J Math Chem (2009) 46:65–85
DOI 10.1007/s10910-008-9399-y

ORIGINAL PAPER

On the Laplacian spectral radii of trees with perfect matchings

Xi-Ying Yuan · Jia-Yu Shao · Chang-Xiang He

Received: 20 March 2008 / Accepted: 10 June 2008 / Published online: 8 July 2008

Abstract Denote by $\mathcal{T}(2k)$ the set of trees of order $2k$ with perfect matchings. GUO [Guo, Linear Algebra Appl. 368:379–385, 2003.] determined the largest value of Laplacian spectral radii $\mu(T)$ of the trees T in $\mathcal{T}(2k)$ and gave the corresponding tree T in $\mathcal{T}(2k)$ whose $\mu(T)$ reaches this largest value. In this paper, we determine the second to the sixth largest values of $\mu(T)$ of the trees T in $\mathcal{T}(2k)$ and also give the corresponding trees T in $\mathcal{T}(2k)$ whose $\mu(T)$ reach these values.

Keywords Tree · Perfect matching · Laplacian spectral radius

1 Introduction

In this paper, all the graphs are finite, undirected and have no loops or multiple edges. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. When v_i and v_j are endpoints of an edge e, we write $e = v_i v_j$. Denote the set of all the neighbors of a vertex v in G by $N_G(v)$ and the degree of v by $d_G(v)$, or simply $N(v)$ and $d(v)$ for convenience.

Let $D(G) = \mathrm{diag}(d(v_1), d(v_2), \ldots, d(v_n))$ be the diagonal matrix of vertex degrees. The Laplacian matrix $L(G)$ of G is defined by $L(G) = D(G) - A(G)$, where $A(G)$ is the (0,1)-adjacency matrix of G. In this paper, the characteristic polynomial $\det(xI - L(G))$ is denoted by $\Phi(G; x)$, or simply $\Phi(G)$. It is well known that

X.-Y. Yuan
Department of Mathematics, Shanghai University, Shanghai 200444, China

J.-Y. Shao (✉)
Department of Mathematics, Tongji University, Shanghai 200092, China
e-mail: jyshao@sh163.net

C.-X. He
College of Science, University of Shanghai for Science and Technology, Shanghai 200093, China

$L(G)$ is positive semi-definite, symmetric and singular. We denote the ith eigenvalue of $L(G)$ by $\mu_i(G)$ and order them in non-increasing order, i.e.,

$$\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_{n-1}(G) \geq \mu_n(G).$$

The eigenvalue $\mu_1(G)$ is called the Laplacian spectral radius of G, denoted by $\mu(G)$.

Eichinger et al. [3] showed that the eigenvalues of the Laplacian matrix of a molecular graph determine the distribution function of the so-called radius of gyration of the molecule, and that the non-zero eigenvalues and their eigenvectors can be used efficiently to compute the scattering functions for Gaussian molecules (see [11]).

Two distinct edges in a graph G are independent if they are not incident with a common vertex in G. A set of pairwise independent edges of G is called a matching of G. A matching M that satisfies $2|M| = |V(G)|$ is called a perfect matching (it is pointed out in [8] that every perfect matching of a HÜCKEL graph is in a one-to-one correspondence with a HÜCKEL structure). Let

$$\mathcal{T}(2k) = \{T \mid T \text{ is a tree of order } 2k \text{ with a perfect matching}\}. \tag{1.1}$$

In chemical graph theory, a tree with a perfect matching can be used to represent a certain hydrocarbon molecule (see [13]), so people are interested in the study of the eigenvalues of the adjacency matrices, as well as the eigenvalues of the Laplacian matrices of the trees in $\mathcal{T}(2k)$. In [14] and [2], the first seven trees in $\mathcal{T}(2k)$ with the largest spectral radii of the adjacency matrices were determined. And in [10] the largest eigenvalues of the adjacency matrices of trees in $\mathcal{T}(2k)$ were studied. In [12], the eigenvalues of the Laplacian matrices of the trees in $\mathcal{T}(2k)$ were studied, and the trees in $\mathcal{T}(2k)$ with the largest algebraic connectivity (i.e., the second smallest eigenvalue of the Laplacian matrix) were determined. In [1], some sufficient conditions for the existence of a perfect matching in a graph in terms of the eigenvalues of the Laplacian matrix were given. In [5], the largest value of the Laplacian spectral radii of the trees in $\mathcal{T}(2k)$ together with the corresponding extremal tree in $\mathcal{T}(2k)$ were determined. In this paper, we determine the second to the sixth largest values of the Laplacian spectral radii $\mu(T)$ of the trees T in $\mathcal{T}(2k)$ together with the corresponding trees T in $\mathcal{T}(2k)$ whose Laplacian spectral radii reach these values.

Let $S_k^1 = K_{1,k-1}$ and S_k^2, S_k^3, S_k^4 be the following trees of order k as shown in Fig. 1.

For any tree H of order k, let $C(H)$ be the tree of order $2k$ obtained from H by adding a new pendant edge at each vertex of H. It is easy to see that $C(H)$ has k pendant vertices and has a perfect matching.

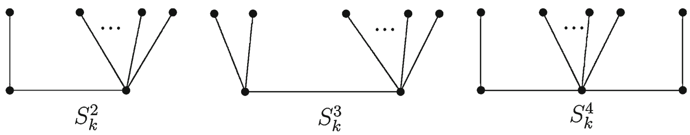


Fig. 1 The trees S_k^2, S_k^3 and S_k^4 (of order k)

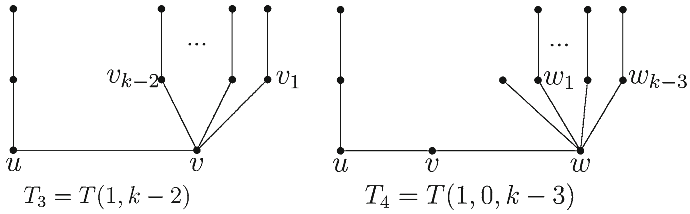


Fig. 2 The trees $T(1, k-2)$ and $T(1, 0, k-3)$ (of order $2k$)

Let T_3 and T_4 be the two trees of order $2k$ as shown in Fig. 2. Then it is easy to see that both T_3 and T_4 have perfect matchings. T_3 and T_4 will also be denoted by $T(1, k-2)$ and $T(1, 0, k-3)$ later in Sect. 4 and Sect. 5, respectively.

The main result of this paper is the following theorem, which will be proved in Sect. 7.

Theorem 7.1 *Let $T_1 = C(K_{1,k-1})$, $T_2 = C(S_k^2)$, T_3 (see Fig. 2), T_4 (see Fig. 2), $T_5 = C(S_k^3)$ and $T_6 = C(S_k^4)$ be the six trees in $\mathcal{T}(2k)$ as defined above. Let $\lambda_1(f_i)$ be the largest (real) root of the equation $f_i(x) = 0$ $(i = 2, 3, \ldots, 6)$, where*

$$f_2(x) = x^6 - (k+8)x^5 + (8k+20)x^4 - (21k+16)x^3 + (22k-2)x^2 - (9k-4)x + k, \tag{1.2}$$

$$f_3(x) = x^4 - (k+5)x^3 + 5(k+1)x^2 - 2(3k-1)x + k, \tag{1.3}$$

$$f_4(x) = x^6 - (k+8)x^5 + (8k+21)x^4 - (22k+18)x^3 + (25k-4)x^2 - (11k-8)x + k, \tag{1.4}$$

$$f_5(x) = x^6 - (k+8)x^5 + (9k+15)x^4 - (25k-4)x^3 + (27k-27)x^2 - (11k-14)x + k, \tag{1.5}$$

$$f_6(x) = x^6 - (k+7)x^5 + (8k+12)x^4 - (21k-4)x^3 + (22k-21)x^2 - (9k-10)x + k. \tag{1.6}$$

Then for $k \geq 6$, we have

(1) $\mu(T_i) = \lambda_1(f_i)$ *for* $i = 2, 3, \ldots, 6$.
(2) $\mu(T_1) > \mu(T_2) > \mu(T_3) > \mu(T_4) > \mu(T_5) > \mu(T_6)$. (1.7)
(3) *For any tree* $T \in \mathcal{T}(2k) \backslash \{T_1, T_2, T_3, T_4, T_5, T_6\}$, *we have*

$$\mu(T) < \mu(T_6). \tag{1.8}$$

2 A basic comparison method

It is well known that if a tree T has a perfect matching, then this matching is unique, and is usually denoted by $M(T)$ (or simply M). It is easy to see that in this case, different pendant vertices of T will be adjacent to different (non-pendant) vertices of T, and each pendant edge of T is in the perfect matching $M(T)$.

