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On the sum of the two largest Laplacian eigenvalues of unicyclic graphs

Yirong Zheng[1,2*], An Chang[2] and Jianxi Li[2,3]

*Correspondence:
yrzheng@xmut.edu.cn
[1]School of Applied Mathematics, Xiamen University of Technology, Xiamen, Fujian, P.R. China
[2]Center for Discrete Mathematics, Fuzhou University, Fuzhou, Fujian, P.R. China
Full list of author information is available at the end of the article

Abstract

Let G be a simple graph and $S_2(G)$ be the sum of the two largest Laplacian eigenvalues of G. Guan *et al.* (J. Inequal. Appl. 2014:242, 2014) determined the largest value for $S_2(T)$ among all trees of order n. They also conjectured that among all connected graphs of order n with m ($n \le m \le 2n-3$) edges, $G_{m,n}$ is the unique graph which has maximal value of $S_2(G)$, where $G_{m,n}$ is a graph of order n with m edges which has $m-n+1$ triangles with a common edge and $2n-m-3$ pendent edges incident with one end vertex of the common edge. In this paper, we confirm the conjecture with $m = n$.

MSC: 05C50; 15A48

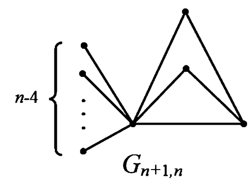
Keywords: Laplacian eigenvalue; sum of eigenvalues; largest eigenvalue; unicyclic graph

1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Its order is $|V(G)|$, denoted by $n(G)$ (or n for short), and its size is $|E(G)|$, denoted by $m(G)$ (or m for short). For a vertex $v \in V(G)$, let $N(v)$ be the set of all neighbors of v in G and let $d(v) = |N(v)|$ be the degree of v. Particularly, denote by $\Delta(G)$ the maximum degree of G. A pendent vertex is a vertex with degree one. The diameter of a connected graph G, denoted by $d(G)$, is the maximum distance among all pairs of vertices in G. Let S_n and P_n be the star and the path of order n, respectively. Let $S_{a,b}^k$ 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 (see Figure 2). For all other notions and definitions, not given here, see, for example, [1] or [2] (for graph spectra).

Let $A(G)$ and $D(G)$ be the adjacency matrix and the diagonal matrix of vertex degrees of G, respectively. The matrix $L(G) = D(G) - A(G)$ is called *Laplacian* matrix of G. The *Laplacian* matrix is an important topic in the theory of graph spectra. We use the notation I_n for the identity matrix of order n and denote by $\phi(G, x) = \det(xI_n - L(G))$ the *Laplacian* characteristic polynomial of G. It is well known that $L(G)$ is positive semidefinite symmetric and singular. Denote its eigenvalues by $\mu_1(G) \ge \mu_2(G) \ge \cdots \ge \mu_n(G)$ (or simply $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n$ sometimes for convenience) which are always enumerated in non-increasing order and repeated according to their multiplicity. Note that each row sum of $L(G)$ is 0 and, therefore, $\mu_n(G) = 0$. Fiedler [3] showed that the second smallest eigenvalue $\mu_{n-1}(G)$ of $L(G)$ is 0 if and only if G is disconnected. Thus the second smallest eigenvalue

Figure 1 $\boldsymbol{G_{n+1,n}}$**.** $G_{m,n}$ is a graph of order n with m edges which has $m-n+1$ triangles with a common edge and $2n-m-3$ pendent edges incident with one end vertex of the common edge.



of $L(G)$ is popularly known as the algebraic connectivity of G. The largest eigenvalue $\mu_1(G)$ of $L(G)$ is usually called the *Laplacian* spectral radius of the graph G. Recently, some of the research has been focused on μ_1, μ_2 or u_{n-1} (see [3–9]).

