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On the k^{th} Eigenvalues of Trees with Perfect Matchings

An Chang¹ and Wai Chee Shiu^{2†}

¹Department of Mathematics, Fuzhou University, Fuzhou, Fujian, 350002, P.R. China.

²Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong, P.R. China.

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Let \mathcal{T}_{2p}^+ be the set of all trees on $2p$ ($p \geq 1$) vertices with perfect matchings. In this paper, we prove that for any tree T in \mathcal{T}_{2p}^+ , the k th largest eigenvalue $\lambda_k(T)$ satisfies $\lambda_k(T) \leq \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor - 1} + \sqrt{\lfloor \frac{p}{k} \rfloor + 3} \right)$ ($k = 1, 2, \dots, p$). This upper bound is known to be best possible when $k = 1$. The set of trees obtained from a tree on p vertices by joining a pendent vertex to each vertex of the tree is denoted by \mathcal{T}_{2p}^* . We also prove that for any tree T in \mathcal{T}_{2p}^* , its k th largest eigenvalue $\lambda_k(T)$ satisfies $\lambda_k(T) \leq \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor - 1} + \sqrt{\lfloor \frac{p}{k} \rfloor + 3} \right)$ ($k = 1, 2, \dots, p$) and show that this upper bound is best possible when $k = 1$ or $p \not\equiv 0 \pmod{k}$. We further give the following inequality

$$\lambda_k^*(2p) > \frac{1}{2} \left(\sqrt{t-1 - \sqrt{\frac{k-1}{t-k}}} + \sqrt{t+3 - \sqrt{\frac{k-1}{t-k}}} \right) \quad t = \lfloor \frac{p}{k} \rfloor,$$

where $\lambda_k^*(2p)$ is the maximum value of the k th largest eigenvalue of the trees in \mathcal{T}_{2p}^* . By this inequality, it is easy to see that the above upper bound on $\lambda_k(T)$ for $T \in \mathcal{T}_{2p}^*$ turns out to be asymptotically tight when $p \equiv 0 \pmod{k}$.

Keywords: tree, eigenvalue, perfect matching.

1 Introduction

Let G be a simple graph, i.e., a graph without loops or multiple edges. Suppose the vertex set of G is $V(G) = \{v_1, v_2, \dots, v_n\}$. The adjacency matrix of G is an $n \times n$ matrix $A(G) = (a_{ij})$, where $a_{ij} = 1$ if v_i is adjacent to v_j , and $a_{ij} = 0$ otherwise. The characteristic polynomial of G is $\det(\lambda I - A(G))$, which is denoted by $P(G; \lambda)$. Since $A(G)$ is symmetric, its eigenvalues are real; moreover, they are independent of the ordering of the vertices of G . As usual, we write them in non-increasing order as $\lambda_1(G) \geq \lambda_2(G) \geq \lambda_3(G) \geq \dots \geq \lambda_n(G)$ and call them the eigenvalues of G . If G is a bipartite graph, then $\lambda_i(G) = -\lambda_{n-i+1}(G)$ for $i = 1, 2, \dots, \lfloor n/2 \rfloor$ (see [6]), where $\lfloor x \rfloor$ denotes the largest integer less than or equal to x , i.e., the floor function of x when x is a real number. Similarly, $\lceil x \rceil$ denotes the least integer greater than or equal to x , i.e., the ceiling function of x .

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Two distinct edges in a graph G incident with the same vertex will be called *adjacent edges*. A *matching* of G is a set of edges in G such that no two of them are adjacent. A largest matching is called a *maximum matching*. The cardinality of a maximum matching of G is commonly known as its *matching number*, denoted by $\mu(G)$. Let M be a matching of G . M is called an *s-matching* of G if M contains exactly s edges of G . A vertex $v \in V(G)$ is said to be *M-saturated* if it is incident with an edge of M , otherwise v is called an *M-unsaturated vertex*. The matching M of G is called a *perfect matching* if all vertices of G are M -saturated. Trees are connected acyclic graphs, and it is obvious that they are also bipartite graphs. So we only need to investigate those eigenvalues $\lambda_k(T)$ of a tree T with n vertices for $k = 1, 2, \dots, \lfloor n/2 \rfloor$.

Throughout this paper, we denote by \mathcal{T}_n and \mathcal{T}_{2p}^+ the set of trees on n vertices and the set of trees on $2p$ vertices with perfect matchings. For simplicity, a tree with n vertices is often called a tree of order n . For symbols and concepts not defined in this paper we refer to the book [2].

