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Graphs with diameter $n - e$ minimizing the spectral radius

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ABSTRACT

The spectral radius $\rho(G)$ of a graph G is the largest eigenvalue of its adjacency matrix $A(G)$. For a fixed integer $e \geq 1$, let $G^{min}_{n,n-e}$ be a graph with minimal spectral radius among all connected graphs on n vertices with diameter $n-e$. Let $P^{m_1,m_2,\ldots,m_t}_{n_1,n_2,\ldots,n_t,p}$ be a tree obtained from a path of p vertices $(0 \sim 1 \sim 2 \sim \cdots \sim (p-1))$ by linking one pendant path P_{n_i} at m_i for each $i \in \{1, 2, \ldots, t\}$. For $e = 1, 2, 3, 4, 5$, $G^{min}_{n,n-e}$ were determined in the literature. Cioabă et al. [2] conjectured for fixed $e \geqslant 6$, $G^{min}_{n,n-e}$ is in the family $\mathcal{P}_{n,e} = \{P^{2,m_2,\ldots,m_{e-4},n-e-2}_{2,1,\ldots,1,2,n-e+1} \mid 2 < m_2 < \cdots < m_{e-4} < n-e-2\}$. For $e = 6, 7$, they conjectured $G^{min}_{n,n-6} = P^{2,\lceil\frac{D-1}{2}\rceil,D-2}_{2,1,2,n-5}$ and $G^{min}_{n,n-7} = P^{2,\lfloor\frac{D+2}{3}\rfloor,D-\lfloor\frac{D+2}{3}\rfloor,D-2}_{2,1,1,2,n-6}$. In this paper, we settle their conjectures positively. Note that any tree in $\mathcal{P}_{n,e}$ is uniquely determined by its internal path lengths. For any $e-4$ non-negative integers $k_1, k_2, \ldots, k_{e-4}$, let $T_{(k_1,k_2,\ldots,k_{e-4})} = P^{2,m_2,\ldots,m_{e-4},n-e-2}_{2,1,\ldots,1,2,n-e+1}$ with $k_i = m_{i+1} - m_i - 1$, for $1 \leqslant i \leqslant e-4$. (Here we assume $m_1 = 2$ and $m_{e-3} = n-e-2$.)

Let $s = \frac{\sum_{i=1}^{e-4} k_i + 2}{e-4}$. For any integer $e \geqslant 6$ and sufficiently large n, we prove that $G^{min}_{n,n-e}$ must be one of the trees $T_{(k_1,k_2,\ldots,k_{e-4})}$ with the parameters satisfying $\lfloor s \rfloor - 1 \leqslant k_j \leqslant \lfloor s \rfloor \leqslant k_i \leqslant \lceil s \rceil + 1$ for $j = 1, e-4$ and $i = 2, \ldots, e-5$. Moreover, $0 \leq k_i - k_j \leq 2$ for $2 \leq i \leq e-5$, $j = 1, e-4$; and $|k_i - k_j| \leq 1$ for $2 \leq i, j \leq e-5$. These results are best possible as shown by cases $e = 6, 7, 8$, where $G^{min}_{n,n-e}$ are completely determined here. Moreover, if $n-6$ is divisible by $e-4$ and n is sufficiently large, then $G^{min}_{n,e} = T_{(k-1,k,k,\ldots,k,k,k-1)}$ where $k = \frac{n-6}{e-4} - 2$.

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1. Introduction

Let $G = (V, E)$ be a simple connected graph, and $A(G)$ be the adjacency matrix of G. The *characteristic polynomial* of G is defined by $\phi_G(\lambda) = \det(\lambda I - A(G))$. The *spectral radius*, denoted by $\rho(G)$, is the largest root of ϕ_G. The problem of determining graphs with small spectral radius can be traced back to Hoffman and Smith [7,8,10]. Smith completely determined all connected graphs G with $\rho(G) \leqslant 2$. The connected graphs with $\rho(G) < 2$ are precisely simple Dynkin Diagrams A_n, D_n, E_6, E_7, and E_8. The connected graphs with $\rho(G) = 2$ are exactly those simple extended Dynkin Diagrams $\tilde{A}_n$, $\tilde{D}_n$, $\tilde{E}_6$, $\tilde{E}_7$, and $\tilde{E}_8$. Note $A_n := P_n$ (paths) and $\tilde{A}_n := C_n$ (cycles). The rest of (extended) Dynkin Diagrams are drawn in Fig. 1 (for the details of Dynkin Diagrams, see [16]).

Cvetković et al. [4] gave a nearly complete description of all graphs G with $2 < \rho(G) \leqslant \sqrt{2+\sqrt{5}}$. Their description was completed by Brouwer and Neumaier [1]. Those graphs are some special trees with at most two vertices of degree 3. Wang et al. [12] studied some graphs with spectral radius close to $\frac{3}{2}\sqrt{2}$. Woo and Neumaier [13] determined the structures of graphs G with $\sqrt{2+\sqrt{5}} \leqslant \rho(G) \leqslant \frac{3}{2}\sqrt{2}$; if G has maximum degree at least 4, then G is a *dagger* (i.e., a path is attached to a leaf of a star S_4); if G is a tree with maximum degree at most 3, then G is an *open quipu* (i.e., the vertices of degree 3 lies on a path); else G is a *closed quipu* (i.e., a unicyclic graph with maximum degree at most 3 satisfies that the vertices of degree 3 lies on a cycle).

Van Dam and Kooij [3] used the following notation to denote an open quipu. Let $P^{m_1,m_2,\ldots,m_t}_{n_1,n_2,\ldots,n_t,p}$ be a tree obtained from a path on p vertices $(0 \sim 1 \sim 2 \sim \cdots \sim (p-1))$ by linking one pendant path P_{n_i} at m_i for $i = 1, 2, \ldots, t$ (see Fig. 2.) The path $0 \sim 1 \sim 2 \sim \cdots \sim (p-1)$ is called *main path*. For $i = 1, \ldots, t-1$, let $P^{(i)}$ be the ith *internal path* $(m_i \sim m_i{+}1 \sim \cdots \sim m_{i+1})$ and $k_i = m_{i+1} - m_i - 1$ be the number of internal vertices on $P^{(i)}$. In general, an *internal path* in G is a path $v_0 \sim v_1 \sim \cdots \sim v_s$ such that $d(v_0) > 2$, $d(v_s) > 2$, and $d(v_i) = 2$, whenever $0 < i < s$. An internal path is *closed* if $v_0 = v_s$.

Van Dam and Kooij [3] asked an interesting question *"which connected graph of order n with a given diameter D has minimal spectral radius*?". The *diameter* of a connected graph is the maximum distance among all pairs of its vertices. They [3] solved this problem explicitly for graphs with diameter

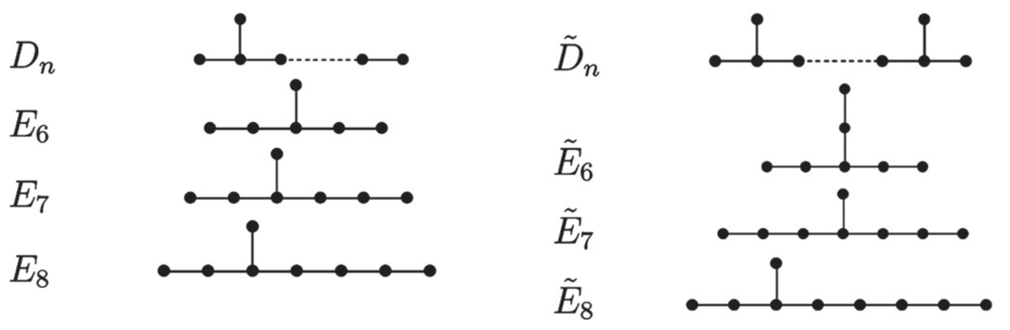

Fig. 1. Dynkin Diagrams.

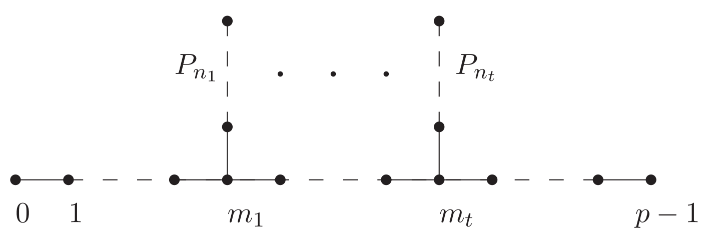

Fig. 2. $P^{m_1,m_2,\ldots,m_t}_{n_1,n_2,\ldots,n_t,p}$

$D \in \{1, 2, \lfloor n/2 \rfloor, n-3, n-2, n-1\}$. The cases $D = 1$ and $D = n-1$ are trivial. A *minimizer* graph, denoted by $G^{min}_{n,D}$, is a graph that has the minimal spectral radius among all the graphs of order n and diameter D. Van Dam and Kooij [3] proved that $G^{min}_{n,2}$ is either a star or a Moore graph; $G^{min}_{n,\lfloor n/2 \rfloor}$ is the cycle C_n; $G^{min}_{n,n-2}$ is the tree $P^1_{1,n-1}$; $G^{min}_{n,n-3}$ is the tree $P^{1,n-4}_{1,1,n-2}$. They conjectured $G^{min}_{n,n-e} = P^{\lfloor \frac{e-1}{2} \rfloor, n-e-\lceil \frac{e-1}{2} \rceil}_{\lfloor \frac{e-1}{2} \rfloor, \lceil \frac{e-1}{2} \rceil, n-e+1}$ for any constant $e \geqslant 1$ and n large enough.

The case $e = 4$ was proved by Yuan et al. [5], and also independently by Cioabă et al. [2]. Cioabă et al. actually proved more results: they settled the case $e = 5$ and disproved the case $e \geqslant 6$. (The case $e \geqslant 6$ was also disproved independently by Sun [11].) Cioabă et al. [2] proved the following theorem.

Theorem 5.2 of [2] *For $e \geq 6$, $\rho(G^{min}_{n,n-e}) \to \sqrt{2+\sqrt{5}}$ as $n \to \infty$. Moreover $G^{min}_{n,n-e}$ is contained in one of the following three families of graphs*

$$\mathcal{P}_{n,e} = \left\{ P^{2,m_2,\ldots,m_{e-4},n-e-2}_{2,1,\ldots,1,2,n-e+1} \mid 2 < m_2 < \cdots < m_{e-4} < n-e-2 \right\},$$
$$\mathcal{P}'_{n,e} = \left\{ P^{2,m_2,\ldots,m_{e-3},n-e-1}_{2,1,\ldots,1,1,n-e+1} \mid 2 < m_2 < \cdots < m_{e-3} < n-e-1 \right\},$$
$$\mathcal{P}''_{n,e} = \left\{ P^{1,m_2,\ldots,m_{e-2},n-e-1}_{1,1,\ldots,1,1,n-e+1} \mid 1 < m_2 < \cdots < m_{e-2} < n-e-1 \right\}.$$

Cioabă et al. [2] made three conjectures.

Conjecture 1 [2, 5.3]. *For fixed $e \geqslant 5$, a minimizer graph with n vertices and diameter $D = n-e$ is in the family $\mathcal{P}_{n,e}$, for n large enough.*

Conjecture 2 [2, 5.4]. *The graph $P^{2,\lceil \frac{D-1}{2} \rceil, D-2}_{2,1,2,n-5}$ is the unique minimizer graph with n vertices and diameter $D = n-6$, for n large enough.*

Conjecture 3 [2, 5.5]. *The graph $P^{2,\lfloor \frac{D+2}{3} \rfloor, D-\lfloor \frac{D+2}{3} \rfloor, D-2}_{2,1,1,2,n-6}$ is the unique minimizer graph with n vertices and diameter $D = n-7$, for n large enough.*[3]

In this paper, we settle these three conjectures positively.

Note that graphs in each family can be determined by the lengths of internal paths (see Fig. 3). The parameters k_i's and m_i's are related as follows. In the first family $\mathcal{P}_{n,e}$, $T_{(k_1,k_2,\ldots,k_{e-4})} = P^{2,m_2,\ldots,m_{e-4},n-e-2}_{2,1,\ldots,1,2,n-e+1}$ if $k_i = m_{i+1} - m_i - 1$ for $1 \leqslant i \leqslant e-4$, where $m_1 = 2$ and $m_{e-3} = n-e-2$. In the second family $\mathcal{P}'_{n,e}$, $T'_{(k_1,k_2,\ldots,k_{e-3})} = P^{2,m_2,\ldots,m_{e-3},n-e-1}_{2,1,\ldots,1,1,n-e+1}$ if $k_i = m_{i+1} - m_i - 1$ for $1 \leqslant i \leqslant e-3$, where $m_1 = 2$ and $m_{e-2} = n-e-1$. In the third family $\mathcal{P}''_{n,e}$, $T''_{(k_1,k_2,\ldots,k_{e-2})} = P^{1,m_2,\ldots,m_{e-2},n-e-1}_{1,1,\ldots,1,1,n-e+1}$ if $k_i = m_{i+1} - m_i - 1$ for $1 \leqslant i \leqslant e-2$, where $m_1 = 1$ and $m_{e-1} = n-e-1$. In all three cases, the summation of all k_i's is always equal to $n-2e$.

