

# 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  $G_{n,n-e}^{min}$  be a graph with minimal spectral radius among all connected graphs on  $n$  vertices with diameter  $n - e$ . Let  $P_{n_1, n_2, \dots, n_t, p}^{m_1, m_2, \dots, m_t}$  be a tree obtained from a path of  $p$  vertices ( $0 \sim 1 \sim 2 \sim \dots \sim (p-1)$ ) by linking one pendant path  $P_{n_i}$  at  $m_i$  for each  $i \in \{1, 2, \dots, t\}$ . For  $e = 1, 2, 3, 4, 5$ ,  $G_{n,n-e}^{min}$  were determined in the literature. Cioabă-van Dam-Koolen-Lee [2] conjectured for fixed  $e \geq 6$ ,  $G_{n,n-e}^{min}$  is in the family  $\mathcal{P}_{n,e} = \{P_{2,1,\dots,1,2,n-e+1}^{2,m_2,\dots,m_{e-4},n-e-2} \mid 2 < m_2 < \dots < m_{e-4} < n - e - 2\}$ . For  $e = 6, 7$ , they conjectured  $G_{n,n-6}^{min} = P_{2,1,2,n-5}^{2, \lceil \frac{D-1}{2} \rceil, D-2}$  and  $G_{n,n-7}^{min} = P_{2,1,1,2,n-6}^{2, \lfloor \frac{D+2}{3} \rfloor, D - \lfloor \frac{D+2}{3} \rfloor, D-2}$ . 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  $k_1, k_2, \dots, k_{e-4}$ , let  $T_{(k_1, k_2, \dots, k_{e-4})} = P_{2,1,\dots,1,2,n-e+1}^{2,m_2,\dots,m_{e-4},n-e-2}$  with  $k_i = m_{i+1} - m_i - 1$ , for  $1 \leq i \leq e - 4$ . (Here we assume  $m_1 = 2$  and  $m_{e-3} = n - e - 2$ .)

Let  $s = \sum_{i=1}^{e-4} k_i + 2$ . For any integer  $e \geq 6$  and sufficiently large  $n$ , we proved that  $G_{n,n-e}^{min}$  must be one of the trees  $T_{(k_1, k_2, \dots, k_{e-4})}$  with the parameters satisfying  $\lfloor s \rfloor - 1 \leq k_j \leq \lfloor s \rfloor \leq k_i \leq \lfloor s \rfloor + 1$  for  $j = 1, e - 4$  and  $i = 2, \dots, e - 5$ . 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  $G_{n,n-e}^{min}$  are completely determined here. Moreover, if  $n - 6$  is divisible by  $e - 4$  and  $n$  is sufficiently large, then  $G_{n,e}^{min} = T_{(k-1, k, k, \dots, k, k, k-1)}$  where  $k = \frac{n-6}{e-4} - 2$ .

## 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  $\phi_G$ . The problem of determining graphs with small spectral radius can be traced back to Hoffman and Smith [10, 7, 8]. They completely determined all connected graphs  $G$  with  $\rho(G) \leq 2$ . 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  $\tilde{E}_8$ . Cvetković et al. [4] gave a nearly complete description of all graphs  $G$  with  $2 < \rho(G) \leq \sqrt{2 + \sqrt{5}}$ . Their description was completed by Brouwer and Neumaier [1]. Those graphs are some special trees with at most two

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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  $\sqrt{2 + \sqrt{5}} \leq \rho(G) \leq \frac{3}{2}\sqrt{2}$ ; 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 quipus* (i.e., the vertices of degree 3 lies on a path); else  $G$  is a *closed quipus* (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 quipus. Let  $P_{n_1, n_2, \dots, n_t, p}^{m_1, m_2, \dots, m_t}$  be a tree obtained from a path on  $p$  vertices ( $0 \sim 1 \sim 2 \sim \dots \sim (p-1)$ ) by linking one pendant path  $P_{n_i}$  at  $m_i$  for  $i = 1, 2, \dots, t$  (see Figure 1.) The path  $0 \sim 1 \sim 2 \sim \dots \sim (p-1)$  is called *main path*. For  $i = 1, \dots, t-1$ , let  $P^{(i)}$  be the  $i$ -th *internal path* ( $m_i \sim m_i+1 \sim \dots \sim m_{i+1}$ ) and  $k_i = m_{i+1} - m_i - 1$  be the the number of internal vertices on  $P^{(i)}$ . In general, an *internal path* in  $G$  is a path  $v_0 \sim v_1 \sim \dots \sim v_s$  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  $v_0 = v_s$ .

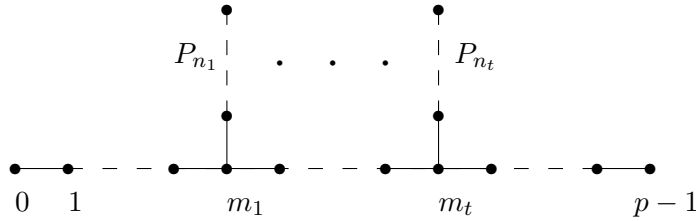


Figure 1:  $P_{n_1, n_2, \dots, n_t, p}^{m_1, m_2, \dots, m_t}$

Recently van Dam and Kooij [3] asked an interesting question “*which connected graph of order  $n$  with a given diameter  $D$  has minimal spectral radius?*”. Here 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  $D \in \{1, 2, \lfloor n/2 \rfloor, n-3, n-2, n-1\}$ . The cases  $D = 1$  and  $D = n-1$  are trivial. A *minimizer* graph, denoted by  $G_{n, D}^{min}$ , is a graph that has the minimal spectral radius among all the graphs of order  $n$  and diameter  $D$ . They proved that  $G_{n, 2}^{min}$  is either a star or a Moore graph;  $G_{n, \lfloor n/2 \rfloor}^{min}$  is the cycle  $C_n$ ;  $G_{n, n-2}^{min}$  is the tree  $P_{1, n-1}^1$ ;  $G_{n, n-3}^{min}$  is the tree  $P_{1, 1, n-2}^{1, n-4}$ . They conjectured  $G_{n, n-e}^{min} = P_{\lfloor \frac{e-1}{2} \rfloor, \lceil \frac{e-1}{2} \rceil, n-e+1}^{\lfloor \frac{e-1}{2} \rfloor, n-e-\lceil \frac{e-1}{2} \rceil}$  for any constant  $e \geq 1$  and  $n$  large enough.

