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Ordering Quasi-Tree Graphs by the Second Largest Signless Laplacian Eigenvalues

Zhen LIN[1], **Shuguang GUO**[2], **Lianying MIAO**[1,*]
1. *School of Mathematics, China University of Mining and Technology, Jiangsu* 221116*, P. R. China;*
2. *School of Mathematics and Statistics, Yancheng Teachers University, Jiangsu* 224002*, P. R. China*

Abstract A connected graph $G=(V,E)$ is called a quasi-tree graph if there exists a vertex $v_0\in V(G)$ such that $G-v_0$ is a tree. In this paper, we determine all quasi-tree graphs of order n with the second largest signless Laplacian eigenvalue greater than or equal to $n-3$. As an application, we determine all quasi-tree graphs of order n with the sum of the two largest signless Laplacian eigenvalues greater than to $2n-\frac{5}{4}$.

Keywords quasi-tree graph; signless Laplacian matrix; second largest eigenvalue; sum of eigenvalues; ordering

MR(2010) Subject Classification 05C50

1. Introduction

Let $G=(V,E)$ be a simple undirected graph with vertex set $V(G)=\{v_0,v_1,\ldots,v_{n-1}\}$ and edge set $E=E(G)$. For a graph G, $A(G)$ is its adjacency matrix and $D(G)$ is the diagonal matrix of its degrees. The matrix $Q(G)=D(G)+A(G)$ is called the signless Laplacian matrix of G. The eigenvalues of $Q(G)$ are called the signless Laplacian eigenvalues of G, and denoted by $q_1(G)\geq q_2(G)\geq\cdots\geq q_{n-1}(G)\geq q_n(G)\geq 0$. The sum of the k largest signless Laplacian eigenvalues of G is denoted by $S_k(G)$.

The second largest signless Laplacian eigenvalue $q_2(G)$ of a graph G is well studied by several authors. Cvetković and Simić [1] proved that algebraic connectivity $a(G)\leq q_2(G)$ for a non-complete connected graph of order $n\geq 2$. Cvetković and Rowlinson et al. [2] gave some conjectures involving algebraic connectivity, the largest signless Laplacian eigenvalue and the second largest signless Laplacian eigenvalue of G. Das [3, 4] proved the conjectures involving second largest signless Laplacian eigenvalue of graphs.

For a graph G of order $n\geq 2$, Chen [5] proved that $q_2(G)\leq n-2$ and the equality holds when G is the complete graph. Wang and Belardo et al. [6] gave a necessary condition on a graph G for which the bound is reached. They raised the problem to characterize all graphs G

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* Corresponding author
E-mail address: lnlinzhen@163.com (Zhen LIN); ychgsg@163.com (Shuguang GUO); miaolianying@cumt.edu.cn (Lianying MIAO)

of order $n \geq 2$ such that $q_2(G) = n - 2$, and gave a partial answer to this question. For the class of bipartite graphs, Aochiche and Hansen et al. [7] gave a complete characterization for $q_2(G) = n - 2$. Lima and Nikiforov [8] gave a necessary and sufficient condition for the equality $q_i(G) = n - 2$ $(2 \leq i \leq n)$. For more results, one may refer to [1,2] and references therein.

A connected graph $G = (V, E)$ is called a quasi-tree graph, if there exists a vertex $v_0 \in V(G)$ such that $G - v_0$ is a tree. Let $\mathcal{Q}_n$ denote the set of all quasi-tree graphs on n vertices with $v_0 \in V(G)$ such that $G - v_0$ is a tree, and H_i^k $(i = 2, 4, 6, \ldots, 14)$ and H_i $(i = 1, 3, 5, \ldots, 15, 16)$ denote the quasi-tree graphs on n vertices shown in Figure 1. In this paper, we prove the following theorem.

Theorem 1.1 *Let $n \geq 47$ and $G \in \mathcal{Q}_n \setminus \{H_1, H_3, H_5, H_2^2\}$. Then*

$$q_2(G) < n - \frac{41}{16} < q_2(H_2^2) < q_2(H_5) < n - \frac{5}{2} < q_2(H_3) = q_2(H_1) = n - 2.$$