We have the following theorem.

Theorem 1.1. *For any $e \geq 6$ and sufficiently large n, $G^{min}_{n,n-e}$ must be a tree $T_{(k_1,k_2,\ldots,k_{e-4})}$ in $\mathcal{P}_{n,e}$ satisfying*

1. $\lfloor s \rfloor - 1 \leqslant k_j \leqslant \lfloor s \rfloor \leqslant k_i \leqslant \lceil s \rceil + 1$ *for $2 \leqslant i \leqslant e-5$ and $j = 1, e-4$, where $s = \frac{n-6}{e-4} - 2$.*
2. $0 \leq k_i - k_j \leq 2$ *for $2 \leq i \leq e-5$ and $j = 1, e-4$.*
3. $|k_i - k_j| \leq 1$ *for $2 \leq i, j \leq e-5$.*

In particular, if $n-6$ is divisible by $e-4$, then $G^{min}_{n,n-e} = T_{(s-1,s,\ldots,s,s-1)}$.

[3] Conjecture 5.5 of [2] contains a typo: "…$P^{2,\lfloor \frac{D-2}{3} \rfloor, D-\lfloor \frac{D-2}{3} \rfloor, D-2}_{2,1,1,2,n-6}$…".

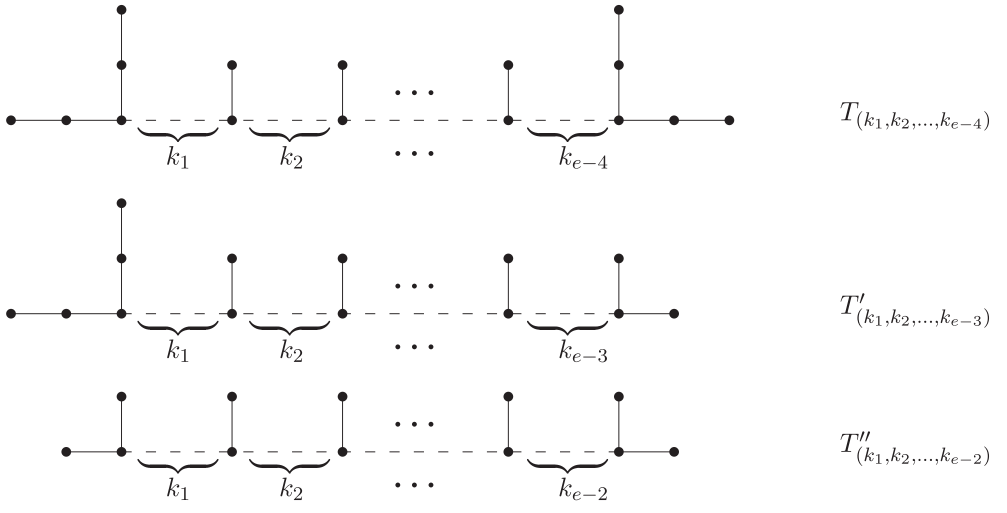

Fig. 3. The three families of graphs: $\mathcal{P}_{n,e}$, $\mathcal{P}'_{n,e}$,$\mathcal{P}''_{n,e}$.

Here we completely determine the $G^{min}_{n,n-e}$ for $e = 6, 7, 8$ and settle the Conjectures 2 and 3 positively.

Theorem 1.2. *For $e = 6$ and n large enough, $G^{min}_{n,n-e}$ is unique up to a graph isomorphism.*

1. *If $n = 2k + 12$, then $G^{min}_{n,n-6} = T_{(k,k)}$.*
2. *If $n = 2k + 13$, then $G^{min}_{n,n-6} = T_{(k,k+1)}$.*

Theorem 1.3. *For $e = 7$ and n large enough, $G^{min}_{n,n-e}$ is unique up to a graph isomorphism.*

1. *If $n = 3k + 14$, then $G^{min}_{n,n-7} = T_{(k,k,k)}$.*
2. *If $n = 3k + 15$, then $G^{min}_{n,n-7} = T_{(k,k+1,k)}$.*
3. *If $n = 3k + 16$, then $G^{min}_{n,n-7} = T_{(k,k+2,k)}$.*

Theorem 1.4. *For $e = 8$ and n large enough, $G^{min}_{n,n-e}$ is determined up to a graph isomorphism as follows.*

1. *If $n = 3k + 16$, then $G^{min}_{n,n-8} = T_{(k,k,k,k)}$, $T_{(k,k,k+1,k-1)}$, or $T_{(k-1,k+1,k+1,k-1)}$; all three trees have the same spectral radius.*
2. *If $n = 3k + 17$, then $G^{min}_{n,n-8} = T_{(k,k+1,k,k)}$.*
3. *If $n = 3k + 18$, then $G^{min}_{n,n-8} = T_{(k,k+1,k+1,k)}$.*
4. *If $n = 3k + 19$, then $G^{min}_{n,n-8} = T_{(k,k+1,k+2,k)}$.*

For $e = 6$, Theorem 1.2 is an easy corollary of Theorem 1.1. Theorem 1.3 and Theorem 1.4 show that the bounds on k_i's in Theorem 1.1 are best possible.

The remaining of the paper is organized as follows. In Section 2, we prove some useful lemmas. The proof of Theorem 1.1 is presented in Section 3 and the proof of Theorem 1.3 and 1.4 are given in Section 4.

2. Basic notations and lemmas

2.1. Preliminary results

For any vertex v in a graph G, let $N(v)$ be the neighborhood of v. Let $G - v$ be the remaining graph of G after deleting the vertex v (and all edges incident to v). Similarly, $G - u - v$ is the remaining graph of G after deleting two vertices u, v. Here are some basic facts found in literature [14,6,7,9,11], which will be used later.

Lemma 2.1 [14]. *Suppose that G is a connected graph. If v is not in any cycle of G, then $\phi_G = \lambda\phi_{G-v} - \sum_{w\in N(v)} \phi_{G-w-v}$. If $e = uv$ is a cut edge of G, then $\phi_G = \phi_{G-e} - \phi_{G-u-v}$.*

Lemma 2.2. *Let G_1 and G_2 be two graphs, then the following statements hold:*

1. *[6] If G_1 is connected and G_2 is a proper subgraph of G_1, then $\rho(G_1) > \rho(G_2)$.*
2. *[15] If G_1 is connected and G_2 is a spanning proper subgraph of G_1, then $\rho(G_1) > \rho(G_2)$ and $\phi_{G_2}(\lambda) > \phi_{G_1}(\lambda)$ for all $\lambda \geq \rho(G_1)$.*
3. *If $\phi_{G_2}(\lambda) > \phi_{G_1}(\lambda)$ for all $\lambda \geq \rho(G_1)$, then $\rho(G_2) < \rho(G_1)$.*
4. *If $\phi_{G_1}(\rho(G_2)) < 0$,then $\rho(G_1) > \rho(G_2)$.*

Lemma 2.3 [11]. *Let G_1 and G_2 be two (possibly single-vertex) connected graphs with $a \in V(G_1)$ and $b \in V(G_2)$, and let H_1 and H_2 be two graphs shown in Fig. 4. Then $\rho(H_1) = \rho(H_2)$.*

Proof. Applying Lemma 2.1 to H_1 with the cut edge v_1v_2, we get

$$\begin{aligned}\phi(H_1) &= \phi(G_1{-}\bullet)\phi(G_1{-}\bullet{-}\bullet{-}G_2) - \phi(G_1)\phi(G_2)\phi(G_1{-}\bullet)\\ &= \phi(G_1{-}\bullet)\left(\phi(G_1{-}\bullet{-}\bullet{-}G_2) - \phi(G_1)\phi(G_2)\right).\end{aligned}$$

Since G_1 and G_2 are connected, H_1 is connected. Note $G_1{-}\bullet$ is a subgraph of H_1. By Lemma 2.2 item 1, we have $\rho(H_1) > \rho(G_1{-}\bullet)$. Thus, $\rho(H_1)$ is the largest root of

$$\phi(G_1{-}\bullet{-}\bullet{-}G_2) - \phi(G_1)\phi(G_2). \tag{1}$$

Note the expression (1) is symmetric on G_1 and G_2. By symmetry, $\rho(H_2)$ is also the largest root of the expression (1). Therefore $\rho(H_1) = \rho(H_2)$. The proof of the lemma is finished. □

Lemma 2.4 [7]. *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 once, i.e., adding a new vertex w and edges wu, wv in $G - uv$. Then the following two properties 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 $G \neq P_{1,1,n}^{1,n-2}$, then $\rho(G_{u,v}) < \rho(G)$.*

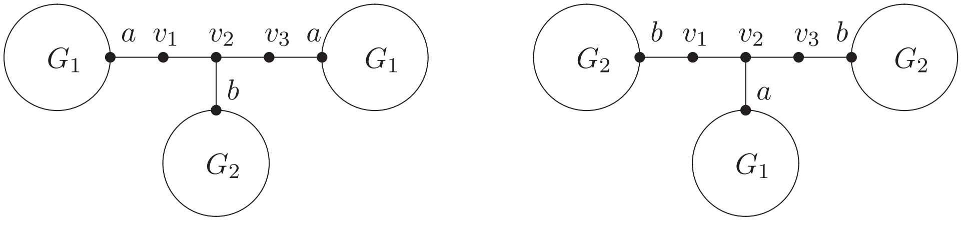

Fig. 4. The graphs H_1 and H_2.

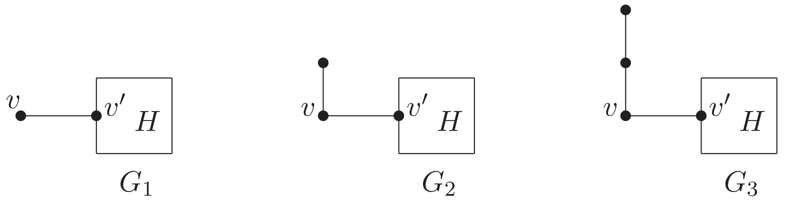

Fig. 5. For $i = 1, 2, 3$, three graphs (G_i, v) are constructed from (H, v').

Theorem 2.1 (Cauchy Interlace Theorem [16])**.** *Let A be a Hermitian matrix of order n, and let B be a principal submatrix of A of order $n-1$. If $\lambda_n \leqslant \lambda_{n-1} \leqslant \cdots \leqslant \lambda_1$ lists the eigenvalues of A and $\mu_{n-1} \leqslant \mu_{n-2} \leqslant \cdots \leqslant \mu_1$ lists the eigenvalues of B, then*

$$\lambda_n \leqslant \mu_{n-1} \leqslant \lambda_{n-1} \leqslant \cdots \leqslant \lambda_2 \leqslant \mu_1 \leqslant \lambda_1.$$

Applying Cauchy Interlace Theorem to the adjacency matrices of graphs, we have the following corollary.

Corollary 2.1. *Suppose G is a connected graph. Let $\lambda_2(G)$ be the second largest eigenvalue of G. For any vertex v, we have*

$$\lambda_2(G) < \rho(G-v) < \rho(G).$$

2.2. Our approach

A *rooted graph* (G, v) is a graph G together with a designated vertex v as a root. For $i = 1, 2, 3$ and a given rooted graph (H, v'), we get a new rooted graph (G_i, v) from H by attaching a path P_i to v' and changing the root from v' to v as shown in Fig. 5.

Note that any tree in the three families $\mathcal{P}_{n,e}, \mathcal{P}'_{n,e}, \mathcal{P}''_{n,e}$ can be built up from a single vertex through a sequence of three operations above. Applying Lemma 2.1, we observe that the pair $(\phi_{G_i}, \phi_{G_i-v})$ linearly depends on $(\phi_H, \phi_{H-v'})$ with coefficients in $\mathbb{Z}[\lambda]$. We can choose proper base to diagonalize the operation from (H, v') to (G_i, v).