This conjecture is proved for  $e = 4$  by Yuan et al. [5] and for  $e = 5$  by Cioabă et al. [2]. However, it is disproved for  $e = 6$  by [11] and any  $e \geq 6$  by [2] when  $n$  large enough. Cioabă-van Dam-Koolen-Lee [2] proved the following theorem.

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

$$\begin{aligned} \mathcal{P}_{n, e} &= \left\{ P_{2, 1, \dots, 1, 2, n-e+1}^{2, m_2, \dots, m_{e-4}, n-e-2} \mid 2 < m_2 < \dots < m_{e-4} < n-e-2 \right\}, \\ \mathcal{P}'_{n, e} &= \left\{ P_{2, 1, \dots, 1, 1, n-e+1}^{2, m_2, \dots, m_{e-3}, n-e-1} \mid 2 < m_2 < \dots < m_{e-3} < n-e-1 \right\}, \\ \mathcal{P}''_{n, e} &= \left\{ P_{1, 1, \dots, 1, 1, n-e+1}^{1, m_2, \dots, m_{e-2}, n-e-1} \mid 1 < m_2 < \dots < m_{e-2} < n-e-1 \right\}. \end{aligned}$$

Cioabă et al. [2] made three conjectures.

**Conjecture 1** ([2], 5.3) For fixed  $e \geq 5$ , 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  $P_{2,1,2,n-5}^{2, \lceil \frac{D-1}{2} \rceil, D-2}$  is the unique minimizer graph with  $n$  vertices and diameter  $D = n - 6$ , for  $n$  large enough.

**Conjecture 3** ([2], 5.5) The graph  $P_{2,1,1,2,n-6}^{2, \lceil \frac{D+2}{3} \rceil, D - \lfloor \frac{D+2}{3} \rfloor, D-2}$  is the unique minimizer graph with  $n$  vertices and diameter  $D = n - 7$ , for  $n$  large enough. <sup>1</sup>

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 Figure 2). The parameters  $k_i$ 's and  $m_i$ 's are related as follows. In the first family  $\mathcal{P}_{n,e}$ ,  $T_{(k_1, k_2, \dots, k_{e-4})} = P_{2,1, \dots, 1, 2, n-e+1}^{2, m_2, \dots, m_{e-4}, n-e-2}$  if  $k_i = m_{i+1} - m_i - 1$  for  $1 \leq i \leq e - 4$ , where  $m_1 = 2$  and  $m_{e-3} = n - e - 2$ . In the second family  $\mathcal{P}'_{n,e}$ ,  $T'_{(k_1, k_2, \dots, k_{e-3})} = P_{2,1, \dots, 1, 1, n-e+1}^{2, m_2, \dots, m_{e-3}, n-e-1}$  if  $k_i = m_{i+1} - m_i - 1$  for  $1 \leq i \leq e - 3$ , where  $m_1 = 2$  and  $m_{e-2} = n - e - 1$ . In the third family  $\mathcal{P}''_{n,e}$ ,  $T''_{(k_1, k_2, \dots, k_{e-2})} = P_{1,1, \dots, 1, 1, n-e+1}^{1, m_2, \dots, m_{e-2}, n-e-1}$  if  $k_i = m_{i+1} - m_i - 1$  for  $1 \leq i \leq e - 2$ , 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  $n - 2e$ .

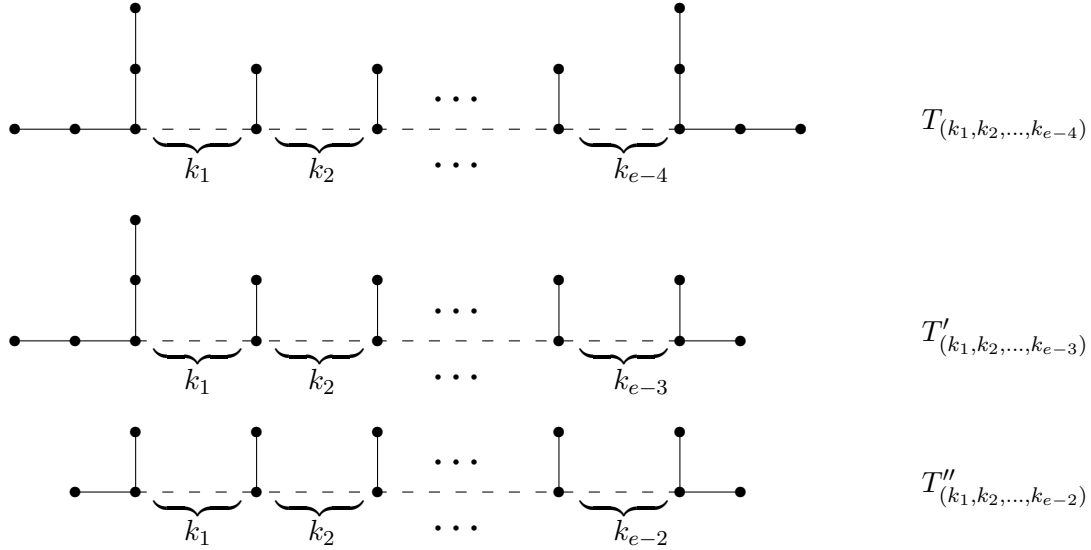


Figure 2: The three families of graphs:  $\mathcal{P}_{n,e}$ ,  $\mathcal{P}'_{n,e}$ ,  $\mathcal{P}''_{n,e}$ .