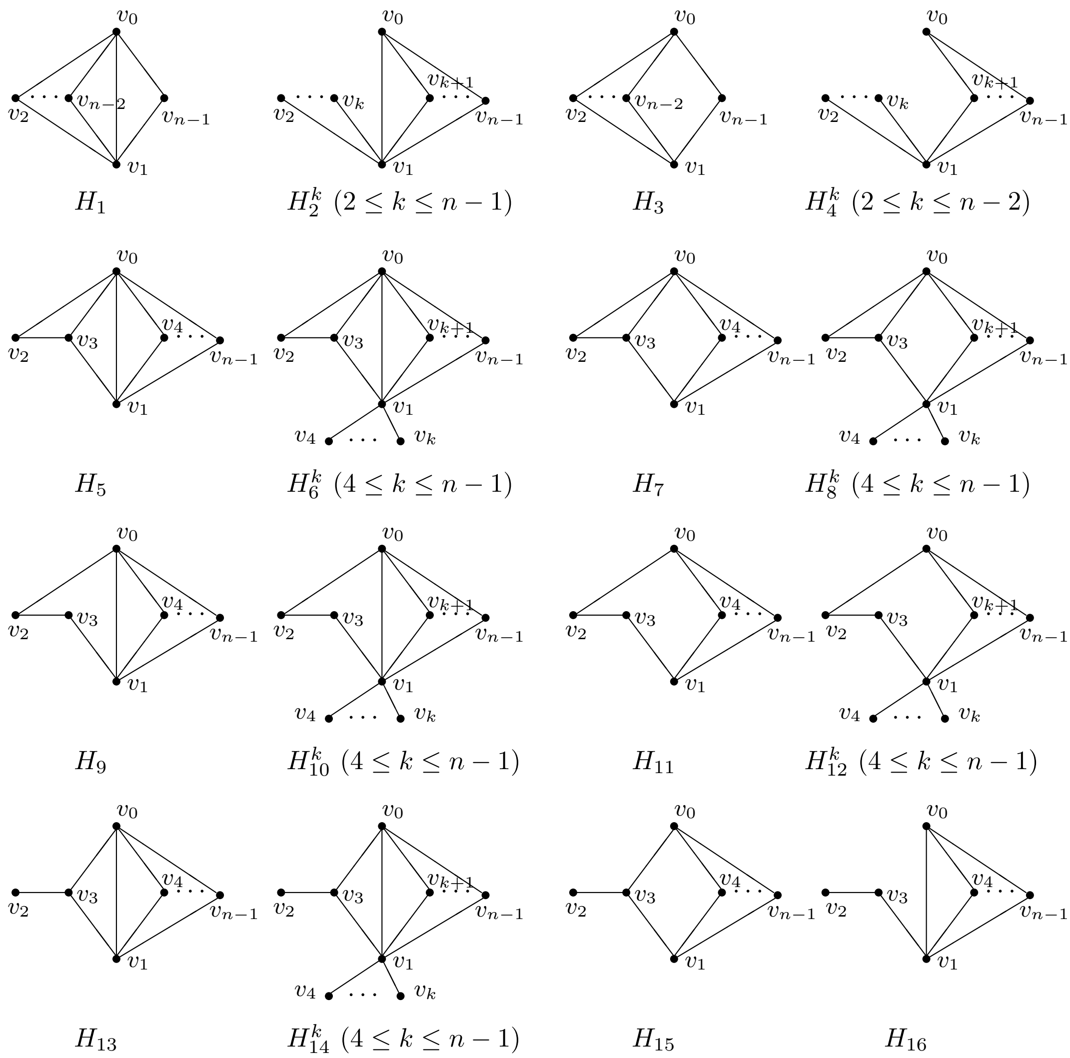

Figure 1 Graphs H_i $(i = 1, 3, 5, \ldots, 15, 16)$, H_i^k $(i = 2, 4, 6, \ldots, 14)$

For any graph G with n vertices, Ashraf et al. [9] conjectured that $S_k(G) \leq e(G) + \binom{k+1}{2}$ for $k = 1, \ldots, n$, and proved the conjecture for $k = 2$ for any graph and for all k for regular graphs. As an application of Theorem 1.1, we prove the following theorem.

Theorem 1.2 *Let $n \geq 47$ and $G \in \mathcal{Q}_n \setminus \{H_1, H_5, H_2^2\}$. Then*

$$S_2(G) < 2n - \frac{5}{4} < S_2(H_2^2) < S_2(H_5) < S_2(H_1).$$

The rest of the paper is organized as follows. In Section 2, we recall some basic notions and lemmas used further, and prove a new lemma. In Section 3, we give a proof of Theorem 1.1. In Section 4, we give a proof of Theorem 1.2.

2. Preliminaries

Let $G - u$ denote the graph that arises from a graph G by deleting the vertex $u \in V(G)$ and all the edges incident with u. The join of two disjoint graphs G and H, denoted by $G \vee H$, is the graph obtained by joining each vertex of G to each vertex of H. For $v \in V(G)$, $N_G(v)$ (or $N(v)$) denotes the neighborhood of v in G, and $d(v) = d_G(v) = |N_G(v)|$ denotes the degree of vertex v in G. We denote by $\Delta(G)$ the maximum degree of the vertices of G. The matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix of G. The largest eigenvalue of $L(G)$ is called the Laplacian spectral radius of G, denoted by $\mu_1(G)$. Two distinct edges in a graph G are independent if they do not have a common end vertex in G. A set of pairwise independent edges of G is called a matching in G, while a matching of maximum cardinality is a maximum matching in G. The matching number $\beta(G)$ of G is the cardinality of a maximum matching of G. The signless Laplacian characteristic polynomial of a graph G is equal to $\det(xI_n - Q(G))$, denoted by $\phi(G, x)$. Let I_p be the $p \times p$ identity matrix and $J_{p,q}$ be the $p \times q$ matrix in which every entry is 1, or simply J_p if $p = q$. Let M be a matrix of order n, $\sigma(M)$ be the spectrum of the matrix M.

Definition 2.1 ([10]) *Let M be a real matrix of order n described in the following block form*

$$\begin{pmatrix} M_{11} & \cdots & M_{1t} \\ \vdots & \ddots & \vdots \\ M_{t1} & \cdots & M_{tt} \end{pmatrix}, \tag{2.1}$$

where the diagonal blocks M_{ii} are $n_i \times n_i$ matrices for any $i \in \{1, 2, \ldots, t\}$ and $n = n_1 + \cdots + n_t$. For any $i, j \in \{1, 2, \ldots, t\}$, let b_{ij} denote the average row sum of M_{ij}, i.e., b_{ij} is the sum of all entries in M_{ij} divided by the number of rows. Then $B(M) = (b_{ij})$ (simply by B) is called the quotient matrix of M.

Lemma 2.2 ([11]) *Let $M = (m_{ij})_{n \times n}$ be defined as (2.1), and for any $i, j \in \{1, 2, \ldots, t\}$, $M_{ii} = l_i J_{n_i} + p_i I_{n_i}$, $M_{ij} = s_{ij} J_{n_i, n_j}$, for $i \neq j$, where l_i, p_i, s_{ij} are real numbers, $B = B(M)$ be the quotient matrix of M. Then*

$$\sigma(M) = \sigma(B) \cup \{p_i^{[n_i - 1]} \mid i = 1, 2, \ldots, t\},$$

where $p_i^{[n_i-1]}$ *means that* p_i *is an eigenvalue with multiplicity* $n_i - 1$.

Lemma 2.3 ([12]) *Suppose* G *is a connected graph with* $n \geq 3$ *vertices. Then*

$$q_1(G) \leq \max\{d(v) + m(v) \,|\, v \in V(G) \text{ and } d(v) > 1\},$$

and equality holds if and only if G *is either a regular graph or a semiregular bipartite graph, where* $m(v) = \sum_{u \in N(v)} d(u)/d(v)$.

Lemma 2.4 ([13]) *Let* G *be a graph of order* n *and* $v \in V(G)$. *Then*

$$q_{i+1}(G) - 1 \leq q_i(G - v) \leq q_i(G)$$

for $i = 1, 2, \ldots, n-1$, *where the right equality holds if and only if* v *is an isolated vertex.*

Let T_m^n $(2m \leq n+1)$ denote the tree of order n obtained from the star $K_{1,\,n-m}$ by joining $m-1$ pendant vertices of $K_{1,\,n-m}$ to $m-1$ isolated vertices by $m-1$ edges.

Lemma 2.5 ([14]) *Let* T *be a tree on* n *vertices with matching number* β. *Then* $\mu_1(T) \leq r$, *where* r *is the maximum root of the equation*

$$x^3 - (n - \beta + 4)x^2 + (3n - 3\beta + 4)x - n = 0.$$

The equality holds if and only if $T = T_\beta^n$.

