Maximizing the signless Laplacian spectral radius of graphs with given diameter or cut vertices

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Maximizing the signless Laplacian spectral radius of graphs with given diameter or cut vertices

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The signless Laplacian matrix of a graph is defined to be the sum of its adjacency matrix and degree matrix. Let $G_{d}^{n}$ be the set of all the connected graphs of order $n$ and diameter $d$ and $G_{n,k}$ the set of all connected graphs with order $n$ and $k$ cut vertices. In this article, we determine the graphs that have the maximal signless Laplacian spectral radius and give the upper bounds of graphs in these two sets.

**Keywords:** adjacency matrix; signless Laplacian; diameter; cut vertices; spectral radius

**AMS Subject Classification:** 05C50

1. Introduction

All graphs considered here are simple. For a graph $G$, let $M$ be a responding graph matrix defined in a prescribed way. The $M$-spectrum of $G$ is a multiset consisting of the eigenvalues of its graph matrix $M$. The $M$-spectral radius (or $M$-index) of $G$ is the largest eigenvalue of its graph matrix $M$. It is well-known that there are several graph matrices two of which named adjacency matrix $A(G)$ and Laplacian matrix $L(G) = D(G) - A(G)$ where $D(G)$ is a diagonal matrix of vertices degrees, are investigated extensively, and the other one named signless Laplacian $Q(G) = A(G) + D(G)$.

Recently, Cvetković et al. [6] intended to build a spectral theory for the signless Laplacian matrices (see [6–9,18] for more results). For this purpose, in this article we will focus our attention on $Q(G)$-spectrum of a graph $G$.

Brualdi and Solheid [4] posed the following problem concerning the spectral radius of graphs:

Given a set $\mathcal{S}$ of graphs, find an upper bound for the spectral radius of graphs in $\mathcal{S}$ and characterize the graphs in which the maximal spectral radius is attained.

Let us call such a graph the maximal graph of $\mathcal{S}$. From then on, this problem has drawn much attention, and some important results have been obtained by many researchers. For the $A(G)$-index of graphs, let the set $\mathcal{S}_{A}$ be \{size, order and size,
diameter, cut vertices cut edges, chromatic number}, then the maximal graph with one of the conditions given in $\mathcal{S}_L$ are studied in [1–3, 5, 10–12, 14–17]. For the $L(G)$-index, let the set $\mathcal{S}_L$ be \{maximal degree, cut edges, diameter\}, the maximal (bipartite) graphs with one of the conditions given in $\mathcal{S}_L$ are investigated in [19–21]. For the $Q$-index, as far as we know, the only result is that Zhai et al. [20] determined the maximal bipartite graphs with given diameter. In this article, for the $Q$-index we will determine the general maximal graphs with given diameter and the graphs with cut vertices and give the upper bounds for $Q$-index. We shall see that the methods in this article can be also extended to the $A(G)$-spectrum, which can be applied to give a new proof of Berman and Zhang’s result [2] and van Dam’s [17] result (see also [12]).

Now we introduce some notation and terminology. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where its order and size are $|V(G)| = n(G) = n$ and $|E(G)| = m(G) = m$, respectively. For $S \subseteq V(G)$, let $G[S]$ be the induced subgraph by $S$, and $E(S, V(G)\setminus S)$ the set of all the edges with one end-vertex in $S$ and the other in $V(G)\setminus S$. Let $N_G(v)$ denote the set of vertices adjacent to the vertex $v$ in $G$ and $d_v$ the degree of $v$. As usual, $P_n$ and $C_n$, respectively, denote the path and the cycle. By $K_{1,n-1}$ and $K_n$ we denote, respectively, the star and the complete graph of order $n$.

Since $Q(G)$ is positive semidefinite and symmetric, we denote the eigenvalues of $Q(G)$ in non-increasing order by $q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G) \geq 0$, where $q_1(G)$ is usually called the $Q$-index of $G$ and is denoted by $\varrho(G) = \varrho$. Moreover, since $Q(G)$ is non-negative, the eigenvector associated with $\varrho(G)$ can be taken to be non-negative. In addition, if $G$ is connected (i.e. if $Q(G)$ is irreducible), then $\varrho(G)$ is of multiplicity one and its corresponding eigenvector can be taken to be positive. Such an eigenvector is called the $Q$-Perron eigenvector of $G$, which is denoted by $x = (x_1, x_2, \ldots, x_n)^T$, where $x_i$ corresponds to the vertex $v_i$ ($1 \leq i \leq n$). Hence, we have

$$\varrho - d_i)x_i = \sum_{j \neq i} x_j \quad (i = 1, 2, \ldots, n),$$

where the summation is over all neighbors $j$ of the vertex $i$. As a matter of fact, (1) is the eigenvalue equation for the $i$-th vertex (associated with the $Q$-index).

This article is organized as follows: In Section 2, some useful results will be introduced. In Section 3, the maximal graphs with order $n$ and diameter $d$ will be determined. In Section 4, the maximal graphs with order $n$ and $k$ cut vertices will be determined.

## 2. Basic results

Applying the Perron–Frobenius theory of non-negative matrices we have the following lemma.

