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A new conjecture on Laplacian eigenvalues and degree sequence of a graph

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Abstract. Let $d_1 \geq d_2 \geq \cdots \geq d_n$ be the degree sequence of a graph G of order n and $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ be the Laplacian eigenvalues of G. In this paper, we propose a new conjecture that for any graph G except for $C_{4k+1}(k \in Z^+)$,

$$\sum_{\mu_i \geq 2} (\mu_i - 2)^2 \leq (1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1).$$

We also prove this conjecture is true for the star, the path, the strongly regular graph, the threshold graph, the barbell graph and the complete bipartite graph, respectively.

1. Introduction

Let G be a graph with n vertices and m edges, and $d_1(G) \geq d_2(G) \geq \cdots \geq d_n(G)$ be the degree sequence of G. Denote by $A(G)$ the adjacency matrix of G and $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ the eigenvalues of $A(G)$. Let $d(v)$ be the degree of vertex v of G, and $L(G) = D(G) - A(G)$ be the Laplacian matrix of G, where $D(G) = diag(d(v_1), d(v_2), \ldots, d(v_n))$ is the diagonal matrix of vertex degrees of G. Let $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$ be the eigenvalues of $L(G)(\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ for short), which are also called the Laplacian eigenvalues of G. It is well known that $L(G)$ is positive semidefinite and so its eigenvalues are nonnegative real numbers. Note that each row sum of $L(G)$ is 0 and, therefore $\mu_n(G) = 0$. Let $Q(G) = D(G) + A(G)$ be the signless Laplacian matrix of G and $q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G)$ be the signless Laplacian eigenvalues of G.

A clique of a graph G is the complete subgraph of the graph G. The order of the maximum clique is called the clique number of the graph G and is denoted by ω. As usual, we denote the complete graph, star, path and cycle with n vertices by K_n, S_n, P_n and C_n, respectively. The complete bipartite graph with the part sizes p and q is denoted by $K_{p,q}$.

Let $S_k(G) = \sum_{i=1}^{k} \mu_i(G), k = 1, 2, \ldots, n$ be the sum of the first k largest Laplacian eigenvalues of G. Let $d_i^T(G) = |\{v \in V(G) : d(v) \geq i\}|$ for $i = 1, 2, \ldots, n$. In 1994, Grone and Merris [10] observed that $S_k(G) \leq \sum_{i=1}^{k} d_i^T(G), k = 1, 2, \ldots, n$. And Bai [2] has proved this, which is called as Grone-Merris-Bai theorem

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now. As an analogue to Grone-Merris-Bai theorem, Brouwer [4] conjectured that $S_k(G) \leq m + \binom{k+1}{2}$ for $k = 1, 2, \ldots, n$. In 2010, Haemers et al. [12] proved that the conjecture holds for all graphs when $k = 2$. There are numerous studies on it (see [5, 6, 9, 13] and the references therein), but it is still open now.

In this paper, we propose a new conjecture on Laplacian eigenvalues related to the degree sequence of a graph.

Conjecture 1.1. *Let G be a graph with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$ and $G \neq C_{4k+1} (k \in Z^+)$. Then*

$$\sum_{\mu_i \geq 2} (\mu_i - 2)^2 \leq (1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1).$$

By using a computer, we check that Conjecture 1.1 holds for connected graphs with at most 9 vertices. It is easy to show that the conjecture holds for complete bipartite graphs. In Section 2, we will assert that to prove Conjecture 1.1, it suffices to consider connected graphs. Furthermore, we prove that Conjecture 1.1 is true for the star, the path, the strongly regular graph, the threshold graph and the barbell graph, respectively. And we also prove Conjecture 1.1 is true for the largest Laplacian eigenvalue, and for the first two largest Laplacian eigenvalues, it is also true for the d-regular($d \geq 3$) graph and the starlike tree, respectively.

Using Cauchy-Schwarz inequality, the weaker conjecture is also proposed.

Conjecture 1.2. *Let G be a graph with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Then for $k = 1, 2, \ldots, n$,*

$$S_k(G) \leq 2k + \sqrt{k(1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1)}.$$

Remark 1: Haemers et al. [12] proved that for all graphs,

$$S_2(G) \leq m + 3. \tag{1}$$

From the Grone-Merris-Bai Theorem, we have

$$S_2(G) \leq d_1^T + d_2^T. \tag{2}$$

From Conjecture 1.2, we conjecture that

$$S_2(G) \leq 4 + \sqrt{2(1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1)}. \tag{3}$$

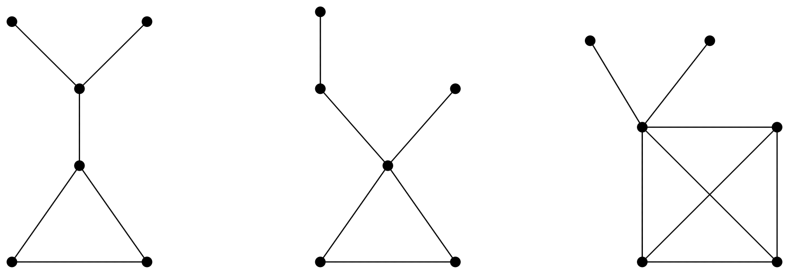
We notice that these three upper bounds (1)-(3) are not comparable. For example, we list three graphs (a), (b) and (c) with 6 vertices as Figure 1. For graph (a), (3) is smaller than (1) and (2). For graph (b), (1) is smaller than (2) and (3). For graph (c), (2) is smaller than (1) and (3).

2. Lemmas and Results

Firstly, we assert that to prove Conjecture 1.1, it will suffice to consider connected graphs.

Lemma 2.1. *If Conjecture 1.1 is true for connected graphs, then Conjecture 1.1 is also true for disconnected graphs.*

Proof. Let G be a graph of order n with connected components $H_1, H_2, \ldots, H_t$, where $1 \leq t \leq n$. Assume that H_i contains n_i vertices, where $i = 1, 2, \ldots, t$. Clearly, $\sum_{i=1}^{t} n_i = n$. It is known that the Laplacian eigenvalues of G is the union of the Laplacian eigenvalues of its connected components and the degree sequence of



(a) (b) (c)

Figure 1: Graphs (a), (b), (c)

G is the union of the degree sequence of its connected components. Since Conjecture 1.1 is true for each connected component H_j $1 \le j \le t$, we have

$$\sum_{\mu_i(H_j)\ge 2}(\mu_i(H_j)-2)^2 \le (1-\frac{1}{d_1(H_j)})\sum_{i=1}^{n_j} d_i(H_j)(d_i(H_j)-1).$$

It follows that

$$\begin{aligned}\sum_{\mu_i(G)\ge 2}(\mu_i(G)-2)^2 &= \sum_{j=1}^{t}\sum_{\mu_i(H_j)\ge 2}(\mu_i(H_j)-2)^2\\ &\le \sum_{j=1}^{t}(1-\frac{1}{d_1(H_j)})\sum_{i=1}^{n_j} d_i(H_j)(d_i(H_j)-1)\\ &\le (1-\frac{1}{d_1(G)})\sum_{j=1}^{t}\sum_{i=1}^{n_j} d_i(H_j)(d_i(H_j)-1)\\ &= (1-\frac{1}{d_1(G)})\sum_{i=1}^{n} d_i(G)(d_i(G)-1).\end{aligned}$$

This completes the proof. □

Next, we state some lemmas which will be used in the subsequent sections.

