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THE SUM OF THE FIRST TWO LARGEST SIGNLESS LAPLACIAN EIGENVALUES OF TREES AND UNICYCLIC GRAPHS*

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Abstract. Let G be a graph on n vertices with $e(G)$ edges. The sum of eigenvalues of graphs has been receiving a lot of attention these years. Let $S_2(G)$ be the sum of the first two largest signless Laplacian eigenvalues of G, and define $f(G) = e(G) + 3 - S_2(G)$. Oliveira et al. (2015) conjectured that $f(G) \geqslant f(U_n)$ with equality if and only if $G \cong U_n$, where U_n is the n-vertex unicyclic graph obtained by attaching $n-3$ pendent vertices to a vertex of a triangle. In this paper, it is proved that $S_2(G) < e(G) + 3 - \frac{2}{n}$ when G is a tree, or a unicyclic graph whose unique cycle is not a triangle. As a consequence, it is deduced that the conjecture proposed by Oliveira et al. is true for trees and unicyclic graphs whose unique cycle is not a triangle.

Key words. The sum of eigenvalues, Signless Laplacian eigenvalues, Laplacian eigenvalues, Trees, Unicyclic graphs.

AMS subject classifications. 05C50, 15A42.

1. Introduction. Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Denote by $n(G)$ and $e(G)$ the numbers of vertices and edges in G, respectively, i.e., $n(G) = |V(G)|$ and $e(G) = |E(G)|$.

The research about the eigenvalues of graphs is the core of spectral graph theory. In particular, the research regarding the sum of eigenvalues of various matrices based on graphs is rather active these years, and a number of results are established, e.g., [1, 5, 6, 8, 11, 13, 14, 15, 16]. This paper will focus on the sum of signless Laplacian eigenvalues of graphs.

The Laplacian matrix of G is defined as $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$, where $\mathbf{D}(G)$ is the diagonal matrix of vertex degrees of G, and $\mathbf{A}(G)$ is the adjacency matrix of G. Let

$$\mu_1(G) \geqslant \mu_2(G) \geqslant \cdots \geqslant \mu_n(G) = 0$$

be the Laplacian eigenvalues of G, i.e., the eigenvalues of $\mathbf{L}(G)$, in the non-increasing order, where $n = n(G)$.

The signless Laplacian matrix of G is defined as $\mathbf{Q}(G) = \mathbf{D}(G) + \mathbf{A}(G)$. Let

$$q_1(G) \geqslant q_2(G) \geqslant \cdots \geqslant q_n(G) \geqslant 0$$

be the signless Laplacian eigenvalues of G, i.e., the eigenvalues of $\mathbf{Q}(G)$, in the non-increasing order, where $n = n(G)$.

Let

$$S_k(G) = \sum_{i=1}^{k} q_i(G),$$

where $k = 1, 2, \ldots, n$.

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Analogous to Brouwer's conjecture [2, 11], Ashraf et al. [1] proposed a conjecture about the sum of the signless Laplacian eigenvalues of graphs.

Conjecture 1.1. [1] *Let G be a graph on n vertices. Then*

$$S_k(G) \leqslant e(G) + \binom{k+1}{2}$$

for $k = 1, 2, \ldots, n$.

In the same paper, Ashraf et al. [1] showed that Conjecture 1.1 is true when $k = 2$, i.e.,

$$S_2(G) \leqslant e(G) + 3.$$

Moreover, this inequality is asymptotically tight [1, 16].

In order to get the best upper bound for $S_2(G)$, Oliveira et al. [16] defined the function

$$f(G) = e(G) + 3 - S_2(G),$$

and proposed a conjecture about $f(G)$.

Conjecture 1.2. [16] *Let G be a graph on $n \geqslant 9$ vertices with $e(G)$ edges. Then*

$$f(G) \geqslant f(U_n)$$

with equality if and only if $G \cong U_n$, where U_n is the n-vertex unicyclic graph obtained by attaching $n-3$ pendent vertices to a vertex of a triangle.

As a preliminary trial, Oliveira et al. [16] showed that Conjecture 1.2 is true for firefly graphs, i.e., the graphs consisting of some triangles, pendent edges and pendent paths of length 2, all of which share the same vertex.

Motivated by [16] and Conjecture 1.2 proposed there, we further research the lower bound of $f(G)$. In this paper, we will show that

$$S_2(G) < e(G) + 3 - \frac{2}{n},$$

or equivalently,

$$f(G) > \frac{2}{n}$$

when G is a tree, or a unicyclic graph whose unique cycle is not a triangle. As a consequence, we deduce that Conjecture 1.2 is true for trees and unicyclic graphs whose unique cycle is not a triangle.

2. Preliminaries.

In this section, we will recall some useful lemmas.

First of all, let us recall a well-known properties for the Laplacian spectrum and signless Laplacian spectrum of bipartite graphs.

Lemma 2.1. [2] *A graph G is bipartite if and only if the Laplacian spectrum and signless Laplacian spectrum of G are equal.*

Let $\lambda_1(\mathbf{A}) \geqslant \lambda_2(\mathbf{A}) \geqslant \cdots \geqslant \lambda_n(\mathbf{A})$ be the eigenvalues of the $n \times n$ symmetric matrix $\mathbf{A}$ in the non-increasing order.

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Lemma 2.2. [7] *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *be two* $n \times n$ *real symmetric matrices. Then*

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

for $k = 1, 2, \ldots, n$.

