On the distance signless Laplacian Estrada index of graphs

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Abstract. The distance signless Laplacian eigenvalues $\rho_1, \rho_2, \ldots, \rho_n$ of a connected graph G are the eigenvalues of the distance signless Laplacian matrix of G, defined as $D^Q(G) = Tr(G)+D(G)$, where $D(G)$ is the distance matrix of G and $Tr(G)$ is the diagonal matrix of vertex transmissions of G. In this paper we define and investigate the distance signless Laplacian Estrada index of the graph G as $D^QEE(G) = \sum_{i=1}^{n} e^{\rho_i}$ and obtain some upper and lower bounds for $D^QEE(G)$ in terms of other graph invariants. We also obtain some relations between $D^QEE(G)$ and the the distance signless Laplacian energy-like invariant of G.

Keywords: Distance signlees Laplacian matrix; distance signlees Laplacian Estrada index; transmission regular graph; distance signless Laplacian energy-like invariant.

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1 Introduction and preliminaries

In this paper, we consider only connected, undirected, simple and finite graphs. A graph is denoted by $G = (V(G), E(G))$, where $V(G)$ is its vertex set and $E(G)$ is its edge set. The *order* of G is the number $n = |V(G)|$ and its *size* is the number $m = |E(G)|$. The set of vertices adjacent to $v \in V(G)$, denoted by $N(v)$, refers to the *neighborhood* of v. The *degree* of v, denoted by $d_G(v)$ (we simply write d_v if it is clear from the context) means the cardinality of $N(v)$. A graph is called *regular* if each of its vertex has the same degree. The *distance* between two vertices $u, v \in V(G)$, denoted by d_{uv}, is defined as the length of a shortest path between u and v in G. The *diameter* of G is the maximum distance between any two vertices of G. The *distance matrix* of G is denoted by $D(G)$ and is defined as $D(G) = (d_{uv})_{u,v \in V(G)}$. The *transmission* $Tr_G(v)$ of a vertex v is defined to be the sum of the distances from v to all other vertices in G, i.e., $Tr_G(v) = \sum\limits_{u \in V(G)} d_{uv}$. A graph G is said to be *k-transmission regular* if $Tr_G(v) = k$, for each $v \in V(G)$. The *transmission* of a graph G, denoted by $\sigma(G)$, is the sum of distances between all unordered pairs of vertices in G. Clearly, $\sigma(G) = \frac{1}{2} \sum\limits_{v \in V(G)} Tr_G(v)$.

For a graph G with $V(G) = \{v_1, v_2, \ldots, v_n\}$, $Tr_G(v_i)$ has been referred as the *transmission degree* Tr_i [27] and hence the *transmission degree sequence* is given by $\{Tr_1, Tr_2, \ldots, Tr_n\}$. Let $Tr(G) = diag(Tr_1, Tr_2, \ldots, Tr_n)$ be the diagonal matrix of vertex transmissions of G. M. Aouchiche and P. Hansen [1, 2] introduced the Laplacian and the signless Laplacian for the distance matrix of a connected graph. The matrix $D^L(G) = Tr(G) - D(G)$ is called the *distance Laplacian matrix* of G, while the matrix $D^Q(G) = Tr(G) + D(G)$ is called the *distance signless Laplacian matrix of* G.

If G is connected, then $D^Q(G)$ is symmetric, nonnegative and irreducible. Hence, all the eigenvalue of $D^Q(G)$ can be arranged as: $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$, where ρ_1 is called the *distance signless Laplacian spectral radius* of G. (From now onwards, we will denote $\rho_1(G)$ by $\rho(G)$). As $D^Q(G)$ is irreducible, by the Perron-Frobenius theorem, $\rho(G)$ is positive, simple and there is a unique positive unit eigenvector X corresponding to $\rho(G)$, which is called the *distance signless Laplacian Perron vector* of G.

Based on investigations on geometric properties of biomolecules [13, 14], Ernesto Estrada considered an expression of the form

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i},$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of a molecular graph G. The mathematical significance of this quantity was recognized short time later [22] and soon it became known under the name "Estrada index" [10]. The mathematical properties of the Estrada index have been intensively studied, see e.g. [6, 8, 10, 23, 24, 34]. There exist a vast literature related to Estrada index and its bounds. We refer the reader to consult the nice surveys [11, 21].

This graph-spectrum-based invariant has also an important role in chemistry and physics. For example, it is used as a measure for the degree of folding of long chain polymeric molecules

[12, 13, 16]. It has found a number of applications in complex networks and characterizes the centrality [14] as well as robustness [35] of complex networks. For the application of the Estrada index in network theory see the book [15].

