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TREES WITH MAXIMUM SUM OF THE TWO LARGEST LAPLACIAN EIGENVALUES*

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Abstract. Let T be a tree of order n and $S_2(T)$ be the sum of the two largest Laplacian eigenvalues of T. Fritscher *et al.* proved that for any tree T of order n, $S_2(T) \leq n+2-\frac{2}{n}$. Guan *et al.* determined the tree with maximum $S_2(T)$ among all trees of order n. In this paper, we characterize the trees with $S_2(T) \geq n+1$ among all trees of order n except some trees. Moreover, among all trees of order n, we also determine the first $\lfloor \frac{n-2}{2} \rfloor$ trees according to their $S_2(T)$. This extends the result of Guan *et al.*

Key words. Tree, Laplacian Eigenvalue, Sum.

AMS subject classification. 05C50.

1. Introduction. Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The order and size of G are $|V(G)| = n(G)$ and $|E(G)| = m(G)$ (or n and m for short), respectively. The set of vertices adjacent to $v_i \in V(G)$, denoted by $N(v_i)$, refers to the neighborhood of v_i. The degree of v_i, denoted by $d(v_i)$, is the cardinality of $N(v_i)$. The maximum and minimum degrees of G are denoted by $\Delta(G)$ and $\delta(G)$, respectively. The *Laplacian* matrix of G is defined as $L(G) = D(G) - A(G)$, where $A(G)$ is the adjacency matrix of G and $D(G) = diag(d(v_1), d(v_2), \ldots, d(v_n))$ is the diagonal matrix of vertex degrees of G. It is well known that $L(G)$ is positive semidefinite, and its eigenvalues are non-negative real number. Moreover, note that each row sum of $L(G)$ is 0, and therefore, $\mu_n(G) = 0$. The eigenvalues of $L(G)$ are called the *Laplacian* eigenvalues of G and denoted by $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) = 0$ (or $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ for short), which are always enumerated in non-increasing order and repeated according to their multiplicities. Let $S_k(G) = \sum_{i=1}^{k} \mu_i$ be the sum of the k largest Laplacian eigenvalues of G. Clearly, $\sum_{i=1}^{n} \mu_i = \sum_{i=1}^{n-1} \mu_i = 2m(G)$ since $\mu_n = 0$. Brouwer [3] conjectured that $S_k(G) \leq m + \binom{k+1}{2}$ for $k = 1, 2, \ldots, n$. This conjecture is interesting and still open. Up to now, for fixed k ($k = 1, 2, n-1, n$) or some given graph classes (trees, regular graphs, *etc.*), this conjecture has been proved (see [3, 7, 5, 4, 11, 14, 19, 10, 20]). In particular, for $k = 2$, Haemers *et al.* [14] proved that $S_2(G) \leq m + 3$ holds for any graph G of order n with m edges. When G is a tree, Fritscher et al.[9] improved this bound by showing $S_2(T) \leq m + 3 - \frac{2}{n}$ (or $n + 2 - \frac{2}{n}$ since $m = n - 1$), which indicates that Haemers' bound is always not attainable for trees. Therefore, it is interesting to know which tree has the maximum value of $S_2(T)$ among all trees of order n. Guan *et al.* [11] determined the tree with maximum

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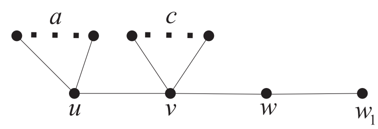

FIGURE 1. $T_{a,1,c}$ *with* $a \geq 1$, $c \geq 2$ *and* $a + c + 4 = n$.

$S_2(T)$ among all trees of order $n \geq 4$ by proving that $S_2(T) \leq S_2\left(S^1_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor}\right)$, and the equality holds if and only if $T \cong S^1_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor}$, where $S^k_{a,b}$ is the tree of order n obtained from two stars S_{a+1}, S_{b+1} by joining a path of length k between their central vertices. Let $\mathscr{T}_n$ be the set of trees of order n and $T_{a,1,c}$ be the tree shown in Fig. 1, where $a \geq 1$, $c \geq 2$ and $a + c + 4 = n$. Let $\mathscr{T}^*_n = \{T \in \mathscr{T}_n | T \neq T_{a,1,c}\}$. In this paper, we further study the maximum values of $S_2(T)$ for trees and characterize trees with $S_2(T) \geq n + 1$ among all trees in $\mathscr{T}^*_n$. Moreover, among all trees in $\mathscr{T}_n$, we also determine the first $\lfloor \frac{n-2}{2} \rfloor$ trees according to their $S_2(T)$. This extends the result of Guan *et al.*

The rest of this paper is organized as follows: in Section 2, we present some useful lemmas. In Section 3, we characterize trees with $S_2(T) \geq n + 1$ among all trees in $\mathscr{T}^*_n$. In Section 4, we determine the first $\lfloor \frac{n-2}{2} \rfloor$ trees according to their $S_2(T)$ among all trees in $\mathscr{T}_n$.