Applying Lemma 2.2 with $k = 2$ to the signless Laplacian matrices of a graph and its subgraphs, we can get the following lemma immediately.

Lemma 2.3. *Let* H *be a proper subgraph of a graph* G. *Then*

$$S_2(G) \leqslant S_2(H) + 2(e(G) - e(H)).$$

The bounds of the signless Laplacian eigenvalues of graphs are of great importance in our subsequent proofs. Let d_v be the degree of vertex v in G.

Lemma 2.4. [4] *Let* G *be a connected graph. Then*

$$q_1(G) \leqslant \max\{d_u + m_u : u \in V(G)\},$$

where $m_u = \frac{1}{d_u} \sum_{uv \in E(G)} d_v$.

Lemma 2.5. [12] *Let* G *be a graph with the second maximum degree* d_2. *Then* $\mu_2(G) \geqslant d_2$.

The following interlacing theorem reveals the relationship about the signless Laplacian spectrum of a graph and its subgraphs.

For a graph G with edge subset $E' \subseteq E(G)$, let $G - E'$ be the graph obtained from G by deleting the edges in E'. If $E' = \{e\}$, then we write $G - e$ for $G - \{e\}$.

Lemma 2.6. [3] *Let* G *be a graph on* n *vertices, and* e *be an edge of* G. *Denote by* $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n$ *and* $s_1 \geqslant s_2 \geqslant \cdots \geqslant s_n$ *the signless Laplacian eigenvalues of* G *and* $G - e$, *respectively. Then*

$$q_1 \geqslant s_1 \geqslant q_2 \geqslant s_2 \geqslant \cdots \geqslant q_n \geqslant s_n \geqslant 0.$$

At this stage, we present some bounds for the signless Laplacian eigenvalues of trees and unicyclic graphs.

Lemma 2.7. [9] *Let* G *be a tree on* n *vertices. Then* $\mu_1(G) \leqslant n$.

Notice that a tree is a bipartite graph. So, from Lemma 2.1, the upper bound n in Lemma 2.7 is not only valid for the maximum Laplacian eigenvalue, but also valid for the maximum signless Laplacian eigenvalue.

Lemma 2.8. *Let* G *be a tree on* n *vertices. Then* $q_1(G) \leqslant n$.

Let S_n be the star on n vertices. Let $S_{a,b}$ be the tree of order $a + b + 2$ obtained by joining an edge between the centers of the two stars S_{a+1} and S_{b+1}, where $a \geqslant b \geqslant 1$, see Figure 1.

Lemma 2.9. [10] *Among the trees on* $n \geqslant 6$ *vertices, the first three maximum signless Laplacian radii are successively attained by* S_n, $S_{n-3,1}$ *and* $S_{n-4,2}$.

Combining Lemmas 2.9 and 2.4, it is easy to get the following two lemmas, we omit the details here.

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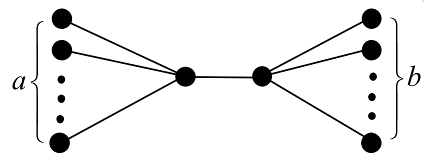

FIGURE 1. *The tree $S_{a,b}$.*

LEMMA 2.10. *Let T be a tree on $n \geqslant 6$ vertices different from S_n. Then*

$$q_1(T) < n - \frac{1}{2} - \frac{2}{n}.$$

LEMMA 2.11. *Let T be a tree on $n \geqslant 6$ vertices different from S_n and $S_{n-3,1}$. Then*

$$q_1(T) \leqslant n - 1 - \frac{2}{n}.$$

LEMMA 2.12. [3] *Let G be a unicyclic graph on $n \geqslant 4$ vertices. Then*

$$q_1(G) \leqslant q_1(U_n).$$

LEMMA 2.13. [16] *For $n \geqslant 7$, we have*

$$q_1(U_n) < n + \frac{1}{n}.$$

Together with Lemmas 2.12 and 2.13, we would conclude with the following result.

LEMMA 2.14. *Let G be a unicyclic graph on $n \geqslant 7$ vertices. Then*

$$q_1(G) < n + \frac{1}{n}.$$

3. Bounds to trees and unicyclic graphs.

Fritscher et al. [8] established an upper bound for the sum of the first k largest Laplacian eigenvalues of trees:

$$\sum_{i=1}^{k} \mu_i(G) \leqslant n + 2k - 2 - \frac{2k-2}{n}.$$

In particular, when $k = 2$, we have

$$\mu_1(G) + \mu_2(G) < n + 2 - \frac{2}{n}.$$

Notice that a tree is a bipartite graph. From Lemma 2.1, we can get an upper bound for $S_2(G)$ when G is a tree.

THEOREM 3.1. [8] *Let G be a tree on n vertices. Then*

$$S_2(G) < n + 2 - \frac{2}{n}.$$

Now we turn to consider $S_2(G)$ when G is a unicyclic graph.

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3.1. The effect of $S_2(G)$ under deleting edges operations. First we present two deleting edges operations, and establish an upper bound for $S_2(G)$.

Let $G \cup H$ be the vertex-disjoint union of the graphs G and H.

LEMMA 3.1. *Let G be a unicyclic graph on $n \geqslant 9$ vertices, and e be an edge outside the unique cycle of G. Suppose that $G - e$ consists of two nontrivial components (i.e., either of them contains at least two vertices), one of which is a unicyclic graph, say G_1. If*

$$S_2(G_1) < n(G_1) + 3 - \frac{2}{n(G_1)},$$

then

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Denote by G_1 and G_2 the two components of $G - e$, i.e., $G - e = G_1 \cup G_2$. It is easily seen that one of them is a unicyclic graph and the other is a tree.

