On Zagreb index, signless Laplacian eigenvalues and signless Laplacian energy of a graph

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Abstract
Let $G$ be a simple graph with order $n$ and size $m$. The quantity $M_1(G) = \sum_{i=1}^{n} d_{v_i}^2$ is called the first Zagreb index of $G$, where $d_{v_i}$ is the degree of vertex $v_i$, for all $i = 1, 2, \ldots, n$. The signless Laplacian matrix of a graph $G$ is $Q(G) = D(G) + A(G)$, where $A(G)$ and $D(G)$ denote, respectively, the adjacency and the diagonal matrix of the vertex degrees of $G$. Let $q_1 \geq q_2 \geq \cdots \geq q_n \geq 0$ be the signless Laplacian eigenvalues of $G$. The largest signless Laplacian eigenvalue $q_1$ is called the signless Laplacian spectral radius or $Q$-index of $G$ and is denoted by $q(G)$. Let $S^+_k(G) = \sum_{i=1}^{k} q_i$ and $L_k(G) = \sum_{i=0}^{k-1} q_{n-i}$, where $1 \leq k \leq n$, respectively denote the sum of $k$ largest and smallest signless Laplacian eigenvalues of $G$. The signless Laplacian energy of $G$ is defined as $QE(G) = \sum_{i=1}^{n} |q_i - \bar{d}|$, where $\bar{d} = \frac{2m}{n}$ is the average vertex degree of $G$. In this article, we obtain upper bounds for the first Zagreb index $M_1(G)$ and show that each bound is best possible. Using these bounds, we obtain several upper bounds for the graph invariant $S^+_k(G)$ and characterize the extremal cases. As a consequence, we find upper bounds for the $Q$-index and lower bounds for the graph invariant $L_k(G)$ in terms of various graph parameters and determine the extremal cases. As an application, we obtain upper bounds for the signless Laplacian energy of a graph and characterize the extremal cases.

Keywords First Zagreb index · Signless Laplacian matrix · Signless Laplacian eigenvalues · Signless Laplacian energy

Mathematics Subject Classification 05C50 · 05C12 · 15A18
1 Introduction

We consider simple graphs $G = G(V, E)$ with order $n$ and size $m$ having vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. As usual, $K_{1,n-1}$ and $K_n$ denote the star on $n$ vertices and the complete graph on $n$ vertices, respectively. The degree of a vertex $v_i \in V(G)$, denoted by $d_{v_i} = d_i$, is the number of edges incident on $v_i$. We will denote by $\Delta(G)$ and $\delta(G)$ the maximum vertex degree and the minimum vertex degree in a graph $G$, respectively. The diameter of a connected graph $G$, denoted by $d(G)$, is the largest distance between any pair of vertices in $G$. We refer the reader to Cvetković et al. (1980) and Pirzada (2012) for other undefined notations and terminology from spectral graph theory.

The adjacency matrix $A(G) = (a_{ij})$ of $G$ is a $(0, 1)$-square matrix of order $n$ whose $(i, j)$-entry is equal to 1, if $v_i$ is adjacent to $v_j$ and equal to 0, otherwise. If $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the adjacency eigenvalues of $G$, the energy Gutman (2001) of $G$ is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. The quantity $E(G)$ introduced by Gutman has well developed mathematical aspect and has noteworthy chemical applications (see Li et al. 2012).