Lemma 2.6 ([15]) *If* G *is connected, then* $\mu_1(G) \leq q_1(G)$, *where the equality holds if and only if* G *is bipartite.*

Lemma 2.7 ([3]) *Let* G *be a connected graph with second maximum degree* $d_2(G)$. *Then*

$$d_2(G) - 1 \leq q_2(G) \leq n - 2.$$

Lemma 2.8 ([2]) *Let* G *be a graph with order* n *and* $e \in E(G)$. *Then*

$$q_1(G) \geq q_1(G - e) \geq q_2(G) \geq q_2(G - e) \geq \cdots \geq q_n(G) \geq q_n(G - e) \geq 0.$$

Lemma 2.9 ([16]) *Let* $n > 3$, $G \in \mathcal{Q}_n$. *Then*

$$q_1(G) < \max\{2 + \frac{d(v_0) + n - 3}{2}, \Delta(G) + \frac{d(v_0) + n - 3}{\Delta(G)}\} + 1.$$

Lemma 2.10 ([17]) *Let* G *be a connected graph and* $q_1(G)$ *be the spectral radius of* $Q(G)$. *Let* u, v *be two vertices of* G *and* $d(v)$ *be the degree of vertex* v. *Suppose* $v_1, v_2, \ldots, v_s$ $(1 \leq s \leq d(v))$ *are some vertices of* $N_G(v) \setminus N_G(u)$ *and* $x = (x_1, x_2, \ldots, x_n)^T$ *is the Perron vector of* $Q(G)$, *where* x_i *corresponds to the vertex* v_i $(1 \leq i \leq n)$. *Let* G^* *be the graph obtained from* G *by deleting the edges* (v, v_i) *and adding the edges* (u, v_i) $(1 \leq i \leq s)$. *If* $x_u \geq x_v$, *then* $q_1(G) < q_1(G^*)$.

Lemma 2.11 *Let* $n \geq 11$ *and* T^k *denote the trees of order* $n-1$ *shown in Figure 2. Then*

$$\begin{aligned}\phi(K_1 \vee T^k, x) = &(x-2)^{n-5}\{x^5 - 2(n+2)x^4 + [n^2 + (k+6)n - k^2 + k + 6]x^3 - \\ &[(k+2)n^2 - (k^2 - 2k - 12)n - k^2 + k - 6]x^2 + [(k+2)n^2 - (k^2 - 9k - 2)n - \\ &8k^2 + 8k - 16]x - 4(3k-2)n + 12k^2 - 12k + 8\}.\end{aligned}$$

Proof It is easy to see that

$$Q(K_1 \vee T^k) = \begin{pmatrix} n-1 & 1 & 1 & 1 & 1 & \cdots & 1 & 1 & 1 & 1 & \cdots & 1 \\ 1 & k & 1 & 1 & 1 & \cdots & 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & n-k+1 & 0 & 0 & \cdots & 0 & 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 0 & 2 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & 0 & 2 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 0 & 0 & 0 & \cdots & 2 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 2 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 2 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 2 \end{pmatrix}.$$

It can be written as follows:

$$Q(K_1 \vee T^k) = \begin{pmatrix} (n-2)J_1 + I_1 & J_1 & J_1 & J_{1,k} & J_{1,n-k-1} \\ J_1 & kJ_1 & J_1 & J_{1,k} & 0 \\ J_1 & J_1 & (n-k+1)J_1 & 0 & J_{1,n-k-1} \\ J_{k-2,1} & J_{k-2,1} & 0 & 2I_{k-2} & 0 \\ J_{n-k-1,1} & 0 & J_{n-k-1,1} & 0 & 2I_{n-k-1} \end{pmatrix}.$$

Let $B(K_1 \vee T^k)$ be the corresponding quotient matrix of $Q(K_1 \vee T^k)$. Then

$$B(K_1 \vee T^k) = \begin{pmatrix} n-1 & 1 & 1 & k-2 & n-k-1 \\ 1 & k & 1 & k-2 & 0 \\ 1 & 1 & n-k+1 & 0 & n-k-1 \\ 1 & 1 & 0 & 2 & 0 \\ 1 & 0 & 1 & 0 & 2 \end{pmatrix}.$$

By Lemma 2.2, we have

$$\sigma(Q(K_1 \vee T^k)) = \sigma(B(K_1 \vee T^k)) \cup \{2^{[n-5]}\}. \tag{2.2}$$

By direct computing, we know the characteristic polynomial of $B(K_1 \vee T^k)$ is as follows:

$$\begin{aligned} \varphi(x) =& x^5 - 2(n+2)x^4 + [n^2 + (k+6)n - k^2 + k + 6)x^3 - [(k+2)n^2 - (k^2 - 2k- \\ & 12)n - k^2 + k - 6]x^2 + [(k+2)n^2 - (k^2 - 9k - 2)n - 8k^2 + 8k - 16]x- \\ & 4(3k-2)n + 12k^2 - 12k + 8. \end{aligned} \tag{2.3}$$

Combining (2.2) and (2.3), we have $\phi(K_1 \vee T^k, x) = (x-2)^{n-5}\varphi(x)$. □

3. The proof of Theorem 1.1

In this section, we determine all quasi-tree graphs of order n with the second largest signless

Laplacian eigenvalue greater than or equal to $n-3$.

Lemma 3.1 *Let $n \geq 11$ and $G \in \mathcal{Q}_n$. If $\Delta(G-v_0) \leq n-6$, then $q_2(G) < n-3$.*

Proof For the tree $G-v_0$ and any $u \in V(G-v_0)$ with $d(u) > 1$, we have

$$\begin{aligned} d(u)+m(u) =& d(u)+\frac{\sum_{v\in N(u)} d(v)}{d(u)} \leq d(u)+\frac{n-2}{d(u)} \\ \leq& \max\{2+\frac{n-2}{2}, \Delta(G-v_0)+\frac{n-2}{\Delta(G-v_0)}\} \\ \leq& \max\{2+\frac{n-2}{2}, n-6+\frac{n-2}{n-6}\} \\ =& n-5+\frac{4}{n-6} < n-4. \end{aligned}$$

By Lemma 2.3, we have $q_1(G-v_0) < n-4$. By Lemma 2.4, we have

$$q_2(G) \leq q_1(G-v_0)+1 < n-4+1 = n-3.$$

This completes the proof. □

Lemma 3.2 *Let $n \geq 11$ and $G \in \mathcal{Q}_n$. If $\beta(G-v_0) \geq 5$, then $q_2(G) < n-3$.*

Proof Let $\beta = \beta(G-v_0)$ and $r = \mu_1(T_\beta^{n-1})$. By Lemma 2.5, we have $\mu_1(G-v_0) \leq r$ and

$$r^3-(n-\beta+3)r^2+(3n-3\beta+1)r-n+1 = 0.$$

It follows that $r > 3$ and

$$\beta = \frac{-r^3+(n+3)r^2-(3n+1)r+n-1}{r^2-3r}.$$

If $\beta \geq 5$, then

$$r^3-(n-2)r^2+(3n-14)r-n+1 \leq 0.$$

Let $f(x) = x^3-(n-2)x^2+(3n-14)x-n+1$. Noting that $f'(x) > 0$ for $x \in [n-4, +\infty)$, we know that $f(x)$ is strictly increasing on $x \in [n-4, +\infty)$. Since $f(n-4) = n^2-11n+25 > 0$ for $n \geq 11$, it follows that $r < n-4$. By Lemma 2.6, we have

$$q_1(G-v_0) = \mu_1(G-v_0) \leq r < n-4.$$

By Lemma 2.4, we have

$$q_2(G) \leq q_1(G-v_0)+1 < n-4+1 = n-3.$$

This completes the proof. □

Lemma 3.3 *Let $n \geq 47$ and $G \in \mathcal{Q}_n$. If $2 \leq \beta(G-v_0) \leq 4$, $\Delta(G-v_0) = n-5$ or $n-4$, then $q_2(G) < n-3$.*

Proof Let T^k, $T^{r,s}$, T_1, T_2 and T_3 denote the trees of order $n-1$ shown in Figure 2, where $r = s$ means $d(v_2) = 2$ for the tree $T^{r,s}$.