Let $m_1 = m_1(T)$ be the number of pendant vertices of T. If $T \in \mathcal{T}(2k)$ (has a perfect matching), then m_1 is equal to the number of pendant edges in $M(T)$, and thus the number of non-pendant edges in $M(T)$ is just equal to $k - m_1$.

Let $m_{12} = m_{12}(T)$ be the number of such pendant vertices of a tree T whose neighbor is a vertex of degree 2. Obviously we have $m_{12}(T) \leq m_1(T)$.

Let $B(G) = D(G) + A(G)$, and $\rho(B(G))$ be the largest eigenvalue of the nonnegative symmetric matrix $B(G)$. It is obvious that

$$B(G) = |D(G) - A(G)| = |L(G)|,$$

where $|Q|$ denotes the (entrywise) absolute value of a matrix Q.

Lemma 2.1 [17] *Let G be a graph. Then $\mu(G) \leq \rho(B(G))$. Moreover, if G is connected, then equality holds if and only if G is a bipartite graph.*

The following Theorem 2.1 is a generalization of a comparison theorem given in [9] (Theorem 2.1) and in [7] (Theorem 3.8), which will be a basic comparison method used in this paper.

Theorem 2.1 *Let G be a connected graph and $u, v_1, v_2, \ldots, v_r$ be vertices of G. Suppose $V_1, V_2, \ldots, V_r$ are pairwise disjoint vertex subsets of G, which are not all empty, and*

$$V_i = \{v_{i1}, v_{i2}, \ldots, v_{ik_i}\} \subseteq N(v_i) \backslash (N(u) \cup \{u\}) \ \ (i = 1, 2, \ldots, r). \tag{2.1}$$

Let G' be the graph with $V(G') = V(G)$ and

$$E(G') = \left(E(G) \backslash \bigcup_{i=1}^{r} \{v_i v_{i1}, \ldots, v_i v_{ik_i}\} \right) \bigcup \left(\bigcup_{i=1}^{r} \{u v_{i1}, \ldots, u v_{ik_i}\} \right). \tag{2.2}$$

Let X be the unit (positive) eigenvector of the nonnegative irreducible (also symmetric) matrix $B(G)$ corresponding to its eigenvalue $\rho(B(G))$. Suppose we have

(1) *Both G' and G are bipartite graphs,*
(2) $x_u \geq max\{x_{v_1}, x_{v_2}, \ldots, x_{v_r}\}$, *where x_u denotes the coordinate of X corresponding to the vertex u.*

Then we have $\mu(G) < \mu(G')$.

Proof From Lemma 2.1 and the hypothesis (1), we know that $\mu(G) = \rho(B(G))$ and $\mu(G') = \rho(B(G'))$. From the well-known results of real symmetric matrices in linear algebra, we have

$$\rho(B(G)) = X^T B(G) X \quad \text{and} \quad \rho(B(G')) \geq X^T B(G') X.$$

So we have

$$\begin{aligned} \rho(B(G')) - \rho(B(G)) &\geq X^T B(G') X - X^T B(G) X \\ &= X^T \left(B(G') - B(G) \right) X \\ &= \sum_{i=1}^{r} \left(\sum_{j=1}^{k_i} \left[(x_u + x_{v_{ij}})^2 - (x_v + x_{v_{ij}})^2 \right] \right) \\ &\geq 0. \end{aligned} \tag{2.3}$$

Next we want to show that the strict inequality holds in (2.3). Namely, we want to show that $\rho(B(G')) - \rho(B(G)) > 0$. Suppose not, then all the equalities hold in (2.3). In particular, we have

$$\rho(B(G)) - \rho(B(G')) = X^T B(G') X - X^T B(G) X = 0,$$

but $\rho(B(G)) = X^T B(G) X$, so we have

$$\rho(B(G')) = \rho(B(G)) = X^T B(G) X = X^T B(G') X,$$

which implies that X is also an eigenvector of $B(G')$ corresponding to $\rho(B(G'))$, namely we also have $B(G')X = \rho(B(G'))X$. Thus

$$\left(B(G') - B(G) \right) X = \rho(B(G'))X - \rho(B(G))X = 0. \tag{2.4}$$

On the other hand, we have

$$\left((B(G') - B(G)) X \right)_u = \left(\sum_{i=1}^{r} k_i \right) x_u + \sum_{i=1}^{r} \left(\sum_{j=1}^{k_i} x_{v_{ij}} \right) > 0.$$

This contradicts (2.4). □

Remark In this paper, we will mostly use the special case $r = 1$ of Theorem 2.1, which is just the result in [9] and [7].

Now we define the following subsets of trees in $\mathcal{T}(2k)$.

$$\mathcal{T}_q(2k) = \{T \in \mathcal{T}(2k) \mid m_1(T) = q\} \ \ (q = 2, 3, \ldots, k)\,. \tag{2.5}$$

The following theorem is also useful in the comparison of Laplacian spectral radii of the trees in $\mathcal{T}(2k)$.

Theorem 2.2 *Let $T \in \mathcal{T}_q(2k)$ with $q \le k-1$. Then there exists $T' \in \mathcal{T}_{q+1}(2k)$ with $m_{12}(T') = m_{12}(T)$ such that $\mu(T) < \mu(T')$.*

Proof Since $m_1(T) = q \le k-1$, there exists some edge $e = uv$ in the perfect matching M of T such that both u and v are non-pendant vertices. Let X be the unit positive eigenvector of $B(T)$ corresponding to $\rho(B(T))$ (where $B(T) = D(T)+A(T)$). Without loss of generality, we may assume that $x_u \ge x_v$ (otherwise we can exchange u and v). Now using Theorem 2.1 on T in the special case $r = 1$, $v_1 = v$ and $V_1 = N(v)\backslash\{u\}$. We obtain a tree T' of order $2k$ with $\mu(T) < \mu(T')$. Also, it is easy to verify that T' has a perfect matching (since $e = uv \in M(T)$) and

$$d_{T'}(v) = 1,\ d_{T'}(u) \ge 3,\ d_{T'}(w) = d_T(w) \text{ for all } w \notin \{u, v\}. \tag{2.6}$$

It follows from (2.6) that $m_1(T') = m_1(T) + 1 = q + 1$ (thus $T' \in \mathcal{T}_{q+1}(2k)$) and $m_{12}(T') = m_{12}(T)$. □

3 Ordering trees in $\mathcal{T}_k(2k)$

In this section, we first determine the structure of the trees in the class $\mathcal{T}_k(2k)$. Then we use this structure to determine the first four trees in $\mathcal{T}_k(2k)$ with the largest Laplacian spectral radii. We also compare the Laplacian spectral radii of the fourth tree in $\mathcal{T}_k(2k)$ with some other classes of trees in $\mathcal{T}(2k)$.

Recall that if H is a tree of order k, then $C(H)$ is the tree of order $2k$ obtained from H by adding a new pendant edge at each vertex of H.

