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Research article

Extremal graphs for the sum of two largest eigenvalues

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Abstract: In this paper, we characterize all connected graphs for which the sum of two largest eigenvalues is less than 4. As an application, we prove that the path graph minimizes this sum among all connected graphs of order $n \geq 467$, thereby solving a conjecture posed by Kumar, Liu, Monterde, Pragada, and Tait in "Maximum spectral sum of graphs (arXiv: 2604.00512v2)".

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1. Introduction

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. Let $n = V(G)$ and $m = |E(G)|$ denote the order and size of G, respectively. Also let $N_G(v_i)$ (or N_i) be the neighbor set of the vertex $v_i \in V(G)$. A closed neighbor set $N_G[v_i]$ of the vertex v_i is defined as the set $N_G(v_i) \cup \{v_i\}$. The degree d_i of a vertex v_i of a graph G is the cardinality of the neighborhood N_i of v_i. The maximum degree is denoted by Δ.

If graph G and H are given such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$, then H is called a subgraph of G, denoted as $H \subseteq G$. Let $S \subset V(G)$ be any subset of vertices of graph G. We use S^c to denote $V(G) \setminus S$. Then the induced subgraph $G[S]$ is the graph whose vertex set is S and whose edge set consists of all the edges in $E(G)$ that have both endpoints in S.

Let P_n, C_n, and $K_{p,q}$ $(p + q = n)$ be the path graph, the cycle graph, and the complete bipartite graph with n vertices, respectively. Let $v_iv_{i+1} \in E(P_n)$ for $i = 1, 2, \ldots, n-1$. Let Y_n be the graph obtained from P_n by deleting the edge v_1v_2 and adding the edge v_1v_3. Let W_n $(n \geq 6)$ be the graph obtained from P_n by deleting the edges v_1v_2 and $v_{n-1}v_n$, and adding the edges v_1v_3 and $v_{n-2}v_n$. The T-shape tree $T_{a,b,c}$ with $a \geq b \geq c \geq 1$ is the tree obtained by identifying one endpoint from each of the three paths P_{a+1}, P_{b+1}, and P_{c+1}. Let U_k be the graph obtained from C_k by attaching a pendant edge uv at u of C_k.

Let M be an $n \times n$ symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. For a graph G, we write $\lambda_i(G) = \lambda_i(A(G))$, where $A(G)$ is the adjacency matrix of graph G. Define $S_k(G) = \sum_{i=1}^{k} \lambda_i(G)$.

Initially, Gernert conjectured that $S_2(G) \leq n$ holds for every n-vertex graph and verified it for several classes of graphs, such as regular graphs and planar graphs. However, Nikiforov [8] disproved this conjecture and established a non-trivial upper bound for $S_2(G)$. Subsequently, Ebrahimi et al. [3] refined this bound to a near-optimal one and extended the result from graphs to general non-negative matrices. Very recently, Kumar et al. [5] proved that $S_2(G) \leq \frac{8n}{7}$ for any n-vertex graph, and this bound is best possible. In the same paper, the authors proposed the following conjecture:

Conjecture 1.1. *[5] For sufficiently large n, the path uniquely minimizes $S_2(G)$ among all connected graphs of order n.*

Inspired by this conjecture, we investigate the characterization of connected n-vertex graphs achieving the minimum $S_2(G)$. For the general case of $S_k(G)$, a wide range of results have been established; see [2, 6, 7] and our recent paper on the symmetric matrix [11].

The remainder of this paper is structured as follows: In Section 2, we present some preliminary results, focusing primarily on properties of the spectral radius of a graph. In Section 3, we give a complete characterization of graphs with $S_2(G) < 4$. As an application, we prove that the path graph minimizes $S_2(G)$ among all connected graphs of order $n \geq 467$, which implies that Conjecture 1.1 holds. Finally, in Section 4, we offer some concluding remarks and directions for further research.

2. Preliminaries

This section reviews several known results essential for the proofs in Section 3. To begin, we give a fundamental result on the sum of the k largest eigenvalues of a symmetric matrix.

