On the largest eigenvalues of trees with perfect matchings

Wenshui Lin and Xiaofeng Guo*

School of Mathematical Sciences, Xiamen University, Xiamen Fujian 361005, China E-mail: xfguo@xmu.edu.cn

Received 21 May 2006; revised 22 June 2006

Let $\lambda_1(G)$ and $\Delta(G)$, respectively, denote the largest eigenvalue and the maximum degree of a graph *G*. Let \mathcal{T}_{2m} be the set of trees with perfect matchings on 2m vertices, and $\mathcal{T}_{2m}^{(\Delta)} = \{T \in \mathcal{T}_{2m} | \Delta(T) = \Delta\}$. Among the trees in $\mathcal{T}_{2m}^{(\Delta)}(m \ge 2)$, we characterize the tree which alone minimizes the largest eigenvalue, as well as the tree which alone maximizes the largest eigenvalue when $\lceil \frac{m}{2} \rceil + 1 \le \Delta \le m$. Furthermore, it is proved that, for two trees T_1 and T_2 in \mathcal{T}_{2m} ($m \ge 4$), if $\lceil \frac{2m}{3} \rceil \le \Delta(T_1) \le m$ and $\Delta(T_1) > \Delta(T_2)$, then $\lambda_1(T_1) > \lambda_1(T_2)$.

KEY WORDS: tree, perfect matching, eigenvalue, spectral radius, maximum degree

1. Introduction

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and A(G)the adjacency matrix of G. The characteristic polynomial of G is just $P(G, \lambda) = \det(\lambda I - A(G))$. Since A(G) is a real symmetric matrix, all of its eigenvalues $\lambda_i(G)$, $i = 1, 2, \ldots, n$, are real. We assume, without loss of generality, that $\lambda_1(G) \ge \lambda_2(G) \ge \cdots \ge \lambda_n(G)$, and call them the eigenvalues (or the spectrum) of G. Particularly, $\lambda_1(G)$ is called the largest eigenvalue (or the spectral radius, or the index) of G. Throughout this paper, we denote the set of trees on n vertices and the set of trees with perfect matchings on 2m vertices by \mathcal{F}_n and \mathcal{T}_{2m} , respectively. Let $d_G(v)$ denote the degree of a vertex v of G, and $\Delta(G)$ the maximum degree of G. Let $\mathcal{F}_n^{(\Delta)} = \{T \in \mathcal{F}_n | \Delta(T) = \Delta\}$ and $\mathcal{T}_{2m}^{(\Delta)} = \{T \in \mathcal{T}_{2m} | \Delta(T) = \Delta\}$.

Spectra of graphs are important graph structural invariants, which have numerous applications in chemistry. In quantum chemistry the skeletons of certain non-saturated hydrocarbon molecules are represented by so-called molecular graphs. In [1, 2] it was recognized that the famous Hückel molecular orbital

*Corresponding author.

(HMO) theory is fully equivalent to the graph spectral theory, namely, the eigenvalues of the adjacency matrix of a molecular graph are identical with Hückel orbital energy levels, and the eigenvectors are identical with the Hückel molecular orbitals. In particular, following a suggestion by Lovász and Pelikán [3], and Cvetković and Gutman [4] proposed that the spectral radius of a molecular graph be used as a measure of branching of the molecule. Therefore, since the fifties last century, eigenvalues of graphs have been intensively investigated (see [5–7]). In particular, the largest eigenvalues of trees, unicyclic graphs and bicyclic graphs were considered (see [8–17]).

Most of the early results of the graph spectral theory are concerned with the relation between spectral and structural properties of a graph. As for the relation between $\lambda_1(G)$ and $\Delta(G)$ for a graph G, it is well known that $\sqrt{\Delta(G)} \leq \lambda_1(G) \leq \Delta(G)$ (see [4]). If G is just a tree, Godsil [13] showed that $\lambda_1(G) < 2\sqrt{\Delta(G)} - 1$. We [14] considered the relation for a tree in \mathcal{F}_n . Let $B_{n,n-\Delta+1}(2 \leq \Delta \leq n-1)$ be a so-called broom (see [18]) and $T_{i,j}^1$ (i + j = n - 2) a double star, as shown in figure 1. We showed that among the trees in $\mathcal{F}_n^{(\Delta)}(n \geq 4)$, $B_{n,n-\Delta+1}$ alone minimizes the largest eigenvalue, as well $T_{\Delta-1,n-\Delta-1}^1$ alone maximizes the largest eigenvalue when $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-1$. Simić et al. [19] completely determined the tree maximizing the largest eigenvalue when $2 \leq \Delta \leq n-1$. Furthermore in [14] we proved the following result:

