + 1)^{r-1} (-1, 1) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 0.$$

Next we prove $\phi_G(\lambda) > 0$ for any $\lambda > \rho_{2k+3}$. When $\lambda > \rho_{2k+3}$, we have $d_2 x_2^{2k+3} - 1 > d_1 x_1^{2k+3} + 1$. Then, by an induction argument on r , one can show

$$\phi_G(\lambda) = \frac{\lambda^2}{(x_2 - x_1)^{r-2}} (-1, 1) \begin{pmatrix} d_1 x_1^{2k+3} & 1 \\ -1 & d_2 x_2^{2k+3} \end{pmatrix}^{r-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} > 0.$$

By Lemmas 2.3 and 3.6, we obtain that ρ_{2k+3} is monotone decreasing in k and $\rho_{2k+3} \rightarrow \sqrt{2 + \sqrt{5}}$ as $k \rightarrow \infty$. $\square$

Let $v_0, v_1, \dots, v_r$ be the sequence of vertices of degree three in $T(k_1, k_2, \dots, k_r)$ from left to right. Let $H(k_1, k_2, \dots, k_j)$ be the graph shown in Fig. 3.4, and for $i = 1, 2, \dots, r-1$, let $L_i = H(k_1, k_2, \dots, k_i)$ (from the left direction); for $j = 2, 3, \dots, r$, let $R_j = H(k_r, k_{r-1}, \dots, k_j)$ (from the right). Moreover, let L_0 be the path of order three with the center v_0 and R_{r+1} be the path of order three with the center v_r . In view of Lemma 2.1 (1), the positivity of functions p and q in the following lemma mimics the property of the characteristic polynomial of subgraphs.

LEMMA 3.8. For $\lambda \geq \rho(T(k_1, k_2, \dots, k_r))$, the following hold:

1. $p_{(L_i, v_i)} \geq 0$ and $q_{(L_i, v_i)} \geq 0$ for $i = 0, 1, \dots, r-1$;
2. $p_{(R_j, v_{j-1})} \geq 0$ and $q_{(R_j, v_{j-1})} \geq 0$ for $j = 2, 3, \dots, r+1$.

Proof. We denote $p_{(L_i, v_i)}$, $q_{(L_i, v_i)}$, $p_{(R_j, v_{j-1})}$, $q_{(R_j, v_{j-1})}$ by p_i , q_i , p'_j , q'_j , respectively for $i = 0, 1, \dots, r-1$ and $j = 2, 3, \dots, r+1$. By our previous definition, for $\lambda > \lambda_0$, we have

$$\begin{aligned} p_0 &= p'_{r+1} = p_{(P_3, v_0)} = \lambda x_1^2 > 0, \\ q_0 &= q'_{r+1} = q_{(P_3, v_0)} = \lambda x_2^2 > 0. \end{aligned}$$

We need consider other situations, namely p_i, q_i, p'_j, q'_j for $i = 1, 2, \dots, r-1$ and $j = 2, 3, \dots, r$. Let μ be the smallest number such that all $p_i(\lambda), q_i(\lambda), p'_j(\lambda), q'_j(\lambda)$ take non-negative values for $\lambda \geq \mu$.

Now our task is to prove such μ exists. By Lemma 3.3, we have $\lim_{\lambda \rightarrow +\infty} q_i(\lambda) = +\infty$ and $\lim_{\lambda \rightarrow +\infty} q'_j(\lambda) = +\infty$. Since $\lim_{\lambda \rightarrow +\infty} p_0 = \lim_{\lambda \rightarrow +\infty} \lambda x_1^2 \geq 0$ and

$$p_i = \frac{1}{x_2 - x_1} \left(d_1 x_1^{k_i} p_{i-1} + x_2^{k_i-1} q_{i-1} \right)$$

by Lemma 3.2, we can get that $\lim_{\lambda \rightarrow +\infty} p_i(\lambda) = +\infty$ by induction on i . Then μ exists.

If $\mu \leq \rho(T(k_1, k_2, \dots, k_r))$, then it is done. Assume that $\mu > \rho(T(k_1, k_2, \dots, k_r))$. It is easily seen that μ is a root of one among $p_i(\lambda), q_i(\lambda), p'_j(\lambda), q'_j(\lambda)$.

Case 1. There exists an i ($1 \leq i \leq r-1$) such that $p_i(\mu) = 0$. Note that

$$p_i = \frac{d_1 x_1^{k_i} p_{i-1} + x_2^{k_i-1} q_{i-1}}{x_2 - x_1}.$$

We have $p_{i-1}(\mu) = q_{i-1}(\mu) = 0$. Applying Lemmas 3.2 and 3.4, we obtain

$$\phi_{T(k_1, k_2, \dots, k_r)}(\mu) = \left[(x_2 - x_1) \left(x_2^{k_i-1} q_{i-1} q'_{i+1} - x_1^{k_i-1} p_{i-1} p'_{i+1} \right) \right] (\mu) = 0,$$

which is contrary to $\mu > \rho(T(k_1, k_2, \dots, k_r))$.

Case 2. There exists a j ($2 \leq j \leq r$) such that $p'_j(\mu) = 0$. This case is similar to Case 1.

Case 3. There exists an i ($1 \leq i \leq r-1$) such that $q_i(\mu) = 0$. Again applying Lemmas 3.2 and 3.4, we obtain

$$\phi_{T(k_1, k_2, \dots, k_r)}(\mu) = \left[(x_2 - x_1) \left(x_2^{k_{i+1}-1} q'_i q'_{i+2} - x_1^{k_{i+1}-1} p_i p'_{i+2} \right) \right] (\mu) \leq 0,$$

which contradicts $\mu > \rho(T(k_1, k_2, \dots, k_r))$.

Case 4. There exists a j ($2 \leq j \leq r$) such that $q'_j(\mu) = 0$. This case is similar to Case 3. $\square$

LEMMA 3.9. Let $r > 1$ be an integer and n be the order of $T(k_1, k_2, \dots, k_r)$. Then

$$d_2 \geq \frac{2x_1^{\frac{n-3}{r-1}-2}}{1 - x_1^{\frac{n-3}{r-1}-1}}$$

for all $\lambda \geq \rho(T(k_1, k_2, \dots, k_r))$, where the equality holds if and only if $k_1 = k_r$ and $k_i = 2k_1 + 3$ for $i = 2, 3, \dots, r-1$ and $\lambda = \rho(T(k_1, k_2, \dots, k_r))$.

Proof. For $i = 0, 1, \dots, r-1$ and $j = 2, 3, \dots, r+1$, we define $t_i = q_i/p_i$ and $t'_j = q'_j/p'_j$. For any $s > 0$, define

$$f_s(t) = \frac{d_2 x_2^{2s} t - x_2}{x_2^{2s-1} t + d_1} = \frac{d_2 x_2 t - x_1^{2s-2}}{t + d_1 x_1^{2s-1}}, \quad t > 0.$$

So by Lemma 3.2, we have

$$t_{s+1} = \frac{q_{s+1}}{p_{s+1}} = f_{k_{s+1}} \left(\frac{q_s}{p_s} \right) = f_{k_{s+1}}(t_s).$$

Consider the fixed point of $f_s(t)$, which satisfies $t^2 - (d_2 x_2 - d_1 x_1^{2s-1})t + x_1^{2s-2} = 0$. When

$$d_2 = 2x_1^s + d_1 x_1^{2s}, \quad (3.2)$$

the above quadratic equation has a unique root x_1^{s-1} . We choose $s = s(\lambda)$ to be the root of Eq. (3.2). The line $y = t$ is tangent to the curve $y = f_s(t)$ at $t = x_1^{s-1}$. Because $f_s(t)$ is an increasing and concave function of t , we have $f_s(t) \leq t$ for any $t > 0$. Then for $i = 1, 2, \dots, r-1$, we have

$$f_{k_i}(t) = f_s \left(x_2^{2(k_i-s)} t \right) \leq x_2^{2(k_i-s)} t. \quad (3.3)$$