2. Preliminaries. In this section, we give notations and collect known results on Laplacian eigenvalues of a graph. A vertex with degree one in G is called a pendent vertex of G. Particularly, denote by $\Delta(G)$ (or Δ for short) the maximum degree of G. Let S_n and P_n be the star and path of order n, respectively. Let $S^k_{a,b}$ be the tree of order n obtained from two stars S_{a+1}, S_{b+1} by joining a path of length k between their central vertices. For all other definitions and notations, not given here, see [6].

We denote by $\Phi(L(G)) = \phi(G, x) = det(xI_n - L(G))$ the *Laplacian* characteristic polynomial of G, where I_n is the identity matrix of order n. For the Laplacian characteristic polynomials of graphs, Guo et al. [13] gave the reduction procedures for computing them respectively.

For $U \subseteq V(G)$, let $L_U(G)$ be the principal submatrix of $L(G)$ formed by deleting the rows and columns corresponding to all vertices in U. If $U = \{v\}$ or $U = \{v, u\}$ when $uv \in E(G)$, then we simply write $L_U(G)$ as $L_v(G)$ or $L_{vu}(G)$. The following result displays the relations between the characteristic polynomials of $L(G)$ and $L_v(G)$.

LEMMA 2.1 ([13]). *Let G be a graph of order n. For $v \in V(G)$, let $\varphi(v)$ be the collection of cycles containing v. Then, the Laplacian characteristic polynomial of G satisfies*

$$\Phi(L(G)) = (x - d(v))\Phi(L_v(G)) - \sum_{w} \Phi(L_{vw}(G)) - 2 \sum_{Z \in \varphi(v)} (-1)^{|Z|} \Phi(L_Z(G)),$$

where the first summation extends over those vertices w adjacent to v, and the second summation extends over all $Z \in \varphi(v)$, $|Z|$ denotes the length of Z.

The following is the special case of Lemma 2.1 when $d(v) = 1$.

COROLLARY 2.2 ([13]). *Let v be a vertex of a graph G with $d(v) = 1$ and $uv \in E(G)$. Then,*

$$\Phi(L(G)) = (x - 1)\Phi(L(G - v)) - x\Phi(L_{uv}(G)).$$

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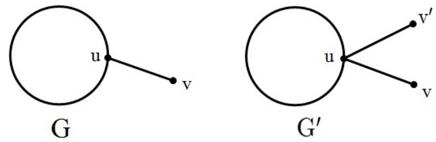

FIGURE 2. *Graphs G and G'.*

The next result displays the relation between the Laplacian characteristic polynomials of G and $G-e$, where $e \in E(G)$.

LEMMA 2.3 ([13]). *Let G be a graph of order n. For $e \in E(G)$, let $\mathscr{C}_G(e)$ be the set of all cycles containing e in G. Then, the Laplacian characteristic polynomial of G satisfies*

$$\Phi(L(G)) = \Phi(L(G-e)) - \Phi(L_u(G-e)) - \Phi(L_v(G-e)) - 2\sum_{Z}(-1)^{|Z|}\Phi(L_Z(G)),$$

where the summation extends over all $Z \in \mathscr{C}_G(e)$.

LEMMA 2.4 ([2]). *Let G be a connected graph of order n with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$ and Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. Then,*

$$\mu_k(G) \geq d_k + 2 - k.$$

Specially, $\mu_1(G) \geq \Delta(G) + 1$ and $\mu_2(G) \geq d_2$.

We now list some known and useful results on μ_1.

LEMMA 2.5 ([1, 17, 16]). *Let G be a graph of order n with m edges. Then,*

(1) $\mu_1(G) \leq n$, *with equality if and only if the complement of G is disconnected;*
(2) $\mu_1(G) \leq \max\{d(v) + \pi(v) | v \in V(G)\}$, *where* $\pi(v) = \sum\limits_{u \in N(v)} \frac{d(u)}{d(v)}$;
(3) $\mu_1(G) < \max\left\{\triangle(G), m - \frac{n-1}{2}\right\} + 2.$

For an eigenvalue x of $L(G)$, let $m_G(x)$ be the multiplicity of it. It is well known that $m_G(1) = n - r(I_n - L(G))$, where $r(I_n - L(G))$ is the rank of $I_n - L(G)$.