Let $S_k(G) = \sum_{i=1}^{i=k} \mu_i(G)$ be the sum of the k largest *Laplacian* eigenvalues of G. Brouwer conjectured that $S_k(G) \leq m(G) + \binom{k+1}{2}$ for $k = 1, 2, \ldots, n$. The conjecture is still open, but some advances on the conjecture have been achieved (see [10–14]). Specially, for $k = 2$, Haemers *et al.* [12] proved that $S_2(G) \leq m(G) + 3$ for any graph G. When G is a tree, Fritscher *et al.* [15] improved this bound by giving $S_2(T) \leq m(T) + 3 - \frac{2}{n(T)}$, which implies that Haemers' bound is always not attainable for trees. Therefore, it is interesting to determine which tree has maximal value of $S_2(T)$ among all trees of order n. Guan *et al.* [11] proved that $S_2(T) \leq S_2(T^1_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor})$ for any tree of order $n \geq 4$, and the equality holds if and only if $T \cong T^1_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor}$. For any graph G of order n with m edges, note that $\mu_1(G) \leq n(G)$. Then Haemers' bound is clearly not attainable when $2n(G) < m(G) + 3$. For $m(G) + 3 \leq 2n(G)$, Guan *et al.* [11] showed that $S_2(G_{m,n}) = m(G_{m,n}) + 3$, where $G_{m,n}$ is a graph of order n size m which has $m-n+1$ triangles with a common edge and $2n-m-3$ pendent edges incident with one end vertex of the common edge ($G_{n+1,n}$ is illustrated in Figure 1). This indicates that Haemers' bound is always sharp for connected graphs ($m \leq 2n-3$) other than trees. The following conjecture on the uniqueness of the extremal graph is also presented in [11].

Conjecture 1.1 [11] *Among all connected graphs of order n with m edges ($n \leq m \leq 2n-3$), $G_{m,n}$ is the unique graph with maximal value of $S_2(G)$, that is, $S_2(G_{m,n}) = m(G_{m,n}) + 3$.*

In this paper, we confirm Conjecture 1.1 with $m = n$.

2 Preliminaries

In this section, we present some lemmas which will be useful in the subsequent sections. For $\mu_1(G)$, the following results are well known.

Lemma 2.1 *Let G be a connected graph of order n, $d_i = d(v_i)$ and $m_i = \sum_{v_j \in N(v_i)} d_j/d_i$. Then*
(1) [4] $\mu_1(G) \leq n(G)$ *with equality if and only if the complement of G is disconnected*;
(2) [8] $\mu_1(G) \leq \max\{d_i + m_i | v_i \in V(G)\}$.

Lemma 2.2 [7] *Let G be a connected graph of order $n \geq 4$ with m edges. Then*

$$\mu_1(G) < \max\left\{\Delta(G), m - \frac{n-1}{2}\right\} + 2.$$

Lemma 2.3 [9] *Let T be a tree of order n with $d(T) \geq 3$. Then $\mu_1(T) < n - 0.5$.*

Lemma 2.4 *Let T be a tree of order n with $d(T) \geq 4$. Then $\mu_1(T) < n - 1$.*

Proof For any tree T of order n with $d(T) \geq 4$, it follows that $n \geq 5$ and $\Delta(T) \leq n-3$. That is, $\Delta(T)+2 \leq n-1$ and $m - \frac{n-1}{2} + 2 = \frac{n-1}{2} + 2 \leq n-1$. Then the result follows from Lemma 2.2. □

The following theorem from matrix theory plays a key role in our proofs. We denote the eigenvalues of a symmetric matrix M of order n by $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$.

Theorem 2.5 [16] *Let A and B be two real symmetric matrices of size n. Then, for any $1 \leq k \leq n$,*

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

From Theorem 2.5, the following lemma is immediate.

Lemma 2.6 *Let $G_1, \ldots, G_r$ be some edge disjoint graphs. Then, for any k,*

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

The following lemma can be found in [2] and is well known as the interlacing theorem of *Laplacian* eigenvalues.