Lemma 3.1 *$T \in \mathcal{T}_k(2k)$ if and only if there exists a tree H of order k such that $T = C(H)$.*

Proof The sufficiency follows easily from the definition of $C(H)$. For necessity, suppose $T \in \mathcal{T}_k(2k)$, let H be the tree of order k obtained from T by deleting its k pendant vertices. Then we can verify that $T = C(H)$, since T has a perfect matching. □

The next lemma gives explicit relations between the Laplacian spectral radii of the trees H and $C(H)$.

Lemma 3.2 *Let $T \in \mathcal{T}_k(2k)$ and $T = C(H)$, where H is a tree of order k. Then we have*

(1) $\Phi(T; x) = (x-1)^k\, \Phi\left(H; x - 1 - \frac{1}{x-1}\right)$ *for $x \neq 1$.*

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

Proof (1) By labelling the vertices of T properly, we can get the following relation between $L(T)$ and $L(H)$,

$$L(T) = \begin{pmatrix} L(H) + I & -I \\ -I & I \end{pmatrix},$$

where I is the identity matrix of order k. Then

$$\Phi(T; x) = \det \begin{pmatrix} (x-1)I - L(H) & I \\ I & (x-1)I \end{pmatrix}.$$

Notice that for $x \neq 1$, we have

$$\begin{pmatrix} (x-1)I - L(H) & I \\ I & (x-1)I \end{pmatrix} \begin{pmatrix} I & 0 \\ -\frac{1}{x-1}I & I \end{pmatrix}$$

$$= \begin{pmatrix} \left(x - 1 - \frac{1}{x-1}\right) I - L(H) & I \\ 0 & (x-1)I \end{pmatrix}.$$

Take the determinants for both sides, we get the desired result.

(2) From (1) and using

$$\Phi(H; y) = \prod_{i=1}^{k} [y - \mu_i(H)],$$

we have

$$\Phi(T; x) = \prod_{i=1}^{k} \left[(x-1)^2 - \mu_i(H)(x-1) - 1\right].$$

So we can see that $\mu(T)$ is the larger root of the equation

$$(x-1)^2 - \mu(H)(x-1) - 1 = 0.$$

Namely,

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

□

The following result follows immediately from Lemma 3.2.

Corollary 3.1 *Let H_1, H_2 be two trees with $\mu(H_1) > \mu(H_2)$. Then*

$$\mu(C(H_1)) > \mu(C(H_2)).$$

Let $\mathbf{T}_k$ be the set of trees of order k. In [5] and [16], the first four trees in $\mathbf{T}_k$ with the largest values of Laplacian spectral radii were determined. They are $S_k^1 = K_{1,k-1}$, S_k^2, S_k^3 and S_k^4 (see Fig. 1).

Actually, in [5] and [16], it is proved that if $k \geq 6$ and $T \in \mathbf{T}_k \backslash \{K_{1,k-1}, S_k^2, S_k^3, S_k^4\}$, then

$$k = \mu(K_{1,k-1}) > \mu(S_k^2) > \mu(S_k^3) > \mu(S_k^4) > \mu(T). \tag{3.1}$$

From (3.1) and Corollary 3.1, we immediately have the following result.

Lemma 3.3 *If $k \geq 6$, then*

(1) $\mu(C(K_{1,k-1})) > \mu(C(S_k^2)) > \mu(C(S_k^3)) > \mu(C(S_k^4))$.
(2) *If $T \in \mathcal{T}_k(2k) \backslash \{C(K_{1,k-1}), C(S_k^2), C(S_k^3), C(S_k^4)\}$, then $\mu(T) < \mu(C(S_k^4))$.*

From Lemma 3.2 and $\mu(K_{1,k-1}) = k$, we have $\mu(C(K_{1,k-1})) = (k+2+\sqrt{k^2+4})/2$. So using Theorem 2.2 and Lemma 3.3, we can easily get the following result.

Corollary 3.2 [5] *Let $T \in \mathcal{T}(2k)$ for $k \geq 1$. Then*

$$\mu(T) \leq \frac{k+2+\sqrt{k^2+4}}{2},$$

with equality if and only if $T = C(K_{1,k-1})$.

If $v \in V(G)$, let $L_v(G)$ be the principal sub-matrix of $L(G)$ obtained by deleting the row and column corresponding to the vertex v. The following two results (Lemma 3.4, 3.5) from [6] and [4], respectively, will play important roles in the proofs of our later results.

Lemma 3.4 [6] *Let $G = G_1u : vG_2$ be the graph obtained by joining the vertex u of the graph G_1 to the vertex v of the graph G_2 by an edge, where G_1 and G_2 are disjoint. Then*

$$\Phi(L(G)) = \Phi(L(G_1))\Phi(L(G_2)) - \Phi(L(G_1))\Phi(L_v(G_2)) - \Phi(L(G_2))\Phi(L_u(G_1)).$$

Lemma 3.5 [4] *Let G be a connected graph of order n with at least one edge, then $\mu(G) \geq \Delta(G)+1$, where $\Delta(G)$ is the maximum degree of the graph G, with equality if and only if $\Delta(G) = n-1$.*

From the above discussions, we already know that the first four trees in the set $\mathcal{T}_k(2k)$ with the largest Laplacian spectral radii are $C(K_{1,k-1})$, $C(S_k^2)$, $C(S_k^3)$ and $C(S_k^4)$. Also $\mu(C(K_{1,k-1})) = (k+2+\sqrt{k^2+4})/2$. The next lemma gives the values of $\mu(C(S_k^2))$, $\mu(C(S_k^3))$ and $\mu(C(S_k^4))$ as the largest roots of certain polynomials.

Lemma 3.6 *If* $k \geq 6$, *then* $\mu(T_i) = \lambda_1(f_i)$ *for* $i = 2, 5, 6$, *where* $T_2 = C(S_k^2)$, $T_5 = C(S_k^3)$, $T_6 = C(S_k^4)$, *and*

$$f_2(x) = x^6 - (k+8)x^5 + (8k+20)x^4 - (21k+16)x^3 \\ +(22k-2)x^2 - (9k-4)x + k, \quad (1.2)$$

$$f_5(x) = x^6 - (k+8)x^5 + (9k+15)x^4 - (25k-4)x^3 \\ +(27k-27)x^2 - (11k-14)x + k, \quad (1.5)$$

$$f_6(x) = x^6 - (k+7)x^5 + (8k+12)x^4 - (21k-4)x^3 \\ +(22k-21)x^2 - (9k-10)x + k. \quad (1.6)$$

Proof Using Lemma 3.4, we have

$$\Phi(T_2; x) = x(x-2)(x^2-3x+1)^{k-4} f_2(x), \quad (3.2)$$

$$\Phi(T_5; x) = x(x-2)(x^2-3x+1)^{k-4} f_5(x), \quad (3.3)$$

$$\Phi(T_6; x) = x(x-2)(x^2-3x+1)^{k-6}(x^4-7x^3+14x^2-8x+1) f_6(x). \quad (3.4)$$

From Lemma 3.5, we know $\mu(T_2) > k \geq 6$, $\mu(T_5) > k-1 \geq 5$, and $\mu(T_6) > k-1 \geq 5$. Also, the largest root of the following polynomial

$$x^4 - 7x^3 + 14x^2 - 8x + 1 = x(x-1)(x-2)(x-4) + 1$$

is less than 4. So we conclude that $\mu(T_i)$ is the largest root of $f_i(x) = 0$, namely, $\mu(T_i) = \lambda_1(f_i)$ for $i = 2, 5, 6$. □

One of our main goals in the later sections 4–7 of this paper is to prove (1.8), namely, $\mu(T) < \mu(C(S_k^4))$ for all $T \in \mathcal{T}(2k)\backslash\{T_1, T_2, T_3, T_4, T_5, T_6\}$. From Lemma 3.3, we already know that $\mu(T) < \mu(C(S_k^4))$ for $T \in \mathcal{T}_k(2k)\backslash\{T_1, T_2, T_5, T_6\}$. Next we will show in Lemma 3.7 that all $T \in \mathcal{T}(2k)\backslash\{C(S_k^4)\}$ with $m_{12}(T) \leq k-3$ satisfy $\mu(T) < \mu(C(S_k^4))$.