LEMMA 2.6. *Let G be a graph of order n. For $v \in V(G)$ with $d(v) = 1$ and $uv \in E(G)$, let G' be the graph obtained from G by adding a new vertex v' and a new edge uv' (see Fig. 2). Then,*

$$m_{G'}(1) = m_G(1) + 1.$$

Proof. Let $L(G)$ and $L(G')$ be the Laplacian matrices of G and G', respectively. It is not difficult to check that $r(I_n - L(G)) = r(I_{n+1} - L(G'))$. Thus, the result follows from the facts that $m_G(1) = n - r(I_n - L(G))$ and $m_{G'}(1) = (n+1) - r(I_{n+1} - L(G'))$. □

LEMMA 2.7 ([18]). *Let G be a graph of order n. For $v \in V(G)$ with $d(v) = 1$, we have*

$$\mu_{n-1}(G) \leq \mu_{n-2}(G - v).$$

Let $\mathscr{T}_{(n,d)}$ be the set of trees of order n with diameter d and $T_{(n,d)}(i)$ be the tree of order n with diameter d obtained from a path $P_{d+1} = v_1v_2\cdots v_dv_{d+1}$ (of length d) by attaching $n-d-1$ new pendant edges $v_{d+2}v_i, \ldots, v_nv_i$ to the vertex v_i (shown in Fig. 3).

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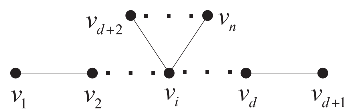

FIGURE 3. $T_{(n,d)}(i)$.

Guo [12] determined the first $\lfloor \frac{d}{2} \rfloor$ trees among trees in $\mathscr{T}_{(n,d)}$ according to their Laplacian spectral radii as follows.

THEOREM 2.8 ([12]). *For $n \geq d+3$ and $d \geq 3$, the first $\lfloor \frac{d}{2} \rfloor$ trees in the set $\mathscr{T}_{(n,d)}$ according to their Laplacian spectral radii are as follows:*

$$T_{(n,d)}\left(\left\lfloor \frac{d}{2} \right\rfloor + 1\right), T_{(n,d)}\left(\left\lfloor \frac{d}{2} \right\rfloor\right), \ldots, T_{(n,d)}(3), T_{(n,d)}(2).$$

From above, we immediately have the following lemma.

LEMMA 2.9. *For $T \in \mathscr{T}_{(n,d)}$ with $d \geq 4$, we have $\mu_1(T) < n - 1.3$.*

Proof. For $T \in \mathscr{T}_{(n,d)}$ with $d \geq 4$, if $d \geq 5$, then $\Delta(T) \leq n-4$. Thus, Lemma 2.5 implies that $\mu_1(T) \leq \Delta(T) + 2 \leq n-2$; if $d = 4$, by Theorem 2.8 and Lemma 2.5, we then have $\mu_1(T) \leq \mu_1(T_{(n,4)}(3)) \leq (n-3) + \frac{n-1}{n-3} \leq (n-2) + \frac{2}{n-3} < n - 1.3$ when $n \geq 6$. And for $n = 5$, a direct calculation shows that $\mu_1(P_5) = 3.618 < 5 - 1.3$, as desired. □

Guan *et al.* [11] gave the following upper bound for $S_2(T)$ for trees in $\mathscr{T}_{(n,d)}$ with $d \geq 4$.

LEMMA 2.10 ([11]). *For $T \in \mathscr{T}_{(n,d)}$ with $d \geq 4$, we have $S_2(T) < n + 1.5$.*

This upper bound is slightly improved by Zheng *et al.* for $T \in \mathscr{T}_{(n,d)}$ with $d \geq 5$ as follows.

LEMMA 2.11 ([21]). *For $T \in \mathscr{T}_{(n,d)}$ with $d \geq 5$, we have $S_2(T) < n + 1$.*

Let M be a real symmetric matrix of order n. Then, all eigenvalues of M are real and can be denoted by $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$ in non-increasing order. The following result in matrix theory plays a key role in our proofs.

LEMMA 2.12 ([8]). *Let A and B be two real symmetric matrices of order n. Then for any $1 \leq k \leq n$,*

$$\sum_{i=1}^{k} \lambda_i(A+B) \leq \sum_{i=1}^{k} \lambda_i(A) + \sum_{i=1}^{k} \lambda_i(B).$$

The next results follows from Lemma 2.12 immediately.

LEMMA 2.13. *Suppose that $G_1, \ldots, G_r$ are edge disjoint graphs on the same vertex set. Then for any k,*

$$S_k(G_1 \cup \cdots \cup G_r) \leq \sum_{i=1}^{r} S_k(G_i).$$

The following results can be found in [10], and Lemma 2.14 is known as the Interlacing Theorem for Laplacian eigenvalues.

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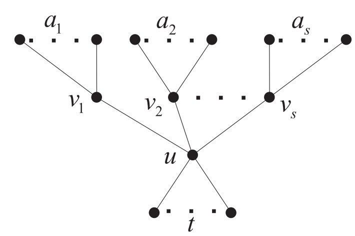

FIGURE 4. $T_{(a_1,a_2,\ldots,a_s;t)}$.