Lemma 2.7 [2] *Let G be a graph of order n and let G' be the graph obtained from G by inserting a new edge into G. Then the Laplacian eigenvalues of G and G' interlace, that is,*

$$\mu_1(G') \geq \mu_1(G) \geq \cdots \mu_n(G') \geq \mu_n(G) = 0.$$

Lemma 2.8 [2] *Let A be a 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 $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_m$. Then the eigenvalues of B interlace the eigenvalues of A, that is, $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i = 1, \ldots, m$. Specially, for $v \in V(G)$, let $L_v(G)$ be the principal submatrix of $L(G)$ formed by deleting the row and column corresponding to vertex v, then the eigenvalues of $L_v(G)$ interlace the eigenvalues of $L(G)$.*

Lemma 2.9 *For any tree T of order n, if there exists an edge $e \in E(T)$ such that $\min\{e(T_1), e(T_2)\} \geq 2$ and $\min\{d(T_1), d(T_2)\} \geq 3$ or $\max\{d(T_1), d(T_2)\} \geq 4$, then $S_2(T) < n(T)+1$, where T_1, T_2 are the two components of $T-e$.*

Proof Let $T - e = T_1 \cup T_2$. By Lemma 2.6, it suffices to show that $S_2(T_1 \cup T_2) < n(T) - 1$. If $\mu_1(T) = \mu_1(T_1)$ and $\mu_2(T) = \mu_2(T_1)$ (or $\mu_1(T) = \mu_1(T_2)$ and $\mu_2(T) = \mu_2(T_2)$), then the result follows since $S_2(T_1 \cup T_2) = S_2(T_i) < m(T_i) + 3 \leq m(T) = n(T) - 1$ for $i = 1, 2$. In what follows, we assume that $S_2(T_1 \cup T_2) = \mu_1(T_1) + \mu_1(T_2)$. If $\min\{d(T_1), d(T_2)\} \geq 3$, then Lemma 2.3 implies that $S_2(T_1 \cup T_2) < (n(T_1) - 0.5) + (n(T_2) - 0.5) = n(T) - 1$. If $\max\{d(T_1), d(T_2)\} \geq 4$, say $d(T_2) \geq 4$, then Lemmas 2.1 and 2.4 imply that $S_2(T_1 \cup T_2) < n(T_1) + (n(T_2) - 1) = n(T) - 1$. This completes the proof. □

Lemma 2.10 *For any tree T of order n with $d(T) = 5$, $S_2(T) < n(T) + 1$.*

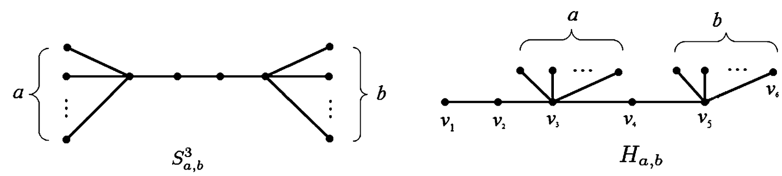


Figure 2 Two trees of order *n*.

Proof Without loss of generality, we assume that $v_1v_2v_3v_4v_5v_6$ is a path of length 5 in T. We now consider the following three cases.

Case 1. $\min\{d(v_3), d(v_4)\} \geq 3$.

Let T_1, T_2 be the two components of $T - v_3v_4$. Then the result follows from Lemma 2.9.

Case 2. $d(v_3) = d(v_4) = 2$.