Assume that G_1 is a unicyclic graph, and G_2 is a tree. From the hypothesis, we have

$$S_2(G_1) < n(G_1) + 3 - \frac{2}{n(G_1)},$$

and from Theorem 3.1, we have

$$S_2(G_2) \leqslant n(G_2) + 2 - \frac{2}{n(G_2)}.$$

If $S_2(G_1 \cup G_2) = S_2(G_1)$, then by Lemma 2.3, we get that

$$\begin{aligned} S_2(G) &\leqslant S_2(G - e) + 2 \\ &= S_2(G_1 \cup G_2) + 2 \\ &= S_2(G_1) + 2 \\ &< \left(n(G_1) + 3 - \frac{2}{n(G_1)}\right) + 2 \\ &< n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

If $S_2(G_1 \cup G_2) = S_2(G_2)$, then by Lemma 2.3, we have

$$\begin{aligned} S_2(G) &\leqslant S_2(G - e) + 2 \\ &= S_2(G_1 \cup G_2) + 2 \\ &= S_2(G_2) + 2 \\ &\leqslant \left(n(G_2) + 2 - \frac{2}{n(G_2)}\right) + 2 \\ &< n + 3 - \frac{2}{n}, \end{aligned}$$

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i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

If $S_2(G_1 \cup G_2) = q_1(G_1) + q_1(G_2)$, then by Lemmas 2.3, 2.14 and 2.8, it follows that

$$\begin{aligned} S_2(G) &\leqslant S_2(G-e) + 2 \\ &= S_2(G_1 \cup G_2) + 2 \\ &= q_1(G_1) + q_1(G_2) + 2 \\ &< \left(n(G_1) + \frac{1}{n(G_1)} \right) + n(G_2) + 2 \\ &= n + 2 + \frac{1}{n(G_1)} \\ &< n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Now the result follows. ∎

Lemma 3.2. *Let G be a unicyclic graph on $n \geqslant 12$ vertices, and e_1 and e_2 be two edges lying on the unique cycle of G. Suppose that $G - \{e_1, e_2\} = G_1 \cup G_2$, where both G_1 and G_2 contain at least two edges, equivalently, both G_1 and G_2 contain at least three vertices. If neither G_1 nor G_2 is a star, or one of G_1 and G_2, say G_1, is a tree different from $S_{n(G_1)}$ and $S_{n(G_1)-3,1}$, then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Notice that both G_1 and G_2 are trees.

If $S_2(G_1 \cup G_2) = S_2(G_1)$, then by Lemma 2.3 and Theorem 3.1, we can get that

$$\begin{aligned} S_2(G) &\leqslant S_2(G - \{e_1, e_2\}) + 4 \\ &= S_2(G_1 \cup G_2) + 4 \\ &= S_2(G_1) + 4 \\ &\leqslant \left(n(G_1) + 2 - \frac{2}{n(G_1)} \right) + 4 \\ &< n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

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If $S_2(G_1 \cup G_2) = S_2(G_2)$, then as above, we have

$$\begin{aligned} S_2(G) &\leqslant S_2(G - \{e_1, e_2\}) + 4 \\ &= S_2(G_1 \cup G_2) + 4 \\ &= S_2(G_2) + 4 \\ &\leqslant \left(n(G_2) + 2 - \frac{2}{n(G_2)}\right) + 4 \\ &< n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Suppose that $S_2(G_1 \cup G_2) = q_1(G_1) + q_1(G_2)$. If neither G_1 nor G_2 is a star, then by Lemmas 2.3 and 2.10, we have

$$\begin{aligned} S_2(G) &\leqslant S_2(G - \{e_1, e_2\}) + 4 \\ &= S_2(G_1 \cup G_2) + 4 \\ &= q_1(G_1) + q_1(G_2) + 4 \\ &< \left(n(G_1) - \frac{1}{2} - \frac{2}{n(G_1)}\right) + \left(n(G_2) - \frac{1}{2} - \frac{2}{n(G_2)}\right) + 4 \\ &< n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

If one of G_1 and G_2, say G_1, is a tree different from $S_{n(G_1)}$ and $S_{n(G_1)-3,1}$, then by Lemmas 2.3, 2.11 and 2.8, we have that

$$\begin{aligned} S_2(G) &\leqslant S_2(G - \{e_1, e_2\}) + 4 \\ &= S_2(G_1 \cup G_2) + 4 \\ &= q_1(G_1) + q_1(G_2) + 4 \\ &\leqslant \left(n(G_1) - 1 - \frac{2}{n(G_1)}\right) + n(G_2) + 4 \\ &< n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Now we get the desired result. □

3.2. $S_2(G)$ **for some particular graphs.** Next we consider $S_2(G)$ for some graphs of particular roles, which will be used in the proofs of our main results.

Let $\phi(G, x)$ be the characteristic polynomial of the signless Laplacian matrix of G.

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Let $S_n^3(a,b)$ be the n-vertex tree obtained by attaching a and b pendent vertices to the two end vertices of the path of length three, respectively, where $a \geqslant b \geqslant 1$ and $a+b = n-4$, see Figure 2.