Theorem 1.1 [14]. Let $T^{(\Delta)}$ be a tree in $\mathcal{F}_n^{(\Delta)}$, $\Delta = 2, 3, \ldots, n-1$ and $n \ge 4$. Then

$$\lambda_1(T^{(n-1)}) > \lambda_1(T^{(n-2)}) > \cdots \lambda_1\left(T^{\left(\left\lceil \frac{2n}{3} \right\rceil\right)}\right) > \lambda_1\left(T^{\left(1\right)}_{\left\lfloor \frac{n}{3} \right\rfloor, \left\lceil \frac{2n}{3} \right\rceil - 2}\right) \ge \lambda_1(T^{(l)}).$$

where $2 \leq l \leq \left\lceil \frac{2n}{3} \right\rceil - 1$, with the equality iff $T^{(l)} \cong T^{1}_{\lfloor \frac{n}{3} \rfloor, \lceil \frac{2n}{3} \rceil - 2}$.

Theorem 1.1 indicates that, the largest eigenvalue of a tree T in \mathcal{F}_n strictly increases with its maximum degree when $\Delta(T) \ge \left\lceil \frac{2n}{3} \right\rceil - 1$.

In the present paper, we investigate the relation between the largest eigenvalue and the maximum degree of a tree with a perfect matching. In quantum chemistry a tree with a perfect matching represents an acyclic Kekulean conjugated hydrocarbon molecule (see [2,20]), so it is significant to investigate the largest eigenvalue of a tree with a perfect matching. Xu [15] and Chang [8] determined the first seven trees with perfect matchings and large largest eigenvalues. Clearly, if a tree T on n vertices has a perfect matching, then n must be even, say n = 2m, and $\Delta(T) \leq m = (\frac{n}{2} \leq \lceil 2n/3 \rceil - 1)$ with the equality iff $T \cong T_{2m}^*$, which is shown in figure 1. Hence though $\mathcal{T}_n \subseteq \mathcal{F}_n$, theorem 1.1 conveys nothing on the relation for a tree in \mathcal{T}_n . In section 3, we determine the trees in $\mathcal{T}_{2m}^{(\Delta)}$ with extreme largest eigenvalues (see theorems 3.1 and 3.2). Furthermore it is shown

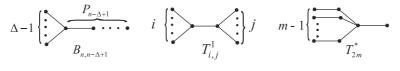


Figure 1. Trees $B_{n,n-\Delta+1}$, $T_{i,j}^1$, and T_{2m}^* .

that the largest eigenvalue of a tree T in T_{2m} also strictly increases with its maximum degree when $\left\lceil \frac{n}{3} \right\rceil = \left\lceil \frac{2m}{3} \right\rceil \leqslant \Delta(T) \leqslant m = n/2$ (see theorem 3.6). To carry out this, some graph transformations are introduced in section 2.

2. Preliminaries

Some groundwork is needed. First, we formulate some useful lemmas as follows, which can be used to compare the largest eigenvalues of two relational graphs. For convenience some transformations based on these lemmas are defined.

Lemma 2.1 [16]. Let *G* be a connected graph, and *G'* a proper subgraph of *G*. Then $\lambda_1(G') < \lambda_1(G)$.

Lemma 2.2 [16, 6]. Let *u* be a vertex of a non-trivial connected graph *G*, and let $G_{k,l}^0$ denote the graph obtained from *G* by adding pendant paths of length *k* and *l* at *u*. If $k \ge l \ge 1$, then $\lambda_1(G_{k,l}^0) > \lambda_1(G_{k+1,l-1}^0)$.

Definition 2.3. We call the transformation from $G_{k,l}^0$ to $G_{k+1,l-1}^0$ the α_0 transformation of $G_{k,l}^0$, that from $G_{k,l}^0$ to $G_{k+2,l-2}^0$ when $k \ge l \ge 2$ the α_0^2 transformation of $G_{k,l}^0$, and that from $G_{k,l}^0$ to $G_{k+l,0}^0$ the α_0^* transformation of $G_{k,l}^0$.

Lemma 2.4 [16]. Let *u* and *v* be two adjacent vertices of *G* such that the degrees of *u* and *v* are both greater than 1 in *G*. Let $G_{k,l}^1$ denote the graph obtained from *G* by adding a pendant path of length *k* (resp. *l*) at vertex *u* (resp. *v*). If $k \ge l \ge 1$, then $\lambda_1(G_{k,l}^1) > \lambda_1(G_{k+1,l-1}^1)$.

Definition 2.5. We call the transformation from $G_{k,l}^1$ to $G_{k+1,l-1}^1$ the α_1 transformation of $G_{k,l}^1$.

Lemma 2.6 [17]. Let w and v be two vertices in a non-trivial connected graph G and suppose that s pendant paths of length 2 are added to G at w, and t pendant paths of length 2 are added to G at v to form $G_{s,t}^2$. Then either $\lambda_1(G_{s+i,t-i}^2) > \lambda_1(G_{s,t}^2)$ $(1 \le i \le t)$ or $\lambda_1(G_{s-i,t+i}^2) > \lambda_1(G_{s,t}^2)$ $(1 \le i \le s)$.