Note that $d(T) = 5$. Then T is isomorphic to $S^3_{a,b}$ (see Figure 2), where $a, b \geq 1$ and $a + b + 4 = n$. By an elementary calculation, we have $\phi(S^3_{a,b}, \lambda) = \lambda(\lambda - 1)^{n-5}f_1(\lambda)$, where $f_1(\lambda) = \lambda^4 - (n+3)\lambda^3 + (5n + ab - 4)\lambda^2 - (6n + 3ab - 10)\lambda + n$. Denoted by $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 > 0$ are the four roots of $f_1(\lambda) = 0$. Then we have $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = n + 3$ since $\sum_{i=1}^{i=n} \mu_i = 2m$. Note that $S^3_{a,b}$ contains P_6 as a subgraph. Then Lemma 2.7 implies that $\lambda_3 \geq \mu_3(P_6) = 2$. Thus, $S_2(T) = \lambda_1 + \lambda_2 = n + 3 - (\lambda_3 + \lambda_4) < n + 3 - \lambda_3 < n - 1$, as desired.

Case 3. $d(v_3) \geq 3$ and $d(v_4) = 2$ (or $d(v_4) \geq 3$ and $d(v_3) = 2$).

Without loss of generality, we assume that $d(v_3) \geq 3$ and $d(v_4) = 2$. If $d(v_2) \geq 3$, let $T - v_2v_3 = T_1 \cup T_2$; if there is $P_3 = uvv_3$ attached to v_3, let $T - v_3v_4 = T_1 \cup T_2$, where $u, v \neq v_i$ $(i = 1, 2, \ldots, 6)$. Then the result follows from Lemma 2.9. We now assume that $d(v_2) = d(v_4) = 2$ and all the neighbors of v_3 except for v_2 and v_4 are pendent vertices. That is, T is isomorphic to $H_{a,b}$, where $H_{a,b}$ (see Figure 2) is the tree of order n obtained from $v_1v_2v_3v_4v_5v_6$ by attaching a and $b - 1$ pendent vertices to v_3 and v_5, respectively, where $a, b \geq 1$ and $a + b + 5 = n$. Note that the matrix $1 \cdot I_n - L(H_{a,b})$ has a and b different identical rows. Then the multiplicity of eigenvalue 1 is at least $n - 7$. Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \lambda_5 \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues. Then $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 + \lambda_7 = n + 5$ since $\sum_{i=1}^{i=n} \mu_i = 2m$. For $a, b \geq 2$, $H_{a,b}$ contains $H_{2,2}$ as a subgraph. Then by Lemma 2.7 we have $\lambda_3 \geq \mu_3(H_{2,2}) = 2.44$ and $\lambda_4 \geq \mu_4(H_{2,2}) = 1.59$. Therefore, $S_2(T) = \lambda_1 + \lambda_2 < n + 5 - (\lambda_3 + \lambda_4) < n + 1$, as required. If $a = 1$, then by Lemmas 2.1 and 2.8 we have $\mu_1(H_{1,b}) \leq (n-5) + \frac{n-4}{n-5}$ and $\mu_2(H_{1,b}) \leq \mu_1(L_{v_5}(H_{1,b})) = 4.26$. That is, $S_2(T) = S_2(H_{1,b}) = \mu_1(H_{1,b}) + \mu_2(H_{1,b}) < n + 1$, as required. Similarly, if $b = 1$, then by Lemmas 2.1 and 2.8 we have $\mu_1(H_{a,1}) \leq (n-4) + \frac{n-2}{n-4}$ and $\mu_2(H_{a,1}) \leq \mu_1(L_{v_3}(H_{a,1})) = 3.0$. It follows that $S_2(T) = S_2(H_{a,1}) = \mu_1(H_{a,1}) + \mu_2(H_{a,1}) < n + 1$, as required.

From the discussion above, the proof is completed. □

Lemma 2.11 *Let T be a tree of order n with $d(T) \geq 6$. Then $S_2(T) < n(T) + 1$.*

Proof We now consider the following two cases.

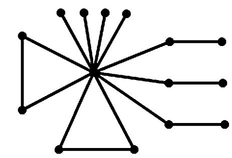
Case 1. $d(T) \geq 7$.