Let $D(G) = \text{diag}(d_1, d_2, \ldots, d_n)$ be the diagonal matrix associated to $G$, where $d_i = d_{v_i}$ is the degree of the vertex $v_i$, for all $i = 1, 2, \ldots, n$. The matrices $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$ are called the Laplacian and the signless Laplacian matrices, respectively. Their spectrum are called the Laplacian spectrum and the signless Laplacian spectrum of the graph $G$, respectively. Both the matrices $L(G)$ and $Q(G)$ are real symmetric, positive semi-definite matrices, therefore their eigenvalues are non-negative real numbers. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n \geq 0$ and $q_1 \geq q_2 \geq \cdots \geq q_n \geq 0$ be the Laplacian spectrum and the signless Laplacian spectrum of the graph $G$, respectively. The eigenvalues of $Q(G)$ are called the $Q$-eigenvalues of $G$. Also, the largest signless Laplacian eigenvalue $q_1$ of $Q(G)$ is called the signless Laplacian spectral radius or $Q$-index of $G$ and is denoted by $q(G)$. For $k = 1, 2, \ldots, n$, let $S_k(G) = \sum_{i=1}^{k} \mu_i$, be the sum of $k$ largest Laplacian eigenvalues of $G$. We note that the sum $S_k(G)$ is of much interest by itself and some exciting details, extensions and open problems about it may be found in the excellent paper of Nikiforov (2015). The well-known Brouwer’s conjecture, due to Brouwer and Haemers (2011) about the sum $S_k(G)$ is stated as follows.

**Conjecture 1** If $G$ is any graph with order $n$ and size $m$, then
\[
S_k(G) \leq m + \binom{k+1}{2}, \quad \text{for any } k \in \{1, 2, \ldots, n\}.
\]

Although Conjecture 1 has been studied extensively but it remains open at large. For the progress on Brouwer’s Conjecture, we refer to Chen (2018), Ganie et al. (2016) and Helmberg and Trevisan (2017) and the references therein.

Let $S_k^+(G) = \sum_{i=1}^{k} q_i$ and $L_k(G) = \sum_{i=0}^{k-1} q_{n-i}$, where $k = 1, 2, \ldots, n$, be the sum of $k$ largest and smallest signless Laplacian eigenvalues of $G$, respectively. Motivated by the studies of Mohar (2009) and Jin et al. (2013) investigated the sum of the $k$ largest signless Laplacian eigenvalues. Motivated by the definition of $S_k(G)$ and Brouwer’s conjecture, Ashraf et al. (2013) proposed the following conjecture about $S_k^+(G)$.

**Conjecture 2** If $G$ is any graph with order $n$ and size $m$, then
\[
S_k^+(G) \leq m + \binom{k+1}{2}, \quad \text{for any } k \in \{1, 2, \ldots, n\}.
\]

To see the progress on this conjecture, we refer to Yang and You (2014) and the references therein.
The rest of the paper is organized as follows. In Sect. 2, we obtain upper bounds for the first Zagreb index $M_1(G)$ and show that the bounds are sharp. Using these investigations, we obtain several upper bounds for the graph invariant $S_k^+(G)$ and determine the extremal graphs. As a consequence, we obtain upper bounds for the $Q$-index and lower bounds for the graph invariant $L_k(G)$ in terms of various graph parameters and determine the extremal cases in each case. In Sect. 3, we find some upper bounds for the signless Laplacian energy $QE(G)$ for a connected graph $G$ and determine the extremal cases.

2 Sum of the signless Laplacian eigenvalues of a graph

The first Zagreb index $M_1(G)$ Nikolić et al. (2003) of a graph $G$ is defined as $M_1(G) = \sum_{i=1}^{n} d_{v_i}^2$, where $d_{v_i}$ is the degree of vertex $v_i$, for all $i = 1, 2, \ldots, n$. The following inequality can be found in Izumino et al. (1998).

Lemma 2.1 (Izumino et al. 1998) Let $a = (a_1, a_2, \ldots, a_n)$ and $b = (b_1, b_2, \ldots, b_n)$ be $n$-tuples of real numbers satisfying $0 \leq m_1 \leq a_i \leq M_1$, $0 \leq m_2 \leq b_i \leq M_2$ with $i = 1, 2, \ldots, n$ and $M_1 M_2 \neq 0$. Let $\alpha = \frac{m_1}{M_1}$ and $\beta = \frac{m_2}{M_2}$. If $(1 + \alpha)(1 + \beta) \geq 2$, then

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left( \sum_{i=1}^{n} a_i b_i \right)^2 \leq \frac{n^2}{4} (M_1 M_2 - m_1 m_2)^2. \quad (2.1)$$

The following result gives an upper bound for the graph invariant $M_1(G)$ in terms of the order $n$, size $m$, $\Delta(G)$ and $\delta(G)$.