**Lemma 2.1** Let $H$ be a proper subgraph of a connected graph $G$. Then $\varrho(H) < \varrho(G)$.

**Lemma 2.2** [6] Let $G$ be a graph with maximal degree $\Delta$ and minimal degree $\delta$. Then

$$2\delta \leq \varrho(G) \leq 2\Delta.$$
LEMMA 2.3 [6] Let $G$ be a graph. Then the following statements hold:

(i) $\rho(G) = 0$ if and only if $G$ has no edges;
(ii) $0 < \rho(G) < 4$ if and only if all components of $G$ are paths;
(iii) For a connected graph $G$, we have $\rho(G) = 4$ if and only if $G$ is a cycle $C_n$ or $K_{1,3}$.

Let $e = st$ and $f = uv$ be two edges of a graph $G$, and assume that the vertices $s$ and $v$, and $t$ and $u$ are non-adjacent. A local switching (with respect to $e$ and $f$) consists of the deletion of edges $e$ and $f$, followed by the addition of edges $e' = sv$ and $f' = tu$.

LEMMA 2.4. [6] Let $H$ be a graph obtained from a connected graph $G$ of order $n$ by a local switching, as given above. Let $x = (x_1, x_2, \ldots, x_n)^T$ be the $Q$-Perron eigenvector of $G$. If $(x_s - x_u)(x_v - x_t) \geq 0$, then $\rho(H) \geq \rho(G)$, with equality if and only if $x_s = x_u$ and $x_v = x_t$.

LEMMA 2.5. [13] Let $G$ be a connected graph and $\rho(G)$ be the spectral radius of $Q(G)$. Let $u, v$ be two vertices of $G$. 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 $Q$-Perron eigenvector. Let $H$ be the graph obtained from $G$ by deleting the edges $vv_i$ and adding the edges $uv_i$ ($1 \leq i \leq s$). If $x_u \geq x_v$, then $\rho(G) < \rho(H)$.

Let $G_{s,t}$ be the graph obtained from a non-trivial connected graph $H$ by attaching pendant paths $P_s$ and $P_t$ at some vertex $u$ in $V(H)$. We, for convenience, write $G_{s,t} = H_u + P_s + P_t$, where $P_s = x_s x_{s-1} \cdots x_2 x_1$, $P_t = y_t y_{t-1} \cdots y_2 y_1$ and $u$ is called the coalescent vertex (Figure 1). Given $H$ and constant $a = s + t$, let $\mathcal{G}_{s,t} = \{G_{s,t} \mid G_{s,t} = H_u + P_s + P_t, s + t = a, u \in V(H)\}$ be the set of all the graphs $G_{s,t}$. Now we pose the following question:

Among all the graphs in the set $\mathcal{G}_{s,t}$, which graph $G_{s,t}$ has the maximal $Q$-index?

Next, we will give a necessary condition for the above problem. Note, any graph $G_{s,t} \in \mathcal{G}_{s,t}$ cannot be a path by the choice of graph $H$. So, by Lemma 2.3 we have the following facts.

**Fact 1** For any graph $G_{s,t} \in \mathcal{G}_{s,t}$, $\rho(G_{s,t}) \geq 4$, and for the coalescent vertex $u$, $d_{G_{s,t}}(u) \geq 3$.

Let $\rho = \rho(G_{s,t})$ and $x$ be the corresponding $Q$-Perron eigenvector whose entries are labelled the same as the vertices $x_i$ and $y_j$ at $P_s$ and $P_t$ (Figure 1).

![Figure 1. $G_{s,t} = H_u + P_s + P_t$.](attachment:image.png)
From (1) it follows that

\[
\begin{align*}
\frac{x_2}{x_1} &= \varrho - 1 \\
\frac{x_3}{x_2} &= \varrho - 2 - \frac{1}{\varrho - 1} \\
\frac{x_4}{x_3} &= \varrho - 2 - \frac{1}{\varrho - 2 - \frac{1}{\varrho - 1}} \\
&\quad \vdots \\
\frac{x_s}{x_{s-1}} &= \varrho - 2 - \frac{1}{\frac{x_{s-1}}{x_{s-2}}} \\
\frac{x_u}{x_s} &= \varrho - 2 - \frac{1}{\frac{x_s}{x_{s-1}}} \\
\end{align*}
\]

and

\[
\begin{align*}
\frac{y_2}{y_1} &= \varrho - 1 \\
\frac{y_3}{y_2} &= \varrho - 2 - \frac{1}{\varrho - 1} \\
\frac{y_4}{y_3} &= \varrho - 2 - \frac{1}{\varrho - 2 - \frac{1}{\varrho - 1}} \\
&\quad \vdots \\
\frac{y_t}{y_{t-1}} &= \varrho - 2 - \frac{1}{\frac{y_{t-1}}{y_{t-2}}} \\
\frac{y_u}{y_t} &= \varrho - 2 - \frac{1}{\frac{y_t}{y_{t-1}}} \\
\end{align*}
\]

(2)

Let \( \{a_i = \frac{x_{i+1}}{x_i} \mid i = 1, 2, \ldots, s \} \) and \( \{b_i = \frac{y_{i+1}}{y_i} \mid i = 1, 2, \ldots, t \} \). By simple observation, we obtain the following facts from (2) and Fact 1.