Lemma 2.1. *[4] Let M be a symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then $\lambda_1 + \lambda_2 + \cdots + \lambda_r = \sup\left\{u_1^T M u_1 + u_2^T M u_2 + \cdots + u_r^T M u_r\right\}$ $(r = 1, 2, \ldots, n)$, where the supremum is taken over all orthonormal vectors $u_1, u_2, \ldots, u_r$.*

Next, we give the eigenvalues of path graph and cycle graph.

Lemma 2.2. *[1] The eigenvalues of path graph P_n are $2\cos\left(\frac{k\pi}{n+1}\right)$ with corresponding eigenvector*

$$\left(\sin\Big(\frac{k\pi}{n+1}\Big), \sin\Big(\frac{2k\pi}{n+1}\Big), \ldots, \sin\Big(\frac{nk\pi}{n+1}\Big)\right)^T, \quad k = 1, 2, 3, \ldots, n.$$

Lemma 2.3. *[1] The eigenvalues of cycle graph C_n are $2\cos(\frac{2k\pi}{n})$, $k = 1, 2, \ldots, n$.*

Here we, list some well-known results on the spectral radius of a graph.

Lemma 2.4. *[1] If H is a subgraph of a graph G, then $\lambda_1(H) \leq \lambda_1(G)$.*

Lemma 2.5. *[9] Let G be a connected graph with order $n \geq 10$. Then*
(i) $\lambda_1(G) < 2$ if and only if $G \in \{P_n, Y_n\}$;
(ii) $\lambda_1(G) = 2$ if and only if $G \in \{C_n, W_n\}$.

Lemma 2.6. *[12] For $x > 0$, we have $x - \frac{x^3}{6} < \sin x < x$.*

The next lemma is the well-known result about the relation between the eigenvalues of a matrix and its principal submatrix.

Lemma 2.7. *[10] Let B be an $n\times n$ symmetric matrix and let B_k be its $k\times k$ leading principal submatrix. Then, for $i = 1, 2, \ldots, k$,*

$$\lambda_i(B) \geq \lambda_i(B_k) \geq \lambda_{n-k+i}(B).$$

By the above result, we have the following result immediately.

Corollary 2.1. *Let G be a graph and let H be its induced subgraph. Then $S_2(G) \geq S_2(H)$.*

3. Extremal graphs with the minimum $S_2(G)$

In this section, we will focus on the characterization of connected graphs with $S_2(G) < 4$. For this, we first give some results on properties on $S_2(G)$.

Lemma 3.1. *Let G be a graph of order n. For any $S \subset V(G)$, we have*

$$S_2(G) \geq \lambda_1(G[S]) + \lambda_1(G[S^c]).$$

Proof. Let $x = (x_1, \ldots, x_{|S|})^T$ and $y = (y_1, \ldots, y_{n-|s|})^T$ be the eigenvectors corresponding to eigenvalues $\lambda_1(G[S])$ of $G[S]$ and $\lambda_1(G[S^c])$ of $G[S^c]$, respectively. Without loss of generality, we assume $S = \{v_1, v_2, \ldots, v_{|s|}\}$. By setting two n-tuple vectors $u_1 = (x_1, \ldots, x_{|S|}, 0, \ldots, 0)^T$ and $u_2 = (0, \ldots, 0, y_1, \ldots, y_{n-|S|})^T$ ($u_1 \perp u_2$) in Lemma 2.1 for $A(G)$, we obtain

$$S_2(G) \geq \frac{u_1^T A(G) u_1}{u_1^T u_1} + \frac{u_2^T A(G) u_2}{u_2^T u_2} = \frac{x^T A(G[S]) x}{x^T x} + \frac{y^T A(G[S^c]) y}{y^T y} = \lambda_1(G[S]) + \lambda_1(G[S^c]),$$

which follows the required result. □

Combining Lemmas 2.4 and 3.1, we immediately obtain the following result.