Lemma 2.2 Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$\sum_{i=1}^{n} d_i^2 \leq \frac{4m^2}{n} + \frac{n}{4} (\Delta(G) - \delta(G))^2. \quad (2.2)$$

Furthermore, the inequality is sharp and is shown by all degree regular graphs.

Proof In Lemma 2.1, taking $a = (d_1, d_2, \ldots, d_n)$, $b = (1, 1, \ldots, 1)$, $M_1 = \Delta(G)$, $m_1 = \delta(G)$ and $M_2 = m_2 = 1$. With these values the condition $(1 + \alpha)(1 + \beta) \geq 2$ in Lemma 2.1 is satisfied. Substituting these values in Inequality 2.1, we get

$$\sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} 1 - \left( \sum_{i=1}^{n} d_i \right)^2 \leq \frac{n^2}{4} (\Delta(G) - \delta(G))^2.$$

Using the fact that $\sum_{i=1}^{n} d_i = 2m$ in the above inequality and simplifying further, we get

$$n \sum_{i=1}^{n} d_i^2 - 4m^2 \leq \frac{n^2}{4} (\Delta(G) - \delta(G))^2,$$

that is,

$$\sum_{i=1}^{n} d_i^2 \leq \frac{4m^2}{n} + \frac{n}{4} (\Delta(G) - \delta(G))^2,$$

which proves the required inequality.
Now, let $G$ be an $r$-regular graph so that $\triangle(G) = \delta(G)$. Clearly, the left hand side of Inequality 2.2 becomes $nr^2$ and the right hand side becomes $\frac{n^2r^2}{n} = nr^2$. This completes the proof.

The next lemma shows that the diameter of a connected graph $G$ can be at most $e(G) - 1$ where $e(G)$ is the number of distinct $Q$-eigenvalues of $G$.

**Lemma 2.3** (Cvetković 2008) Let $G$ be a connected graph of diameter $d(G)$ and $e(G)$ distinct $Q$-eigenvalues. Then $d(G) \leq e(G) - 1$.

In the next lemma, we show that the complete graph is the unique connected graph having only two distinct $Q$-eigenvalues.

**Lemma 2.4** Let $G$ be a connected graph on $n$ vertices with $e(G)$ distinct $Q$-eigenvalues. Then $e(G) = 2$ if and only if $G \cong K_n$.

**Proof** Assume that $e(G) = 2$. Then, from Lemma 2.3, we have $D(G) = 1$, which shows that $G \cong K_n$.

Conversely, suppose that $G \cong K_n$. The proof follows by observing that the $Q$-spectrum of $K_n$ is $\{2n-2, n-2, \ldots, n-2\}$.

A simpler version of classical Cauchy–Schwarz Inequality is as follows.

**Lemma 2.5** Let $(a_1, a_2, \ldots, a_n)$ be a sequence of non-negative real numbers. Then

$$\left( \sum_{i=1}^{n} a_i \right)^2 \leq n \sum_{i=1}^{n} a_i^2$$

with equality if and only if $a_1 = a_2 = \cdots = a_n$.

Now, we obtain an upper bound for $S_k^+(G)$ in terms of $n, m, \triangle(G)$ and $\delta(G)$ and characterize the extremal graphs.

**Theorem 2.6** Let $G$ be a connected graph with $n$ vertices and $m$ edges. If $1 \leq k \leq n - 1$, then

$$S_k^+(G) \leq \frac{2mk}{n} + \frac{\sqrt{k(n-k)\left(8mn + n^2(\triangle(G) - \delta(G))^2\right)}}{2n}$$

with equality if and only if $G \cong K_n$ and $k = 1$. Equality always holds when $k = n$.