By Lemmas 3.2 and 3.4,

$$\phi_{T(k_1, k_2, \dots, k_r)} = (x_2 - x_1) \left(x_2^{k_r-1} q_{r-1} q'_{r+1} - x_1^{k_r-1} p_{r-1} p'_{r+1} \right).$$

Since $\phi_{T(k_1, k_2, \dots, k_r)}(\lambda) \geq 0$ for any $\lambda \geq \rho(T(k_1, k_2, \dots, k_r))$, we have

$$t_{r-1}t'_{r+1}x_2^{2(k_r-1)} \geq 1. \quad (3.4)$$

Note that $t'_{r+1} = t_0 = q_3/p_3 = x_2^4$. By Eqs. (3.3) and (3.4),

$$\begin{aligned} 1 &\leq x_2^4 x_2^{2(k_r-1)} t_{r-1} \\ &= x_2^{2(k_r+1)} f_{k_{r-1}}(f_{k_{r-2}}(\cdots(f_{k_1}(t_0))\cdots)) \\ &\leq x_2^{2(k_r+1)} x_2^{2(k_{r-1}-s)} \cdots x_2^{2(k_1-s)} x_2^4 \\ &= x_2^{2[n-2r-1-(r-1)s]}, \end{aligned}$$

as $\sum_{i=1}^r k_i = n - 2r - 4$. Since $x_2 > 1 > x_1$, we get $n - 2r - 1 - (r - 1)s \geq 0$. Thus, $s \leq \frac{n-3}{r-1} - 2$, and the equality holds if and only if $k_1 = k_r = \frac{s-3}{2}$, $k_i = s$ for $i = 2, 3, \dots, r - 1$ and $\lambda = \rho(T(k_1, k_2, \dots, k_r))$. By the choice of s , we have

$$d_2 = 2x_1^s + d_1 x_1^{2s} \geq 2x_1^{\frac{n-3}{r-1}-2} + d_1 x_1^{\frac{2(n-3)}{r-1}-4}.$$

Hence, by Remark 3.1, we get

$$d_2 \geq \frac{2x_1^{\frac{n-3}{r-1}-2}}{1 - x_1^{\frac{n-3}{r-1}-1}}$$

for all $\lambda \geq \rho(T(k_1, k_2, \dots, k_r))$. $\square$

LEMMA 3.10. Let T^* be the tree minimizing the spectral radius of $T(k_1, k_2, \dots, k_r)$ of order n and fixed integer $r > 1$. Then

$$d_2 \leq \frac{2x_1^{2\lfloor \frac{s+1}{2} \rfloor - 1}}{1 - x_1^{2\lfloor \frac{s+1}{2} \rfloor}}$$

at $\lambda = \rho(T^*)$, where $s = \frac{n-3}{r-1} - 2$.

Proof. (I) When $\lfloor s \rfloor$ is odd, observe that we can always subdivide some edges on internal paths of $T\left(\frac{\lfloor s \rfloor - 3}{2}, \lfloor s \rfloor, \dots, \lfloor s \rfloor, \frac{\lfloor s \rfloor - 3}{2}\right)$ to get a tree $T := T(k_1, k_2, \dots, k_r)$ of order n for some k_i , $i = 1, 2, \dots, r$. By Lemma 2.3, we have

$$\rho(T^*) \leq \rho(T) \leq \rho\left(T\left(\frac{\lfloor s \rfloor - 3}{2}, \lfloor s \rfloor, \dots, \lfloor s \rfloor, \frac{\lfloor s \rfloor - 3}{2}\right)\right) = \rho_{\lfloor s \rfloor}.$$

By Lemma 3.7, $\rho_{\lfloor s \rfloor}$ is the root of $d_2 = \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}}$.

Since d_2 is an increasing function and $\frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}}$ is a decreasing function for $\lambda > \sqrt{2 + \sqrt{5}}$, we have

$$d_2(\rho(T^*)) \leq d_2(\rho_{\lfloor s \rfloor}) = \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}} \bigg|_{\rho_{\lfloor s \rfloor}} \leq \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}} \bigg|_{\rho(T^*)} = \frac{2x_1^{2\lfloor \frac{s+1}{2} \rfloor - 1}}{1 - x_1^{2\lfloor \frac{s+1}{2} \rfloor}} \bigg|_{\rho(T^*)}.$$

(II) When $\lfloor s \rfloor$ is even, observe that we can always subdivide some edges on internal paths of $T(\lfloor s \rfloor/2 - 2, \lfloor s \rfloor - 1, \dots, \lfloor s \rfloor - 1, \lfloor s \rfloor/2 - 2)$ to get a tree $T' := T(k'_1, k'_2, \dots, k'_r)$ of order n for some k'_i , $i = 1, 2, \dots, r$. By Lemma 2.3, we have

$$\rho(T^*) \leq \rho(T') \leq \rho(T(\lfloor s \rfloor/2 - 2, \lfloor s \rfloor - 1, \dots, \lfloor s \rfloor - 1, \lfloor s \rfloor/2 - 2)) = \rho_{\lfloor s \rfloor - 1}.$$

By Lemma 3.7, $\rho_{\lfloor s \rfloor - 1}$ is the root of $d_2 = \frac{2x_1^{\lfloor s \rfloor - 1}}{1 - x_1^{\lfloor s \rfloor}}$.

Since d_2 is an increasing function and $\frac{2x_1^{\lfloor s \rfloor - 1}}{1 - x_1^{\lfloor s \rfloor}}$ is a decreasing function for $\lambda > \sqrt{2 + \sqrt{5}}$, we have

$$d_2(\rho(T^*)) \leq d_2(\rho_{\lfloor s \rfloor - 1}) = \frac{2x_1^{\lfloor s \rfloor - 1}}{1 - x_1^{\lfloor s \rfloor}} \Big|_{\rho_{\lfloor s \rfloor - 1}} \leq \frac{2x_1^{\lfloor s \rfloor - 1}}{1 - x_1^{\lfloor s \rfloor}} \Big|_{\rho(T^*)} = \frac{2x_1^{2\lfloor \frac{s+1}{2} \rfloor - 1}}{1 - x_1^{2\lfloor \frac{s+1}{2} \rfloor}} \Big|_{\rho(T^*)}. \quad \square$$

COROLLARY 3.11. Let T^* and s be as in Lemma 3.10. Then

$$\frac{2x_1^s}{1 - x_1^{s+1}} \leq d_2 \leq \frac{2x_1^{2\lfloor \frac{s+1}{2} \rfloor - 1}}{1 - x_1^{2\lfloor \frac{s+1}{2} \rfloor}}$$

holds at $\lambda = \rho(T^*)$. In particular, $\rho(T^*) = \sqrt{2 + \sqrt{5}} + O\left(\left(\frac{\sqrt{5}-1}{2}\right)^{\lfloor \frac{s+1}{2} \rfloor - \frac{1}{2}}\right)$.

