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## ON THE LARGEST DISTANCE (SIGNLESS LAPLACIAN) EIGENVALUE OF NON-TRANSMISSION-REGULAR GRAPHS\*

SHUTING LIU<sup>†</sup>, JINLONG SHU<sup>†</sup>, AND JIE XUE<sup>†</sup>

**Abstract.** Let  $G = (V(G), E(G))$  be a connected graph with  $n$  vertices and  $m$  edges. Let  $D(G)$  be the distance matrix and  $\lambda_1(D)$  be the distance spectral radius of  $G$ , respectively. The transmission  $\text{Tr}(v_i)$  of  $v_i \in V(G)$  is the sum of distances from  $v_i$  to all other vertices of  $G$ , i.e., the row sum  $D_i$  of  $D(G)$  indexed by vertex  $v_i$ . Let  $\text{Tr}(G)$  be the  $n \times n$  diagonal matrix whose  $(i, i)$ -entry is equal to  $\text{Tr}(v_i)$ . The distance signless Laplacian matrix of  $G$  is defined as  $D^Q(G) = \text{Tr}(G) + D(G)$  and its spectral radius is denoted by  $\rho_1(D^Q)$ . A connected graph  $G$  is  $t$ -transmission-regular if  $\text{Tr}(v_i) = t$  for every vertex  $v_i \in V(G)$ ; otherwise,  $G$  is non-transmission-regular. Suppose  $D_1$  is the maximum row sum of  $D(G)$ . In this paper,  $D_1 - \lambda_1(D)$  and  $2D_1 - \rho_1(D^Q)$  are estimated in different ways for a  $k$ -connected non-transmission-regular graph. These obtained results are compared, and it is conjectured that  $D_1 - \lambda_1(D) > \frac{1}{n+1}$ . Moreover, it is shown that the conjecture holds for trees.

**Key words.** Distance (signless Laplacian) spectral radius, Maximum row sum, Connectivity, Non-transmission-regular graph.

**AMS subject classifications.** 05C50.

**1. Introduction.** Unless stated otherwise, we follow [2] for the terminology and notation and consider finite connected simple graphs throughout this article. Let  $G = (V(G), E(G))$  be a connected graph with  $n$  vertices and  $m$  edges. The *vertex degree* of  $v_i \in V(G)$ , denoted by  $d(v_i)$ , is the number of edges incident with  $v_i$ . We use  $N(v_i)$  or  $N_G(v_i)$  to denote the neighbor set of vertex  $v_i \in V(G)$ . The *distance* between the vertices  $v_i$  and  $v_j$  is the length of a shortest path between them, and is denoted by  $d(v_i, v_j)$  (or  $d_{ij}$ ). The *diameter* of  $G$ , denoted by  $\text{diam}(G)$  or  $d$ , is the maximum distance between any pair of vertices of  $G$ . The (*vertex*) *connectivity*  $\kappa(G)$  of  $G$  is the minimum number of vertices whose removal from  $G$  results in a disconnected or trivial graph. A graph  $G$  is  $k$ -connected if  $\kappa(G) \geq k$ .

The *distance matrix* of  $G$  is the  $n \times n$  matrix  $D(G) = (d(v_i, v_j))$ , where  $v_i, v_j \in V(G)$ . The spectrum of distance matrix, arose from a data communication problem studied in [7] by Graham and Pollack in 1971, has been studied extensively (see [1, 9, 10, 11, 12, 13, 22]). The eigenvalues, eigenvectors and spectrum of  $D(G)$  are the  $D$ -eigenvalues,  $D$ -eigenvectors and  $D$ -spectrum of  $G$ , respectively. The distance matrix  $D(G)$  is symmetric, so all of its eigenvalues are real, say  $\lambda_i(D)$ ,  $i = 1, 2, \dots, n$ . Then the distance eigenvalues have an ordering  $\lambda_1(D) \geq \lambda_2(D) \geq \dots \geq \lambda_n(D)$ . The largest eigenvalue of the distance matrix is called the *distance spectral radius*, denoted by  $\lambda_1(D)$ . The unique unit positive eigenvector corresponding to  $\lambda_1(D)$  is called the *principal eigenvector* of  $D(G)$ .

For  $v_i \in V(G)$ , the *transmission* of  $v_i$  in  $G$ , denoted by  $\text{Tr}(v_i)$ , is the sum of distances from  $v_i$  to all other vertices of  $G$ , i.e., the row sum  $D_i(G)$  of  $D(G)$  indexed by vertex  $v_i$ , i.e.,

$$\text{Tr}(v_i) = \sum_{v_j \in V(G)} d(v_i, v_j).$$

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For convenience, we suppose  $\text{Tr}(v_1) = D_1(G) \geq \dots \geq D_n(G) = \text{Tr}(v_n)$ . A connected graph  $G$  is *t-transmission-regular* if  $\text{Tr}(v_i) = t$  for every vertex  $v_i \in V(G)$ ; otherwise,  $G$  is *non-transmission-regular*. The *Wiener index* ([8]) of  $G$ , denoted by  $W(G)$ , is given by  $W(G) = \frac{1}{2} \sum_{i=1}^n D_i(G)$ .

Let  $\text{Tr}(G)$  be the  $n \times n$  diagonal matrix with its  $(i, i)$ -entry equal to  $\text{Tr}(v_i)$ . The distance signless Laplacian matrix of  $G$  is defined by Aouchiche and Hansen in [1] as  $D^Q(G) = \text{Tr}(G) + D(G)$ . The largest eigenvalue of the distance signless Laplacian matrix is called the *distance signless Laplacian spectral radius*, and is denoted by  $\rho_1(D^Q)$ . The unique unit positive eigenvector corresponding to  $\rho_1(D^Q)$  is called the *principal eigenvector* of  $\rho_1(D^Q)$ .