Lemma 3.7 *If* $T \in \mathcal{T}(2k)\backslash\{C(S_k^4)\}$ *with* $m_{12}(T) \leq k-3$, *then* $\mu(T) < \mu(C(S_k^4))$.

Proof By using Theorem 2.2 several times, we can obtain a tree $T' \in \mathcal{T}_k(2k)$ with $m_{12}(T') = m_{12}(T) \leq k-3$ such that

$$\mu(T) \leq \mu(T'). \quad (3.5)$$

Now $m_{12}(T') \leq k-3$ implies that $T' \in \mathcal{T}_k(2k)\backslash\{C(K_{1,k-1}), C(S_k^2), C(S_k^3)\}$. So from Lemma 3.3 we have

$$\mu(T') \leq \mu(C(S_k^4)). \quad (3.6)$$

Since $T \neq C(S_k^4)$, we can see that $T \neq T'$ or $T' \neq C(S_k^4)$ holds. So at least one strict inequality in (3.5) and (3.6) holds. Thus $\mu(T) < \mu(C(S_k^4))$. □

Corollary 3.3 *If $T \in \mathcal{T}_q(2k)$ with $q \leq k-3$, then $\mu(T) < \mu(C(S_k^4))$.*

Proof The result follows from the fact that $m_{12}(T) \leq m_1(T) = q \leq k-3$ and Lemma 3.7. □

From the above results we see that in order to prove (1.8), namely, $\mu(T) < \mu(C(S_k^4))$ for all $T \in \mathcal{T}(2k)\backslash\{T_1, T_2, T_3, T_4, T_5, T_6\}$, we are only left the following three classes of trees in $\mathcal{T}(2k)$ to be considered.

Class $(C1)$: The trees in $\mathcal{T}_{k-1}(2k)$ with $m_{12}(T) = k-1$.
Class $(C2)$: The trees in $\mathcal{T}_{k-1}(2k)$ with $m_{12}(T) = k-2$.
Class $(C3)$: The trees in $\mathcal{T}_{k-2}(2k)$ with $m_{12}(T) = k-2$.

In the following, we will consider Class $(C1)$ in Sect. 4, Class $(C2)$ in Sect. 5 and Class $(C3)$ in Sect. 6.

4 The trees T in $\mathcal{T}_{k-1}(2k)$ with $m_{12}(T) = k-1$

In this section, we first determine the structure of the trees in Class $(C1)$. Then we give a complete ordering of all the trees in Class $(C1)$ according to their Laplacian spectral radii by using the basic comparison method given in Theorem 2.1. We then show that all the trees in Class $(C1)$, except the first one, satisfy $\mu(T) < \mu(C(S_k^4))$.

Let $T(i, j)$ be a tree of order $2k$ obtained from P_2 by attaching i new paths of length 2 to one vertex of P_2 and attaching j new paths of length 2 to the other vertex of P_2, where $1 \leq i \leq j,\ i+j = k-1$ (see Fig. 3).

Recall that in Sect. 1 (Fig. 2), we have denoted the tree $T(1, k-2)$ by T_3.

The tree which is obtained from P_2 by attaching i new pendant edges at one vertex of P_2 and attaching j new pendant edges at the other vertex of P_2 is called a double star graph, and is denoted $S(i, j)$.

Lemma 4.1 *$T \in \mathcal{T}_{k-1}(2k)$ with $m_{12}(T) = k-1$ if and only if $T = T(i, j)$ for some $1 \leq i \leq j,\ i+j = k-1$.*

Proof The sufficiency part is obvious. We now consider the necessity.

Since $m_1(T) = k-1$ and $m_{12}(T) = k-1$, we may write

$$M(T) = \{uv, x_1y_1, x_2y_2, \ldots, x_{k-1}y_{k-1}\}$$

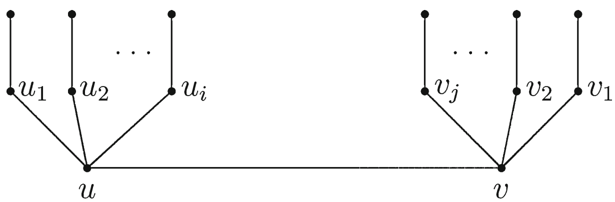


Fig. 3 The tree $T(i, j)$ (of order $2k$)

with $d(u) \geq 2, d(v) \geq 2, d(x_t) = 1$ and $d(y_t) = 2$ for $t = 1, 2, \ldots, k-1$. Let $G = T - \{x_1, x_2, \ldots, x_{k-1}\}$, then G is a sub-tree of T of order $k+1$. Furthermore, $uv \in E(G), d_G(u) \geq 2, d_G(v) \geq 2$, and $d_G(y_t) = 1$ for $t = 1, 2, \ldots, k-1$. So we can see that $G = S(i, j)$ with $1 \leq i \leq j,\ i + j = k - 1$. Thus $T = T(i, j)$. □

Lemma 4.2 *If* $1 \leq i < j \leq \lfloor \frac{k-1}{2} \rfloor$, *then we have*

$$\mu(T(i, k-1-i)) > \mu(T(j, k-1-j)).$$

Proof Let $T = T(j, k-1-j)$ and u, v be the two non-pendant vertices of T which are not adjacent to any pendant vertices. Let $N(u) = \{u_1, u_2, \ldots, u_j, v\}$, $N(v) = \{v_1, v_2 \ldots, v_{k-1-j}, u\}$. Let X be the unit positive eigenvector of $B(T)$ corresponding to $\rho(B(T))$ (where $B(T) = D(T) + A(T)$ as defined in Sect. 2). By hypothesis, we have $k - 1 - j \geq j > i$. We distinguish the following cases.

Case 1. $x_u \geq x_v$.

Let $t = k - 1 - j - i \geq 1$. Now using Theorem 2.1 on T to take

$$T' = T - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}.$$

Then we have $T' = T(i, k-1-i)$ and $\mu(T) < \mu(T')$.

Case 2. $x_v > x_u$.

Let $s = j - i \geq 1$. Also using Theorem 2.1 on T to take

$$T' = T - \{uu_1, uu_2, \ldots, uu_s\} + \{vu_1, vu_2, \ldots, vu_s\}.$$

Then we have $T' = T(i, k-1-i)$ and $\mu(T) < \mu(T')$. □

Lemma 4.3 $\mu(T(2, k-3)) < \mu(C(S_k^4))$ *for* $k \geq 6$.

Proof By direct calculations, we have

$$\Phi(T(2, k-3); x) = x(x-2)(x^2 - 3x + 1)^{k-3} g(x),$$

where

$$g(x) = x^4 - (k+5)x^3 + (6k+1)x^2 - (8k-10)x + k.$$

Furthermore, we can see that $\mu(T(2, k-3))$ is the largest root of $g(x) = 0$. From Lemma 3.6, we get $\mu(C(S_k^4)) = \lambda_1(f_6)$, where

$$\begin{aligned} f_6(x) = x^6 - (k+7)x^5 + (8k+12)x^4 - (21k-4)x^3 \\ +(22k-21)x^2 - (9k-10)x + k. \end{aligned} \tag{1.6}$$

Let

$$h(x) = x^2 - (k+2)x + k. \tag{4.1}$$

Then we can verify that

$$f_6(x) = (x-1)^2 g(x) + x h(x). \tag{4.2}$$

Let $\mu(T(2, k-3)) = a$. By Lemma 3.5 and Corollary 3.2, we have

$$\frac{k+2-\sqrt{k^2+4}}{2} < 1 < a < \mu(C(K_{1,k-1})) = \frac{k+2+\sqrt{k^2+4}}{2}.$$

So from (4.1) we have $h(a) < 0$. It follows from (4.2) that $f_6(a) < 0$. So $\mu(C(S_k^4)) = \lambda_1(f_6) > a = \mu(T(2, k-3))$. □

Combining Lemma 4.1, 4.2 and 4.3, we see that all the trees in Class $(C1)$ except $T_3 = T(1, k-2)$ satisfy $\mu(T) < \mu(C(S_k^4))$.