**Fact 2** \( \varrho > a_i, b_j > 1 \). In addition, \( a_i = b_i \) for \( i = 1, 2, \ldots, \min \{s, t\} \).

**Fact 3** The sequences \( \{a_i \mid i = 1, 2, \ldots, s\} \) and \( \{b_i \mid i = 1, 2, \ldots, t\} \) are decreasing.

**Proof** By induction on \( i \) we prove \( a_i > a_{i+1} \), where \( i = 1, 2, \ldots, s \). For \( i = 1 \), we have \( a_1 - a_2 = 1 + \frac{1}{\varrho - 1} \), and so \( a_1 > a_2 \) by \( \varrho \geq 4 \). Suppose that the result is true for \( i - 1 \), i.e., \( a_{i-1} > a_i \). For \( i \), we get \( a_i - a_{i+1} = \frac{1}{a_i} - \frac{1}{a_{i-1}} \), and thus \( a_i > a_{i+1} \) by the inductive assumption. The same argument can be applied to show that \( \{b_i \mid i = 1, 2, \ldots, t\} \) is decreased.

**Lemma 2.6** Let \( G_{s,t}^* \subseteq \mathcal{G}_{s,t} \) be the maximal graph. If \( t \geq s + 2 \), then

\[ x_u > y_I > \cdots > y_{s+1} > x_s > y_s > x_{s-1} > \cdots > y_3 > x_2 > y_2 > x_1 > y_1. \]

**Proof** From Lemma 2.5, we first claim that \( x_u > x_i, y_j \) for \( 1 \leq i \leq s \) and \( 1 \leq j \leq t \). By Fact 1 we have,

\[
\frac{x_{i+1}}{x_i} = \frac{y_{i+1}}{y_I}, \quad \text{where } i = 1, 2, \ldots, s.
\]

Taking \( i = s \), we have \( \frac{x_s}{x_1} = \frac{x_{s+1}}{y_I} \) and so \( \frac{y_I}{x_1} = \frac{x_{s+1}}{x_s} \). Since \( x_u > y_{s+1} \), then \( x_1 > y_1 \). If \( x_1 \geq y_2 \), by resetting \( P_s = x_u x_s \cdots x_1 y_1 \) and \( P_I = x_u y_I \cdots y_3 y_2 \) we know that the \( Q \)-index increases by Lemma 2.5, and thus \( y_2 > x_1 \). Again, taking \( i = 1 \) in (3) we get \( \frac{x_1}{x_s} = \frac{y_1}{y_I} \), and so \( x_2 > y_2 \). By Fact 2 we have \( x_{i+1} > x_i \) and \( y_{i+1} > y_I \). If \( y_3 \leq x_2 \), then \( (x_2 - y_3) (y_2 - x_1) \geq 0 \). By setting

\[ G = G_{s,t}^* - x_1 x_2 - y_2 y_3 + x_1 y_3 + x_2 y_2, \]

we get, by Lemma 2.4, that \( G \in \mathcal{G}_{s,t} \) and \( \varrho(G) > \varrho(G^*) \), which contradicts our assumption. Hence \( y_3 > x_2 > y_2 > x_1 \).

By induction on \( i \) we will show \( y_{i+2} > x_{i+1} > y_{i+1} > x_i \), where \( i \leq s - 1 \). For \( i = 1 \), we have finished. Suppose that it is true for \( i = k - 1 \), i.e., \( y_{k+1} > x_k > y_k > x_{k-1} \).
For $i = k$, since $\frac{x_{k+1}}{x_k} = \frac{y_{k+1}}{y_k}$, then $x_{k+1} > y_{k+1}$, if $y_{k+2} \leq x_{k+1}$, then $(x_{k+1} - y_{k+2}) (y_{k+1} - x_k) \geq 0$. By setting

$$G = G^*_s - x_k y_{k+1} - y_{k+1} y_{k+2} + x_k y_{k+2} + x_{k+1} y_{k+1},$$

we obtain, by Lemma 2.4 again, that $G \in \mathcal{G}_{s,t}$ and $\varphi(G) > \varphi(G^*)$, which contradicts our assumption. Hence, we get $y_{k+2} > x_{k+1} > y_{k+1} > x_k$.

**Theorem 2.1** Let $G^*_s, t \in \mathcal{G}_{s,t}$ be the maximal graph. Then $|s - t| \leq 1$.

**Proof** Fact 1 indicates that $\varphi(G^*_s, t) \geq 4$ and $d_{\mathcal{G}_{s,t}}(u) \geq 3$, where $u$ is the coalescent vertex. Suppose that $s + t \leq 2$. We conclude that $s = t = 1$. Otherwise, without loss of generality, set $t > s$ and so $t = 2$, $s = 0$. Since $x_u > y_2$, by setting $G = G^*_s, t + P_1 + P_1$ we get from Lemma 2.5 that $\varphi(G) > \varphi(G^*_s, t)$, a contradiction. Thus, the theorem holds.