LEMMA 2.14 ([10]). *Let G be a graph of order n. For $e \in E(G)$, let $G' = G - e$ be the graph obtained by deleting e from G. Then, the Laplacian eigenvalues of G and G' interlace, that is,*

$$\mu_1(G) \geq \mu_1(G') \geq \mu_2(G) \geq \cdots \geq \mu_{n-1}(G') \geq \mu_n(G) \geq \mu_n(G') = 0.$$

LEMMA 2.15 ([10]). *Let A be a real symmetric matrix of order n with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and B be a principal submatrix of A of order m with eigenvalues $\lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_m$. Then, the eigenvalues of B interlace the eigenvalues of A, that is $\lambda_i \geq \lambda'_i \geq \lambda_{n-m+i}$ for $i = 1, \ldots, m$. Specially, for $v \in V(G)$, the eigenvalues of $L_v(G)$ interlace the eigenvalues of $L(G)$.*

3. Trees with $S_2(T) \geq n(T)+1$. In this section, we study the sum of two largest Laplacian eigenvalues of trees and characterize the trees with $S_2(T) \geq n + 1$ among all trees in $\mathscr{T}_n^*$. First, we consider $S_2(T)$ for $T \in \mathscr{T}_{(n,4)}$. Note that $T \cong T_{(a_1,a_2,\ldots,a_s;t)}$ (shown in Fig. 4) for $T \in \mathscr{T}_{(n,4)}$, where $a_1 \geq a_2 \geq \cdots \geq a_s \geq 1$, $s \geq 2$, $t \geq 0$ and $a_1 + a_2 + \cdots + a_s + s + t + 1 = n$.

THEOREM 3.1. *Let $T_{(a_1,a_2,\ldots,a_s;t)}$ be the tree as shown in Fig. 4. If $s \geq 3$, then $S_2(T_{(a_1,a_2,\ldots,a_s;t)}) < n+1$.*

Proof. Let T_1 and T_2 be the two components of $T_{(a_1,a_2,\ldots,a_s;t)} - uv_1$, where T_1 (T_2) contains $v_1(u)$. Note that $d(T_2) = 4$ since $s \geq 3$. Hence, Lemma 2.9 implies that $\mu_1(T_2) < n(T_2) - 1.3$ and Lemma 2.10 implies that $S_2(T_2) < n(T_2) + 1.5$. We now consider the following two cases.

Case 1 $a_1 \geq 2$.

If $S_2(T_1 \cup T_2) = S_2(T_2)$, then Lemma 2.13 implies that $S_2(T_{(a_1,a_2,\ldots,a_s;t)}) \leq S_2(T_1 \cup T_2) + 2 = S_2(T_2) + 2 < \underbrace{(n(T_2) + 1.5) + 2 \leq n(T_{(a_1,a_2,\ldots,a_s;t)}) + 0.5}_{\text{since } n(T_1) \geq 3} < n + 1$, as desired; if $S_2(T_1 \cup T_2) = \mu_1(T_1) + \mu_1(T_2)$, then Lemma 2.13 implies that $S_2(T_{(a_1,a_2,\ldots,a_s;t)}) \leq S_2(T_1 \cup T_2) + 2 = \mu_1(T_1) + \mu_1(T_2) + 2 < n(T_1) + (n(T_2) - 1.3) + 2 = n(T_{(a_1,a_2,\ldots,a_s;t)}) + 0.7 < n + 1$, as desired.

Case 2 $a_1 = 1$.

Note that the eigenvalues of $L_u(T_{(1,1,\ldots,1;t)})$ are $\underbrace{\frac{3+\sqrt{5}}{2}, \ldots, \frac{3+\sqrt{5}}{2}}_{s}, \underbrace{1, \ldots, 1}_{t}, \underbrace{\frac{3-\sqrt{5}}{2}, \ldots, \frac{3-\sqrt{5}}{2}}_{s}$ by a direct computation. Then, Lemma 2.15 implies that $\frac{3+\sqrt{5}}{2} \leq \mu_2(T_{(1,1,\ldots,1;t)}) \leq \frac{3+\sqrt{5}}{2}$ since $s \geq 3$. That is $\mu_2(T_{(1,1,\ldots,1;t)}) = \frac{3+\sqrt{5}}{2} \doteq 2.618$. Moreover, Lemma 2.5(3) implies that $\mu_1(T_{(1,1,\ldots,1;t)}) < \Delta(T_{(1,1,\ldots,1;t)}) + 2 \leq n(T_{(1,1,\ldots,1;t)}) - 2$ since $\Delta(T_{(1,1,\ldots,1;t)}) \leq n - 4$. Thus, we have $S_2(T_{(1,1,\ldots,1;t)}) < n(T_{(1,1,\ldots,1;t)}) - 2 + 2.618 < n + 1$, as desired.

