



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

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**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.,

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

\*Received by the editors on June 30, 2017. Accepted for publication on June 12, 2018. Handling Editor: Bryan L. Shader. Corresponding Author: Jinlong Shu.

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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

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

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.  $\square$

**Acknowledgments.** The authors are grateful to the anonymous referees for their valuable comments and useful suggestions, which have considerably improved the presentation of this paper. This work was supported by the National Natural Science Foundation of China (no. 11471121) and China Scholarship Council (no. 201706140137).

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