Let λ_0 be the constant $\sqrt{2+\sqrt{5}} = 2.058\ldots$. In this paper, we consider only the range $\lambda \geqslant \lambda_0$. Let x_1 and x_2 be two roots of the equation $x^2 - \lambda x + 1 = 0$. We have

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

and

$$x_1 + x_2 = \lambda, \quad x_1 x_2 = 1. \tag{2}$$

For any vertex v in a graph G, we define two functions (of λ) $p_{(G,v)}$ and $q_{(G,v)}$ satisfying

$$\phi_G = p_{(G,v)} + q_{(G,v)},$$
$$\phi_{G-v} = x_2 p_{(G,v)} + x_1 q_{(G,v)}.$$

This definition can be written in the following matrix form:

$$\begin{pmatrix} \phi_G \\ \phi_{G-v} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix} \begin{pmatrix} p_{(G,v)} \\ q_{(G,v)} \end{pmatrix}. \tag{3}$$

Using Eq. (2), we can solve $p_{(G,v)}$ and $q_{(G,v)}$ and get

$$\begin{pmatrix} p_{(G,v)} \\ q_{(G,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1 & 1 \\ x_2 & -1 \end{pmatrix} \begin{pmatrix} \phi_G \\ \phi_{G-v} \end{pmatrix}. \tag{4}$$

For example, let v be the center of the odd path P_{2k+1}. We have

$$\begin{pmatrix} p_{(P_1,v)} \\ q_{(P_1,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1^2 \\ x_2^2 \end{pmatrix}, \tag{5}$$

$$\begin{pmatrix} p_{(P_3,v)} \\ q_{(P_3,v)} \end{pmatrix} = \lambda \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}, \tag{6}$$

$$\begin{pmatrix} p_{(P_5,v)} \\ q_{(P_5,v)} \end{pmatrix} = \frac{\lambda^2 - 1}{x_2 - x_1} \begin{pmatrix} (\lambda - x_1^3)x_1 \\ (x_2^3 - \lambda)x_2 \end{pmatrix}. \tag{7}$$

We have the following lemma.

Lemma 2.5. *For any tree G and any vertex v, we have*

$$\lim_{\lambda \to +\infty} q_{(G,v)}(\lambda) = +\infty. \tag{8}$$

Proof. From Lemma 2.1, we have

$$\phi_G = \lambda \phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v}.$$

By Eq. (4), we get

$$\begin{aligned} q_{(G,v)} &= \frac{1}{x_2 - x_1}(x_2\phi_G - \phi_{G-v}) \\ &= \frac{1}{x_2 - x_1}\left(x_2\left(\lambda\phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v}\right) - \phi_{G-v}\right) \\ &= \frac{1}{x_2 - x_1}\left((\lambda x_2 - 1)\phi_{G-v} - x_2 \sum_{w \in N(v)} \phi_{G-w-v}\right) \\ &= \frac{x_2}{x_2 - x_1}\left(x_2\phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v}\right). \end{aligned}$$

Note that ϕ_{G-v} is a polynomial of degree $n-1$ with highest coefficient 1 while ϕ_{G-w-v} is a polynomial of degree $n-2$ with highest coefficient 1. Since $x_2 > 1 > x_1$, we have $x_2\phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v}$ goes to infinity as λ approaches infinity. □

Lemma 2.6. *Let G_1, G_2, G_3 be the graphs shown in Fig. 5. Then the following equations hold:*

1. $$\begin{pmatrix} p_{(G_1,v)} \\ q_{(G_1,v)} \end{pmatrix} = \begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}.$$

2. $\begin{pmatrix} p_{(G_2,v)} \\ q_{(G_2,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} \lambda - x_1^3 & x_1 \\ -x_2 & x_2^3 - \lambda \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}$.

3. $\begin{pmatrix} p_{(G_3,v)} \\ q_{(G_3,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1^4 + \lambda^2 - 1 & \lambda x_1 \\ -\lambda x_2 & x_2^4 - \lambda^2 + 1 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}$.

Proof. By Lemma 2.1, we have

$$\begin{pmatrix} \phi_{G_1} \\ \phi_{G_1 - v} \end{pmatrix} = \begin{pmatrix} \lambda & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \phi_H \\ \phi_{H-v'} \end{pmatrix}.$$

Combining it with Eqs. (3) and (4), we get

$$\begin{aligned} \begin{pmatrix} p_{(G_1,v)} \\ q_{(G_1,v)} \end{pmatrix} &= \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix}^{-1} \begin{pmatrix} \lambda & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix} \\ &= \frac{1}{x_2 - x_1} \begin{pmatrix} 2 - \lambda x_1 & x_1^2 - \lambda x_1 + 1 \\ -x_2^2 + \lambda x_2 - 1 & \lambda x_2 - 2 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix} \\ &= \begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}. \end{aligned}$$

The proofs of items 2 and 3 are similar as that of item 1. □

We denote the three matrices by A, B, and C. Namely,

$$A = \begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix}, \quad B = \frac{1}{x_2 - x_1} \begin{pmatrix} \lambda - x_1^3 & x_1 \\ -x_2 & x_2^3 - \lambda \end{pmatrix},$$
$$C = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1^4 + \lambda^2 - 1 & \lambda x_1 \\ -\lambda x_2 & x_2^4 - \lambda^2 + 1 \end{pmatrix}.$$

The diagonal elements of B are very useful parameters. To simplify our notations later, we define two parameters d_1 and d_2 as follows:

$$d_1 = \lambda - x_1^3, \tag{9}$$
$$d_2 = x_2^3 - \lambda. \tag{10}$$

Note that $d_2 = 0$ if $\lambda = \lambda_0$. The Eq. (7) can be written as

$$\begin{pmatrix} p_{(P_5,v)} \\ q_{(P_5,v)} \end{pmatrix} = \frac{\lambda^2 - 1}{x_2 - x_1} \begin{pmatrix} d_1 x_1 \\ d_2 x_2 \end{pmatrix}. \tag{11}$$

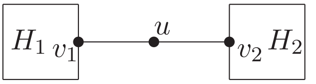

Fig. 6. The graph $(H_1, v_1) \cdot P_1 \cdot (H_2, v_2)$.

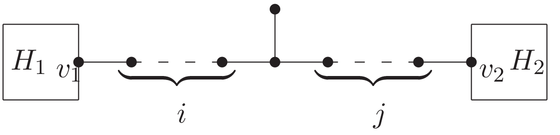

Fig. 7. The graph $G_{i,j}$.

From the definitions of d_1 and d_2, we can derive the following identity:

$$d_1x_2 - d_2x_1 = 2. \tag{12}$$

Given two rooted graphs (H_1, v_1) and (H_2, v_2), we define some new graphs. Denote by $(H_1, v_1) \cdot P_i$, the graph consisting of the graph H_1 and a path P_i linking one of its ends at the vertex v_1. Similarly denote by $(H_1, v_1) \cdot P_i \cdot (H_2, v_2)$ the graph consisting of graphs H_1, H_2 and a path P_i linking the two ends at v_1, v_2 respectively.

Lemma 2.7. $\phi_{(H_1,v_1)\cdot P_1\cdot(H_2,v_2)}(\lambda) = (x_2 - x_1)(q_{(H_1,v_1)}q_{(H_2,v_2)} - p_{(H_1,v_1)}p_{(H_2,v_2)})$.

Proof. By Lemmas 2.1 and Eq. (3), we have

$$\begin{aligned}
&\phi_{(H_1,v_1)\cdot P_1\cdot(H_2,v_2)}(\lambda)\\
&\quad= \lambda\phi_{H_1}\phi_{H_2} - \phi_{H_1-v_1}\phi_{H_2} - \phi_{H_2-v_2}\phi_{H_1}\\
&\quad= (x_1 + x_2)(p_{(H_1,v_1)} + q_{(H_1,v_1)})(p_{(H_2,v_2)} + q_{(H_2,v_2)}) - (p_{(H_1,v_1)}x_2 + q_{(H_1,v_1)}x_1)\\
&\qquad(p_{(H_2,v_2)} + q_{(H_2,v_2)}) - (p_{(H_1,v_1)} + q_{(H_1,v_1)})(p_{(H_2,v_2)}x_2 + q_{(H_2,v_2)}x_1)\\
&\quad= (p_{(H_2,v_2)} + q_{(H_2,v_2)})(p_{(H_1,v_1)}x_1 + q_{(H_1,v_1)}x_2) - (p_{(H_1,v_1)} + q_{(H_1,v_1)})(p_{(H_2,v_2)}x_2 + q_{(H_2,v_2)}x_1)\\
&\quad= p_{(H_2,v_2)}p_{(H_1,v_1)}x_1 + q_{(H_2,v_2)}q_{(H_1,v_1)}x_2 - p_{(H_2,v_2)}p_{(H_1,v_1)}x_2 - q_{(H_2,v_2)}q_{(H_1,v_1)}x_1\\
&\quad= (x_2 - x_1)(q_{(H_1,v_1)}q_{(H_2,v_2)} - p_{(H_1,v_1)}p_{(H_2,v_2)}). \quad \square
\end{aligned}$$

Lemma 2.8. *Let $G_{i,j}$ be the graph shown in Fig. 7 where i, j are the numbers of included vertices. Then*

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

Proof. By Lemma 2.1, we have

$$\begin{aligned}
\phi_{G_{i,j}} &= \lambda\phi_{(H_1,v_1)\cdot P_{i+j+1}\cdot(H_2,v_2)} - \phi_{(H_1,v_1)\cdot P_i}\phi_{(H_2,v_2)\cdot P_j},\\
\phi_{G_{i+1,j-1}} &= \lambda\phi_{(H_1,v_1)\cdot P_{i+j+1}\cdot(H_2,v_2)} - \phi_{(H_1,v_1)\cdot P_{i+1}}\phi_{(H_2,v_2)\cdot P_{j-1}}.
\end{aligned}$$

Thus, we get

$$\begin{aligned}\phi_{G_{i,j}} - \phi_{G_{i+1,j-1}} &= \phi_{(H_1,v_1)\cdot P_{i+1}}\phi_{(H_2,v_2)\cdot P_{j-1}} - \phi_{(H_1,v_1)\cdot P_i}\phi_{(H_2,v_2)\cdot P_j} \\ &= \left(p_{(H_1,v_1)}x_1^{i+1} + q_{(H_1,v_1)}x_2^{i+1}\right)\left(p_{(H_2,v_2)}x_1^{j-1} + q_{(H_2,v_2)}x_2^{j-1}\right) \\ &\quad - \left(p_{(H_1,v_1)}x_1^{i} + q_{(H_1,v_1)}x_2^{i}\right)\left(p_{(H_2,v_2)}x_1^{j} + q_{(H_2,v_2)}x_2^{j}\right) \\ &= p_{(H_1,v_1)}q_{(H_2,v_2)}\left(x_1^{i+1}x_2^{j-1} - x_1^i x_2^j\right) + q_{(H_1,v_1)}p_{(H_2,v_2)}\left(x_1^{j-1}x_2^{i+1} - x_1^j x_2^i\right) \\ &= x_1^i x_2^i\left[p_{(H_1,v_1)}q_{(H_2,v_2)}(x_1x_2^{j-i-1} - x_2^{j-i}) + q_{(H_1,v_1)}p_{(H_2,v_2)}(x_1^{j-i-1}x_2 - x_1^{j-i})\right] \\ &= (x_1 - x_2)\left(p_{(H_1,v_1)}q_{(H_2,v_2)}x_2^{j-i-1} - q_{(H_1,v_1)}p_{(H_2,v_2)}x_1^{j-i-1}\right).\end{aligned}$$

The proof is completed. □

Lemma 2.9. *Suppose G_1 and G_2 are two connected graphs satisfying $G_1 - u_1 = G_2 - u_2$ for some vertices $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$. If $\phi_{G_2}(\rho(G_1)) > 0$, then $\rho(G_1) > \rho(G_2)$.*

Proof. Let $G = G_1 - u_1 = G_2 - u_2$. By Corollary 2.1, we have

$$\rho(G_i) > \rho(G) \geqslant \lambda_2(G_i) \quad \text{for } i = 1, 2.$$

Here $\lambda_2(G_i)$ is the second largest eigenvalue of G_i. We have $\rho(G_1) > \lambda_2(G_2)$.

Since $\rho(G_2)$ is a simple root and $\lim_{\lambda\to\infty} \phi_{G_2}(\lambda) = +\infty$, we have

$$\phi_{G_2}(\lambda) < 0 \quad \text{for } \lambda \in (\lambda_2(G_2), \rho(G_2)).$$

Since $\phi_{G_2}(\rho(G_1)) > 0$ and $\rho(G_1) > \lambda_2(G_2)$, we must have $\rho(G_1) > \rho(G_2)$. □

2.3. A special tree $T_{(k-1,k,\ldots,k,k-1)}$

The tree $T_{(k-1,k,\ldots,k,k-1)}$ ($\in \mathcal{P}_{n,e}$) plays an important role in this paper. We have the following lemma.