**Proof** Using the fact that the sum of the eigenvalues of a matrix equals its trace, we have

$$2m = \sum_{v_i \in V(G)} d_{v_i} = q_1 + q_2 + \cdots + q_n,$$

that is,

$$2m + \sum_{v_i \in V(G)} d_{v_i}^2 = \sum_{v_i \in V(G)} (d_{v_i}^2 + d_{v_i}) = q_1^2 + q_2^2 + \cdots + q_n^2.$$

Let $S_k^+(G) = S_k^+$. Using the above equations with Lemma 2.5, we get
\[(q_{k+1} + \cdots + q_n)^2 = (2m - S_k^+)^2 \leq (n - k)(q_{k+1}^2 + \cdots + q_n^2)\]
\[= (n - k) \left( 2m + \sum_{v_i \in V(G)} d_{v_i}^2 - (q_1^2 + \cdots + q_n^2) \right) \]
\[\leq (n - k) \left( 2m + \sum_{v_i \in V(G)} d_{v_i}^2 - \frac{S_k^2}{k} \right).\]

Simplifying further, we get
\[S_k^+ + \frac{4mkS_k^+}{n} + \frac{4m^2k}{n} - \frac{k(n - k)}{n} \left( 2m + \sum_{v_i \in V(G)} d_{v_i}^2 \right) \leq 0,
\]
that is,
\[S_k^+ \leq \frac{2mk}{n} + \sqrt{\frac{4m^2k^2 - 4knm^2 + nk(n - k)}{n}} \left( 2m + \sum_{v_i \in V(G)} d_{v_i}^2 \right).
\]

or
\[S_k^+ \leq \frac{2mk}{n} + \frac{k(n - k)}{n} \left( n(2m + \sum_{v_i \in V(G)} d_{v_i}^2) - 4m^2 \right) \]
and this proves the required inequality.

Using Lemma 2.2 in Inequality (2.4), we get
\[S_k^+ \leq \frac{2mk}{n} + \frac{\sqrt{k(n - k) \left( 2mn + 4m^2 + \frac{n^2}{4}(\triangle(G) - \delta(G))^2 - 4m^2 \right)}}{n},\]
and this proves the required inequality.

Now, suppose that the equality holds in Inequality 2.3. Then, from the above proof, equality must hold in Lemmas 2.5 and 2.2. Thus, we must have \(q_{k+1} = q_{k+2} = \cdots = q_n\) and \(q_1 = q_2 = \cdots = q_k\), from Lemma 2.5. These two equalities show that \(G\) has exactly two distinct \(Q\)-eigenvalues. Thus, by Lemma 2.4, \(G \cong K_n\) and we know that \(K_n\) is a regular graph. Lastly, \(k = 1\) follows from the \(Q\)-spectrum of \(K_n\).

Conversely, it is easy to see that the equality holds in Inequality 2.3 if \(G \cong K_n\) and \(k = 1\).

Furthermore, if \(k = n\) then the left hand side of Inequality 2.3 is \(q_1 + \cdots + q_n = 2m\) and the right hand side becomes \(\frac{2mn}{n} = 2m\). Thus, equality always holds when \(k = n\). 

Proceeding and using arguments similar to those used in Theorem 2.6, we get the following lower bound for \(L_k(G)\).
Theorem 2.7 Let $G$ be a connected graph with $n$ vertices and $m$ edges. If $1 \leq k \leq n - 1$, then

$$L_k(G) \geq \frac{2mk}{n} - \frac{\sqrt{k(n-k)\left(8mn + n^2(\Delta(G) - \delta(G))^2\right)}}{2n}$$

with equality if and only if $G \cong K_n$ and $k = n - 1$. Equality always holds when $k = n$.

Taking $k = 1$ in Theorem 2.6, we obtain the following upper bound for the signless Laplacian spectral radius in terms of $m$, $n$, $\Delta(G)$ and $\delta(G)$.