Lemma 2.2 ([10]). *If G is a connected graph on n vertices with at least an edge, then $\mu_1 \ge d_1 + 1$, with equality if and only if $d_1 = n - 1$.*

Lemma 2.3 ([1]). *Let G be a connected graph with $n \ge 2$ vertices, then $\mu_1(G) \le n$ with equality if and only if the complement of G is disconnected.*

Lemma 2.4 ([7]). *If G is a graph with $n \ge 2$ vertices and $\overline{G}$ is its complement, then $\mu_n(\overline{G}) = 0$ and $\mu_i(\overline{G}) = n-\mu_{n-i}(G)$ $(i = 1, 2, \ldots, n-1)$.*

We next list the Laplacian eigenvalues of some graphs.

Lemma 2.5 ([4]). *Let n be a natural number.*
(1) *The Laplacian eigenvalues of K_n are n with multiplicity $n-1$, 0.*
(2) *The Laplacian eigenvalues of S_n are n, 1 with multiplicity $n-2$, 0.*

(3) *The Laplacian eigenvalues of* P_n *are* $2 - 2\cos\frac{\pi i}{n}$ *for* $i = 0, \ldots, n-1$.
(4) *The Laplacian eigenvalues of* C_n *are* $2 - 2\cos\frac{2\pi i}{n}$ *for* $i = 0, \ldots, n-1$.
(5) *The Laplacian eigenvalues of* $K_{p,q}$ *are* $p + q$, p *with multiplicity* $q - 1$, q *with multiplicity* $p - 1$, 0.

Nikiforov obtained the following assertion by using Motzkin-Straus inequality.

Lemma 2.6 ([16]). *Let G be a graph with clique number* ω *and m edges. Then* $\lambda_1^2(G) \leq \frac{2(\omega-1)m}{\omega}$.

Considering the matrix A^2 and using the fact that the sum of the eigenvalues of a matrix is equal to the sum of its diagonal elements, we have the following lemma.

Lemma 2.7. *Let* $A = (a_{ij})_{n\times n}$ *be a real symmetric matrix with eigenvalues* $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. *Then* $\sum_{i=1}^{n}\lambda_i^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij}^2$.

A graph (simple, undirected, and loopless) of order n is called strongly regular with parameters n, d, λ, μ whenever it is not complete or edgeless and

1. each vertex is adjacent to d vertices,
2. for each pair of adjacent vertices there are λ vertices adjacent to both,
3. for each pair of nonadjacent vertices there are μ vertices adjacent to both.

We call an eigenvalue restricted if it has an eigenvector perpendicular to the all-1 vector **1**. For strongly regular graph $G(n, d, \lambda, \mu)$, $A(G)$ has precisely two distinct restricted eigenvalues[4]. And they have the following properties.

Lemma 2.8 ([4]). *Let G be a strong regular graph* $G(n, d, \lambda, \mu)$ *with restricted eigenvalues* $r, s (r > s)$ *and let* f, g *be their respective multiplicities. Then* $f, g = \frac{1}{2}(n - 1 \mp \frac{(r+s)(n-1)+2d}{r-s})$.

Denote by $\Phi(B) = \Phi(B; x) = det(xI - B)$ the characteristic polynomial of B. If $v \in G$, let $L_v(G)$ be the principal submatrix of $L(G)$ formed by deleting the row and column corresponding to vertex v. If $G = v$, then suppose that $\Phi(L_v(G)) = 1$.

Lemma 2.9 ([11]). *Let* $G = G_1u : vG_2$ *be the graph obtained by joining the vertex u of the graph* G_1 *to the vertex v of the graph* G_2 *by an edge. Then*

$$\Phi(L(G)) = \Phi(L(G_1))\Phi(L(G_2)) - \Phi(L(G_1))\Phi(L_v(G_2)) - \Phi(L(G_2))\Phi(L_u(G_1)).$$

For $i = 1, 2, \ldots, n$ the conjugate degree $d_i^T(G) = |\{v \in V(G) : d(v) \geq i\}|$ gives the number of nodes of G of degree at least i. Each degree sequence satisfying $d_i^T = d_i + 1$ for $i = 1, \ldots, h$ with trace $h = max\{i : d_i \geq i\}$ uniquely defines a graph and these graphs form the so called threshold graphs [15].

Lemma 2.10 ([14]). *Let G be a threshold graph. Then* $\mu_i(G) = d_i^T(G)$ *for* $i = 1, \ldots, n$.

A tree is said to be starlike if exactly one of its vertices has degree greater than two. By $S(n_1, n_2, \ldots, n_k)$ we denote the starlike tree which has a vertex v_1 of degree $k \geq 3$ and which has the property $S(n_1, n_2, \ldots, n_k) - v_1 = P_{n_1} \cup P_{n_2} \cup \cdots \cup P_{n_k}$. We assume that $n_1 \geq n_2 \geq \cdots \geq n_k \geq 1$. Das [8] gave the upper bound of $\mu_1(G)$ and $\mu_2(G)$ for starlike trees as follows.

Lemma 2.11 ([8]). *Let G be a starlike tree* $S(n_1, n_2, \ldots, n_k)$, $n_1 \geq n_2 \geq \cdots \geq n_k \geq 1$. *Then*
(1) $\mu_1(G) < k + 1 + \frac{1}{k-1}$.
(2) $\mu_2(G) \leq 2 + 2\cos\frac{2\pi}{2n_1+1}$.