LEMMA 3.12. Let $T^* = T(k_1, k_2, \dots, k_r)$ be the minimal tree as in Lemma 3.10 and let $\rho_0 = \rho(T^*)$ and $c = (\rho_0 + \sqrt{\rho_0^2 + 4d_1d_2})/2$. Then at $\lambda = \rho_0$,

$$cx_1^{k_i+1} \leq d_2 \leq cx_1^{k_i-1} \quad \text{for } i = 2, 3, \dots, r-1; \quad (3.5)$$

$$cx_1^{2(k_j+2)} \leq d_2 \leq cx_1^{2(k_j+1)} \quad \text{for } j = 1, r. \quad (3.6)$$

Proof. We also use our former notation $L_i, p_i, q_i, t_i, R_j, p'_j, q'_j, t'_j$ for $i = 0, 1, \dots, r-1$ and $j = 2, 3, \dots, r+1$ and $f_s(t)$, which are introduced from Lemmas 3.8 and 3.9. By Lemma 3.4, we have

$$t_i t'_{i+2} x_2^{2(k_{i+1}-1)} = 1 \quad (3.7)$$

at $\lambda = \rho_0$ for $i = 1, 2, \dots, r-1$. Note that at $\lambda = \rho_0$,

$$t_i = f_{k_i}(t_{i-1}) = \frac{d_2 x_2 t_{i-1} - x_1^{2(k_i-1)}}{t_{i-1} + d_1 x_1^{2k_i-1}}. \quad (3.8)$$

Combining Eqs. (3.7) and (3.8), we get

$$\frac{d_2 x_2 t_{i-1} - x_1^{2(k_i-1)}}{t_{i-1} + d_1 x_1^{2k_i-1}} t'_{i+2} x_2^{2(k_{i+1}-1)} = 1. \quad (3.9)$$

Let $T = T(k_1, \dots, k_i + 1, k_{i+1} - 1, \dots, k_r)$. We conclude that $\phi_T(\rho_0) \leq 0$, lest we are led to the contradiction with the minimality of T^* by applying Lemma 2.9 to T^* and T .

Applying Lemma 3.5 and evaluating the difference at $\lambda = \rho_0$, we get

$$(\phi_{T^*} - \phi_T)(\rho_0) = \left[(x_1 - x_2) \left(p_{i-1} q'_{i+2} x_2^{k_{i+1} - k_i - 1} - q_{i-1} p'_{i+2} x_1^{k_{i+1} - k_i - 1} \right) \right] (\rho_0) \geq 0.$$

Then at $\lambda = \rho_0$,

$$\frac{t'_{i+2}}{t_{i-1}} \leq x_1^{2(k_{i+1} - k_i - 1)}. \quad (3.10)$$

In the rest of our proof, all expressions are evaluated at $\lambda = \rho_0$.

(I) By Eq. (3.10), we get $t'_{i+2} \leq t_{i-1} x_1^{2(k_{i+1} - k_i - 1)}$. Substituting this to Eq. (3.9) and simplifying, we have

$$d_2 t_{i-1}^2 - x_1^{2k_i} \rho_0 t_{i-1} - d_1 x_1^{4k_i} \geq 0.$$

As $c = (\rho_0 + \sqrt{\rho_0^2 + 4d_1 d_2})/2$, solving the quadratic inequality, we get

$$t_{i-1} \geq c x_1^{2k_i} / d_2, \quad i = 1, 2, \dots, r-1.$$

By symmetry, we have

$$t'_{i+1} \geq c x_1^{2k_i} / d_2, \quad i = 2, 3, \dots, r.$$

(II) Again by Eq. (3.10), we have

$$t_{i-1} \geq t'_{i+2} x_2^{2(k_{i+1} - k_i - 1)}. \quad (3.11)$$

By Eq. (3.9), we obtain that

$$t_{i-1} = \frac{d_1 x_1^{2k_i - 1} + t'_{i+2} x_2^{2(k_{i+1} - k_i)}}{d_2 t'_{i+2} x_2^{2k_{i+1} - 1} - 1}. \quad (3.12)$$

Combining Eqs. (3.11) and (3.12) and simplifying, we get

$$d_2 t_{i+2}'^2 - x_1^{2(k_{i+1} - 1)} \rho_0 t'_{i+2} - d_1 x_1^{4(k_{i+1} - 1)} \geq 0.$$

It follows that

$$t'_{i+2} \leq c x_1^{2(k_{i+1} - 1)} / d_2, \quad i = 1, 2, \dots, r-1.$$

Hence,

$$t'_{i+1} \leq c x_1^{2(k_i - 1)} / d_2, \quad i = 2, 3, \dots, r.$$

Similarly, we have

$$t_{i-1} \leq cx_1^{2(k_i-1)}/d_2, \quad i = 1, 2, \dots, r-1.$$

In short, we obtain

$$cx_1^{2k_i}/d_2 \leq t_{i-1} \leq cx_1^{2(k_i-1)}/d_2, i = 1, 2, \dots, r-1, \quad (3.13)$$

$$cx_1^{2k_i}/d_2 \leq t'_{i+1} \leq cx_1^{2(k_i-1)}/d_2, i = 2, 3, \dots, r. \quad (3.14)$$

By Lemma 3.4, we have

$$t_{i-1}t'_{i+1}x_2^{2(k_i-1)} = 1. \quad (3.15)$$

Then Eq. (3.5) follows easily from Eqs. (3.13), (3.14) and (3.15). Eq. (3.6) follows easily from $cx_1^{2k_j}/d_2 \leq t_0 = t'_{r+1} = x_2^4 \leq cx_1^{2(k_j-1)}/d_2$ for $j = 1, r$. $\square$

Proof of Theorem 1.3. By Lemma 2.7, $T^*(n, 3, l)$ must be an open quipu. Then by Lemmas 2.1 (1) and 2.3, we have that $T^*(n, 3, l) \cong T(k_1, k_2, \dots, k_{l-1})$ for some $k_i \in \mathbb{N}$, $i = 1, 2, \dots, l-1$. Let $r = l-1$. All expressions in the proof will be evaluated at $\lambda = \rho_0 := \rho(T^*(n, 3, l))$.

Proof of Item 1. By Lemma 3.12, for $2 \leq i \leq r-1$, we have

$$cx_1^{k_i+1} \leq d_2 \leq cx_1^{k_i-1}.$$

By the definition of c , we have

$$2d_2x_2^{k_i-1} \leq \rho_0 + \sqrt{\rho_0^2 + 4d_1d_2} \leq 2d_2x_2^{k_i+1}.$$

Combining the property $d_1x_2 - d_2x_1 = 2$ we mentioned before, after solving for d_2 and simplifying, we obtain

$$\frac{\rho_0x_1^{k_i+1} + 2x_1^{2k_i+3}}{1 - x_1^{2(k_i+2)}} \leq d_2 \leq \frac{\rho_0x_1^{k_i-1} + 2x_1^{2k_i-1}}{1 - x_1^{2k_i}}.$$

Since $\rho_0x_1 = 1 + x_1^2 < 2 < \rho_0$, we get

$$\frac{2x_1^{k_i+1}}{1 - x_1^{k_i+2}} < \frac{\rho_0x_1^{k_i+1} + 2x_1^{2k_i+3}}{1 - x_1^{2(k_i+2)}}$$

and

$$\frac{\rho_0x_1^{k_i-1} + 2x_1^{2k_i-1}}{1 - x_1^{2k_i}} < \frac{2x_1^{k_i-2} + 2x_1^{2k_i-1}}{1 - x_1^{2k_i}} < \frac{2x_1^{k_i-2} + 2x_1^{2k_i-3}}{1 - x_1^{2k_i-2}} = \frac{2x_1^{k_i-2}}{1 - x_1^{k_i-1}},$$

So, for $2 \leq i \leq r-1$,

$$\frac{2x_1^{k_i+1}}{1 - x_1^{k_i+2}} < d_2 < \frac{2x_1^{k_i-2}}{1 - x_1^{k_i-1}}. \quad (3.16)$$

By Corollary 3.11, we obtain that when $\lfloor s \rfloor$ is odd,

$$\frac{2x_1^s}{1-x_1^{s+1}} \leq d_2 \leq \frac{2x_1^{\lfloor s \rfloor}}{1-x_1^{\lfloor s \rfloor+1}}. \quad (3.17)$$

