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, ..., 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 $q_1 \ge q_2 \ge \cdots \ge q_n \ge 0$ 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 $1 \le k \le n$, respectively denote the sum of k largest and smallest signless Laplacian eigenvalues of G. The signless Laplacian energy of G is defined as $QE(G) = \sum_{i=1}^n |q_i - \overline{d}|$, where $\overline{d} = \frac{2m}{n}$ 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

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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 [7,21] 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 $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$ are the adjacency eigenvalues of G, the energy [13] of G is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. The quantity E(G) introduced by I. Gutman has well developed mathematical aspect and has noteworthy chemical applications (see [17]).

Let $D(G) = diag(d_1, d_2, \ldots, d_n)$ 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 $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n \ge 0$ and $q_1 \ge q_2 \ge \cdots \ge q_n \ge 0$ 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 [19]. The well-known Brouwer's conjecture, due to Brouwer [3] about the sum $S_k(G)$ is stated as follows.

Conjecture 1 If G is any graph with order n and size m, then

$$S_k(G) \le m + \binom{k+1}{2}$$
, for any $k \in \{1, 2, \dots, n\}$

Although Conjecture 1 has been studied extensively but it remains open at large. For the progress on Brouwer's Conjecture, we refer to [5, 11, 14] 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, ..., n, be the sum of k largest and smallest signless Laplacian eigenvalues of G, respectively. Motivated by the studies of Mohar [18], Jin et al. [16] 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. [2] proposed the following conjecture about $S_k^+(G)$.

Conjecture 2 If G is any graph with order n and size m, then

$$S_k^+(G) \le m + \binom{k+1}{2}$$
, for any $k \in \{1, 2, ..., n\}$.

To see the progress on this conjecture, we refer to [24] and the references therein.

The rest of the paper is organized as follows. In Section 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 Section 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 $M_1(G)$ [20] 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, ..., n. The following inequality can be found in [15].

Lemma 2.1 [15] 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 $0 \le m_1 \le a_i \le M_1$, $0 \le m_2 \le b_i \le M_2$ with $i = 1, 2, \ldots, n$ and $M_1M_2 \ne 0$. Let $\alpha = \frac{m_1}{M_1}$ and $\beta = \frac{m_2}{M_2}$. If $(1 + \alpha)(1 + \beta) \ge 2$, then

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

$$\sum_{i=1}^{n} d_i^2 \le \frac{4m^2}{n} + \frac{n}{4} (\triangle(G) - \delta(G))^2.$$
(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 $(1 + \alpha)(1 + \beta) \ge 2$ in Lemma 2.1 is satisfied. Substituting these values in Inequality 2.1, we get

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

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

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

that is,

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

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 nk^2 and the right hand side becomes $\frac{n^2k^2}{n} = nk^2$. This completes the proof.

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

Lemma 2.3 Let G be a connected graph of diameter D and e(G) distinct Q-eigenvalues. Then $D \le e(G) - 1$.

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 $\{2n-2, \underbrace{n-2, \ldots, n-2}_{n-1}\}$.

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

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

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 $n, m, \Delta(G)$ and $\delta(G)$ and characterize the extremal graphs.

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

$$S_{k}^{+}(G) \le \frac{2mk}{n} + \frac{\sqrt{k(n-k)\left(8mn + n^{2}(\triangle(G) - \delta(G))^{2}\right)}}{2n}$$
(2.3)

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

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

that is,

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

Let $S_k^+(G) = S_k^+$. Using the above equations with Lemma 2.5, we get

$$(q_{k+1} + \dots + q_n)^2 = (2m - S_k^+)^2 \le (n - k)(q_{k+1}^2 + \dots + q_n^2)$$
$$= (n - k)\left(2m + \sum_{v_i \in V(G)} d_{v_i}^2 - (q_1^2 + \dots + q_k^2)\right)$$
$$\le (n - k)\left(2m + \sum_{v_i \in V(G)} d_{v_i}^2 - \frac{S_k^{+2}}{k}\right).$$