Definition 2.7. We call the transformation from $G_{s,t}^2$ to G_1 , where $G_1 \cong G_{s+t,0}^2$ or $G_{0,s+t}^2$ such that $\lambda_1(G_1) > \lambda_1(G_{s,t}^2)$, the β transformation of $G_{s,t}^2$.

Let G be a connected graph with perfect matchings, as shown in figure 2, consisting of a connected subgraph H with a tree T added to a vertex r of H. Let |V(T)| be the number of vertices of T, including the vertex r. Suppose $v(T) \ge 3$. If v is a vertex of T furthest from r, then it is easy to see that v is a pendant vertex of G and adjacent to a vertex u of degree 2. Let G_1 be the graph obtained from G - u - v by adding a pendant path of length 2 to r. If |V(T - u - v)| is greater than 3, we can repeat above transformation on G_1 . Finally we get a graph G_0 when |V(T)| is even or a graph H_0 when |V(T)| is odd. G_0 and H_0 are shown in figure 2.

Lemma 2.8 [10]. Let G, G₀, and H₀ be the above three graphs shown in figure 2. Then $\lambda_1(G_0) > \lambda_1(G)$ and $\lambda_1(H_0) > \lambda_1(G)$, respectively.

Definition 2.9. We call the transformation from G to G_0 or H_0 the γ transformation of G (on T).

Definition 2.10 [15]. Let T be a tree in \mathcal{F}_n , and $n \ge 4$. Let e = uv be a non-pendent edge of T. T_0 is the graph obtained from T in the following way:

- (1) Contract the edge e = uv.
- (2) Add a pendant edge to the vertex u(=v).

The procedures (1) and (2) are called the edge-growing transformation of T (on edge e), or e.g.t of T (on edge e) for short.

Lemma 2.11 [15]. Let T be a tree with at least a non-pendent edge in \mathcal{F}_n , and $n \ge 4$. If T can be transformed into T_0 by carrying out a step of e.g.t, then $\lambda_1(T_0) > \lambda_1(T)$.

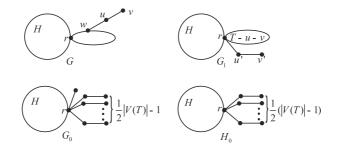


Figure 2. Graphs G, G_1, G_0 , and H_0 .

We will use $\alpha_0, \alpha_0^2, \alpha_0^*, \alpha_1, \beta, \gamma$ transformations and e.g.t to compare the largest eigenvalues of two trees in \mathcal{T}_{2m} . Note that if a tree T has a perfect matching, then T has a unique perfect matching. Denote the unique perfect matching of T by M(T). Clearly if T' is obtained from a tree T in \mathcal{T}_{2m} by a step of $\alpha_0^2, \alpha_0^*, \beta$ or γ transformation, then $T' \in \mathcal{T}_{2m}$, i.e., T' still has a perfect matching. But α_0, α_1 transformations and e.g.t do not always have this property. For α_0 transformation of a tree $T \cong G_{k,l}^0$ in $\mathcal{T}_{2m}, T' = G_{k+1,l-1}^0 \in \mathcal{T}_{2m}$ iff $P_{k+1} \cup P_{l+1}$ is an M(T)-alternating path, where P_{k+1} and P_{l+1} denote the two pendant paths added to G at u. For α_1 transformation of a tree $T \cong G_{k,l}^1$ in $\mathcal{T}_{2m}, T' = G_{k+1,l-1}^1 \in \mathcal{T}_{2m}$ iff $P_{k+1} \cup \{uv\} \cup P_{l+1}$ is an M(T)-alternating path, where P_{k+1} and P_{l+1} denote the two pendant paths added to G at u. For α_1 transformation of a tree $T \cong G_{k,l}^1$ in $\mathcal{T}_{2m}, T' = G_{k+1,l-1}^1 \in \mathcal{T}_{2m}$ iff $P_{k+1} \cup \{uv\} \cup P_{l+1}$ is an M(T)-alternating path, where P_{k+1} and P_{l+1} denote the two pendant paths added to G at u and v, respectively. Finally if T' is obtained from a tree T in \mathcal{T}_{2m} by a step of e.g.t, then $T' \in \mathcal{T}_{2m}$ iff the e.g.t is carried out on an (non-pendant) edge in M(T).

We summarize the above discussions and lemmas 2.2, 2.4, 2.6, 2.8 and 2.11 into the following.

Corollary 2.12. Let T be a tree in T_{2m} .

