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

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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 kth largest eigenvalue $\lambda_k(T)$ satisfies $\lambda_k(T) \leq \frac{1}{2}\left(\sqrt{\lceil\frac{p}{k}\rceil - 1} + \sqrt{\lceil\frac{p}{k}\rceil + 3}\right)$ $(k = 1, 2, \ldots, p)$. 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 kth largest eigenvalue $\lambda_k(T)$ satisfies $\lambda_k(T) \leq \frac{1}{2}\left(\sqrt{\lfloor\frac{p}{k}\rfloor - 1} + \sqrt{\lfloor\frac{p}{k}\rfloor + 3}\right)$ $(k = 1, 2, \ldots, p)$ 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

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

where $\lambda_k^*(2p)$ is the maximum value of the kth 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 $V(G) = \{v_1, v_2, \ldots, v_n\}$. 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 $\lambda_1(G) \geq \lambda_2(G) \geq \lambda_3(G) \geq \cdots \geq \lambda_n(G)$ and call them the eigenvalues of G. If G is a bipartite graph, then $\lambda_i(G) = -\lambda_{n-i+1}(G)$ for $i = 1, 2, \ldots, \lfloor n/2 \rfloor$ (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 $k = 1, 2, \ldots, \lfloor n/2 \rfloor$.

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 kth 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*

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

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*

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

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

$$V(G \odot H) = V(G) \cup \bigcup_{i \in V(G)} V(H_i),$$
$$E(G \odot H) = E(G) \cup \bigcup_{i \in V(G)} \Big(E(H_i) \cup \{iu_i \mid u_i \in V(H_i)\}\Big),$$

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.

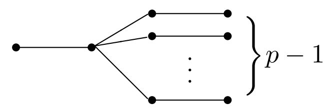

Fig. 1.1: The tree T^1_{2p}

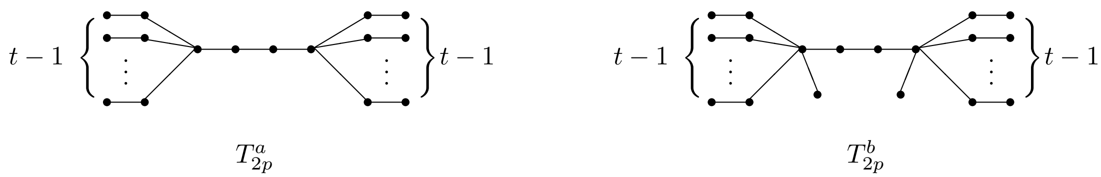

Fig. 1.2: Two graphs T^a_{2p} and $T^b_{2p}(= T^{2'}_{2p})$

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

$$\lambda_1(T) \le \frac{1}{2}(\sqrt{p-1} + \sqrt{p+3}) = \lambda_1(\mathcal{T}^1_{2p}) \qquad p = 1, 2, 3, \ldots.$$

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

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

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

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 $T \cong T^a_{2p}$, and equality holds in the second inequality if and only if $T \cong T^b_{2p}$, where T^a_{2p} and T^b_{2p} 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.

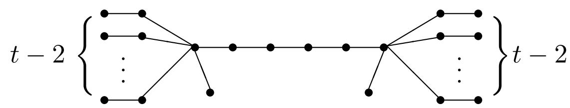

Fig. 1.3: The tree T_{2p}^2

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

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

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 kth 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 kth eigenvalue of trees.

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

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

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

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 wv 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 wv 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 $T_0 \supset T_1 \supset \cdots \supset T_h$ and vertices $v_1, \ldots, v_h$ (not necessary distinct) such that all components of

$T-\{v_1, v_2, \ldots, v_h\}$ 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 $n_i \leq n_{i-1} - s,\ (i = 1, 2, \ldots, h)$,

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

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 $\{v_1, v_2, \ldots, v_h\}$ 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. □

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*

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

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 $T_1, T_2, \ldots, T_q$, 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

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

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. □

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].* □

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 kth 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 kth eigenvalue of T for $k = 1, 2, \ldots, p$,