Lemma 2.10. *The spectral radius of the tree $T_{(k-1,k,\ldots,k,k-1)}$ is the unique root ρ_k of the equation $d_2 = \frac{2x_1^k}{1-x_1^{k+1}}$ in the interval $\left(\sqrt{2+\sqrt{5}}, \infty\right)$.*

Remark 1. The following equations are equivalent to one another.

$$\begin{aligned}&d_2 = \frac{2x_1^k}{1 - x_1^{k+1}}, \\ &d_2x_2^k - d_1x_1^k = 2, \\ &d_2 = d_1x_1^{k-1}, \\ &d_2x_2^{\frac{k-1}{2}} = d_1x_1^{\frac{k-1}{2}}, \\ &d_2 = 2x_1^k + d_1x_1^{2k}.\end{aligned}$$

If "=" is replaced by "⩾", then these inequalities are still equivalent to each other. These equivalences can be proved by Eq. (12). The details are omitted.

Remark 2. For any $k \geqslant 4$, we have $\rho_k \leq \rho_4 < \frac{3}{2}\sqrt{2}$. For any $e \geqslant 6$ and $n \geqslant (k+2)(e-4)+6$, we can obtain a tree T on n vertices and diameter $n-e$ by subdividing some edges on internal paths of

$T_{(k-1,k,\ldots,k,k-1)}$. By Lemma 2.4, we have

$$\rho(T) \leqslant \rho(T_{(k-1,k,\ldots,k,k-1)}) = \rho_k < \frac{3}{2}\sqrt{2}.$$

In particular, for $e \geqslant 6$ and $n \geqslant (k+2)(e-4)+6 = |T_{(k-1,k,\ldots,k,k-1)}|$, we have $\rho(G^{min}_{n,n-e}) < \frac{3}{2}\sqrt{2}$. In the set of graphs with spectral radius at most $\sqrt{2+\sqrt{5}}$ (see [1]), there is no graph with diameter $n-e$ for $e \geqslant 6$. Thus, $\rho(G^{min}_{n,n-e}) \geqslant \sqrt{2+\sqrt{5}}$.

Proof of Lemma 2.10. Let $G = T_{(k-1,k,\ldots,k,k-1)}$ and v be the leftmost vertex. Note that G can be built up from a single vertex with a series of three operations as specified in Lemma 2.6. We have

$$\begin{aligned}
\phi_G &= (1,1)\begin{pmatrix} p_{(T_{(k-1,k,\ldots,k,k-1)},v)} \\ q_{(T_{(k-1,k,\ldots,k,k-1)},v)} \end{pmatrix} \\
&= (1,1)A^2CA^{k-1}BA^k\ldots BA^{k-1}CA\begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix}^{-1}\begin{pmatrix} \lambda \\ 1 \end{pmatrix} \\
&= \frac{(\lambda^2-1)^2}{x_2-x_1}(-d_1,d_2)A^{k-1}BA^k\ldots BA^{k-1}\begin{pmatrix} d_1x_1 \\ d_2x_2 \end{pmatrix} \\
&= \frac{(\lambda^2-1)^2}{x_2-x_1}(-d_1,d_2)A^{k-1}BA^k\ldots BA^k\begin{pmatrix} d_1 \\ d_2 \end{pmatrix}.
\end{aligned}$$

Let $l = \frac{k-1}{2}$; l does not have to be an integer. Define $A^l = \begin{pmatrix} x_1^l & 0 \\ 0 & x_2^l \end{pmatrix}$. We can write ϕ_G as

$$\phi_G = \frac{(\lambda^2-1)^2}{x_2-x_1}(-d_1x_1^l, d_2x_2^l)(A^lBA^{l+1})^{r-1}\begin{pmatrix} d_1x_1^l \\ d_2x_2^l \end{pmatrix}. \tag{13}$$

It is easy to calculate

$$A^lBA^{l+1} = \frac{1}{x_2-x_1}\begin{pmatrix} d_1x_1^k & 1 \\ -1 & d_2x_2^k \end{pmatrix}. \tag{14}$$

Now we prove that ρ_k is a root of ϕ_G. At $\lambda = \rho_k$, we have $d_1x_1^l = d_2x_2^l$ and $d_1x_1^k + 1 = d_2x_2^k - 1$. Thus

$$\begin{aligned}
(A^lBA^{l+1})\begin{pmatrix} 1 \\ 1 \end{pmatrix} &= \frac{1}{x_2-x_1}\begin{pmatrix} d_1x_1^k & 1 \\ -1 & d_2x_2^k \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\
&= \frac{d_1x_1^k+1}{x_2-x_1}\begin{pmatrix} 1 \\ 1 \end{pmatrix}.
\end{aligned}$$

We have

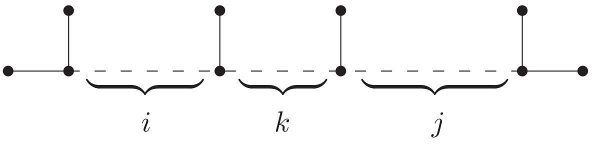

Fig. 8. The graphs $T''_{(i,k,j)}$.

$$\begin{aligned}\phi_G(\rho_k) &= \frac{(\lambda^2-1)^2}{x_2-x_1}(-d_1x_1^l, d_2x_2^l)(A^lBA^{l+1})^{r-1}\begin{pmatrix} d_1x_1^l \\ d_2x_2^l \end{pmatrix} \\ &= \frac{(\lambda^2-1)^2}{(x_2-x_1)^r}(d_1x_1^k+1)^{r-1}d_1^2x_1^{k-1}(-1,1)\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ &= 0.\end{aligned}$$

It remains to prove $\phi_G(\lambda) > 0$ for any $\lambda > \rho_k$. When $\lambda > \rho_k$, we have $d_2x_2^k - 1 > d_1x_1^k + 1$ (and $d_2x_2^l > d_1x_1^l$). It is easy to check A^lBA^{l+1} maps the region $\{(z_1, z_2) : z_2 \geqslant z_1 > 0\}$ to $\{(z_1, z_2) : z_2 > z_1 > 0\}$. By induction on r, $(A^lBA^{l+1})^{r-1}$ maps the region $\{(z_1, z_2) : z_2 \geqslant z_1 > 0\}$ to $\{(z_1, z_2) : z_2 > z_1 > 0\}$. Let

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = (A^lBA^{l+1})^{r-1}\begin{pmatrix} d_1x_1^l \\ d_2x_2^l \end{pmatrix}.$$

Since $d_2x_2^l > d_1x_1^l > 0$, we have $z_2 > z_1 > 0$. From Eq. (13), we get

$$\begin{aligned}\phi_G &= \frac{(\lambda^2-1)^2}{x_2-x_1}(-d_1x_1^l, d_2x_2^l)(A^lBA^{l+1})^{r-1}\begin{pmatrix} d_1x_1^l \\ d_2x_2^l \end{pmatrix} \\ &= \frac{(\lambda^2-1)^2}{x_2-x_1}(-d_1x_1^l, d_2x_2^l)\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \\ &= \frac{(\lambda^2-1)^2}{x_2-x_1}(d_2x_2^lz_2 - d_1x_1^lz_1) \\ &> 0.\end{aligned}$$

The proof of the lemma is finished. □

2.4. Limit points of some graphs

Using the tools developed in the previous section, we can compute the limit point of the spectral radius of some graphs.

Lemma 2.11. *Let $T''_{(i,k,j)}$ be the tree shown in Fig. 8 and ρ''_k be the unique root of $d_2 = x_1^k$ in the interval $\left(\sqrt{2+\sqrt{5}}, +\infty\right)$. Then $\lim_{i,j\to\infty} \rho(T''_{(i,k,j)}) = \rho''_k$.*

Proof. By Lemma 2.4, we have

$$\rho(T''_{(i,k,i)}) \geqslant \rho(T''_{(i,k,j)}) \geqslant \rho(T''_{(j,k,j)}) \quad \text{if } i \leqslant j.$$

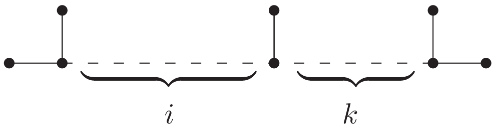

Fig. 9. The graph $T''(k, i)$.

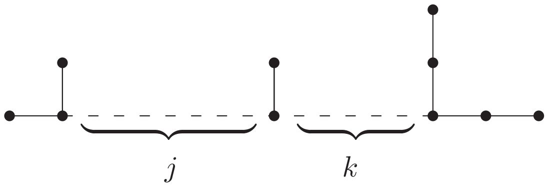

Fig. 10. The graph $T'(k, j)$.

It suffices to show $\lim_{l\to\infty} \rho(T''_{(l,k,l)}) = \rho''_k$. Let v be the leftmost vertex of $T''_{(l,k,l)}$. A simple calculation shows

$$\begin{aligned}\phi_{T''_{(l,k,l)}} &= (1, 1)\begin{pmatrix} p_{(T''_{(l,k,l)},v)} \\ q_{(T''_{(l,k,l)},v)} \end{pmatrix} \\ &= (1, 1)ABA^lBA^kBA^lB\begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix}^{-1}\begin{pmatrix} \lambda \\ 1 \end{pmatrix} \\ &= \frac{x_2^{2l-k+1}(d_2x_2 + x_1^2)^2}{(x_2 - x_1)^5}\Big[((d_2x_2^k)^2 - 1) - 2x_1^{2l-k+3}(d_1x_1^k + d_2x_2^k) \\ &\qquad -x_1^{2(2l-k+3)}((d_1x_1^k)^2 - 1)\Big].\end{aligned}$$

As l goes to infinity, $\lim_{l\to\infty} \rho(T''_{(l,k,l)})$ is the largest root of $(d_2x_2^k)^2 - 1 = 0$; namely $d_2 = x_1^k$. The proof is completed. □

We have the following corollary from Lemma 2.11.

Corollary 2.2. *Let $T''_{(k,i)}$ be the tree shown in Fig. 9. We have* $\lim_{i\to\infty} \rho(T''_{(k,i)}) = \rho''_{2k+3}$.

Proof. By Lemma 2.3, we have $\rho(T''_{(k,i)}) = \rho(T''_{(i,2k+3,i)})$. Thus $\lim_{i\to\infty} \rho(T''_{(k,i)}) = \lim_{i\to\infty} \rho(T''_{(i,2k+3,i)}) = \rho''_{2k+3}$. □

Lemma 2.12. *Let $T'_{(k,j)}$ be the tree shown in Fig. 10 and ρ'_k be the unique root of $d_2 = d_1^{\frac{1}{2}}x_1^{k+\frac{1}{2}}$ in the interval $\left(\sqrt{2+\sqrt{5}}, +\infty\right)$. Then $\lim_{j\to\infty} \rho(T'_{(k,j)}) = \rho'_k$.*

Proof. Similarly, we have

$$\begin{aligned}\phi_{T'_{(k,j)}} &= (1,1)\begin{pmatrix} p_{(T'_{(k,j)},v)} \\ q_{(T'_{(k,j)},v)} \end{pmatrix} \\ &= (1,1)ABA^jBA^kCA\begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix}^{-1}\begin{pmatrix} \lambda \\ 1 \end{pmatrix} \\ &= \frac{x_2^{j+k+1}(\lambda^2-1)(d_2x_2+x_1^3)}{(x_2-x_1)^3}\left(d_2^2 - d_1x_1^{2k+1} - d_2x_1^{2j+3} - d_1^2x_1^{2j+2k+4}\right).\end{aligned}$$

As j goes to infinity, $\lim_{l\to\infty}\rho(T'_{(k,j)})$ is the largest root of $d_2^2 = d_1x_1^{2k+1}$; namely $d_2 = d_1^{\frac{1}{2}}x_1^{k+\frac{1}{2}}$. The proof is completed. □

2.5. Comparison of ρ_k, ρ'_k, and ρ''_k

Observe that ρ_k, ρ'_k, and ρ''_k satisfy similar equations. Since $1 < \sqrt{d_1x_1} < \frac{2}{1-x_1^{k+1}}$, we have

$$\rho''_k \leqslant \rho'_k \leqslant \rho_k.$$

For $\lambda \in [\lambda_0, \frac{3}{2}\sqrt{2}]$, x_2, d_2, and d_1x_1 are increasing while x_1 is decreasing. Using these facts, it is easy to check that for $k \geqslant 7$, ρ_k, ρ'_k, and ρ''_k are in the interval $(\lambda_0, \frac{3}{2}\sqrt{2})$.

We have the following lemma.