5 The trees T in $\mathcal{T}_{k-1}(2k)$ with $m_{12}(T) = k-2$

In this section, we first determine the structure of the trees in Class $(C2)$ (namely, the trees in $\mathcal{T}_{k-1}(2k)$ with $m_{12}(T) = k-2$.) Then we use this structure to show that all the trees in Class $(C2)$, except the tree T_4, satisfy $\mu(T) < \mu(C(S_k^4))$.

Let $T(\ell_1, \ell_2, \ell_3)$ be a tree of order $2k$ obtained from $P_3 : u\,v\,w$ by attaching ℓ_1 new paths of length 2 to the vertex u, attaching ℓ_2 new paths of length 2 to the vertex v and attaching ℓ_3 new paths of length 2 and one pendant edge to the vertex w, where $\ell_1 \geq 1$, $\ell_3 \geq 1$ and $\ell_1 + \ell_2 + \ell_3 = k-2$ (see Fig. 4).

Recall that in Sect. 1 (Fig. 2), we have denoted the tree $T(1, 0, k-3)$ by T_4.

Lemma 5.1 *$T \in \mathcal{T}_{k-1}(2k)$ with $m_{12}(T) = k-2$ if and only if $T = T(\ell_1, \ell_2, \ell_3)$ for some $\ell_1 \geq 1$, $\ell_3 \geq 1$ and $\ell_1 + \ell_2 + \ell_3 = k-2$.*

Proof The sufficiency part is obvious. Now we consider the necessity.

Since $m_1(T) = k-1$ and $m_{12}(T) = k-2$, we may write

$$M(T) = \{uv, x_1 y_1, x_2 y_2, \ldots, x_{k-1} y_{k-1}\}$$

with $d(u) \geq 2$, $d(v) \geq 2$, $d(x_t) = 1$ for $t = 1, 2, \ldots, k-1$, $d(y_t) = 2$ for $t = 1, 2, \ldots, k-2$, and $d(y_{k-1}) \geq 3$.

Let $G = T - \{x_1, x_2, \ldots, x_{k-1}\}$. Then G is a sub-tree of T of order $k+1$. Furthermore, G contains exactly 3 vertices which are non-pendant vertices, that is u, v, y_{k-1}.

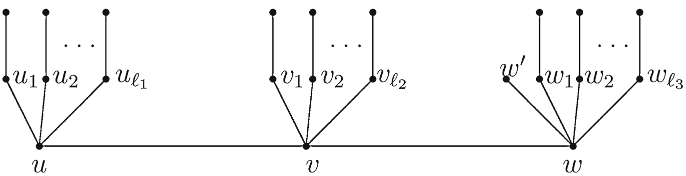


Fig. 4 The tree $T(\ell_1, \ell_2, \ell_3)$ (of order $2k$)

Since $G - \{y_1, y_2, \ldots, y_{k-2}\}$ is also a tree (of order 3), y_{k-1} is adjacent to u or v, but y_{k-1} can not be adjacent to both u and v, since $uv \in E(T)$. Without loss of generality, we assume y_{k-1} is adjacent to v. Since $d_T(y_{k-1}) \geq 3$, y_{k-1} is adjacent to at least one of $\{y_1, y_2, \ldots, y_{k-2}\}$. Let

$$\{y_1, y_2, \ldots, y_{k-2}\} = Y_1 \dot{\cup} Y_2 \dot{\cup} Y_3,$$

and $\ell_t = |Y_t|$ for $t = 1, 2, 3$, where the vertices in Y_1 are adjacent to u, the vertices in Y_2 are adjacent to v, and the vertices in Y_3 are adjacent to y_{k-1}. From the above discussions, we conclude that $T = T(\ell_1, \ell_2, \ell_3)$ with $\ell_1 + \ell_2 + \ell_3 = k - 2$. Furthermore, $\ell_1 \geq 1$ follows from $d(u) \geq 2$, and $\ell_3 \geq 1$ follows from $Y_3 \neq \emptyset$. □

Let $T_4 = T(1, 0, k-3)$ as in Sect. 1, and let

$$G_1 = T(k-3, 0, 1), \;\; G_2 = T(1, k-4, 1),$$
$$G_3 = T(2, 0, k-4), \;\; G_4 = T(1, 1, k-4).$$

Lemma 5.2 *If $T = T(\ell_1, \ell_2, \ell_3)$ with $\ell_1 \geq 1, \ell_3 \geq 1, \ell_1 + \ell_2 + \ell_3 = k - 2$, and $T \notin \{G_1, G_2, G_3, G_4, T_4\}$, then $\mu(T) < max\{\mu(G_1), \mu(G_2), \mu(G_3), \mu(G_4)\}$.*

Proof Let u, v and w be three vertices of T as shown in Fig. 4, and $N(u) = \{u_1, u_2, \ldots, u_{\ell_1}, v\}$, $N(v) = \{v_1, v_2, \ldots, v_{\ell_2}, u, w\}$, $N(w) = \{w_1, w_2, \ldots, w_{\ell_3}, v, w'\}$. Let X be the unit positive eigenvector of $B(T)$ corresponding to $\rho(B(T))$ (where $B(T) = D(T) + A(T)$ as defined in Sect. 2). We distinguish the following cases.

Case 1. $\max\{x_u, x_v, x_w\} = x_u$.

Take

$$T' = T - \{vv_1, vv_2, \ldots, vv_{\ell_2}\} - \{ww_2, ww_3, \ldots, ww_{\ell_3}\}$$
$$+\{uv_1, uv_2, \ldots, uv_{\ell_2}\} + \{uw_2, uw_3, \ldots, uw_{\ell_3}\}.$$

Then we have $T' = G_1$. Since $T \neq G_1$, we have $\mu(T) < \mu(T')$ by Theorem 2.1. So $\mu(T) < \mu(G_1)$.

Case 2. $\max\{x_u, x_v, x_w\} = x_v$.

Take

$$T' = T - \{uu_2, uu_3, \ldots, uu_{\ell_1}\} - \{ww_2, ww_3, \ldots, ww_{\ell_3}\}$$
$$+\{vu_2, vu_3, \ldots, vu_{\ell_1}\} + \{vw_2, vw_3, \ldots, vw_{\ell_3}\}.$$

Then we have $T' = G_2$. Since $T \neq G_2$, we have $\mu(T) < \mu(T')$ by Theorem 2.1. So $\mu(T) < \mu(G_2)$.

Case 3. $\max\{x_u, x_v, x_w\} = x_w$.

Subcase 3.1. $\ell_1 \geq 2$.

Take

$$T' = T - \{uu_3, uu_4, \ldots, uu_{\ell_1}\} - \{vv_1, vv_2, \ldots, vv_{\ell_2}\}$$
$$+\{wu_3, wu_4, \ldots, wu_{\ell_1}\} + \{wv_1, wv_2, \ldots, wv_{\ell_2}\}.$$

Then we have $T' = G_3$. Since $T \neq G_3$, we have $\mu(T) < \mu(T')$ by Theorem 2.1. So $\mu(T) < \mu(G_3)$.

Subcase 3.2. $\ell_1 = 1$.