The investigation on the eigenvalues of trees in \mathcal{T}_n is one of the oldest problems in the spectral theory of graphs and has been intensively studied by many authors (see [1, 6, 11, 12, 13, 15]). A classic result is that for any $T \in \mathcal{T}_n$, $\lambda_1(T) \leq \sqrt{n-1}$ and equality holds if and only if T is the star $K_{1,n-1}$. In particular, H. Yuan [12] studied the k th eigenvalue of a tree $T \in \mathcal{T}_n$ and obtained the following upper bound.

Theorem 1.1 ([12]) *Let T be a tree in \mathcal{T}_n . Then*

$$\lambda_k(T) \leq \sqrt{\left\lfloor \frac{n-2}{k} \right\rfloor} \quad \left(2 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor\right)$$

and the upper bound is best possible if $n \equiv 1 \pmod{k}$.

J.Y. Shao [15] improved the above result.

Theorem 1.2 ([15]) *Let T be a tree in \mathcal{T}_n . Then*

$$\lambda_k(T) \leq \sqrt{\left\lfloor \frac{n}{k} \right\rfloor} - 1 \quad \left(1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor\right).$$

Moreover, the bound is best possible when $n \not\equiv 0 \pmod{k}$ and it is an asymptotically tight bound when $n \equiv 0 \pmod{k}$ ($2 \leq k \leq \lfloor n/2 \rfloor$).

Concerning the trees in \mathcal{T}_{2p}^+ there are lots of results on the first two largest eigenvalues (see [3, 4, 5, 8, 9, 10, 16, 17, 18]).

Frucht and Harary [7] gave the following construction of graphs. Given two graphs G and H , the *corona of G with H* , denoted by $G \odot H$, is the graph with

$$\begin{aligned} V(G \odot H) &= V(G) \cup \bigcup_{i \in V(G)} V(H_i), \\ E(G \odot H) &= E(G) \cup \bigcup_{i \in V(G)} \left(E(H_i) \cup \{iu_i \mid u_i \in V(H_i)\} \right), \end{aligned}$$

where $H_i \cong H$ for all $i \in V(G)$.

Let $T_{2p}^1 = K_{1,p-1} \odot N_1$ (see Fig. 1.1), where N_s is the null graph (i.e., edgeless graph) of order s . G.H. Xu [17] got the following initial result.

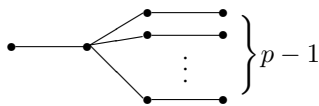


Fig. 1.1: The tree T_{2p}^1

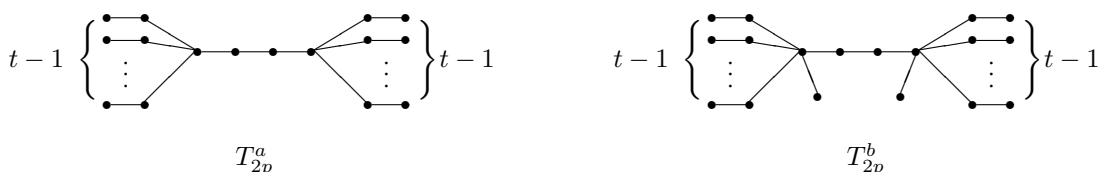


Fig. 1.2: Two graphs T_{2p}^a and $T_{2p}^b (= T_{2p}^{2'})$

Theorem 1.3 ([17]) Let T be a tree in \mathcal{T}_{2p}^+ . Then

$$\lambda_1(T) \leq \frac{1}{2}(\sqrt{p-1} + \sqrt{p+3}) = \lambda_1(T_{2p}^1) \quad p = 1, 2, 3, \dots$$

and equality holds if and only if $T \cong T_{2p}^1$.

A. Chang [3] studied bounds for the second largest eigenvalue of trees in \mathcal{T}_{2p}^+ and proposed the following conjecture:

Let p be a positive integer, and T be a tree in \mathcal{T}_{2p}^+ . Then

$$\lambda_2(T) \leq \begin{cases} r' & \text{if } p = 2t \\ r'' & \text{if } p = 2t + 1 \end{cases} \quad \text{for } t = 1, 2, 3, \dots,$$

where r' and r'' are the maximum positive roots of the equations $x^3 - (t+1)x + 1 = 0$ and $x^4 - (t+2)x^2 + x + 1 = 0$, respectively. Equality holds in the first inequality if and only if $T \cong T_{2p}^a$, and equality holds in the second inequality if and only if $T \cong T_{2p}^b$, where T_{2p}^a and T_{2p}^b are the trees shown in Fig. 1.2

More recently, J-M. Guo and S-W. Tan [9] proved that the second inequality holds but the first one does not hold. A correct version of the first inequality was given by J-M. Guo and S-W. Tan in [10]. Their results can be stated as follows.