Lemma 2.13. *For $k \geqslant 7$, we have $\rho_k < \rho''_{k-4}$ and $\rho_k < \rho'_{k-3}$.*

Proof. Recall that ρ''_{k-4} is the root of $d_2 = x_1^{k-4}$ and ρ_k is the root of $d_2 = \frac{2x_1^k}{1-x_1^{k+1}}$. We need to show $2 < x_2^4(1-x_1^{k+1})$ for $\lambda \in [\lambda_0, \frac{3}{2}\sqrt{2}]$. For $k \geqslant 7$, we have

$$\begin{aligned}x_2^4(1-x_1^{k+1}) &\geqslant x_2^4 - x_1^4 \\ &\geqslant (x_2^4 - x_1^4)|_{\lambda_0} \\ &> 2.\end{aligned}$$

Note that ρ'_{k-3} is the root of $d_2 = \sqrt{d_1x_1}x_1^{k-3}$. It suffices to show $2 < \sqrt{d_1x_1}x_2^3(1-x_1^{k+1})$ for $\lambda \in [\lambda_0, \frac{3}{2}\sqrt{2}]$. We have

$$\begin{aligned}\sqrt{d_1x_1}x_2^3(1-x_1^{k+1}) &\geqslant \sqrt{d_1x_1}x_2^3(1-x_1^8) \\ &\geqslant \sqrt{d_1x_1}x_2^3(1-x_1^8)|_{\lambda_0} \\ &> 2.\end{aligned}$$

The proof is completed. □

3. Proof of Theorem 1.1

The proof of Theorem 1.1 can be naturally divided into two parts. In the first part, we prove that $G^{min}_{n,n-e} \in \mathcal{P}_{n,e}$. In the second part, we prove the other statements in Theorem 1.1.

3.1. Part 1

Let $\rho^{min}_{n,n-e} = \rho(G^{min}_{n,n-e})$ in the rest part of this paper. Now we prove the following theorem, which implies the first part of Theorem 1.1.

Theorem 3.1. *If $e \geqslant 6$ and $n \geqslant 10e^2 - 74e + 142$, then $G^{min}_{n,n-e} \in \mathcal{P}_{n,e}$.*

Proof. By Theorem 5.2 of [2] (see page 2825), it suffices to show $G^{min}_{n,n-e} \notin \mathcal{P}'_{n,e}$ and $G^{min}_{n,n-e} \notin \mathcal{P}''_{n,e}$.

Suppose $G^{min}_{n,n-e} = T'_{(k_1,k_2,\ldots,k_{e-3})} \in \mathcal{P}'_{n,e}$. Note that $T'_{(k_1,k_2,\ldots,k_{e-3})}$ contains sub-trees of type $T'_{(k_1,*)}$, $T''_{(k_{e-3},*)}$, and $T''_{(*,k_i,*)}$ for $2 \leqslant i \leqslant e-4$. By Lemma 2.4, Lemma 2.11, Corollary 2.2, and Lemma 2.12, we have

$$\rho^{min}_{n,n-e} > \rho'_{k_1},$$
$$\rho^{min}_{n,n-e} > \rho''_{2k_{e-3}+3},$$
$$\rho^{min}_{n,n-e} > \rho''_{k_i}, \quad \text{for } 2 \leqslant i \leqslant e-4.$$

Next, we show that at least one of $k_1, k_2, \ldots, k_{e-3}$ is small. Let $l_1 = \lceil \frac{n-3e+5}{e-3.5} \rceil$. We claim

$$k_1 \leq l_1 + 1 \quad \text{or} \quad k_{e-3} \leq \frac{l_1 - 3}{2} \quad \text{or} \quad \exists i \in \{2, 3, \ldots, e-4\}\ s.t.\ k_i \leqslant l_1.$$

Otherwise, we have

$$k_1 \geqslant l_1 + 2 \quad \text{and} \quad k_{e-3} \geqslant \frac{l_1 - 2}{2} \quad \text{and} \quad k_2, \ldots, k_{e-4} \geqslant l_1 + 1.$$

We get

$$n = \sum_{i=1}^{e-3} k_i + 2e \geqslant l_1 + 2 + \frac{l_1 - 2}{2} + (l_1 + 1)(e-5) + 2e = (e - 3.5)l_1 + 3e - 4 \geq n + 1.$$

Contradiction!

If $k_1 \leqslant l_1 + 1$, then we have $\rho^{min}_{n,n-e} > \rho'_{l_1+1} > \rho_{l_1+4}$; if $k_{e-3} \leqslant \frac{l_1-3}{2}$, then we have $\rho^{min}_{n,n-e} > \rho''_{2k_{e-3}+3} > \rho''_{l_1} > \rho_{l_1+4}$; if $k_i \leqslant l_1$ for some $i \in \{2, \ldots, e-4\}$, then we have $\rho^{min}_{n,n-e} > \rho''_{k_i} \geqslant \rho''_{l_1} > \rho_{l_1+4}$. In all cases, we have

$$\rho^{min}_{n,n-e} > \rho_{l_1+4}.$$

Let $k = \lfloor \frac{n-2e+2}{e-4} \rfloor$. There exists a tree $T \in \mathcal{P}_{n,e}$, which can be obtained by subdividing some edges on internal paths of $T_{(k-1,k,\ldots,k,k-1)}$. Since $n \geqslant 10e^2 - 74e + 142$, we have

$$l_1 + 4 = \left\lceil \frac{n - 3e + 5}{e - 3.5} \right\rceil + 4 \leqslant \left\lfloor \frac{n - 2e + 2}{e - 4} \right\rfloor = k.$$

We get

$$\rho^{min}_{n,n-e} > \rho_{l_1+4} \geqslant \rho(T_{(k-1,k,\ldots,k,k-1)}) \geqslant \rho(T).$$

Contradiction!

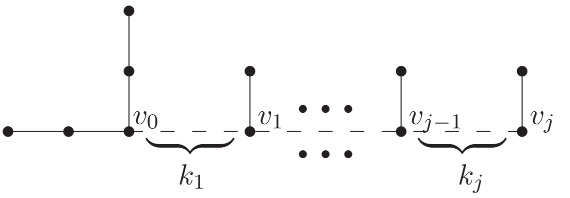

Fig. 11. The graphs $H_{(k_1,\dots,k_j)}$.

Now we assume $G^{min}_{n,n-e} = T''_{(k_1,k_2,\dots,k_{e-2})} \in \mathcal{P}''_{n,e}$. This is very similar to previous case. We must have

$$k_1 \le \frac{l_2-3}{2} \quad \text{or} \quad k_{e-2} \le \frac{l_2-3}{2} \quad \text{or} \quad \exists i \in \{2,\dots,e-3\}\ s.t.\ k_i \le l_2,$$

where $l_2 = \lceil \frac{n-3e+7}{e-3} \rceil$. A similar argument shows $\rho^{min}_{n,n-e} > \rho_{l_2+4}$. Here we omit the detail.

Let $k = \lfloor \frac{n-2e+2}{e-4} \rfloor$. There exists a tree $T \in \mathcal{P}_{n,e}$, which can be obtained by subdividing some edges on internal paths of $T_{(k-1,k,\dots,k,k-1)}$.

Since $e \geqslant 5$ and $n \geqslant 10e^2 - 74e + 142$, we have $n > 5e^2 - 31e + 50$; thus,

$$l_2 + 4 = \left\lceil \frac{n-3e+7}{e-3} \right\rceil + 4 \leqslant \left\lfloor \frac{n-2e+2}{e-4} \right\rfloor = k.$$

We get

$$\rho^{min}_{n,n-e} > \rho_{l_2+4} \geqslant \rho(T_{(k-1,k,\dots,k,k-1)}) \geqslant \rho(T).$$

Contradiction! □

Remark 3. Assume $G^{min}_{n,n-e} = T_{(k_1,\dots,k_r)} \in P_{n,e}$. Let $\bar{k} = \frac{\sum_{i=1}^r k_i}{r}$. By Lemma 2.13, we can get $k_i \ge \lfloor \bar{k} + \frac{2}{r} \rfloor - 3$ for $2 \le i \le r-1$ and $k_i \ge \lfloor \bar{k} + \frac{2}{r} \rfloor - 2$ for $i = 1, r$ whenever $n \ge 9e - 30$.

3.2. Part 2

From now on, we only consider a tree $T_{(k_1,k_2,\dots,k_r)}$ in $\mathcal{P}_{n,e}$. (Here $r = e-4$ through the remaining of the paper.) Let $v_0, v_1, \dots, v_r$ be the list (from left to right) of all degree 3 vertices in $T_{(k_1,k_2,\dots,k_r)} \in \mathcal{P}_{n,e}$. Let $H_{(k_1,k_2,\dots,k_j)}$ be the graph shown in Fig. 11.

Now we define two families of sub-trees of $T_{(k_1,k_2,\dots,k_r)}$. For $i = 1,\dots,r-1$, let $L_i = H_{(k_1,k_2,\dots,k_i)}$ (from the left direction). For $j = 2,\dots,r$, let $R_j = H_{(k_r,k_{r-1},\dots,k_j)}$ (from the right direction). We also define $L_0 = P_5$ and $R_{r+1} = P_5$.

Lemma 3.1. *For any $\lambda \ge \rho(T_{(k_1,k_2,\dots,k_r)})$, we have*

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

Proof. For simplicity, we also write $p_i = p_{(L_i,v_i)}$, $q_i = q_{(L_i,v_i)}$ for $i = 0,1,2,\dots,r-1$, and $p'_j = p_{(R_j,v_{j-1})}$, $q'_j = q_{(R_j,v_{j-1})}$ for $j = 2,\dots,r+1$. From Eq. (11), we have $p'_{r+1} = p_0 = p_{(P_5,v_0)} = \frac{d_1x_1(\lambda^2-1)}{x_2-x_1} > 0$ and $q'_{r+1} = q_0 = q_{(P_5,v_0)} = \frac{d_2x_2(\lambda^2-1)}{x_2-x_1} > 0$ for any $\lambda > \lambda_0$.

It remains to consider p_i, q_i for $i = 1,2,\dots,r-1$, and p'_j, q'_j for $j = 2,\dots,r$. Let μ be the least number such that these functions $p_i(\lambda), q_i(\lambda)\ p'_j(\lambda), q'_j(\lambda)$ take non-negative values for all $\lambda \geqslant \mu$.

We need to show such μ exists. By Lemma 2.5, we have $\lim_{\lambda\to+\infty} q_i(\lambda) = +\infty$ and $\lim_{\lambda\to+\infty} q'_j(\lambda) = +\infty$. Since $\lim_{\lambda\to+\infty} p_0 = \lim_{\lambda\to+\infty} \frac{d_1x_1(\lambda^2-1)}{x_2-x_1} = +\infty$ and $p_i = \frac{1}{x_2-x_1}(d_1x_1^{k_i}p_{i-1}+x_2^{k_i-1}q_{i-1})$ (see Lemma 2.6), by induction on i, we have $\lim_{\lambda\to+\infty} p_i(\lambda) = +\infty$. Similarly, we have $\lim_{\lambda\to+\infty} p'_j(\lambda) = +\infty$. Thus μ is well-defined.

If $\mu \leqslant \rho(T_{(k_1,k_2,\ldots,k_r)})$, then we are done. Otherwise, we assume $\mu > \rho(T_{(k_1,k_2,\ldots,k_r)})$. Note that μ is always a root of one of those $p_i(\lambda)$, $q_i(\lambda)$, $p'_j(\lambda)$, $q'_j(\lambda)$.

Case (1). There exists an i $(1 \leqslant i \leqslant r-1)$ such that $p_i(\mu) = 0$. Since $p_i = \frac{1}{x_2-x_1}(d_1x_1^{k_i}p_{i-1} + x_2^{k_i-1}q_{i-1})$, we must have $p_{i-1}(\mu) = q_{i-1}(\mu) = 0$. By Lemma 2.7, we have

$$\phi_{T_{(k_1,k_2,\ldots,k_r)}}(\mu) = (x_2-x_1)(x_2^{k_i-1}q_{i-1}q'_{i+1} - x_1^{k_i-1}p_{i-1}p'_{i+1})\mid_{\mu}= 0.$$

It contradicts to the assumption $\mu > \rho(T_{(k_1,k_2,\ldots,k_r)})$.
Case (2). There exists a j $(2 \leqslant j \leqslant r)$ such that $p'_j(\mu) = 0$. This case is symmetric to Case (1).
Case (3). There exists an i $(1 \leqslant i \leqslant r-1)$ such that $q_i(\mu) = 0$. By Lemma 2.7, we have

$$\phi_{T_{(k_1,k_2,\ldots,k_r)}}(\mu) = (x_2-x_1)(x_2^{k_{i+1}-1}q_iq'_{i+2} - x_1^{k_{i+1}-1}p_ip'_{i+2})\mid_{\mu}\leqslant 0.$$

It contradicts to $\mu > \rho(T_{(k_1,k_2,\ldots,k_r)})$.
Case (4). There exists a j $(2 \leqslant j \leqslant r)$ such that $q'_j(\mu) = 0$. This case is symmetric to Case (3).