Theorem 2.8 Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$\varrho(G) \leq \frac{2m}{n} + \frac{\sqrt{(n-1)\left(8mn + n^2(\Delta(G) - \delta(G))^2\right)}}{2n}$$

with equality if and only if $G \cong K_n$.

The following inequality can be seen in Polya and Szegö (1972).

Lemma 2.9 (Polya and Szegö 1972) If $a_i$ and $b_i$, $1 \leq i \leq n$, are positive real numbers, then

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 \leq \frac{1}{4}\left(\frac{M_1 M_2}{m_1 m_2} + \sqrt{m_1 m_2} \frac{M_1 M_2}{m_1 m_2}\right)^2 \left(\sum_{i=1}^{n} a_i b_i\right)^2,$$

where $M_1 = \max\{a_i : 1 \leq i \leq n\}$, $m_1 = \min\{a_i : 1 \leq i \leq n\}$, $M_2 = \max\{b_i : 1 \leq i \leq n\}$ and $m_2 = \min\{b_i : 1 \leq i \leq n\}$.

Now, we obtain a different upper bound for the sum of squares of the vertex degrees of a connected graph $G$ in terms of the same parameters as in Lemma 2.2.

Lemma 2.10 Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$\sum_{i=1}^{n} d_i^2 \leq \frac{m^2 (\Delta(G) + \delta(G))^2}{n\Delta(G)\delta(G)}.$$  \hspace{1cm} (2.5)

Moreover, the inequality is sharp and is shown by all degree regular graphs.

Proof In Lemma 2.9, take $a_i = d_{v_i} = d_i$ ($1 \leq i \leq n$), $b_i = 1$ ($1 \leq i \leq n$), $M_1 = \Delta(G)$, $m_1 = \delta(G)$ and $M_2 = m_2 = 1$, we get

$$\sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} 1 \leq \frac{1}{4}\left(\sqrt{\frac{\Delta(G)}{\delta(G)}} + \sqrt{\frac{\delta(G)}{\Delta(G)}}\right)^2 \left(\sum_{i=1}^{n} d_i\right)^2.$$

Using $\sum_{i=1}^{n} d_i = 2m$ in the above inequality, we get

$$\sum_{i=1}^{n} d_i^2 \leq \frac{m^2 (\Delta(G) + \delta(G))^2}{n\Delta(G)\delta(G)},$$

which is the required inequality.

For the equality part, let $G$ be $r$-regular. Then the left hand side of Inequality 2.5 becomes $nr^2$ and the right hand side becomes $\frac{4r^4n^2}{4nr^2} = nr^2$. Thus equality holds in Inequality 2.5 whenever $G$ is a regular graph. \qed
Now, we will use the Lemma 2.10 to get the following upper bound for the graph invariant $S_k^+(G)$.

**Theorem 2.11** Let $G$ be a connected graph with $n$ vertices and $m$ edges. If $1 \leq k \leq n - 1$, then

$$S_k^+(G) \leq \frac{2mk}{n} + \frac{\sqrt{mk(n-k)\left(2\Delta(G)\delta(G)(n-2m) + m(\Delta(G) + \delta(G))^2\right)}}{n\sqrt{\Delta(G)\delta(G)}}$$

(2.6)

with equality if and only if $G \cong K_n$ and $k = 1$. Equality always holds when $k = n$.

**Proof** Proceeding similarly as in Theorem 2.6 upto Inequality 2.4 and using Lemma 2.10, we get

$$S_k^+ \leq \frac{2mk}{n} + \frac{\sqrt{k(n-k)\left(n\left(2m + \frac{m^2(\Delta(G) + \delta(G))^2}{n\Delta(G)\delta(G)}\right) - 4m^2\right)}}{n}$$

or

$$S_k^+ \leq \frac{2mk}{n} + \frac{\sqrt{mk(n-k)\left(2\Delta(G)\delta(G)(n-2m) + m(\Delta(G) + \delta(G))^2\right)}}{n\sqrt{\Delta(G)\delta(G)}}.$$

This proves Inequality 2.6.