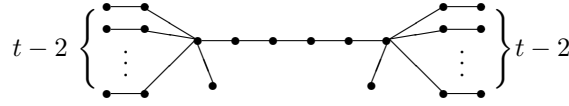


Fig. 1.3: The tree T_{2p}^2

Theorem 1.4 ([9, 10]) Let p be a positive integer, and T be a tree in \mathcal{T}_{2p}^+ . Then

$$\lambda_2(T) \leq \begin{cases} r_1 & \text{if } p = 2t \\ r_2 & \text{if } p = 2t + 1 \end{cases} \text{ for } t = 2, 3, \dots,$$

where r_1 and r_2 are the maximum positive roots of the equations $(x^4 - (t + 1)x^2 + 1)(x^2 + x - 1) + x = 0$ and $x^4 - (t + 2)x^2 + x + 1 = 0$, respectively. Equality holds in the first inequality if and only if $T \cong T_{2p}^2$, and equality holds in the second inequality if and only if $T \cong T_{2p}^{2'}$, where T_{2p}^2 and $T_{2p}^{2'} \cong T_{2p}^b$ are the trees shown in Fig. 1.3 and 1.2, respectively.

It is natural to consider the problem of determining upper and lower bounds of the k th eigenvalues of the trees in \mathcal{T}_{2p}^+ . This is the purpose of our paper.

2 Main results

We need some groundwork before giving the main result. Before we recall the well-known *Cauchy Interlacing Theorem* [6, Theorem 0.10], we introduce some notation and terminology first. A vertex subset with k vertices is called a k -vertex subset. Suppose V' is a subset of vertices. $G - V'$ is the subgraph of G obtained by deleting all vertices in V' together with their incident edges. Cauchy Interlacing Theorem usually plays an important role in the estimation of the k th eigenvalue of trees.

Theorem 2.1 (Cauchy Interlacing Theorem) For every graph G and every k -vertex subset V' we have

$$\lambda_i(G) \geq \lambda_i(G - V') \geq \lambda_{i+k}(G), \quad i = 1, 2, \dots, n - k.$$

Lemma 2.2 ([1]) Let G be a graph and H a subgraph of G . Then $\lambda_1(H) \leq \lambda_1(G)$.

Lemma 2.3 ([15]) Let T be a tree in \mathcal{T}_n . Then for any positive integer s , there exists a vertex $v \in V(T)$ such that the largest component of $T - v$ has order at most $\max\{n - 1 - s, s\}$ and all other components of $T - v$ have orders at most s .

It is worth mentioning that when the tree T considered in Lemma 2.3 is in \mathcal{T}_{2p}^+ , i.e., T is a tree with a perfect matching, then obviously all components of $T - v$ but one have perfect matchings. The only component without perfect matching, say T_0 , has matching number $\mu(T_0) = \frac{1}{2}(V(T_0) - 1)$, and the only unsaturated vertex of T_0 is the vertex w which is adjacent with v in T and wv is an edge of the perfect matching of T . This fact leads us to get the following useful lemma.

Lemma 2.4 *Let $T \in \mathcal{T}_n^+$, and let s be a positive even integer not greater than n . Then there exist a vertex $v \in V(T)$ and a subtree U of T such that*

1. U has a perfect matching;
2. either U is a component of $T - v$ when $v \notin V(U)$, or $U - v$ is a component of $T - v$ when $v \in V(U)$;
3. $|V(U)| \leq \max\{n - s, s\}$;
4. all components of $(T - V(U)) - v$ have order at most s , and all but at most one of them have a perfect matching.

Proof: Let M be a perfect matching of T . By Lemma 2.3, there exists a vertex $v \in V(T)$ such that one component T' of $T - v$ has order $|V(T')| \leq \max\{n - 1 - s, s\}$, and all other components of $T - v$ have orders not exceeding s . We know that only one component, say T_0 , has no perfect matching and all the others have perfect matchings.

Suppose $T' \neq T_0$. Then $M \cap E(T')$ is a perfect matching of T' . Since s and n are even, $|V(T')| \leq \max\{n - 2 - s, s\}$. Let $U = T'$. Then T_0 is a component of $(T - V(U)) - v$ and its matching number is $\mu(T_0) = \frac{1}{2}(|V(T_0)| - 1)$. Let w be the only unsaturated vertex of T_0 which is adjacent with v in T and vw is an edge of M . Now let T'_0 be the tree obtained from T_0 by joining a pendant vertex u to w . Actually, we can view this vertex u as the removed vertex v . Obviously, T'_0 has a perfect matching $(E(T_0) \cap M) \cup \{vw\}$ and order $|V(T'_0)| = |V(T_0)| + 1 \leq s$, and T'_0 is a subtree of T .