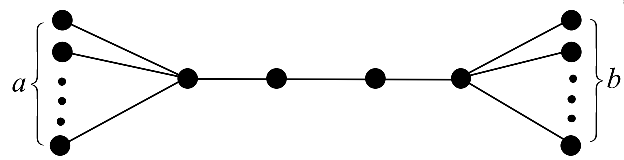

FIGURE 2. *The tree $S_n^3(a,b)$.*

LEMMA 3.3. *For $n \geqslant 7$ and $a \geqslant b \geqslant 1$, we have*

$$S_2(S_n^3(a,b)) < n + 1 - \frac{2}{n}.$$

Proof. By direct calculation, we have

$$\phi(S_n^3(a,b),x) = x(x-1)^{n-5} f(x),$$

where

$$f(x) = x^4 - (n+3)x^3 + (5n + ab - 4)x^2 - (6n + 3ab - 10)x + n.$$

Let $x_1 \geqslant x_2 \geqslant x_3 \geqslant x_4 > 0$ be the roots of $f(x) = 0$. Clearly,

$$x_1 + x_2 + x_3 + x_4 = n + 3.$$

In the following, we will show that $x_3 + x_4 > 2 + \frac{2}{n}$.

If $(a,b) = (2,1)$ or $(3,1)$, then $x_3 + x_4 > 2 + \frac{2}{n}$ follows from direct calculations easily.

Note that $S_n^3(a,b)$ is a bipartite graph. By Lemmas 2.1 and 2.5, we have

$$q_2(S_n^3(a,b)) = \mu_2(S_n^3(a,b)) \geqslant b + 1 \geqslant 2,$$

and noting that $f(1) = -a-b-2ab < 0$, thus $x_3 > 1$. So, the first three largest signless Laplacian eigenvalues of $S_n^3(a,b)$ are successively x_1, x_2 and x_3.

First suppose that $a \geqslant b = 1$. Assume that $a \geqslant 4$, i.e., $n \geqslant 9$, thus $S_9^3(4,1)$ is a subgraph of $S_n^3(a,b)$. So, by Lemma 2.6, we have

$$x_3 = q_3(S_n^3(a,b)) \geqslant q_3(S_9^3(4,1)) > 2.275,$$

and then

$$x_3 + x_4 > x_3 > 2.275 > 2 + \frac{2}{n}$$

for $n \geqslant 9$.

Next suppose that $a \geqslant b \geqslant 2$. Clearly, $n \geqslant 8$. Note that $S_8^3(2,2)$ is a subgraph of $S_n^3(a,b)$, thus by Lemma 2.6,

$$x_3 = q_3(S_n^3(a,b)) \geqslant q_3(S_8^3(2,2)) > 2.47,$$

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and then

$$x_3 + x_4 > x_3 > 2.47 > 2 + \frac{2}{n}$$

for $n \geqslant 8$.

Now we have showed that

$$x_3 + x_4 > 2 + \frac{2}{n}.$$

So,

$$S_2(S_n^3(a,b)) = x_1 + x_2 = n + 3 - (x_3 + x_4) < n + 3 - \left(2 + \frac{2}{n}\right) = n + 1 - \frac{2}{n},$$

i.e.,

$$S_2(S_n^3(a,b)) < n + 1 - \frac{2}{n},$$

as desired. □

Let $U_n^1(a,b)$ be the n-vertex unicyclic graph obtained by attaching a and b pendent vertices to two non-adjacent vertices of a pentagon, respectively, where $a + b = n - 5$, $n \geqslant 6$, $a \geqslant b \geqslant 0$, see Figure 3. In particular, if $b = 0$, then $a = n - 5$, and $U_n^1(n-5, 0)$ is the n-vertex unicyclic graph obtained by attaching $n - 5$ vertices to a vertex of a pentagon.

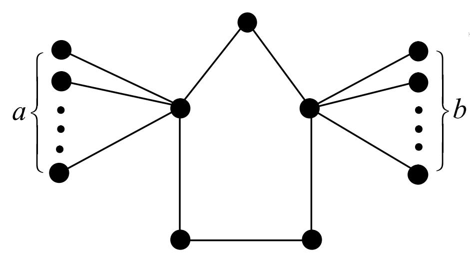

FIGURE 3. *The unicyclic graph $U_n^1(a,b)$.*

Let C_n be the cycle on $n \geqslant 3$ vertices.

LEMMA 3.4. *Let G be a unicyclic graph on $n \geqslant 9$ vertices obtained by identifying two trees (possibly trivial trees) with two non-adjacent vertices of a pentagon, respectively. Then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Assume that the unique cycle of G is $C_5 = v_1v_2v_3v_4v_5v_1$, and G is a unicyclic graph obtained by identifying two trees (possibly trivial trees) with v_1 and v_3, respectively. Moreover, we may assume that $d_{v_1} \geqslant d_{v_3}$. It implies that $d_{v_1} \geqslant 3$, $d_{v_3} \geqslant 2$ and $d_{v_2} = d_{v_4} = d_{v_5} = 2$.

We partition our proofs into two cases.

Case 1. Every edge outside the unique cycle of G is a pendent edge.

In this case, note that $G \cong U_n^1(d_{v_1} - 2, d_{v_3} - 2)$.