- (1) If T' can be obtained from T by a step of α_0^2 or α_0^* transformation, then $T' \in \mathcal{T}_{2m}$ and $\lambda_1(T') < \lambda_1(T)$.
- (2) If $T \cong G_{k,l}^0$ and $P_{k+1} \cup P_{l+1}$ is an M(T)-alternating path, then $T' = G_{k+1,l-1}^0 \in \mathcal{T}_{2m}$ and $\lambda_1(T') < \lambda_1(T)$.
- (3) If $T \cong G_{k,l}^1$ and $P_{k+1} \cup \{uv\} \cup P_{l+1}$ is an M(T)-alternating path, then $T' = G_{k+1,l-1}^1 \in \mathcal{T}_{2m}$ and $\lambda_1(T') < \lambda_1(T)$.
- (4) If T' can be obtained from T by a step of β or γ transformation, or by a step of e.g.t on a non-pendant edge in M(T), then $T' \in \mathcal{T}_{2m}$ and $\lambda_1(T') > \lambda_1(T)$.

We also need the following partition of \mathcal{T}_{2m} introduced by Chang [1]. Let X_{2m} be the set of the trees on 2m vertices obtained from a tree \hat{T} on m vertices by adding one pendant edge to each of the m vertices of \hat{T} . Then $X_{2m} \subseteq \mathcal{T}_{2m} \subseteq \mathcal{F}_{2m}$. If $T \in X_{2m}$ is obtained from \hat{T} , then T is denoted by $C(\hat{T})$. Clearly every pendant edge of a tree T in X_{2m} belongs to M(T), i.e., M(T) consists of the pendant edges of T. Let $X_{2m}^t = \{T \in \mathcal{T}_{2m}|$ there are exactly t non-pendant edges, which belong to M(T)}. Then $X_{2m}^0 = X_{2m}$, $X_{2m}^{m-2} = \{P_{2m}\}$ and $\mathcal{T}_{2m}| = \bigcup_{t=0}^{m-2} X_{2m}^t$. It is not difficult to see that any $T \in X_{2m}^t$ ($t = 1, 2, \ldots, m-2$) can be transformed into a tree in X_{2m}^{t-1} by a step of e.g.t on a non-pendant edge in M(T).

Lemma 2.13 [8]. Let $C(\hat{T})$ be a tree in X_{2m} . Then

$$\lambda_1(T) = \frac{1}{2} \left[\sqrt{\lambda_1^2(\hat{T}) + 4} + \lambda_1(\hat{T}) \right].$$

1062 W. Lin and X. Guo / On the largest eigenvalues of trees with perfect matchings

Lemma 2.14 [9].
$$\lambda_1(T_{1,n-3}^1) > \lambda_1(T_{2,n-4}^1) > \cdots > \lambda_1\left(T_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}^1\right)$$
.

Lemma 2.15 [15]. Let T be a tree in $\mathcal{T}_{2m}|$. Then $\lambda_1(T) \leq \frac{1}{2}(\sqrt{m-1} + \sqrt{m+3}), m = 1, 2, 3, \ldots$, with the equality iff $T \cong T_{2m}^*$.

3. Main results

For convenience, we introduce more notations. Let G and H be two graphs whose vertex sets are disjoint. If v is a vertex of G and w a vertex of H, then G(v, w)H denotes the graph obtained from G and H by identifying the vertices v and w. Let $K_{1,\Delta}$ be a star with center v, and $v_1, v_2, \ldots, v_{\Delta}$ the pendant vertices of $K_{1,\Delta}$. Let H_i be a tree with maximum degree at most Δ, u_i a vertex of H_i with $d_{H_i}(u_i) \leq \Delta - 1$, $n_i = |V(H_i)| \geq 1$ (including the vertex u_i), $i = 1, 2, ..., \Delta$, and $\sum_{i=1}^{\Delta} n_i = n - 1$. Then simply denote $K_{1,\Delta}(v_1, u_1)H_1(v_2, u_2)H_2, \ldots, (v_{\Delta}, u_{\Delta})H_{\Delta}$ by $T(n, \Delta; H_1, H_2, \ldots, H_{\Delta})$. If H_i is a pendant path P_{n_i} with an end vertex u_i , then write H_i as P_{n_i} ; if H_i consists of $\left|\frac{n_i-1}{2}\right|$ pendant paths of length 2 and $n_i - 1 - 2\left|\frac{n_i-1}{2}\right|$ (= 0 or 1) pendant path of length 1 with a common end vertex u_i , then write H_i as C_{n_i} . Thus $\mathcal{F}_n^{(\Delta)}$ is just the set of $T(n, \Delta; H_1, H_2, \ldots, H_\Delta)$ s. And of course each $T \in \mathcal{T}_{2m}^{(\Delta)}$ has the form $T(2m, \Delta; H_1, H_2, \ldots, H_{\Delta})$. Moreover, there is exactly one of the n_i s is odd, since T has a perfect matching. Without loss of generality, assume that n_1 is odd. Then in fact, $\mathcal{T}_{2m}^{(\Delta)}$ is just the set of $T(2m, \Delta; H_1, H_2, \dots, H_{\Delta})$'s such that $n_1 \ge 1$ is odd, $n_i \ge 2$ is even for $i = 2, 3, \dots, \Delta, \sum_{i=1}^{\Delta} n_i = 2m - 1, H_1 - u_1$ and $H_i(i = 2, 3, ..., \Delta)$ have perfect matchings. Without loss of generality assume $n_2 \leqslant n_3 \leqslant \cdots \leqslant n_\Delta.$