In what follows we suppose $s + t \geq 3$. Assume, by way of contradiction, that $t \geq s + 2$. Let $q = s + 2$ and $p = s + 1$. Let $x$ be the corresponding $Q$-Perron eigenvector of $G^*_s, t$ whose entries are labelled the same as the vertices $x_i$ and $y_j$ at $P_s$ and $P_t$ (Figure 1). We have $x_u > y_q > y_p > x_s$ by Lemma 2.6. Let

$$\begin{align*}
P_{p-p+s} &= x_u y_1 \cdots y_q x_s \cdots x_2 x_1, \\
P_p &= x_u y_p \cdots y_3 y_2 y_1,
\end{align*}$$

and $G(t-p)+s, p = H_u + P_{p-p+s} + P_p$. Let $Q$ and $Q'$ be the signless Laplacians of $G^*_s, t$ and $G(t-p)+s, p$, respectively. Then

$$x^T Q x - x^T Q' x = x_u x_s + y_p y_q - (y_q x_s + x_u y_p)$$

$$= x_s (x_u - y_q) + y_p (y_q - x_u)$$

$$= (x_u - y_q) (x_s - y_p) < 0,$$

which gives that $\varphi(G(t-p)+s, p) \geq x^T Q' x > x^T Q x = \varphi(G^*_s, t)$, a contradiction. 

We will see that this method is helpful to show Theorem 2.2. Let $G_{s_1, s_2, \ldots, s_k}$ be the graph obtained from a nontrivial connected graph $H$ by attaching $k$ pendant paths $P_{s_1}, P_{s_2}, \ldots, P_{s_k}$ at some vertex $u \in V(H)$. According to Theorem 2.1, we have the following generalization.

**Corollary 2.1** If $s_1 + s_2 + \cdots + s_k = a$ is a constant, then the maximal $Q$-index of $G_{s_1, s_2, \ldots, s_k}$ is attained at $|s_i - s_j| \leq 1$ for $1 \leq i, j \leq k$.

Let $G_{s, t}^{u, v} = H + P_{s}^{u} + P_{t}^{v}$ be the graph of order $n$ such that $u \in V(H)$ connects one end-vertex of $P_{s}$ and $v \in V(H)$ connects one end-vertex of $P_{t}$ (Figure 2), where $H$ is a nontrivial connected graph. Similarly, given $H = H_{u, v}$ and constant $a = s + t$, let

![Figure 2. $G_{s, t}^{u, v} = H_{u, v} + P_{s}^{u} + P_{t}^{v}$](image)

...
\[ \mathcal{G}_{H,a}^{u,v} = \{G_{s,t}^{u,v} = H_{u,v} + P_s + P_t | s + t = a, u, v \in V(H) \} \]

be the set of all the graphs \( G_{s,t}^{u,v} \). Naturally, we ask; which graph in \( \mathcal{G}_{H,a}^{u,v} \) has maximal \( Q \)-index? In the following, we shall provide a theorem similar to Theorem 2.1.

Suppose that \( G^* \in \mathcal{G}_{H,a}^{u,v} \) is the maximal graph, i.e. \( \varrho(G^*) \geq \varrho(G_{s,t}^{u,v}) \) for any graph \( G_{s,t}^{u,v} \in \mathcal{G}_{H,a}^{u,v} \), and the vertices \( x_i \) and \( y_j \) are regarded as the entries of \( Q \)-Perron eigenvector at that vertex (Figure 2). First, it is easy to see that Facts 1–3 still hold.

**Fact 4** Let \( G^* \in \mathcal{G}_{H,a}^{u,v} \) be the maximal graph. Then

\[ y_2 > x_1, \quad x_2 > y_1, \quad x_u > x_3 > \cdots > x_2 > x_1 \quad \text{and} \quad y_t > y_1 > \cdots > y_2 > y_1. \]

**Proof** If \( x_1 \geq y_2 \), then \( G = G^* - y_1y_2 + x_1y_1 \) is a graph in \( \mathcal{G}_{H,a}^{u,v} \) that has larger \( Q \)-index than \( G^* \) by Lemma 2.5. Similarly, \( x_2 > y_1 \). The last two inequalities follows from Facts 2 and 3.

**Fact 5** Let \( G^* \in \mathcal{G}_{H,a}^{u,v} \) be a maximal graph. If \( x_u > y_v \), then \( x_1 > y_2 \); If \( y_v > x_u \), then \( y_t > x_1 \).

**Proof** Let \( G = G^* - x_uy_3 - y_2y_1 + x_1y_1 + y_2x_3 \). Then \( \varrho(G^*) \geq \varrho(G) \), and so

\[ x^T Q(G^*) x - x^T Q(G) x = x_u x_3 + y_v y_1 - (x_u y_1 + y_v x_3) = (x_u - y_u)(x_t - y_t) \geq 0, \]

which gives the results.

