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# On resolvent signless Laplacian Estrada index of graphs

Ramin Nasiri<sup>1</sup>

Department of Mathematics, Faculty of Sciences, Imam Hossein Comprehensive University, Tehran, Iran

Ali Nakhaei Amroodi

Department of Computer, network and communications, Imam Hossein Comprehensive University, Tehran, Iran

#### Abstract

For a simple non-complete graph G on n vertices, the resolvent signless Laplacian Estrada index of G is defined as  $SLEE_r(G) = \sum_{i=1}^n \left(1 - \frac{q_i}{2n-2}\right)^{-1}$ , where  $q_1 \ge q_2 \ge \ldots \ge q_n$  are the eigenvalues of the signless Laplacian matrix of G. In this work, we introduce the extremal trees with respect to this consept, finally we establish some lower bounds for  $SLEE_r$ .

Keywords: resolvent signless Laplacian Estrada index, spectral moment, eigenvalues.

# 1 Introduction

For a simple graph G of order n, the adjacency matrix  $\mathbf{A} = [a_{ij}]$  of G is the  $n \times n$  matrix in which  $a_{ij} = 1$  if the vertices i and j are adjacent, and  $a_{ij} = 0$  otherwise. The matrix  $\mathbf{Q}(G) = \mathbf{D}(G) + \mathbf{A}(G)$  is called the signless Laplacian matrix of G, where  $\mathbf{D}(G) = diag(d_1, d_2, \dots, d_n)$  is the diagonal matrix of G. The set of all eigenvalues of  $\mathbf{Q}(G)$  are denoted by  $\mathbf{Q}-Spec(G) = \{q_1, \dots, q_n\}, q_1 \ge q_2 \ge \dots \ge q_n \ge 0$ .

It is well-known that  $q_1 = 2n - 2$  if and only if G is a complete graph  $K_n$ . Hence, we have to consider non-complete graphs in definition of resolvent signless Laplacian Estrada index of G. The resolvent signless Laplacian Estrada index of G is defined as:

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

One can see that we can write this quantity as:

$$SLEE_r(G) = tr\left(\mathbf{I} - \frac{1}{2n-2}\mathbf{Q}(G)\right)^{-1}.$$
 (2)

Notice that if  $G \not\cong K_n$ , then for each i = 0, 1, ..., n,  $q_i < 2n - 2$ , and therefore  $0 \le \frac{q_i}{2n-2} < 1$ . Thus, we may use the Maclaurin series for  $(1 - \frac{q_i}{2n-2})^{-1}$  to evaluate  $SLEE_r(G)$ . In an exact phrase,

$$SLEE_r(G) = \sum_{k \ge 0} \frac{T_k(G)}{(2n-2)^k},$$
(3)

 $^{1}\mathrm{speaker}$ 

where  $T_k(G)$  denotes to the k-th signless Laplacian spectral moment of the graph G, i.e.  $T_k(G) = \sum_{i=1}^n q_i^k$ . It is well-known that  $T_k(G)$  equals to the number of closed semi-edge walks of length k, see [?] and so for some small values of k, it is possible to evaluate  $T_k(G)$  in terms of some graph parameters. For example,  $T_0(G) = n$ ,  $T_1(G) = 2m$ ,  $T_2(G) = Zg_1(G) + 2m$  and  $T_3(G) = 6t + 3Zg_1(G) + \sum_{v \in V(G)} d^3(v)$ , where  $Zg_1(G)$ and  $Zg_2(G)$  are the first and second Zagreb indices of garph G.

### 2 Main results

In this section, some results for the resolvent signless Laplacian Estrada index are presented. Assume that G is a simple *n*-vetex graph with signless Laplacian eigenvalues  $q_1 \ge q_2 \ge \ldots \ge q_n$ . In the following Lemma, the resolvent signless Laplacian Estrada index is computed by the characteristic polynomial of  $\mathbf{Q}$ .