The proof of the remaining part of the theorem follows by using similar arguments as in Theorem 2.6. \qed

Taking $k = 1$ in Theorem 2.11, we obtain an upper bound for the signless Laplacian spectral radius as follows.

**Theorem 2.12** Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$q(G) \leq \frac{2m}{n} + \frac{\sqrt{m(n-1)\left(2\Delta(G)\delta(G)(n-2m) + m(\Delta(G) + \delta(G))^2\right)}}{n\sqrt{\Delta(G)\delta(G)}}$$

with equality if and only if $G \cong K_n$.

Proceeding and using arguments similar to those used in Theorem 2.12, we get the following lower bound for $L_k(G)$.

**Theorem 2.13** Let $G$ be a connected graph with $n$ vertices and $m$ edges. If $1 \leq k \leq n - 1$, then

$$L_k(G) \geq \frac{2mk}{n} - \frac{\sqrt{mk(n-k)\left(2\Delta(G)\delta(G)(n-2m) + m(\Delta(G) + \delta(G))^2\right)}}{n\sqrt{\Delta(G)\delta(G)}}$$

with equality if and only if $G \cong K_n$ and $k = n - 1$. Equality always holds when $k = n$.

### 3 Signless Laplacian energy of a graph

The Laplacian energy of a graph $G$ is defined as $LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|$. This quantity, which is an extension of graph-energy concept (Li et al. 2012), has found remarkable chemical...
applications beyond the molecular orbital theory of conjugated molecules (see Radenkovic and Gutman 2007).

In analogy to Laplacian energy, the signless Laplacian energy $QE(G)$ of $G$ is defined as

$$QE(G) = \sum_{i=1}^{n} |q_i - \frac{2m}{n}|.$$ 

To see the basic properties of this quantity, including various upper and lower bounds, we refer to Abreu et al. (2011), Das and Mojallal (2016), Ganie and Pirzada (2017) and Ganie et al. (2018). We start with the following lemma which gives an upper bound for the $Q$-index $q(G)$ of a connected graph $G$ in terms of the order $n$ and size $m$.

**Lemma 3.1** (Feng and Yu 2009) Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$q(G) \leq \frac{2m}{n} + n - 2$$

with equality if and only if $G$ is $K_{1,n-1}$ or $K_n$.

Now, we obtain an upper bound for $QE(G)$ of a connected graph $G$ in terms of the order $n$, size $m$, maximum vertex degree $\Delta(G)$, minimum vertex degree $\delta(G)$ and $Q$-index $q(G)$ of $G$.

**Theorem 3.2** Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$QE(G) \leq \frac{2m}{n(n-1)} + n - 2 + \sqrt{(n-1) \left(2m + \frac{n}{4}(\Delta(G) - \delta(G))^2 - \left(q(G) - \frac{2m}{n}\right)^2\right)}$$

(3.1)

with equality if and only if $G \cong K_n$.

**Proof** It is easy to see that

$$q_1 = q(G) \geq \frac{2m}{n}, \quad \sum_{i=1}^{n} |q_i - \frac{2m}{n}|^2 = \sum_{i=1}^{n} q_i^2 - \frac{4m^2}{n} \quad \text{and} \quad \sum_{i=1}^{n} q_i^2 = 2m + \sum_{i=1}^{n} d_i^2.$$ 

Using this observations and Lemma 2.5, we get

$$QE(G) = \sum_{i=1}^{n} |q_i - \frac{2m}{n}| = q_1 - \frac{2m}{n} + \sum_{i=2}^{n} |q_i - \frac{2m}{n}|$$

$$\leq q_1 - \frac{2m}{n} + \sqrt{(n-1) \sum_{i=2}^{n} |q_i - \frac{2m}{n}|^2}$$

$$= q_1 - \frac{2m}{n} + \sqrt{(n-1) \left(\sum_{i=1}^{n} q_i^2 - \frac{4m^2}{n} \right) - \left(q_1 - \frac{2m}{n}\right)^2}$$