We have the following theorem.

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

1.  $\lfloor s \rfloor - 1 \leq k_j \leq \lfloor s \rfloor \leq k_i \leq \lceil s \rceil + 1$  for  $2 \leq i \leq e - 5$  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  $G_{n,n-e}^{\min} = T_{(s-1, s, \dots, s, s-1)}$ .

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

<sup>1</sup>Conjecture 5.5 of [2] contains a typo: "... $P_{2,1,1,2,n-6}^{2, \lceil \frac{D-2}{3} \rceil, D - \lfloor \frac{D-2}{3} \rfloor, D-2}$  ...".

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

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

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

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

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

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

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 proofs 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 [6, 7, 9, 11], which will be used later.

**Lemma 2.1** [6] 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** [6] Let  $G_1$  and  $G_2$  be two graphs, then the following statements hold.

1. If  $G_2$  is a proper subgraph of  $G_1$ , then  $\rho(G_1) > \rho(G_2)$ .
2. If  $G_2$  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  $\rho(G_1) > \rho(G_2)$ .

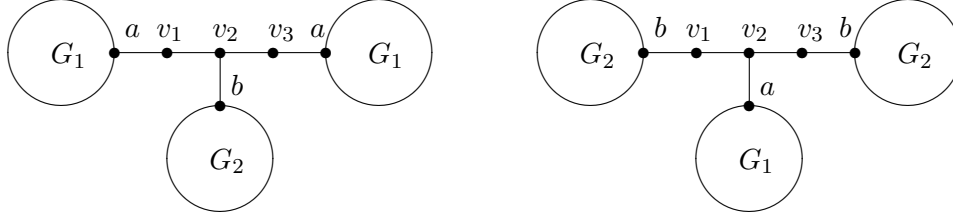


Figure 3: The graphs  $H_1$  and  $H_2$

**Lemma 2.3** [11] *Let  $G_1$  and  $G_2$  be two (possibly empty) 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 Figure 3. Then  $\rho(H_1) = \rho(H_2)$ .*

**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  $\rho(G_{u,v}) < \rho(G)$ .*

**Theorem 2.1 (Cauchy Interlace Theorem (see p.183, [9]))** *Let  $A$  be a Hermitian matrix of order  $n$ , and let  $B$  be a principal submatrix of  $A$  of order  $n - 1$ . If  $\lambda_n \leq \lambda_{n-1} \leq \dots \leq \lambda_1$  lists the eigenvalues of  $A$  and  $\mu_{n-1} \leq \mu_{n-2} \leq \dots \leq \mu_1$  the eigenvalues of  $B$ , then*

$$\lambda_n \leq \mu_{n-1} \leq \lambda_{n-1} \leq \dots \leq \lambda_2 \leq \mu_1 \leq \lambda_1.$$

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 by Figure 4.

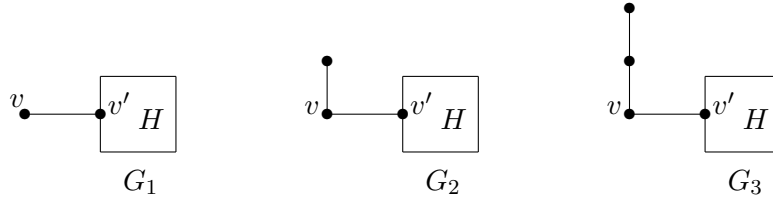


Figure 4: For  $i = 1, 2, 3$ , three graphs  $(G_i, v)$  are constructed from  $(H, v')$ .

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  $(G_1, v)$ .

Let  $\lambda_0$  be the constant  $\sqrt{2 + \sqrt{5}} = 2.058\dots$ . In this paper, we consider only the range  $\lambda \geq \lambda_0$ . 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

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

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

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

This definition can be written in the following matrix form:

$$\begin{pmatrix} \phi_G \\ \phi_{G-v} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix} \begin{pmatrix} p_{(G,v)} \\ q_{(G,v)} \end{pmatrix}. \quad (2)$$

Using Equation (1), we can solve  $p_{(G,v)}$  and  $q_{(G,v)}$  and get

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

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

$$\begin{pmatrix} p_{(P_1,v)} \\ q_{(P_1,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1^2 \\ x_2^2 \end{pmatrix}, \quad (4)$$

$$\begin{pmatrix} p_{(P_3,v)} \\ q_{(P_3,v)} \end{pmatrix} = \lambda \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}, \quad (5)$$

$$\begin{pmatrix} p_{(P_5,v)} \\ q_{(P_5,v)} \end{pmatrix} = \frac{\lambda^2 - 1}{x_2 - x_1} \begin{pmatrix} (\lambda - x_1^3)x_1 \\ (x_2^3 - \lambda)x_2 \end{pmatrix}. \quad (6)$$

We have the following lemma.