**Lemma 2.1.** Let G be a non-complete n-vertex graph. Then,

$$SLEE_r(G) = (2n-2)\frac{\Phi'_G(2n-2)}{\Phi_G(2n-2)},$$

where  $\Phi_G(x)$  is the characteristic polynomial of the matrix **Q**.

In the following, the quantity  $SLEE_r$  for some trees are computed. We start by an example applicable in chemistry.

**Example 2.2.** Apply Lemma ??, we can calculate the resolvent signless Laplacian Estrada index of graphs by their **Q**-polynomial. As an example, one can easily seen that  $\Phi_{CH_4}(x) = x^5 - 8x^4 + 18x^3 - 16x^2 + 5x$  and  $\Phi_{C_2H_6}(x) = x^8 - 14x^7 + 73x^6 - 182x^5 + 244x^4 - 182x^3 + 73x^2 - 14x + 1$ , where  $CH_4$  and  $C_2H_6$ , Figure 1, are molecular graphs of the Methane and Ethane molecules, respectively.



Figure 1: Molecular graphs of Methane and Ethane

Hence, by Lemma ??,

$$SLEE_{r}(CH_{4}) = 8 \cdot \frac{5x^{4} - 32x^{3} + 54x^{2} - 32x + 5}{x^{5} - 8x^{4} + 18x^{3} - 16x^{2} + 5x} \Big|_{x=8} \simeq 7.09524$$
  

$$SLEE_{r}(C_{2}H_{6}) = 14 \cdot \frac{8x^{7} - 98x^{6} + 438x^{5} - 910x^{4} + 976x^{3} - 546x^{2} + 146x - 14}{x^{8} - 14x^{7} + 73x^{6} - 182x^{5} + 244x^{4} - 182x^{3} + 73x^{2} - 14x + 1} \Big|_{x=14}$$
  

$$\simeq 9.37856.$$

**Lemma 2.3.** Let G be a graph and  $e \in E(G)$ . Then  $SLEE_r(G-e) < SLEE_r(G)$ .

**Lemma 2.4.** Let T be a tree on n vertices, also  $P_n$  and  $S_n$  are the path and star trees, respectively. Then

$$\sum_{i=1}^{n} \frac{n-1}{n-2-\cos(\frac{\pi i}{n})} = SLEE_r(P_n) \le SLEE_r(T) \le SLEE_r(S_n) = \frac{2n^3 - 4n^2 - n + 4}{2n^2 - 7n + 6},$$

with left equality if and only if  $T \cong P_n$  and right equality if and only if  $T \cong S_n$ .

**Lemma 2.5.** Let G be a non-complete graph on n vertices. Then,

$$n = SLEE_r(\overline{K_n}) \le SLEE_r(G) \le SLEE_r(K_n - e).$$

Moreover, if G is a connected non-complete graph on n vertices, then

$$SLEE_r(P_n) \leq SLEE_r(G) \leq SLEE_r(K_n - e).$$

Up to now, many lower and upper bounds for the largest and least signless Laplacian eigenvalues  $q_1$  and  $q_n$  were given. In [?, ?], bounds on the signless Laplacian spectral radius  $q_1(G)$  in terms of n and m of a connected graph G are investigated as:

$$\frac{4m}{n} \le q_1(G) \le \frac{2m}{n-1} + n - 2 \tag{4}$$

and left equality holds if and only if G is a regular graph and right equality holds if and only if G is  $S_n$  or  $K_n$ . Also, for the least **Q**-eigenvalue  $q_n(G)$  are the following [?, ?]:

$$\frac{2m}{n-2} - n + 1 \le q_n(G) < \delta.$$
<sup>(5)</sup>

It is well known that the empty graph  $\overline{K_n}$  is the unique graph with exactly one  $\mathbf{Q}$ -eigenvalue. Cvetković [?] proved that if G is a connected graph with r distinct signless Laplacian eigenvalues and diameter d, then  $d \leq r - 1$ . On the other hand, we know that the complete graph  $K_n$  is the unique connected graph with diameter one. Therefore, we can deduce that the complete graph  $K_n$  is the unique connected graph with exactly two  $\mathbf{Q}$ -eigenvalues. In the following Lemma, connected graphs which have three distinct  $\mathbf{Q}$ -eigenvalues are characterized.