$$L_{2m}^{(\Delta)} = T(2m, \Delta; P_1, P_2, \dots, P_2, P_{2m-2\Delta+2}), U_{2m}^{(\Delta)} = C(T_{\Delta-2,m-\Delta}^1) \left(\Delta \geqslant \left\lceil \frac{m-2}{2} \right\rceil\right),$$

and let $N(\Delta - 1, m - \Delta)$ denote the tree obtained from $T^{1}_{\Delta - 1, m - \Delta}$ by adding a pendant edge to each pendant vertex of $T^{1}_{\Delta - 1, m - \Delta}$.

Then

$$\Delta(L_{2m}^{(\Delta)}) = \Delta(U_{2m}^{(\Delta)}) = \Delta \text{ and } \Delta(N(\Delta - 1, m - \Delta))$$
$$= \max\{\Delta, m - \Delta + 1\}.$$
$$L_{2m}^{(\Delta)}, U_{2m}^{(\Delta)}$$

and $N(\Delta - 1, m - \Delta)$ are shown in figure 3.

Theorem 3.1. $L_{2m}^{(\Delta)}$ is the unique tree in $\mathcal{T}_{2m}^{(\Delta)}$, which has the minimum largest eigenvalue, where $2 \leq \Delta \leq m$.

$$\Delta - 2 \left\{ \underbrace{\begin{array}{c} & & \\$$

Proof. Let $T = T(2m, \Delta; H_1, H_2, ..., H_{\Delta})$ be a tree in $T_{2m}^{(\Delta)}$ and $T \not\cong L_{2m}^{(\Delta)}$. First T can be transformed into $T' = T(2m, \Delta; P_{n_1}, P_{n_2}, ..., P_{n_{\Delta}})$ by repeatedly carrying out α_0^* transformation on T, so $\lambda_1(T') \leq \lambda_1(T)$, with the equality iff $T' \cong T$ by corollary 2.12. (1). Moreover by α_0 and α_0^2 transformations, T' can be transformed into $L_{2m}^{(\Delta)}$. The conclusion follows from corollary 2.12. (1) and (2).

Theorem 3.2. $U_{2m}^{(\Delta)}$ is the unique tree in $T_{2m}^{(\Delta)}$, which has the maximum largest eigenvalue, where $\lceil \frac{m}{2} \rceil + 1 \leq \Delta \leq m$ and $m \geq 2$.

Proof. Let $T = T(2m, \Delta; H_1, H_2, ..., H_{\Delta})$ be a tree in $T_{2m}^{(\Delta)}$ and $T \not\cong U_{2m}^{(\Delta)}$. First T can be transformed into $T' = T(2m, \Delta; C_{n_1}, C_{n_2}, ..., C_{n_{\Delta}})$ by a step of γ transformation to T on each $H_i, i = 1, 2, ..., \Delta$, so $\lambda_1(T) \leq \lambda_1(T')$, with the equality iff $T' \cong T$ by corollary 2.12. (4). Moreover T' can be transformed into $T'' = U_{2m}^{(\Delta)}$ or $N(\Delta - 1, m - \Delta)$ by β transformations. Since $\Delta \geq \lceil \frac{m}{2} \rceil + 1$, $\Delta(T'') = \Delta$. Noting that $N(\Delta - 1, m - \Delta)$ can be obtained from $U_{2m}^{(\Delta)}$ by a step of α_1 transformation, the proof is completed.

Lemma 3.3.
$$\lambda_1(U_{2m}^{(m)}) > \lambda_1\left(U_{2m}^{(m-1)}\right) > \cdots > \lambda_1\left(U_{2m}^{\left(\left\lceil \frac{m}{2} \right\rceil + 1\right)}\right).$$

Proof. Recall that $U_{2m}^{(\Delta)} = C(T_{\Delta-2,m-\Delta}^1)$. From lemma 2.13, we have $\lambda_1(U_{2m}^{(\Delta)})$ strictly increases with $\lambda_1(T_{\Delta-2,m-\Delta}^1)$, and so the conclusion follows from lemma 2.14.