Suppose $T' = T_0$. Then T' has a maximum matching $M_1 = E(T') \cap M$ and its matching number is $\mu(T') = \frac{1}{2}(|V(T')| - 1)$. Since s is even, $|V(T')| \leq \max\{n - 1 - s, s - 1\}$. Let $w \in V(T')$ be the only M_1 -unsaturated vertex. Then vw is an edge of M . Let U be the tree obtained from T' by joining a pendant vertex u to w . Actually, we can view this vertex u as the removed vertex v . Then U is a subtree of T and is of order not greater than $\max\{n - s, s\}$. Clearly, $M_1 \cup \{vw\}$ is a perfect matching of U and $U - v = T'$. □

Lemma 2.5 *Let T be a tree in \mathcal{T}_{2p}^+ . Then for any positive integer k with $1 \leq k \leq p$, there exists a $(k - 1)$ -vertex subset $V' \subset V(T)$ such that all components of $T - V'$ have the largest eigenvalues not greater than $\lambda_1(T_{2t}^1)$, where T_{2t}^1 is the tree shown in Fig. 1.1 and $t = \lceil p/k \rceil$.*

Proof: When $k = 1$, the result is actually Theorem 1.3. So we may assume that $k \geq 2$. Let $s = 2t = 2\lceil p/k \rceil$, and $T_0 = T$, $n_0 = 2p$. Since $k \geq 2$, we have $n_0 > s$. We perform the following procedure:

By Lemma 2.4, there are a vertex $v_1 \in V(T)$ and a subtree T_1 of order not greater than $\max\{n_0 - s, s\}$ such that T_1 has a perfect matching, $T_1 - v_1$ is a component of $T - v_1$ and the other components of $T - v_1$ have orders not greater than s . Note that v_1 may not be a vertex of T_1 .

Let $n_1 = |V(T_1)|$. If all components of $T - v_1$ and T_1 are of orders not greater than s , then we stop the procedure. If not, then $n_1 > s$. By applying Lemma 2.4 to T_1 there are a vertex $v_2 \in V(T_1)$ and a subtree T_2 of T_1 such that the order of T_2 is not greater than $\max\{n_1 - s, s\}$, T_2 has a perfect matching, $T_2 - v_2$ is a component of $T_1 - v_2$ and the other components of $T_1 - v_2$ have orders not greater than s .

Let $n_2 = |V(T_2)|$. If all components of $T - \{v_1, v_2\}$ and T_2 are of orders not greater than s , then we stop the procedure. If not, we continue to perform the above procedure. Since n_0 is finite, there are h subtrees $T_0 \supset T_1 \supset \dots \supset T_h$ and vertices v_1, \dots, v_h (not necessary distinct) such that all components of

$T - \{v_1, v_2, \dots, v_h\}$ are of orders not greater than s , $n_i = |V(T_i)| \leq \max\{n_{i-1} - s, s\}$ and $v_i \in V(T_{i-1})$ for $1 \leq i \leq h$. Hence we have $n_i > s$ for $1 \leq i \leq h - 1$. Since $s = 2\lceil p/k \rceil$,

$$ks = 2k\lceil p/k \rceil \geq 2k(p/k) = 2p.$$

Since $n_i \leq n_{i-1} - s$, ($i = 1, 2, \dots, h$),

$$n_{h-1} - n_0 = \sum_{i=1}^{h-1} (n_i - n_{i-1}) \leq -(h-1)s.$$

Hence

$$s < n_{h-1} \leq 2p - (h-1)s \leq ks - hs + s = (k-h+1)s.$$

Thus $h \leq k - 1$.

Now we may choose a $(k - 1)$ -vertex subset V' containing $\{v_1, v_2, \dots, v_h\}$ such that the components of $T - V'$ are of orders not exceeding s . By Lemma 2.2 and Theorem 1.3, all components of $T - V'$ have their largest eigenvalues not great than $\lambda_1(T_{2t}^1)$. The proof is completed. \square

Combining Lemma 2.5 with the Cauchy Interlacing Theorem, we obtain the following main result.

Theorem 2.6 *Let T be a tree in \mathcal{T}_{2p}^+ . Then for any positive integer k with $1 \leq k \leq p$, we have*

$$\lambda_k(T) \leq \frac{1}{2} \left(\sqrt{\lceil \frac{p}{k} \rceil - 1} + \sqrt{\lceil \frac{p}{k} \rceil + 3} \right) \tag{2.1}$$

and this upper bound is best possible when $k = 1$.