Corollary 3.1. *Let G be a connected graph of order n and let G_1 and G_2 be disjoint graphs such that $G_1 \bigcup G_2$ is a subgraph of G. Then*

$$S_2(G) \geq \lambda_1(G_1) + \lambda_1(G_2).$$

Let $K'_{1,9}$ denote the connected graph of order 17 obtained from the star $K_{1,9}$ by attaching one new vertex to each of seven pendant vertices of $K_{1,9}$.

Proposition 3.1. *Let G be a connected graph of order $n \geq 17$ with maximum degree Δ. If $\Delta \geq 9$, then $S_2(G) \geq 4$.*

Proof. If $G \cong K_n$, then $\lambda_1(G) = n - 1$ and $\lambda_2(G) = -1$. Thus, we have

$$S_2(G) = \lambda_1(G) + \lambda_2(G) = n - 2 \geq 15 > 4.$$

Otherwise, $G \ncong K_n$. Then there exists a pair of vertices v_i and v_j such that $v_i v_j \notin E(G)$ and hence $\lambda_2(G) \geq 0$. If $\Delta \geq 16$, then G contains $K_{1,16}$ as $n \geq 17$. Then $S_2(G) \geq 4$ by Corollary 3.1.

Otherwise, $9 \leq \Delta \leq 15$. Since G is connected, for $10 \leq \Delta \leq 15$, G contains $K_{1,9} \bigcup K_2$ as $n \geq 17$. Again by Corollary 3.1, we have $S_2(G) \geq 3 + 1 = 4$. Now consider $\Delta = 9$. If G contains $K_{1,8} \bigcup K_{1,2}$, we have

$$S_2(G) \geq \lambda_1(G) + \lambda_2(G) \geq \sqrt{8} + \sqrt{2} > 4.$$

Otherwise, $G \cong K'_{1,9}$. Then we obtain

$$S_2(G) \geq \lambda_1(G) + \lambda_2(G) > 4.$$

This completes the proof. □

Now we characterize the graphs with $S_2(G) < 4$ among all connected graphs that contain at least a cycle.

Lemma 3.2. *Let G be a connected graph with $m \geq n \geq 467$. Then $S_2(G) < 4$ if and only if $G \cong C_n$.*

Proof. Since G is connected with $m \geq n$, G contains at least one cycle, say C_k. If $k = n$, then $G \cong C_n$ and $S_2(G) = 2 + 2\cos(\frac{2\pi}{n}) < 4$. Otherwise, $k < n$. In this case, the set $V(G) \setminus V(C_k)$ is not empty. Thus, G contains U_k as a subgraph. Next, we consider the following two cases:

Case 1. $k \geq 26$. Then $T_{5,5,1} \bigcup P_{k-11}$ is a subgraph of G. By Corollary 3.1, we have

$$S_2(G) \geq \lambda_1(T_{5,5,1}) + \lambda_1(P_{k-11}) \geq \lambda_1(T_{5,5,1}) + \lambda_1(P_{15}) > 4,$$

where $\lambda_1(T_{5,5,1}) > 2.042$ and $\lambda_1(P_{15}) > 1.961$ by SAGE.

Case 2. $3 \leq k \leq 25$. Let $V(U_k) = \{v_1, \ldots, v_{k+1}\}$ such that $v_{k+1} \notin V(C_k)$. Let $d'_i = |N_G(v_i) \setminus V(U_k)|$ and let $\Delta' = \max\left\{d'_i \,|\, 1 \leq i \leq k\right\}$. Without loss of generality, we let $d'_1 = \Delta'$. It is clear that $d'_i \leq d_i - 2$ for $1 \leq i \leq k$ and $d'_{k+1} \leq d_{k+1} - 1$. From Proposition 3.1, we have $S_2(G) \geq 4$ if $\Delta \geq 9$. Otherwise, $\Delta \leq 8$. Thus, $d'_i \leq 6\,(1 \leq i \leq k)$ and $d'_{k+1} \leq 7$.

Claim 1. If $S_2(G) < 4$, then $\sum_{i=1}^{k+1} d'_i \leq 40$.