The pioneering papers [13, 14] further proposes the study of graphs with an analogue of the Estrada index defined with respect to other (than adjacency) matrices. Because of the evident success of the graph Estrada index, this proposal has been put into effect and Estrada index based of the eigenvalues of other graph matrices have, one-by-one, been introduced: Estrada index based invariant with respect to distance matrix, as well as Estrada index based invariant with respect to Laplacian matrix, have been introduced and studied, see e.g. [7,9,25,26,28,31–33,37]. Quite recently, in full analogy with the Estrada index, the signless Laplacian Estrada index of a connected graph G was introduced and studied [4, 5].

From this respect, we define the distance signless Laplacian Estrada index $D^Q EE(G)$, based on distance signless Laplacian matrix of the graph G as the following:

$$D^Q EE(G) = \sum_{i=1}^{n} e^{\rho_i}. \tag{1.1}$$

where $\rho_1, \rho_2, \ldots, \rho_n$ are the distance signlees Laplacian eigenvalues of a graph G.
Let

$$M_k = \sum_{i=1}^{n} (\rho_i)^k.$$

Recalling the power series expansion of e^x we have another expression of distance signless Laplacian Estrada index as the following

$$D^Q EE(G) = \sum_{k\geq 0} \frac{M_k}{k!} = \sum_{k\geq 0} \frac{tr(D^Q(G))}{k!}. \tag{1.2}$$

In this paper, not only we obtain some upper and lower bounds for $D^Q EE(G)$ in terms of other graph invariants, but also characterize the extremal graphs. We also present some relations between distance signless Laplacian Estrada index and the the distance signless Laplacian energy-like invariant of G.

2 Bounds for the distance signless Laplacian Estrada index

We start by mentioning the following lemmas, they will be useful to derive our main results in the sequel.

Lemma 2.1 [3, Theorem 2.7] If G is graph of order n, having maximum degree Δ_1 and second maximum degree Δ_2, then

$$\rho_1 \geq 4n - 4 - \Delta_1 - \Delta_2,$$

with equality holding if and only if G is a regular graph with diameter less than or equal to 2.

Lemma 2.2 [3, Theorem 2.2] If the transmission degree sequence of G is $\{Tr_1, Tr_2, \ldots, Tr_n\}$, then

$$\rho_1 \geq 2\sqrt{\frac{\sum_{i=1}^{n} Tr_i^2}{n}},$$

with equality holding if and only if G is transmission regular.

Lemma 2.3 [36, Lemma 2.2] If G is a connected graph of order n, then

$$\rho_1 \geq \frac{4\sigma(G)}{n},$$

with equality holding if and only if G is transmission regular.

Lemma 2.4 *A connected graph G has two distinct D^Q-eigenvalues if and only if G is a complete graph.*

The proof is analogous to that of [29, Lemma 2].

Theorem 2.5 *Let G be an r-regular graph of diameter 2, and let its adjacency spectrum be $spec_A(G) = \{r, \lambda_2, \ldots, \lambda_n\}$. Then $spec_{D^Q}(G) = \{2(2n-r-2), 2n-\lambda_2-r-4, \ldots, 2n-\lambda_n-r-4\}$.*

The result follows from the fact that the D^Q-matrix of G is $A + 2\bar{A} + (2n-2)I - Diag(Deg)$, where $\bar{A} = J - I - A$, A is the adjacency matrix of G, $\bar{A}$ is the adjacency matrix of G, J is a matrix whose all entries are equal to 1 and I is an identity matrix.

We first present some bounds for the distance signless Laplacian Estrada index.

Theorem 2.6 *Let G be a connected graph with n vertices. Then*

$$D^Q EE(G) \geq e^{\frac{4\sigma(G)}{n}} + (n-1)e^{\frac{2\sigma(G)(n-2)}{n(n-1)}}, \tag{2.3}$$

with equality holds if and only if $G = K_n$.