Combining Eqs. (3.16) and (3.17), we have

$$\begin{aligned} \frac{2x_1^{k_i+1}}{1-x_1^{k_i+2}} &< \frac{2x_1^{\lfloor s \rfloor}}{1-x_1^{\lfloor s \rfloor+1}}, \\ \frac{2x_1^{k_i-2}}{1-x_1^{k_i-1}} &> \frac{2x_1^s}{1-x_1^{s+1}}. \end{aligned}$$

Therefore, when $\lfloor s \rfloor$ is odd, we get $\lfloor s \rfloor - 1 < k_i < s + 2$ for $2 \leq i \leq r - 1$, and thus, $\lfloor s \rfloor \leq k_i \leq \lfloor s \rfloor + 1$. Similarly, one can show that when $\lfloor s \rfloor$ is even, $\lfloor s \rfloor - 1 \leq k_i \leq \lfloor s \rfloor + 1$ for $2 \leq i \leq r - 1$, and thus, $2\lfloor \frac{s+1}{2} \rfloor - 1 \leq k_i \leq \lfloor s \rfloor + 1$ for $2 \leq i \leq r - 1$.

For $j = 1, r$, combining Eqs. (3.6) and (3.17), we obtain that when $\lfloor s \rfloor$ is odd,

$$\begin{aligned} \frac{cx_1^{2(k_j+2)}}{2} &\leq \frac{x_1^{\lfloor s \rfloor}}{1-x_1^{\lfloor s \rfloor+1}}, \\ \frac{cx_1^{2(k_j+1)}}{2} &\geq \frac{x_1^s}{1-x_1^{s+1}}. \end{aligned}$$

By Lemma 3.6, we get that $d_2 \rightarrow 0$, $d_1 \rightarrow 2x_1$, and $c \rightarrow \lambda_0$ as $n \rightarrow \infty$. Note that $\frac{\ln(\lambda_0/2)}{\ln x_2(\lambda_0)} = 0.119 \dots$. For n large enough, we have $2x_2^{0.1} < \lambda_0 < 2x_2^{0.12}$ and then

$$x_1^{2k_j+3.9} < x_1^{\lfloor s \rfloor}, \quad x_1^{2k_j+1.88} > x_1^s.$$

Thus, when $\lfloor s \rfloor$ is odd, we obtain that $(\lfloor s \rfloor - 3)/2 \leq k_j < (s - 1.88)/2$. Similarly, when $\lfloor s \rfloor$ is even, we have $\lfloor s \rfloor/2 - 2 \leq k_j < (s - 1.88)/2$. So $\lfloor (s - 3)/2 \rfloor \leq k_j < (s - 1.88)/2$ for $j = 1, r$.

Proof of Item 2. By Lemma 3.12, we have

$$\begin{aligned} cx_1^{k_i+1} &\leq d_2 \leq cx_1^{k_i-1} \quad \text{for } i = 2, 3, \dots, r - 1, \\ cx_1^{2(k_j+2)} &\leq d_2 \leq cx_1^{2(k_j+1)} \quad \text{for } j = 1, r. \end{aligned}$$

Therefore,

$$\begin{aligned} cx_1^{k_i+1} &\leq cx_1^{2(k_j+1)}, \\ cx_1^{2(k_j+2)} &\leq cx_1^{k_i-1}, \end{aligned}$$

for $i = 2, 3, \dots, r - 1$ and $j = 1, r$. So, we get $1 \leq k_i - 2k_j \leq 5$.

Proof of Item 3. Again by Lemma 3.12, we have $cx_1^{k_j+1} \leq d_2 \leq cx_1^{k_i-1}$ for $2 \leq i, j \leq r-1$. This implies that $|k_i - k_j| \leq 2$ for $2 \leq i, j \leq r-1$. Now we show it is impossible that $|k_i - k_j| = 2$ for any i and j . If not, without loss of generality, we assume there exist such two indices i and j with $k_j - k_i = 2$, such that $2 \leq i < j \leq r-1$ and $j - i$ is as small as possible. Let $k = k_i$. Then $k_j = k + 2$ and $k_h = k + 1$ for $i < h < j$. Applying Lemma 3.12 to k_i and k_j , we have

$$cx_1^{k+1} = cx_1^{k_i+1} \leq d_2 \leq cx_1^{k_j-1} = cx_1^{k+1}.$$

Combining this with Eqs. (3.13) and (3.14), we have $d_2 = cx_1^{k+1}$, $t_{i-1} = t'_{i+1} = x_1^{k-1}$, and $t_{j-1} = t'_{j+1} = x_1^{k+1}$.

Now we consider the function $f(t) := f_k(x_1^{2k}t) = \frac{d_2t - x_2}{x_1t + d_1}$. Note that

$$x_2^{k+1} = c/d_2 = \frac{\rho_0 + \sqrt{\rho_0^2 + 4d_1d_2}}{2d_2}.$$

It is easy to verify that $f(x_2^{k+1}) = x_1^{k+1}$.

Next, by induction, we show that

$$t_h = x_1^{k+1} \quad \text{for } i \leq h \leq j-1. \quad (3.18)$$

For $h = i$, we have

$$t_i = f_k(t_{i-1}) = f_k(x_1^{k-1}) = f(x_2^{k+1}) = x_1^{k+1}.$$

By the induction hypothesis on $h > i$, we get

$$t_h = f_{k+1}(t_{h-1}) = f_{k+1}(x_1^{k+1}) = f(x_2^{k+1}) = x_1^{k+1}.$$

This completes the proof of (3.18).

By Lemma 3.4, we have $t_{j-2}t'_jx_2^{2k} = 1$. As $t_{j-2} = x_1^{k+1}$, we get $t'_j = x_1^{k-1}$. But we also have

$$t'_j = f_{k+2}(t'_{j+1}) = f_{k+2}(x_1^{k+1}) = f(x_2^{k+3}) \neq x_1^{k-1}.$$

This contradiction completes the proof of Item 3.

In particular, if $n - 5l + 7$ is divisible by $2(l - 2)$, then

$$\frac{s-3}{2} = \frac{1}{2} \left(\frac{n-2l+1}{l-2} - 3 \right) = \frac{n-5l+7}{2(l-2)} \in \mathbb{N}.$$

By the above results, we get $k_j = \frac{s-3}{2}$ for $j = 1, l-1$, and $s \leq k_i \leq s+1$ for $i = 2, 3, \dots, l-2$. Also note that

$$\sum_{i=1}^{l-1} k_i = n - 2l - 2 = (l-2)s - 3.$$

Then we obtain that $T^*(n, 3, l) \cong T\left(\frac{s-3}{2}, s, \dots, s, \frac{s-3}{2}\right)$.

If $n = 2(k+2)(l-2) + 2$, $k \in \mathbb{N}$ and $3 \leq l \leq 10$, then

$$\left\lfloor \frac{s-3}{2} \right\rfloor = \left\lfloor \frac{1}{2} \left(\frac{n-2l+1}{l-2} - 3 \right) \right\rfloor = \left\lfloor k - \frac{l-1}{2(l-2)} \right\rfloor = k-1,$$

$$\frac{s-1.88}{2} = \frac{1}{2} \left(\frac{n-2l+1}{l-2} - 1.88 \right) = k + 0.06 - \frac{1}{2(l-2)} < k.$$

Thus, $k_j = k-1$ for $j = 1, l-1$. For $l > 3$, we have

$$\lceil s \rceil = \left\lceil \frac{n-2l+1}{l-2} \right\rceil = \left\lceil 2k+2 - \frac{1}{l-2} \right\rceil = 2k+2,$$

$$\left\lfloor \frac{s+1}{2} \right\rfloor = \left\lfloor \frac{1}{2} \left(\frac{n-2l+1}{l-2} + 1 \right) \right\rfloor = \left\lfloor k+2 - \frac{l-3}{2(l-2)} \right\rfloor = k+1.$$

Thus, $2k+1 \leq k_i \leq 2k+3$ for $i = 2, 3, \dots, l-2$. Also note that

$$\sum_{i=1}^{l-1} k_i = n - 2l - 2 = 2(k+1)(l-2) - 4.$$

Then we get that $T^*(n, 3, l) \cong T(k-1, 2k+2, \dots, 2k+2, k-1)$.