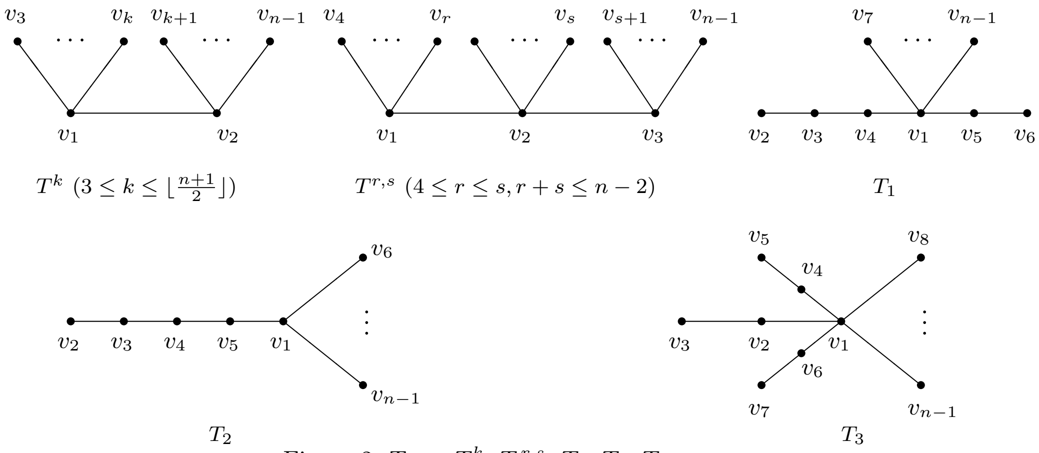

Figure 2 Trees T^k, $T^{r,s}$, T_1, T_2, T_3

Next, we distinguish five cases to show $q_2(G) < n-3$.

Case 1. $\beta(G-v_0) = 2$ and $\Delta(G-v_0) = n-4$. Then $G-v_0$ must be T^4 or $T^{4,4}$ shown in Figure 2. By Lemma 2.8, we have $q_2(G) \le q_2(K_1 \vee T^4)$ or $q_2(G) \le q_2(K_1 \vee T^{4,4})$.

By Lemma 2.11, we have $\phi(K_1 \vee T^4, x) = (x-2)^{n-5} f_1(x)$, where

$$f_1(x) = x^5 - 2(n+2)x^4 + (n^2+10n-6)x^3 - 2(3n^2+2n-9)x^2 + (6n^2+22n-112)x - 40n + 152.$$

By Lemma 2.7, we have $q_2(K_1 \vee T^4) \in [n-4, n-2]$. Therefore, $q_2(K_1 \vee T^4)$ is the second largest root of the polynomial $f_1(x)$. Taking the derivative of $f_1(x)$ with respect to x, we know that $f_1'(x) < 0$ on the interval $[n-4, n-2]$. Therefore, $f_1(x)$ is strictly decreasing on $[n-4, n-2]$. Since $f_1(n-4) = (n-24)(4n^2+24n+992) + 23032 > 0$ and $f_1(n-3) = -(n-5)(n-7)^2 < 0$, it follows that $q_2(K_1 \vee T^4) < n-3$. It follows that $q_2(G) \le q_2(K_1 \vee T^4) < n-3$.

By a similar reasoning as the proof of Lemma 2.11, we can obtain that $\phi(T^{4,4}, x) = (x-2)^{n-7} f_2(x)$, where

$$\begin{aligned} f_2(x) =& x^7 - 2(n+4)x^6 + (n^2+18n+15)x^5 - (10n^2+54n-26)x^4 + \\ & (35n^2+81n-207)x^3 - (51n^2+143n-654)x^2 + \\ & (26n^2+250n-1016)x - 160n + 560. \end{aligned}$$

By Lemma 2.7, we have $q_2(K_1 \vee T^{4,4}) \in [n-4, n-2]$. Therefore, $q_2(K_1 \vee T^{4,4})$ is the second largest root of the polynomial $f_2(x)$. Taking the derivative of $f_2(x)$ with respect to x, we know that $f_2'(x) < 0$ on the interval $[n-4, n-2]$. Therefore, $f_2(x)$ is strictly decreasing on the interval $[n-4, n-2]$. Since $f_2(n-4) = 4(n-5)(n^2-13n+41)(n-6)^2 > 0$ and $f_2(n-3) = -(n-5)^2[(n-35)(n^2+16n+675)+23404] < 0$, it follows that $q_2(K_1 \vee T^{4,4}) < n-3$. It follows that $q_2(G) \le q_2(K_1 \vee T^{4,4}) < n-3$.

Case 2. $\beta(G-v_0) = 2$ and $\Delta(G-v_0) = n-5$. Then $G-v_0$ must be T^5 or $T^{5,5}$ shown in Figure 2. By Lemma 2.8, we have $q_2(G) \le q_2(K_1 \vee T^5)$ or $q_2(G) \le q_2(K_1 \vee T^{5,5})$.

By a similar reasoning as the proof of Lemma 2.11, we can obtain that $\phi(K_1 \vee T^5, x) =$

$(x-2)^{n-5}f_3(x)$, where

$$f_3(x) = x^5 - 2(n+2)x^4 + (n^2+11n-14)x^3 - (7n^2-3n-26)x^2 + (7n^2+22n-176)x - 52n + 248.$$

By Lemma 2.7, we have $q_2(K_1 \vee T^5) \in [n-5, n-2]$. Therefore, $q_2(K_1 \vee T^5)$ is the second largest root of the polynomial $f_3(x)$. Taking the derivative of $f_3(x)$ with respect to x, we know that $f_3'(x) < 0$ on the interval $[n-5, n-2]$. Therefore, $f_3(x)$ is strictly decreasing on $[n-5, n-2]$. Since $f_3(n-5) = (n-22)(6n^2+927)+18297$ and $f_3(n-3) = -(n-22)(4n^2+16n+775) - 16229 < 0$, it follows that $q_2(K_1 \vee T^5) < n-3$. It follows that $q_2(G) \le q_2(K_1 \vee T^5) < n-3$.