The proof of this Lemma is finished. □

The following Lemma gives the lower bound for the spectral radius of a general tree $T_{(k_1,k_2,\ldots,k_r)} \in \mathcal{P}_{n,e}$.

Lemma 3.2. *Let $\bar{k} = \frac{\sum_{i=1}^r k_i}{r}$. We have*

$$d_2 \geq \frac{2x_1^{\bar{k}+\frac{2}{r}}}{1-x_1^{\bar{k}+\frac{2}{r}+1}}$$

for all $\lambda \geq \rho(T_{(k_1,k_2,\ldots,k_r)})$, where the equality holds if and only if $k_1+1 = k_2 = \cdots = k_{r-1} = k_r+1$ and $\lambda = \rho(T_{(k_1,k_2,\ldots,k_r)})$.

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

$$f_s(t) = \frac{d_2x_2^{2s}t - x_2}{x_2^{2s-1}t + d_1} = \frac{d_2x_2t - x_1^{2s-2}}{t + d_1x_1^{2s-1}}, \quad t > 0.$$

We consider the fixed point of $f_s(t)$, which satisfies

$$t^2 - (d_2x_2 - d_1x_1^{2s-1})t + x_1^{2s-2} = 0.$$

This quadratic equation has a unique root x_1^{s-1} when

$$d_2 = 2x_1^s + d_1x_1^{2s}. \tag{15}$$

We choose $s = s(\lambda)$ to be the root of Eq. (15). 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

$$f_s(t) \le t, \quad \forall t > 0.$$

For $i = 1, \ldots, r$, we have

$$f_{k_i}(t) = f_s(x_2^{2(k_i-s)}t) \le x_2^{2(k_i-s)}t. \tag{16}$$

By Lemma 2.7, we get

$$\phi_{T_{(k_1,k_2,\ldots,k_r)}} = (x_2 - x_1)(x_2^{k_r-1}q_{r-1}q'_{r+1} - x_1^{k_r-1}p_{r-1}p'_{r+1}).$$

Since $\phi_{T_{(k_1,k_2,\ldots,k_r)}} \geqslant 0$ for all $\lambda \ge \rho(T_{(k_1,k_2,\ldots,k_r)})$, we get

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

Note $t'_{r+1} = t_0 = \frac{d_2x_2}{d_1x_1} = \frac{d_2}{d_1}x_2^2$. Applying inequality (16) recursively, we have

$$\begin{aligned}
1 &\leqslant \frac{d_2}{d_1}x_2^2 \cdot x_2^{2(k_r-1)}\frac{q_{r-1}}{p_{r-1}} \\
&= \frac{d_2}{d_1}x_2^{2k_r}f_{k_{r-1}}(f_{k_{r-2}}(\ldots(f_{k_1}(t_0)\ldots))) \\
&\le \frac{d_2}{d_1}x_2^{2k_r}x_2^{2(k_{r-1}-s)}x_2^{2(k_{r-2}-s)}\ldots x_2^{2(k_1-s)}t_0 \\
&= \frac{d_2}{d_1}x_2^{2k_r}x_2^{2(k_{r-1}-s)}x_2^{2(k_{r-2}-s)}\ldots x_2^{2(k_1-s)}\frac{d_2}{d_1}x_2^2 \\
&= \frac{d_2^2}{d_1^2}x_2^{2(r\bar{k}-(r-1)s+1)}.
\end{aligned}$$

We get $d_2 \geqslant d_1x_1^{r\bar{k}-(r-1)s+1}$; and the equality holds if and only if $k_1 + 1 = k_2 = \cdots = k_{r-1} = k_r + 1 = s$ and $\lambda = \rho(T_{(k_1,k_2,\ldots,k_r)})$. By Remark 1, $d_2 \geqslant d_1x_1^{r\bar{k}-(r-1)s+1}$ is equivalent to

$$d_2 \geqslant 2x_1^{r\bar{k}-(r-1)s+2} + d_1x_1^{2(r\bar{k}-(r-1)s+2)}. \tag{17}$$

Comparing this inequality with Eq. (15), we must have $s \le r\bar{k}-(r-1)s+2$. Solving s, we get $s \le \bar{k}+\frac{2}{r}$. Thus,

$$d_2 = 2x_1^s + d_1x_1^{2s} \ge 2x_1^{\bar{k}+\frac{2}{r}} + d_1x_1^{2(\bar{k}+\frac{2}{r})}.$$

Applying Remark 1 one more time, we get

$$d_2 \ge \frac{2x_1^{\bar{k}+\frac{2}{r}}}{1 - x_1^{\bar{k}+\frac{2}{r}+1}}.$$

The proof is completed. □

Lemma 3.3. *Let $G^{min}_{n,n-e} = T_{(k_1,k_2,\ldots,k_r)}$ and $\overline{k} = \frac{\sum_{i=1}^r k_i}{r}$. Then*

$$d_2 \le \frac{2x_1^{\lfloor \overline{k}+\frac{2}{r}\rfloor}}{1 - x_1^{\lfloor \overline{k}+\frac{2}{r}\rfloor+1}}$$

holds at $\lambda = \rho^{min}_{n,n-e}$.

Proof. Let $s = \overline{k} + \frac{2}{r}$. Observe that we can always subdivide some edges on internal paths of $T_{(\lfloor s\rfloor-1,\lfloor s\rfloor,\ldots,\lfloor s\rfloor,\lfloor s\rfloor-1)}$ to get a tree T on n vertices and diameter $n-e$. By Lemma 2.4, we have

$$\rho^{min}_{n,n-e} \le \rho(T) \leqslant \rho(T_{(\lfloor s\rfloor-1,\lfloor s\rfloor,\ldots,\lfloor s\rfloor,\lfloor s\rfloor-1)}) = \rho_{\lfloor s\rfloor}.$$

By Lemma 2.10, $\rho_{\lfloor s\rfloor}$ is the root of

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

Since $d_2(\lambda)$ is increasing while $\frac{2x_1^{\lfloor s\rfloor}}{1-x_1^{\lfloor s\rfloor+1}}$ is decreasing on $\left(\sqrt{2+\sqrt{5}}, \infty\right)$, we get

$$d_2(\rho^{min}_{n,n-e}) \le d_2(\rho_{\lfloor s\rfloor}) = \left.\frac{2x_1^{\lfloor s\rfloor}}{1 - x_1^{\lfloor s\rfloor+1}}\right|_{\rho_{\lfloor s\rfloor}} \le \left.\frac{2x_1^{\lfloor s\rfloor}}{1 - x_1^{\lfloor s\rfloor+1}}\right|_{\rho^{min}_{n,n-e}}.$$

The proof is completed. □

We get the following corollary.

Corollary 3.1. *Let $G^{min}_{n,n-e} = T_{(k_1,k_2,\ldots,k_r)} \in \mathcal{P}_{n,e}$ and $s = \frac{1}{r}\sum_{i=1}^r k_i + \frac{2}{r} = \frac{n-2e+2}{e-4}$. We have*

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

holds at $\lambda = \rho(G^{min}_{n,n-e})$. In particular, $\rho(G^{min}_{n,n-e}) = \sqrt{2+\sqrt{5}} + O\left((\frac{\sqrt{5}-1}{2})^{s/2}\right)$.

Lemma 3.4. *Assume $G^{min}_{n,n-e} = T_{(k_1,\ldots,k_i,k_{i+1},\ldots,k_r)}$ and $\overline{c} = \frac{\rho^{min}_{n,n-e}+\sqrt{(\rho^{min}_{n,n-e})^2+4d_1d_2}}{2}$. Then the following equalities hold at the point $\lambda = \rho^{min}_{n,n-e}$.*

$$\overline{c}x_1^{k_i+1} \le d_2 \le \overline{c}x_1^{k_i-1} \quad \text{for } i = 2, \ldots, r-1; \tag{18}$$

$$\sqrt{\overline{c}d_1}x_1^{k_i+1} \le d_2 \le \sqrt{\overline{c}d_1}x_1^{k_i} \quad \text{for } i = 1, r. \tag{19}$$

Proof. We reuse notations L_i, p_i, q_i, t_i (for $i = 0, 1, \ldots, r-1$) and R_j, p'_j, q'_j, t'_j (for $j = 2, \ldots, r+1$), which are introduced in Lemma 3.1 and Lemma 3.2.

Choosing any $i \in \{1, \ldots, r-1\}$, by Lemma 2.7 we have

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

at $\lambda = \rho^{min}_{n,n-e}$. This means

$$\frac{d_2x_2t_{i-1} - x_1^{2(k_i-1)}}{t_{i-1} + d_1x_1^{2k_i-1}} t'_{i+2}x_2^{2(k_{i+1}-1)} = 1.$$

We can rewrite it as

$$\left(t_{i-1} - \frac{x_1^{2k_i-1}}{d_2}\right)\left(t'_{i+2} - \frac{x_1^{2k_{i+1}-1}}{d_2}\right) = \frac{d_1d_2+1}{d_2^2}x_1^{2(k_i+k_{i+1}-1)}. \tag{20}$$

Note $t_i = f_{k_i}(t_{i-1}) = \frac{d_2x_2t_{i-1}-x_1^{2(k_i-1)}}{t_{i-1}+d_1x_1^{2k_i-1}} > 0$. We have

$$t_{i-1} > \frac{x_1^{2k_i-1}}{d_2}. \tag{21}$$

For $i=1, \ldots, r-1$, we apply Lemma 2.9 to $G_1 = T_{(k_1,\ldots,k_i,k_{i+1},\ldots,k_r)}$ and $G_2 = T_{(k_1,\ldots,k_i+1,k_{i+1}-1,\ldots,k_r)}$, where both trees contain a common induced subtree $T_{(k_1,\ldots,k_i+k_{i+1}+1,\ldots,k_r)}$ (after removing one leaf vertex). If $\phi_{G_2}(\rho(G_1)) > 0$, then $\rho(G_1) > \rho(G_2)$. This contradicts to the assumption $G_1 = G^{min}_{n,n-e}$.

We get $\phi_{G_2}(\rho(G_1)) \leqslant 0$, i.e., $\phi_{T_{(k_1,\ldots,k_i+1,k_{i+1}-1,\ldots,k_r)}}(\rho^{min}_{n,n-e}) \leqslant 0$.

We apply Lemma 2.8 and obtain the difference of characteristic polynomials of $T_{(k_1,\ldots,k_i,k_{i+1},\ldots,k_r)}$ and $T_{(k_1,\ldots,k_i+1,k_{i+1}-1,\ldots,k_r)}$,

$$\phi_{T_{(k_1,\ldots,k_i,k_{i+1},\ldots,k_r)}} - \phi_{T_{(k_1,\ldots,k_i+1,k_{i+1}-1,\ldots,k_r)}} = (x_1-x_2)\left(p_{i-1}q'_{i+2}x_2^{k_{i+1}-k_i-1} - q_{i-1}p'_{i+2}x_1^{k_{i+1}-k_i-1}\right).$$

Evaluating the function above at $\lambda = \rho^{min}_{n,n-e}$, we have

$$(x_1 - x_2)\left(p_{i-1}q'_{i+2}x_2^{k_{i+1}-k_i-1} - q_{i-1}p'_{i+2}x_1^{k_{i+1}-k_i-1}\right)\Big|_{\rho^{min}_{n,n-e}} \geq 0.$$

Since $q_{i-1} \geqslant 0$ and $p'_{i+2} \geqslant 0$ (from Lemma 3.1), we get $\frac{t'_{i+2}}{t_{i-1}} \leq x_1^{2(k_{i+1}-k_i-1)}$ at $\lambda = \rho^{min}_{n,n-e}$. In the rest of the proof, all expressions are evaluated at $\lambda = \rho^{min}_{n,n-e}$. The notation "$|_{\rho^{min}_{n,n-e}}$" is omitted for simplicity.