Since $T \neq T_4$, we have $\ell_2 \geq 1$. Take

$$T' = T - \{uu_2, uu_3, \ldots, uu_{\ell_1}\} - \{vv_2, vv_3, \ldots, vv_{\ell_2}\}$$
$$+\{wu_2, wu_3, \ldots, wu_{\ell_1}\} + \{wv_2, wv_3, \ldots, wv_{\ell_2}\}.$$

Then we have $T' = G_4$. Since $T \neq G_4$, we have $\mu(T) < \mu(T')$ by Theorem 2.1. So $\mu(T) < \mu(G_4)$. □

Lemma 5.3 *If $k \geq 6$, and G_1, G_2, G_3, G_4 are as above, then we have*

(1) $\mu(G_1) < \mu(T(2, k-3))$.
(2) $\mu(G_2) < \mu(T(2, k-3))$.
(3) $\mu(G_3) < \mu(T(2, k-3))$.
(4) $\mu(G_4) < \mu(T(2, k-3))$.

Proof By direct calculations using Lemma 3.4, we have

$$\Phi(G_1; x) = x(x-2)(x^2 - 3x + 1)^{k-4} r_1(x), \tag{5.1}$$

$$\Phi(G_2; x) = x(x-2)(x^2 - 3x + 1)^{k-5} r_2(x), \tag{5.2}$$

$$\Phi(G_3; x) = x(x-2)(x^2 - 3x + 1)^{k-4} r_3(x), \tag{5.3}$$

$$\Phi(G_4; x) = x(x-2)(x^2 - 3x + 1)^{k-5} r_4(x), \tag{5.4}$$

where

$$\begin{aligned} r_1(x) &= x^6 - (k+8)x^5 + (9k+17)x^4 - (27k-2)x^3 + (32k-32)x^2 \\ &\quad -(13k-16)x + k, \\ r_2(x) &= x^8 - (k+11)x^7 + (12k+42)x^6 - (55k+57)x^5 + (121k-17)x^4 \\ &\quad -(132k-98)x^3 + (67k-60)x^2 - (14k-8)x + k, \\ r_3(x) &= x^6 - (k+8)x^5 + (9k+17)x^4 - (27k-2)x^3 + (33k-37)x^2 \\ &\quad -(15k-26)x + k, \\ r_4(x) &= x^8 - (k+11)x^7 + (12k+42)x^6 - (55k+57)x^5 + (122k-22)x^4 \\ &\quad -(137k-123)x^3 + (74k-95)x^2 - (16k-18)x + k. \end{aligned}$$

From (5.1) to (5.4), it is easy to see that $\mu(G_i)$ is the largest root of the equation $r_i(x) = 0$ for $i = 1, 2, 3, 4$. Now let

$$g(x) = x^4 - (k+5)x^3 + (6k+1)x^2 - (8k-10)x + k.$$

From the proof of the Lemma 4.3, we know that $\mu(T(2, k-3))$ is the largest root of the equation $g(x) = 0$. By calculations we also have

$$
\begin{aligned}
r_1(x) &= (x^2 - 3x + 1)g(x) + h_1(x), \ \text{ where } h_1(x) = (k-3)x(x-2),\\
r_2(x) &= (x^2 - 3x + 1)^2 g(x) + h_2(x), \ \text{ where } \ h_2(x) = x(x-2)[x^2 - (k-1)x + 1],\\
r_3(x) &= (x^2 - 3x + 1)g(x) + h_3(x), \ \text{ where } h_3(x) = 2(k-4)x(x-2),\\
r_4(x) &= (x^2 - 3x + 1)^2 g(x) + h_4(x), \ \text{ where } h_4(x) = (k-4)x(x-2)(x^2 - 4x + 1).
\end{aligned}
$$

Notice from Lemma 3.5 that $\mu(G_i) \geq \Delta(G_i) + 1 \geq k - 1 \geq 5$, so we can easily see that $h_i(\mu(G_i)) > 0$. So from the above relations and the fact that $r_i(\mu(G_i)) = 0$, we can conclude that $g(\mu(G_i)) < 0$. So we have $\mu(G_i) < \lambda_1(g) = \mu(T(2, k-3))$ for $i = 1, 2, 3, 4$ as desired. □

Combining Lemma 5.1, 5.2, 5.3, we see that all the trees in Class $(C2)$ except $T_4 = T(1, 0, k-3)$ satisfy $\mu(T) < \mu(T(2, k-3)) < \mu(C(S_k^4))$.

6 The trees T in $\mathcal{T}_{k-2}(2k)$ with $m_{12}(T) = k - 2$

In this section, we first determine the structure of the trees in Class $(C3)$ (namely, the trees in $\mathcal{T}_{k-2}(2k)$ with $m_{12}(T) = k-2$.) Then we use this structure and the comparison method given in Theorem 2.1 together with another useful comparison method given in Lemma 6.3 to show that all the trees in Class $(C3)$ satisfy $\mu(T) < \mu(C(S_k^4))$.

Let $T(\ell_1, \ell_2, \ell_3, \ell_4)$ be a tree of order $2k$ obtained from $P_4 : u_1\, u_2\, u_3\, u_4$ by attaching ℓ_i new paths of length 2 to the vertex u_i for $i = 1, 2, 3, 4$, respectively, where $\ell_1 \geq 1, \ell_4 \geq 1$ and $\ell_1 + \ell_2 + \ell_3 + \ell_4 = k - 2$ (see Fig. 5). It is easy to see that $T(\ell_1, \ell_2, \ell_3, \ell_4) = T(\ell_4, \ell_3, \ell_2, \ell_1)$.

Lemma 6.1 *$T \in \mathcal{T}_{k-2}(2k)$ with $m_{12}(T) = k-2$ if and only if $T = T(\ell_1, \ell_2, \ell_3, \ell_4)$ for some $\ell_1 \geq 1, \ell_4 \geq 1$ and $\ell_1 + \ell_2 + \ell_3 + \ell_4 = k - 2$.*

Proof The sufficiency is obvious. Now we consider the necessity.

Since $m_1(T) = k-2$ and $m_{12}(T) = k-2$, we may write

$$M(T) = \{u_1u_2, u_3u_4, x_1y_1, x_2y_2, \ldots, x_{k-2}y_{k-2}\}$$

with $d(u_i) \geq 2$ for $i = 1, 2, 3, 4$, $d(x_j) = 1$ and $d(y_j) = 2$ for $j = 1, 2, \ldots, k-2$. Let $G_1 = T - \{x_1, x_2, \ldots, x_{k-2}\}$. Then G_1 is a sub-tree of T of order $k+2$. Furthermore, $y_1, y_2, \ldots, y_{k-2}$ are pendant vertices of G_1. Let $G_2 = G_1 - \{y_1, y_2, \ldots, y_{k-2}\}$.

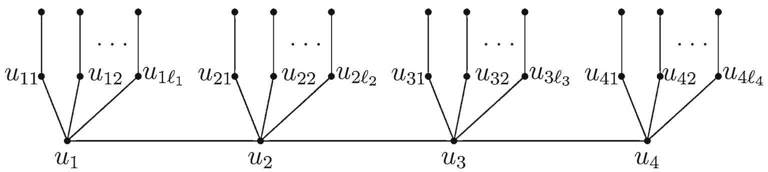


Fig. 5 The tree $T(\ell_1, \ell_2, \ell_3, \ell_4)$ (of order $2k$)

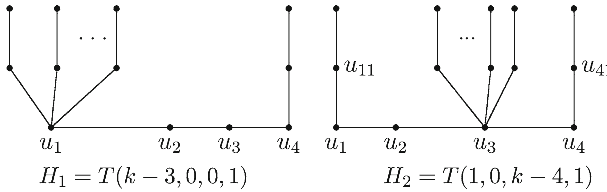


Fig. 6 The trees H_1 and H_2 (of order $2k$)

It is easy to see that G_2 is a tree of order 4 with a perfect matching. Note that P_4 is the unique tree of order 4 with a perfect matching. Then $G_2 = P_4$. From this we can easily get $T = T(\ell_1, \ell_2, \ell_3, \ell_4)$ for some $\ell_1 \geq 1$, $\ell_4 \geq 1$ and $\ell_1 + \ell_2 + \ell_3 + \ell_4 = k - 2$. □

Now let $H_1 = T(k-3, 0, 0, 1)$ and $H_2 = T(1, 0, k-4, 1)$, which are shown in Fig. 6.