Moreover, it follows from Corollary 3.11 that $\rho(T^*(n, 3, l)) \rightarrow \sqrt{2 + \sqrt{5}}$ as $n \rightarrow \infty$. $\square$

In order to simplify the proof of Corollary 1.4, we introduce the following short

notation with expressions which can be obtained by Lemma 3.2.

$$\begin{aligned}
 \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} &= \begin{pmatrix} p_{(L_0, v_0)} \\ q_{(L_0, v_0)} \end{pmatrix} = \lambda \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}, \\
 \begin{pmatrix} p_{(k-1)} \\ q_{(k-1)} \end{pmatrix} &:= \begin{pmatrix} p_{(H(k-1), v_1)} \\ q_{(H(k-1), v_1)} \end{pmatrix} = \frac{\lambda}{x_2 - x_1} \begin{pmatrix} d_1 x_1^{k+1} + x_2^k \\ d_2 x_2^{k+1} - x_1^k \end{pmatrix}, \\
 \begin{pmatrix} p_{(k)} \\ q_{(k)} \end{pmatrix} &:= \begin{pmatrix} p_{(H(k), v_1)} \\ q_{(H(k), v_1)} \end{pmatrix} = \frac{\lambda}{x_2 - x_1} \begin{pmatrix} d_1 x_1^{k+2} + x_2^{k+1} \\ d_2 x_2^{k+2} - x_1^{k+1} \end{pmatrix}, \\
 \begin{pmatrix} p_{(k-1, 2k+3)} \\ q_{(k-1, 2k+3)} \end{pmatrix} &:= \begin{pmatrix} p_{(H(k-1, 2k+3), v_2)} \\ q_{(H(k-1, 2k+3), v_2)} \end{pmatrix} \\
 &= \frac{\lambda}{(x_2 - x_1)^2} \begin{pmatrix} d_1^2 x_1^{3k+4} + d_1 x_1^{k+3} + d_2 x_2^{3k+3} - x_2^{k+2} \\ d_2^2 x_2^{3k+4} - d_2 x_2^{k+3} - d_1 x_1^{3k+3} - x_1^{k+2} \end{pmatrix}, \\
 \begin{pmatrix} p_{(k, 2k+2)} \\ q_{(k, 2k+2)} \end{pmatrix} &:= \begin{pmatrix} p_{(H(k, 2k+2), v_2)} \\ q_{(H(k, 2k+2), v_2)} \end{pmatrix} \\
 &= \frac{\lambda}{(x_2 - x_1)^2} \begin{pmatrix} d_1^2 x_1^{3k+4} + d_1 x_1^{k+1} + d_2 x_2^{3k+3} - x_2^k \\ d_2^2 x_2^{3k+4} - d_2 x_2^{k+1} - d_1 x_1^{3k+3} - x_1^k \end{pmatrix}, \\
 \begin{pmatrix} p_{(k, 2k+3)} \\ q_{(k, 2k+3)} \end{pmatrix} &:= \begin{pmatrix} p_{(H(k, 2k+3), v_2)} \\ q_{(H(k, 2k+3), v_2)} \end{pmatrix} \\
 &= \frac{\lambda}{(x_2 - x_1)^2} \begin{pmatrix} d_1^2 x_1^{3k+5} + d_1 x_1^{k+2} + d_2 x_2^{3k+4} - x_2^{k+1} \\ d_2^2 x_2^{3k+5} - d_2 x_2^{k+2} - d_1 x_1^{3k+4} - x_1^{k+1} \end{pmatrix}.
 \end{aligned}$$

Proof of Corollary 1.4. We consider $T^*(n, 3, l)$ for $l = 3, 4, 5$ one by one. Firstly, The case of $l = 3$ follows easily from Theorem 1.3.

Next consider $l = 4$, the case for $n = 4k + 10$, $4k + 13$ can directly be achieved by Theorem 1.3. Then we only need to check two cases according to the value of n .

Case 1. $n = 4k + 11$.

By Theorem 1.3, we know that $T^*(n, 3, 4)$ is isomorphic to one of the three trees $T(k-1, 2k+3, k-1)$, $T(k-1, 2k+2, k)$, and $T(k, 2k+1, k)$. For brevity, we denote them by T_1 , T_2 , and T_3 , respectively. Next we prove $\rho(T_1) = \rho(T_2) = \rho(T_3)$.

By Lemma 2.6, we have $\rho(T_1) = \rho(T(k-1, k)) = \rho(T_3)$. By Lemma 3.4, we have

$$\begin{aligned}
 \phi_{T_1} &= (x_2 - x_1)x_2^{2k+2} \left(q_{(k-1)}^2 - p_{(k-1)}^2 x_1^{4k+4} \right), \\
 \phi_{T_2} &= (x_2 - x_1)x_2^{2k+1} \left(q_{(k-1)}q_{(k)} - p_{(k-1)}p_{(k)}x_1^{4k+2} \right), \\
 \phi_{T_3} &= (x_2 - x_1)x_2^{2k} \left(q_{(k)}^2 - p_{(k)}^2 x_1^{4k} \right).
 \end{aligned}$$

Let $\rho = \rho(T_1) = \rho(T_3)$ and $\rho' = \rho(T_2)$. Then ρ is the root of both equations $q_{(k-1)}^2 -$

$p_{(k-1)}^2 x_1^{4k+4} = 0$ and $q_{(k)}^2 - p_{(k)}^2 x_1^{4k} = 0$. Thus, at ρ ,

$$q_{(k-1)}q_{(k)} = p_{(k-1)}p_{(k)}x_1^{4k+2}.$$

It follows that $\phi_{T_2}(\rho) = 0$ and $\rho' \geq \rho$.

If $\rho' > \rho$, then $\phi_{T_1}(\rho') > 0$ and $\phi_{T_3}(\rho') > 0$. It follows that at ρ' , $q_{(k-1)} - p_{(k-1)}x_1^{2k+2} > 0$ and $q_{(k)} - p_{(k)}x_1^{2k} > 0$. Thus,

$$\phi_{T_2}(\rho') = (x_2 - x_1)x_2^{2k-1}(q_{(k-1)}q_{(k)} - p_{(k-1)}p_{(k)}x_1^{4k+2}) > 0,$$

which is contrary to $\rho' = \rho(T_2)$. This gives that $\rho = \rho'$.

Case 2. $n = 4k + 12$.

By Theorem 1.3, we know that $T^*(n, 3, 4)$ is isomorphic to either $T(k-1, 2k+3, k)$ or $T(k, 2k+2, k)$. For brevity, we denote them by T_4 and T_5 , respectively. By Lemma 3.5, we have

$$\begin{aligned} \phi_{T_4} - \phi_{T_5} &= (x_1 - x_2)(p_0q_{(k)}x_2^{k+3} - q_0p_{(k)}x_1^{k+3}) \\ &= \lambda^2 [x_1^{k+1}(d_1x_1^{k+2} + x_2^{k+1}) - x_2^{k+1}(d_2x_2^{k+2} - x_1^{k+1})] \\ &= \lambda^2 (d_1x_1^{2k+3} - d_2x_2^{2k+3} + 2). \end{aligned}$$

Next we prove $T^*(n, 3, 4) \cong T_5$. Assume to the contrary that $T^*(n, 3, 4) \cong T_4$. Then by Lemma 3.12, $d_2 = cx_1^{2k+2}$ at $\lambda = \rho(T_4)$ and by Lemma 3.6, $c \rightarrow \lambda_0$, $d_1 \rightarrow 2x_1$ as $n \rightarrow \infty$. Note that $x_1 < 1 < x_2$. When n is large enough, we have $\phi_{T_5}(\rho(T_4)) > 0$. By Lemma 2.9, we get $\rho(T_4) > \rho(T_5)$, contrary to the minimality assumption of T_4 . So $T^*(n, 3, 4) \cong T(k, 2k+2, k)$.