**Lemma 2.6.** [?] Let G be a connected graph of order  $n \ge 4$ . Then G has a Q-eigenvalue of multiplicity n-2 if and only if G is one of the graphs  $K_n - e, S_n, K_{\frac{n}{2}, \frac{n}{2}}, \overline{K_3 + S_4}$  or  $\overline{K_1 + 2K_3}$ .

**Example 2.7.** In what follows, we compute the signless laplacian spectrum of graphs which are mentioned in the above lemma.

$$\begin{aligned} \mathbf{Q} - Spec(K_n - e) &= \left\{ [\frac{3n - 6 \pm \sqrt{n^2 + 4n - 12}}{2}]^1, [n - 2]^{n-2} \right\} \\ \mathbf{Q} - Spec(S_n) &= \left\{ [n]^1, [1]^{n-2}, [0]^1 \right\} \\ \mathbf{Q} - Spec(K_{\frac{n}{2}, \frac{n}{2}}) &= \left\{ [n]^1, [\frac{n}{2}]^{n-2}, [0]^1 \right\} \\ \mathbf{Q} - Spec(\overline{K_3 + S_4}) &= \left\{ [9]^1, [4]^{n-2}, [1]^1 \right\} ; n = 7 \\ \mathbf{Q} - Spec(\overline{K_1 + 2K_3}) &= \left\{ [9]^1, [4]^{n-2}, [1]^1 \right\} ; n = 7 \end{aligned}$$

We are now ready to present some lower bounds for resolvent signless Laplacian Estrada index of graphs. Lemma 2.8. Let G be a graph with n vertices and m edges, and let  $I \subseteq \{1, 2, ..., n\}$ , then

$$SLEE_r(G) \geq \sum_{j \in I} \frac{2n-2}{2n-2-q_j} + \frac{(2n-2)(n-n')^2}{(2n-2)(n-n')-2m + \sum_{j \in I} q_j}$$

where n' = n(I), and equality holds if and only if  $q_i = q_j$ , for all  $i, j \notin I$ .

**Theorem 2.9.** Let G be a non-complete connected graph or empty graph with n vertices, m edges, maximum degree  $\Delta$ , minimum degree  $\delta$  and average degree  $\overline{d}$ . also let  $1 \leq s < r \leq n$ . Then,

0

$$\begin{aligned} (1). \ SLEE_r(G) &\geq \frac{n^2 (n-1)}{n (n-1) - m} \\ (2). \ SLEE_r(G) &\geq \frac{n (n-1)}{n (n-1) - 2m} + \frac{n (n-1)^3}{n (n-1)^2 + 2m - mn} \\ (3). \ SLEE_r(G) &\geq \frac{2n-2}{2n-2-q_2} + \frac{2n-2}{2n-2-q_s} + \frac{(2n-2) (n-2)^2}{(2n-2)(n-2) - 2m + q_r + q_s} \\ (4). \ SLEE_r(G) &> \frac{2n-2}{2n-2-2\overline{d}} + \frac{2n-2}{2n-1-\overline{d}} + \frac{(2n-2) (n-2)^2}{(2n-2) (n-2) - 2m + n - 2 + 2\Delta} \\ &\geq \frac{2n-2}{2n-2-2\delta} + \frac{2n-2}{2n-1-\delta} + \frac{(2n-2) (n-2)^2}{(2n-2) (n-2) - 2m + n - 2 + 2\Delta} \end{aligned}$$

The equalities in parts (1) and (2) hold if and only if  $G \cong \overline{K_n}$ , and in (3) holds if and only if  $G \cong \overline{K_n}$ ,  $K_n - e, S_n, K_{\frac{n}{2}, \frac{n}{2}}, \overline{K_3 + S_4}$  or  $\overline{K_1 + 2K_3}$ .

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e-mail: rnasiri@ihu.ac.ir e-mail: Kpnakhaei@ihu.ac.ir