Let G be a graph with $V(G) = \{1, \ldots, n\}$ and $E(G) = \{e_1, \ldots, e_m\}$. The (vertex-edge) incidence matrix of G, which we denote by $M(G)$, or simply by M, is the $n \times m$ matrix defined as follows. The rows and the columns of M are indexed by $V(G)$ and $E(G)$, respectively. The (i, j)-entry of M is 0 if vertex i and edge e_j are not incident, and otherwise it is 1. Then $Q(G) = MM'$, where M' is the transpose of M. Let $\mathscr{L}(G)$ be the line graph of G. Note that $A(\mathscr{L}(G)) + 2I = M'M$ [3]. Then $Q(G)$ and $A(\mathscr{L}(G)) + 2I$ have the same nonzero eigenvalues.

We next prove Conjecture 1.1 is true for the largest Lapalcian eigenvalue, and so we give a new upper bound for the largest Laplacian eigenvalue.

Theorem 2.12. *Let G be a graph on n vertices and $m \geq 1$ edges with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Then $\mu_1 \leq 2 + \sqrt{(1 - \frac{1}{d_1}) \sum_{i=1}^n d_i(d_i - 1)}$.*

Proof. Consider the line graph $\mathscr{L}(G)$ of G. Then $\omega(\mathscr{L}(G)) = d_1$. By Lemma 2.6, $\lambda_1(\mathscr{L}(G))^2 \leq 2(1 - \frac{1}{d_1})m(\mathscr{L}(G))$. Since $\lambda_1(\mathscr{L}(G)) = q_1(G) - 2$ and $m(\mathscr{L}(G)) = \frac{\sum_{i=1}^n d_i(d_i-1)}{2}$, we have $(q_1(G) - 2)^2 \leq 2(1 - \frac{1}{d_1})\frac{\sum_{i=1}^n d_i(d_i-1)}{2}$. Then $\mu_1 \leq q_1 \leq 2 + \sqrt{(1 - \frac{1}{d_1}) \sum_{i=1}^n d_i(d_i - 1)}$. □

The following results show that the equality of Conjecture 1.1 holds for the star, the path and the even cycle, respectively.

Theorem 2.13. *Let G be a graph of order n.*
(1) If G is a star, then $\sum_{\mu_i \geq 2}(\mu_i - 2)^2 = (1 - \frac{1}{d_1}) \sum_{i=1}^n d_i(d_i - 1)$.
(2) If G is a path, then $\sum_{\mu_i \geq 2}(\mu_i - 2)^2 = (1 - \frac{1}{d_1}) \sum_{i=1}^n d_i(d_i - 1)$.

Proof. (1)For the star graph S_n, by Lemma 2.5, $\sum_{\mu_i \geq 2}(\mu_i - 2)^2 = (n-2)^2$. Since $(1 - \frac{1}{d_1}) \sum_{i=1}^n d_i(d_i - 1) = (n-2)^2$, the theorem holds.
(2)For the path P_n, since $\sum_{\mu_i \geq 2}(\mu_i - 2)^2 = \sum_{\mu_i > 2}(\mu_i - 2)^2$, we only consider Laplacian eigenvalues greater than 2. By Lemma 2.5, the Laplacian eigenvalues of P_n are $2 - 2\cos\frac{\pi i}{n}$ for $i = 0, \ldots, n-1$. Hence $\mu_i > 2$ if and only if $\cos\frac{\pi i}{n} < 0$. This implies $\frac{n}{2} < i < n$.

If $n = 2k (k \in Z^+)$, then $k < i < 2k$. We need to show that

$$\sum_{i=k+1}^{2k-1}(2 - 2\cos\frac{\pi i}{2k} - 2)^2 = 2k - 2.$$

After simplification, the previous equality is equivalent to

$$\sum_{i=k+1}^{2k-1}\cos\frac{\pi i}{k} = 0.$$

Since $\sum_{i=1}^n \mu_i = 2m$, by Lemma 2.5, using the Laplacian eigenvalues of the cycle, we have $\sum_{i=0}^{n-1}(2 - 2\cos\frac{2\pi i}{n}) = 2n$. Then we have $\sum_{i=0}^{n-1}\cos\frac{2\pi i}{n} = 0$. It follows that

$$\begin{aligned}\sum_{i=k+1}^{2k-1}\cos\frac{\pi i}{k} &= \sum_{i=0}^{2k-1}\cos\frac{2\pi i}{2k} - 1 - \sum_{i=1}^{k-1}\cos\frac{2\pi i}{2k} - \cos\frac{2\pi k}{2k} \\ &= -\sum_{i=1}^{k-1}\cos\frac{2\pi i}{2k} \\ &= -\sum_{i=k+1}^{2k-1}\cos\frac{2\pi i}{2k}.\end{aligned}$$

Therefore, $\sum_{i=k+1}^{2k-1} \cos \frac{\pi i}{k} = 0$.

If $n = 2k + 1 (k \in Z^+)$, then $k + \frac{1}{2} < i < 2k + 1$. We need to show that

$$\sum_{i=k+1}^{2k} (2 - 2\cos \frac{\pi i}{2k+1} - 2)^2 = 2k - 1.$$

After simplification, the previous equality is equivalent to

$$\sum_{i=k+1}^{2k} \cos \frac{2\pi i}{2k+1} = -\frac{1}{2}.$$

Since $\sum_{i=0}^{n-1} \cos \frac{2\pi i}{n} = 0$, we have $\sum_{i=1}^{2k} \cos \frac{2\pi i}{2k+1} = \sum_{i=0}^{2k} \cos \frac{2\pi i}{2k+1} - 1 = -1$. On the other hand, $\sum_{i=1}^{2k} \cos \frac{2\pi i}{2k+1} = 2\sum_{i=k+1}^{2k} \cos \frac{2\pi i}{2k+1}$. Then $\sum_{i=k+1}^{2k} \cos \frac{2\pi i}{2k+1} = -\frac{1}{2}$. □

Theorem 2.14. *Let C_n be a cycle. If $n \neq 4k + 1 (k \in Z^+)$, then $\sum_{\mu_i \geq 2} (\mu_i - 2)^2 \leq (1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1)$, with equality if and only if n is even.*

Proof. Since $\sum_{\mu_i \geq 2} (\mu_i - 2)^2 = \sum_{\mu_i > 2} (\mu_i - 2)^2$, we only consider Laplacian eigenvalues greater than 2. By Lemma 2.5, the Laplacian eigenvalues of C_n are $2 - 2\cos \frac{2\pi i}{n}$ for $i = 0, \ldots, n-1$. Hence $\mu_i > 2$ if and only if $\cos \frac{2\pi i}{n} < 0$. This implies $\frac{n}{4} < i < \frac{3n}{4}$.