On the one hand, by inequality (21), we can substitute $t'_{i+2} \leq t_{i-1}x_1^{2(k_{i+1}-k_i-1)}$ into Eq. (20) and get

$$\left(t_{i-1} - \frac{x_1^{2k_i-1}}{d_2}\right)\left(x_1^{2(k_{i+1}-k_i-1)}t_{i-1} - \frac{x_1^{2k_{i+1}-1}}{d_2}\right) \geq \frac{d_1d_2+1}{d_2^2}x_1^{2(k_i+k_{i+1}-1)}.$$

After simplification, we have

$$d_2t_{i-1}^2 - x_1^{2k_i}\rho^{min}_{n,n-e}t_{i-1} - d_1x_1^{4k_i} \geq 0.$$

Recall $\bar{c} = \frac{\rho^{min}_{n,n-e} + \sqrt{(\rho^{min}_{n,n-e})^2 + 4d_1d_2}}{2}$. Solving this quadratic inequality, since $t_{i-1} > 0$, we get

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

By symmetry, we have

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

On the other hand, we substitute $t_{i-1} \geq t'_{i+2}x_2^{2(k_{i+1}-k_i-1)}$ into Eq. (20). By the similar calculation, we get

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

Changing the index $i+2$ to $i+1$, we have

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

By symmetry, we have

$$t_{i-1} \leq \bar{c}x_1^{2(k_i-1)}/d_2, \quad i = 1, \ldots, r-1.$$

Combining the inequalities above, we get

$$\frac{\bar{c}}{d_2}x_1^{2k_i} \leq t_{i-1} \leq \frac{\bar{c}}{d_2}x_1^{2(k_i-1)}, \quad i = 1, \ldots, r-1, \tag{22}$$

$$\frac{\bar{c}}{d_2}x_1^{2k_i} \leq t'_{i+1} \leq \frac{\bar{c}}{d_2}x_1^{2(k_i-1)}, \quad i = 2, \ldots, r. \tag{23}$$

Now we apply Lemma 2.7 and get

$$t_{i-1}t'_{i+1}x_2^{2(k_i-1)} = 1. \tag{24}$$

Taking product of inequalities (22), (23), and then substituting $t_{i-1}t'_{i+1}$ into Eq. (24). After simplification, wet get inequality (18).

When $i = 1$ or r, we have

$$\frac{\bar{c}}{d_2}x_1^{2k_i} \leq t_0 = t'_{r+1} = \frac{d_2}{d_1}x_2^2 \leq \frac{\bar{c}}{d_2}x_1^{2(k_i-1)}.$$

Solving for d_2, we get inequality (19). The proof of this lemma is completed. □

Proof of the second part of Theorem 1.1. As in the proof of Lemma 3.4, all expressions in this proof are evaluated at $\lambda = \rho_{n,n-e}^{min}$ and "$|_{\rho_{n,n-e}^{min}}$" is omitted for simplicity.

By Lemma 3.4, for $2 \leq i \leq r-1$, we have

$$\bar{c}x_1^{k_i+1} \leq d_2 \leq \bar{c}x_1^{k_i-1}.$$

By the definition of $\bar{c}$, we get

$$2d_2x_1^{k_i+1} \leq \rho_{n,n-e}^{min} + \sqrt{(\rho_{n,n-e}^{min})^2 + 4d_1d_2} \leq 2d_2x_1^{k_i-1}.$$

After solving for d_2 and simplifying, we have

$$\frac{\rho_{n,n-e}^{min}x_1^{k_i+1} + 2x_1^{2k_i+3}}{1 - x_1^{2(k_i+2)}} \leq d_2 \leq \frac{\rho_{n,n-e}^{min}x_1^{k_i-1} + 2x_1^{2k_i-1}}{1 - x_1^{2k_i}}.$$

Since $\rho_{n,n-e}^{min} > 2 > 1 + x_1^2 = \rho_{n,n-e}^{min} x_1$, we observe

$$\frac{2x_1^{k_i+1}}{1-x_1^{k_i+2}} < \frac{\rho_{n,n-e}^{min} x_1^{k_i+1} + 2x_1^{2k_i+3}}{1-x_1^{2(k_i+2)}}$$

and

$$\frac{\rho_{n,n-e}^{min} x_1^{k_i-1} + 2x_1^{2k_i-1}}{1-x_1^{2k_i}} < \frac{2x_1^{k_i-2}}{1-x_1^{k_i-1}}.$$

We obtain

$$\frac{2x_1^{k_i+1}}{1-x_1^{k_i+2}} < d_2 < \frac{2x_1^{k_i-2}}{1-x_1^{k_i-1}} \quad \text{for } 2 \le i \le r-1. \tag{25}$$

From Theorem 3.1, we have

$$\frac{2x_1^{s}}{1-x_1^{s+1}} \le d_2 \le \frac{2x_1^{\lfloor s \rfloor}}{1-x_1^{\lfloor s \rfloor+1}}. \tag{26}$$

Combining inequalities (25) and (26), we get

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

Thus, $\lfloor s \rfloor - 1 < k_i < s + 2$. So $\lfloor s \rfloor < k_i \le \lceil s \rceil + 1$ where $i = 2, \ldots, r-1$.

For $j = 1$ or r, combining inequalities (19) and (26), we have

$$\frac{\sqrt{\bar{c}d_1}}{2} x_1^{k_j+1} \le \frac{x_1^{\lfloor s \rfloor}}{1-x_1^{\lfloor s \rfloor+1}},$$
$$\frac{\sqrt{\bar{c}d_1}}{2} x_1^{k_j} \ge \frac{x_1^{s}}{1-x_1^{s+1}}.$$

Note that $d_1 \to 2x_1$ and $\bar{c} \to \lambda_0$ as n approaches infinity. For sufficiently large n, we have $x_2^{0.1} < \frac{\lambda_0}{2} < x_2^{0.2}$. We get

$$x_1^{k_j+1+0.45} \le x_1^{\lfloor s \rfloor} \quad \text{and} \quad x_1^{k_j+0.4} > x_1^{s}.$$

So $\lfloor s \rfloor - 1 \le k_j \le \lfloor s \rfloor$ for n large enough.

In conclusion, we get

$$\lfloor s \rfloor - 1 \le k_j \le \lfloor s \rfloor \leqslant k_i \leqslant \lceil s \rceil + 1$$

for $2 \leqslant i \leqslant r-1$ and $j = 1, r$.

Now we will prove item 2. It suffices to show $k_i - k_j \leqslant 2$, for $2 \leqslant i \leqslant r-1$ and $j = 1, r$. Suppose that there exist i, j with $i \in \{2, \ldots, r-1\}$ and $j \in \{1, r\}$ so that $k_i \geq k_j + 3$. By Lemma 3.4, we have

$$\sqrt{\bar{c}d_1}x_1^{k_j+1} \leq d_2 \leq \bar{c}x_1^{k_j+2}.$$

Since $\lambda x_2^2 = (1+x_1^2)x_1 < 2x_1 \leq d_1$ for $\lambda \geq \lambda_0$ and $\bar{c} \to \lambda_0$ as n approaches infinity, we have $\bar{c}x_1^{k_j+2} < \sqrt{\bar{c}d_1}x_1^{k_j+1}$ for n large enough. Contradiction!

Now we will prove item 3. By Lemma 3.4, we have $\bar{c}x_1^{k_j+1} \leq d_2 \leq \bar{c}x_1^{k_i-1}$ for all $2 \leq i, j \leq r-1$. This implies $|k_i - k_j| \leq 2$. It is sufficient to show that there are no i, j with $|k_i - k_j| = 2$. Otherwise, suppose there exist $i, j \in \{2, \ldots, r-1\}$ such that $k_i = k$ and $k_j = k+2$. Without loss of generality, we can assume that $i < j$ and in addition i, j are mostly close to each other. Namely, $k_l = k+1$ for all integer l between i and j.

Applying inequality (18) to $k_i = k$ and $k_j = k+2$, we have

$$d_2 \geqslant \bar{c}x_1^{k_i+1} = \bar{c}x_1^{k+1},$$
$$d_2 \leqslant \bar{c}x_1^{k_j-1} = \bar{c}x_1^{k+1}.$$

Two inequalities above force $d_2 = \bar{c}x_1^{k+1}$. These equalities force $t_{i-1} = t'_{i+1} = x_1^{k-1}$, $t_{j-1} = t'_{j+1} = x_1^{k+1}$ by inequalities (22) and (23).

Consider the function $f(t) = \frac{d_2t - x_2}{x_1t + d_1} = f_k(x_1^{2k}t)$ and let $c = \bar{c}/d_2 = x_2^{k+1}$. It is easy to check $f(c) = \frac{1}{c}$. We claim

$$t_l = x_1^{k+1} \quad \text{for } i \leqslant l \leqslant j-1.$$

For $l = i$, we have

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

By induction on l, we have

$$t_l = f_{k+1}(t_{l-1}) = f_{k+1}(x_1^{k+1}) = f(x_2^{k+1}) = f(c) = \frac{1}{c} = x_1^{k+1}.$$

By Lemma 2.7, we have

$$t_{j-2}t'_jx_2^{2k} = 1.$$

Since $t_{j-2} = x_1^{k+1}$, it implies $t'_j = x_1^{k-1}$. However, we also have

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

Contradiction!

If $n-6$ is divisible by $e-4$, then $s = \frac{n-6}{e-2} - 4$ is an integer. In this case, the only possible sequence $(k_1, k_2, \ldots, k_r)$ satisfying items 1-3 is $(s-1, s, \ldots, s, s-1)$. In particular, we have $G_{n,n-e}^{min} = T_{(s-1,s,\ldots,s,s-1)}$.

The proof is completed. □

4. Proof of Theorems 1.3 and 1.4

4.1. e=7

Let $G^{min}_{n,n-7} = T_{(k_1,k_2,k_3)} \in \mathcal{P}_{n,7}$. Note $k_1 + k_2 + k_3 = n - 14$. By Theorem 1.1, here are all the possible graphs for $G^{min}_{n,n-7}$.

Case 1. $\sum_{i=1}^{3} k_i = 3k$. We have $(k_1, k_2, k_3) = (k, k, k)$ or $(k, k+1, k-1)$.
Case 2. $\sum_{i=1}^{3} k_i = 3k+1$. We have $(k_1, k_2, k_3) = (k, k+1, k)$.
Case 3. $\sum_{i=1}^{3} k_i = 3k+2$. We have $(k_1, k_2, k_3) = (k, k+2, k)$ or $(k, k+1, k+1)$.

To simplify the proof of Theorem 1.3, we introduce the following short notations. We have

$$p_0 := p_{(L_0,v_0)} = \frac{\lambda^2-1}{x_2-x_1} d_1x_1,$$

$$q_0 := q_{(L_0,v_0)} = \frac{\lambda^2-1}{x_2-x_1} d_2x_2,$$

$$p^{(k-1)} := p_{(H_{(k-1)},v_1)} = \frac{\lambda^2-1}{(x_2-x_1)^2}(d_1^2x_1^k + d_2x_2^{k-1}),$$

$$q^{(k-1)} := q_{(H_{(k-1)},v_1)} = \frac{\lambda^2-1}{(x_2-x_1)^2}(d_2^2x_2^k - d_1x_1^{k-1}),$$

$$p^{(k)} := p_{(H_{(k)},v_1)} = \frac{\lambda^2-1}{(x_2-x_1)^2}(d_1^2x_1^{k+1} + d_2x_2^{k}),$$

$$q^{(k)} := q_{(H_{(k)},v_1)} = \frac{\lambda^2-1}{(x_2-x_1)^2}(d_2^2x_2^{k+1} - d_1x_1^{k}),$$

$$p^{(k+1)} := p_{(H_{(k+1)},v_1)} = \frac{\lambda^2-1}{(x_2-x_1)^2}(d_1^2x_1^{k+2} + d_2x_2^{k+1}),$$

$$q^{(k+1)} := q_{(H_{(k+1)},v_1)} = \frac{\lambda^2-1}{(x_2-x_1)^2}(d_2^2x_2^{k+2} - d_1x_1^{k+1}),$$

$$p^{(k,k+1)} := p_{(H_{(k,k+1)},v_2)} = \frac{\lambda^2-1}{(x_2-x_1)^3}(d_1^3x_1^{2k+2} + d_1d_2x_1 + d_2^2x_2^{2k+1} - d_1),$$

$$q^{(k,k+1)} := q_{(H_{(k,k+1)},v_2)} = \frac{\lambda^2-1}{(x_2-x_1)^3}(d_2^3x_2^{2k+2} - d_1d_2x_2 - d_1^2x_1^{2k+1} - d_2).$$

Proof of Theorem 1.3. We will compare the spectral radius of the possible graphs listed above in three cases separately.

Case 1. $\sum_{i=1}^{3} k_i = 3k$.
By Lemma 2.8, we have

$$\phi_{T_{(k,k,k)}} - \phi_{T_{(k,k+1,k-1)}} = (x_1 - x_2)\left(p^{(k)}q_0x_1 - q^{(k)}p_0x_2\right)$$
$$= -\frac{(\lambda^2-1)^2}{(x_2-x_1)^2}\left[(d_2x_1+1)d_1^2x_1^k - (d_1x_2-1)d_2^2x_2^k\right]$$
$$= \frac{(d_2x_1+1)(\lambda^2-1)^2}{(x_2-x_1)^2}\left(d_2^2x_2^k - d_1^2x_1^k\right).$$

In the last step, we applied the fact $d_2x_1 + 1 = d_1x_2 - 1$.