Proof of Claim 1. First, we assume that $3 \leq k \leq 5$. Then $\sum_{i=1}^{k+1} d'_i \leq 6k + 7 \leq 37 < 40$ as $d'_i \leq 6\,(1 \leq i \leq k)$ and $d'_{k+1} \leq 7$. Next, we assume that $6 \leq k \leq 25$. If $5 \leq d'_1$ or $6 \leq d'_{k+1}$, then G contains $K_{1,7} \bigcup P_3$ as a subgraph. By Corollary 3.1, we have

$$S_2(G) \geq \lambda_1(K_{1,7}) + \lambda_1(P_3) = \sqrt{7} + \sqrt{2} > 4,$$

which contradicts the given condition. Otherwise, $d'_1 \leq 4$ and $d'_{k+1} \leq 5$. For $d'_1 = 4$, $d'_i = 0$ for $i = 4, 5, \ldots, k-2$ (Otherwise, $K_{1,6} \bigcup K_{1,3}$ is a subgraph of G, and then by Corollary 3.1, we obtain $S_2(G) \geq \sqrt{6} + \sqrt{3} > 4$, a contradiction). Hence, we have $\sum_{i=1}^{k+1} d'_i \leq 4\times5+5 = 25$. For $d'_1 = 3$, similarly we have $d'_i \leq 1$ for $i = 4, 5, \ldots, k-2$ as $\sqrt{5}+\sqrt{4} > 4$. Thus, $\sum_{i=1}^{k+1} d'_i \leq 3\times5+(k-5)+5 \leq 40$. For $d'_1 = 2$, similarly we have $d'_i \leq 1$ for $i = 4, 5, \ldots, k-2$ as $\sqrt{4}+\sqrt{4} = 4$. Thus, $\sum_{i=1}^{k+1} d'_i \leq 2\times5+(k-5)+5 \leq 35$. For $d'_1 \leq 1$, $\sum_{i=1}^{k+1} d'_i \leq k + 5 \leq 30$, which completes the proof of Claim 1. □

By Claim 1, we have $S_2(G) \geq 4$ if $\sum_{i=1}^{k+1} d'_i > 40$. Otherwise, $\sum_{i=1}^{k+1} d'_i \leq 40$. Let $G[V^c(U_k)] = H_1 \cup H_2 \cup \cdots \cup H_t$, where H_i is a connected graph with order n_i $(1 \leq i \leq t)$ and $n_1 \geq n_2 \geq \cdots \geq n_t$. Then,

$$t \leq \left|\bigcup_{i=1}^{k+1} N_G(v_i)\backslash V(U_k)\right| = \sum_{i=1}^{k+1} d'_i \leq 40.$$

Thus, $n_1 \geq \frac{n-k-1}{t} > 11$ as $n \geq 467$, that is, $n_1 \geq 12$ as n_1 is integer. Note that G contains $U_k \bigcup H_{n_1}$ as a subgraph, where $k \leq 25$ and $n_1 \geq 12$. By Corollary 3.1, we have

$$S_2(G) \geq \lambda_1(U_k) + \lambda_1(H_{n_1}).$$

By SAGE, we confirm that $\lambda_1(U_k) \geq \lambda_1(U_{25}) > 2.0586$ for $k \leq 25$. Combining these results with the well-known fact that $\lambda_1(H) \geq \lambda_1(P_n)$ for any connected n-vertex graph H, we have

$$S_2(G) \geq \lambda_1(U_{25}) + \lambda_1(P_{n_1}) \geq \lambda_1(U_{25}) + \lambda_1(P_{12}) > 4$$

as $\lambda_1(P_{12}) > 1.9418$. This completes the proof. □

Next, we characterize all the n-vertex trees with $S_2(G) < 4$.