$$= q_1 - \frac{2m}{n} + \sqrt{(n-1) \left(2m + \sum_{i=1}^{n} d_i^2 - \frac{4m^2}{n} \right) - \left(q_1 - \frac{2m}{n}\right)^2}$$

$$\leq q_1 - \frac{2m}{n} + \sqrt{(n-1) \left(2m + \frac{4m^2}{n} + \frac{n}{4}(\Delta(G) - \delta(G))^2 - \frac{4m^2}{n} \right) - \left(q_1 - \frac{2m}{n}\right)^2}.$$
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(by using Lemma 2.2)
\[ \leq \frac{2m}{n-1} + n - 2 - \frac{2m}{n} + \sqrt{(n-1)\left(2m + \frac{n}{4}(\Delta(G) - \delta(G))^2 - \left(q_1 - \frac{2m}{n}\right)^2\right)} \]
(by using Lemma 3.1)
\[ = \frac{2m}{n(n-1)} + n - 2 + \sqrt{(n-1)\left(2m + \frac{n}{4}(\Delta(G) - \delta(G))^2 - \left(q(G) - \frac{2m}{n}\right)^2\right)}. \]

This proves the required inequality.

Assume that equality holds in Inequality 3.1. Then equality must hold in all the above inequalities, that is, equality must hold simultaneously in Lemmas 2.5, 2.2 and 3.1. We consider the following cases.

**Case 1.** Equality holds in Lemma 2.5 if \[ \left| q_2 - \frac{2m}{n} \right| = \left| q_3 - \frac{2m}{n} \right| = \cdots = \left| q_n - \frac{2m}{n} \right|. \]

**Case 2.** Equality holds in Lemma 3.1 if \( G \) is either \( K_{1,n-1} \) or \( K_n \). But \( K_{1,n-1} \) does not satisfy Case 1. \( K_n \) satisfies Case 1 and also equality holds in Lemma 2.2 when \( G \cong K_n \) as \( K_n \) is a regular graph.

All these arguments show that if equality holds in Inequality 3.1, then \( G \cong K_n \).

Conversely, if \( G \cong K_n \), then it is easy to see that the equality holds in Inequality 3.1. \( \square \)

The next lemma due to Caen (1998) gives the upper bound for the sum of the squares of vertex degrees in a graph.

**Lemma 3.3** (Caen 1998) Let \( G \) be a graph with \( n \) vertices and \( m \) edges. Then
\[ \sum_{u \in V(G)} d_u^2 \leq m\left(\frac{2m}{n-1} + n - 2\right). \]
Moreover, if \( G \) is connected, then equality holds if and only if \( G \) is either a star \( K_{1,n-1} \) or a complete graph \( K_n \).

Proceeding and using arguments similar to Theorem 3.2 and using Lemma 3.3 in place of Lemma 2.2, we get the following upper bound for \( QE(G) \) in terms of order \( n \), size \( m \) and \( Q \)-index \( q(G) \) of \( G \).

**Theorem 3.4** Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges. Then
\[ QE(G) \leq \frac{2m}{n(n-1)} + n - 2 + \sqrt{(n-1)\left(mn + \frac{2m^2(2-n)}{n(n-1)} - \left(q(G) - \frac{2m}{n}\right)^2\right)} \]
with equality if and only if \( G \cong K_n \).

We require the following lemma (Ning et al. 2013).

**Lemma 3.5** Let \( G \) be a graph of order \( n \) with \( m \) edges. Then \( q_1 \geq \frac{4m}{n} \) with equality if and only if \( G \) is regular.

For a graph \( G \) on \( n \) vertices and \( m \) edges with signless Laplacian spectrum \( q_1 \geq q_2 \geq \ldots \geq q_n \), let \( v \) \((1 \leq v \leq n)\) be the largest positive integer such that \( q_v \geq \frac{2m}{n} \).