Proof: Suppose that $T \in \mathcal{T}_{2p}^+$. By Lemma 2.5, we have a $(k - 1)$ -vertex subset $V' \subset V(T)$ such that all components, say T_1, T_2, \dots, T_q , of $T - V'$ are trees with the largest eigenvalues not exceeding $\lambda_1(T_{2t}^1)$, $t = \lceil \frac{p}{k} \rceil$. By Theorems 2.1 and 1.3, we obtain

$$\begin{aligned} \lambda_k(T) &\leq \lambda_1(T - V') = \max_{1 \leq i \leq q} \lambda_1(T_i) \\ &\leq \max_{1 \leq i \leq s} \frac{1}{2} \left(\sqrt{\frac{|V(T_i)|}{2} - 1} + \sqrt{\frac{|V(T_i)|}{2} + 3} \right) \\ &\leq \frac{1}{2} \left(\sqrt{\lceil \frac{p}{k} \rceil - 1} + \sqrt{\lceil \frac{p}{k} \rceil + 3} \right) \end{aligned}$$

This proves the upper bound (2.1). Obviously, for $k = 1$, (2.1) is just the upper bound $\lambda_1(T) \leq \frac{1}{2}(\sqrt{p-1} + \sqrt{p+3})$ in Theorem 1.3, and it is best possible upper bound. \square

Example 2.1 *For any $T \in \mathcal{T}_{10}^+$, from Theorem 2.6 we get that $\lambda_1(T) \leq \frac{1}{2}(\sqrt{4} + \sqrt{8}) \approx 2.414$, $\lambda_2(T) \leq \frac{1}{2}(\sqrt{2} + \sqrt{6}) \approx 1.932$, $\lambda_3(T) \leq \frac{1}{2}(1 + \sqrt{5}) \approx 1.618$, $\lambda_4(T) \leq \frac{1}{2}(1 + \sqrt{5}) \approx 1.618$ and $\lambda_5(T) \leq 1$. We find that $\lambda_1(T)$ and $\lambda_5(T)$ are tight, which can be verified by the table of the spectra of all trees with n vertices ($2 \leq n \leq 10$) in [6]. \square*

There is a relationship between the characteristic polynomial $P(G \odot N_s; \lambda)$ of $G \odot N_s$ and that of G as follows.

Lemma 2.7 ([6]) $P(G \odot N_s; \lambda) = \lambda^{ps} P(G; \lambda - \frac{s}{\lambda})$.

Let \mathcal{T}_{2p}^* be the set of the coronas of trees of order p with N_1 , i.e.,

$$\mathcal{T}_{2p}^* = \{T \odot N_1 \mid T \in \mathcal{T}_p\}.$$

Obviously, any graph in \mathcal{T}_{2p}^* is a tree and has a perfect matching. Thus we have $\mathcal{T}_{2p}^* \subset \mathcal{T}_{2p}^+$. Note that for any $T^* \in \mathcal{T}_{2p}^*$, there is a unique tree T with $T^* = T \odot N_1$. The tree T is called the *contracted tree* of the tree T^* . Now we prove an upper bound on the k th eigenvalue of trees in \mathcal{T}_{2p}^* .

Lemma 2.8 *Let $T^* \in \mathcal{T}_{2p}^*$ and let T be the contracted tree of T^* . Then*

$$\lambda_k(T^*) = \frac{1}{2} \left(\sqrt{\lambda_k(T)^2 + 4} + \lambda_k(T) \right).$$

Proof: By Lemma 2.7, we have $P(T^*; \lambda) = \lambda^p P(T; \lambda - \frac{1}{\lambda})$. Since $\lambda_k(T)$ is the k th eigenvalue of T for $k = 1, 2, \dots, p$,

$$P(T^*; \lambda) = \lambda^p \prod_{i=1}^p \left(\lambda - \frac{1}{\lambda} - \lambda_i(T) \right) = \prod_{i=1}^p (\lambda^2 - \lambda_i(T)\lambda - 1).$$

So the positive eigenvalues of T^* are $\frac{1}{2}(\sqrt{\lambda_i(T)^2 + 4} + \lambda_i(T))$, $i = 1, 2, \dots, p$. Since $f(x) = \frac{1}{2}(\sqrt{x^2 + 4} + x)$ is an increasing function of the variable x , the result follows immediately. \square

Theorem 2.9 *Let T^* be a tree in \mathcal{T}_{2p}^* . Then*

$$\lambda_k(T^*) \leq \frac{1}{2} \left(\sqrt{\left\lfloor \frac{p}{k} \right\rfloor - 1 + \sqrt{\left\lfloor \frac{p}{k} \right\rfloor + 3}} \right), \tag{2.2}$$

for $k = 1, 2, \dots, p$. Moreover, this upper bound is best possible when $k = 1$ or $p \not\equiv 0 \pmod{k}$.