Lemma 3.3. *Let T be a tree with order $n \geq 378$. Then $S_2(T) < 4$ if and only if $T \in \{Y_n, W_n, P_n\}$.*

Proof. It is easy to confirm that $S_2(T) < 4$ if $T \in \{Y_n, W_n, P_n\}$ since $\lambda_2(Y_n) < \lambda_1(Y_n) < 2$, $\lambda_2(P_n) < \lambda_1(P_n) < 2$ and $\lambda_2(W_n) < \lambda_1(W_n) = 2$. Next we assume that $S_2(T) < 4$. Without loss of generality, we let v_1 be the vertex such that $\Delta = d_1$. By Proposition 3.1, we have $\Delta \leq 8$ as $n \geq 378$. Let $L_i = \{v_j | d_T(v_1, v_j) = i\}$ for $i \geq 1$ and let $L_0 = \{v_1\}$, where $d_T(v_1, v_j)$ is the distance between v_1 and v_j of T.

Case 1. $5 \leq \Delta \leq 8$. In this case, $|L_1| = d_1 \leq 8$ and $|L_2| \leq d_1(d_1 - 1) \leq 56$. Note that $T[(L_0 \cup L_1)^c] = H_1 \cup H_2 \cup \cdots \cup H_{|L_2|}$, where H_i is the tree with order n_i ($1 \leq i \leq |L_2|$) and $n_1 \geq n_2 \geq \cdots \geq n_{|L_2|}$. Then $K_{1,d_1} \cup H_1$ is a subgraph of T and $n_1 \geq \frac{n-1-|L_1|}{|L_2|} \geq \frac{n-9}{56} > 6$ as $n \geq 378$. Combining the above results with Corollary 3.1, we have

$$S_2(T) \geq \lambda_1(K_{1,d_1}) + \lambda_1(H_1) \geq \sqrt{d_1} + \lambda_1(P_{n_1}) > \sqrt{5} + \lambda_1(P_6) > 4,$$

a contradiction.

Case 2. $\Delta = 4$. Then $|L_1| = 4$, $|L_2| \leq 12$, and $|L_3| \leq 36$. Note that $T[(L_0 \cup L_1 \cup L_2)^c] = Q_1 \cup Q_2 \cup \cdots \cup Q_{|L_3|}$, where Q_i is the tree with order n_i ($1 \leq i \leq |L_3|$) and $n_1 \geq n_2 \geq \cdots \geq n_{|L_3|}$. Let Q' be the tree obtained from $K_{1,4} \cup K_1$ by adding an edge between the pendent vertex and the isolated vertex. Then $Q' \cup Q_1$ is a subgraph of T and $n_1 \geq \frac{n-1-|L_1|-|L_2|}{|L_3|} \geq \frac{n-17}{36} > 10$ as $n \geq 378$. Combining the above results with Corollary 3.1, we have

$$S_2(T) \geq \lambda_1(Q') + \lambda_1(Q_1) > 2.074 + \lambda_1(P_{n_1}) \geq 2.074 + \lambda_1(P_{11}) > 4,$$

a contradiction.

Case 3. $\Delta \leq 3$. If $\Delta = 2$, $T \cong P_n$. Otherwise, $\Delta = 3$, that is, $|L_1| = 3$. Then $T[L_0^c] = T_1 \cup T_2 \cup T_3$, where T_i is the tree with order n_i and $n_1 \geq n_2 \geq n_3$.

Subcase 3.1. $n_3 \geq 2$. Then $T_{2,2,2}$ is a subgraph of $T[L_0 \cup L_1 \cup L_2]$. As $\Delta = 3$, $|L_2| \leq 6$ and $|L_3| \leq 12$. Then $T[(L_0 \cup L_1 \cup L_2)^c]$ contains at most 12 subtrees. Among these subtrees, let T' be the subtree with the maximum order n'. As $n \geq 378$, we have

$$n' \geq \frac{n-1-|L_1|-|L_2|}{|L_3|} \geq \frac{n-10}{12} > 30.$$

Combining the above results with Corollary 3.1, we have

$$S_2(T) \geq \lambda_1(T_{2,2,2}) + \lambda_1(T') > 2.028 + \lambda_1(P_{n'}) > 2.028 + \lambda_1(P_{30}) > 4,$$

a contradiction.