It is easy to see that the adjacency spectral radius, denoted by  $\mu_1(A)$ , of a regular graph is the maximum degree  $\Delta$  with  $(1, 1, \dots, 1)^T$  as a corresponding eigenvector.  $\Delta - \mu_1(A)$  has been considered as a measure of irregularity for a graph  $G$  ([6], p. 242). Some estimates on  $\Delta - \mu_1(A)$  for a connected irregular graph  $G$  have been obtained in many papers. Next we will list some of these known estimates on  $\Delta - \mu_1(A)$ . Let  $G$  be a  $k$ -connected irregular graph with  $n$  vertices,  $m$  edges, diameter  $d$ , maximum degree  $\Delta$  and minimum degree  $\delta$ . In [21], Stevanović first derived

$$(1.1) \quad \Delta - \mu_1(A) > \frac{1}{2n(n\Delta - 1)\Delta^2}.$$

Later, Zhang [23] showed that

$$(1.2) \quad \Delta - \mu_1(A) > \frac{\Delta + \delta - 2\sqrt{\Delta\delta}}{nd\Delta} \geq \frac{2\Delta - 1 - 2\sqrt{\Delta(\Delta - 1)}}{n(n - 1)\Delta},$$

and improved Stevanović's bound in (1.1). Liu, Shen and Wang in [16] obtained the following bound:

$$(1.3) \quad \Delta - \mu_1(A) \geq \frac{\Delta + 1}{n(3n + 2\Delta - 4)}.$$

Later, bound (1.3) was improved by Liu and Li in [15] as follows:

$$(1.4) \quad \Delta - \mu_1(A) > \frac{\Delta + 1}{n(3n + \Delta - 8)}.$$

Furthermore, Liu, Huang and You in [14] established the following bound which improves (1.4), i.e.,

$$\Delta - \mu_1(A) > \frac{\Delta + 1}{n(3n + \Delta - 3\delta - 5)}.$$

Cioabă, Gregory and Nikiforov in [5] showed that

$$\Delta - \mu_1(A) > \frac{n\Delta - 2m}{n(d(n\Delta - 2m) + 1)} \geq \frac{1}{n(d + 1)},$$

which improves bounds (1.1) and (1.2). Moreover, the authors in [5] conjectured that

$$(1.5) \quad \Delta - \mu_1(A) > \frac{1}{nd}.$$

Later, Cioabă [4] confirmed the conjecture. In [19], Shi pointed out that there is no much room to improve bound (1.5) with an example. However, considering degree parameters, he established another strong inequality as follows:

$$(1.6) \quad \Delta - \mu_1(A) > \left[ (n - \delta)d + \frac{1}{\Delta - d} - \binom{d}{2} \right]^{-1},$$

where  $\bar{d}$  is the average degree of  $G$ . Taking connectivity parameter into account, Chen and Hou [3] gave the following bound, which sometimes improves (1.5) and (1.6):

$$(1.7) \quad \Delta - \mu_1(A) > \frac{(n\Delta - 2m)k^2}{(n\Delta - 2m)[n^2 - 2(n - k)] + nk^2}.$$

Let  $q_1(Q)$  be the signless Laplacian spectral radius of  $G$ . It is known that  $q_1(Q) \leq 2\Delta$  and equality holds if and only if  $G$  is a regular graph. Let  $G$  be a  $k$ -connected irregular graph with  $n$  vertices,  $m$  edges, diameter  $d$ , maximum degree  $\Delta$ . Ning et al. in [18] proved that

$$(1.8) \quad 2\Delta - q_1(Q) > \frac{1}{n(d - \frac{1}{4})}.$$

In [20], Wai Chee Shiu et al. established a lower bound on  $2\Delta - q_1(Q)$  similar to (1.7), i.e.,

$$(1.9) \quad 2\Delta - q_1(Q) > \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - (\Delta - k + 2)(n - k)) + nk^2}.$$

The authors in [20] also indicated that when  $k \geq \sqrt{n}$ , the bound in (1.9) is better than the bound in (1.8) and with the same arguments they improved the bound in (1.8), which were given in their remarks.

**2. Main results.** Motivated by these known estimates on  $\Delta - \mu_1(A)$  and  $2\Delta - q_1(Q)$  and some methods used in estimating them, we pose and consider the following two natural questions:

How small can  $D_1(G) - \lambda_1(D)$  be when  $G$  is non-transmission-regular?

How small can  $2D_1(G) - \rho_1(D^Q)$  be when  $G$  is non-transmission-regular?

Meanwhile, we give some estimates on them in different ways and compare these obtained results in this paper.

Let  $x = (x_1, x_2, \dots, x_n)^T$  be the principal eigenvector of  $D(G)$ . Suppose that  $u, v$  are two vertices satisfying  $x_u = \max_{1 \leq i \leq n} \{x_i\}$  and  $x_v = \min_{1 \leq i \leq n} \{x_i\}$ , respectively. Suppose  $u = 0, 1, \dots, s = v$  are consecutive vertices of a shortest path  $P_{uv}$  from  $u$  to  $v$  in  $G$  and the length of  $P_{uv}$  is  $s$ . Then we have the following theorems. Indicate that the proofs of those will be given in Section 3.