Starting with the equation (1.1) and using arithmetic-geometric mean inequality, we get

$$\begin{aligned} D^{Q}EE(G) &= e^{\rho_1} + e^{\rho_2} + \cdots + e^{\rho_n} \\ &\geq e^{\rho_1} + (n-1)\left(\prod_{i=2}^{n} e^{\rho_i}\right)^{\frac{1}{n-1}} && (2.4) \\ &= e^{\rho_1} + (n-1)\left(e^{2\sigma(G)-\rho_1}\right)^{\frac{1}{n-1}}. && (2.5) \end{aligned}$$

Consider the following function

$$f(x) = e^{x} + \frac{n-1}{e^{\frac{x-2\sigma(G)}{n-1}}}$$

for $x > \frac{2\sigma(G)}{n}$. We have

$$f'(x) = e^{x} - e^{\frac{2\sigma(G)-x}{n-1}} > 0$$

for $x > \frac{2\sigma(G)}{n}$. It is easy to see that f is an increasing function for $x > \frac{2\sigma(G)}{n}$. From the equation (2.5) and Lemma 2.3, we obtain

$$D^{Q}EE(G) \geq e^{\frac{4\sigma(G)}{n}} + \frac{n-1}{e^{\frac{2\sigma(G)(2-n)}{n(n-1)}}}. \tag{2.6}$$

This completes the first part of the proof. Now we suppose that the equality holds in (2.3). Then all inequalities in the above argument must be equalities. From (2.6) we have $\rho_1 = \frac{4\sigma(G)}{n}$, which implies G is a transmission regular graph. From (2.4) and Arithmetic-Geometric Mean inequality we get $\rho_2 = \rho_3 = \cdots = \rho_n$. Therefore G has exactly two distinct eigenvalues, by Lemma 2.4, G is the complete graph K_n.

Conversely, one can easily see that the equality holds in (2.3) for the complete graph K_n. This completes the proof.

Lemma 2.7 *Let G be a connected graph with n vertices. Then*

$$D^{Q}EE(G) \leq n + 2\sigma(G) - 1 - \sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2} + e^{\sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2}}.$$

For $k \geq 3$,

$$\begin{aligned} \left(\sum_{i=1}^{n} \rho_i^2\right)^{k} &\geq \sum_{i=1}^{n} \rho_i^{2k} + k \sum_{1\leq i<j\leq n} \left(\rho_i^2 \rho_j^{2(k-1)} + \rho_i^{2(k-1)} \rho_j^2\right) \\ &\geq \sum_{i=1}^{n} \rho_i^{2k} + 2k \sum_{1\leq i<j\leq n} \rho_i^k \rho_j^k \geq \left(\sum_{i=1}^{n} \rho_i^k\right)^2, \end{aligned}$$

and then

$$\sum_{i=1}^{n}\rho_i^k \leq \left(\sum_{i=1}^{n}\rho_i^2)^{\frac{k}{2}} = (2\sum_{1\leq i<j\leq n}(d_{ij})^2+\sum_{i=1}^{n}Tr_i^2\right)^{\frac{k}{2}}.$$

It is easily seen that

$$\begin{aligned} D^QEE(G) &= n+2\sigma(G)+\sum_{k\geq 2}\frac{1}{k!}\sum_{i=1}^{n}\rho_i^k \leq n+2\sigma(G)+\sum_{k\geq 2}\frac{1}{k!}\left(\sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2+\sum_{i=1}^{n}Tr_i^2}\right)^k \\ &= n+2\sigma(G)-1-\sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2+\sum_{i=1}^{n}Tr_i^2}+e^{\sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2+\sum_{i=1}^{n}Tr_i^2}}. \end{aligned}$$

Theorem 2.8 *Let G be a connected graph of order n and diameter d. Then*

$$\sqrt{2n^3-n+(n-1)e^{2(n-1)}} \leq D^QEE(G) \leq n-1+e^{\sqrt{n(n-1)d^2+\frac{n^3(n-1)^2}{4}}}. \tag{2.7}$$

Equality holds on both sides of (2.7) if and only if $G\cong K_1$.

Lower bound: Directly from Eq. (1.1) we get

$$D^QEE^2(G)=\sum_{i=1}^{n}e^{2\rho_i}+2\sum_{i<j}e^{\rho_i}e^{\rho_j}. \tag{2.8}$$

By the arithmetic-geometric mean inequality, we get

$$\begin{aligned} 2\sum_{i<j}e^{\rho_i}e^{\rho_j} &\geq n(n-1)\left(\prod_{i>j}e^{\rho_i}e^{\rho_j}\right)^{\frac{2}{n(n-1)}} \\ &= n(n-1)\left[\left(\prod_{i=1}^{n}e^{\rho_i}\right)^{n-1}\right]^{\frac{2}{n(n-1)}} \\ &= n(n-1)(e^{2\sigma(G)})^{\frac{2}{n}} \\ &= n(n-1)e^{\frac{4\sigma(G)}{n}}. \end{aligned} \tag{2.9}$$