At last, we consider $l = 5$. The case when $n - 6k = 12, 13, 14, 15$ can directly be achieved by Theorem 1.3. Then only two cases are left.

Case I. $n = 6k + 16$.

By Theorem 1.3, we know that $T^*(n, 3, 5)$ is isomorphic to one of the four trees $T(k-1, 2k+3, 2k+3, k-1)$, $T(k-1, 2k+2, 2k+3, k)$, $T(k-1, 2k+3, 2k+2, k)$, and $T(k, 2k+2, 2k+2, k)$. We also denote the four trees by G_i , $i = 1, 2, 3, 4$, respectively.

By Lemma 3.5, we have

$$\begin{aligned}
 \phi_{G_3} - \phi_{G_1} &= (x_1 - x_2) (p_{(k-1, 2k+3)} q_0 x_1^{k+3} - p_0 q_{(k-1, 2k+3)} x_2^{k+3}) \\
 &= \frac{\lambda^2}{x_1 - x_2} [x_1^{k+1} (d_1^2 x_1^{3k+4} + d_1 x_1^{k+3} + d_2 x_2^{3k+3} - x_2^{k+2}) \\
 &\quad - x_2^{k+1} (d_2^2 x_2^{3k+4} - d_2 x_2^{k+3} - d_1 x_1^{3k+3} - x_1^{k+2})] \\
 &= \frac{\lambda^2}{x_1 - x_2} (d_1^2 x_1^{4k+5} + d_1 x_1^{2k+4} + d_2 x_2^{2k+2} - x_2 - d_2^2 x_2^{4k+5} \\
 &\quad + d_2 x_2^{2k+4} + d_1 x_1^{2k+2} + x_1), \\
 \phi_{G_2} - \phi_{G_3} &= (x_1 - x_2) (p_{(k-1)} q_{(k)} - q_{(k-1)} p_{(k)}) \\
 &= \frac{\lambda^2}{x_1 - x_2} [(d_1 x_1^{k+1} + x_2^k) (d_2 x_2^{k+2} - x_1^{k+1}) \\
 &\quad - (d_2 x_2^{k+1} - x_1^k) (d_1 x_1^{k+2} + x_2^{k+1})] \\
 &= \lambda^2 (d_1 d_2 + 1) (x_1 - x_2), \\
 \phi_{G_3} - \phi_{G_4} &= (x_1 - x_2) (p_0 q_{(k, 2k+2)} x_2^{k+3} - q_0 p_{(k, 2k+2)} x_1^{k+3}) \\
 &= \frac{\lambda^2}{x_1 - x_2} [x_2^{k+1} (d_2^2 x_2^{3k+4} - d_2 x_2^{k+1} - d_1 x_1^{3k+3} - x_1^k) \\
 &\quad - x_1^{k+1} (d_1^2 x_1^{3k+4} + d_1 x_1^{k+1} + d_2 x_2^{3k+3} - x_2^k)] \\
 &= \frac{\lambda^2}{x_1 - x_2} (d_2^2 x_2^{4k+5} - 2d_2 x_2^{2k+2} - 2d_1 x_1^{2k+2} - d_1^2 x_1^{4k+5} + x_1 - x_2).
 \end{aligned}$$

Then $\phi_{G_2}(\rho(G_3)) < 0$, and by Lemma 2.1, we get $\rho(G_2) > \rho(G_3)$.

Next we prove that $T^*(n, 3, 5)$ can neither be isomorphic to G_1 nor to G_3 . Assume to the contrary that $T^*(n, 3, 5) \cong G_1$. Then by Lemma 3.12, $d_2 = cx_1^{2k+2}$ at $\lambda = \rho(G_1)$, and by Lemma 3.6, $c \rightarrow \lambda_0$, $d_1 \rightarrow 2x_1$ as $n \rightarrow \infty$. Also note that $x_1 < 1 < x_2$. For n large enough, $\phi_{G_3}(\rho(G_1)) > 0$. Thus, by Lemma 2.9, we get $\rho(G_1) > \rho(G_3)$, contrary to the minimality of G_1 . Assume that $T^*(n, 3, 5) \cong G_3$. Then by Lemma 3.12, we also get $d_2 = cx_1^{2k+2}$ at $\lambda = \rho(G_3)$, and by Lemma 3.6, $c \rightarrow \lambda_0$, $d_1 \rightarrow 2x_1$ as $n \rightarrow \infty$. Again note that $x_1 < 1 < x_2$. For n large enough, $\phi_{G_4}(\rho(G_3)) > 0$. Thus, by Lemma 2.9, we get $\rho(G_3) > \rho(G_4)$, contrary to the minimality of G_3 . Therefore we must have that $T^*(n, 3, 5) \cong G_4 = T(k, 2k+2, 2k+2, k)$.

Case II. $n = 6k + 17$.

By Theorem 1.3, we know that $T^*(n, 3, 5)$ is isomorphic to either $T(k-1, 2k+3, 2k+3, k)$ or $T(k, 2k+2, 2k+3, k)$. We also denote them by G_5 and G_6 , respectively.

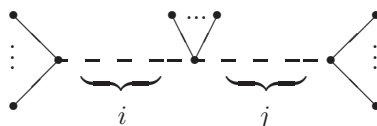


FIG. 4.1. The graph $R(\Delta; i, j)$.

Similarly as above, we have

$$\begin{aligned} \phi_{G_5} - \phi_{G_6} &= (x_1 - x_2) (p_0 q_{(k, 2k+3)} x_2^{k+3} - q_0 p_{(k, 2k+3)} x_1^{k+3}) \\ &= \frac{\lambda^2}{x_1 - x_2} [x_2^{k+1} (d_2^2 x_2^{3k+5} - d_2 x_2^{k+2} - d_1 x_1^{3k+4} - x_1^{k+1}) \\ &\quad - x_1^{k+1} (d_1^2 x_1^{3k+5} + d_1 x_1^{k+2} + d_2 x_2^{3k+4} - x_2^{k+1})] \\ &= \frac{\lambda^2}{x_1 - x_2} (d_2^2 x_2^{4k+6} - 2d_2 x_2^{2k+3} - 2d_1 x_1^{2k+3} - d_1^2 x_1^{4k+6}). \end{aligned}$$

Next we prove $T^*(n, 3, 5) \cong G_6$. Assume to the contrary that $T^*(n, 3, 5) \cong G_5$. Then by Lemma 3.12, $d_2 = cx_1^{2k+2}$ at $\lambda = \rho(G_5)$, and by Lemma 3.6, $c \rightarrow \lambda_0$, $d_1 \rightarrow 2x_1$ as $n \rightarrow \infty$. Again note that $x_1 < 1 < x_2$. For n large enough, $\phi_{G_6}(\rho(G_5)) > 0$. Thus, by Lemma 2.9, we get $\rho(G_5) > \rho(G_6)$, contrary to the minimality of G_5 . Hence, we have that $T^*(n, 3, 5) \cong T(k, 2k+2, 2k+3, k)$. $\square$

4. Minimal trees $T^*(n, \Delta, 3)$. In this section, we characterize the minimal trees with at most three vertices of maximum degree. Let $T_0(\Delta, k)$ denote a *broom* of order $\Delta + k$ with maximum degree Δ , i.e., a path with a star attached to an end vertex. Then $T_0(4, k)$ is a *dagger* for instance. Let $T_1(\Delta, k)$ denote a tree consisting of a path of length $2k$ with a star of order $\Delta - 1$ the center of which is attached to the center of the path. Let $R(\Delta; i, j)$ denote the tree obtained by linking two distinct brooms $T_0(\Delta, i)$ and $T_0(\Delta, j)$ to the center of a star as depicted in Fig. 4.1. It is clear by the definitions that $T_0(\Delta, k)$ is a subgraph of $T_1(\Delta, k)$ which in turn is a subgraph of $R(\Delta; k, k)$.