**THEOREM 2.1.** *Let  $G$  be a connected non-transmission-regular graph with  $n$  vertices, Wiener index  $W$ , and maximum row sum  $D_1$  of  $D(G)$ . Then we have the following statements.*

- (1) If  $s = 1$ , then  $D_1 - \lambda_1(D) > \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n}$ .
- (2) If  $s \geq 2$  is even, then  $D_1 - \lambda_1(D) > \frac{5(nD_1 - 2W)}{[2(nD_1 - 2W) + 5]n}$ .
- (3) If  $s \geq 3$  is odd, then  $D_1 - \lambda_1(D) > \frac{4(nD_1 - 2W)}{(nD_1 - 2W + 4)n}$ .

**THEOREM 2.2.** *Let  $G$  be a connected non-transmission-regular graph with  $n$  vertices, Wiener index  $W$ , and maximum row sum  $D_1$  of  $D(G)$ . Then*

$$(2.10) \quad D_1 - \lambda_1(D) > \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n}.$$

Furthermore,

$$(2.11) \quad D_1 - \lambda_1(D) > \frac{1}{2n}.$$

Particularly, if  $n \mid 2W$ , then

$$(2.12) \quad D_1 - \lambda_1(D) > \frac{1}{n+1}.$$

By Theorem 2.2, we get  $D_1 - \lambda_1(D) > \frac{1}{2n} \geq \frac{1}{dn}$ . Thus, we have the following result that is similar to Cioabă's [4] about the adjacency spectral radius and the maximum degree.

COROLLARY 2.3. *If  $G$  is a connected non-transmission-regular graph with  $n$  vertices and diameter  $d$ , then*

$$D_1 - \lambda_1(D) > \frac{1}{dn}.$$

Let  $K_{n_1, \dots, n_k}$  denote the complete  $k$ -partite graph. Let  $G = K_{1, 2, \dots, 2}$  with  $n = 2k - 1$  and  $D_1 = n$ . By a simple calculation, we have  $\lambda_1(D(G)) = k - 1 + \sqrt{k^2 - 1}$ . Then

$$D_1 - \lambda_1(D) = k - \sqrt{k^2 - 1} = \frac{1}{k + \sqrt{k^2 - 1}} < \frac{1}{2k - 1} = \frac{1}{n}.$$

On the other hand, we have  $D_1 - \lambda_1(D) > \frac{1}{n+1}$ . Combining with Theorem 2.2, it is natural to conjecture the following.

CONJECTURE 2.4. *Let  $G$  be a connected non-transmission-regular graph with  $n$  vertices. Then*

$$D_1 - \lambda_1(D) > \frac{1}{n+1}.$$

We will show that the conjecture holds for trees.

THEOREM 2.5. *Let  $T$  be a tree with  $n \geq 3$  vertices and maximum row sum  $D_1$  of distance matrix  $D$ . Then we have*

$$D_1 - \lambda_1(D) > \frac{1}{n+1}.$$

Taking connectivity parameter and Wiener index of  $G$  into account, we have the following theorem.

THEOREM 2.6. *Let  $G$  be a  $k$ -connected non-transmission-regular graph with  $n$  vertices and Wiener index  $W$ . Then*

$$(2.13) \quad D_1 - \lambda_1(D) > \frac{(nD_1 - 2W)k^2}{(nD_1 - 2W)(n^2 - 3n + k + 2) + nk^2}.$$

Similar to the estimates on  $D_1 - \lambda_1(D)$ , we give the results on  $2D_1 - \rho_1(D^Q)$  as follows.

Let  $x = (x_1, x_2, \dots, x_n)^T$  be the principal eigenvector corresponding to  $\rho_1(D^Q)$ . and  $u, v$  be two vertices such that  $x_u = \max_{1 \leq i \leq n} \{x_i\}$  and  $x_v = \min_{1 \leq i \leq n} \{x_i\}$ , respectively. Suppose  $u = 0, 1, \dots, s = v$  are consecutive vertices of a shortest path  $P_{uv}$  from  $u$  to  $v$  in  $G$  and the length of  $P_{uv}$  is  $s$ . Then we present the following theorems. Indicate that the proofs of those will be given in Section 3.

THEOREM 2.7. *Let  $G$  be a connected non-transmission-regular graph with  $n$  vertices, maximum row sum  $D_1$  of  $D(G)$ , and Wiener index  $W$ . Then the following hold:*

$$(1) \text{ If } s = 1, \text{ then } 2D_1 - \rho_1(D^Q) > \frac{2(nD_1 - 2W)}{[2(nD_1 - 2W) + 1]n}.$$

(2) If  $s \geq 2$  is even, then  $2D_1 - \rho_1(D^Q) > \frac{10(nD_1 - 2W)}{[4(nD_1 - 2W) + 5]n}$ .

(3) If  $s \geq 3$  is odd, then  $2D_1 - \rho_1(D^Q) > \frac{4(nD_1 - 2W)}{(nD_1 - 2W + 2)n}$ .

**THEOREM 2.8.** *Let  $G$  be a connected non-transmission-regular graph with  $n$  vertices, maximum row sum  $D_1$  of  $D(G)$ , and Wiener index  $W$ . Then*

$$(2.14) \quad 2D_1 - \rho_1(D^Q) > \frac{2(nD_1 - 2W)}{[2(nD_1 - 2W) + 1]n}.$$

Furthermore,

$$2D_1 - \rho_1(D^Q) > \frac{2}{3n}.$$

Particularly, if  $n \mid 2W$ , then

$$2D_1 - \rho_1(D^Q) > \frac{2}{2n + 1}.$$

**THEOREM 2.9.** *Let  $G$  be a  $k$ -connected non-transmission-regular graph with  $n$  vertices and Wiener index  $W$ . Then*

$$(2.15) \quad 2D_1 - \rho_1(D^Q) > \frac{2(nD_1 - 2W)k^2}{2(nD_1 - 2W)(n^2 - 3n + k + 2) + nk^2}.$$

For convenience, we use the symbol *Bound* (1)  $\succ$  *Bound* (2) to assert that Bound (1) is better than Bound (2). We use the symbol *Bound* (1)  $\succeq$  *Bound* (2) to assert that Bound (1) is good as or better than Bound (2).