Proof: Suppose that T is the contracted tree of the tree T^* . Then T is a tree of order p . By Theorem 1.2, Lemma 2.8 and its proof, we have

$$\begin{aligned} \lambda_k(T^*) &= \frac{1}{2} \left(\sqrt{\lambda_k(T)^2 + 4} + \lambda_k(T) \right) \\ &\leq \frac{1}{2} \left(\sqrt{\left\lfloor \frac{p}{k} \right\rfloor - 1 + \sqrt{\left\lfloor \frac{p}{k} \right\rfloor + 3}} \right) \end{aligned}$$

for $k \leq \lfloor \frac{p}{2} \rfloor$. For $k > \lfloor \frac{p}{2} \rfloor$, since $\lambda_k(T) \leq 0$, we have $\lambda_k(T^*) \leq 1$. The Equation (2.2) holds, since the right hand side of (2.2) is equal to 1.

When $k = 1$, it is known that this bound is best possible. To show tightness for $k \geq 2$ and $p \not\equiv 0 \pmod{k}$, we shall construct a corona of a tree with N_1 . First, we write $p = \lfloor p/k \rfloor k + r$, where $1 \leq r \leq k - 1$. Set $t = 2\lfloor p/k \rfloor$ and thus $2p = tk + 2r$. Let T be the tree obtained by joining edges from the

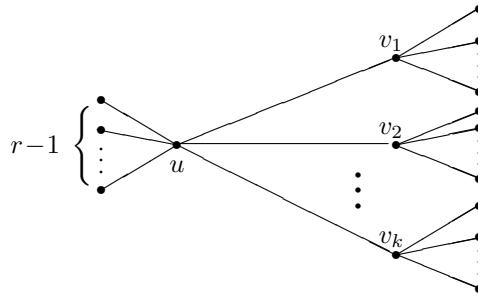


Fig. 2.1: A tree T in the proof of Theorem 2.9

center u of a star $K_{1,r-1}$ to the centers v_1, v_2, \dots, v_k of k disjoint stars $K_{1, \frac{t}{2}-1}$ (see Fig. 2.1). Then let $T^* = T \odot N_1 \in \mathcal{T}_{2p}^*$. It is easy to see that

$$\lambda_1(T - u) = \lambda_2(T - u) = \dots = \lambda_k(T - u) = \lambda_1(K_{1, \frac{t}{2}-1}) = \sqrt{\frac{t}{2} - 1}.$$

By Lemma 2.2 and the Cauchy Interlacing Theorem we have

$$\lambda_k(T - u) \leq \lambda_k(T) \leq \lambda_{k-1}(T - u).$$

Therefore,

$$\lambda_k(T) = \sqrt{\frac{t}{2} - 1}.$$

By Lemma 2.8, we have

$$\lambda_k(T^*) = \frac{1}{2} \left(\sqrt{\frac{t}{2} - 1} + \sqrt{\frac{t}{2} + 3} \right) = \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor - 1} + \sqrt{\lfloor \frac{p}{k} \rfloor + 3} \right).$$

This shows that the upper bound (2.2) is best possible when $p \not\equiv 0 \pmod{k}$. □

Example 2.2 For any tree $T^* \in \mathcal{T}_{10}^*$, by Theorem 2.6 we have $\lambda_1(T^*) \leq \frac{1}{2}(\sqrt{4} + \sqrt{8}) \approx 2.414$, $\lambda_2(T^*) \leq \frac{1}{2}(1 + \sqrt{5}) \approx 1.618$, $\lambda_3(T^*) \leq 1$, $\lambda_4(T^*) \leq 1$ and $\lambda_5(T^*) \leq 1$. It can be verified from the table of the spectra of all trees with n vertices ($2 \leq n \leq 10$) in [6] that these bounds are tight. □

Example 2.3 For any tree $T^* \in \mathcal{T}_8^*$, by Theorem 2.6 we have $\lambda_1(T^*) \leq \frac{1}{2}(\sqrt{3} + \sqrt{7}) \approx 2.189$, $\lambda_2(T^*) \leq \frac{1}{2}(1 + \sqrt{5}) \approx 1.618$, $\lambda_3(T^*) \leq 1$ and $\lambda_4(T^*) \leq 1$. We know that the upper bounds on λ_1 and λ_3 are tight but on λ_2 and λ_4 they are not. Actually, the maximum values of λ_2 and λ_4 are approximately 1.356 and 0.477, respectively. □