If $n = 4k (k \in Z^+)$, then $k < i < 3k$. We need to show that

$$\sum_{i=k+1}^{3k-1} (2 - 2\cos \frac{2\pi i}{4k} - 2)^2 = 4k.$$

After simplification, the previous equality is equivalent to

$$\sum_{i=k+1}^{3k-1} \cos \frac{\pi i}{k} = 1.$$

Since $\sum_{i=k}^{3k} \cos \frac{\pi i}{k} = -1$, we have $\sum_{i=k+1}^{3k-1} \cos \frac{\pi i}{k} = -1 - cos\pi - cos3\pi = 1$.

If $n = 4k + 2 (k \in Z^+)$, then $k + \frac{1}{2} < i < 3k + \frac{3}{2}$. We need to show that

$$\sum_{i=k+1}^{3k+1} (2 - 2\cos \frac{2\pi i}{4k+2} - 2)^2 = 4k + 2.$$

After simplification, the previous equality is equivalent to

$$\sum_{i=k+1}^{3k+1} \cos \frac{2\pi i}{2k+1} = 0.$$

Since $\sum_{i=0}^{n-1} \cos \frac{2\pi i}{n} = 0$, we have

$$\begin{aligned}
\sum_{i=k+1}^{3k+1} \cos \frac{2\pi i}{2k+1} &= \sum_{i=k+1}^{2k+1} \cos \frac{2\pi i}{2k+1} + \sum_{i=2k+2}^{3k+1} \cos \frac{2\pi i}{2k+1} \\
&= \sum_{i=k+1}^{2k+1} \cos \frac{2\pi i}{2k+1} + \sum_{i=1}^{k} \cos \frac{2\pi i}{2k+1} \\
&= \sum_{i=1}^{2k+1} \cos \frac{2\pi i}{2k+1} \\
&= 0.
\end{aligned}$$

If $n = 4k + 3 (k \in Z^+)$, then $k + \frac{3}{4} < i < 3k + \frac{9}{4}$. We need to show that

$$\sum_{i=k+1}^{3k+2} (2 - 2\cos\frac{2\pi i}{4k+3} - 2)^2 < 4k + 3.$$

After simplification, the previous inequality is equivalent to

$$\sum_{i=k+1}^{3k+2} \cos\frac{4\pi i}{4k+3} < -\frac{1}{2}.$$

Using a computer we have

$$\begin{aligned}
\sum_{i=k+1}^{3k+2} \cos\frac{4\pi i}{4k+3} &= \frac{\sin\frac{(12k+10)\pi}{4k+3} - \sin\frac{(4k+2)\pi}{4k+3}}{2\sin\frac{2\pi}{4k+3}} \\
&= \frac{\sin(3\pi + \frac{\pi}{4k+3}) - \sin(\pi - \frac{\pi}{4k+3})}{2\sin\frac{2\pi}{4k+3}} \\
&= -\frac{2\sin\frac{\pi}{4k+3}}{2\sin\frac{2\pi}{4k+3}} \\
&= -\frac{\sin\frac{\pi}{4k+3}}{2\sin\frac{\pi}{4k+3}\cos\frac{\pi}{4k+3}} \\
&= -\frac{1}{2\cos\frac{\pi}{4k+3}} \\
&< -\frac{1}{2}.
\end{aligned}$$

This completes the proof. □

Remark 2: When $n = 4k + 1 (k \in Z^+)$, for cycle C_n, we conclude that $\sum_{\mu_i \geq 2}(\mu_i - 2)^2 > (1 - \frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i - 1)$. Otherwise, assume that $\sum_{\mu_i \geq 2}(\mu_i - 2)^2 \leq (1 - \frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i - 1)$. By the theorem above, $\mu_i > 2$ implies that $k + \frac{1}{4} < i < 3k + \frac{3}{4}$. Then we need to show that

$$\sum_{i=k+1}^{3k} (2 - 2\cos\frac{2\pi i}{4k+1} - 2)^2 \leq 4k + 1.$$

After simplification, the previous inequality is equivalent to

$$\sum_{i=k+1}^{3k} \cos\frac{4\pi i}{4k+1} \leq \frac{1}{2}.$$

Using a computer we have

$$\begin{aligned}\sum_{i=k+1}^{3k}\cos\frac{4\pi i}{4k+1} &= \frac{\sin\frac{(12k+2)\pi}{4k+1}-\sin\frac{(4k+2)\pi}{4k+1}}{2\sin\frac{2\pi}{4k+1}}\\ &= \frac{\sin(3\pi-\frac{\pi}{4k+1})-\sin(\pi+\frac{\pi}{4k+1})}{2\sin\frac{2\pi}{4k+1}}\\ &= \frac{2\sin\frac{\pi}{4k+1}}{2\sin\frac{2\pi}{4k+1}}\\ &= \frac{\sin\frac{\pi}{4k+1}}{2\sin\frac{\pi}{4k+1}\cos\frac{\pi}{4k+1}}\\ &= \frac{1}{2\cos\frac{\pi}{4k+1}}\\ &> \frac{1}{2},\end{aligned}$$

a contradiction.

Theorem 2.15. *Let G be a strong regular graph $G(n,d,\lambda,\mu)(d \geq 3)$ with restricted eigenvalues $r > s$. Then $\sum_{\mu_i\geq 2}(\mu_i-2)^2 \leq (1-\frac{1}{d_1})\sum_{i=1}^n d_i(d_i-1)$.*

Proof. By Lemma 2.8, the eigenvalues of G are d, r with multiplicity f and s with multiplicity g, where $f=\frac{1}{2}(n-1-\frac{(r+s)(n-1)+2d}{r-s})$ and $g=\frac{1}{2}(n-1+\frac{(r+s)(n-1)+2d}{r-s})$. Since $L(G)=D(G)-A(G)$, the Laplacian eigenvalues of G is $d-s$ with multiplicity g, $d-r$ with multiplicity f and 0. If $d-r\geq 2$, we will show that

$$g(d-s-2)^2+f(d-r-2)^2 \leq n(d-1)^2.$$

Since $\sum_{i=1}^n \lambda_i = 0$ and $\sum_{i=1}^n \lambda_i^2 = \sum_{i=1}^n d_i$, we have $gs+fr=-d$ and $gs^2+fr^2+d^2=nd$. Then

$$\begin{aligned}g(d-s-2)^2+f(d-r-2)^2 &= g((d-2)^2-2s(d-2)+s^2)+f((d-2)^2-2r(d-2)+r^2)\\ &= (g+f)(d-2)^2-2(d-2)(gs+fr)+gs^2+fr^2\\ &= (n-1)(d-2)^2+2d(d-2)+nd-d^2.\end{aligned}$$

Then we only need to show that

$$(n-1)(d-2)^2+2d(d-2)+nd-d^2 \leq n(d-1)^2.$$

That is

$$4+n(d-3)\geq 0.$$

The inequality holds if $d\geq 3$. If $d-r<2$, it easily follows that $g(d-s-2)^2 < g(d-s-2)^2+f(d-r-2)^2 \leq n(d-1)^2$. This completes the proof. □

The barbell graph $B_{s,t}$ is constructed by connecting two complete graphs $K_s(s\geq 1)$ and $K_t(t\geq 1)$ by a bridge.