**THEOREM 2.10.** *Let  $G$  be a connected non-transmission-regular graph of order  $n$  with connectivity  $\kappa$  and Wiener index  $W$ . Let  $k = \kappa$  in Bounds (2.13) and (2.15).*

(1) If  $1 \leq \kappa \leq \frac{1 + \sqrt{4n(n^2 - 3n + 2) + 1}}{2n}$ , then *Bound* (2.10)  $\succeq$  *Bound* (2.13) and *Bound* (2.14)  $\succeq$  *Bound* (2.15);

(2) If  $\frac{1 + \sqrt{4n(n^2 - 3n + 2) + 1}}{2n} < \kappa < n - 1$ , then *Bound* (2.13)  $\succ$  *Bound* (2.10) and *Bound* (2.15)  $\succ$  *Bound* (2.14).

**3. Proofs.** A reformulation of inequalities from the theory of nonnegative matrices ([17], Chapter 2) yields the lemma as follows.

**LEMMA 3.1.** [17] *If  $A$  is a nonnegative irreducible  $n \times n$  matrix with largest eigenvalue  $\lambda_1(A)$  and row sums  $S_1, S_2, \dots, S_n$ , then*

$$\min_{1 \leq i \leq n} \{S_i\} \leq \lambda_1(A) \leq \max_{1 \leq i \leq n} \{S_i\}.$$

Moreover, one of the equalities holds if and only if the row sums of  $A$  are all equal.

The following simple observation, due to Shi [19], will be used frequently in the subsequent proofs.

**LEMMA 3.2.** [19] *If  $a, b > 0$ , then  $a(x - y)^2 + by^2 \geq abx^2 / (a + b)$  with equality if and only if  $y = ax / (a + b)$ .*

The following easily proven result will be used frequently. We state it as our lemma.

LEMMA 3.3. Let  $x = (x_1, \dots, x_n)^T \in R^n$  with  $\|x\|_2 = 1$ . Then for any connected graph  $G$ ,

$$\lambda_1(D) \geq 2 \sum_{i>j} d_{ij} x_i x_j$$

with equality if and only if  $x$  is an eigenvector corresponding to  $\lambda_1(D)$ . And

$$\rho_1(D^Q) \geq \sum_{i>j} d_{ij} (x_i + x_j)^2$$

with equality if and only if  $x$  is an eigenvector corresponding to  $\rho_1(D^Q)$ .

*Proof of Theorem 2.1.* Let  $x = (x_1, x_2, \dots, x_n)^T$  be the principal eigenvector corresponding to  $\lambda_1(D)$ . Obviously,  $\sum_{i=1}^n x_i^2 = 1$ . Suppose that  $u, v$  are two vertices of  $G$  satisfying  $x_u = \max_{1 \leq i \leq n} \{x_i\}$  and  $x_v = \min_{1 \leq i \leq n} \{x_i\}$ . Since  $G$  is non-transmission-regular, we get  $x_u > \frac{1}{\sqrt{n}} > x_v$ . Moreover, by Lemma 3.3, we have

$$\begin{aligned} D_1 - \lambda_1(D) &= D_1 - 2 \sum_{i>j} d_{ij} x_i x_j \\ (3.16) \quad &= \sum_i (D_1 - D_i) x_i^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\ &\geq (nD_1 - 2W) x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij}. \end{aligned}$$

Suppose  $u = 0, 1, \dots, s = v$  are consecutive vertices of a shortest path  $P_{uv}$  from  $u$  to  $v$  in  $G$  and the length of  $P_{uv}$  is  $s$ .

*Case 1.*  $s = 1$ . By Lemma 3.2 and inequality (3.16), we obtain

$$\begin{aligned} D_1 - \lambda_1(D) &\geq (nD_1 - 2W) x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\ &\geq (nD_1 - 2W) x_v^2 + (x_u - x_v)^2 d_{uv} \\ &\geq \frac{nD_1 - 2W}{nD_1 - 2W + 1} x_u^2 \\ &> \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n}, \end{aligned}$$

which proves statement (1).

*Case 2.*  $s \geq 2$ . For the shortest path  $P_{uv}$ , let  $i$  ( $1 \leq i \leq s-1$ ) be a vertex of  $P_{uv}$ . By the Cauchy-Schwarz inequality, we get

$$(3.17) \quad \begin{aligned} (x_i - x_0)^2 d_{0i} + (x_i - x_s)^2 d_{is} &\geq \min\{i, s-i\} [(x_i - x_0)^2 + (x_s - x_i)^2] \\ &\geq \frac{1}{2} \min\{i, s-i\} (x_s - x_0)^2. \end{aligned}$$

Suppose  $f(t) = \frac{(nD_1 - 2W)t}{(8(nD_1 - 2W) + t)n}$ . Then  $f(t)$  is a monotonically increasing function on  $t > 0$ .