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

$$\lim_{\lambda \rightarrow +\infty} q_{(G,v)}(\lambda) = +\infty. \quad (7)$$

**Proof** From Lemma 2.1, we have

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

By Equation (3), 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  $\phi_{G-v}$  is a polynomial of degree  $n - 1$  with highest coefficient 1 while  $\phi_{G-w-v}$  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  $\lambda$  approaches infinity.  $\square$

**Lemma 2.6** *Let  $G_1, G_2, G_3$  be the graphs shown in Figure 4. 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 equations (2) (3), 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.  $\square$

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

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

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:

$$d_1 = \lambda - x_1^3, \tag{8}$$

$$d_2 = x_2^3 - \lambda. \tag{9}$$

Note that  $d_2 = 0$  if  $\lambda = \lambda_0$ . The equation (6) can be written as

$$\begin{pmatrix} p_{(P_5,v)} \\ q_{(P_5,v)} \end{pmatrix} = \frac{\lambda^2 - 1}{x_2 - x_1} \begin{pmatrix} d_1 x_1 \\ d_2 x_2 \end{pmatrix}. \tag{10}$$

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

$$d_1 x_2 - d_2 x_1 = 2. \tag{11}$$

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.

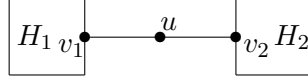


Figure 5: The graph  $(H_1, v_1) \cdot P_1 \cdot (H_2, v_2)$

**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 2.6, we have

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

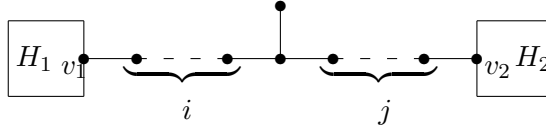


Figure 6: The graph  $G_{i,j}$

**Lemma 2.8** Let  $G_{i,j}$  be the graph shown in Figure 6 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

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

The proof is completed.  $\square$



**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

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

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  $\lim_{\lambda \rightarrow \infty} \phi_{G_2}(\lambda) = +\infty$ , 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 $T_{(k-1, k, \dots, k, k-1)}$

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

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

**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 “ $\geq$ ”, then these inequalities are still equivalent to each other. These equivalences can be proved by equation (11). The details are omitted.

**Remark 2:** For any  $k \geq 4$ , we have  $\rho_k \leq \rho_4 < \frac{3}{2}\sqrt{2}$ . For any  $e \geq 6$  and  $n \geq (k+2)(e-4) + 6$ , we can obtain a tree  $T$  on  $n$  vertices and diameter  $n-e$  by subdividing some edges on internal paths of  $T_{(k-1, k, \dots, k, k-1)}$ . By Lemma 2.4, we have

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

In particular, for  $e \geq 6$  and  $n \geq (k+2)(e-4) + 6 = |T_{(k-1, k, \dots, k, k-1)}|$ , we have  $\rho(G_{n, n-e}^{min}) < \frac{3}{2}\sqrt{2}$ . 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  $e \geq 6$ . Thus,  $\rho(G_{n, n-e}^{min}) \geq \sqrt{2+\sqrt{5}}$ .

**Proof of Lemma 2.10.** Let  $G = T_{(k-1, k, \dots, k, k-1)}$  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

$$\begin{aligned}
\phi_G &= (1, 1) \begin{pmatrix} p(T_{(k-1, k, \dots, k, k-1), v}) \\ q(T_{(k-1, k, \dots, k, k-1), v}) \end{pmatrix} \\
&= (1, 1) A^2 C A^{k-1} B A^k \dots B A^{k-1} C A \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix}^{-1} \begin{pmatrix} \lambda \\ 1 \end{pmatrix} \\
&= \frac{(\lambda^2 - 1)^2}{x_2 - x_1} (-d_1, d_2) A^{k-1} B A^k \dots B A^{k-1} \begin{pmatrix} d_1 x_1 \\ d_2 x_2 \end{pmatrix} \\
&= \frac{(\lambda^2 - 1)^2}{x_2 - x_1} (-d_1, d_2) A^{k-1} B A^k \dots B A^k \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}.
\end{aligned}$$

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  $\phi_G$  as

$$\phi_G = \frac{(\lambda^2 - 1)^2}{x_2 - x_1} (-d_1 x_1^l, d_2 x_2^l) (A^l B A^{l+1})^{r-1} \begin{pmatrix} d_1 x_1^l \\ d_2 x_2^l \end{pmatrix}. \quad (12)$$

It is easy to calculate

$$A^l B A^{l+1} = \frac{1}{x_2 - x_1} \begin{pmatrix} d_1 x_1^k & 1 \\ -1 & d_2 x_2^k \end{pmatrix}. \quad (13)$$

Now we prove that  $\rho_k$  is a root of  $\phi_G$ . At  $\lambda = \rho_k$ , we have  $d_1 x_1^l = d_2 x_2^l$  and  $d_1 x_1^k + 1 = d_2 x_2^k - 1$ . Thus

$$\begin{aligned}
(A^l B A^{l+1}) \begin{pmatrix} 1 \\ 1 \end{pmatrix} &= \frac{1}{x_2 - x_1} \begin{pmatrix} d_1 x_1^k & 1 \\ -1 & d_2 x_2^k \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\
&= \frac{d_1 x_1^k + 1}{x_2 - x_1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.
\end{aligned}$$

We have

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

It remains to prove  $\phi_G(\lambda) > 0$  for any  $\lambda > \rho_k$ . When  $\lambda > \rho_k$ , we have  $d_2 x_2^k - 1 > d_1 x_1^k + 1$  (and  $d_2 x_2^l > d_1 x_1^l$ ). It is easy to check  $A^l B A^{l+1}$  maps the region  $\{(z_1, z_2) : z_2 \geq z_1 > 0\}$  to  $\{(z_1, z_2) : z_2 > z_1 > 0\}$ . By induction on  $r$ ,  $(A^l B A^{l+1})^{r-1}$  maps the region  $\{(z_1, z_2) : z_2 \geq z_1 > 0\}$  to  $\{(z_1, z_2) : z_2 > z_1 > 0\}$ . Let