By means of a power-series expansion, we obtain

$$\sum_{i=1}^{n}e^{2\rho_i}=\sum_{i=1}^{n}\sum_{k\geq 0}\frac{(2\rho_i)^k}{k!}=n+4\sigma(G)+4\sum_{1\leq i<j\leq n}(d_{ij})^2+2\sum_{i=1}^{n}Tr_i^2+\sum_{i=1}^{n}\sum_{k\geq 3}\frac{(2\rho_i)^k}{k!}.$$

Since we want to get as good a lower bound as possible, it looks reasonable to replace $\sum_{k\geq 3}\frac{(2\rho_i)^k}{k!}$ by $4\sum_{k\geq 3}\frac{(\rho_i)^k}{k!}$. However, we use a multiplier $t\in[0,4]$ instead of $4=2^2$, so as to arrive at

$$\begin{aligned}
\sum_{i=1}^{n} e^{2\rho_i} &\geq n+4\sigma(G)+4\sum_{1\leq i<j\leq n}(d_{ij})^2+2\sum_{i=1}^{n}Tr_i^2+t\sum_{i=1}^{n}\sum_{k\geq 3}\frac{(\rho_i)^k}{k!}\\
&= n+4\sigma(G)+4\sum_{1\leq i<j\leq n}(d_{ij})^2+2\sum_{i=1}^{n}Tr_i^2-tn-2t\sigma(G)-t\sum_{1\leq i<j\leq n}(d_{ij})^2\\
&- \frac{t}{2}\sum_{i=1}^{n}Tr_i^2+t\sum_{i=1}^{n}\sum_{k\geq 0}\frac{(\rho_i)^k}{k!}\\
&= n(1-t)+2\sigma(G)(2-t)+(4-t)\sum_{1\leq i<j\leq n}(d_{ij})^2+(2-\frac{t}{2})\sum_{i=1}^{n}Tr_i^2+tD^QEE(G).
\end{aligned}$$

Since $\sigma(G)\geq\frac{n(n-1)}{2}$, $\sum_{1\leq i<j\leq n}(d_{ij})^2\geq\frac{n(n-1)}{2}$ and $\sum_{i=1}^{n}Tr_i^2\geq n(n-1)^2$, then we have

$$\begin{aligned}
\sum_{i=1}^{n} e^{2\rho_i} &\geq n(1-t)+n(n-1)(2-t)+(4-t)\frac{n(n-1)}{2}\\
&+ (2-\frac{t}{2})(n(n-1)^2)+tD^QEE(G).
\end{aligned} \tag{2.10}$$

By substituting (2.9) and (2.10) back in to (2.8), and solving for $D^QEE(G)$, we get

$$D^QEE(G)\geq\frac{1}{2}(t+\sqrt{t^2+8n^3-4n-2tn^2(n+1)+4n(n-1)e^{2(n-1)}}).$$

It is easy to see that for $n\geq 2$ the function

$$f(x):=\frac{1}{2}(x+\sqrt{x^2+8n^3-4n-2xn^2(n+1)+4n(n-1)e^{2(n-1)}}).$$

monotonically decreases in the interval $[0,4]$. As a result, the best bound for $D^QEE(G)$ is attained for $t=0$. This gives us the first part of the Theorem.

Upper bound: Starting from the following inequality, we get

$$\begin{aligned}
D^Q EE(G) &= n + \sum_{i=1}^{n} \sum_{k\geq 1} \frac{(\rho_i)^k}{k!} \\
&= n + \sum_{i=1}^{n} \sum_{k\geq 1} \frac{|\rho_i|^k}{k!} \\
&= n + \sum_{k\geq 1} \frac{1}{k!} \sum_{i=1}^{n} (\rho_i^2)^{\frac{k}{2}} \\
&\leq n + \sum_{k\geq 1} \frac{1}{k!} [\sum_{i=1}^{n} (\rho_i^2)]^{\frac{k}{2}} \\
&= n + \sum_{k\geq 1} \frac{1}{k!} [2 \sum_{1\leq i<j\leq n} (d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2]^{\frac{k}{2}} \\
&= n - 1 + \sum_{k\geq 0} \frac{(\sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2})^k}{k!} \\
&= n - 1 + e^{\sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2}}.
\end{aligned}$$

Since, $d_{ij} \leq d$ for $i \neq j$ and there are $\frac{n(n-1)}{2}$ pairs of vertices in G, we have $2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2 \leq 2\frac{n(n-1)}{2} d^2 + \frac{n^3(n-1)^2}{4}$, then

$$D^Q EE(G) \leq n - 1 + e^{\sqrt{n(n-1)d^2 + \frac{n^3(n-1)^2}{4}}}.$$

Hence we get the right-hand side of inequality of (2.7).
From the derivation of (2.7) it is clear that equality holds if and only if the graph G has all zero D^Q-eigenvalues. Since G is a connected graph, this only happens in the case of $G \cong K_1$. Hence we get the proof.