*Subcase 2.1.*  $s \geq 2$  is even. Based on inequality (3.17), we have

$$\begin{aligned} \sum_{i>j} (x_i - x_j)^2 d_{ij} &\geq [2 \times \frac{1}{2} (1 + 2 + \dots + \frac{s}{2}) - \frac{s}{2} \times \frac{1}{2} + s] (x_s - x_0)^2 \\ (3.18) \quad &= [\frac{s}{2} (\frac{s}{2} + 1) / 2 - \frac{s}{4} + s] (x_s - x_0)^2 \\ &= \frac{s^2 + 8s}{8} (x_u - x_v)^2. \end{aligned}$$

Using Lemma 3.2 and the monotonicity of the function  $f(t)$ , and combining (3.16) and (3.18), we have

$$\begin{aligned} D_1 - \lambda_1(D) &\geq (nD_1 - 2W)x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\ &\geq (nD_1 - 2W)x_v^2 + \frac{s^2 + 8s}{8}(x_u - x_v)^2 \\ &> \frac{(nD_1 - 2W)(s^2 + 8s)}{[8(nD_1 - 2W) + (s^2 + 8s)]n} \\ &\geq \frac{20(nD_1 - 2W)}{[8(nD_1 - 2W) + 20]n} \\ &= \frac{5(nD_1 - 2W)}{[2(nD_1 - 2W) + 5]n}, \end{aligned}$$

which proves statement (2).

*Subcase 2.2.*  $s \geq 3$  is odd. Based on inequality (3.17), we find

$$\begin{aligned} \sum_{i>j} (x_i - x_j)^2 d_{ij} &\geq [2 \times \frac{1}{2}(1 + 2 + \dots + \lfloor \frac{s}{2} \rfloor) + s](x_s - x_0)^2 \\ (3.19) \quad &= (\frac{\lfloor \frac{s}{2} \rfloor(\lfloor \frac{s}{2} \rfloor + 1)}{2} + s)(x_s - x_0)^2 \\ &= \frac{s^2 + 8s - 1}{8}(x_u - x_v)^2. \end{aligned}$$

By Lemma 3.2 and the monotonicity of the function  $f(t)$ , from inequalities (3.16) and (3.19) we obtain

$$\begin{aligned} D_1 - \lambda_1(D) &\geq (nD_1 - 2W)x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\ &> \frac{(nD_1 - 2W)(s^2 + 8s - 1)}{[8(nD_1 - 2W) + (s^2 + 8s - 1)]n} \\ &\geq \frac{32(nD_1 - 2W)}{[8(nD_1 - 2W) + 32]n} \\ &= \frac{4(nD_1 - 2W)}{(nD_1 - 2W + 4)n}, \end{aligned}$$

which proves statement (3). □

*Proof of Theorem 2.2.* Let  $G$  be a connected non-transmission-regular graph with  $n$  vertices and maximum row sum  $D_1$  of  $D(G)$ . Note that the non-transmission regularity of  $G$  implies that  $nD_1 > 2W$ . So  $nD_1 - 2W \geq 1$  follows. Suppose  $f_1(nD_1 - 2W) = \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n}$ ,  $f_2(nD_1 - 2W) = \frac{5(nD_1 - 2W)}{[2(nD_1 - 2W) + 5]n}$ , and  $f_3(nD_1 - 2W) = \frac{4(nD_1 - 2W)}{(nD_1 - 2W + 4)n}$ . Since  $f_i(nD_1 - 2W)$ , where  $i = 1, 2, 3$ , are monotonically increasing functions on  $nD_1 - 2W$ , by Theorem 2.1, we get

$$\begin{aligned} D_1 - \lambda_1(D) &> \min \left\{ \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n}, \frac{5(nD_1 - 2W)}{[2(nD_1 - 2W) + 5]n}, \frac{4(nD_1 - 2W)}{(nD_1 - 2W + 4)n} \right\} \\ &= \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n} \\ &\geq \frac{1}{2n}, \end{aligned}$$

completing the proofs of inequalities (2.10) and (2.11).



Now we prove inequality (2.12). If  $n \mid 2W$ , combining with the non-transmission regularity of  $G$ , then we have  $nD_1 - 2W \geq n$ . Since  $f_1(nD_1 - 2W) = \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n}$  is a monotonically increasing function on  $nD_1 - 2W$ , inequality (2.10) implies that

$$\begin{aligned} D_1 - \lambda_1(D) &> \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n} \\ &\geq \frac{1}{n + 1}. \quad \square \end{aligned}$$

*Proof of Theorem 2.5.* Let  $T$  be a tree with  $n \geq 3$  vertices, diameter  $d$ , Wiener index  $W$  and maximum row sum  $D_1$  of  $D(T)$ . We consider two cases in the following based on the diameter  $d$  of the tree  $T$ .

*Case 1.*  $d = 2$ . Then  $T \cong K_{1,n-1}$ . By a simple calculation, we have  $\lambda_1(D(K_{1,n-1})) = n - 2 + \sqrt{n^2 - 3n + 3}$  and  $D_1(K_{1,n-1}) = 2n - 3$ . Then

$$\begin{aligned} D_1 - \lambda_1(D) &= 2n - 3 - (n - 2 + \sqrt{n^2 - 3n + 3}) \\ &= n - 1 - \sqrt{n^2 - 3n + 3} \\ &= \frac{n - 2}{n - 1 + \sqrt{n^2 - 3n + 3}} \\ &> \frac{1}{n + 1}. \end{aligned}$$

*Case 2.*  $d \geq 3$ . If  $T \cong P_4$ , by a calculation, we have  $D_1(P_4) - \lambda_1(D(P_4)) \approx 6 - 5.16 > 0.2$ . Next we will prove that the result holds for  $T \not\cong P_4$ .