By a similar reasoning as the proof of Lemma 2.11, we can obtain that $\phi(K_1 \vee T^{5,5}, x) = (x-2)^{n-7}f_4(x)$, where

$$f_4(x) = x^7 - 2(n+4)x^6 + (n^2+19n+8)x^5 - (11n^2+53n-68)x^4 + (41n^2+58n-340)x^3 - (62n^2+120n-1032)x^2 + (32n^2+296n-1632)x - 208n + 896.$$

By Lemma 2.7, we have $q_2(K_1 \vee T^{5,5}) \in [n-5, n-2]$. Therefore, $q_2(K_1 \vee T^5)$ is the second largest root of the polynomial $f_4(x)$. Taking the derivative of $f_4(x)$ with respect to x, we know that $f_4'(x) < 0$ on $[n-5, n-2]$. Therefore, $f_4(x)$ is strictly decreasing on $[n-5, n-2]$. Since $f_4(n-5) = (n-7)[(n-41)(6n^3+72n^2+4821n+188837)+7757793] > 0$ and $f_4(n-3) = -(n-5)[(n-41)(4n^3+72n^2+3733n+150155)+6160316] < 0$, it follows that $q_2(K_1 \vee T^{5,5}) < n-3$. Therefore, $q_2(G) \le q_2(K_1 \vee T^{5,5}) < n-3$.

Case 3. $\beta(G-v_0) = 3$ and $\Delta(G-v_0) = n-4$. Then $G-v_0$ must be $T^{4,n-2}$ shown in Figure 2. By Lemma 2.8, we have $q_2(G) \le q_2(K_1 \vee T^{4,n-2})$.

By a similar reasoning as the proof of Lemma 2.11, we have $\phi(K_1 \vee T^{4,n-2}, x) = (x-2)^{n-7}f_5(x)$, where

$$f_5(x) = x^7 - 2(n+4)x^6 + (n^2+18n+15)x^5 - (10n^2+54n-26)x^4 + (35n^2+80n-201)x^3 - (50n^2+156n-696)x^2 + (25n^2+280n-1160)x - 180n + 680.$$

By Lemma 2.7, we have $q_2(K_1 \vee T^{4,n-2}) \in [n-4, n-2]$. Therefore, $q_2(K_1 \vee T^{4,n-2})$ is the second largest root of the polynomial $f_5(x)$. Taking the derivative of $f_5(x)$ with respect to x, we know that $f_5'(x) < 0$ on $[n-4, n-2]$. Therefore, $f_5(x)$ is strictly decreasing on $x \in [n-4, n-2]$. Since $f_5(n-4) = 4(n-6)(n^2-11n+29)(n^2-13n+41) > 0$ and $f_5(n-3) = -(n-7)(n^2-11n+29)(n^2-11n+31) < 0$, it follows that $q_2(K_1 \vee T^{4,n-2}) < n-3$. Therefore, $q_2(G) \le q_2(K_1 \vee T^{4,n-2}) < n-3$.

Case 4. $\beta(G-v_0) = 3$ and $\Delta(G-v_0) = n-5$. Then $G-v_0 \in \{T^{4,5}, T^{4,n-3}, T_1, T_2\}$, where $T^{4,5}, T^{4,n-3}, T_1, T_2$ are shown in Figure 2. By Lemma 2.8, $q_2(G) \le q_2(K_1 \vee T^{4,5})$ or $q_2(G) \le q_2(K_1 \vee T^{4,n-3})$ or $q_2(G) \le q_2(K_1 \vee T_1)$ or $q_2(G) \le q_2(K_1 \vee T_2)$.

By a similar reasoning as the proof of Lemma 2.11, we have $q_2(K_1 \vee T^{4,5})$, $q_2(K_1 \vee T^{4,n-3})$, $q_2(K_1 \vee T_1)$, $q_2(K_1 \vee T_2)$ are the second largest root of the following polynomials $f_i(x)$ ($i =$

$6, 7, 8, 9)$, respectively,

$$f_6(x) = x^7 - 2(n+4)x^6 + (n^2+19n+8)x^5 - (11n^2+53n-68)x^4 + (41n^2+57n-334)x^3 - (61n^2+133n-1074)x^2 + (31n^2+326n-1776)x - 228n + 1016,$$

$$f_7(x) = x^7 - 2(n+4)x^6 + (n^2+19n+8)x^5 - (11n^2+53n-68)x^4 + (41n^2+56n-326)x^3 - (60n^2+148n-1130)x^2 + (30n^2+358n-1968)x - 248n + 1176,$$

$$f_8(x) = x^8 - 2(n+5)x^7 + (n^2+23n+25)x^6 - (13n^2+93n-50)x^5 + (64n^2+170n-468)x^4 - (148n^2+260n-1768)x^3 + (160n^2+649n-4167)x^2 - (65n^2+977n-5000)x + 504n - 2248,$$

$$f_9(x) = x^6 - 2(n+3)x^5 + (n^2+15n-3)x^4 - (9n^2+25n-62)x^3 + (24n^2+11n-215)x^2 - (17n^2+105n-632)x + 120n - 520.$$

By Lemma 2.7, we have $q_2(K_1 \vee T^{4,5}) \in [n-5, n-2]$. Noting that $n \geq 41$, by derivative we know that $f_6'(x) < 0$ for $x \in [n-5, n-2]$. Therefore, $f_6(x)$ is strictly decreasing on $x \in [n-5, n-2]$. Since $f_6(n-5) = (n-41)(6n^4+30n^3+4314n^2+155034n+6433145)+263651816 > 0$ and $f_6(n-3) = -(n-7)[(n-41)(4n^3+80n^2+3938n+159180)+6529319] < 0$, it follows that $q_2(K_1 \vee T^{4,5}) < n-3$. If $d_G(v_0) < n-1$ and $G - v_0 = T^{4,5}$, by Lemma 2.8, we have $q_2(G) \leq q_2(K_1 \vee T^{4,5}) < n-3$.

By Lemma 2.7, we have $q_2(K_1 \vee T^{4,n-3}) \in [n-5, n-2]$. Noting that $n \geq 41$, by derivative we know that $f_7'(x) < 0$ for $x \in [n-5, n-2]$. Therefore, $f_7(x)$ is strictly decreasing on $x \in [n-5, n-2]$. Since $f_7(n-5) = (n-7)[(n-41)(6n^3+72n^2+4815n+188689)+7751336] > 0$ and $f_7(n-3) = -(n-41)(4n^4+52n^3+3383n^2+131728n+5420269) - 222209432 < 0$, it follows that $q_2(K_1 \vee T^{4,n-3}) < n-3$. If $d_G(v_0) < n-1$ and $G - v_0 = T^{4,n-3}$, by Lemma 2.8, we have $q_2(G) \leq q_2(K_1 \vee T^{4,n-3}) < n-3$.

By Lemma 2.7, we have $q_2(K_1 \vee T_1) \in [n-5, n-2]$. Noting that $n \geq 47$, by derivative we know that $f_8'(x) < 0$ for $x \in [n-5, n-2]$. Therefore, $f_8(x)$ is strictly decreasing on $x \in [n-5, n-2]$. Since $f_8(n-5) = (n-7)[(n-47)(6n^4+66n^3+6192n^2+269066n+12723617)+597901238] > 0$ and $f_8(n-3) = -(n-7)[(n-47)(4n^4+84n^3+5030n^2+230784n+10861453)+510473164] < 0$, it follows that $q_2(K_1 \vee T_1) < n-3$. If $d_G(v_0) < n-1$ and $G - v_0 = T_1$, by Lemma 2.8, we have $q_2(G) \leq q_2(K_1 \vee T_1) < n-3$.