**Fact 6** Let \( G^* \in \mathcal{G}_{H,a}^{u,v} \) be the maximal graph. If \( y_v > x_u \), then \( t \geq s \).

**Proof** From Fact 2 we know that \( \frac{x_{s+1}}{X_t} = \frac{y_{s+1}}{Y_t} \) for \( i = 1, 2, \ldots \). If \( s \geq t \), then \( \frac{x_{s+1}}{X_t} = \frac{y_{s+1}}{Y_t} \), which gives by Fact 4 that \( \frac{x_{s+1}}{X_t} = \frac{y_{s+1}}{Y_t} \), and so \( y_t > x_1 \). Since \( \frac{x_1}{x_t} = \frac{y_1}{y_t} \), then \( y_2 > x_2 \).

By Fact 4 again we get \( y_2 > x_2 > y_1 > x_1 \). Consequently, as the proof of Lemma 2.6, we obtain

\[ x_u > \cdots > y_v > x_{t+1} > y_t > x_1 > y_{t-1} > x_{t-1} > \cdots > y_2 > x_2 > y_1 > x_1, \]

which contradicts the condition that \( y_v > x_u \).

**Theorem 2.2** Let \( G^* \in \mathcal{G}_{H,a}^{u,v} \) be the maximal graph. Then \( |s - t| \leq 1 \).

**Proof** If \( x_u = y_v \), then our result holds by the proof of Theorem 2.1. Without loss of generality, we assume that \( y_v > x_u \). By way of contradiction, we may assume, according to Fact 6, that \( t \geq s + 2 \), and thus (4) becomes

\[ y_v > y_1 > \cdots > y_{s+1} > x_u > y_s > x_2 > \cdots > y_2 > x_2 > y_1 > x_1, \]

similar to the proof of Theorem 2.1, we produce a contradiction from (5). Thus, \( s + 1 \geq t \geq s \) and it follows our result.

Given a graph \( H \) and \( u_1, u_2, \ldots, u_k \in V(H) \), where the \( u_i \) is not necessary to be distinct, let \( G_{u_1 u_2 \ldots u_k}^{a} \) be a graph obtained from \( H \) by joining \( u_i \) with pendant path \( P_{a_i}(i = 1, 2, \ldots, k) \) at its end. According to the above proof, we can generalize Theorem 2.2 as follows.

**Corollary 2.2** If \( s_1 + s_2 + \cdots + s_k = a \) is a constant, then the maximal radius of \( G_{s_1 s_2 \ldots s_k}^{a} \) is attained at \( |s_i - s_j| \leq 1 \) for \( 1 \leq i, j \leq k \).
3. The maximal graphs with order $n$ and diameter $d$

Let $\mathcal{G}_n^d$ be the family of all the connected graphs of order $n$ and diameter $d$. Let $P_{d+1}$ be a path of order $d+1$ whose vertices are successively labelled by $1, 2, \ldots, d, d+1$. Now we construct a graph, denoted by $K_{d-i}^{n-d-1}$, which is obtained from the complete graph $K_{d-i}$ and the path $P_{d+1}$ by joining each vertex of $K_{d-i}$ to the vertices $i$, $i+1$ and $i+2$ of $P_{d+1}$. Obviously, $K_{d-i}^{n-d-1} \in \mathcal{G}_n^d$ for $2 \leq i \leq d-2$. Especially, for $i = \lceil \frac{d}{2} \rceil$ the graph $K_{\lceil \frac{d}{2} \rceil}^{n-d-1}$ is shown in Figure 3.

**Theorem 3.1** In the set $\mathcal{G}_n^d$, the maximum $Q$-index is attained by the following graphs:

The complete graph $K_n$ for $d = 1$ and the graph $K_{\lceil \frac{d}{2} \rceil}^{n-d-1}$ for $2 \leq d < n$.

**Proof** Since the complete graph $K_n$ is the unique graph with order $n$ and $d = 1$, then the theorem holds for $d = 1$. Since $P_n \cong K_{\lceil \frac{n}{2} \rceil}$ and it is the unique graph with order $n$ and $d = n - 1$, the theorem holds for $d = n - 1$.

For $2 \leq d \leq n - 2$, assume that $K^* \in \mathcal{G}_n^d$ is the maximal graph. Let $P_{d+1} = u_1 u_2 \cdots u_d u_{d+1}$ be the path of $K^*$ that connects $x$ and $y$, where $x = u_1$ and $y = u_{d+1}$, and let $S = V(K^*) \setminus V(P_{d+1})$. Clearly, $n > d + 1$ and thus $|S| = |V(K^*)| - |V(P_{d+1})| = n - (d + 1) > 0$. Since $K^*$ is connected, $E(S, V(P_{d+1})) \neq \emptyset$. For $s \in S$, set $N_{V(P_{d+1})}(s) = \{u_i \in V(P_{d+1}) | su_i \in E(K^*)\}$. We will prove $K^* \cong K_{\lceil \frac{d}{2} \rceil}^{n-d-1}$ by the following claims.

**Claim 1** The set $S$ induces a clique $K_{n-d-1}$ in $K^*$.

It follows the fact that adding edges to a connected graph increases the $Q$-index.