Let $v_1v_2v_3v_4v_5v_6v_7v_8$ be a path of length 7 in T and $T - v_4v_5 = T_1 \cup T_2$. Then the result follows from Lemma 2.9.

Case 2. $d(T) = 6$.

If $T = P_7$, then the result follows since $S_2(P_7) < 8$. If $T \neq P_7$, let $v_1v_2v_3v_4v_5v_6v_7$ be a path of length 6 in T. If $d(v_4) \geq 3$, let $T - v_3v_4 = T_1 \cup T_2$; if $d(v_3) \geq 3$ (or $d(v_5) \geq 3$), let $T - v_3v_4 =$

Figure 3 An example of firefly graph.



$T_1 \cup T_2$ (or $T - v_4v_5 = T_1 \cup T_2$); if $d(v_2) \geq 3$ (or $d(v_6) \geq 3$), let $T - v_2v_3 = T_1 \cup T_2$ (or $T - v_5v_6 = T_1 \cup T_2$). In each of the above cases, by Lemma 2.9, we have $S_2(T) < n(T) + 1$. This completes the proof. □

A firefly graph $F_{s,t,n-2s-2t-1}$ ($s \geq 0$, $t \geq 0$ and $n - 2s - 2t - 1 \geq 0$) is a graph with n vertices that consists of s triangles, t pendent paths of length 2 and $n - 2s - 2t - 1$ pendent edges, sharing a common vertex. An example of a firefly graph $F_{2,3,4}$ is illustrated in Figure 3. Clearly $F_{0,0,n-1} \cong S_n$ and $F_{1,0,n-3} \cong G_{n,n}$.

Lemma 2.12 [6] *The second largest Laplacian eigenvalue of* $F_{1,t,n-2t-3}$ *satisfies* $\mu_2(F_{1,t,n-2t-3}) = 3$.

Note that for $t \geq 1$, the complement of $F_{1,t,n-2t-3}$ is connected. Hence Lemma 2.1 implies that $\mu_1(F_{1,t,n-2t-3}) < n(F_{1,t,n-2t-3})$. This together with Lemma 2.12 implies the following lemma.

Lemma 2.13 *For* $t \geq 1$, $S_2(F_{1,t,n-2t-3}) < n(F_{1,t,n-2t-3}) + 3$.

3 Main result

A unicyclic graph is a connected graph whose number of edges m is equal to the number of vertices n. It is easy to see that each unicyclic graph can be obtained by attaching rooted trees to the vertices of a cycle C_k for some k. Thus if $R_1, \dots, R_k$ are k rooted trees (of orders $n_1, \dots, n_k$, say), then we adopt the notation $U(R_1, \dots, R_k)$ to denote the unicyclic graph G (of order $n = n_1 + \cdots + n_k$) obtained by attaching the rooted tree R_i to the vertex v_i of a cycle $C_k = v_1v_2 \cdots v_kv_1$ (*i.e.*, by identifying the root of R_i with the vertex v_i for $i = 1, \dots, k$). Denote by $e(v_i)$ the maximum distance between v_i and any vertex of R_i. In the special case when R_i is a rooted star K_{1,a_i} with the center of the star as its root (that is, $e(v_i) = 1$), we will simplify the notation by replacing R_i by the number a_i.

The following lemma is immediate from Lemmas 2.6, 2.10 and 2.11.

Lemma 3.1 *For any unicyclic graph G of order n with m edges, if there exists an edge $e \in E(G)$ such that $G - e$ is a tree with $d(G - e) \geq 5$, then $S_2(G) < m(G) + 3$.*

Let $uvwu$ be a triangle and $T_{a,b,c}$ be the graph obtained by attaching a, b, c pendent vertices to u, v, w, respectively, where $a + b + c = n - 3$ and $a \geq b \geq c \geq 0$. Note that $T_{n-3,0,0} \cong G_{n,n}$. Denote by $Q_{a,b}$ the graph obtained by attaching a and b pendent vertices to two nonadjacent vertices of a quadrangle, respectively, where $a + b = n - 4$ and $a \geq b \geq 0$. $T_{a,b,c}$ and $Q_{a,b}$ are illustrated in Figure 4.