The proof is completed. ∎

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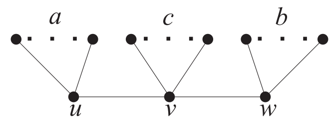

FIGURE 5. $T_{a,b,c}$.

For $s = 2$, for convenience, we use $T_{a,b,c}$ (shown in Fig. 5) instead of $T_{(a_1,a_2;t)}$, where $a \geq b \geq 1$ and $c \geq 0$. In particular, $T_{a,b,0} \cong S^2_{a,b}$.

THEOREM 3.2. *For $T_{a,b,c}$ with $a \geq b \geq 1$ and $c \geq 0$,*

(1) *if $c = 0$, then $S_2(T_{a,b,0}) > n(T_{a,b,0}) + 1$;*
(2) *if $c = 1$, then $S_2(T_{a,b,1}) < n(T_{a,b,1}) + 1$;*
(3) *if $c \geq 2$ and $b \geq 2$, then $S_2(T_{a,b,c}) < n(T_{a,b,c}) + 1$.*

Proof. (1) For $c = 0$, by Lemma 2.1 and some elementary calculations, we get that the Laplacian characteristic polynomial of $T_{a,b,0}$ is that $\phi(T_{a,b,0}, x) = (x-1)^{n-5}g(x)$ where $g(x) = (x-2)(x^2-(a+2)x+1)(x^2-(b+2)x+1)-(x-1)(x^2-(b+2)x+1)-(x-1)(x^2-(a+2)x+1)$. Let $x_1 \geq x_2 \geq x_3 \geq x_4 > x_5 = 0$ be the roots of $g(x) = 0$. If $a \geq b+1$, then Lemma 2.4 implies that $x_1 \geq \Delta+1 = a+2$. Moreover, note that $g(a+2) = -(a-b+1)(a+2) < 0$ and $g(b+2) = (a-b-1)(b+2) \geq 0$ since $a \geq b+1$. Thus, $x_1 > a+2$ and $x_2 \geq b+2$. That is $S_2(T_{a,b,0}) = x_1 + x_2 > (a+2)+(b+2) = n+1$; if $a = b$, then by some elementary calculations, we have $\phi(T_{a,b,0}, x) = x(x-1)^{n-5}h(x)$, where $h(x) = (x^2-(a+2)x+1)(x^2-(a+4)x+(2a+3))$. Then the largest two roots of $h(x) = 0$ are $\frac{(a+2)+\sqrt{a^2+4a}}{2}$ and $\frac{(a+4)+\sqrt{a^2+4}}{2}$. Hence, we have $S_2(T_{a,b,0}) = \frac{(a+2)+\sqrt{a^2+4a}}{2} + \frac{(a+4)+\sqrt{a^2+4}}{2} > 2a+4 = n+1$ since $2a+3 = n$, as desired.

In what follows, we assume that $c \geq 1$. Note that Lemma 2.6 implies that $m_{T_{a,b,c}}(1) \geq n-6$. Then, the Laplacian characteristic polynomial of $T_{a,b,c}$ can be written as $\phi(T_{a,b,c}, x) = (x-1)^{n-6}k(x)$. Let $x_1 \geq x_2 \geq x_3 \geq x_4 \geq x_5 > x_6 = 0$ be the six roots of $k(x) = 0$. Note that $x_1+x_2+x_3+x_4+x_5 = n+4$ since $\sum_{i=1}^{n} \mu_i = 2m = 2n-2$. So, in order to prove $S_2(T_{a,b,c}) = x_1+x_2 < n+1$, we only need to prove that $x_3 \geq 3$.

(2) $c = 1$.

If $b = 1$, note that the eigenvalues of $L_u(T_{a,1,1})$ are $3.9563, 2.2091, \underbrace{1, \ldots 1}_{n-5}, 0.6717$ and 0.1729 by a direct calculation. Then, Lemma 2.15 implies that $x_2 \leq \lambda_1(L_u(T_{a,1,1})) \doteq 3.9563 < 3.96$. Moreover, Lemma 2.5 implies that $x_1 \leq \max\{d(v)+\pi(v)\} = (n-4)+\frac{n-2}{n-4}$. Hence, $x_1+x_2 < (n-4)+\frac{n-2}{n-4}+3.96 \leq n+1$ when $n \geq 54$. Moreover, with the aid of the *newGRAPH* software, we can check that $S_2(T_{a,1,1}) < n+1$ holds for $n < 54$.