Theorem 2.16. *Let G be the barbell graph $B_{s,t}(s\geq 1, t\geq 1)$. Then $\sum_{\mu_i\geq 2}(\mu_i-2)^2 \leq (1-\frac{1}{d_1})\sum_{i=1}^n d_i(d_i-1)$.*

Proof. We may assume that $s+t\geq 10$ and $s\geq t$. Let $u\in K_s$, $v\in K_t$ and uv be the bridge of $B_{s,t}$.

If $s=t=1$, then $G=K_2$. The result holds. If $s\geq 2$ and $t=1$, then by Lemma 2.9, the characteristic polynomial of $L(G)$ is as follows:

$$\begin{aligned}\Phi(L(G)) =&\Phi(L(K_s))\Phi(L(K_1))-\Phi(L(K_s))\Phi(L_v(K_1))-\Phi(L(K_1))\Phi(L_u(K_s))\\ =&x(x-s)^{s-1}x-x(x-s)^{s-1}-x(x-1)(x-s)^{s-2}\\ =&x(x-1)(x-s)^{s-2}(x-s-1).\end{aligned}$$

Then the Laplacian spectrum of G are 0, 1, s with multiplicity $s-2$, and $s+1$. Then

$$\sum_{\mu_i \geq 2} (\mu_i - 2)^2 = (s-1)^2 + (s-2)^3$$

and

$$(1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1) = (s-1)^2 + \frac{s-2}{s}(s-1)^3.$$

It is easy to check that the result holds.

If $s \geq t \geq 2$, then by Lemma 2.9, the characteristic polynomial of $L(G)$ is as follows:

$$\begin{aligned}
\Phi(L(G)) =& \Phi(L(K_s))\Phi(L(K_t)) - \Phi(L(K_s))\Phi(L_v(K_t)) - \Phi(L(K_t))\Phi(L_u(K_s)) \\
=& x(x-s)^{s-1}x(x-t)^{t-1} - x(x-s)^{s-1}(x-1)(x-t)^{t-2} \\
& - x(x-t)^{t-1}(x-1)(x-s)^{s-2} \\
=& x(x-s)^{s-2}(x-t)^{t-2}(x^3 - (s+t+2)x^2 + (st+s+t+2)x - (s+t)) \\
\triangleq& x(x-s)^{s-2}(x-t)^{t-2}g(x).
\end{aligned}$$

Let $x_1 \geq x_2 \geq x_3$ be the roots of the equation $g(x) = 0$. Then the Laplacian spectrum of G are x_1, s with multiplicity $s-2$, x_2, t with multiplicity $t-2$, x_3 and 0. Since

$$\begin{aligned}
& g(0) = -s - t < 0, g(1) = st - (s+t) + 1 > 0, \\
& g(t) = (t-1)(s-t) \geq 0, g(t+1) = -s + 1 < 0, \\
& g(s) = (s-1)(t-s) \leq 0, g(s+2) = s^2 + (3-t)s - 3t + 4 > 0,
\end{aligned}$$

we have $0 < x_3 < 1$, $t \leq x_2 < t+1$, and $s \leq x_1 < s+2$. Then

$$\sum_{\mu_i \geq 2} (\mu_i - 2)^2 \leq s^2 + (s-2)^3 + (t-1)^2 + (t-2)^3.$$

The degree sequence of the barbell graph $B_{s,t}$ is $(s, t, \underbrace{s-1, \ldots, s-1}_{s-1}, \underbrace{t-1, \ldots, t-1}_{t-1})$. Then

$$(1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1) = \frac{s-1}{s}(s(s-1) + (s-1)^2(s-2) + t(t-1) + (t-1)^2(t-2)).$$

Hence, it suffices to prove

$$s^2 + (s-2)^3 + (t-1)^2 + (t-2)^3 \leq \frac{s-1}{s}(s(s-1) + (s-1)^2(s-2) + t(t-1) + (t-1)^2(t-2)).$$

Cancelling and rearranging shows that the previous inequality is equivalent to

$$0 \leq s^3 - 5s^2 + (2t^2 - 6t + 7)s - t^3 + 3t^2 - 4t + 4.$$

Consider the polynomial $f(s,t) = s^3 - 5s^2 + (2t^2 - 6t + 7)s - t^3 + 3t^2 - 4t + 4$. If $s = t$, which implies that $s = t \geq 5$, then $f(s,t) = f(s) = 2s^3 - 8s^2 + 3s + 4$. It is easy to check that $f(s)$ increases as s increases when $s \geq 5$. Then $f(s) \geq f(5) > 0$. If $s > t$, let $s = t + a$, $a \geq 1$. Let $h(a,t) = f(t+a,t) = a^3 + (3t-5)a^2 + (5t^2 - 16t + 7)a + 2t^3 - 8t^2 + 3t + 4$. We next prove $h(a,t) \geq 0$ for $t \geq 1$.

If $t = 1$, which implies that $a \geq 8$, then $h(a,1) = a^3 - 2a^2 - 4a + 1$. It is easy to check that $h(a,1)$ increases as a increases when $a \geq 8$. Then $h(a,1) \geq h(8,1) > 0$. If $t = 2$, which implies that $a \geq 6$, then $h(a,2) = a^3 + a^2 - 5a - 6$. It is easy to check that $h(a,2)$ increases as a increases when $a \geq 6$. Then $h(a,2) \geq h(6,2) > 0$. If $t \geq 3$, the derivative of $h(a,t)$ with respect to a is $h_a(a,t) = 3a^2 + 2(3t-5)a + 5t^2 - 16t + 7$. The derivative of $h_a(a,t)$

with respect to a is $h_{aa}(a,t) = 6a + 6t - 10$. Since $a \geq 1$ and $t \geq 3$, $h_{aa}(a,t) > 0$. We have $h_a(a,t)$ increases as a when $a \geq 1$, then $h_a(a,t) > h_a(1,t) = 5t^2 - 10t > 0$. Then $h(a,t)$ increases as a when $a \geq 1$. Hence $h(a,t) \geq h(1,t) = 2t^3 - 3t^2 - 10t + 7$. It is easy to check that $h(1,t) = 2t^3 - 3t^2 - 10t + 7$ increases as t increases when $t \geq 3$. Thus, $h(a) \geq h(1,3) > 0$. □

A vertex is called dominating if it is adjacent to every other vertex. One way to characterize threshold graphs is through an iterative process which starts with an isolated vertex, and where, at each step, either a new isolated vertex is added, or a dominating vertex is added.