Lemma 2.9 *Let G be a k-transmission regular graph with n vertices. Then*

$$D^Q EE(G) \geq ne^k. \tag{2.11}$$

Note that the distance signless Laplacian spectrum of the graph G consists of $k+\mu_1 \geq k+\mu_2 \geq \cdots \geq k+\mu_n$, where $\mu_1 \geq \cdots \geq \mu_n$ are the distance spectrum of G. Then $D^Q EE(G) = \sum_{i=1}^{n} e^{k+\mu_i}$ and thus by the arithmetic-geometric mean inequality,

$$D^Q EE(G)e^{-k} = \sum_{i=1}^{n} e^{\mu_i} \geq ne^{\frac{1}{n}\sum_{i=1}^{n}\mu_i} = n,$$

from which we arrive at the inequality (2.11).

Theorem 2.10 *Let G be a connected graph on $n \geq 2$ vertices with maximum degree Δ_1 and second maximum degree Δ_2. Then*

$$D^Q EE(G) \geq e^{4n-4-\Delta_1-\Delta_2} + (n-1)e^{\frac{2\sigma(G)-4n+4+\Delta_1+\Delta_2}{n-1}}, \tag{2.12}$$

and equality holds if and only if $G = K_n$.

Using the arithmetic-geometric mean inequality, we obtain

$$\begin{aligned} D^Q EE(G) &= e^{\rho_1} + \sum_{i=2}^{n} e^{\rho_i} \\ &\geq e^{\rho_1} + (n-1)(e^{\sum_{i=2}^{n}\rho_i})^{\frac{1}{n-1}} \\ &= e^{\rho_1} + (n-1)e^{\frac{2\sigma(G)-\rho_1}{n-1}}, \end{aligned}$$

with equality if and only if $\rho_2 = \rho_3 = \cdots = \rho_n$.
For $x > \frac{2\sigma(G)}{n}$, define $f(x) = e^x + (n-1)e^{\frac{2\sigma(G)-x}{n-1}}$. It is easy to see that $f'(x) = e^x - e^{\frac{2\sigma(G)-x}{n-1}} > 0$ for any $x > \frac{2\sigma(G)}{n}$. Then by Lemma 2.1, we have

$$D^Q EE(G) \geq f(\rho_1) \geq f(4n-4-\Delta_1-\Delta_2),$$

and (2.12) follows. Note that the complete graph K_n has distance signless Laplacian spectrum $\{2n-2, n-2, n-2, \ldots, n-2\}$. Hence, if $G = K_n$, we obtain $D^Q EE(G) = e^{2n-2} + (n-1)e^{n-2}$, and the equality holds in (2.12).

Conversely, if the equality holds in (2.12) then G must be a regular graph, say $r-$regular, with diameter at most 2 by Lemma 2.1. Then $D^Q(G) = 2(J-I) - A + (2n-2)I - Diag(Deg)$. Employing Theorem 2.6 and the fact that $\rho_2 = \rho_3 = \cdots = \rho_n$, we conclude that $\rho_1(A) = r, \rho_2(A) = \cdots = \rho_n(A)$. Since the trace of A is zero, we know that $\rho_1(A) > \rho_2(A)$. It is well known that a connected graph with two distinct adjacency eigenvalues must be complete, which completes the proof.

Theorem 2.11 *Let G be an r-regular graph of diameter 2. Then*

$$D^Q EE(G) = e^{4n-2r-4} - e^{3n-2r-4} + e^{2n-r-3} EE(\bar{G}).$$

It is well known that (see [17]) the adjacency eigenvalues of $\bar{G}$ are $\{n-r-1, -1-\lambda_2(A)), -1-\lambda_3(A), \ldots, -1-\lambda_n(A)\}$. Hence $EE(\bar{G}) = \sum_{i=1}^{n} e^{\lambda_i(A(\bar{G}))} = e^{n-r-1} + e^{-1-\lambda_2(A)} + \ldots + e^{-1-\lambda_n}$. Then by Theorem 2.6, we have

$$\begin{aligned} D^Q EE(G) &= \sum_{i=1}^{n} e^{\rho_i} = e^{2(2n-r-2)} + e^{2n-\lambda_2-r-4} + \ldots + e^{2n-\lambda_n-r-4} \\ &= e^{4n-2r-4} - e^{3n-2r-4} + e^{2n-r-3} EE(\bar{G}). \end{aligned}$$

Let $M(G)=(\prod_{i=1}^{n}Tr_i)^{\frac{1}{n}}$ be the geometric mean of the transmission degrees sequence. Then $\frac{2\sigma(G)}{n}\geq M(G)$ holds, and equality is attained if and only if $Tr_1=\cdots=Tr_n$ (i.e., the graph G is transmission regular (Hilano Nomura, 1984)).