Lemma 3.2 *For* $T_{a,b,c}$, $S_2(T_{a,b,c}) \leq m(T_{a,b,c}) + 3$ *with equality if and only if* $a = n - 3$ (*that is*, $T_{a,b,c} \cong G_{n,n}$).

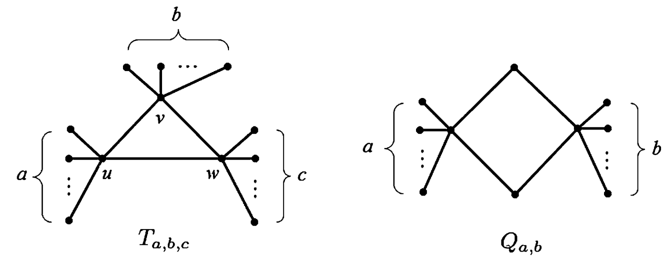


Figure 4 Two unicyclic graphs of order *n*. $T_{a,b,c}$ is a unicyclic graph of order n obtained by attaching a, b, c pendent vertices to three vertices of a triangle uvw, respectively, and $Q_{a,b}$ is a unicyclic graph of order n obtained by attaching a and b pendent vertices to two non-adjacent vertices of a quadrangle, respectively.

Proof Note that the matrix $1 \cdot I_n - L(T_{a,b,c})$ has a, b and c different identical rows. So the multiplicity of eigenvalue 1 is at least $n-6$. Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \lambda_5 > \lambda_6 = 0$ be the other six eigenvalues of $L(T_{a,b,c})$. Then we have $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 = n + 6$ since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. For $c \geq 2$, $T_{a,b,c}$ contains $T_{2,2,2}$ as a subgraph. Then by Lemma 2.7 we have $\lambda_3 \geq \mu_3(T_{2,2,2}) = 3.0$. Therefore, $S_2(T_{a,b,c}) = \lambda_1 + \lambda_2 = n + 6 - (\lambda_3 + \lambda_4 + \lambda_5) < n + 6 - \lambda_3 \leq n + 3 = m(T_{a,b,c}) + 3$, as required. For $c = 1$ and $b \geq 4$, $T_{a,b,c}$ contains $T_{4,4,1}$ as a subgraph. Then by Lemma 2.7 we have $\lambda_3 \geq \mu_3(T_{4,4,1}) = 3.0$. That is, $S_2(T_{a,b,1}) = n + 6 - (\lambda_3 + \lambda_4 + \lambda_5) < n + 6 - \lambda_3 \leq n + 3 = m(T_{a,b,c}) + 3$, as required. If $c = 1$ and $b = 3$, then by Lemmas 2.1 and 2.8, we have $\mu_1(T_{a,3,1}) \leq n - 4 + \frac{6}{n-5}$ and $\mu_2(T_{a,3,1}) \leq \mu_1(L_u(T_{a,3,1})) = 5.88$. It follows that $S_2(T_{a,3,1}) = \mu_1(T_{a,3,1}) + \mu_2(T_{a,3,1}) < m(T_{a,3,1}) + 3$, as required. If $c = 1$ and $b = 2$, then by Lemmas 2.1 and 2.8, we have $\mu_1(T_{a,2,1}) \leq n - 3 + \frac{5}{n-4}$ and $\mu_2(T_{a,2,1}) \leq \mu_1(L_u(T_{a,2,1})) = 5.05$. That is, $S_2(T_{a,2,1}) = \mu_1(T_{a,2,1}) + \mu_2(T_{a,2,1}) < m(T_{a,2,1}) + 3$ for $n \geq 10$ (that is, $a \geq 4$), as required. A direct calculation shows that $S_2(T_{3,2,1}) < m(T_{3,2,1}) + 3$ (or $S_2(T_{2,2,1}) < m(T_{2,2,1}) + 3$). Similarly, if $c = 1$ and $b = 1$, then by Lemmas 2.1 and 2.8, we have $\mu_1(T_{a,1,1}) \leq n - 2 + \frac{4}{n-3}$ and $\mu_2(T_{a,1,1}) \leq \mu_1(L_u(T_{a,1,1})) = 4.30$. That is, $S_2(T_{a,1,1}) = \mu_1(T_{a,1,1}) + \mu_2(T_{a,1,1}) < m(T_{a,1,1}) + 3$, for $n \geq 9$ (that is, $a \geq 4$), as required. A direct calculation shows that $S_2(T_{3,1,1}) < m(T_{3,1,1}) + 3$ (or $S_2(T_{2,1,1}) < m(T_{2,1,1}) + 3$ or $S_2(T_{1,1,1}) < m(T_{1,1,1}) + 3$). Next, we assume $c = 0$. By an elementary calculation, we have $\phi(T_{a,b,0}, \lambda) = \lambda(\lambda - 1)^{n-5} f_2(\lambda)$, where $f_2(\lambda) = \lambda^4 - (n+5)\lambda^3 + (5n + ab + 7)\lambda^2 - (7n + 2ab + 3)\lambda + 3n$. Let $x_1 \geq x_2 \geq x_3 \geq x_4$ be the roots of $f_2(\lambda) = 0$. Then