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = (A^l B A^{l+1})^{r-1} \begin{pmatrix} d_1 x_1^l \\ d_2 x_2^l \end{pmatrix}.$$

Since  $d_2 x_2^l > d_1 x_1^l > 0$ , we have  $z_2 > z_1 > 0$ . From equation (12), we get

$$\begin{aligned}
\phi_G &= \frac{(\lambda^2 - 1)^2}{x_2 - x_1} (-d_1 x_1^l, d_2 x_2^l) (A^l B A^{l+1})^{r-1} \begin{pmatrix} d_1 x_1^l \\ d_2 x_2^l \end{pmatrix} \\
&= \frac{(\lambda^2 - 1)^2}{x_2 - x_1} (-d_1 x_1^l, d_2 x_2^l) \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \\
&= \frac{(\lambda^2 - 1)^2}{x_2 - x_1} (d_2 x_2^l z_2 - d_1 x_1^l z_1) \\
&> 0.
\end{aligned}$$

The proof of the Lemma is finished.  $\square$

## 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.

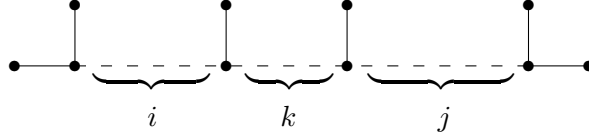


Figure 7: The graphs  $T''_{(i,k,j)}$

**Lemma 2.11** *Let  $T''_{(i,k,j)}$  be the tree shown in Figure 7 and  $\rho''_k$  be the unique root of  $d_2 = x_1^k$  in the interval  $(\sqrt{2 + \sqrt{5}}, +\infty)$ . Then  $\lim_{i,j \rightarrow \infty} \rho(T''_{(i,k,j)}) = \rho''_k$ .*

**Proof** By Lemma 2.4, we have

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

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

$$\begin{aligned} & \phi_{T''_{(l,k,l)}} \\ &= (1, 1) \begin{pmatrix} p_{(T''_{(l,k,l)}, v)} \\ q_{(T''_{(l,k,l)}, v)} \end{pmatrix} \\ &= (1, 1) ABA^l BA^k BA^l B \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix}^{-1} \begin{pmatrix} \lambda \\ 1 \end{pmatrix} \\ &= \frac{x_2^{2l-k+1} (d_2 x_2 + x_1^2)^2}{(x_2 - x_1)^5} \left[ ((d_2 x_2^k)^2 - 1) - 2x_1^{2l-k+3} (d_1 x_1^k + d_2 x_2^k) - x_1^{2(2l-k+3)} ((d_1 x_1^k)^2 - 1) \right]. \end{aligned}$$

As  $l$  goes to infinity,  $\lim_{l \rightarrow \infty} \rho(T''_{(l,k,l)})$  is the largest root of  $(d_2 x_2^k)^2 - 1 = 0$ ; namely  $d_2 = x_1^k$ . The proof is completed.  $\square$

We have the following Corollary from Lemma 2.11.

**Corollary 2.2** *Let  $T''_{(k,i)}$  be the tree shown in Figure 8. We have  $\lim_{i \rightarrow \infty} \rho(T''_{(k,i)}) = \rho''_{2k+3}$ .*

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

**Lemma 2.12** *Let  $T'_{(k,j)}$  be the tree shown in Figure 9 and  $\rho'_k$  be the unique root of  $d_2 = d_1^{\frac{1}{2}} x_1^{k+\frac{1}{2}}$  in the interval  $(\sqrt{2 + \sqrt{5}}, +\infty)$ . Then  $\lim_{j \rightarrow \infty} \rho(T'_{(k,j)}) = \rho'_k$ .*

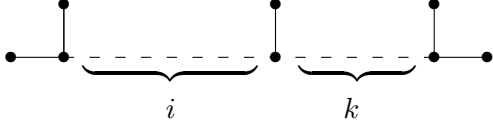


Figure 8: The graph  $T''(k, i)$

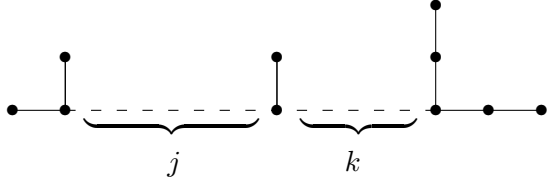


Figure 9: The graph  $T'(k, j)$

**Proof** Similarly, we have

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

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

## 2.5 Comparison of $\rho_k$ , $\rho'_k$ , and $\rho''_k$

Observe that  $\rho_k$ ,  $\rho'_k$ , and  $\rho''_k$  satisfy similar equations. Since  $1 < \sqrt{d_1 x_1} < \frac{2}{1-x_1^{k+1}}$ , we have

$$\rho''_k \leq \rho'_k \leq \rho_k.$$

For  $\lambda \in [\lambda_0, \frac{3}{2}\sqrt{2}]$ ,  $x_2$ ,  $d_2$ , and  $d_1 x_1$  are increasing while  $x_1$  is decreasing. Using these facts, it is easy to check that for  $k \geq 7$ ,  $\rho_k$ ,  $\rho'_k$ , and  $\rho''_k$  are in the interval  $(\lambda_0, \frac{3}{2}\sqrt{2})$ .

We have the following lemma.