Lemma 3.4. Let $T^{(\Delta)}$ be a tree in $\mathcal{T}_{2m}^{(\Delta)}$, where $m \ge 4$ and $\left\lceil \frac{2m}{3} \right\rceil + 1 \le \Delta \le m$. Then $\lambda_1(T^{(\Delta-1)}) < \lambda_1(T^{(\Delta)})$.

Proof. Since $\left\lceil \frac{2m}{3} \right\rceil \ge \left\lceil \frac{m}{2} \right\rceil + 1$ when $m \ge 4$, by theorems 3.1 and 3.2, it suffices to show that $\lambda_1(U_{2m}^{(\Delta-1)}) < \lambda_1(L_{2m}^{(\Delta)})$ for $\left\lceil \frac{2m}{3} \right\rceil + 1 \le \Delta \le m$. When $\Delta = m$, since $L_{2m}^{(\Delta)} = T_{2m}^*$, the conclusion holds from lemma 2.15. So assume $\Delta \le m - 1$. Thus $L_{2m}^{(\Delta)}$ contains $T_{2\Delta}^*$ as a proper subgraph, and by lemmas 2.1 and 2.15

$$\lambda_1(L_{2m}^{(\Delta)}) > \lambda_1(T_{2\Delta}^*) = \frac{1}{2}[\sqrt{\Delta - 1} + \sqrt{\Delta + 3}].$$

1064 W. Lin and X. Guo / On the largest eigenvalues of trees with perfect matchings

Since $U_{2m}^{(\Delta-1)} = C(T_{\Delta-3,m-\Delta+1}^1)$, by lemma 2.13,

$$\lambda_1(U_{2m}^{(\Delta-1)}) = \frac{1}{2} \left[\sqrt{\lambda_1^2(T_{\Delta-3,m-\Delta+1}^1) + 4} + \lambda_1(T_{\Delta-3,m-\Delta+1}^1) \right].$$

And from the proof of theorem 3.1 in [9], we have

$$\lambda_1(T^1_{\Delta-3,m-\Delta+1}) = \sqrt{\frac{1}{2}(m-1+\sqrt{(m-1)^2-4(\Delta-3)(m-\Delta+1)})}.$$

So we are done by verifying that

$$\frac{1}{2}[\sqrt{\Delta-1} + \sqrt{\Delta+3}] \ge \lambda_1(U_{2m}^{(\Delta-1)}) \Leftrightarrow \Delta \ge \lambda_1^2(T_{\Delta-3,m-\Delta+1}^1) + 1$$
$$\Leftrightarrow \Delta \ge \left\lceil \frac{2m}{3} \right\rceil + 1.$$

Lemma 3.5. Let *T* be a tree in \mathcal{T}_{2m} , where $2 \leq \Delta(T) \leq \left\lceil \frac{2m}{3} \right\rceil$ and $m \geq 4$. Then $\lambda_1(T) \leq \lambda_1\left(U_{2m}^{\left(\left\lceil \frac{2m}{3} \right\rceil\right)}\right)$, with the equality iff $T \cong U_{2m}^{\left(\left\lceil \frac{2m}{3} \right\rceil\right)}$.

Proof. We distinguish the following three cases.

Case 1. $\lfloor \frac{m}{3} \rfloor + 2 \leq \Delta = \Delta(T) \leq \lceil \frac{2m}{3} \rceil$. Suppose $T = T(2m, \Delta; H_1, H_2, \dots, H_\Delta)$. First *T* can be transformed into $T' = T(2m, \Delta; C_{n_1}, C_{n_2}, \dots, C_{n_\Delta})$ by a step of γ transformation to *T* on each $H_i, i = 1, 2, \dots, \Delta$. Moreover by β transformations we can obtain a tree *T''*, where $T'' = C(T_{\Delta-2,m-\Delta}^1)$ or $N(\Delta - 1, m - \Delta)$. Thus $\Delta(T'') = \max\{\Delta, m - \Delta + 2\}$. Since $m - \Delta + 2 \leq m - \lfloor \frac{m}{3} \rfloor = \lceil \frac{2m}{3} \rceil$, we have $\lfloor \frac{m}{3} \rfloor + 2 \leq \Delta(T'') \leq \lceil \frac{2m}{3} \rceil$. Noting that $N(\Delta - 1, m - \Delta)$ can be obtained from $C(T_{\Delta-2,m-\Delta}^1)$ by a step of α_1 transformation, by corollary 2.12. (3), (4), and lemma 3.3, we have

$$\lambda_{1}(T) \leq \lambda_{1}(T') \leq \lambda_{1}(T'') \leq \lambda_{1}(C(T^{1}_{\Delta-2,m-\Delta})) \leq \lambda_{1}\left(U^{\left(\left\lceil\frac{2m}{3}\right\rceil\right)}_{2m}\right)$$

with all the equalities iff $T \cong U_{2m}^{\left(\left\lceil \frac{2m}{3} \right\rceil\right)}$. Case 2. $\Delta = \left\lfloor \frac{m}{3} \right\rfloor + 1$.