By Lemma 2.10 and Remark 1, $\rho(T_{(k,k+1,k)})$ $(= \rho_{k+1})$ satisfies $d_2x_2^{k/2} = d_1x_1^{k/2}$. The largest root of $\phi_{T_{(k,k,k)}} - \phi_{T_{(k,k+1,k-1)}} = 0$ is ρ_{k+1}.

Noting that $d_2^2x_2^k - d_1^2x_1^k$ is an increasing function of $\lambda \in \left(\sqrt{2+\sqrt{5}}, \frac{3}{2}\sqrt{2}\right)$ for sufficiently large k. By Lemma 2.4, we have $\rho_{k+1} = \rho(T_{(k,k+1,k)}) < \rho(T_{(k,k,k)})$. Evaluating $\phi_{T_{(k,k,k)}} - \phi_{T_{(k,k+1,k-1)}}$ at $\lambda = \rho(T_{(k,k,k)})$, we get $\phi_{T_{(k,k+1,k-1)}}(\rho(T_{(k,k,k)})) < 0$. Thus, by Lemma 2.2, $\rho(T_{(k,k,k)}) < \rho(T_{(k,k+1,k-1)})$ and $G^{min}_{n,n-7} = T_{(k,k,k)}$.

Case 2. $\sum_{i=1}^{3} k_i = 3k + 1$. We must have $G^{min}_{n,n-7} = T_{(k,k+1,k)}$.

Case 3. $\sum_{i=1}^{3} k_i = 3k + 2$.

Similarly by Lemma 2.8, we have

$$\phi_{T_{(k,k+1,k+1)}} - \phi_{T_{(k,k+2,k)}} = \frac{(d_2x_1+1)(\lambda^2-1)^2}{(x_2-x_1)^2}\left(d_2^2x_2^k - d_1^2x_1^k\right).$$

Noting that $d_2^2x_2^k - d_1^2x_1^k$ is an increasing function of $\lambda \in \left(\sqrt{2+\sqrt{5}}, \frac{3}{2}\sqrt{2}\right)$ for sufficiently large k. We have $\phi_{T_{(k,k+1,k+1)}}(\lambda) < \phi_{T_{(k,k+2,k)}}(\lambda)$ for any $\sqrt{2+\sqrt{5}} \leqslant \lambda < \rho_{k+1}$. By Lemma 2.4, we get $\rho(T_{(k,k+2,k)}) < \rho(T_{(k,k+1,k)}) = \rho_{k+1}$. Thus, $\phi_{T_{(k,k+1,k+1)}}(\rho(T_{(k,k+2,k)})) < 0$. It follows $\rho(T_{(k,k+1,k+1)}) > \rho(T_{(k,k+2,k)})$. So $G^{min}_{n,n-7} = T_{(k,k+2,k)}$.

The proof of Theorem 1.3 is completed. □

4.2. e=8

Now we let $G^{min}_{n,n-8} = T_{(k_1,k_2,k_3,k_4)} \in \mathcal{P}_{n,8}$. By Theorem 1.1, all the possible graphs for $G^{min}_{n,n-8}$ are as follows.

Case 1. If $\sum_{i=1}^{4} k_i = 4k$, then $(k_1, k_2, k_3, k_4) = (k, k, k, k)$, $(k, k, k+1, k-1)$, $(k, k+1, k, k-1)$, or $(k-1, k+1, k+1, k-1)$.

Case 2. If $\sum_{i=1}^{4} k_i = 4k+1$, then $(k_1, k_2, k_3, k_4) = (k, k+1, k, k)$ or $(k, k+1, k+1, k-1)$.

Case 3. If $\sum_{i=1}^{4} k_i = 4k+2$, then $(k_1, k_2, k_3, k_4) = (k, k+1, k+1, k)$.

Case 4. If $\sum_{i=1}^{4} k_i = 4k+3$, then $(k_1, k_2, k_3, k_4) = (k, k+1, k+1, k+1)$ or $(k, k+1, k+2, k)$.

Proof of Theorem 1.4. Similarly, we denote $p^{(k,k)} = P_{(H_{(k,k)},v_2)}$, $q^{(k,k)} = q_{(H_{(k,k)},v_2)}$, $p^{(k-1,k+1)} = P_{(H_{(k-1,k+1)},v_2)}$, and $q^{(k-1,k+1)} = q_{(H_{(k-1,k+1)},v_2)}$.

We will compare the spectral radius of all possible graphs listed in four cases above.

Case 1. $\sum_{i=1}^{4} k_i = 4k$.

First we prove

$$\rho(T_{(k,k,k,k)}) = \rho(T_{(k,k,k+1,k-1)}) = \rho(T_{(k-1,k+1,k+1,k-1)}).$$

By Lemma 2.3, it is easy to see

$$\rho(T_{(k,k,k,k)}) = \rho(T_{(k-1,k)}) = \rho(T_{(k-1,k+1,k+1,k-1)}).$$

Applying Lemma 2.7 to these graphs, we get

$$\begin{aligned}
\phi_{T_{(k,k,k,k)}} &= p^{(k,k)}q^{(k)}x_2^{k-1}(x_2 - x_1)\left(\frac{q^{(k,k)}}{p^{(k,k)}} - \frac{p^{(k)}}{q^{(k)}}x_1^{2k-2}\right),\\
\phi_{T_{(k,k,k+1,k-1)}} &= p^{(k,k)}q^{(k-1)}x_2^{k}(x_2 - x_1)\left(\frac{q^{(k,k)}}{p^{(k,k)}} - \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}\right),\\
\phi_{T_{(k,k,k+1,k-1)}} &= p^{(k-1,k+1)}q^{(k)}x_2^{k-1}(x_2 - x_1)\left(\frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}} - \frac{p^{(k)}}{q^{(k)}}x_1^{2k-2}\right),\\
\phi_{T_{(k-1,k+1,k+1,k-1)}} &= p^{(k-1,k+1)}q^{(k-1)}x_2^{k}(x_2 - x_1)\left(\frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}} - \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}\right).
\end{aligned}$$

Let $\rho = \rho(T_{(k,k,k,k)}) = \rho(T_{(k-1,k+1,k+1,k-1)})$ and $\rho' = \rho(T_{(k,k,k+1,k-1)})$. Write $J(\lambda) = p^{(k,k)} q^{(k-1)}x_2^k(x_2 - x_1)$ and $K(\lambda) = p^{(k-1,k+1)}q^{(k)}x_2^{k-1}(x_2 - x_1)$. By Lemma 3.1, $J(\rho) > 0$ and $K(\rho) > 0$.

Note that ρ is the root of both equations

$$\frac{q^{(k,k)}}{p^{(k,k)}} = \frac{p^{(k)}}{q^{(k)}}x_1^{2k-2} \quad \text{and} \quad \frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}} = \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}. \tag{27}$$

Note that ρ' is the root of both equations

$$\frac{q^{(k,k)}}{p^{(k,k)}} = \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k} \quad \text{and} \quad \frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}} = \frac{p^{(k)}}{q^{(k)}}x_1^{2k-2}. \tag{28}$$

We have

$$\begin{aligned}
\phi_{T_{(k,k,k+1,k-1)}}(\rho) &= J(\rho)\left(\frac{p^{(k)}}{q^{(k)}}x_1^{2k-2} - \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}\right)\Bigg|_{\rho}\\
&= K(\rho)\left(\frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k} - \frac{p^{(k)}}{q^{(k)}}x_1^{2k-2}\right)\Bigg|_{\rho}.
\end{aligned}$$

Thus, $\phi_{T_{(k,k,k+1,k-1)}}(\rho)^2 = -J(\rho)K(\rho)\left(x_1^{2k-2}\frac{p^{(k)}}{q^{(k)}} - \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}\right)^2\Big|_{\rho} \leqslant 0$. We get $\phi_{T_{(k,k,k+1,k-1)}}(\rho) = 0$. Similarly, we can prove $\phi_{T_{(k,k,k,k)}}(\rho') = 0$. Hence, we get $\rho = \rho'$.

Now we prove $\rho(T_{(k,k,k+1,k-1)}) < \rho(T_{(k,k+1,k,k-1)})$. By Lemma 2.8, we have

$$\phi_{T_{(k,k,k+1,k-1)}} - \phi_{T_{(k,k+1,k,k-1)}} = (x_1 - x_2)\left(p^{(k)}q^{(k-1)} - q^{(k)}p^{(k-1)}\right) = d_1d_2\lambda^2(\lambda^2 - 1)^2 > 0$$

for any $\lambda > \lambda_0$. So $\rho(T_{(k,k,k+1,k-1)}) < \rho(T_{(k,k+1,k,k-1)})$. We are done in this case.

Case 2. $\sum_{i=1}^{4} k_i = 4k+1$.

Similarly, by Lemma 2.8, we have

$$\begin{aligned}\phi_{T_{(k,k+1,k,k)}} - \phi_{T_{(k,k+1,k+1,k-1)}} &= (x_1 - x_2)\left(p^{(k,k+1)}q_0 - q^{(k,k+1)}p_0\right)\\ &= \frac{(d_2x_1+1)(\lambda^2-1)^2x_2^{2k+1}}{(x_2-x_1)^3}\left(d_2^3 - 2d_1d_2x_1^{2k+1} - d_1^3x_1^{4k+2}\right).\end{aligned}$$

Here we use proof by contradiction. Suppose $G_{n,n-8}^{min} = T_{(k,k+1,k+1,k-1)}$. By Lemma 3.4, $d_2 = \sqrt{\bar{c}d_1}x_1^k$ at $\lambda = \rho(T_{(k,k+1,k+1,k-1)})$. Note $\bar{c} \to \lambda_0$ as $n \to \infty$. When n is large enough, we will get $\bar{c} > (2+\epsilon)x_1$ for some constant $\epsilon > 0$. Thus, we get

$$d_2^2 = \bar{c}d_1x_1^{2k} > (2+\epsilon)d_1x_1^{2k+1}.$$

For n large enough, we have $\phi_{T_{(k,k+1,k,k)}} - \phi_{T_{(k,k+1,k+1,k-1)}} > 0$ at $\lambda = \rho(T_{(k,k+1,k+1,k-1)})$. Equivalently $\phi_{T_{(k,k+1,k,k)}}(\rho(T_{(k,k+1,k+1,k-1)})) > 0$. By Lemma 2.9, we get $\rho(T_{k,k+1,k,k}) < \rho(T_{k,k+1,k+1,k-1})$. Contradiction! Hence, we have $G_{n,n-8}^{min} = T_{k,k+1,k,k}$.

Case 3. $\sum_{i=1}^{4} k_i = 4k+2$. There is only one possible graph $T_{(k,k+1,k+1,k)}$.

Case 4. $\sum_{i=1}^{4} k_i = 4k+3$.

Similarly by Lemma 2.8, we have

$$\begin{aligned}\phi_{T_{(k,k+1,k+1,k+1)}} - \phi_{T_{(k,k+1,k+2,k)}} &= (x_1 - x_2)\left(p^{(k,k+1)}q_0 - q^{(k,k+1)}p_0\right)\\ &= \frac{(d_2x_1+1)(\lambda^2-1)^2x_2^{2k+1}}{(x_2-x_1)^3}\left(d_2^3 - 2d_1d_2x_1^{2k+1} - d_1^3x_1^{4k+2}\right)\\ &< \frac{(d_2x_1+1)(\lambda^2-1)^2x_2^{2k+1}}{(x_2-x_1)^3}\left(d_2^3 - 2d_1d_2x_1^{2k+1}\right)\\ &= \frac{d_2(d_2x_1+1)(\lambda^2-1)^2x_2^{2k+1}}{(x_2-x_1)^3}\left(d_2^2 - 2d_1x_1^{2k+1}\right).\end{aligned}$$

We now suppose $G_{n,n-8}^{min} = T_{(k,k+1,k+1,k+1)}$ in this case. By Lemma 3.4, $d_2 = \sqrt{\bar{c}d_1}x_1^{k+1}$ at $\lambda = \rho(T_{(k,k+1,k+1,k+1)})$. Recall that $\bar{c} \to \lambda_0$ as $n \to \infty$. When n is large enough, we get $\bar{c} < 2x_2$. Thus $d_2 = \sqrt{\bar{c}d_1}x_1^{k+1} < \sqrt{2d_1x_2}x_1^{k+1}$. We get $\phi_{T_{(k,k+1,k+2,k)}}(\rho(T_{(k,k+1,k+1,k+1)})) > 0$. Applying Lemma 2.9 with $G_2 = T_{(k,k+1,k+2,k)}$ and $G_1 = T_{(k,k+1,k+1,k+1)}$, we have $\rho(T_{k,k+1,k+2,k}) < \rho(T_{k,k+1,k+1,k+1})$. Contradiction! Hence $G_{n,n-8}^{min} = T_{k,k+1,k+2,k}$. The proof is completed. □

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