LEMMA 4.1. For each integer $\Delta > 2$, the following holds:

$$\lim_{k \rightarrow \infty} \rho(T_0(\Delta, k)) = \frac{\Delta - 1}{\sqrt{\Delta - 2}} < \sqrt{2 + \sqrt{4 + (\Delta - 2)^2}} = \lim_{k \rightarrow \infty} \rho(T_1(\Delta, k)).$$

Proof. This follows easily by solving the algebraic equation $Ax = \rho x$ for the spectral radius ρ and its eigenvector $x > 0$, noting that x has equal entries for vertices equivalent under a symmetry of the graph. For details, applying Lemma 2.4 to

$T_0(\Delta, k)$ with

$$A_{-1} = \begin{pmatrix} 0 & e \\ e^T & 0 \end{pmatrix} \quad \text{and} \quad A_0 = \begin{pmatrix} 0 & e & 0 \\ e^T & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

where $e = (1, 1, \dots, 1)^T$, together with $\phi(A_0) = \lambda^{\Delta-1}(\lambda^2 - \Delta)$ and $\phi(A_{-1}) = \lambda^{\Delta-2}(\lambda^2 - \Delta + 1)$, we get $\lim_{k \rightarrow \infty} \rho(T_0(\Delta, k))$ is the largest root of

$$f(\lambda) := \frac{1}{2} \left(\lambda + \sqrt{\lambda^2 - 4} \right) \phi(A_0) - \phi(A_{-1}).$$

Let $\lambda = 2 \sec \alpha$, $\alpha \in (0, \pi/2)$. Then

$$\begin{aligned} f(\lambda) &= \frac{1}{2} \lambda^{\Delta-2} \left[\lambda(\lambda^2 - \Delta) \left(\lambda + \sqrt{\lambda^2 - 4} \right) - 2(\lambda^2 - \Delta + 1) \right] \\ &= (2 \sec \alpha)^{\Delta-2} [2 \sec \alpha (4 \sec^2 \alpha - \Delta) (\sec \alpha + \tan \alpha) - 4 \sec^2 \alpha + \Delta - 1] \\ &= 2^{\Delta-2} \sec^{\Delta+2} \alpha [2(4 - \Delta \cos^2 \alpha)(1 + \sin \alpha) - 4 \cos^2 \alpha + (\Delta - 1) \cos^4 \alpha] \\ &= 2^{\Delta-2} \sec^{\Delta+2} \alpha [(4 - \Delta \cos^2 \alpha)(2 + 2 \sin \alpha - \cos^2 \alpha) - \cos^4 \alpha] \\ &= 2^{\Delta-2} \sec^{\Delta+2} \alpha [(4 - \Delta \cos^2 \alpha)(1 + \sin \alpha)^2 - (1 - \sin^2 \alpha)^2] \\ &= 2^{\Delta-2} \sec^{\Delta+2} \alpha (1 + \sin \alpha)^2 [4 - \Delta \cos^2 \alpha - (1 - \sin \alpha)^2] \\ &= 2^{\Delta-2} \sec^{\Delta+2} \alpha (1 + \sin \alpha)^2 [(\Delta - 1) \sin^2 \alpha + 2 \sin \alpha + 3 - \Delta] \\ &= 2^{\Delta-2} \sec^{\Delta+2} \alpha (1 + \sin \alpha)^3 [(\Delta - 1) \sin \alpha + 3 - \Delta]. \end{aligned}$$

So the largest root of f satisfies $\sin \alpha = \frac{\Delta-3}{\Delta-1}$, and $\lim_{k \rightarrow \infty} \rho(T_0(\Delta, k)) = 2 \sec \alpha = \frac{\Delta-1}{\sqrt{\Delta-2}}$.

Similarly, applying Lemma 2.4 to $T_1(\Delta, k)$ with

$$A'_{-1} = \begin{pmatrix} 0 & e \\ e^T & 0 \end{pmatrix} \quad \text{and} \quad A'_0 = \begin{pmatrix} 0 & e & 0 \\ e^T & 0 & 2 \\ 0 & 1 & 0 \end{pmatrix}$$

together with $\phi(A'_0) = \lambda^{\Delta-2}(\lambda^2 - \Delta)$ and $\phi(A'_{-1}) = \lambda^{\Delta-3}(\lambda^2 - \Delta + 2)$, we get $\lim_{k \rightarrow \infty} \rho(T_1(\Delta, k))$ is the largest root of

$$g(\lambda) := \frac{1}{2} \left(\lambda + \sqrt{\lambda^2 - 4} \right) \phi(A'_0) - \phi(A'_{-1}).$$

Let $\lambda = 2 \sec \beta$, $\beta \in (0, \pi/2)$. Then

$$\begin{aligned} g(\lambda) &= \frac{1}{2} \lambda^{\Delta-3} \left[\lambda(\lambda^2 - \Delta) \left(\lambda + \sqrt{\lambda^2 - 4} \right) - 2(\lambda^2 - \Delta + 2) \right] \\ &= (2 \sec \beta)^{\Delta-3} [2 \sec \beta (4 \sec^2 \beta - \Delta) (\sec \beta + \tan \beta) - 4 \sec^2 \beta + \Delta - 2] \\ &= 2^{\Delta-3} \sec^{\Delta+1} \beta (1 + \sin \beta)^2 [(\Delta - 2) \sin^2 \beta + 4 \sin \beta + 2 - \Delta]. \end{aligned}$$

So the largest root of g satisfies

$$\sin \beta = \frac{\sqrt{4 + (\Delta - 2)^2} - 2}{\Delta - 2},$$

and therefore,

$$\lim_{k \rightarrow \infty} \rho(T_1(\Delta, k)) = 2 \sec \beta = \sqrt{2 + \sqrt{4 + (\Delta - 2)^2}}. \quad \square$$

LEMMA 4.2. For $\Delta \geq 3$ and $j - i \geq 2$, $\Delta, i, j, k \in \mathbb{N}$, $\rho(Y(\Delta; i, j, k)) > \rho(Y(\Delta; i + 1, j - 1, k))$.