**Claim 2** Let $s \in S$. Then $N_{V(P_{d+1})}(s) = \{u_i \} \text{ for some } 3 \leq i \leq d - 1$.

If $N_{V(P_{d+1})}(s) = \{u_j\}$, where $j \leq \frac{d}{2}$ by symmetry, then $K^* + su_j \in \mathcal{G}_n^d$ will contain $K^*$ as a proper subgraph, which is impossible. Thus there exists at least $u_j, u_k \in N_{V(P_{d+1})}(s)$, and say $j < k$. Clearly, $k \leq j + 2$ since $P_{d+1}$ is the shortest path between $x$ and $y$. Suppose that $N_{V(P_{d+1})}(s) = \{u_j, u_k\}$. If $k = j + 1$ then, by setting $l = j + 2$, $K^* + su_l \in \mathcal{G}_n^d$ will contains $K^*$ as a proper subgraph; If $k = j + 2$ then, by setting $l = j + 1$, $K^* + su_l \in \mathcal{G}_n^d$ will contains $K^*$ as a proper subgraph; Therefore, $N_{V(P_{d+1})}(s) = \{u_j, u_j, u_{j+1}\}$ for some $1 \leq j \leq d$.

**Claim 3** $N_{V(P_{d+1})}(s) = N_{V(P_{d+1})}(t)$ for $s, t \in S$ and $s \neq t$.

By Claim 2, we can set $N_{V(P_{d+1})}(s) = \{u_{j-1}, u_j, u_{j+1}\}$ and $N_{V(P_{d+1})}(t) = \{u_{j-1}, u_j, u_{j+1}\}$. Assume, by way of contradiction, that $N_{V(P_{d+1})}(s) \neq N_{V(P_{d+1})}(t)$. Hence,

$$|N_{V(P_{d+1})}(s) \cap N_{V(P_{d+1})}(t)| \leq 2.$$ 

Note, Claim 1 shows that $st \in E(K^*)$. Thus if $|N_{V(P_{d+1})}(s) \cap N_{V(P_{d+1})}(t)| \leq 1$, then the diameter of $K^*$ will decrease, and so $|N_{V(P_{d+1})}(s) \cap N_{V(P_{d+1})}(t)| = 2$ which must
yield, without loss of generality, that $N_{V(P_{n+1})}(t) = \{u_i, u_{i+1}, u_{i+2}\}$. Let $x = (x_1, x_2, \ldots, x_n)$ be the $Q$-Perron eigenvector, where the entries $x_i$, $x_{i+1}$ and $x_{i+2}$ correspond to the vertices $u_i$, $u_{i+1}$ and $u_{i+2}$, respectively. Without loss of generality, set $x_{i-1} \geq x_{i+2}$. By constructing $G = K^* - tu_{i+2} + tu_{i-1}$ we obtain that $G \in \mathcal{G}_n^d$ and $\varphi(G) > \varphi(K^*)$ by Lemma 2.5, a contradiction.

**Claim 4** $K^* = K_n^{n-d-1}$.

From Claims 2 and 3, we get $N(S) = \{y \in V(K^*) \setminus S \mid ys \in E(K^*), s \in S\} = \{u_{i-1}, u_{i}, u_{i+1}\}$. By Claim 1 and Theorem 2.1, we have that $K^* \cong K_n^{n-d-1}$. By Claim 1 and Theorem 2.1, we have that $K^* \cong K_n^{n-d-1}$.

**Theorem 3.2** Let $n - d$ be a fixed constant. Then

$$\lim_{n \to \infty} \varphi\left(K_n^{n-d-1}\right) = \frac{4(n-d)^2}{2(n-d) - 1}.$$  

**Proof** Since $n - d = s$ is a constant, $Q_{n,d} = \varphi(K_n^{n-d-1})$ is an increasing function of order $n$ and diameter $d$, and $\varphi_{n,d} \leq 2\Delta(K_n^{n-d-1})$ by Lemma 2.2. Hence $\lim_{n \to \infty} \varphi_{n,d} = \lim_{d \to \infty} \varphi_{n,d} = \varphi$ exists. Note that $\varphi(K_n^{n-d-1}) \leq \varphi(K_n^{n-d-1})$, since $K_n^{n-d-1}$ is a subgraph of $K_n^{n-d-1}$. Now we consider the graph $K_{r,r}^{n-d-1}$, where $r = \lfloor \frac{n}{2} \rfloor$. As labelled in Figure 3, by (1) we get

$$\begin{align*}
(Q_{n,d} - 2)x_2 &= x_1 + x_3, \\
\ldots &
\ldots\ldots \\
(Q_{n,d} - 2)x_{r-1} &= x_{r-2} + x_r.
\end{align*}$$