If $b = 2$, then $n \geq 8$. For $n = 8$, by a direct calculation, we have $x_1+x_2 = \mu_1(T_{2,2,1})+\mu_2(T_{2,2,1}) \doteq 4.8136+3.7321 = 8.5457 < 8+1$. For $n \geq 9$, note that the eigenvalues of $L_u(T_{a,2,1})$ are $4.4458, 2.7968, \underbrace{1, \ldots 1}_{n-5}, 0.6297$ and 0.1277 by a direct calculation. Then, Lemma 2.15 implies that $x_2 \leq \lambda_1(L_u(T_{a,2,1})) \doteq 4.4458 < 4.5$. Moreover, Lemma 2.5 implies that $x_1 \leq max\{d(v)+\pi(v)\} = (n-5)+\frac{n-3}{n-5}$. Hence, $x_1+x_2 < (n-5)+\frac{n-3}{n-5}+4.5 < n+1$ for $n \geq 9$.

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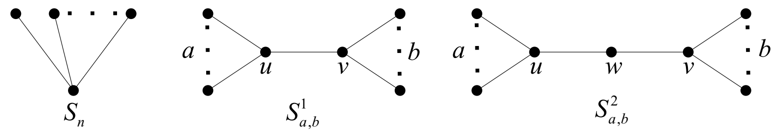

FIGURE 6. S_n, $S^1_{a,b}$ and $S^2_{a,b}$.

If $b = 3$, note that $T_{a,b,1}$ contains $T_{8,3,1}$ as a subgraph for $n \geq 15$. Then, Lemma 2.14 implies that $x_3 \geq \mu_3(T_{8,3,1}) = 3.0$. Hence, it follows that $S_2(T_{a,3,1}) < n(T_{a,3,1}) + 1$ for $n \geq 15$. Moreover, for $n < 15$, we check that $S_2(T_{a,3,1}) < n(T_{a,3,1}) + 1$ by the aid of the *newGRAPH* software.

If $b \geq 4$, note that $T_{a,b,1}$ contains $T_{4,4,1}$ as a subgraph. Then, Lemma 2.14 implies that $x_3 \geq \mu_3(T_{4,4,1}) = 3.0$. Hence, it follows that $S_2(T_{a,b,1}) < n + 1$.

(3) For $a \geq b \geq 2$, note that $T_{a,b,c}$ contains $T_{2,2,2}$ as a subgraph. Then, Lemma 2.14 implies that $x_3 \geq \mu_3(T_{2,2,2}) = 3.0$. Hence, it follows that $S_2(T_{a,b,c}) < n + 1$.

The proof is completed. ☐

REMARK 3.3. From the argument in Theorem 3.2, for $T_{a,b,c}$ with $a \geq b \geq 1$ and $c \geq 0$, the remaining case is $a \geq b = 1$ and $c \geq 2$. That is $T_{a,1,c}$ with $a \geq 1$, $c \geq 2$ and $a + c + 4 = n$ (shown in Fig. 1). We now have the following observations for $S_2(T_{a,1,c})$. Firstly, by Lemma 2.3, it follows that the Laplacian characteristic polynomial of $T_{a,1,c}$ is $\phi(T_{a,1,c}, x) = x(x-1)^{n-6}g(x)$, where $a + c + 4 = n$ and $g(x) = x^5 - (a+c+8)x^4 + (ac+6a+5c+23)x^3 - (3ac+11a+8c+30)x^2 + (ac+7a+5c+18)x - (a+c+4)$. Let $x_1 \geq x_2 \geq \cdots \geq x_5 > 0$ be the roots of $g(x) = 0$.

(1) Let $T_{a,1,c} - uv = T_1 \cup T_2$, where T_1 (T_2) contains u (v) and $n(T_1) = n_1$ and $n(T_2) = n_2$. Then, Lemma 2.5 implies that $\mu_1(T_1) = n_1$ and $\mu_1(T_2) \leq (n_2 - 2) + \frac{n_2-1}{n_2-2} = (n_2 - 1) + \frac{1}{n_2-2}$. Moreover, by Lemma 2.13, we have $S_2(T_{a,1,c}) \leq S_2(T_1 \cup T_2) + 2 = \mu_1(T_1) + \mu_1(T_2) + 2 \leq n_1 + (n_2 - 1) + \frac{1}{n_2-2} + 2 = n + 1 + \frac{1}{n_2-2} \to n + 1\ (n_2 \to \infty)$.