Lemma 6.2 *If $T = T(\ell_1, \ell_2, \ell_3, \ell_4)$ with $\ell_1 \geq 1$, $\ell_4 \geq 1$, $\ell_1 + \ell_2 + \ell_3 + \ell_4 = k - 2$ and $T \notin \{H_1, H_2\}$. Then $\mu(T) < max\{\mu(H_1), \mu(H_2)\}$.*

Proof Let u_1, u_2, u_3 and u_4 be the four vertices of T as shown in Fig. 5, and let

$$\begin{aligned} N(u_1) &= \{u_{11}, u_{12}, \ldots, u_{1\ell_1}, u_2\}, \\ N(u_2) &= \{u_{21}, u_{22}, \ldots, u_{2\ell_2}, u_1, u_3\}, \\ N(u_3) &= \{u_{31}, u_{32}, \ldots, u_{3\ell_3}, u_2, u_4\}, \\ N(u_4) &= \{u_{41}, u_{42}, \ldots, u_{4\ell_4}, u_3\}. \end{aligned}$$

Let X be the unit positive eigenvector of $B(T)$ corresponding to $\rho(B(T))$, where $B(T) = D(T) + A(T)$. We distinguish the following cases.

Case 1. max $\{x_{u_1}, x_{u_2}, x_{u_3}, x_{u_4}\} = x_{u_1}$ or x_{u_4}, say x_{u_1}.

Take

$$\begin{aligned} T' = T &- \{u_2u_{21}, \ldots, u_2u_{2\ell_2}\} - \{u_3u_{31}, \ldots, u_3u_{3\ell_3}\} - \{u_4u_{42}, \ldots, u_4u_{4\ell_4}\} \\ &+ \{u_1u_{21}, \ldots, u_1u_{2\ell_2}\} + \{u_1u_{31}, \ldots, u_1u_{3\ell_3}\} + \{u_1u_{42}, \ldots, u_1u_{4\ell_4}\} \end{aligned}$$

Then we have $T' = H_1$. Since $T \neq H_1$, we have $\mu(T) < \mu(T')$ by Theorem 2.1. So $\mu(T) < \mu(H_1)$.

Case 2. max $\{x_{u_1}, x_{u_2}, x_{u_3}, x_{u_4}\} = x_{u_2}$ or x_{u_3}, say x_{u_3}.

Take

$$\begin{aligned} T' = T &- \{u_1u_{12}, \ldots, u_1u_{1\ell_1}\} - \{u_2u_{21}, \ldots, u_2u_{2\ell_2}\} - \{u_4u_{42}, \ldots, u_4u_{4\ell_4}\} \\ &+ \{u_3u_{12}, \ldots, u_3u_{1\ell_1}\} + \{u_3u_{21}, \ldots, u_3u_{2\ell_2}\} + \{u_3u_{42}, \ldots, u_3u_{4\ell_4}\} \end{aligned}$$

Then we have $T' = H_2$. Since $T \neq H_2$, we have $\mu(T) < \mu(T')$ by Theorem 2.1. So $\mu(T) < \mu(H_2)$. □

The following Lemma 6.3 is also a useful comparison method for Laplacian spectral radii, which will be used in Lemma 6.4 and later in Lemma 7.2.

Lemma 6.3 *[15] Let $T_{k,l}(u)$ be the tree obtained from a tree T by attaching two new paths of length k and l to a vertex u, respectively. If $k \geq l \geq 1$, then $\mu(T_{k+1,l-1}(u)) < \mu(T_{k,l}(u))$.*

Lemma 6.4 *If $k \geq 6$, then we have*

(1) $\mu(H_1) < \mu(T(2, k-3))$.
(2) $\mu(H_2) < \mu(T(2, k-3))$.

Proof (1) Let T^* be a tree of order $2k-4$ as shown in Fig. 7. Then we have $T(2, k-3) = T^*_{2,2}(u)$ and $H_1 = T(1, 0, 0, k-3) = T^*_{4,0}(u)$. So by Lemma 6.3 we have $\mu(H_1) < \mu(T(2, k-3))$.

(2) Let X be the unit positive eigenvector of $B(H_2)$ corresponding to $\rho(B(H_2))$. We distinguish the following cases.

Case 1. $x_{u_1} \geq x_{u_4}$.

Take $T' = H_2 - \{u_4u_{41}\} + \{u_1u_{41}\}$. Then $T' = G_3 = T(2, 0, k-4)$. So $\mu(H_2) < \mu(T') = \mu(G_3)$ by Theorem 2.1. Furthermore, $\mu(H_2) < \mu(T(2, k-3))$ by Lemma 5.3 (3).

Case 2. $x_{u_4} > x_{u_1}$.

Take $T' = H_2 - \{u_1u_{11}\} + \{u_4u_{11}\}$. Then $T' = T(2, k-3)$. So $\mu(H_2) < \mu(T') = \mu(T(2, k-3))$ by Theorem 2.1. □

Combining Lemma 6.1, 6.2 and 6.4, we can see that all the trees in Class $(C3)$ satisfy $\mu(T) < \mu(T(2, k-3)) < \mu(C(S_k^4))$.

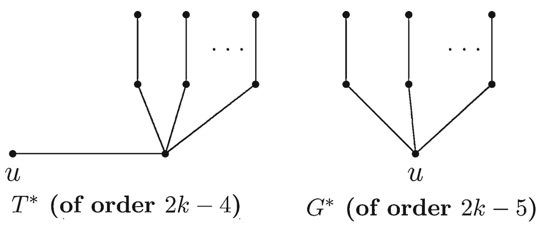
7 Main results

In this section, we will prove our main result. We first give the values of $\mu(T_3)$ and $\mu(T_4)$ (as the largest roots of the equations $f_3(x) = 0$ and $f_4(x) = 0$, respectively). Then we compare $\mu(T_2)$, $\mu(T_3)$, $\mu(T_4)$ and $\mu(T_5)$ in Lemma 7.2, 7.3 and 7.4. Finally, we obtain our main result in Theorem 7.1.

Lemma 7.1 *Let $T_3 = T(1, k-2)$ and $T_4 = T(1, 0, k-3)$ as defined in Sect. 1. Then we have $\mu(T_3) = \lambda_1(f_3)$, $\mu(T_4) = \lambda_1(f_4)$, where*

$$f_3(x) = x^4 - (k+5)x^3 + 5(k+1)x^2 - 2(3k-1)x + k, \tag{1.3}$$

Fig. 7 The trees T^* and G^*



and

$$f_4(x) = x^6 - (k+8)x^5 + (8k+21)x^4 - (22k+18)x^3 \\ +(25k-4)x^2 - (11k-8)x + k. \tag{1.4}$$

Proof By direct calculations, we have

$$\Phi(T_3; x) = x(x-2)(x^2-3x+1)^{k-3} f_3(x), \tag{7.1}$$

$$\Phi(T_4; x) = x(x-2)(x^2-3x+1)^{k-4} f_4(x). \tag{7.2}$$

From (7.1) and (7.2), it follows easily that $\mu(T_i)$ is the largest root of the equation $f_i(x) = 0$ for $i = 3, 4$. □

Next we use the comparison method given in Lemma 6.3 to compare $\mu(T_4)$ and $\mu(T_3)$.

Lemma 7.2 $\mu(T_4) < \mu(T_3)$ *for* $k \geq 4$.

Proof Let G^* be a tree of order $2k-5$ as shown in Fig. 7. Then we have $T(1, k-2) = G^*_{3,2}(u)$ and $T(1, 0, k-3) = G^*_{4,1}(u)$. So by Lemma 6.3, we have $\mu(T_4) < \mu(T_3)$ for $k \geq 4$. □

Lemma 7.3 $\mu(T_3) < \mu(T_2)$ *for* $k \geq 4$.