Simplifying further, we get

$$S_k^{+2} - \frac{4mkS_k^+}{n} + \frac{4m^2k}{n} - \frac{k(n-k)}{n} \Big(2m + \sum_{v_i \in V(G)} d_{v_i}^2\Big) \le 0,$$

that is,

$$S_k^+ \le \frac{2mk}{n} + \frac{\sqrt{4m^2k^2 - 4knm^2 + nk(n-k)\left(2m + \sum_{v_i \in V(G)} d_{v_i}^2\right)}}{n}$$

or

$$S_k^+ \le \frac{2mk}{n} + \frac{\sqrt{k(n-k)\left(n(2m+\sum_{v_i \in V(G)} d_{v_i}^2) - 4m^2\right)}}{n}.$$
(2.4)

Using Lemma 2.2 in Inequality (2.4), we get

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

or

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

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 Lemma 2.5 and Lemma 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 $1 \le k \le n-1$, then

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

with equality if and only if $G \cong K_n$ and k = 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

$$q(G) \le \frac{2m}{n} + \frac{\sqrt{(n-1)\left(8mn + n^2(\triangle(G) - \delta(G))^2\right)}}{2n}$$

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

The following inequality can be seen in [22].

Lemma 2.9 [22] If a_i and b_i , $1 \le i \le n$, are positive real numbers, then

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

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

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

$$\sum_{i=1}^{n} d_i^2 \le \frac{m^2 \left(\triangle(G) + \delta(G)\right)^2}{n \triangle(G) \delta(G)}.$$
(2.5)

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

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

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

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

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

which is the required inequality.

For the equality part, let G be k-regular. Then the left hand side of Inequality 2.5 becomes nk^2 and the right hand side becomes $\frac{4k^4n^2}{4nk^2} = nk^2$. Thus equality holds in Inequality 2.5 whenever G is a regular graph.

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 $1 \le k \le n-1$, then

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

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

or

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

This proves Inequality 2.6.

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

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

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

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 $1 \le k \le n-1$, then

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

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 [17], has found remarkable chemical applications beyond the molecular orbital theory of conjucated molecules (see [23]).

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

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

To see the basic properties of this quantity, including various upper and lower bounds, we refer to [1,8,10,12]. 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 [9] Let G be a connected graph with n vertices and m edges. Then

$$q(G) \le \frac{2m}{n-1} + n - 2$$

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

$$QE(G) \le \frac{2m}{n(n-1)} + n - 2 + \sqrt{(n-1)\left(2m + \frac{n}{4}(\triangle(G) - \delta(G))^2 - \left(q(G) - \frac{2m}{n}\right)^2\right)}$$
(3.7)

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

Proof. It is easy to see that

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

Using this observations and Lemma 2.5, we get

$$\leq \frac{2m}{n-1} + n - 2 - \frac{2m}{n} + \sqrt{(n-1)\left(2m + \frac{n}{4}(\triangle(G) - \delta(G))^2 - \left(q_1 - \frac{2m}{n}\right)^2\right)}$$

(by using Lemma 3.1)

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

This proves the required inequality.

Assume that equality holds in Inequality 3.7. 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 3.7, then $G \cong K_n$.

Conversely, if $G \cong K_n$, then it is easy to see that the equality holds in Inequality 3.7.

The next lemma due to Cean [4] gives the upper bound for the sum of the squares of vertex degrees in a graph.

Lemma 3.3 [4] Let G be a graph with n vertices and m edges. Then

$$\sum_{u \in V(G)} d_u^2 \le m \left(\frac{2m}{n-1} + n - 2\right).$$

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

$$QE(G) \le \frac{2m}{n(n-1)} + n - 2 + \sqrt{(n-1)\left(mn + \frac{2m^2(2-n)}{n(n-1)} - \left(q(G) - \frac{2m}{n}\right)^2\right)}$$

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

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Data availability Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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