Subcase 3.2. $n_3 = 1$. By the result in Subcase 3.1, we conclude that every vertex of degree 3 is adjacent to at least one vertex of degree 1. Then $|L_1| = 3$ and $|L_i| \leq 4$ for $i \geq 2$. If $n_2 \geq 2$, then $T_{6,2,1}$ is a subgraph of $T[\cup_{i=0}^{6} L_i]$. Moreover, $T[(\cup_{i=0}^{6} L_i)^c]$ contains two subtrees and two isolated vertices at most. Among these subtrees, let T^* be the subtree with the maximum order n^*. As $n \geq 378$, we have

$$n^* \geq \frac{n - 2 - \sum_{i=0}^{6} |L_i|}{2} \geq \frac{n - 26}{2} > 39.$$

Combining the above results with Corollary 3.1, we have

$$S_2(T) \geq \lambda_1(T_{6,2,1}) + \lambda_1(T^*) > 2.0065 + \lambda_1(P_{n^*}) > 2.0065 + \lambda_1(P_{39}) > 4,$$

a contradiction. Otherwise, $n_2 = 1$. This means that every vertex of degree 3 is adjacent to exactly two pendent vertices. Hence, $T \cong W_n$ or $T \cong Y_n$. This completes the proof. □

By combining Lemmas 3.2 and 3.3, we have the following result immediately.

Theorem 3.1. *Let G be a connected graph of order $n \geq 467$. Then $S_2(G) < 4$ if and only if $G \in \{Y_n, W_n, P_n, C_n\}$.*

Next, we will compare $S_2(G)$ for $G \in \{Y_n, W_n, P_n, C_n\}$.

Lemma 3.4. *For $n \geq 7$, we have $S_2(Y_n) > S_2(P_n)$ and $S_2(W_n) > S_2(P_n)$.*

Proof. If $7 \leq n \leq 10$, the required results are directly confirmed by SAGE. Otherwise, $n \geq 11$. Let $x = (x_1, \ldots, x_n)^T$ and $y = (y_1, \ldots, y_n)^T$ be the eigenvectors corresponding to eigenvalues $\lambda_1(P_n)$ and $\lambda_2(P_n)$ of P_n, respectively. By Lemma 2.2, we have $x_i = \sin(\frac{\pi i}{n+1})$ and $y_i = \sin(\frac{2\pi i}{n+1})$ for $1 \leq i \leq n$. Note that $x \perp y$. We will first prove $S_2(Y_n) > S_2(P_n)$. By Lemma 2.1, we have

$$\begin{aligned}
S_2(Y_n) &\geq \frac{x^T A(Y_n) x}{x^T x} + \frac{y^T A(Y_n) y}{y^T y} \\
&= \frac{x^T A(P_n) x + 2x_1(x_3 - x_2)}{x^T x} + \frac{y^T A(P_n) y + 2y_1(y_3 - y_2)}{y^T y} \\
&= S_2(P_n) + \frac{2\sin(\frac{\pi}{n+1})(\sin(\frac{3\pi}{n+1}) - \sin(\frac{2\pi}{n+1}))}{x^T x} + \frac{2\sin(\frac{2\pi}{n+1})(\sin(\frac{6\pi}{n+1}) - \sin(\frac{4\pi}{n+1}))}{y^T y} \\
&> S_2(P_n), \quad \text{as } n \geq 11.
\end{aligned}$$

By a similar way, we also have

$$\begin{aligned}
S_2(W_n) &\geq \frac{x^T A(W_n) x}{x^T x} + \frac{y^T A(W_n) y}{y^T y} \\
&= \frac{x^T A(P_n) x + 2x_1(x_3 - x_2) + 2x_n(x_{n-2} - x_{n-1})}{x^T x} + \frac{y^T A(P_n) y + 2y_1(y_3 - y_2) + 2y_n(y_{n-2} - y_{n-1})}{y^T y}
\end{aligned}$$

$$= \quad S_2(P_n) + \frac{2x_1(x_3 - x_2) + 2x_n(x_{n-2} - x_{n-1})}{x^T x} + \frac{2y_1(y_3 - y_2) + 2y_n(y_{n-2} - y_{n-1})}{y^T y}.$$