Let  $D_1 \geq D_2 \geq \dots \geq D_n$  be the row sums of  $D(T)$ , we have

$$(3.20) \quad nD_1 - 2W = \sum_{i=1}^n (D_1 - D_i).$$

We use  $D_{v_i}$  to denote the row sum of  $D(T)$  indexed by the vertex  $v_i$ . Suppose that  $P_{v_0 v_d} = v_0 v_1 \dots v_{d-1} v_d$  is a diametrical path of  $T$ . Without loss of generality, we assume  $D_{v_0} \geq D_{v_d}$ . Obviously,  $v_0$  is a pendant vertex of  $T$ . We obtain that

$$(3.21) \quad D_{v_0} - D_{v_1} = n - 2.$$

Since  $G \not\cong K_{1,n-1}$ , we have  $d(v_1) \leq n - 2$ . If  $d(v_1) = n - 2$ , then  $d(T) = 3$ . Furthermore,  $T \not\cong P_4$  implies that  $D_{v_0} < D_{v_3}$ , a contradiction to the assumption. Therefore,  $d(v_1) \leq n - 3$ . Then we have

$$(3.22) \quad \begin{aligned} D_{v_0} - D_{v_2} &\geq 2[n - (d(v_1) + 1)] \\ &\geq 2[n - (n - 3 + 1)] \\ &= 4. \end{aligned}$$

Combining (3.20), (3.21) and (3.22), we deduce that  $nD_1 - 2W \geq n - 2 + 4 > n$ . Furthermore, by Theorem 2.2 and the monotonicity of the function  $f(nD_1 - 2W) = \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n}$  on  $nD_1 - 2W$ , we obtain

$$D_1 - \lambda_1(D) > \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n} > \frac{1}{n + 1}. \quad \square$$

*Proof of Theorem 2.6.* Let  $x = (x_1, x_2, \dots, x_n)^T$  be the principal eigenvector corresponding to  $\lambda_1(D)$ . Obviously,  $\sum_{i=1}^n x_i^2 = 1$ . Let  $u, v$  be two vertices of  $G$  such that  $x_u = \max_{1 \leq i \leq n} \{x_i\}$  and  $x_v = \min_{1 \leq i \leq n} \{x_i\}$ , respectively. Since  $G$  is non-transmission-regular, we have  $x_u > \frac{1}{\sqrt{n}} > x_v$ . Furthermore, we get

$$(3.23) \quad D_1 - \lambda_1(D) \geq (nD_1 - 2W)x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij}.$$

Since  $G$  is  $k$ -connected, by Menger's Theorem ([2]), there are at least  $k$  internally vertex-disjoint paths connecting  $u$  and  $v$ . We choose  $k$  paths and denote them by  $P_1, P_2, \dots, P_k$ . Note that  $\sum_{t=1}^k |V(P_t) - 2| \leq n - 2$ . Following the argument in [3], by the Cauchy-Schwarz inequality, we have

$$(3.24) \quad \begin{aligned} \sum_{i>j} (x_i - x_j)^2 d_{ij} &\geq \sum_{t=1}^k \sum_{ij \in E(P_t)} (x_i - x_j)^2 \cdot 1 \\ &\geq \sum_{t=1}^k \frac{1}{|V(P_t)|-1} (\sum_{ij \in E(P_t)} (x_i - x_j))^2 \\ &= \sum_{t=1}^k \frac{1}{|V(P_t)|-1} (x_u - x_v)^2 \\ &\geq \frac{k^2}{\sum_{t=1}^k (|V(P_t)|-1)} (x_u - x_v)^2 \\ &\geq \frac{k^2}{n+k-2} (x_u - x_v)^2. \end{aligned}$$

Combining (3.23) and (3.24), from Lemma 3.2 we obtain

$$(3.25) \quad \begin{aligned} D_1 - \lambda_1(D) &\geq (nD_1 - 2W)x_v^2 + \frac{k^2}{n+k-2} (x_u - x_v)^2 \\ &\geq \frac{(nD_1 - 2W)k^2}{(nD_1 - 2W)(n+k-2) + k^2} x_u^2. \end{aligned}$$

Let

$$C = \frac{(nD_1 - 2W)k^2}{(nD_1 - 2W)(n^2 - 3n + k + 2) + nk^2}.$$

We can choose  $k$  vertices in  $N_G(v)$  and denote them as  $\{v_1, v_2, \dots, v_k\}$ , since  $k \leq \delta(G) \leq d(v)$ . If  $x_v^2 \geq C/(nD_1 - 2W)$ , by (3.23), we have  $D_1 - \lambda_1(D) > (nD_1 - 2W)x_v^2 \geq C$ , and thus, (2.13) holds. If  $\sum_{t=1}^k x_{v_t}^2 > C[1 + k/(nD_1 - 2W)]$ , then it follows from (3.23) and Lemma 3.2 that

$$\begin{aligned} D_1 - \lambda_1(D) &\geq (nD_1 - 2W)x_v^2 + \sum_{t=1}^k (x_{v_t} - x_v)^2 \\ &= \sum_{t=1}^k \left[ \frac{nD_1 - 2W}{k} x_v^2 + (x_{v_t} - x_v)^2 \right] \\ &\geq \sum_{t=1}^k \frac{nD_1 - 2W}{nD_1 - 2W + k} x_{v_t}^2 \\ &> C. \end{aligned}$$

Thus, (2.13) holds as well. Now it remains to consider the case that

$$x_v^2 < C/(nD_1 - 2W) \quad \text{and} \quad \sum_{t=1}^k x_{v_t}^2 \leq C[1 + k/(nD_1 - 2W)].$$