Proof From Lemma 3.6 and Lemma 7.1, we have $\mu(T_i) = \lambda_1(f_i)$ for $i = 2, 3$, where

$$f_2(x) = x^6 - (k+8)x^5 + (8k+20)x^4 - (21k+16)x^3 \\ +(22k-2)x^2 - (9k-4)x + k, \tag{1.2}$$

and

$$f_3(x) = x^4 - (k+5)x^3 + 5(k+1)x^2 - 2(3k-1)x + k. \tag{1.3}$$

Let

$$h(x) = x(x-2)(x^2 - kx + 1).$$

Then it can be easily verified that

$$f_2(x) = (x^2 - 3x + 1) f_3(x) - h(x).$$

Note that $h(x) > 0$ for $x \geq k$. Let $\mu(T_3) = a$, then from Lemma 3.5 we have $a > \Delta(T_3) + 1 = k$, so $h(a) > 0$. It follows that $f_2(a) = -h(a) < 0$, since $f_3(a) = 0$. So the largest root of $f_2(x) = 0$ is larger than a. Thus $\mu(T_2) = \lambda_1(f_2) > \mu(T_3)$ as desired. □

Lemma 7.4 $\mu(T_5) < \mu(T_4)$ *for* $k \geq 6$.

Proof From Lemma 3.6 and Lemma 7.1, we have $\mu(T_i) = \lambda_1(f_i)$ for $i = 4, 5$, where

$$f_4(x) = x^6 - (k+8)x^5 + (8k+21)x^4 - (22k+18)x^3 \\ +(25k-4)x^2 - (11k-8)x + k, \tag{1.4}$$

and

$$f_5(x) = x^6 - (k+8)x^5 + (9k+15)x^4 - (25k-4)x^3 \\ +(27k-27)x^2 - (11k-14)x + k. \tag{1.5}$$

Let

$$h(x) = (k-6)x^3 + (-3k+22)x^2 + (2k-23)x + 6.$$

Then it can be easily verified that

$$f_5(x) = f_4(x) + xh(x). \tag{7.3}$$

Now

$$h(x) = (x-5)\Big[(k-6)x^2 + (2k-8)x + (12k-63)\Big] + 60k - 309. \tag{7.4}$$

Let $b = \mu(T_5)$. Then by Lemma 3.5 we have $b > \Delta(T_5) + 1 = k - 1 \geq 5$. So from (7.4) we have $h(b) > 0$. It follows from (7.3) and the fact that $f_5(b) = 0$ that $f_4(b) < 0$. Thus we have $\mu(T_4) = \lambda_1(f_4) > b = \mu(T_5)$ as desired. □

Now we are ready to obtain our main result.

Theorem 7.1 *Let* $T_1 = C(K_{1,k-1})$, $T_2 = C(S_k^2)$, T_3*(see Fig. 2)*, T_4*(see Fig. 2)*, $T_5 = C(S_k^3)$ *and* $T_6 = C(S_k^4)$ *be the six trees in* $\mathcal{T}(2k)$ *as defined above. Let* $\lambda_1(f_i)$ *be the largest (real) root of the equation* $f_i(x) = 0$ $(i = 2, 3, \ldots, 6)$, *where*

$$f_2(x) = x^6 - (k+8)x^5 + (8k+20)x^4 - (21k+16)x^3 \\ +(22k-2)x^2 - (9k-4)x + k, \tag{1.2}$$

$$f_3(x) = x^4 - (k+5)x^3 + 5(k+1)x^2 - 2(3k-1)x + k, \tag{1.3}$$

$$f_4(x) = x^6 - (k+8)x^5 + (8k+21)x^4 - (22k+18)x^3 \\ +(25k-4)x^2 - (11k-8)x + k, \tag{1.4}$$

$$f_5(x) = x^6 - (k+8)x^5 + (9k+15)x^4 - (25k-4)x^3 \\ +(27k-27)x^2 - (11k-14)x + k, \tag{1.5}$$

$$f_6(x) = x^6 - (k+7)x^5 + (8k+12)x^4 - (21k-4)x^3 \\ +(22k-21)x^2 - (9k-10)x + k. \tag{1.6}$$

Then for $k \geq 6$, we have

(1) $\mu(T_i) = \lambda_1(f_i)$ for $i = 2, 3, \ldots, 6$.
(2)

$$\mu(T_1) > \mu(T_2) > \mu(T_3) > \mu(T_4) > \mu(T_5) > \mu(T_6). \tag{1.7}$$

(3) For any tree $T \in \mathcal{T}(2k)\backslash\{T_1, T_2, T_3, T_4, T_5, T_6\}$, we have

$$\mu(T) < \mu(T_6). \tag{1.8}$$

Proof (1) By Lemma 3.6 and Lemma 7.1.
(2) By Lemma 3.3 (1), Lemma 7.2, 7.3 and 7.4.
(3) By Lemma 3.3 (2), Lemma 3.7, Corollary 3.3; Lemma 4.1, 4.2, 4.3; Lemma 5.1, 5.2, 5.3; Lemma 6.1, 6.2 and 6.4. □

Acknowledgements The authors would like to thank the anonymous referees for their valuable suggestions and comments on an earlier version of this paper. Jia-Yu Shao research was supported by the National Natural Science Foundation of China 10731040.

References

1. A.E. Brouwer, W.H. Haemers, Eigenvalues and perfect matchings, Linear Algebra Appl. **395**, 155–162 (2005)
2. A. Chang, On the largest eigenvalue of a tree with perfect matchings, Discrete Math. **269**, 45–63 (2003)
3. B.E. Eichinger, J.E. Martin, Distribution functions for Gaussian molecules. II. Reduction of the Kirchhoff matrix for large molecules, J. Chem. Phys. **69**(10), 4595–4599 (1978)
4. R. Grone, R. Merris, V.S. Sunder, Then Laplacian spectrum of a graph, SIAM J. Matrix Anal. Appl. **11**(2), 218–238 (1990)
5. J.M. Guo, On the Laplacian spectral radius of a tree, Linear Algebra Appl. **368**, 379–385 (2003)
6. J.M. Guo, On the second largest Laplacian eigenvalue of the trees, Linear Algebra Appl. **404**, 251–261 (2005)
7. J.M. Guo, The effect on the Laplacian spectral radius of a graph by adding or grafting edges, Linear Algebra Appl. **413**, 59–71 (2006)
8. I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry* (Springer-Verlag, Berlin Heidelberg, 1986)
9. Y. Hong, X.D. Zhang, Sharp upper and lower bounds for largest eigenvalue of the Laplacian matrices of trees, Discrete Math. **296**, 187–197 (2005)
10. W.S. Lin, X.F. Guo, On the largest eigenvalues of trees with perfect matchings, J. Math. Chem. **42**, 1057–1067 (2007)
11. B. Mohar, *The Laplacian spectrum of graphs, Graph Theory, Combinatorics, and Applications*, vol. 2 (Wiley, 1991), pp. 871–898

12. J.J. Molitiernoa, M. Neumannb, On trees with perfect matchings, Linear Algebra Appl. **362**, 75–85 (2003)
13. D. Rouvray, in *Chemical Applications of Graph Theory* ed. by A.T. Balaban (Academic Press, 320 New York, 1976) (Chapter 7)
14. G.H. Xu, in *Combinatorics and Graph Theory* (World Scientific, Singapore, 1997)
15. X.Y. Yuan, B.F. Wu, E.L. Xiao, The modifications of trees and the Laplacian spectrum (in Chinese), J. East China Norm. Univ. (Natur. Sci). (2) 13–18 (2004)
16. X.D. Zhang, J.S. Li, The two largest eigenvalues of the Laplacian matrices of trees (in Chinese), J. China Univ. Sci. Technol. **28**, 513–518 (1998)
17. X.D. Zhang, R. Luo, The spectral radius of triangle-free graphs, Austraslas. J. Combin. **26**, 33–39 (2002)