Note that $x_n(x_{n-2} - x_{n-1}) = x_1(x_3 - x_2) > 0$ and $y_n(y_{n-2} - y_{n-1}) = y_1(y_3 - y_2) > 0$ for $n \geq 11$. Combining the above results, we obtain that $S_2(W_n) > S_2(P_n)$. It completes the proof. □

Lemma 3.5. *For $n \geq 3$, we have $S_2(C_n) > S_2(P_n)$.*

Proof. Let $a = \frac{2\pi}{n}$ and $b = \frac{\pi}{n+1}$. By Lemmas 2.2 and 2.3, it is equivalent to prove

$$1 + \cos a - \cos b - \cos 2b > 0.$$

Since $\cos 2b = 2\cos^2 b - 1 = 1 - 2\sin^2 b$ and $\cos a - \cos b = -2\sin\left(\frac{a+b}{2}\right)\sin\left(\frac{a-b}{2}\right)$, the above inequality simplifies to

$$\sin^2 b > \sin\left(\frac{a+b}{2}\right)\sin\left(\frac{a-b}{2}\right). \tag{3.1}$$

If $3 \leq n \leq 9$, the above inequality is easily confirmed by SAGE. Otherwise, $n \geq 10$. Let $f(n) = b^2 - \frac{b^4}{3} - \frac{a^2-b^2}{4}$. As $a = \frac{2\pi}{n}$, $b = \frac{\pi}{n+1}$, and $n \geq 10$,

$$f(n) = \frac{5\pi^2}{4(n+1)^2} - \frac{\pi^4}{3(n+1)^4} - \frac{\pi^2}{n^2} = \frac{\pi^2(3n^4 - 18n^3 - 57n^2 - 4\pi^2 n^2 - 48n - 12)}{12n^2(n+1)^4} > 0. \tag{3.2}$$

By Lemma 2.6, we have

$$\sin^2 b > \left(b - \frac{b^3}{6}\right)^2 = b^2 - \frac{b^4}{3} + \frac{b^6}{36} > b^2 - \frac{b^4}{3},$$

and

$$\sin\left(\frac{a+b}{2}\right)\sin\left(\frac{a-b}{2}\right) < \frac{a^2 - b^2}{4}.$$

Combining the above results with (3.2), we confirm that the inequality in (3.1) holds. Hence, we complete the proof. □

By Theorem 3.1, Lemmas 3.4 and 3.5, we get the following result directly.

Theorem 3.2. *Let G be a connected graph of order $n \geq 467$. Then $S_2(G) \geq S_2(P_n)$ with the equality holding if and only if $G \cong P_n$.*

4. Conclusions

In this paper, we characterized all connected graphs with $S_2(G) < 4$. Moreover, we proved that the path graph minimizes $S_2(G)$ among all connected graphs with order $n \geq 467$, which implies that Conjecture 1.1 holds. It is then natural to investigate the case for arbitrary n, which motivates the following problem:

Problem 4.1. *For each positive integer n, characterize the graphs with minimum $S_2(G)$ among all connected graphs with order n.*

Using SAGE, we confirmed that the star graph minimizes $S_2(G)$ for $n \leq 10$. Extending this observation, numerical results suggest the following answer to Problem 4.1: The extremal graph is $K_{1,n-1}$ when $n \leq 15$ and P_n, otherwise.

Author contributions

Shaowei Sun: Writing–review & editing, Writing–original draft, Software, Methodology, Investigation, Conceptualization; Yaping Min: Writing–review & editing, Writing–original draft, Software, Methodology, Investigation, Formal analysis; Kinkar Chandra Das: Writing–review & editing, Software, Methodology, Investigation, Formal analysis.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare no conflict of interest.

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