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

**Proof** Recall that  $\rho''_{k-4}$  is the root of  $d_2 = x_1^{k-4}$  and  $\rho_k$  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  $k \geq 7$ , we have

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

Note that  $\rho'_{k-3}$  is the root of  $d_2 = \sqrt{d_1 x_1} x_1^{k-3}$ . It suffices to show  $2 < \sqrt{d_1 x_1} x_2^3(1-x_1^{k+1})$  for  $\lambda \in [\lambda_0, \frac{3}{2}\sqrt{2}]$ . We have

$$\begin{aligned}
\sqrt{d_1 x_1} x_2^3(1-x_1^{k+1}) &\geq \sqrt{d_1 x_1} x_2^3(1-x_1^8) \\
&\geq \sqrt{d_1 x_1} x_2^3(1-x_1^8)|_{\lambda_0} \\
&> 2.
\end{aligned}$$

The proof is completed.  $\square$

### 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  $G_{n,n-e}^{min} \in \mathcal{P}_{n,e}$ . In the second part, we prove the other statements in Theorem 1.1.

#### 3.1 Part 1

Let  $\rho_{n,n-e}^{min} = \rho(G_{n,n-e}^{min})$  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  $e \geq 6$  and  $n \geq 10e^2 - 74e + 142$ , then  $G_{n,n-e}^{min} \in \mathcal{P}_{n,e}$ .*

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

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

$$\begin{aligned} \rho_{n,n-e}^{min} &> \rho'_{k_1}, \\ \rho_{n,n-e}^{min} &> \rho''_{2k_{e-3}+3}, \\ \rho_{n,n-e}^{min} &> \rho''_{k_i}, \quad \text{for } 2 \leq i \leq e-4. \end{aligned}$$

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

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

Otherwise, we have

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

We get

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

Contradiction!

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

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

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  $T_{(k-1, k, \dots, k, k-1)}$ . Since  $n \geq 10e^2 - 74e + 142$ , we have

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

We get

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

Contradiction!

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

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

where  $l_2 = \lceil \frac{n-3e+7}{e-3} \rceil$ . A similar argument shows  $\rho_{n,n-e}^{min} > \rho_{l_2+4}$ . 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  $e \geq 5$  and  $n \geq 10e^2 - 74e + 142$ , we have  $n > 5e^2 - 31e + 50$ ; thus,

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

We get

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

Contradiction! □

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

### 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 Figure 10.

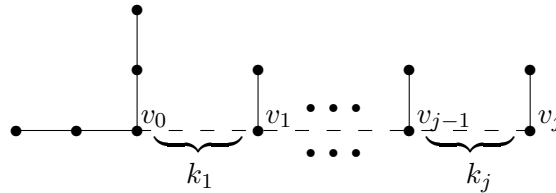


Figure 10: The graphs  $H_{(k_1, \dots, k_j)}$

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  $\lambda \geq \rho(T_{(k_1, k_2, \dots, k_r)})$ , we have

1.  $p_{(L_i, v_i)}(\lambda) \geq 0$  and  $q_{(L_i, v_i)}(\lambda) \geq 0$  for  $i = 0, 1, 2, \dots, r-1$ ;
2.  $p_{(R_j, v_{j-1})}(\lambda) \geq 0$  and  $q_{(R_j, v_{j-1})}(\lambda) \geq 0$  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 equation (10), we have  $p'_{r+1} = p_0 = p(P_5, v_0) = \frac{d_1 x_1 (\lambda^2 - 1)}{x_2 - x_1} > 0$  and  $q'_{r+1} = q_0 = q(P_5, v_0) = \frac{d_2 x_2 (\lambda^2 - 1)}{x_2 - x_1} > 0$  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  $\mu$  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  $\lambda \geq \mu$ .

We need to show such  $\mu$  exists. By Lemma 2.5, we have  $\lim_{\lambda \rightarrow +\infty} q_i(\lambda) = +\infty$  and  $\lim_{\lambda \rightarrow +\infty} q'_j(\lambda) = +\infty$ . Since  $\lim_{\lambda \rightarrow +\infty} p_0 = \lim_{\lambda \rightarrow +\infty} \frac{d_1 x_1 (\lambda^2 - 1)}{x_2 - x_1} = +\infty$  and  $p_i = \frac{1}{x_2 - x_1} (d_1 x_1^{k_i} p_{i-1} + x_2^{k_i - 1} q_{i-1})$  (see Lemma 2.6), by induction on  $i$ , we have  $\lim_{\lambda \rightarrow +\infty} p_i(\lambda) = +\infty$ . Similarly, we have  $\lim_{\lambda \rightarrow +\infty} p'_j(\lambda) = +\infty$ . Thus  $\mu$  is well-defined.

If  $\mu \leq \rho(T_{(k_1, k_2, \dots, k_r)})$ , then we are done. Otherwise, we assume  $\mu > \rho(T_{(k_1, k_2, \dots, k_r)})$ . Note that  $\mu$  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  $i$  ( $1 \leq i \leq r - 1$ ) such that  $p_i(\mu) = 0$ . Since  $p_i = \frac{1}{x_2 - x_1} (d_1 x_1^{k_i} p_{i-1} + x_2^{k_i - 1} q_{i-1})$ , we must have  $p_{i-1}(\mu) = q_{i-1}(\mu) = 0$ . By Lemma 2.7, we have

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

It contradicts to the assumption  $\mu > \rho(T_{(k_1, k_2, \dots, k_r)})$ .