$$x_1 + x_2 + x_3 + x_4 = n + 5, \tag{3.1}$$

$$x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_2x_4 + x_3x_4 = 5n + ab + 7, \tag{3.2}$$

$$x_2x_3x_4 + x_1x_3x_4 + x_1x_2x_4 + x_1x_2x_3 = 7n + 2ab + 3. \tag{3.3}$$

If

$$x_1 + x_2 = n + 3, \tag{3.4}$$

then, by (3.1), we have

$$x_3 + x_4 = 2. \tag{3.5}$$

From (3.2)-(3.5) it follows that

$$x_1x_2 + x_3x_4 = 3n + ab + 1, \tag{3.6}$$

$$(n+3)x_3x_4 + 2x_1x_2 = 7n + 2ab + 3. \tag{3.7}$$

By (3.6) and (3.7), we have

$$x_3x_4 = 1. \tag{3.8}$$

Combining (3.5) and (3.8), we have

$$x_3 = x_4 = 1. \tag{3.9}$$

Then $f_2(1) = -2ab = 0$, which implies that $b = 0$. Therefore, if $b \geq 1$, then $S_2(T_{a,b,0}) < m(T_{a,b,0}) + 3$. A direct calculation shows that $S_2(T_{n-3,0,0}) = m(T_{n-3,0,0}) + 3$. This completes the proof. □

Lemma 3.3 *For* $Q_{a,b}$, $S_2(Q_{a,b}) < m(Q_{a,b}) + 3$.