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First suppose that $d_{v_3} = 2$. Clearly, $G - v_1v_2 \cong S_n^3(d_{v_1} - 2, 1)$. Notice that $d_{v_1} \geqslant 6$ since $n \geqslant 9$. By Lemmas 2.3 and 3.3, we have

$$\begin{aligned} S_2(G) &\leqslant S_2(G - v_1v_2) + 2 \\ &= S_2(S_n^3(d_{v_1} - 2, 1)) + 2 \\ &< \left(n + 1 - \frac{2}{n}\right) + 2 \\ &= n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Next suppose that $d_{v_3} \geqslant 3$. Clearly, $G - v_2v_3 \cong S_n^3(d_{v_1} - 1, d_{v_3} - 2)$. Note that $d_{v_1} \geqslant 3$, then by Lemmas 2.3 and 3.3, we have

$$\begin{aligned} S_2(G) &\leqslant S_2(G - v_2v_3) + 2 \\ &= S_2(S_n^3(d_{v_1} - 1, d_{v_3} - 2)) + 2 \\ &< \left(n + 1 - \frac{2}{n}\right) + 2 \\ &= n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Case 2. There is some edge outside C_5 which is not a pendent edge of G.

Denote by $t(G)$ the number of edges outside C_5 which are not the pendent edges of G.

In this case, we will prove the result, i.e.,

$$S_2(G) < n + 3 - \frac{2}{n} \tag{3.1}$$

by induction on $t(G)$.

Actually, in case 1, we have shown that the result holds when $t(G) = 0$. Now suppose that $t(G) \geqslant 1$ and the result holds for all nonnegative integers less than $t(G)$.

Let e be an edge outside C_5 which is not a pendent edge of G. Assume that $G - e = G_1 \cup G_2$, where G_1 is a unicyclic graph. Note that $t(G_1) < t(G)$, thus by induction, we know that (3.1) holds for G_1, i.e.,

$$S_2(G_1) < n(G_1) + 3 - \frac{2}{n(G_1)}.$$

Clearly, G_2 contains at least two vertices, since e is not a pendent edge of G. Now applying Lemma 3.1,

$$S_2(G) < n + 3 - \frac{2}{n}$$

can be deduced. The result follows. ∎

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Let $U_n^2(a,b)$ be the n-vertex unicyclic graph obtained by attaching a and b pendent vertices to two non-adjacent vertices of a quadrangle, respectively, where $a+b=n-4$, $n \geqslant 5$, $a \geqslant b \geqslant 0$, see Figure 4. In particular, if $b=0$, then $a=n-4$, and $U_n^2(n-4,0)$ is the n-vertex unicyclic graph obtained by attaching $n-4$ vertices to a vertex of a quadrangle.

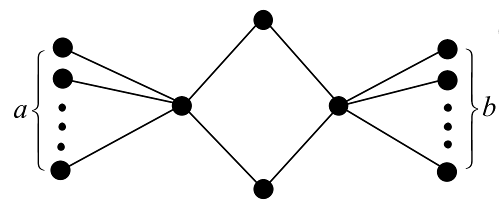

FIGURE 4. *The unicyclic graph $U_n^2(a,b)$.*

LEMMA 3.5. *Let G be a unicyclic graph on $n \geqslant 9$ vertices obtained by identifying two trees (possibly trivial trees) with two non-adjacent vertices of a quadrangle, respectively. Then*

$$S_2(G) < n+3-\frac{2}{n}.$$

Proof. Assume that the unique cycle of G is $C_4 = v_1v_2v_3v_4v_1$, and G is a unicyclic graph obtained by identifying two trees (possibly trivial trees) with v_1 and v_3, respectively. Moreover, we may assume that $d_{v_1} \geqslant d_{v_3}$. It implies that $d_{v_1} \geqslant 3$, $d_{v_3} \geqslant 2$ and $d_{v_2} = d_{v_4} = 2$.

We partition our proofs into two cases.

Case 1. Every edge outside the unique cycle of G is a pendent edge.

In this case, note that $G \cong U_n^2(a,b)$, where $a = d_{v_1}-2$ and $b = d_{v_3}-2$.

By direct calculation, we have

$$\phi(U_n^2(a,b),x) = x(x-2)(x-1)^{n-6}f(x),$$

where

$$f(x) = x^4-(n+4)x^3+(5n+ab+1)x^2-(6n+2ab-2)x+2n.$$

Let $x_1 \geqslant x_2 \geqslant x_3 \geqslant x_4 > 0$ be the roots of $f(x)=0$. Clearly,

$$x_1+x_2+x_3+x_4 = n+4.$$

First we consider the case $a \geqslant b \geqslant 1$. Note that $U_n^2(a,b)$ is a bipartite graph. By Lemmas 2.1 and 2.5, we have

$$q_2(U_n^2(a,b)) = \mu_2(U_n^2(a,b)) \geqslant b+2 \geqslant 3.$$

Moreover, noting that $f(2) = 2n-8 > 0$ and $f(1) = -ab < 0$, thus $1 < x_3 < 2$. So, the first four largest signless Laplacian eigenvalues of $U_n^2(a,b)$ are successively $x_1, x_2, 2, x_3$.