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

**Case (3)** There exists an  $i$  ( $1 \leq i \leq r - 1$ ) such that  $q_i(\mu) = 0$ . By Lemma 2.7, we have

$$\phi_{T_{(k_1, k_2, \dots, k_r)}}(\mu) = (x_2 - x_1)(x_2^{k_{i+1} - 1} q_i q'_{i+2} - x_1^{k_{i+1} - 1} p_i p'_{i+2})|_{\mu} \leq 0.$$

It contradicts to  $\mu > \rho(T_{(k_1, k_2, \dots, k_r)})$ .

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

The proof of this Lemma is finished.  $\square$

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

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

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

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

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

$$t^2 - (d_2 x_2 - d_1 x_1^{2s-1}) t + x_1^{2s-2} = 0.$$

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

$$d_2 = 2x_1^s + d_1 x_1^{2s}. \quad (14)$$

We choose  $s = s(\lambda)$  to be the root of Equation (14). 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

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

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

$$f_{k_i}(t) = f_s(x_2^{2(k_i-s)}t) \leq x_2^{2(k_i-s)}t. \quad (15)$$

By Lemma 2.7, we get

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

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

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

Note  $t'_{r+1} = t_0 = \frac{d_2 x_2}{d_1 x_1} = \frac{d_2}{d_1} x_2^2$ . Applying inequality (15) recursively, we have

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

We get  $d_2 \geq d_1 x_1^{r\bar{k}-(r-1)s+1}$ ; and the equality holds if and only if  $k_1 + 1 = k_2 = \dots = k_{r-1} = k_r + 1 = s$  and  $\lambda = \rho(T_{(k_1, k_2, \dots, k_r)})$ . By Remark 1,  $d_2 \geq d_1 x_1^{r\bar{k}-(r-1)s+1}$  is equivalent to

$$d_2 \geq 2x_1^{r\bar{k}-(r-1)s+2} + d_1 x_1^{2(r\bar{k}-(r-1)s+2)}. \quad (16)$$

Comparing this inequality with equation (14), we must have  $s \leq r\bar{k} - (r-1)s + 2$ . Solving  $s$ , we get  $s \leq \bar{k} + \frac{2}{r}$ . Thus,

$$d_2 = 2x_1^s + d_1 x_1^{2s} \geq 2x_1^{\bar{k} + \frac{2}{r}} + d_1 x_1^{2(\bar{k} + \frac{2}{r})}.$$

Applying Remark 1 one more time, we get

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

The proof is completed. □

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

$$d_2 \leq \frac{2x_1^{\lceil \bar{k} + \frac{2}{r} \rceil}}{1 - x_1^{\lceil \bar{k} + \frac{2}{r} \rceil + 1}}$$

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



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

$$\rho_{n, n-e}^{\min} \leq \rho(T) \leq \rho(T_{([s]-1, [s], \dots, [s], [s]-1)}) = \rho_{[s]}.$$

By Lemma 2.10,  $\rho_{[s]}$  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  $(\sqrt{2 + \sqrt{5}}, \infty)$ , we get

$$d_2(\rho_{n, n-e}^{\min}) \leq d_2(\rho_{[s]}) = \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}} \Bigg|_{\rho_{[s]}} \leq \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}} \Bigg|_{\rho_{n, n-e}^{\min}}.$$

The proof is completed.  $\square$

We get the following corollary.

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

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

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

**Lemma 3.4** Assume  $G_{n, n-e}^{\min} = T_{(k_1, \dots, k_i, k_{i+1}, \dots, k_r)}$  and  $\bar{c} = \frac{\rho_{n, n-e}^{\min} + \sqrt{(\rho_{n, n-e}^{\min})^2 + 4d_1 d_2}}{2}$ . Then the following equalities hold at the point  $\lambda = \rho_{n, n-e}^{\min}$ .

$$\bar{c}x_1^{k_i+1} \leq d_2 \leq \bar{c}x_1^{k_i-1} \quad \text{for } i = 2, \dots, r-1; \quad (17)$$

$$\sqrt{\bar{c}d_1}x_1^{k_i+1} \leq d_2 \leq \sqrt{\bar{c}d_1}x_1^{k_i} \quad \text{for } i = 1, r. \quad (18)$$

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

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

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

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

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

We can rewrite it as

$$\left(t_{i-1} - \frac{x_1^{2k_i-1}}{d_2}\right) \left(t'_{i+2} - \frac{x_1^{2k_{i+1}-1}}{d_2}\right) = \frac{d_1 d_2 + 1}{d_2^2} x_1^{2(k_i+k_{i+1}-1)}. \quad (19)$$

Note  $t_i = f_{k_i}(t_{i-1}) = \frac{d_2 x_2 t_{i-1} - x_1^{2(k_i-1)}}{t_{i-1} + d_1 x_1} > 0$ . We have

$$t_{i-1} > \frac{x_1^{2k_i-1}}{d_2}. \quad (20)$$

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

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

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

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

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

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

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

On the one hand, by inequality (20), we can substitute  $t'_{i+2} \leq t_{i-1} x_1^{2(k_{i+1}-k_i-1)}$  into equation(19) and get

$$\left( t_{i-1} - \frac{x_1^{2k_i-1}}{d_2} \right) \left( x_1^{2(k_{i+1}-k_i-1)} t_{i-1} - \frac{x_1^{2k_{i+1}-1}}{d_2} \right) \geq \frac{d_1 d_2 + 1}{d_2^2} x_1^{2(k_i+k_{i+1}-1)}.$$

After simplification, we have

$$d_2 t_{i-1}^2 - x_1^{2k_i} \rho_{n, n-e}^{min} t_{i-1} - d_1 x_1^{4k_i} \geq 0.$$

Recall  $\bar{c} = \frac{\rho_{n, n-e}^{min} + \sqrt{(\rho_{n, n-e}^{min})^2 + 4d_1 d_2}}{2}$ . Solving this quadratic inequality, since  $t_{i-1} > 0$ , we get