Theorem 2.17. *Let G be a threshold graph of order n. Then* $\sum_{\mu_i \geq 2}(\mu_i - 2)^2 \leq (1 - \frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i - 1)$.

Proof. We prove this by induction on the number of vertices n. Let G_n be the threshold graph of order n. Suppose the Laplacian spectrum of G_n is $\mu_1(G_n) \geq \cdots \geq \mu_n(G_n) = 0$. The degree sequence of G_n is $d_1(G_n) \geq \cdots \geq d_n(G_n)$. For $n = 1$, it is obvious that the conclusion is true for $G_1 = K_1$. Assume the result is true for $n = k$ for some $k \in Z^+$, that is,

$$\sum_{\mu_i(G_k) \geq 2}(\mu_i(G_k) - 2)^2 \leq (1 - \frac{1}{d_1(G_k)})\sum_{i=1}^{k} d_i(G_k)(d_i(G_k) - 1).$$

From this assumption we want to deduce the truth of

$$\sum_{\mu_i(G_{k+1}) \geq 2}(\mu_i(G_{k+1}) - 2)^2 \leq (1 - \frac{1}{d_1(G_{k+1})})\sum_{i=1}^{k+1} d_i(G_{k+1})(d_i(G_{k+1}) - 1).$$

If G_{k+1} is obtained by adding an isolated vertex to G_k, using the induction hypothesis we have

$$\begin{aligned}\sum_{\mu_i(G_{k+1}) \geq 2}(\mu_i(G_{k+1}) - 2)^2 &= \sum_{\mu_i(G_k) \geq 2}(\mu_i(G_k) - 2)^2\\ &\leq (1 - \frac{1}{d_1(G_k)})\sum_{i=1}^{k} d_i(G_k)(d_i(G_k) - 1)\\ &= (1 - \frac{1}{d_1(G_{k+1})})\sum_{i=1}^{k+1} d_i(G_{k+1})(d_i(G_{k+1}) - 1).\end{aligned}$$

Next suppose that G_{k+1} is obtained by adding a dominating vertex to G_k. The degree sequence of G_{k+1} is $k \geq d_1(G_k) + 1 \geq d_2(G_k) + 1 \geq \cdots \geq d_k(G_k) + 1$. By Lemma 2.4, the Laplacian spectrum of $\overline{G_{k+1}}$ is $\{k - \mu_{k-1}(G_k), k - \mu_{k-2}(G_k), \ldots, k - \mu_1(G_k), 0, 0\}$. Then by Lemma 2.4, the Laplacian spectrum of G_{k+1} is $k+1 \geq \mu_1(G_k)+1 \geq \mu_2(G_k)+1 \geq \cdots \geq \mu_{k-1}(G_k)+1 \geq 0$. By Lemma 2.10, the Laplacian spectrum of a threshold graph is integral. Then the Laplacian eigenvalues of G_k less than 2 are 0 and 1. Let $t = max\{j|\mu_j(G_k) \geq 2\}$, $s = |\{j|\mu_j(G_k) = 1\}|$. Then using the induction hypothesis,

$$\begin{aligned}\sum_{\mu_i(G_{k+1}) \geq 2}(\mu_i(G_{k+1}) - 2)^2 &= (k + 1 - 2)^2 + \sum_{i=1}^{t}(\mu_i(G_k) + 1 - 2)^2 + \sum_{i=1}^{s}(2 - 2)^2\\ &= (k - 1)^2 + \sum_{i=1}^{t}(\mu_i(G_k) - 2)^2 + 2\sum_{i=1}^{t}(\mu_i(G_k) - 2) + t\\ &\leq (k - 1)^2 + (1 - \frac{1}{d_1(G_k)})\sum_{i=1}^{k} d_i(G_k)(d_i(G_k) - 1) + 2\sum_{i=1}^{t}\mu_i(G_k) - 3t\\ &\leq (k - 1)^2 + (1 - \frac{1}{k})\sum_{i=1}^{k} d_i(G_k)(d_i(G_k) - 1) + 2\sum_{i=1}^{t}\mu_i(G_k) - 3t.\end{aligned}$$

On the other hand,

$$(1-\frac{1}{d_1(G_{k+1})})\sum_{i=1}^{k+1} d_i(G_{k+1})(d_i(G_{k+1})-1) = (1-\frac{1}{k})(k(k-1)+\sum_{i=1}^{k} d_i(G_k)(d_i(G_k)+1))$$
$$= (k-1)^2 + (1-\frac{1}{k})\sum_{i=1}^{k} d_i(G_k)(d_i(G_k)+1).$$

Then we need to show that

$$(1-\frac{1}{k})\sum_{i=1}^{k} d_i(G_k)(d_i(G_k)-1) + 2\sum_{i=1}^{t}\mu_i(G_k) - 3t \le (1-\frac{1}{k})\sum_{i=1}^{k} d_i(G_k)(d_i(G_k)+1).$$

Using $\sum_{i=1}^{n}\mu_i = \sum_{i=1}^{n} d_i$ and simplifying previous inequality, we need to show that

$$2\sum_{i=1}^{t}\mu_i(G_k) - 3t \le 2(1-\frac{1}{k})\sum_{i=1}^{k}\mu_i(G_k)$$
$$= 2\sum_{i=1}^{t}\mu_i(G_k) + 2s - \frac{2}{k}\sum_{i=1}^{t}\mu_i(G_k) - \frac{2s}{k}.$$

We next need to show that $\frac{2}{k}\sum_{i=1}^{t}\mu_i(G_k) + \frac{2s}{k} \le 3t + 2s$. By Lemma 2.3, $\mu_i(G_k) \le \mu_1(G_k) \le k$ for $1 \le i \le k$. Then $\sum_{i=1}^{t}\mu_i(G_k) \le kt$. Since $k \ge 1$, we have $\frac{2}{k}\sum_{i=1}^{t}\mu_i(G_k) + \frac{2s}{k} \le 2t + \frac{2s}{k} \le 3t + 2s$. □

Theorem 2.18. *Let G be a d-regular graph ($d \ge 3$) of order n. Then $(\mu_1-2)^2 + (\mu_2-2)^2 \le (1-\frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i-1)$.*