Proof. Recall that P_i is a path of order i . By Lemma 2.2, we have

$$\begin{aligned} \phi_{T_0(\Delta, i)} &= \lambda^{\Delta-2} (\lambda \phi_{P_{i+1}} - (\Delta - 1) \phi_{P_i}), \\ \phi_{T_0(\Delta, i)} \phi_{T_0(\Delta, j)} &= \lambda^{2(\Delta-2)} [\lambda^2 \phi_{P_{i+1}} \phi_{P_{j+1}} - (\Delta - 1) \lambda (\phi_{P_{i+1}} \phi_{P_j} + \phi_{P_i} \phi_{P_{j+1}}) \\ &\quad + (\Delta - 1)^2 \phi_{P_i} \phi_{P_j}], \\ \phi_{T_0(\Delta, i+1)} \phi_{T_0(\Delta, j-1)} &= \lambda^{2(\Delta-2)} [\lambda^2 \phi_{P_{i+2}} \phi_{P_j} - (\Delta - 1) \lambda (\phi_{P_{i+2}} \phi_{P_{j-1}} + \phi_{P_{i+1}} \phi_{P_j}) \\ &\quad + (\Delta - 1)^2 \phi_{P_{i+1}} \phi_{P_{j-1}}]. \end{aligned}$$

By induction, it is easy to verify that $\phi_{P_i} \phi_{P_j} - \phi_{P_{i-1}} \phi_{P_{j+1}} = \phi_{P_{j-i}}$ for $j - i \geq 0$. Thus,

$$\begin{aligned} \phi_{T_0(\Delta, i+1)} \phi_{T_0(\Delta, j-1)} - \phi_{T_0(\Delta, i)} \phi_{T_0(\Delta, j)} &= \lambda^{2(\Delta-2)} [\lambda^2 \phi_{P_{j-i-2}} - (\Delta - 1) \lambda (\phi_{P_{j-i-3}} + \phi_{P_{j-i-1}}) + (\Delta - 1)^2 \phi_{P_{j-i-2}}] \\ &= \lambda^{2(\Delta-2)} [(2 - \Delta) \lambda^2 + (\Delta - 1)^2] \phi_{P_{j-i-2}}. \end{aligned}$$

By Lemma 2.2, we also get

$$\begin{aligned} \phi_{Y(\Delta; i, j, k)} &= \phi_{T_0(\Delta, k)} \phi_{T^*(2\Delta+i+j+1, \Delta, 2)} - \phi_{T_0(\Delta, i)} \phi_{T_0(\Delta, j)} \phi_{T_0(\Delta, k-1)}, \\ \phi_{Y(\Delta; i+1, j-1, k)} &= \phi_{T_0(\Delta, k)} \phi_{T^*(2\Delta+i+j+1, \Delta, 2)} - \phi_{T_0(\Delta, i+1)} \phi_{T_0(\Delta, j-1)} \phi_{T_0(\Delta, k-1)}. \end{aligned}$$

Taking the difference, we obtain

$$\begin{aligned} \phi_{Y(\Delta; i, j, k)} - \phi_{Y(\Delta; i+1, j-1, k)} &= \phi_{T_0(\Delta, k-1)} (\phi_{T_0(\Delta, i+1)} \phi_{T_0(\Delta, j-1)} - \phi_{T_0(\Delta, i)} \phi_{T_0(\Delta, j)}) \\ &= \lambda^{2(\Delta-2)} [(2 - \Delta) \lambda^2 + (\Delta - 1)^2] \phi_{P_{j-i-2}} \phi_{T_0(\Delta, k-1)}. \end{aligned}$$

Note that $T_0(\Delta, k)$ is a proper subgraph of the subdivision of $Y(\Delta; i, j, k)$. By Lemmas 2.3 and 4.1, we have $\rho(Y(\Delta; i, j, k)) > \frac{\Delta-1}{\sqrt{\Delta-2}}$. Since P_{j-i-2} and $T_0(\Delta, k-1)$ are both proper subgraphs of $Y(\Delta; i+1, j-1, k)$, we have $\phi_{P_{j-i-2}}(\rho(Y(\Delta; i+1, j-1, k))) > 0$ and $\phi_{T_0(\Delta, k-1)}(\rho(Y(\Delta; i+1, j-1, k))) > 0$ by Lemma 2.1. Thus, $\phi_{Y(\Delta; i, j, k)}(\rho(Y(\Delta; i+1, j-1, k))) < 0$, and the result follows from Lemma 2.1 (2). $\square$

Proof of Theorem 1.5. (1) It follows easily from Lemmas 2.1 and 2.3 that $T^*(n, \Delta, 2)$ consists of two stars linked by a path. By Lemmas 2.5 and 4.1, we have $\lim_{n \rightarrow \infty} \rho(T^*(n, \Delta, 2)) = \lim_{n \rightarrow \infty} T_0(\Delta, n) = \frac{\Delta-1}{\sqrt{\Delta-2}}$.

(2) The three vertices of maximum degree are either on a path or connected by three distinct paths to a common vertex. Hence, by Lemmas 2.1 and 2.3, $T^*(n, \Delta, 3)$ must be of type either $R(\Delta; i, j)$ or $Y(\Delta; i, j, k)$. Let $S(i, j, k)$ denote the starlike tree consisting of three distinct paths of length i, j, k respectively with a common end. Then $S(i, j, k)$ is a subgraph of $Y(\Delta; i, j, k)$. As a special case of [13, Remark], $\lim_{k \rightarrow \infty} \rho(S(k, k, k)) = 3/\sqrt{2}$. By Lemma 2.1, if $h \leq i, j, k \leq l$ then $\rho(S(h, h, h)) \leq \rho(S(i, j, k)) \leq \rho(S(l, l, l))$, so the limit of $\rho(S(i, j, k))$ exists and

$$\lim_{i, j, k \rightarrow \infty} \rho(S(i, j, k)) = \lim_{k \rightarrow \infty} \rho(S(k, k, k)) = 3/\sqrt{2}.$$

By Lemmas 2.5 and 4.1, we obtain that for $\Delta \geq 4$,

$$\begin{aligned} \lim_{i, j, k \rightarrow \infty} \rho(Y(\Delta; i, j, k)) &= \max \left\{ \lim_{i \rightarrow \infty} T_0(\Delta, i), \lim_{i, j, k \rightarrow \infty} \rho(S(i, j, k)) \right\} = \frac{\Delta-1}{\sqrt{\Delta-2}} \\ &< \sqrt{2 + \sqrt{4 + (\Delta-2)^2}} = \max_{i=0,1} \lim_{k \rightarrow \infty} \rho(T_i(\Delta, k)) \\ &= \lim_{i, j \rightarrow \infty} \rho(R(\Delta; i, j)). \end{aligned}$$

This implies that if i, j, k are all large enough, then $\rho(Y(\Delta; i, j, k)) < \rho(R(\Delta; i', j'))$. Thus, $T^*(n, \Delta, 3)$ is of type $Y(\Delta; i, j, k)$. Then the result follows from Lemma 4.2. $\square$

5. Final remarks. Since every connected graph has a spanning tree as a subgraph, by Lemma 2.1, for $n \gg l\Delta$, $T^*(n, \Delta, l)$ also minimizes the spectral radius of all *connected graphs* of order n with exactly l vertices of maximum degree Δ . So it is also interesting to know which graph *maximizes* the spectral radius of all connected graphs instead of all trees considered in this paper.

By the result of Wu et al. [17] or Corollary 1.4, $T^*(n, 3, 3) \cong T(\lfloor n/2 \rfloor - 4, \lceil n/2 \rceil - 4)$. Meanwhile, $T^*(n, \Delta, 3) \cong Y(\Delta; i, j, k)$ for $\Delta \geq 4$ by Theorem 1.5. This shows that the minimal trees have a phase transition at the maximum degree changing from three to four for exactly three vertices of maximum degree. Actually the phase transition also occurs for any number of vertices of maximum degree greater than three. Analogous to the proof of Theorem 1.5 for instance, we can show that $T^*(n, 4, 4)$ must be a subdivision of the tree consisting of $T(0)$ and four 3-claws each attached to a leaf of $T(0)$. Also analogous to Lemma 4.2, one can show that $T^*(n, 4, 4)$ has some symmetry. However, we are unable to figure out which subdivision it is. It can be shown that there are exactly $l-2$ vertices of degree three in $T^*(n, 4, l)$, and it can also be imagined that $T^*(n, \Delta, l)$ must all be symmetric in some sense. To characterize them for $\Delta, l \geq 4$, however, remains open and definitely needs some new idea.

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