Subcase 2.1. $T \in X_{2m}$. Then T = C(F) for some F in \mathcal{F}_m with $\Delta(F) = \Delta - 1 = \lfloor \frac{m}{3} \rfloor$. From Lemma 2. 13, we know that $\lambda_1(C(F))$ strictly increases with $\lambda_1(F)$,

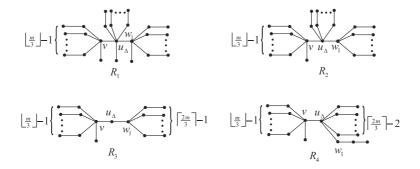


Figure 4. Trees R_1 , R_2 , R_3 , and R_4 in the proof of lemma 3.2.

so from lemma 2. 14, we have

$$\lambda_{1}(T) \leqslant \lambda_{1} \left(C \left(T_{\lfloor \frac{m}{3} \rfloor, \lceil \frac{2m}{3} \rceil - 2}^{1} \right) \right) = \lambda_{1} \left(U_{2m}^{\left(\lceil \frac{2m}{3} \rceil \right)} \right),$$

with the equality iff $T \cong U_{2m}^{\left(\left|\frac{2m}{3}\right|\right)}$.

Subcase 2.2. $T \in X_{2m}^t$, $t \ge 1$. Suppose $T = T(2m, \Delta; H_1, H_2, \ldots, H_\Delta)$. Since $n_i = n(H_i) \ge 2, i = 2, 3, \ldots, \Delta$, and $\sum_{i=1}^{\Delta} n_i = 2m-1, n_1 \le 2m-1-2\lfloor \frac{m}{3} \rfloor = 2 \lceil \frac{2m}{3} \rceil - 1$. Similarly $n_\Delta \le 2 \lceil \frac{2m}{3} \rceil$. If $n_\Delta \le 2 \lceil \frac{2m}{3} \rceil - 2$, then by a step of γ transformation of T on each H_i we obtain $T_1 = K_{1,\Delta}(v_1, u_1)C_{n_1}(v_2, u_2)C_{n_2}\cdots(v_\Delta, u_\Delta)C_{n_\Delta}$. Then $\lfloor \frac{m}{3} \rfloor + 1 \le \Delta(T_1) \le \lceil \frac{2m}{3} \rceil$ and $T_1 \in X_{2m}$, and we are done by corollary 2.12. (4), case 1 and subcase 2.1. So assume $n_\Delta = 2 \lceil \frac{2m}{3} \rceil$. Then by a simple calculation we have $n_1 = 1, n_i = 2, i = 2, 3, \ldots, \Delta - 1$, and there is a path of length at least 3 with an end vertex u_Δ in H_Δ . Let $u_\Delta w_1 w_2, \ldots, w_s, s \ge 3$, be such a path. Let I_1 and I_2 be the two components of $H_\Delta - u_\Delta w_1$. Then by a step of γ transformation of T on each of I_1 and I_2 we obtain a tree R_1 or R_2 , as shown in figure 4. If R_1 is obtained, then since $\lfloor \frac{m}{3} \rfloor + 1 \le \Delta(R_1) \le \lceil \frac{2m}{3} \rceil$ and $\lambda_1(T) \le \lambda_1(R)$ with equality iff $T \cong R$. Both R_3 and R_4 are shown in figure 4. Noting that $\Delta(R) = \Delta(R_3) = \Delta(R_4) = \lceil \frac{2m}{3} \rceil$ we are done by Case 1.

Case 3. $\Delta \leq \lfloor \frac{m}{3} \rfloor$.

Subcase 3.1. $T \in X_{2m}$. Similar to the discussions in subcase 2.1.

Subcase 3.2. $T \in X_{2m}^t$, $t \ge 1$. Then there is a nonpendant edge $e \in M(T)$. Obtain $T_1 \in X_{2m}^{t-1}$ from T by a step of e.g.t on e. Thus $\Delta(T_1) \le 2\Delta - 1 \le 2\lfloor \frac{m}{3} \rfloor - 1 < 2\lfloor \frac{m}{3} \rfloor$

 $\left\lceil \frac{2m}{3} \right\rceil$. If $T_1 \notin X_{2m}$ and $\Delta(T_1) \leqslant \lfloor \frac{m}{3} \rfloor$, then we can repeat the above discussion to obtain trees T_2, T_3, \ldots, T_l , such that $T_l \in X_{2m}$ or $\Delta(T_l) \geqslant \lfloor \frac{m}{3} \rfloor + 1$. Hence the conclusion holds by case 1, case 2 or subcase 3.1.

The proof is thus completed.

We are now in a position to state our main result.