Since $a \geqslant b \geqslant 1$, $U_6^2(1,1)$ is a subgraph of $U_n^2(a,b)$, by Lemma 2.6, we have

$$x_3+x_4 > x_3 = q_4(U_n^2(a,b)) \geqslant q_4(U_6^2(1,1)) > 1.26.$$

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Now it follows that

$$S_2(U_n^2(a,b)) = x_1 + x_2 = n + 4 - (x_3 + x_4) < n + 2.74 < n + 3 - \frac{2}{n}$$

for $n \geqslant 9$, i.e.,

$$S_2(U_n^2(a,b)) < n + 3 - \frac{2}{n}.$$

Next we consider the case $b = 0$, i.e., $a = n - 4$. In this case,

$$f(x) = (x-1)(x^3 - (n+3)x^2 + (4n-2)x - 2n),$$

i.e.,

$$\phi(U_n^2(n-4,0),x) = x(x-2)(x-1)^{n-6}f(x) = x(x-2)(x-1)^{n-5}g(x),$$

where

$$g(x) = x^3 - (n+3)x^2 + (4n-2)x - 2n.$$

Let $y_1 \geqslant y_2 \geqslant y_3 > 0$ be the roots of $g(x) = 0$. Clearly,

$$y_1 + y_2 + y_3 = n + 3.$$

Note that $U_n^2(n-4,0)$ is a bipartite graph. By Lemmas 2.1 and 2.5, we have

$$q_2(U_n^2(n-4,0)) = \mu_2(U_n^2(n-4,0)) \geqslant 2.$$

Note that $g(2) = 2n-8 > 0$. So, y_1 and y_2 are successively the first two largest signless Laplacian eigenvalues of $U_n^2(n-4,0)$. Moreover, it is easily verified that

$$g\left(\frac{2}{n}\right) = -2n + 8 + \frac{8}{n^3} - \frac{12}{n^2} - \frac{8}{n} < 0,$$

which implies that $y_3 > \frac{2}{n}$. Now it follows that

$$S_2(U_n^2(n-4,0)) = y_1 + y_2 = n + 3 - y_3 < n + 3 - \frac{2}{n},$$

i.e.,

$$S_2(U_n^2(n-4,0)) < n + 3 - \frac{2}{n}.$$

Case 2. There is some edge outside C_4 which is not a pendent edge of G.

Similar to the arguments in the proof of case 2 of Lemma 3.4, we can get

$$S_2(G) < n + 3 - \frac{2}{n}$$

similarly. The result follows. □

Let $U_n^3(a,b)$ be the n-vertex unicyclic graph obtained by attaching a and b pendent vertices to two non-adjacent vertices of a quadrangle, respectively, and attaching a pendent vertex to another vertex of the quadrangle, where $a + b = n - 5$, $n \geqslant 7$, $a \geqslant b \geqslant 1$, see Figure 5.

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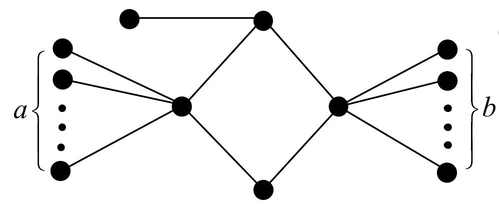

FIGURE 5. *The unicyclic graph* $U_n^3(a,b)$.

LEMMA 3.6. *Let G be a unicyclic graph on $n \geqslant 9$ vertices obtained by identifying two nontrivial trees (i.e., either of them contains at least two vertices) with two non-adjacent vertices of a quadrangle, respectively, and attaching a pendent vertex to another vertex of the quadrangle. Then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Assume that the unique cycle of G is $C_4 = v_1v_2v_3v_4v_1$, and G is a unicyclic graph obtained by identifying two nontrivial trees with v_1 and v_3, respectively, and attaching a pendent vertex to v_2. Moreover, we may assume that $d_{v_1} \geqslant d_{v_3}$. It implies that $d_{v_1} \geqslant d_{v_3} \geqslant 3$, $d_{v_2} = 3$ and $d_{v_4} = 2$.

We partition our proofs into two cases.

Case 1. Every edge outside the unique cycle of G is a pendent edge.

In this case, note that $G \cong U_n^3(a,b)$, where $a = d_{v_1} - 2$ and $b = d_{v_3} - 2$.

By direct calculation, we have

$$\phi(U_n^3(a,b), x) = x(x-1)^{n-7} f(x),$$

where

$$\begin{aligned} f(x) = {} & x^6 - (n+7)x^5 + (9n + ab + 10)x^4 - (28n + 6ab - 16)x^3 \\ & + (37n + 10ab - 39)x^2 - (21n + 4ab - 19)x + 4n. \end{aligned}$$

Let $x_1 \geqslant x_2 \geqslant x_3 \geqslant x_4 \geqslant x_5 \geqslant x_6 > 0$ be the roots of $f(x) = 0$. Clearly,

$$x_1 + x_2 + x_3 + x_4 + x_5 + x_6 = n + 7.$$

Note that $U_n^3(a,b)$ is a bipartite graph. By Lemmas 2.1 and 2.5, we have

$$q_2(U_n^3(a,b)) = \mu_2(U_n^3(a,b)) \geqslant b + 2 \geqslant 3.$$

Moreover, noting that $f(2) = -2n + 10 < 0$ and $f(1) = ab > 0$, thus $x_4 > 1$. So, the first four largest signless Laplacian eigenvalues of $U_n^3(a,b)$ are successively x_1, x_2, x_3, x_4.

Since $a \geqslant b \geqslant 1$, $U_7^3(1,1)$ is a subgraph of $U_n^3(a,b)$, thus by Lemma 2.6, we have

$$x_3 = q_3(U_n^3(a,b)) \geqslant q_3(U_7^3(1,1)) > 2.86$$

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and

$$x_4 = q_4(U_n^3(a,b)) \geqslant q_4(U_7^3(1,1)) > 1.42,$$

thus

$$x_3 + x_4 + x_5 + x_6 > x_3 + x_4 > 4.28.$$

Now it follows that

$$S_2(U_n^3(a,b)) = x_1 + x_2 = n + 7 - (x_3 + x_4 + x_5 + x_6) < n + 2.72 < n + 3 - \frac{2}{n}$$

for $n \geqslant 9$, i.e.,

$$S_2(U_n^3(a,b)) < n + 3 - \frac{2}{n}.$$

Case 2. There is some edge outside C_4 which is not a pendent edge of G.