Lemma 2.12 [38] Let $a_1,a_2,\ldots,a_n$ be nonnegative numbers. Then

$$n\left[\frac{1}{n}\sum_{i=1}^{n}a_i-\left(\prod_{i=1}^{n}a_i\right)^{\frac{1}{n}}\right]\leq n\sum_{i=1}^{n}a_i-\left(\sum_{i=1}^{n}a_i^{\frac{1}{2}}\right)^2$$

Theorem 2.13 *Let G be a connected graph. Then*

$$D^QEE(G)\geq e^{2\sqrt{\frac{4\sigma^2(G)-M^2(G)n}{n(n-1)}}}+\frac{n-1}{e^{\frac{1}{n-1}\left[2\sqrt{\frac{4\sigma^2(G)-M^2(G)n}{n(n-1)}}-2\sigma(G)\right]}},$$

and equality holds if and only $G=K_n$.

Using the arithmetic-geometric mean inequality, we obtain

$$\begin{aligned} D^QEE(G) &= \sum_{i=1}^{n}e^{\rho_i} \\ &\geq e^{\rho_1}+(n-1)e^{\frac{2\sigma(G)-\rho_1}{n-1}}. \end{aligned} \tag{2.13}$$

By Lemma 2.2, $\rho_1\geq 2\sqrt{\frac{\sum_{i=1}^{n}Tr_i^2}{n}}$. Setting $\sqrt{a_i}=Tr_i$ in Lemma 2.12, we get

$$n^2\left[\frac{\sum_{i=1}^{n}Tr_i^2}{n}-\left(\frac{2\sigma(G)}{n}\right)^2\right]\geq\sum_{i=1}^{n}Tr_i^2-n\left(\prod_{i=1}^{n}Tr_i^2\right)^{\frac{1}{n}}.$$

Combining this with Lemma 2.2, yields

$$\rho_1\geq 2\sqrt{\frac{4\sigma^2(G)-M^2(G)n}{n(n-1)}}\geq 0. \tag{2.14}$$

Clearly $4\sigma^2(G)=M^2(G)n$, if and only if $n=1$. Similar to the Theorem 2.10, we get the result. Note that when $G=K_n$ we have $\rho_1=2n-2,\rho_2=\cdots=\rho_n=n-2$, $\sigma(G)=\frac{n(n-1)}{2}$ and $M(G)=n-1$. Hence, $D^QEE(G)=e^{2n-2}+(n-1)e^{n-2}$ and the equality holds.

Conversely, suppose that the equality holds, then from (2.13) we have $\rho_2=\cdots=\rho_n$. It follows from (2.14) that $\rho_1\geq 0$. Then G has exactly two distinct D^Q-eigenvalues, and Lemma 2.4 indicates that G is the complete graph K_n.

Let G be a k-transmission regular graph. Then $\sigma(G)=\frac{nk}{2}$ and $M(G)=k$, and hence the following result is immediate.

Corollary 2.14 *Let G be k-transmission regular. Then*

$$D^Q EE(G) \geq e^{2k} + (n-1)e^{\frac{k(n-2)}{n-1}},$$

with equality holds if and only $G = K_n$.

The concept of energy of a graph was defined in 1978 by Ivan Gutman [19] and have its origin in theoretical chemistry. Let G be a simple graph of order n with adjacency matrix $A(G)$ having eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then the *energy* of a graph G, denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$ (see [20] for details and recent survey). Recently, many results have been obtained about the energy of different graph structures. The pioneering paper [19] further proposes the study of energy in graphs with an analogue of the energy defined with respect to other (than adjacency) matrices assigned to the graphs. This proposal has been put into effect and extended: the energy of a graph with respect to Laplacian matrix as well as the energy of a graph with respect to distance matrix, have been introduced and studied (see [26, 30] for more details in this subject). For distance signless Laplacian matrix, we define the sum of its eigenvalues as the distance signless Laplacian energy-like invariant of G and denote by $E_{D^Q}(G)$. In the sequel, we obtain some relations between $D^Q EE(G)$ and $E_{D^Q}(G)$ for a simple connected graph G.