Proof. We may assume that $n \ge 8$. Let $A = (a_{ij})_{n\times n}$ be the adjacency matrix of G, and $D = dI$ be the degree diagonal matrix. Consider the matrix $B = (b_{ij})_{n\times n}$, where $B = D - A - 2I$. Let $\lambda_1^2(B) \ge \lambda_2^2(B) \ge \cdots \ge \lambda_n^2(B)$ be the eigenvalues of B^2. By Lemma 2.7,

$$\sum_{i=1}^{n}\lambda_i^2(B) = \sum_{i=1}^{n}\sum_{j=1}^{n} {b_{ij}}^2$$
$$= n(d-2)^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} {a_{ij}}^2$$
$$= n(d-2)^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}$$
$$= n(d-2)^2 + nd$$
$$= nd^2 - 3nd + 4n.$$

Then,

$$(\mu_1-2)^2 + (\mu_2-2)^2 \le \lambda_1^2(B) + \lambda_2^2(B) = nd^2 - 3nd + 4n - \sum_{i=3}^{n}\lambda_i^2(B).$$

We have to show that

$$nd^2 - 3nd + 4n - \sum_{i=3}^{n}\lambda_i^2(B) \le n(d-1)^2.$$

That is

$$\sum_{i=3}^{n}\lambda_i^2(B) \ge 3n - nd.$$

Since $d \ge 3$, $3n - nd \le 0 \le \sum_{i=3}^{n}\lambda_i^2(B)$ is true. This completes the proof. □

For 2-regular graph $C_n (n \geq 8)$, by Lemma 2.5, we have $\mu_2 \leq \mu_1 \leq 4$. Then $(\mu_1 - 2)^2 + (\mu_2 - 2)^2 \leq 8 \leq n = (1 - \frac{1}{d_1(C_n)}) \sum_{i=1}^{n} d_i(C_n)(d_i(C_n) - 1)$. For 1-regular graph K_2, by Lemma 2.5, $\mu_1 + \mu_2 = 2 < 4$. Then we have the following corollary.

Corollary 2.19. *Let G be a d-regular graph. Then $S_2(G) \leq 4 + (d-1)\sqrt{2n}$.*

Remark 3: The upper bound in Corollary 2.19 is better than the Brouwer Conjecture's bound for regular graph when $n \geq 8$. That is $nd/2 + 3 - (d-1)\sqrt{2n} - 4 \geq 0$. Let $f(n,d) = nd/2 + 3 - (d-1)\sqrt{2n} - 4$. If $n = 8$, $f(8,d) = 3 > 0$. If $n > 8$, we find that $f(n,d) > 0$ when $d \geq \frac{2-2\sqrt{2n}}{n-2\sqrt{2n}}$. Then $f(n,d) > 0$ for all $d \geq 1$ since $\frac{2-2\sqrt{2n}}{n-2\sqrt{2n}} < 1$.

Lemma 2.20. *Let G be a starlike tree of order $n (n \geq 10)$.*
(i) If $G \cong S(3,1,\ldots,1)$, then $\mu_1 < n - 2 + \frac{3}{n^2}$ and $(\mu_1 - 2)^2 + (\mu_2 - 2)^2 \leq (1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1)$.
(ii) If $G \cong S(2,2,1,\ldots,1)$, then $\mu_1 < n - 2 + \frac{5}{n^2}$ and $(\mu_1 - 2)^2 + (\mu_2 - 2)^2 \leq (1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1)$.
(iii) If $G \cong S(2,1,\ldots,1)$, then $\mu_1 < n - 1 + \frac{2}{n^2}$ and $(\mu_1 - 2)^2 + (\mu_2 - 2)^2 \leq (1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1)$.

Proof. (1) By direct calculation, the characteristic polynomial of $L(G)$ is

$$\Phi(x) = x(x-1)^{n-5}(x^4 - (n+3)x^3 + (5n-4)x^2 - (6n-10)x + n).$$

Let $f(x) = (x^4 - (n+3)x^3 + (5n-4)x^2 - (6n-10)x + n)$. Then $f(n-2+\frac{3}{n^2}) = \frac{2n^9 - 29n^8 + 114n^7 - 99n^6 - 198n^5 + 342n^4 + 81n^3 - 297n^2 + 81}{n^8}$. Let $g(n) = 2n^9 - 29n^8 + 114n^7 - 99n^6 - 198n^5 + 342n^4 + 81n^3 - 297n^2 + 81$. Then $g(n)$ is increasing when $n \geq 9$. Hence $g(n) \geq g(9) > 0$. So $\Phi(n - 2 + \frac{3}{n^2}) > 0$. Since $\Phi(n-2) = 4 - n < 0$, and by Lemmas 2.2 and 2.11, $\mu_1 \geq n - 2$ and $\mu_2 \leq 4$, we have $\mu_1 < n - 2 + \frac{3}{n^2}$.

Therefore, by Lemma 2.11,

$$\begin{aligned}(\mu_1 - 2)^2 + (\mu_2 - 2)^2 &\leq (n - 2 + \frac{3}{n^2} - 2)^2 + 4\cos^2(\frac{2\pi}{7}) \\ &\leq (n-4)^2 + 6\frac{n-4}{n^2} + \frac{9}{n^4} + 1.555.\end{aligned}$$

And we have

$$(1 - \frac{1}{d_1}) \sum_{i=1}^{n} d_i(d_i - 1) = (n-4)^2 + 4\frac{n-4}{n-3}.$$

It suffices to show that

$$6\frac{n-4}{n^2} + \frac{9}{n^4} + 1.555 \leq 4\frac{n-4}{n-3}.$$

It is true for $n \geq 5$. This completes the proof.

(2) By direct calculation, the characteristic polynomial of $L(G)$ is

$$\Phi(x) = x(x-1)^{n-6}(x^2 - 3x + 1)(x^3 - (n+1)x^2 + (3n-5)x - n).$$

Let $f(x) = x^3 - (n+1)x^2 + (3n-5)x - n$, and $x_1 \geq x_2 \geq x_3$ be the roots of $f(x)$. The Laplacian eigenvalues of G are $x_1, x_2, x_3, \frac{3+\sqrt{5}}{2}, \frac{3-\sqrt{5}}{2}, 0, 1$ with multiplicity $n-6$. By Lemmas 2.2 and 2.11, $\mu_1 \geq n-2$ and $\mu_2 \leq 4$. Then $\mu_1 = x_1$. By simple calculation, $f(n-2+\frac{5}{n^2}) = \frac{3n^6 - 35n^5 + 55n^4 + 50n^3 - 175n^2 + 125}{n^6}$. Let $g(n) = 3n^6 - 35n^5 + 55n^4 + 50n^3 - 175n^2 + 125$. Then $g(n)$ is increasing when $n \geq 10$. Hence $g(n) \geq g(10) > 0$. So $f(n - 2 + \frac{5}{n^2}) > 0$. Since $f(n-2) = -2 < 0$, $\mu_1 = x_1 < n - 2 + \frac{5}{n^2}$.