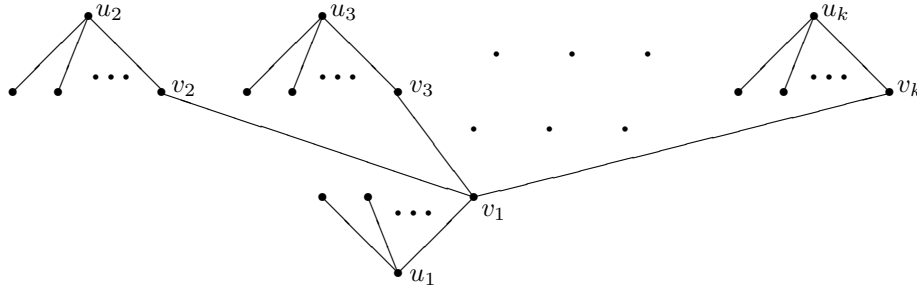


Fig. 2.2: The tree T in Lemma 2.10

Example 2.3 shows that for those k satisfying $p \equiv 0 \pmod{k}$, we usually only have

$$\lambda_k(T^*) < \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor} - 1 + \sqrt{\lfloor \frac{p}{k} \rfloor + 3} \right),$$

and especially, the upper bound is not as good as that in Theorem 1.2 when $k = 2$. However, the upper bound in Theorem 2.6 will be shown to be asymptotically tight when $p \equiv 0 \pmod{k}$.

Lemma 2.10 ([14]) *Let v be a vertex of G , and $\mathcal{C}(v)$ be the set of all cycles containing v . Then the characteristic polynomial of G satisfies*

$$P(G; \lambda) = \lambda P(G - v; \lambda) - \sum_{uv \in E(G)} P(G - v - u; \lambda) - 2 \sum_{Z \in \mathcal{C}(v)} P(G - V(Z); \lambda).$$

We first take k copies of the star $K_{1, t-1}$ (say S_1, S_2, \dots, S_k) with centers u_1, u_2, \dots, u_k , respectively, and choose $v_i \in V(S_i) \setminus \{u_i\}$ ($i = 1, 2, \dots, k$). Then add the edges $v_1 v_i$ ($i = 2, 3, \dots, k$) to obtain tree T with tk vertices as shown in Fig. 2.2

The next lemma follows by direct calculation from Lemma 2.10 with $v = v_1$, observing that the last term in the lemma becomes zero because there are no cycles containing v_1 .

Lemma 2.11 ([15]) *Denoting $f(x) = x^3 + (t-k)x^2 - 2(k-1)x - (k-1)$, the characteristic polynomial of the tree T shown in Fig. 2.2 is*

$$P(T; \lambda) = \lambda^{tk-2(k+1)} (\lambda^2 - t + 1)^{k-2} f(\lambda^2 - t + 1)$$

and the k th eigenvalue of T satisfies

$$\lambda_k(T) = \sqrt{t-1 + \lambda_2(f)} > \sqrt{t-1 - \sqrt{\frac{k-1}{t-k}}},$$

where $\lambda_2(f)$ is the second largest root of the equation $f(x) = 0$.

Denote the maximum value of the k th largest eigenvalue of the trees in \mathcal{T}_{2p}^* by $\lambda_k^*(2p)$. Then Theorem 2.9 tells us that $\lambda_k^*(2p) \leq \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor - 1 + \sqrt{\lfloor \frac{p}{k} \rfloor + 3}} \right)$. We shall give a lower bound for $\lambda_k^*(2p)$, which shows that as k gets large, the upper bound in Theorem 2.6 is asymptotically tight for the value of $\lambda_k^*(2p)$ when $p \equiv 0 \pmod{k}$.

Theorem 2.12 *Let p and k be integers with $1 \leq k \leq p$. If $t = \lfloor \frac{p}{k} \rfloor > k$, then*

$$\lambda_k^*(2p) > \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor - 1 - \sqrt{\frac{k-1}{t-k}}} + \sqrt{\lfloor \frac{p}{k} \rfloor + 3 - \sqrt{\frac{k-1}{t-k}}} \right).$$

Proof: Let $T^* = T \odot N_1 \in \mathcal{T}_{2tk}^*$ by taking the tree T with tk vertices described in Fig. 2.2 From Lemma 2.11, it is easy to see that the second largest root $\lambda_2(f)$ of $f(x) = 0$ is negative. Note that $f(0) = -(k-1) < 0$, $f\left(-\sqrt{\frac{k-1}{t-k}}\right) > 0$ and $\lim_{x \rightarrow -\infty} f(x) = -\infty$. So we know that $\lambda_2(f) > -\sqrt{\frac{k-1}{t-k}}$. Moreover, the expression $\lambda = \frac{1}{2} \left(\sqrt{t-1+\alpha} + \sqrt{t+3+\alpha} \right)$ can be regarded as a strictly increasing function of the variable α . Thus, by Lemmas 2.8 and 2.11, we have

$$\begin{aligned} \lambda_k(T^*) &= \frac{1}{2} \left(\sqrt{t-1+\lambda_2(f)} + \sqrt{t+3+\lambda_2(f)} \right) \\ &> \frac{1}{2} \left(\sqrt{t-1-\sqrt{\frac{k-1}{t-k}}} + \sqrt{t+3-\sqrt{\frac{k-1}{t-k}}} \right). \end{aligned}$$