(2) For $a = c + 1 = \frac{n-3}{2}$ and $n \geq 7$ is even, note that the Laplacian characteristic polynomial of $T_{\frac{n-3}{2},1,\frac{n-5}{2}} - ww_1$ is $\phi(T_{\frac{n-3}{2},1,\frac{n-5}{2}} - ww_1, x) = x^2(x-1)^{n-5}h(x)$, where $h(x) = x^3 - (n+1)x^2 + \left(\frac{(n-3)^2}{4} + 2n - 1\right)x - (n-1)$. Let $y_1 \geq y_2 \geq y_3 > 0$ be the roots of $h(x) = 0$. Then, Lemma 2.4 implies that $\mu_1(T_{\frac{n-3}{2},1,\frac{n-5}{2}} - ww_1) = y_1$ and $\mu_2(T_{\frac{n-3}{2},1,\frac{n-5}{2}} - ww_1) = y_2 > 1$. Moreover, note that $h(\frac{4}{n}) = \frac{64}{n^3} - \frac{16}{n^2} - \frac{11}{n} + 3 > 0$ for $n \geq 7$. It follows that $y_3 < \frac{4}{n}$. That is $S_2(T_{\frac{n-3}{2},1,\frac{n-5}{2}} - ww_1) = y_1 + y_2 = (n+1) - y_3 > (n+1) - \frac{4}{n}$. Then, Lemma 2.14 implies that $S_2(T_{\frac{n-3}{2},1,\frac{n-5}{2}}) \geq S_2(T_{\frac{n-3}{2},1,\frac{n-5}{2}} - ww_1) > n + 1 - \frac{4}{n} \to n + 1\ (n \to \infty)$.

(3) With the aid of the computer programming, we check that $S_2(T_{a,1,c}) = x_1 + x_2 < n+1$ for $n \leq 1000$. But it seems difficult to give a standard mathematical proof for $n > 1000$.

Now we give the main result of this section.

THEOREM 3.4. *For any $T \in \mathscr{T}_n^*$, if $S_2(T) \geq n + 1$, then if and only if $T \in \{S_n, S^1_{a,b}, S^2_{a,b}\}$, where S_n, $S^1_{a,b}$ and $S^2_{a,b}$ are shown in Fig. 6, respectively.*

Proof. For $T \in \mathscr{T}_n$, we will discuss according to its diameter d.

(1) If $d = 1$, then $T = K_2$. Hence, $S_2(K_2) = 2 < n + 1$.

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(2) If $d = 2$, then $T \cong S_n$ and it is known that $S_2(S_n) = n + 1$.

(3) If $d = 3$, then $T \cong S^1_{a,b}$ (see Fig. 6), where $S^1_{a,b}$ is a tree of order n obtained from an edge uv by attaching a and b pendent edges to u and v, respectively, here a and b are positive integers and $a + b + 2 = n$. By Lemma 2.3 and a direct calculation, the Laplacian characteristic polynomial of $S^1_{a,b}$ is

$$\phi(S^1_{a,b}, x) = x(x-1)^{n-4} f_{a,b}(x),$$

where

$$f_{a,b}(x) = x^3 - (n+2)x^2 + (ab + 2n + 1)x - n. \tag{3.1}$$

By Lemma 2.14, we have $\mu_2(S^1_{a,b}) \geq \mu_2(S^1_{1,1}) = 2$. Moreover, it is known that for any tree T, $\alpha(T) \leq 1$, with equality if and only if $T \cong S_n$. These imply that $\mu_1(S^1_{a,b})$, $\mu_2(S^1_{a,b})$ and $\alpha(S^1_{a,b})$ are the three roots of $f_{a,b}(x) = 0$. As follows from Eq. (3.1), we have $\mu_1(S^1_{a,b}) + \mu_2(S^1_{a,b}) + \alpha(S^1_{a,b}) = n + 2$. When $n \geq 6$, $S^1_{a,b}$ contains $S^1_{1,3}$ or $S^1_{2,2}$ as a subgraph. By Lemma 2.7 and the facts that $\alpha(S^1_{1,3}) = 0.486$ and $\alpha(S^1_{2,2}) = 0.438$, we have $\alpha(S^1_{a,b}) < 0.5$. It follows that $\mu_1(S^1_{a,b}) + \mu_2(S^1_{a,b}) > n + 1.5$ when $n \geq 6$. For $n = 4$ or $n = 5$, we easy get that $\mu_1(S^1_{a,b}) + \mu_2(S^1_{a,b}) > n + 1.4$ by direct calculation.

(4) If $d = 4$, then the result follows from Theorems 3.1 and 3.2 since $T_{a,b,0} \cong S^2_{a,b}$ (see Fig. 6).

(5) If $d \geq 5$, then the result follows from Lemma 2.11.

The proof is completed. ∎

4. Ordering trees according to their $S_2(T)$. Guan *et al.* [11] determined the tree with maximum value of $S_2(T)$ among all trees in $\mathscr{T}_n$ by proving that for any tree $T \in \mathscr{T}_n$, $S_2(T) \leq S_2(S^1_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor})$ with equality if and only if $T \cong S^1_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor}$. In this section, we extend their result by determining the first $\lfloor \frac{n-2}{2} \rfloor$ trees according to their $S_2(T)$.