Setting $Q_{n,d} = 2 \cosh t = e^t + e^{-t}$ and solving the above difference equations system, we have

$$x_2 = \frac{cx_1 + ax_r}{b} \quad \text{and} \quad x_{r-1} = \frac{ax_1 + cx_r}{b},$$

where $a = \sinh t$, $b = \sinh(r-1)t$, $c = \sinh(r-2)t$ and $t = \ln \frac{Q_{n,d} - 2 + \sqrt{(Q_{n,d} - 2)^2 - 4}}{2}$. By the symmetry of $K_n^{n-d-1}$, we have $(Q_{n,d} - 1)x_1 = x_2$ and $(Q_{n,d} - (s+1))x_r = x_{r-1} + x_r$. Combing the above two equalities we get

$$Q_{n,d} - 2s - 1 - \left(\frac{a}{b}\right)^2Q_{n,d} - 1 - \frac{c}{b} = 0.$$  

Since $\lim_{r \to \infty} \frac{a}{b} = 0$ and $\lim_{r \to \infty} \frac{c}{b} = \frac{2}{e^2 + \sqrt{(e-2)^2 - 4}}$, from the above equality we arrive at

$$Q - 2s - 1 - \frac{2}{Q - 2 + \sqrt{(Q - 2)^2 - 4}} = 0.$$  

Hence,

$$Q = \frac{4s^2}{2s - 1} = \frac{4(n-d)^2}{2(n-d) - 1}.$$  

This ends the proof.
THEOREM 4.1
Proof

Let $G_n$ be a maximum graph in the set $\mathcal{G}_n$. Clearly, $G_n$ is the maximal graph in the set $\mathcal{G}_n$. Next, we will show that $G_n$ is the maximal graph in the set $\mathcal{G}_n$.

THEOREM 4.1 In the set $\mathcal{G}_n$, the graph $G_n$ is the maximal graph.

Proof Let $G^*$ be a maximum graph in $\mathcal{G}_n$. We first show the following claims.

CLAIM 1 Each cut vertex of $G^*$ is precisely in two blocks, and all of these blocks are cliques.

For a connected graph, its signless Laplacian is irreducible. Thus, adding edges to this graph will increase its $Q$-index. On the other hand, adding the edge to a block does not change the order of $G$ and the number of cut vertices of $G$. Since $G^*$ is the maximal graph, then the claim holds.

CLAIM 2 Let a vertex $u \in V(G^*)$ be such that it lies in two maximal cliques $G_1$ and $G_2$. Then $u$ must be a cut vertex, and at least one of $G_1$ and $G_2$ is the complete graph $K_2$.

By Claim 1 we know that any vertex, which is not a cut vertex, must be contained in an unique clique, and thus $u$ is a cut vertex. Assume, by way of contradiction, that $G_1 = K_p$ and $G_2 = K_q$, where $p, q \geq 3$. Let $u_1 \in V(K_p)$ and $u_2 \in V(K_q)$. Let $x$ be the $Q$-Perron eigenvector of $G^*$ whose entries are labelled by the vertices. Without loss of generality, suppose that $x_{u_1} \geq x_{u_2}$. Set $G = G^* - \sum_{w \in N_G(u_2) \setminus u} u_2 w + \sum_{w \in N_G(u_1) \setminus u} u_1 w$. It is easy to see that $G \in \mathcal{G}_n$. But $\varrho(G) > \varrho(G^*)$ by Lemma 2.5, a contradiction.

CLAIM 3 There is at most one clique with order at least three in $G^*$.

Assume, by way of contradiction, that $K_p$ and $K_q$ are two cliques, where $p, q \geq 3$. Claim 2 indicates that these two cliques have no common vertex. Thus, there exists a path $P_k = u_1 v_1 v_2 \cdots v$ connecting $K_p$ and $K_q$, where $k \geq 2$, $u \in V(K_p)$ and $v \in V(K_q)$. Choose $u' \in V(K_p)$ and $v' \in V(K_q)$ such that $u' \neq u$ and $v' \neq v$. Without loss of generality, set $x_{u} \geq x_{v}$. Let $v''$ (if any) be a vertex in $N_{G^*}(v)$ other than the vertex in $K_q$. Let $G = G^* - \sum_{z \in N_{G^*}(v'') \setminus \{v, v''\}} v'' z + \sum_{z \in N_{G^*}(v') \setminus \{v, v''\}} u' z$. It is easy to see that $G \in \mathcal{G}_n$ and $\varrho(G) > \varrho(G^*)$ by Lemma 2.5. It is a contradiction.
Now, we are at the stage of finishing of this proof of this theorem. Obviously, a connected graph of order $n$ has at most $n - 2$ cut vertices. If $G^*$ has $k = n-2$ cut vertices then it is the unique path $P_n = G_{n,n-2}$, and so our result holds. Assume now that $k \leq n - 3$. This implies that $G^*$ has a vertex $u$ of degree no less than three. By the latter part of Claim 1, there is a clique $K$ with order at least three containing $u$. By Claim 3, $G^*$ must be a graph constructed from $K$ by adding some pendant paths on it. By the former part Claim 1, any vertex not in $K$ is pendant or in at most one path. Then by Corollary 2.2 we obtain that $G^* \cong G_{n,k}$.