Theorem 2.15 *Let G be a connected graph of order n with diameter d. Then*

$$D^Q EE(G) - E_{D^Q}(G) \leq n - 1 - \sqrt{n(n-1)d^2 + \frac{n^3(n-1)^2}{4}} + e^{\sqrt{n(n-1)d^2 + \frac{n^3(n-1)^2}{4}}}. \tag{2.15}$$

or

$$D^Q EE(G) \leq n - 1 + e^{E_{D^Q}(G)}. \tag{2.16}$$

Equality holds in (2.15) or (2.16) if and only if $G \cong K_1$.

From the proof of Theorem 2.8, we have

$$D^Q EE(G) = n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{(\rho_i)^k}{k!} \leq n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{|\rho_i|^k}{k!}.$$

Taking into account the definition of the distance signless Laplacian energy-like invariant, we get

$$D^Q EE(G) \leq n + E_{D^Q}(G) + \sum_{i=1}^{n} \sum_{k \geq 2} \frac{|\rho_i|^k}{k!},$$

which leads to

$$\begin{aligned} D^QEE(G) - E_{D^Q}(G) &\leq n + \sum_{i=1}^{n}\sum_{k\geq 2}\frac{|\rho_i|^k}{k!} \\ &\leq n - 1 - \sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2} + e^{\sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2+\sum_{i=1}^{n} Tr_i^2}}. \end{aligned}$$

One can easily see that the function $f(x) = e^x - x$ monotonically increases for $x \geq 0$. Therefore the best upper bound for $D^QEE(G) - E_{D^Q}(G)$ is obtained for $2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2 \leq 2\frac{n(n-1)}{2}d^2 + \frac{n^3(n-1)^2}{4}$, then we get

$$D^QEE(G) - E_{D^Q}(G) \leq n - 1 - \sqrt{n(n-1)d^2 + \frac{n^3(n-1)^2}{4}} + e^{\sqrt{n(n-1)d^2+\frac{n^3(n-1)^2}{4}}}.$$

Another route to connect $D^QEE(G)$ and $E_{D^Q}(G)$ as follows:

$$\begin{aligned} D^QEE(G) &\leq n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{|\rho_i|^k}{k!} \\ &\leq n + \sum_{k\geq 1}\frac{1}{k!}(\sum_{i=1}^{n}|\rho_i|^k) \\ &= n + \sum_{k\geq 1}\frac{(E_{D^Q}(G))^k}{k!} \\ &= n - 1 + \sum_{k\geq 0}\frac{(E_{D^Q}(G))^k}{k!}, \end{aligned}$$

implying

$$D^QEE(G) \leq n - 1 + e^{E_{D^Q}}(G).$$

Also, equality holds in (2.15) or (2.16) if and only $G \cong K_1$.

We recall Holder inequality. Let $a_1, \ldots, a_n, b_1, \ldots, b_n$ be non-negative real numbers, $p, q > 1$ and $\frac{1}{p} + \frac{1}{q} = 1$. Then

$$\sum_{i=1}^{n} a_ib_i \leq \left(\sum_{i=1}^{n} a_i^p\right)^{\frac{1}{p}}\left(\sum_{i=1}^{n} b_i^q\right)^{\frac{1}{q}}.$$

Here we give the lower bound for $D^QEE(G)$ in terms of n and $\sigma(G)$.

Theorem 2.16 *Let G be a connected graph with n vertices. Then*

$$D^QEE(G) > n + 2\sigma(G) + \frac{2(n+1)}{n^2}\sigma^2(G).$$

By (1.2) we have,

$$D^Q EE(G) > n + tr(D^Q) + \frac{tr(D^{Q^2})}{2}.$$

By Holder inequality for $p = q = 2$, we have $2\sigma(G) = \sum_{i=1}^{n} Tr_i \leq \sqrt{n}(\sum_{i=1}^{n} Tr_i^2)^{\frac{1}{2}}$. Hence

$$\sum_{i=1}^{n} Tr_i^2 \geq \frac{4\sigma^2(G)}{n}. \tag{2.17}$$

Now by Cauchy-Schwartz inequality we have

$$Tr_i^2 = \left(\sum_{j=1}^{n} d_{ij}\right)^2 \leq n \sum_{j=1}^{n} d_{ij}^2.$$