THEOREM 4.1. *For $T, T' \in \mathscr{T}_n$, if $d(T') = 3$ and $d(T) \neq 3$, then we have $S_2(T) < S_2(T')$.*

Proof. Note that for any $T' \in \mathscr{T}_{(n,3)}$, we have $T' \cong S^1_{a,b}$ for some a and b with $a + b + 2 = n$. For $T \in \mathscr{T}^*_n$, recall that $T \neq T_{a,1,c}$, where $a \geq 1$, $c \geq 2$ and $a + c + 4 = n \geq 7$. If $T \cong S^2_{a,b}$, then from the proof of Theorem 3.4 and Lemma 2.10, we have $S_2(T') = S_2(S^1_{a,b}) > n + 1.5 > S_2(S^2_{a,b}) = S_2(T)$; if $T \neq S^2_{a,b}$, then from the proofs of Theorems 3.4 and 3.2 and Lemma 2.10, we have $S_2(T') = S_2(S^1_{a,b}) > n + 1.5 > S_2(S^2_{a,b}) > n + 1 = S_2(S_n) > S_2(T)$ for $n \geq 7$. Moreover, it is also true by a direct check for $n \leq 6$. For $T \cong T_{a,1,c}$, by the fact of Remark 3.3(1) since $n_2 \geq 5$, we then have that $S_2(T') = S_2(S^1_{a,b}) > n + 1.5 > S_2(T_{a,1,c}) = S_2(T)$, as desired. ∎

In what follows, we will compare the values of sum of the two largest Laplacian eigenvalues of two different trees with $d(T) = 3$.

THEOREM 4.2. *For $S^1_{a,b}, S^1_{a+1,b-1} \in \mathscr{T}_{(n,3)}$, if $a \geq b \geq 2$, then we have $S_2(S^1_{a,b}) > S_2(S^1_{a+1,b-1})$.*

Proof. Recall that the Laplacain characteristic polynomial of $S^1_{a,b}$ is $\phi(S^1_{a,b}, x) = x(x-1)^{n-4} f_{a,b}(x)$, where

$$f_{a,b}(x) = x^3 - (n+2)x^2 + (ab + 2n + 1)x - n.$$

Similarly, the Laplacian characteristic polynomial of $S^1_{a+1,b-1}$ is

$$\phi(S^1_{a+1,b-1}, x) = x(x-1)^{n-4} f_{a+1,b-1}(x),$$

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where

$$f_{a+1,b-1}(x) = x^3 - (n+2)x^2 + (ab - (a-b) - 1 + 2n + 1)x - n.$$

Let $x_1 \geq x_2 \geq x_3 > 0$ and $x_1' \geq x_2' \geq x_3' > 0$ be three roots of $f_{a,b}(x) = 0$ and $f_{a+1,b-1}(x) = 0$, respectively. Clearly, $S_2(S^1_{a,b}) = x_1 + x_2$ and $S_2(S^1_{a+1,b-1}) = x_1' + x_2'$.

Note that $f_{a,b}(x) - f_{a+1,b-1}(x) = (a-b+1)x > 0$ for $x > 0$. It follows that $x_3' > x_3$. This together with the fact that $x_1 + x_2 + x_3 = n + 2 = x_1' + x_2' + x_3'$ implies that $x_1 + x_2 > x_1' + x_2'$, as desired. □

By Theorems 4.1 and 4.2, we now come to the main result of this section.

THEOREM 4.3. *Among all trees in $\mathscr{T}_n$, the first $\lfloor \frac{n-2}{2} \rfloor$ trees according to their $S_2(T)$ are as follows:*

$$S^1_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor},\ S^1_{\lceil \frac{n-2}{2} \rceil+1, \lfloor \frac{n-2}{2} \rfloor-1},\ S^1_{\lceil \frac{n-2}{2} \rceil+2, \lfloor \frac{n-2}{2} \rfloor-2},\ \ldots,\ S^1_{n-4,2},\ S^1_{n-3,1}.$$

REMARK 4.4. Here we determine the first $\lfloor \frac{n-2}{2} \rfloor$ trees among all trees in $\mathscr{T}_n$ according to their $S_2(T)$, which extend the result of Guan et al., they determined the tree with maximum value of $S_2(T)$. Moreover, it is known that the Laplacian matrix $L(G)$ and the signless Laplacian matrix $Q(G)$ are similar when G is a bipartite graph [6]. That is, for any $T \in \mathscr{T}_n$, we have $q_i(T) = \mu_i(T)$ for $i = 1, 2, \ldots, n$. Hence, Theorem 4.3 also holds for the sum of two largest signless Laplacian eigenvalues of trees.

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