**Theorem 4.2** Let $\tau = 2(n-k-1)$. If $k \leq \frac{n}{2}$, then

$$\varphi(G_{n,k}) < \tau + \frac{2\tau k}{\tau^2 - 2n}.$$  

**Proof** Since $k \leq \frac{n}{2}$, $G_{n,k}$ is the graph with $V(G_{n,k}) = \{v_1, v_2, \ldots, v_n\}$, $G_{n,k}[\{v_1, \ldots, v_{n-k}\}] = K_{n-k}$ and $v_i v_{n-k+i} \in E(G_{n,k})$ for $i = 1, \ldots, k$. Let $x = (x_1, x_2, \ldots, x_n)$ be the $Q$-Perron eigenvector of $G_{n,k}$, where $x_i$ denote the entry of $x$ at vertex $v_i$. By the symmetry of $G_{n,k}$, we have from (1) and $\varphi(G_{n,k}) = \varphi$ that

$$\begin{align*}
(q - 1)x_{n-k-1} &= x_1, \\
(q - (n-k-1))x_{n-k} &= kx_1 + (n - 2k - 1)x_{n-k}, \\
(q - (n-k))x_1 &= (k-1)x_1 + x_{n-k+1} + (n - 2k)x_{n-k},
\end{align*}$$

which leads to

$$\varphi^3 - (3n - 3k - 2)\varphi^2 - [(n+2) - 2(n-k)^2]\varphi - 2(n-k-1)(n-k-2) = 0. \quad (6)$$

Since $G_{n,k}$ contains a proper subgraph $K_{n-k}$, by Lemma 2.2 we get $\varphi(G_{n-k}) > \varphi(K_{n-k}) = 2(n-k-1)$. Thus, substituting $\varphi = 2(n-k-1) + \epsilon$, where $\epsilon > 0$, into Equation (6) we have

$$\epsilon^3 + [3(n-k) - 4]\epsilon^2 + [2(n-k)^2 - 5n + 4k + 2]\epsilon - 2k(n-k-1) = 0,$$

which indicates that

$$\epsilon < \frac{2k(n-k-1)}{2(n-k)^2 - 5n + 4k + 2} = \frac{2k(n-k-1)}{2(n-k-1)^2 - n} = \frac{2\tau k}{\tau^2 - 2n}.$$

Hence the theorem holds.

**Theorem 4.3** Let $n-k$ be a fixed constant and $\tau = 2(n-k-1)$. If $\frac{n}{2} < k \leq n-3$, then

$$\lim_{n \to \infty} \varphi(G_{n,k}) = \tau + \frac{\tau}{\tau - 1}.$$  

**Proof** Since $\frac{n}{2} < k \leq n-3$, $G_{n,k}$ is the graph obtained from $K_{n-k}$ by identifying each of its vertex $v_i$ with one pendant vertex of the path $P_l$, where $|l_i - l| \leq 1$ and $1 \leq i, j \leq n-k$. For convenience, write $G_{n,k} = G_{l_1, \ldots, l_{n-k}}$. Since $n-k$ is constant, the $Q$-index of $G_{n,k}$ is an increasing function of order $n$ of $G_{n,k}$ and $\varphi_n = \varphi(G_{n,k}) \leq \Delta(G_{n,k})$ by Lemma 2.2, which implies that $\lim_{n \to \infty} \varphi_n = \varphi$ exists. Let $l = \max\{l_i | 1 \leq i \leq n-k\}$. Then $\varphi(G_{l_1, \ldots, l_{n-k}}) \leq \varphi(G_{l_1, \ldots, l_{n-k}})$, since $G_{l_1, \ldots, l_{n-k}}$ is the subgraph of $G_{l_1, \ldots, l_{n-k}}$. Now we consider
the graph $G_{l,...,l}^{n,k}$, where the vertices of $P_l$ are labelled as $v_1, v_2, \ldots, v_l$. Let $x=(x_1, x_2, \ldots, x_n)$ be the $Q$-Perron eigenvector of $G_{l,...,l}^{n,k}$. From (1) it follows that

$$(\rho_n - 2)x_1 = x_2, \ldots, (\rho_n - 2)x_{l-1} = x_{l-2} + x_l,$$

which has the following solutions

$$x_2 = \frac{cx_1 + ax_l}{b} \quad \text{and} \quad x_{l-1} = \frac{ax_1 + cx_l}{b},$$

where $a = \sinh t$, $b = \sinh(l-1)t$, $c = \sinh(l-2)t$ and $t = \ln \frac{\rho_n - 2 + \sqrt{(\rho_n - 2)^2 - 4}}{2}$. By the symmetry of $G_{l,...,l}^{n,k}$ we get 

$$(\rho_n - (n-k))x_1 = x_2 \quad \text{and} \quad (\rho_n - (n-k))x_l = x_{l-1} + (n-k-1)x_l$$

which, together with the above two equalities, yields

$$\rho_n - 2(n-k) + 1 - \frac{c}{b} - \left(\frac{a}{b}\right)^2 \frac{1}{\rho_n - 1 - \frac{c}{b}} = 0.$$

Since $\lim_{l \to \infty} \frac{c}{b} = 0$ and $\lim_{l \to \infty} \frac{a}{b} = \frac{2}{\rho - 2 + \sqrt{(\rho - 2)^2 - 4}}$, from the above equality we arrive at

$$\rho - 2(n-k) + 1 - \frac{2}{\rho - 2 + \sqrt{(\rho - 2)^2 - 4}} = 0.$$

Hence

$$\rho = \frac{4(n-k-1)^2}{2(n-k) - 3} = 2(n-k-1) + \frac{2(n-k-1)}{2(n-k) - 3 - 1} = \tau + \frac{\tau}{\tau - 1}.$$
References