Note that  $k \leq n - 2$  and  $\sum_{i=1}^n x_i^2 = 1$ . Then

$$x_u^2 \geq \left(1 - x_v^2 - \sum_{t=1}^k x_{v_t}^2\right) / (n - k - 1) > \left(1 - \frac{nD_1 - 2W + k + 1}{nD_1 - 2W} C\right) / (n - k - 1).$$

Combining with (3.25), we obtain

$$\begin{aligned}
 D_1 - \lambda_1(D) &\geq \frac{(nD_1 - 2W)k^2}{(nD_1 - 2W)(n + k - 2) + k^2} x_u^2 \\
 &> \frac{(nD_1 - 2W)k^2}{[(nD_1 - 2W)(n + k - 2) + k^2](n - k - 1)} \left(1 - \frac{nD_1 - 2W + k + 1}{nD_1 - 2W} C\right) \\
 &= \frac{(nD_1 - 2W)k^2}{(nD_1 - 2W)(n^2 - 3n + k + 2) + nk^2} \\
 &= C. \quad \square
 \end{aligned}$$

*Proof of Theorem 2.7.* Let  $x = (x_1, x_2, \dots, x_n)^T$  be the principal eigenvector corresponding to  $\rho_1(D^Q)$  of  $G$ . Immediately,  $\sum_{i=1}^n x_i^2 = 1$ . We choose two vertices  $u, v \in V(G)$  so that  $x_u = \max_{1 \leq i \leq n} \{x_i\}$  and  $x_v = \min_{1 \leq i \leq n} \{x_i\}$ , respectively. The non-transmission-regularity of  $G$  implies that  $x_u > \frac{1}{\sqrt{n}} > x_v$ . Furthermore, by Lemma 3.3, we get

$$\begin{aligned}
 (3.26) \quad 2D_1 - \rho_1(D^Q) &= 2D_1 - \sum_{i>j} d_{ij}(x_i + x_j)^2 \\
 &= 2\sum_i D_1 x_i^2 - 2\sum_{i>j} (x_i^2 + x_j^2) d_{ij} + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\
 &\geq 2\sum_i (D_1 - D_i) x_i^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\
 &= 2(nD_1 - 2W)x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij}.
 \end{aligned}$$

Suppose  $u = 0, 1, \dots, s = v$  are consecutive vertices of a shortest path  $P_{uv}$  between  $u$  and  $v$  in  $G$  and the length of  $P_{uv}$  is  $s$ .

*Case 1.*  $s = 1$ . By Lemma 3.2 and inequality (3.26), we find that

$$\begin{aligned}
 2D_1 - \rho_1(D^Q) &\geq 2(nD_1 - 2W)x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\
 &\geq 2(nD_1 - 2W)x_v^2 + (x_u - x_v)^2 \times 1 \\
 &\geq \frac{2(nD_1 - 2W)}{2(nD_1 - 2W) + 1} x_u^2 \\
 &> \frac{2(nD_1 - 2W)}{[2(nD_1 - 2W) + 1]n}.
 \end{aligned}$$

Thus, we complete the proof of statement (1).

*Case 2.*  $s \geq 2$ . In this case, by the same argument for  $\sum_{i>j} (x_i - x_j)^2 d_{ij}$  as Case 2 in the proof of Theorem 2.1, we will prove statements (2) and (3).

Let  $f(t) = \frac{2(nD_1 - 2W)t}{(16(nD_1 - 2W) + t)n}$ . Then  $f(t)$  is a monotonically increasing function on  $t > 0$ .

*Subcase 2.1.*  $s \geq 2$  is even. We have

$$(3.27) \quad \sum_{i>j} (x_i - x_j)^2 d_{ij} \geq \frac{s^2 + 8s}{8} (x_u - x_v)^2.$$

Combining (3.26) and (3.27) and using Lemma 3.2 and the monotonicity of the function  $f(t)$ , we obtain

$$\begin{aligned} 2D_1 - \rho_1(D^Q) &\geq 2(nD_1 - 2W)x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\ &\geq 2(nD_1 - 2W)x_v^2 + \frac{s^2 + 8s}{8}(x_u - x_v)^2 \\ &> \frac{2(nD_1 - 2W)(s^2 + 8s)}{[16(nD_1 - 2W) + (s^2 + 8s)]n} \\ &\geq \frac{10(nD_1 - 2W)}{[4(nD_1 - 2W) + 5]n}, \end{aligned}$$

which gives the required result in statement (2).

*Subcase 2.2.  $s \geq 3$  is odd.* Since

$$\sum_{i>j} (x_i - x_j)^2 d_{ij} \geq \frac{s^2 + 8s - 1}{8}(x_u - x_v)^2,$$

by Lemma 3.2 and the monotonicity of the function  $f(t)$ , from (3.26) we have

$$\begin{aligned} 2D_1 - \rho_1(D^Q) &\geq 2(nD_1 - 2W)x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij} \\ &\geq 2(nD_1 - 2W)x_v^2 + \frac{s^2 + 8s - 1}{8}(x_u - x_v)^2 \\ &> \frac{2(nD_1 - 2W)(s^2 + 8s - 1)}{[16(nD_1 - 2W) + (s^2 + 8s - 1)]n} \\ &\geq \frac{4(nD_1 - 2W)}{(nD_1 - 2W + 2)n}, \end{aligned}$$

which gives the required result in statement (3). □

*Proof of Theorem 2.9.* Let  $x = (x_1, x_2, \dots, x_n)^T$  be the principal eigenvector corresponding to  $\rho_1(D^Q)$  of  $G$ . We choose two vertices  $u, v \in V(G)$  so that  $x_u = \max_{1 \leq i \leq n} \{x_i\}$  and  $x_v = \min_{1 \leq i \leq n} \{x_i\}$ , respectively. Since  $G$  is non-transmission-regular, we obtain  $x_u > \frac{1}{\sqrt{n}} > x_v$ . Furthermore, we get

$$(3.28) \quad 2D_1 - \rho_1(D^Q) \geq 2(nD_1 - 2W)x_v^2 + \sum_{i>j} (x_i - x_j)^2 d_{ij}.$$