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

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

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 $k = 1, 2, \ldots, p$. 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 $k \leq \left\lfloor \frac{p}{2} \right\rfloor$. For $k > \left\lfloor \frac{p}{2} \right\rfloor$, 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

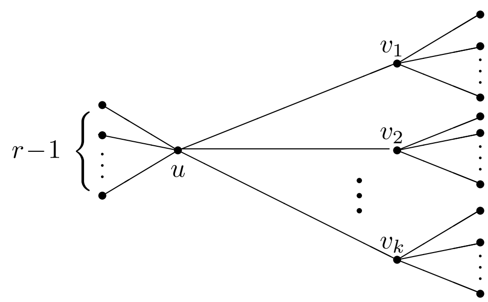

Fig. 2.1: A tree T in the proof of Theorem 2.9

center u of a star $K_{1,r-1}$ to the centers $v_1, v_2, \ldots, v_k$ 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

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

By Lemma 2.2 and the Cauchy Interlacing Theorem we have

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

Therefore,

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

By Lemma 2.8, we have

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

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 $\lambda_1(T^*) \le \frac{1}{2}(\sqrt{4}+\sqrt{8}) \approx 2.414$, $\lambda_2(T^*) \le \frac{1}{2}(1+\sqrt{5}) \approx 1.618$, $\lambda_3(T^*) \le 1$, $\lambda_4(T^*) \le 1$ and $\lambda_5(T^*) \le 1$. It can be verified from the table of the spectra of all trees with n vertices $(2 \le n \le 10)$ in [6] that these bounds are tight.* □

Example 2.3 *For any tree $T^* \in \mathcal{T}^*_8$, by Theorem 2.6 we have $\lambda_1(T^*) \le \frac{1}{2}(\sqrt{3}+\sqrt{7}) \approx 2.189$, $\lambda_2(T^*) \le \frac{1}{2}(1+\sqrt{5}) \approx 1.618$, $\lambda_3(T^*) \le 1$ and $\lambda_4(T^*) \le 1$. 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.* □

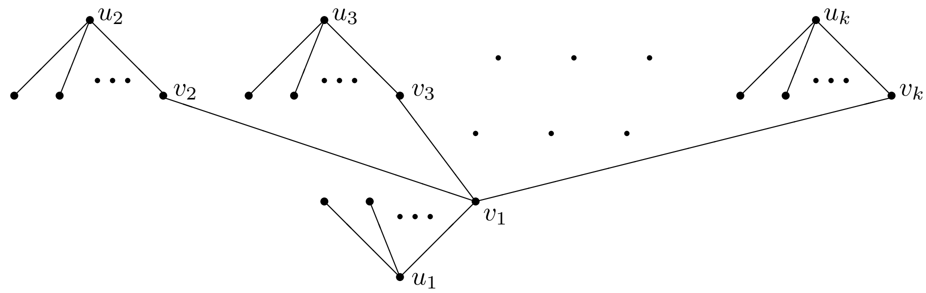

Fig. 2.2: The tree T in Lemma 2.10

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

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

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 $S_1, S_2, \ldots, S_k$) with centers $u_1, u_2, \ldots, u_k$, respectively, and choose $v_i \in V(S_i)\setminus\{u_i\}$ $(i = 1, 2, \ldots, k)$. Then add the edges v_1v_i $(i = 2, 3, \ldots, k)$ 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 kth 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 kth largest eigenvalue of the trees in $\mathcal{T}_{2p}^*$ by $\lambda_k^*(2p)$. Then Theorem 2.9 tells us that $\lambda_k^*(2p) \le \frac{1}{2}\left(\sqrt{\lfloor\frac{p}{k}\rfloor - 1} + \sqrt{\lfloor\frac{p}{k}\rfloor + 3}\right)$. 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 $1 \le k \le p$. If $t = \lfloor\frac{p}{k}\rfloor > k$, then*

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

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 $\lim_{x\to-\infty} f(x) = -\infty$. 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

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

Thus we get the theorem. □

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

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

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