Then

$$\sum_{i=1}^{n} Tr_i^2 \leq n \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij}^2,$$

then by (2.17) we get

$$\sum_{1\leq i<j\leq n} d_{ij}^2 \geq \frac{1}{2n} \sum_{i=1}^{n} Tr_i^2 \geq \frac{1}{2n}.\frac{4\sigma^2(G)}{n} = \frac{2\sigma^2(G)}{n^2}.$$

Thus we have,

$$\begin{aligned} D^Q EE(G) &> n + 2\sigma(G) + \sum_{1\leq i<j\leq n} (d_{ij})^2 + \frac{1}{2}\sum_{i=1}^{n} Tr_i^2 \\ &\geq n + 2\sigma(G) + \frac{2\sigma^2(G)}{n^2} + \frac{2\sigma^2(G)}{n} \\ &= n + 2\sigma(G) + \frac{2(n+1)}{n^2}\sigma^2(G). \end{aligned}$$

Corollary 2.17 *Let G be a connected graph with n vertices, then*

$$D^Q EE(G) > \frac{n^3 + n^2 - n + 1}{2}.$$

Since $d_{ij} \geq 1$ for $i \neq j$ and there are $\frac{n(n-1)}{2}$ pairs of vertices in G, from the lower bound of Theorem 2.16, we get

$$\begin{aligned} D^Q EE(G) &> n + 2\sigma(G) + \frac{2(n+1)}{n^2}\sigma^2(G) \geq n + n(n-1) + \frac{(n+1)(n-1)^2}{2} \\ &= \frac{n^3 + n^2 - n + 1}{2}. \end{aligned}$$

Hence the result.

By the Taylor's Theorem, for any real $x \neq 0$, there is a real η between x and 0 such that $e^x = 1 + x + \frac{x^2}{2!} + e^\eta \frac{x^3}{3!}$. So we have the following.

Lemma 2.18 *For any real $x \neq 0$, one has $e^x > 1 + x + \frac{x^2}{2!}$.*

Theorem 2.19 *Let G be a connected graph with n vertices. Then*

$$D^Q EE(G) > \sqrt{4\sigma(G)(\sigma(G)+n) + n\left[n + 2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n} Tr_i^2\right]}.$$

Using Lemma 2.18, we have

$$\begin{aligned} D^Q EE(G)^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n} e^{\rho_i+\rho_j} \\ &> \sum_{i=1}^{n}\sum_{j=1}^{n}\left(1+\rho_i+\rho_j+\frac{(\rho_i+\rho_j)^2}{2}\right) \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}\left(1+\rho_i+\rho_j+\frac{\rho_i^2}{2}+\frac{\rho_j^2}{2}+\rho_i\rho_j\right). \end{aligned}$$

Now, we have

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\rho_i+\rho_j) = n\sum_{i=1}^{n}\rho_i + n\sum_{j=1}^{n}\rho_j = 4n\sigma(G),$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\rho_i\rho_j = \left(\sum_{i=1}^{n}\rho_i\right)^2 = 4\sigma^2(G).$$

Also,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{\rho_i^2}{2}+\frac{\rho_j^2}{2}\right) = \frac{n}{2}\sum_{i=1}^{n}\rho_i^2 + \frac{n}{2}\sum_{j=1}^{n}\rho_j^2 = n\left[2\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sum_{i=1}^{n}Tr_i^2\right].$$

Combining the above relations, we have

$$D^Q EE(G)^2 > n^2 + 4n\sigma(G) + 4\sigma^2(G) + 2n\sum_{1\leq i<j\leq n}(d_{ij})^2 + n\sum_{i=1}^{n}Tr_i^2.$$

Corollary 2.20 *Let G be a connected graph with n vertices, then*

$$D^Q EE(G) > n\sqrt{n(2n-1)}.$$

Since $d_{ij} \geq 1$ for $i \neq j$ and there are $\frac{n(n-1)}{2}$ pairs of vertices in G, from the lower bound of Theorem 2.19, we get

$$\begin{aligned} D^QEE(G) &> \sqrt{4\sigma(G)(\sigma(G)+n)+n\left[n+2\sum_{1\leq i<j\leq n}(d_{ij})^2+\sum_{i=1}^{n}Tr_i^2\right]} \\ &\geq \sqrt{2n(n-1)\left(\frac{n(n-1)}{2}+n\right)+n\left[n+2\left(\frac{n(n-1)}{2}\right)+n(n-1)^2\right]} \\ &= n\sqrt{n(2n-1)}. \end{aligned}$$

Hence the result.

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