With the same argument for  $\sum_{i>j} (x_i - x_j)^2 d_{ij}$  as (3.24), we have

$$(3.29) \quad \sum_{i>j} (x_i - x_j)^2 d_{ij} \geq \frac{k^2}{n+k-2}(x_u - x_v)^2.$$

Using (3.28), (3.29) and Lemma 3.2, we obtain

$$(3.30) \quad \begin{aligned} 2D_1 - \rho_1(D^Q) &\geq 2(nD_1 - 2W)x_v^2 + \frac{k^2}{n+k-2}(x_u - x_v)^2 \\ &\geq \frac{2(nD_1 - 2W)k^2}{2(nD_1 - 2W)(n+k-2) + k^2} x_u^2. \end{aligned}$$

Define

$$C = \frac{2(nD_1 - 2W)k^2}{2(nD_1 - 2W)(n^2 - 3n + k + 2) + nk^2}.$$

We can choose  $k$  vertices in  $N_G(v)$  and denote them as  $\{v_1, v_2, \dots, v_k\}$ , since  $k \leq \delta(G) \leq d(v)$ . If  $x_v^2 \geq \frac{C}{2(nD_1 - 2W)}$ , from (3.28) we obtain  $2D_1 - \rho_1(D^Q) > 2(nD_1 - 2W)x_v^2 \geq C$  as desired. If  $\sum_{i=1}^k x_{v_i}^2 > C[1 + \frac{k}{2(nD_1 - 2W)}]$ , then using (3.28) and Lemma 3.2 we find

$$\begin{aligned} 2D_1 - \rho_1(D^Q) &\geq 2(nD_1 - 2W)x_v^2 + \sum_{t=1}^k (x_{v_t} - x_v)^2 \\ &= \sum_{t=1}^k \left[ \frac{2(nD_1 - 2W)}{k} x_v^2 + (x_{v_t} - x_v)^2 \right] \\ &\geq \sum_{t=1}^k \frac{2(nD_1 - 2W)}{2(nD_1 - 2W) + k} x_{v_t}^2 \\ &> C. \end{aligned}$$

Therefore, (2.15) holds as well. Now we focus on the remaining case that

$$x_v^2 < \frac{C}{2(nD_1 - 2W)} \quad \text{and} \quad \sum_{t=1}^k x_{v_t}^2 \leq C \left[ 1 + \frac{k}{2(nD_1 - 2W)} \right].$$

This implies that

$$x_u^2 \geq \left( 1 - x_v^2 - \sum_{t=1}^k x_{v_t}^2 \right) / (n - k - 1) > \left( 1 - \frac{2(nD_1 - 2W) + k + 1}{2(nD_1 - 2W)} C \right) / (n - k - 1).$$

By (3.30), we get

$$\begin{aligned} 2D_1 - \rho_1(D^Q) &\geq \frac{2(nD_1 - 2W)k^2}{2(nD_1 - 2W)(n + k - 2) + k^2} x_u^2 \\ &> \frac{2(nD_1 - 2W)k^2}{[2(nD_1 - 2W)(n + k - 2) + k^2](n - k - 1)} \left( 1 - \frac{2(nD_1 - 2W) + k + 1}{2(nD_1 - 2W)} C \right) \\ &= \frac{2(nD_1 - 2W)k^2}{2(nD_1 - 2W)(n^2 - 3n + k + 2) + nk^2} \\ &= C. \quad \square \end{aligned}$$

*Proof of Theorem 2.10.* (1) Denote bound (2.10) in Theorem 2.2 and bound (2.13) in Theorem 2.6 as the functions  $g_1(\kappa)$  and  $g_2(\kappa)$  respectively, i.e.,

$$\begin{aligned} g_1(\kappa) &= \frac{nD_1 - 2W}{(nD_1 - 2W + 1)n} = \frac{nD_1 - 2W}{n(nD_1 - 2W) + n}; \\ g_2(\kappa) &= \frac{(nD_1 - 2W)\kappa^2}{(nD_1 - 2W)(n^2 - 3n + \kappa + 2) + n\kappa^2} = \frac{(nD_1 - 2W)}{\frac{n^2 - 3n + \kappa + 2}{\kappa^2}(nD_1 - 2W) + n}. \end{aligned}$$

And we denote  $h_1 = n$ , and  $h_2 = \frac{n^2 - 3n + \kappa + 2}{\kappa^2}$ . Set  $h_2 - h_1 = \frac{n^2 - 3n + \kappa + 2}{\kappa^2} - n = \frac{n^2 - 3n + \kappa + 2 - n\kappa^2}{\kappa^2}$ . If  $1 \leq \kappa \leq \frac{1 + \sqrt{4n(n^2 - 3n + 2) + 1}}{2n}$ , then  $h_2 \geq h_1$ , and thus, Bound (2.10)  $\succeq$  Bound (2.13). If  $\frac{1 + \sqrt{4n(n^2 - 3n + 2) + 1}}{2n} < \kappa < n - 1$ , then  $h_1 > h_2$ , and thus, Bound (2.13)  $\succ$  Bound (2.10).

(2) Similar to the comparison between Bound (2.10) and Bound (2.13), we can compare the bounds (2.14) and (2.15) easily. So we omit the proof here.  $\square$

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