By Lemma 2.7, we have $q_2(K_1 \vee T_2) \in [n-5, n-2]$. Noting that $n \geq 34$, by derivative we know that $f_9'(x) < 0$ for $x \in [n-5, n-2]$. Therefore, $f_9(x)$ is strictly decreasing on $x \in [n-5, n-2]$. Since $f_9(n-5) = (n-34)(6n^3+30n^2+2895n+89532)+3059783 > 0$ and $f_9(n-3) = -(n-7)(2n-11)(2n^2-21n+53) < 0$, it follows that $q_2(K_1 \vee T_2) < n-3$. If $d_G(v_0) < n-1$ and $G - v_0 = T_2$, by Lemma 2.8, we have $q_2(G) \leq q_2(K_1 \vee T_2) < n-3$.

Case 5. $\beta(G - v_0) = 4$ and $\Delta(G - v_0) = n-5$. Then $G - v_0$ must be T_3 shown in Figure 2. It is easy to see that $q_2(K_1 \vee T_3)$ is the second largest root of the following polynomial,

$$f_{10}(x) = x^5 - 2(n+1)x^4 + (n^2+7n-10)x^3 - (5n^2-n-20)x^2 + (5n^2+20n-136)x - 44n + 208.$$

By Lemma 2.7, we have $q_2(K_1 \vee T_3) \in [n-5, n-2]$. Noting that $n \geq 27$, by derivative we know that $f'_{10}(x) < 0$ for $x \in [n-5, n-2]$. Therefore, $f_{10}(x)$ is strictly decreasing on $x \in [n-5, n-2]$. Since $f_{10}(n-5) = (n-27)(6n^2+42n+1929)+50346 > 0$ and $f_{10}(n-3) = -(n-27)(4n^2+44n+1539)-40892 < 0$, it follows that $q_2(K_1 \vee T_3) < n-3$. If $d_G(v_0) < n-1$ and $G - v_0 = T_3$, by Lemma 2.8, we have $q_2(G) \leq q_2(K_1 \vee T_3) < n-3$.

Combining the above arguments, we have $q_2(G) < n-3$. The proof is completed. □

Lemma 3.4 *Let $n \geq 47$ and $G \in \mathcal{Q}_n$. If $\Delta(G - v_0) = n-2$ or $n-3$, then*

(i) $q_2(G) < n-3$ for $G \in \mathcal{Q}_n \setminus \{H_1, H_2^2, H_3, H_4^2, H_5, H_6^4, H_7, H_8^4, H_9, H_{11}, H_{13}, H_{15}\}$, where $H_1, H_2^2, H_3, H_4^2, H_5, H_6^4, H_7, H_8^4, H_9, H_{11}, H_{13}$, and H_{15} are shown in Figure 1;

(ii) $n-3 \leq q_2(G) < n-\frac{41}{16}$ for $G \in \{H_4^2, H_6^4, H_7, H_8^4, H_9, H_{11}, H_{13}, H_{15}\}$ with equality if and only if $G = H_{13}$ or H_{15};

(iii) $n-\frac{41}{16} < q_2(G) < n-\frac{5}{2}$ for $G \in \{H_2^2, H_5\}$;

(iv) $q_2(H_1) = q_2(H_3) = n-2$.

Proof In the case when $\Delta(G - v_0) = n-2$, $G - v_0$ must be the $K_{1,n-2}$ and $\beta(G - v_0)$=1. It follows that G must be one of H_1, H_2^k $(2 \leq k \leq n-1)$, H_3 and H_4^k $(2 \leq k \leq n-2)$ shown in Figure 1. In the case when $\Delta(G - v_0) = n-3$, $G - v_0$ must be the T^3 shown in Figure 2 and $\beta(G - v_0)$=2. It follows that G must be one of H_i $(i = 5, 7, 9, 11, 13, 15, 16)$ and H_i^k $(i = 6, 8, 10, 12, 14)$ shown in Figure 1. By a similar reasoning as the proof of Lemma 2.11, we have

$$(1)\ \phi(H_2^k, x) = (x-1)^{k-1}(x-2)^{n-k-2}[x^3 - (2n-k+1)x^2 + (n^2 - nk + n)x - 4n + 4k + 4],$$

$$(2)\ \phi(H_4^k, x) = x(x-1)^{k-2}(x-2)^{n-k-2}[x^3 - (2n-k)x^2 + (n^2 - kn + n - 2)x - n^2 + kn + n],$$

$$(3)\ \phi(H_5, x) = (x-2)^{n-5}[x^5 - 2(n+2)x^4 + (n^2+9n)x^3 - (5n^2+9n-12)x^2 + (5n^2+20n-64)x - 28n + 80],$$

$$(4)\ \phi(H_6^k, x) = (x-1)^{k-4}(x-2)^{n-k-1}[x^5 - (2n-k+8)x^4 + (n^2 - kn + 13n - 5k + 19)x^3 - (5n^2 - 5kn + 27n - 8k + 24)x^2 + (4n^2 - 4kn + 40n - 24k + 24)x - 24n + 24k - 24,$$

$$(5)\ \phi(H_7, x) = (x-2)^{n-5}[x^5 - 2(n+1)x^4 + (n^2+7n-9)x^3 - (5n^2-5n-6)x^2 + (5n^2-10n-4)x - 8n + 24],$$

$$(6)\ \phi(H_8^k, x) = (x-1)^{k-3}(x-2)^{n-k-2}[x^5 - (2n-k+6)x^4 + (n^2 - kn + 11n - 4k + 6)x^3 - (5n^2 - 5kn + 13n)x^2 + (4n^2 - 4kn + 12n - 4k + 4)x - 8n + 8k - 8,$$

$$(7)\ \phi(H_9, x) = (x-2)^{n-5}[x^2 - (n-2)x + n - 4][x^3 - (n+4)x^2 + (3n+8)x - 16],$$

$$(8)\ \phi(H_{10}^k, x) = (x-1)^{k-4}(x-2)^{n-k-2}[x^6 - (2n-k+6)x^5 + (n^2 - kn + 11n$$