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

By symmetry, we have

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

On the other hand, we substitute  $t_{i-1} \geq t'_{i+2} x_1^{2(k_{i+1}-k_i-1)}$  into equation (19). By the similar calculation, we get

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

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

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

By symmetry, we have

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

Combining the inequalities above, we get

$$\frac{\bar{c}}{d_2} x_1^{2k_i} \leq t_{i-1} \leq \frac{\bar{c}}{d_2} x_1^{2(k_i-1)}, \quad i = 1, \dots, r-1, \quad (21)$$

$$\frac{\bar{c}}{d_2} x_1^{2k_i} \leq t'_{i+1} \leq \frac{\bar{c}}{d_2} x_1^{2(k_i-1)}, \quad i = 2, \dots, r. \quad (22)$$

Now we apply Lemma 2.7 and get

$$t_{i-1} t'_{i+1} x_2^{2(k_i-1)} = 1. \quad (23)$$

Taking product of inequalities (21), (22), and then substituting  $t_{i-1} t'_{i+1}$  into equation (23). After simplification, we get inequality (17).

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 (18). The proof of this lemma is completed.  $\square$

**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

$$2d_2 x_1^{k_i+1} \leq \rho_{n,n-e}^{\min} + \sqrt{(\rho_{n,n-e}^{\min})^2 + 4d_1 d_2} \leq 2d_2 x_1^{k_i-1}.$$

After solving  $d_2$  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

$$\frac{2x_1^{k_i+1}}{1 - x_1^{k_i+2}} < d_2 < \frac{2x_1^{k_i-2}}{1 - x_1^{k_i-1}} \quad \text{for } 2 \leq i \leq r-1. \quad (24)$$

From Theorem 3.1, we have

$$\frac{2x_1^s}{1 - x_1^{s+1}} \leq d_2 \leq \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}}. \quad (25)$$

Combining inequalities (24) and (25), we get

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

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

For  $j = 1$  or  $r$ , combining inequalities (18) and (25), we have

$$\begin{aligned}\frac{\sqrt{\bar{c}d_1}}{2}x_1^{k_j+1} &\leq \frac{x_1^{\lfloor s \rfloor}}{1-x_1^{\lfloor s \rfloor+1}}, \\ \frac{\sqrt{\bar{c}d_1}}{2}x_1^{k_j} &\geq \frac{x_1^s}{1-x_1^{s+1}}.\end{aligned}$$

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

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

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

In conclusion, we get

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

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

Now we will prove item 2. It suffices to show  $k_i - k_j \leq 2$ , for  $2 \leq i \leq r - 1$  and  $j = 1, r$ . Suppose that there exist  $i, j$  with  $i \in \{2, \dots, r - 1\}$  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  $\lambda x_1^2 = (1 + x_1^2)x_1 < 2x_1 \leq d_1$  for  $\lambda \geq \lambda_0$  and  $\bar{c} \rightarrow \lambda_0$  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  $i, j \in \{2, \dots, r - 1\}$  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 (17) to  $k_i = k$  and  $k_j = k + 2$ , we have

$$\begin{aligned}d_2 &\geq \bar{c}x_1^{k_i+1} = \bar{c}x_1^{k+1}, \\ d_2 &\leq \bar{c}x_1^{k_j-1} = \bar{c}x_1^{k+1}.\end{aligned}$$

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 (21) and (22).

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

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

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  $(k_1, k_2, \dots, k_r)$  satisfying items 1-3 is  $(s - 1, s, \dots, s, s - 1)$ . In particular, we have  $G_{n,n-e}^{min} = T_{(s-1, s, \dots, s, s-1)}$ .

The proof is completed.  $\square$

## 4 Proofs of Theorems 1.3 and 1.4

### 4.1 $e=7$

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

**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

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

**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

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

In the last step, we applied the fact  $d_2 x_1 + 1 = d_1 x_2 - 1$ .

By Lemma 2.10 and Remark 1,  $\rho(T_{(k, k+1, k)}) (= \rho_{k+1})$  satisfies  $d_2 x_2^{k/2} = d_1 x_1^{k/2}$ . The largest root of  $\phi_{T_{(k, k, k)}} - \phi_{T_{(k, k+1, k-1)}} = 0$  is  $\rho_{k+1}$ .

Noting that  $d_2^2 x_2^k - d_1^2 x_1^k$  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  $G_{n, n-7}^{min} = T_{(k, k, k)}$ .

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

**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  $\sqrt{2 + \sqrt{5}} \leq \lambda < \rho_{k+1}$ . 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  $G_{n,n-7}^{min} = T_{(k,k+2,k)}$ .

The proof of Theorem 1.3 is completed.  $\square$

## 4.2 e=8

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

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

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  $\rho$  is the root of both equations

$$\frac{q^{(k,k)}}{p^{(k,k)}} = \frac{p^{(k)}}{q^{(k)}}x_1^{2k-2} \quad \text{and} \quad \frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}} = \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}. \quad (26)$$

Note that  $\rho'$  is the root of both equations

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

We have

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

Thus,  $\phi_{T_{(k,k,k+1,k-1)}}(\rho)^2 = -J(\rho)K(\rho) \left( x_1^{2k-2} \frac{p^{(k)}}{q^{(k)}} - \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k} \right)^2 \Big|_{\rho} \leq 0$ . 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  $\bar{c} \rightarrow \lambda_0$  as  $n \rightarrow \infty$ . 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

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

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  $\bar{c} \rightarrow \lambda_0$  as  $n \rightarrow \infty$ . 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.  $\square$

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