Therefore, by Lemma 2.11,

$$\begin{aligned}(\mu_1 - 2)^2 + (\mu_2 - 2)^2 &\leq (n - 2 + \frac{5}{n^2} - 2)^2 + 4\cos^2(\frac{2\pi}{5}) \\ &\leq (n-4)^2 + 10\frac{n-4}{n^2} + \frac{25}{n^4} + 0.382.\end{aligned}$$

And we have

$$(1-\frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i-1) = (n-4)^2 + 4\frac{n-4}{n-3}.$$

It suffices to show that

$$10\frac{n-4}{n^2} + \frac{25}{n^4} + 0.382 \le 4\frac{n-4}{n-3}.$$

It is true for $n \ge 5$. This completes the proof.

(3) By direct calculation, the characteristic polynomial of $L(G)$ is

$$\Phi(x) = x(x-1)^{n-4}(x^3 - (n+2)x^2 + (3n-2)x - n).$$

Let $f(x) = x^3 - (n+2)x^2 + (3n-2)x - n$. Then $f(n-1+\frac{2}{n^2}) = \frac{n^6-10n^5+10n^4+8n^3-20n^2+8}{n^6}$. Let $g(n) = n^6 - 10n^5 + 10n^4 + 8n^3 - 20n^2 + 8$. Then $g(n)$ is increasing when $n \ge 9$. Hence $g(n) \ge g(9) > 0$. So $f(n-1+\frac{2}{n^2}) > 0$. Since $f(n-1) = -1 < 0$, and by Lemmas 2.2 and 2.11, $\mu_1 \ge n-1$ and $\mu_2 \le 4$, we have $\mu_1 < n-1+\frac{2}{n^2}$.

Therefore, by Lemma 2.11,

$$\begin{aligned}(\mu_1-2)^2 + (\mu_2-2)^2 &\le (n-1+\frac{2}{n^2}-2)^2 + 4\cos^2(\frac{2\pi}{5})\\ &\le (n-3)^2 + 4\frac{n-3}{n^2} + \frac{4}{n^4} + 0.382.\end{aligned}$$

And we have

$$(1-\frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i-1) = (n-3)^2 + 2\frac{n-3}{n-2}.$$

It suffices to show that

$$4\frac{n-3}{n^2} + \frac{4}{n^4} + 0.382 \le 2\frac{n-3}{n-2}.$$

It is true for $n \ge 4$. This completes the proof. □

Theorem 2.21. *Let G be a starlike tree of order $n(n = \sum_{i=1}^{k} n_i + 1)(k \ge 3)$. Then $(\mu_1-2)^2 + (\mu_2-2)^2 \le (1-\frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i-1)$.*

Proof. By Theorem 2.13, we may assume $n_1 \ge 2$. By Lemma 2.11, we have

$$\begin{aligned}(\mu_1-2)^2 + (\mu_2-2)^2 &< (k+1+\frac{1}{k-1}-2)^2 + 4\cos^2\frac{2\pi}{2n_1+1}\\ &= (k-1)^2 + 2 + \frac{1}{(k-1)^2} + 2 + 2\cos\frac{4\pi}{2n_1+1}\\ &\le (k-1)^2 + \frac{17}{4} + 2\cos\frac{4\pi}{2n_1+1}.\end{aligned}$$

By the definition of the starlike tree, we can easily obtain that

$$\begin{aligned}(1-\frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i-1) &= \frac{k-1}{k}(k(k-1) + 2(n_1-1) + \ldots + 2(n_k-1))\\ &= (k-1)^2 + 2\frac{k-1}{k}(n-1-k).\end{aligned}$$

Hence it suffices to prove that

$$(k-1)^2 + \frac{17}{4} + 2\cos\frac{4\pi}{2n_1+1} \le (k-1)^2 + 2\frac{k-1}{k}(n-1-k).$$

That is,

$$\frac{17}{8} + \cos\frac{4\pi}{2n_1+1} \le \frac{k-1}{k}(n-1-k).$$

Since $2 \le n_1 \le n-k$, $\cos\frac{4\pi}{2n_1+1}$ is increasing as n_1 increases. So $\cos\frac{4\pi}{2n_1+1} \le \cos\frac{4\pi}{2(n-k)+1}$. Then it suffices to show that

$$\frac{17}{8} + \cos\frac{4\pi}{2(n-k)+1} \le \frac{k-1}{k}(n-1-k). \tag{4}$$

If $n-k \ge 6$, $\frac{k-1}{k}(n-1-k) \ge \frac{2}{3}\times 5 = \frac{10}{3}$. Then (4) holds since $\frac{17}{8} + \cos\frac{4\pi}{2(n-k)+1} \le \frac{25}{8} < \frac{10}{3}$. If $n-k = 5$, then $\frac{17}{8} + \cos\frac{4\pi}{2(n-k)+1} \approx 2.54$. Thus $\frac{k-1}{k}(n-1-k) \ge \frac{2}{3}\times 4 = \frac{8}{3} > 2.54$. If $n-k = 4$, we may assume $k \ge 5$. Then $\frac{17}{8} + \cos\frac{4\pi}{2(n-k)+1} \approx 2.3$. Thus $\frac{k-1}{k}(n-1-k) \ge \frac{4}{5}\times 3 = 2.4 > 2.3$. If $n-k = 3$, then G is isomorphic to $S(3,1,\dots,1)$ or $S(2,2,1,\dots,1)$, by Lemma 2.20, the theorem holds. If $n-k = 2$, then G is isomorphic to $S(2,1,\dots,1)$, by Lemma 2.20, the theorem holds. This completes the proof. □

At the end, we also propose the following conjecture in terms of signless Laplacian eigenvalues and the degree sequence of a graph.

Conjecture 2.22. *Let G be a graph with degree sequence $d_1 \ge d_2 \ge \cdots \ge d_n$. Then*

$$\sum_{q_i \ge 2}(q_i-2)^2 \le (1-\frac{1}{d_1})\sum_{i=1}^{n} d_i(d_i-1).$$

Remark 4: It is a well known fact that if G is a bipartite graph, then $L(G)$ and $Q(G)$ have the same eigenvalues. So if G is a bipartite graph, then Conjecture 1 is equivalent to Conjecture 3.

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