$$\begin{aligned}
&4k+10)x^4-(5n^2-5kn+23n-6k-2)x^3+(7n^2-7kn+35n-\\
&18k-26)x^2-(3n^2-3kn+37n-32k-32)x+16n-16k-16],\\
(9)\ &\phi(H_{11},x)=(x-2)^{n-5}[x^2-(n-2)x+n-4][x^3-(n+2)x^2+(3n-2)x-4],\\
(10)\ &\phi(H_{12}^k,x)=(x-1)^{k-4}(x-2)^{n-k-2}[x^6-(2n-k+4)x^5+(n^2-kn+9n-3k-\\
&1)x^4-(5n^2-5kn+9n+2k-16)x^3+(7n^2-7kn+n+5k-15)x^2-\\
&(3n^2-3kn+3n-4k-4)x+4n-4k-4],\\
(11)\ &\phi(H_{13},x)=(x-2)^{n-5}(x-n+3)[x^4-(n+5)x^3+(4n+10)x^2-(2n+20)x+8],\\
(12)\ &\phi(H_{14}^k,x)=(x-1)^{k-4}(x-2)^{n-k-2}[x^6-(2n-k+6)x^5+(n^2-kn+11n-4k+\\
&9)x^4-(5n^2-5kn+21n-5k)x^3+(6n^2-6kn+32n-17k-11)x^2-\\
&(2n^2-2kn+28n-24k-4)x+8n-8k],\\
(13)\ &\phi(H_{15},x)=x(x-2)^{n-5}(x-n+3)[x^3-(n+3)x^2+(4n-2)x-2n],\\
(14)\ &\phi(H_{16},x)=(x-2)^{n-5}[x^5-2nx^4+(n^2+3n-6)x^3-(3n^2-3n-12)x^2+\\
&(n^2+10n-48)x-4n+16].
\end{aligned}$$

By a similar reasoning as the proof of Lemma 3.3, we can obtain the results as follows:

$$\begin{aligned}
n-\frac{5}{2} &>q_2(H_2^2)>n-\frac{41}{16}>n-3>q_2(H_2^k)\ \text{ for } k\geq 3;\\
n-\frac{41}{16} &>q_2(H_4^2)>n-3>q_2(H_4^k)\ \text{ for } k\geq 3;\\
n-\frac{5}{2} &>q_2(H_5)>n-\frac{41}{16}>n-3;\\
n-\frac{41}{16} &>q_2(H_6^4)>n-3>q_2(H_6^k)\ \text{ for } k\geq 5;\\
n-\frac{41}{16} &>q_2(H_7)>n-3;\\
n-\frac{41}{16} &>q_2(H_8^4)>n-3>q_2(H_8^k)\ \text{ for } k\geq 5;\\
n-\frac{41}{16} &>q_2(H_9)=q_2(H_{11})>n-3;
\end{aligned}$$

$q_2(H_{13})=q_2(H_{15})=n-3$; $q_2(H_{12}^k)\leq q_2(H_{10}^k)<n-3$ for $k\geq 4$; $q_2(H_{14}^k)<n-3$ for $k\geq 4$; $q_2(H_{16})<n-3$. Combining the above arguments, we have the proof of (i), (ii) and (iii).

By a similar reasoning as the proof of Lemma 2.11, we have

$$\begin{aligned}
\phi(H_1,x)&=(x-n+2)(x-2)^{n-3}[x^2-(n+2)x+4],\\
\phi(H_3,x)&=x(x-2)^{n-3}(x-n)(x-n+2).
\end{aligned}$$

Thus $q_2(H_1)=q_2(H_3)=n-2$. This completes the proof. $\square$

Proof of Theorem 1.1 For $G\in\mathcal{Q}_n\setminus\{H_1,H_2^2,H_3,H_4^2,H_5,H_6^4,H_7,H_8^4,H_9,H_{11},\ H_{13},H_{15}\}$, by Lemmas 3.1–3.4, we have $q_2(G)<n-3$. For $G\in\{H_4^2,H_6^4,H_7,H_8^4,\ H_9,H_{11},H_{13},H_{15}\}$, by Lemma 3.4, we have $n-3\leq q_2(G)<n-\frac{41}{16}$ and the equality holds if and only if $G=H_{13}$ or H_{15}. For $G\in\{H_2^2,H_5\}$, by Lemma 3.4, we have $n-\frac{41}{16}<q_2(G)<n-\frac{5}{2}$. For $G=H_1$ or H_3,

we have $q_2(H_1) = q_2(H_3) = n - 2$.

Now we give the ordering of the graphs in $\{H_2^2, H_5\}$ by the second largest Q-eigenvalue. By the proof of Lemma 3.4, we have

$$\phi(H_2^2, x) = (x-2)^{n-5} f(x), \quad \phi(H_5, x) = (x-2)^{n-5} g(x),$$

where

$$\begin{aligned} f(x) =& x^5 - 2(n+1)x^4 + (n^2+5n-1)x^3 - (3n^2+5n-14)x^2 + \\ & (2n^2+10n-36)x - 8n + 24. \\ g(x) =& x^5 - 2(n+2)x^4 + (n^2+9n)x^3 - (5n^2+9n-12)x^2 + \\ & (5n^2+20n-64)x - 28n + 80. \end{aligned}$$

Obviously, $q_2(H_2^2)$ and $q_2(H_5)$ are the second largest root of $f(x)$ and $g(x)$, respectively. Let $\psi(x) = f(x) - g(x) = 2x^4 - (4n+1)x^3 + (2n^2+4n+2)x^2 - (3n^2+10n-28)x + 20n - 56$, and α denote the second largest root of $\psi(x)$. Since $\psi(0) = 2n - 56 > 0$, $\psi(1) = -(n-5)^2 < 0$, $\psi(n-3) = 4n^2 - 33n + 67 > 0$, $\psi(n - \frac{5}{2}) = -\frac{1}{4}(n^2 - 27n + 79) < 0$ and $\psi(n+2) = 4n^2 + 72n + 32 > 0$ for $n \geq 47$, it follows that $n - 3 < \alpha < n - \frac{5}{2}$.

It is easy to see that $f(x) = \frac{1}{4}(2x-3)\psi(x) + r(x)$ and $g(x) = \frac{1}{4}(2x-7)\psi(x) + r(x)$, where $r(x) = -\frac{11}{4}x^3 + (3n + \frac{3}{2})x^2 - (\frac{1}{4}n^2 + \frac{15}{2}n - 13)x + 7n - 18$. By derivative, we know that $r(x)$ is strictly decreasing on $[n-3, n-\frac{5}{2}]$. Since

$$f(\alpha) = g(\alpha) = r(\alpha) \geq r(n - \frac{5}{2}) = \frac{1}{32}(8n^2 - 50n + 59) > 0$$

for $n \geq 47$, it follows that $q_2(H_2^2)$, $q_2(H_5) \in (\alpha, n - \frac{5}{2})$. Moreover, since $\psi(x)$ is strictly decreasing in the interval $[n-3, n-\frac{5}{2}]$, it follows that $\psi(x) < \psi(\alpha) = 0$ when $\alpha < x < n - \frac{5}{2}$. This implies that $f(x) < g(x)$ when $\alpha < x < n - \frac{5}{2}$. Thus, $q_2(H_5) > q_2(H_2^2)$.