Proof By a direct calculation, we have $\phi(Q_{a,b},\lambda) = \lambda(\lambda-1)^{n-6}f_3(\lambda)$, where $f_3(\lambda) = (\lambda - 2)(\lambda^4 - (n+4)\lambda^3 + (5n+ab+1)\lambda^2 - (6n+2ab-2)\lambda + 2n)$. Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \lambda_5 > 0$ be the five roots of $f_3(\lambda) = 0$. Then we have $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 = n + 6$ since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. For $b \geq 1$, $Q_{a,b}$ contains $Q_{1,1}$ as a subgraph. Then by Lemma 2.7 we have $\lambda_3 \geq \mu_3(Q_{1,1}) = 2$ and $\lambda_4 \geq \mu_4(Q_{1,1}) = 1.26$. Therefore, $S_2(Q_{a,b}) = \lambda_1 + \lambda_2 = n + 6 - \lambda_3 - \lambda_4 - \lambda_5 < n + 3$. In what follows, we assume $b = 0$. Since $f_3(1) = 0$, we can rewrite $\phi(Q_{a,0},\lambda) = \lambda(\lambda-1)^{n-5}f_4(\lambda)$, where $f_3(\lambda) = (\lambda-1)f_4(\lambda)$. Let $\lambda'_1 \geq \lambda'_2 \geq \lambda'_3 \geq \lambda'_4 > 0$ be the four roots of $f_4(\lambda) = 0$. Then we have $\lambda'_1 + \lambda'_2 + \lambda'_3 + \lambda'_4 = n + 5$ since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. For $a \geq 1$, $Q_{a,0}$ contains $Q_{1,0}$ as a subgraph. Then by Lemma 2.7 we have $\lambda'_3 \geq \mu_3(Q_{1,0}) = 2$. Thus, $S_2(Q_{a,b}) = \lambda'_1 + \lambda'_2 = n + 5 - \lambda'_3 - \lambda'_4 < n + 3$. If $a = 0$, then $S_2(Q_{a,b}) = S_2(C_4) < m(C_4) + 3$ by a straight calculation. This completes the proof. □

Now, we come to the main results of this paper.

Theorem 3.4 *For any unicyclic graph* G, $S_2(G) \leq m(G) + 3$ *with equality if and only if* $G \cong T(n-3,0,0)$.

Proof For any unicyclic graph G, we assume that $C_k = v_1v_2\cdots v_kv_1$ is the unique cycle in G (for some k) and G has the form $U(R_1,\ldots,R_k)$. For $k \geq 5$, $G - v_1v_2$ is a tree with $d(G - v_1v_2) \geq 5$. Then by Lemma 3.1 we have $S_2(G) < m(G) + 3$. We now consider the following two cases.

Case 1. $k = 4$.

Let $C_4 = v_1v_2v_3v_4v_1$ be the unique cycle in G. If there exist $e(v_i) \geq 2$, say $e(v_1) \geq 2$, then $G - v_1v_2$ is a tree with $d(G - v_1v_2) \geq 5$; if there are two adjacent vertices in $C_4 = v_1v_2v_3v_4v_1$, say v_1 and v_2, such that $e(v_1) \geq 1$ and $e(v_2) \geq 1$, then $G - v_1v_2$ is a tree with $d(G - v_1v_2) \geq 5$. Then by Lemma 3.1 we have $S_2(G) < m(G) + 3$. We now assume $G \cong Q_{a,b}$ (see Figure 4). Then the result follows from Lemma 3.3.

Case 2. $k = 3$.

If $\max\{e(v_1), e(v_2), e(v_3)\} \geq 3$, say $e(v_1) \geq 3$, then $G - v_1v_2$ is a tree with $d(G - v_1v_2) \geq 5$; if there are two vertices in $C_3 = v_1v_2v_3v_1$, say v_1 and v_2, such that $e(v_1) = 2$ and $e(v_2) \geq 1$, then $G - v_1v_2$ is a tree with $d(G - v_1v_2) \geq 5$. Therefore, Lemma 3.1 implies that $S_2(G) <$

$m(G) + 3$. We now assume $G \cong F_{1,t,n-2t-3}$ $(t \geq 1)$ or $G \cong T_{a,b,c}$. Then the result follows from Lemma 2.13 or Lemma 3.2.

This completes the proof. □

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
YZ carried out the proofs of the main results in the manuscript. AC and JL participated in the design of the study and drafted the manuscript. All the authors read and approved the final manuscript.

Author details
[1]School of Applied Mathematics, Xiamen University of Technology, Xiamen, Fujian, P.R. China. [2]Center for Discrete Mathematics, Fuzhou University, Fuzhou, Fujian, P.R. China. [3]School of Mathematics and Statistics, Minnan Normal University, Zhangzhou, Fujian, P.R. China.

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