Similar to the arguments in the proof of case 2 of Lemma 3.4, we can get

$$S_2(G) < n + 3 - \frac{2}{n}$$

similarly. The result follows. □

LEMMA 3.7. *Let G be a unicyclic graph on $n \geqslant 9$ vertices obtained by identifying two nontrivial trees (i.e., either of them contains at least two vertices) with two adjacent vertices of a quadrangle, respectively. Then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Assume that the unique cycle of G is $C_4 = v_1v_2v_3v_4v_1$, and G is a unicyclic graph obtained by identifying two nontrivial trees with v_1 and v_2, respectively. Moreover, we may assume that $d_{v_1} \geqslant d_{v_2}$. It implies that $d_{v_1} \geqslant d_{v_2} \geqslant 3$ and $d_{v_3} = d_{v_4} = 2$.

We partition our proofs into two cases.

Case 1. Every edge outside the unique cycle of G is a pendent edge.

Clearly, $G - v_1v_2 \cong S_n^3(d_{v_1} - 2, d_{v_2} - 2)$, where $d_{v_1} \geqslant d_{v_2} \geqslant 3$. By Lemmas 2.3 and 3.3, we have

$$\begin{aligned} S_2(G) &\leqslant S_2(G - v_1v_2) + 2 \\ &= S_2(S_n^3(d_{v_1} - 2, d_{v_2} - 2)) + 2 \\ &< \left(n + 1 - \frac{2}{n}\right) + 2 \\ &= n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Case 2. There is some edge outside the unique cycle of G which is not a pendent edge.

Similar to the arguments in the proof of case 2 of Lemma 3.4, we can get the desired result. □

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3.3. $S_2(G)$ for unicyclic graphs in terms of the girth. In order to conclude with our main results, we need to consider the upper bound for $S_2(G)$ when G is a unicyclic graph, in terms of the length of the unique cycle of G.

LEMMA 3.8. *For $n \geqslant 6$, we have*

$$S_2(C_n) < n + 3 - \frac{2}{n}.$$

Proof. It is well-known that the first two largest signless Laplacian eigenvalues of C_n are successively 4 and $2 + 2\cos\frac{2\pi}{n}$ (e.g., see [2]), and thus,

$$S_2(C_n) = 6 + 2\cos\frac{2\pi}{n}.$$

Clearly,

$$S_2(C_n) < 8 < n + 3 - \frac{2}{n}$$

for $n \geqslant 6$. ∎

LEMMA 3.9. *Let G be a unicyclic graph on $n \geqslant \max\{k+1, 12\}$ vertices whose unique cycle is of length $k \geqslant 7$. Then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Denote by $C_k = v_1v_2 \cdots v_kv_1$ the unique cycle of G. Assume that v_1 is a vertex of maximum degree in C_k, i.e., $d_{v_1} \geqslant 3$.

Note that $G - \{v_1v_2, v_4v_5\}$ contains two components, say $G - \{v_1v_2, v_4v_5\} = G_1 \cup G_2$, where G_1 is the component containing v_1. Clearly, both G_1 and G_2 contain at least two edges, and G_1 is a tree different from $S_{n(G_1)}$ and $S_{n(G_1)-3,1}$. Using Lemma 3.2 by setting $e_1 = v_1v_2$ and $e_2 = v_4v_5$, we can get that

$$S_2(G) < n + 3 - \frac{2}{n},$$

as desired. ∎

LEMMA 3.10. *Let G be a unicyclic graph on $n \geqslant 12$ vertices whose unique cycle is of length six. Then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Denote by $C_6 = v_1v_2v_3v_4v_5v_6v_1$ the unique cycle of G. Assume that v_1 is a vertex of maximum degree in C_6. Clearly, $d_{v_1} \geqslant 3$.

Suppose that there is some edge outside C_6 which is not a pendent edge of G. We may assume that there is some edge outside C_6 incident with v_1 which is not a pendent edge of G. Using Lemma 3.2 by setting $e_1 = v_1v_2$ and $e_2 = v_1v_6$, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Now we may assume that every edge outside C_6 is a pendent edge of G.

If $d_{v_2} \geqslant 3$ or $d_{v_5} \geqslant 3$, then using Lemma 3.2 by setting $e_1 = v_1v_2$ and $e_2 = v_5v_6$, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

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If $d_{v_3} \geqslant 3$ or $d_{v_6} \geqslant 3$, then using Lemma 3.2 by setting $e_1 = v_1v_6$ and $e_2 = v_2v_3$, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

So, in the following, we may assume that $d_{v_2} = d_{v_3} = d_{v_5} = d_{v_6} = 2$.