Combining the above arguments, we have

$$q_2(G) < n - \frac{41}{16} < q_2(H_2^2) < q_2(H_5) < n - \frac{5}{2} < q_2(H_3) = q_2(H_1) = n - 2.$$

The proof is completed. □

4. The proof of Theorem 1.2

We consider the following three cases.

Case 1. $\Delta(G) \leq n - 2$. We will show that $S_2(G) < 2n - \frac{3}{2}$. By Lemma 2.9, we have

$$\begin{aligned} q_1(G) <& \max\{2 + \frac{d(v_0) + n - 3}{2}, \Delta(G) + \frac{d(v_0) + n - 3}{\Delta(G)}\} + 1 \\ \leq& \max\{2 + \frac{n - 2 + n - 3}{2}, \Delta(G) + \frac{n - 2 + n - 3}{\Delta(G)}\} + 1 \\ \leq& \max\{2 + \frac{2n-5}{2}, n - 2 + \frac{2n-5}{n-2}\} + 1 < n + 1. \end{aligned}$$

By Theorem 1.1, we have $q_2(G) < n - \frac{5}{2}$ except for H_3. Thus $S_2(G) < 2n - \frac{3}{2}$ except for H_3.

For H_3, by the proof of Lemma 3.4, we have

$$\phi(H_3, x) = x(x-2)^{n-3}(x-n)(x-n+2).$$

It follows that $S_2(H_3) = n + n - 2 = 2n - 2 < 2n - \frac{3}{2}$.

Case 2. There exists $v \in V(G - v_0)$ such that $\Delta(v) = n - 1$. Then $G - v_0 = K_{1,n-2}$ and $G = H_1$ or H_2^k $(2 \le k \le n-1)$. We will show that $S_2(G) < 2n - \frac{5}{4} < S_2(H_2^2) < S_2(H_1)$ for $G \in \mathcal{Q}_n \setminus \{H_1, H_2^2\}$. For $k \ge 4$, by Theorem 1.1 and Lemma 2.8, we have

$$q_2(H_1) > q_2(H_2^2) > n - 3 > q_2(H_2^3) \ge q_2(H_2^k);$$

by Lemma 2.8, we have $q_1(H_1) > q_1(H_2^2) > q_1(H_2^3) > q_1(H_2^k)$. These imply that $S_2(H_1) > S_2(H_2^2) > S_2(H_2^3) > S_2(H_2^k)$ for $k \ge 4$.

By the proof of Lemma 3.4, we know that $q_1(H_2^2)$ and $q_2(H_2^2)$ are the two largest roots of the polynomial

$$h(x) = x^3 - (2n-1)x^2 + (n^2 - n)x - 4n + 12.$$

Let q be the other root of $h(x)$. By derivative, we know that $h'(x) > 0$ for $x \in [0, \frac{1}{4}]$. Thus $h(x)$ is strictly increasing in the interval $[0, \frac{1}{4}]$. Since $h(0) = -4n+12 < 0$ and $h(\frac{1}{4}) = \frac{1}{4}n^2 - \frac{35}{8}n + \frac{773}{64} > 0$ for $n \ge 47$, it follows that $q \in (0, \frac{1}{4})$. By the Vieta Theorem, we have

$$S_2(H_2^2) = q_1(H_2^2) + q_2(H_2^2) = 2n - 1 - q > 2n - \frac{5}{4}.$$

By the proof of Lemma 3.4, we know that $q_1(H_2^3)$ and $q_2(H_2^3)$ are the two largest roots of the polynomial

$$p(x) = x^3 - (2n-2)x^2 + (n^2 - 2n)x - 4n + 16.$$

Let q' be the other root of $p(x)$. Since $q' \ge 0$, by the Vieta Theorem, we have

$$S_2(H_2^3) = q_1(H_2^3) + q_2(H_2^3) = 2n - 2 - q' \le 2n - 2 < 2n - \frac{5}{4}.$$

From the above arguments, we have $S_2(G) < 2n - \frac{5}{4} < S_2(H_2^2) < S_2(H_1)$ for $G \in \mathcal{Q}_n \setminus \{H_1, H_2^2\}$.

Case 3. $d(v_0) = n - 1$. Then $G = K_1 \vee T$, where T is a tree of order $n - 1$. We will show $S_2(G) < 2n - \frac{5}{4} < S_2(H_5) < S_2(H_1)$ for $G \in \mathcal{Q}_n \setminus \{H_1, H_5\}$. Employing Lemma 2.10 to vertices v_1 and v_3 of H_5, we have $q_1(H_5) < q_1(H_1)$. For $G \in \mathcal{Q}_n \setminus \{H_1, H_5\}$, employing Lemma 2.10 repeatedly, we can prove $q_1(G) < q_1(H_5) < q_1(H_1)$. By Theorem 1.1, we have $q_2(G) < n - 3 < q_2(H_5) < q_2(H_1)$ for $G \in \mathcal{Q}_n \setminus \{H_1, H_5\}$. These imply that $S_2(G) < S_2(H_5) < S_2(H_1)$ for $G \in \mathcal{Q}_n \setminus \{H_1, H_5\}$.

Now we show that $S_2(G) < 2n - \frac{5}{4}$ for $G \in \mathcal{Q}_n \setminus \{H_1, H_5\}$. By the proof of Lemma 3.4, we have $\phi(H_5, x) = (x-2)^{n-5}u(x)$, where

$$u(x) = x^5 - 2(n+2)x^4 + (n^2 + 9n)x^3 - (5n^2 + 9n - 12)x^2 + (5n^2 + 20n - 64)x - 28n + 80.$$

It is easy to see that $q_1(H_5)$ and $q_2(H_5)$ are the two largest roots of $u(x)$.

By derivative, we know that $u(x)$ is strictly increasing on $[n,+\infty)$. Since $u(n)=-4n(n-47)(n+39)-7424n+80<0$ and $u(n+\frac{7}{4})=\frac{1}{1024}[n(n-47)(832n+58768)+2708908n-16745]>0$ for $n\geq 47$, it follows that $q_1(H_5)<n+\frac{7}{4}$. Therefore

$$S_2(G)=q_1(G)+q_2(G)<n+\frac{7}{4}+n-3<2n-\frac{5}{4}.$$

Next we show $S_2(H_5)>S_2(H_2^2)>2n-\frac{5}{4}$. From the proof of Theorem 1.1, we know that $q_1(H_2^2)$ and $q_1(H_5)$ are the largest roots of $f(x)$ and $g(x)$, respectively. By a similar reasoning as the proof of Theorem 1.1, we have $q_1(H_5)>q_1(H_2^2)$.

By Theorem 1.1, we have $q_2(H_5)>q_2(H_2^2)$. Thus $S_2(H_5)>S_2(H_2^2)>2n-\frac{5}{4}$.

Combining the above arguments, we have

$$S_2(G)<2n-\frac{5}{4}<S_2(H_2^2)<S_2(H_5)<S_2(H_1).$$

This completes the proof. □

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