There is a tree U of order p containing T described above. Hence $U^* = U \odot N_1 \in \mathcal{T}_{2p}^*$ and

$$\begin{aligned} \lambda_k(U^*) &\geq \lambda_k(T^*) > \frac{1}{2} \left(\sqrt{t-1-\sqrt{\frac{k-1}{t-k}}} + \sqrt{t+3-\sqrt{\frac{k-1}{t-k}}} \right) \\ &= \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor - 1 - \sqrt{\frac{k-1}{t-k}}} + \sqrt{\lfloor \frac{p}{k} \rfloor + 3 - \sqrt{\frac{k-1}{t-k}}} \right). \end{aligned}$$

Thus we get the theorem. □

Remark: If we let $t \rightarrow \infty$ (that is, $2p \rightarrow \infty$) for a fixed k , then $\sqrt{\frac{k-1}{t-k}} \rightarrow 0$, i.e.,

$$\lambda_k^*(2p) \rightarrow \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor - 1 + \sqrt{\lfloor \frac{p}{k} \rfloor + 3}} \right) \text{ as } t \rightarrow \infty.$$

So we can say that our upper bound (2.2) is asymptotically tight. Of course, if we denote the maximum value of the k th eigenvalues of trees in \mathcal{T}_{2p}^+ by $\lambda_k^+(2p)$, then by Theorem 2.9, we have $\lambda_k^+(2p) \geq \frac{1}{2} \left(\sqrt{\lfloor \frac{p}{k} \rfloor - 1 + \sqrt{\lfloor \frac{p}{k} \rfloor + 3}} \right)$. So the upper bound (2.1) is also asymptotically tight in a sense.

References

- [1] N.L. Biggs, *Algebraic Graph Theory, 2nd Ed.*, Cambridge University Press, Cambridge, 1993.
- [2] J.A. Bondy and U.S.R. Murty, *Graph Theory with Applications*, MacMillan Press Ltd., 1976.
- [3] A. Chang, Bounds on the second largest eigenvalue of a tree with perfect matchings, *Linear Algebra and its Applications*, **283** (1998), 247-255.
- [4] A. Chang, The sublargest value and quasi-smallest value of the largest eigenvalue of the tree with perfect matchings (in Chinese), *Applied Mathematics – A Journal of Chinese Universities*. **14(4)** (1999), 397-403.
- [5] A. Chang, On the largest eigenvalue of a tree with perfect matchings, *Discrete Mathematics*, **269** (2003), 45-63.
- [6] D. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs -Theory and Applications*, Academic Press, New York, 1980.
- [7] R. Frucht and F. Harary, On the corona of two graphs, *Aequationes Mathematicae*, **4** (1970), 322-325.
- [8] C.D. Godsil, Inverse of trees, *Combinatorica*, **5** (1985), 33-39.
- [9] J-M. Guo and S-W. Tan, A conjecture on the second largest eigenvalue of a tree with perfect matchings, *Linear Algebra and its Applications*, **347** (2002), 9-15.
- [10] J-M. Guo and S-W. Tan, A note on the second largest eigenvalue of a tree with perfect matchings, *Linear Algebra and its Applications*, **380** (2004), 125-134.
- [11] M. Hofmeister, On the two largest eigenvalues of trees, *Linear Algebra and its Applications*, **260** (1997), 43-59.
- [12] Y. Hong, The k th largest eigenvalue of a tree, *Linear Algebra and its Applications*, **73** (1986), 151-155.
- [13] A. Neumaier, The second largest eigenvalue of a tree, *Linear Algebra and its Applications*, **46** (1982), 9-25.
- [14] A.J. Schwenk, Computing the characteristic polynomial of a graph, In: *Graphs and Combinatorics* (Lecture Notes in Mathematics, 406), edited by R.A. Bari, F. Harary, Springer-Verlag, New York, 1974, 153-173.
- [15] J.Y. Shao, Bounds on the k th eigenvalues of trees and forests, *Linear Algebra and its Applications*, **149** (1991), 19-34.
- [16] J.Y. Shao and Y. Hong, Bounds on the smallest positive eigenvalue of trees with a perfect matching (in Chinese), *Science Bulletin*, **18** (1991), 1361-1364.
- [17] G.H. Xu, On the spectral radius of trees with perfect matchings, in: *Combinatorics and Graph Theory*, World Scientific, Singapore, 1997.
- [18] F. Zhang and A. Chang, Acyclic molecules with greatest HOMO-LUMO separation, *Discrete Applied Mathematics*, **98** (1999), 165-171.