Clearly, $G - v_2v_3 \cong S_n^3(d_{v_1} - 1, d_{v_4} - 1)$, where $d_{v_1} \geqslant 3$ and $d_{v_4} \geqslant 2$. Now by Lemmas 2.3 and 3.3, we get that

$$\begin{aligned} S_2(G) &\leqslant S_2(G - v_2v_3) + 2 \\ &= S_2(S_n^3(d_{v_1} - 1, d_{v_4} - 1)) + 2 \\ &< \left(n + 1 - \frac{2}{n}\right) + 2 \\ &= n + 3 - \frac{2}{n}, \end{aligned}$$

i.e.,

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Now the result follows. □

Lemma 3.11. *Let G be a unicyclic graph on $n \geqslant 12$ vertices whose unique cycle is of length five. Then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Denote by $C_5 = v_1v_2v_3v_4v_5v_1$ the unique cycle of G. Assume that v_1 is a vertex of maximum degree in C_5. Clearly, $d_{v_1} \geqslant 3$.

Case 1. $d_{v_2} \geqslant 3$.

If $d_{v_3} \geqslant 3$ or $d_{v_5} \geqslant 3$, then using Lemma 3.2 by setting $e_1 = v_1v_5$ and $e_2 = v_2v_3$, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

If $d_{v_4} \geqslant 3$, then using Lemma 3.2 by setting $e_1 = v_1v_2$ and $e_2 = v_4v_5$, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Now we may assume that $d_{v_3} = d_{v_4} = d_{v_5} = 2$. Furthermore, in view of Lemma 3.2 by setting $e_1 = v_1v_2$ and $e_2 = v_1v_5$, we may assume that $d_{v_1} = 3$, and the unique neighbor of v_1 outside C_5 is a pendent vertex of G, and in view of Lemma 3.2 by setting $e_1 = v_1v_2$ and $e_2 = v_2v_3$, we may assume that $d_{v_2} = 3$, and the unique neighbor of v_2 outside C_5 is a pendent vertex of G. Now G is the unicyclic graph of order 7 obtained from $C_5 = v_1v_2v_3v_4v_5v_1$ by attaching a pendent vertex to v_1 and a pendent vertex to v_2, which is a contradiction to $n \geqslant 12$.

Case 2. $d_{v_5} \geqslant 3$.

Due to the symmetry of v_2 and v_5 in C_5, similar to the arguments in case 1, the result follows similarly.

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Case 3. $d_{v_2} = d_{v_5} = 2$.

If $d_{v_3}, d_{v_4} \geqslant 3$, then using Lemma 3.2 by setting $e_1 = v_1v_2$ and $e_2 = v_3v_4$, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

If $d_{v_3} = 2$ or $d_{v_4} = 2$, then by Lemma 3.4, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

The result follows. ∎

LEMMA 3.12. *Let G be a unicyclic graph on $n \geqslant 12$ vertices whose unique cycle is of length four. Then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. Denote by $C_4 = v_1v_2v_3v_4v_1$ the unique cycle of G. Assume that v_1 is a vertex of maximum degree in C_4. Clearly, $d_{v_1} \geqslant 3$.

Case 1. $d_{v_2} \geqslant 3$.

Suppose that $d_{v_3} \geqslant 3$. In view of Lemma 3.2 by setting $e_1 = v_1v_2$ and $e_2 = v_2v_3$, we may assume that $d_{v_2} = 3$, and the unique neighbor of v_2 outside C_4 is a pendent vertex of G. Now by Lemma 3.6, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

If $d_{v_4} \geqslant 3$, due to the symmetry of v_3 and v_4 in C_4, similar to the arguments about the case $d_{v_3} \geqslant 3$, the result follows similarly.

If $d_{v_3} = d_{v_4} = 2$, then by Lemma 3.7, the result follows also.

Case 2. $d_{v_4} \geqslant 3$.

Similar to the arguments in case 1, the result follows similarly.

Case 3. $d_{v_2} = d_{v_4} = 2$.

By Lemma 3.5, we have

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Then the result follows. ∎

Now we come to the concluding result for unicyclic graphs.

THEOREM 3.2. *Let G be a unicyclic graph on $n \geqslant 12$ vertices whose unique cycle is not a triangle. Then*

$$S_2(G) < n + 3 - \frac{2}{n}.$$

Proof. If G is a cycle, then the result follows from Lemma 3.8, while if G is not a cycle, then the result follows from Lemmas 3.9, 3.10, 3.11 and 3.12. ∎

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4. Main results. Finally, let us present our main results.

Combining Theorems 3.1 and 3.2, we have

THEOREM 4.1. *Let G be a tree, or a unicyclic graph whose unique cycle is not a triangle on $n \geqslant 12$ vertices with $e(G)$ edges. Then*

$$S_2(G) < e(G) + 3 - \frac{2}{n},$$

equivalently,

$$f(G) > \frac{2}{n}.$$

On the other hand, let us recall that $q_1(U_n) > n$ and $q_2(U_n) > 3 - \frac{2}{n}$ (from a similar method as [16, Lemma 3.1]), which would result in that $f(U_n)$ is less than $\frac{2}{n}$.

LEMMA 4.1. [16] *For $n \geqslant 10$, we have*

$$S_2(U_n) > e(U_n) + 3 - \frac{2}{n},$$

equivalently,

$$f(U_n) < \frac{2}{n}.$$

Combining Theorem 4.1 and Lemma 4.1, we would have the following conclusion.

THEOREM 4.2. *Let G be a tree, or a unicyclic graph whose unique cycle is not a triangle on $n \geqslant 12$ vertices. Then*

$$f(G) > f(U_n).$$

Actually, from Theorem 4.2, we can know that Conjecture 1.2 is true for trees and unicyclic graphs whose unique cycle is not a triangle.

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