**Lemma 3.6** There exists no graph \( G \) with signless Laplacian spectrum \( q_1 \geq q_2 \geq \cdots \geq q_n \) such that \( q_i \geq \frac{2m}{n} \) for all \( 1 \leq i \leq n \).
If possible, let $q_i \geq \frac{2m}{n}$ for all $1 \leq i \leq n$. Using these inequalities and Lemma 3.5, we get $\sum_{i=1}^{n} q_i \geq q_1 + (n - 1) \frac{2m}{n}$, which implies that $\sum_{i=1}^{n} q_i \geq \frac{4m}{m} + (n - 1) \frac{2m}{n}$, further implies that $\sum_{i=1}^{n} q_i \geq 2m + \frac{2m}{n}$, which is a contradiction to the fact that $\sum_{i=1}^{n} q_i = 2m$. This proves the result. \hfill $\Box$

In the following result, we obtain an upper bound for $QE(G)$ of a connected graph $G$ in terms of the order $n$, size $m$, maximum vertex degree $\Delta(G)$, minimum vertex degree $\delta(G)$ and $v$.

**Theorem 3.7** Let $G$ be a connected graph of order $n$ with $m$ edges. Then

$$QE(G) \leq \sqrt{v(n - v) \left(8mn + n^2(\Delta(G) - \delta(G))^2\right)}$$

with equality if and only if $G \cong K_n$.

**Proof** Let $v$ be the largest positive integer such that $q_v \geq \frac{2m}{n}$, with $1 \leq v \leq n - 1$ because of Lemma 3.6. Now, we have

$$QE(G) = \sum_{i=1}^{n} \left| q_i - \frac{2m}{n} \right|$$

$$= \sum_{i=1}^{v} q_i - v \times \frac{2m}{n} + (n - v) \times \frac{2m}{n} - \sum_{i=v+1}^{n} q_i$$

$$= \sum_{i=1}^{v} q_i - \frac{4mv}{n} + 2m - \sum_{i=1}^{v} q_i + \sum_{i=1}^{v} q_i$$

$$= 2 \sum_{i=1}^{v} q_i - \frac{4mv}{n} + 2m - 2m = 2 \sum_{i=1}^{v} q_i - \frac{4mv}{n}.$$ 

Thus, $QE(G) = 2 \sum_{i=1}^{v} q_i - \frac{4mv}{n}$.

Using Theorem 2.6 in the above equality, we get

$$QE(G) \leq \frac{4mv}{n} + \sqrt{v(n - v) \left(8mn + n^2(\Delta(G) - \delta(G))^2\right)} - \frac{4mv}{n}$$

or

$$QE(G) \leq \sqrt{v(n - v) \left(8mn + n^2(\Delta(G) - \delta(G))^2\right)}$$

with equality if and only if equality holds in Theorem 2.6. For $1 \leq v \leq n - 1$, equality holds in Theorem 2.6 if and only if $G \cong K_n$ and $v = 1$. Clearly, for the complete graph $K_n$, $\frac{2m}{n} = \frac{n(n - 1)}{n} = n - 1$. Since signless Laplacian spectrum of $K_n$ is $\{2n - 2, (n - 2)^{n-1}\}$, therefore, it is clear that only the largest signless Laplacian eigenvalue $2n - 2$ of $K_n$ is greater than $n - 1$ and all the remaining are less than $n - 1$. This shows that $v = 1$ for the complete graph $K_n$. Therefore, equality holds in the main inequality if and only if $G \cong K_n$. This completes the proof. \hfill $\Box$
If we use Theorem 2.11 in place of Theorem 2.6 in Theorem 3.7, we get the following result.

**Theorem 3.8** Let $G$ be a connected graph of order $n$ with $m$ edges. Then

$$QE(G) \leq \frac{2\sqrt{m\nu(n - \nu)}\left(2\Delta(G)\delta(G)(n - 2m) + m(\Delta(G) + \delta(G))^2\right)}{n\sqrt{\Delta(G)\delta(G)}}$$

with equality if and only if $G \cong K_n$.

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**Declarations**

**Conflicts of interest** The authors declared that they have no conflict of interest.

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