Theorem 3.6. Let $T^{(\Delta)}$ be a tree in $\mathcal{T}_{2m}^{(\Delta)}|, \Delta = 2, 3, \ldots, m$ and $m \ge 4$. Then

$$\lambda_1\left(T^{(m)}\right) > \lambda_1\left(T^{(m-1)}\right) > \cdots \lambda_1\left(T^{\left(\left\lceil \frac{2m}{3}\right\rceil + 1\right)}\right) > \lambda_1\left(U_{2m}^{\left(\left\lceil \frac{2m}{3}\right\rceil\right)}\right) \geqslant \lambda_1\left(T^{(l)}\right),$$

where $2 \leq l \leq \left\lceil \frac{2m}{3} \right\rceil$, with the equality iff $T^{(l)} \cong U_{2m}^{\left(\left\lceil \frac{2m}{3} \right\rceil \right)}$). Furthermore the bound $\left\lceil \frac{2m}{3} \right\rceil$ is best possible.

Proof. The first part follows immediately from lemmas 3.4 and 3.5. To see the bound $\left\lceil \frac{2m}{3} \right\rceil$ is best possible, let 2m = 16. Then

$$\begin{bmatrix} \frac{2m}{3} \end{bmatrix} = 6, U_{16}^{(5)} \in \mathcal{T}_{16}^{(5)} \text{ and } L_{16}^{(6)} \in \mathcal{T}_{16}^{(6)},$$

but $\lambda_1(U_{16}^{(5)}) \approx 2.6764 > \lambda_1(L_{16}^{(6)}) \approx 2.6254.$

Acknowledgments

The project is supported by the National Natural Science Foundation of China. The author would like to thank Prof. Fuji Zhang for his valuable suggestions and his revision on this paper.

References

- Hs. H. Günthard and H. Primas, Zusammenhang von Graphentheorie und MO-Theorie von Molekeln mit Systemen konjugierter Bindungen, Helv. Chim. Acta 39 (1956) 1645–1653.
- [2] A. Graovac, I. Gutman and N. Trinajstić, *Topological Approch to the Chemistry of Conjugated Molecules* (Springer, Berlin, 1977).
- [3] L. Lovász and J. Pelikán, On the eigenvalues of trees, Period. Math. Hung. 3 (1973) 175-182.
- [4] D. Cvetković and I. Gutman, Note on branching, Croat. Chem. Acta 49 (1977) 115-121.
- [5] D. Cvetković, M. Doob and H. Sachs, Spectra of Graphs-Theory and Applications, 3rd edn (Johann Ambrosius Barth Verlag, Heidelberg-Leipzig, 1995).
- [6] D. Cvetković, P. Rowlinson and S. Simic, *Eigenspaces of Graphs* (Cambridge University Press, Cambridge, 1997).

- [7] A.J. Schwenk and R.J. Wilsion, On the eigenvalues of a graph, in: *Selected Topics in Graph Theory* eds. L.W. Beineke, R.J. Wilson (Academic Press, New York, 1978) pp. 307–336.
- [8] A. Chang, On the largest eigenvalue of a tree with perfect matchings, Discrete Math. 269 (2003) 45–63.
- [9] A. Chang, Q. Huang, Ordering trees by their largest eigenvalues, Linear Algebra Appl. 370 (2003) 175–184.
- [10] A. Chang and F. Tian, On the spectral radius of unicyclic graphs with perfect matchings, Linear Algebra Appl. 370 (2003) 237–250.
- [11] A. Chang, F. Tian and A.M. Yu, On the index of bicyclic graphs with perfect matchings, Discrete Math. 283 (2004) 51–59.
- [12] M. Hofmeister, On the two largest eigenvalues of trees, Linear Algebra Appl. 260 (1997) 43–59.
- [13] C.D. Godsil, Spectra of trees, Ann. Discrete Math. 20 (1984) 151-159.
- [14] W.S. Lin and X.F. Guo, Ordering trees by their largest eigenvalues, Linear Algebra Appl. (in press).
- [15] G.H. Xu, On the spectral radius of trees with perfect matchings, in: *Combinatorics and Graph Theory* (World Scientific, Singapore, 1997).
- [16] Q. Li and K.Q. Feng, On the largest eigenvalues of graphs, Acta Math. Appl. Sinica 2 (1979) 167–175 (in Chinese).
- [17] J.M., Guo and S.W. Tan, On the spectral radius of trees, Linear Algebra Appl. 329 (2001) 1-8.
- [18] R.A. Brualdi and J.L. Goldwasser, Permanent of the Laplacian matrix of trees and bipartite graphs, Discrete Math. 48 (1984) 1–21.
- [19] S.K. Simić and D.V. Tošić, The index of trees with specified maximum degree, MATCH Commun. Math. Comput. Chem. 54 (2005) 351–362.
- [20] D. Rouvary, in: Chemical Applications of Graph Theory ed. A.T. Balaban (Academic Press, New York, 1976) (Chapter 7).