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Normalized Laplacian Eigenvalues and Energy of Trees

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Abstract. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. For any vertex $v_i \in V(G)$, let d_i denote the degree of v_i. The normalized Laplacian matrix of the graph G is the matrix $\mathcal{L} = (\mathcal{L}_{ij})$ given by

$$\mathcal{L}_{ij} = \begin{cases} 1 & \text{if } i = j \text{ and } d_i \neq 0 \\ -\frac{1}{\sqrt{d_i\, d_j}} & \text{if } v_iv_j \in E(G) \\ 0 & \text{otherwise.} \end{cases}$$

In this paper, we obtain some bounds on the second smallest normalized Laplacian eigenvalue of tree T in terms of graph parameters and characterize the extremal trees. Utilizing these results we present some lower bounds on the normalized Laplacian energy (or Randić energy) of tree T and characterize trees for which the bound is attained.

1. Introduction

Let $G = (V, E)$ be a connected graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set $E = E(G)$ ($|E(G)| = m$). Also let d_i be the degree of vertex v_i for $i = 1, 2, \dots, n$. The maximum degree and the second maximum degree of G are denoted by $\Delta_1 = \Delta_1(G)$ and $\Delta_2 = \Delta_2(G)$, respectively. Let $N_G(v_i)$ be the neighbor set of the vertex $v_i \in V(G)$. The distance $d_G(v_i, v_j)$ between the vertices v_i and v_j of the graph G is equal to the length of (number of edges in) the shortest path that connects v_i and v_j. The diameter of a graph G, denoted by d, is the maximum distance between any two vertices of G. If vertices v_i and v_j are adjacent, we denote that by $v_iv_j \in E(G)$. Let $A(G)$ and $D(G)$ be the adjacency matrix and the diagonal matrix of vertex degrees of G, respectively. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. The normalized Laplacian matrix $\mathcal{L}(G)$ of G is defined as $D^{-1/2}(G)L(G)D^{-1/2}(G)$. Let $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} \geq \rho_n = 0$ denote the eigenvalues of $\mathcal{L}(G)$. Denote by $\mathrm{Spec}(G) = \{\rho_1, \rho_2, \dots, \rho_n\}$ the spectrum of $\mathcal{L}(G)$, i.e., the normalized

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Laplacian spectrum of G. Then we have $\sum_{i=1}^{n} \rho_i = n$. When the graph G is disconnected, $\rho_{n-1} = \rho_n = 0$.

For a subset U of $V(G)$, let $G - U$ be the subgraph of G obtained by deleting the vertices of U and the edges incident with them. If $U = \{v_i\}$, the subgraph $G - U$ will be written as $G - v_i$ for short. For any two adjacent vertices v_i and v_j in graph G, we use $G - v_i v_j$ to denote the graph obtained by deleting an edge $v_i v_j$ from graph G. As usual, K_n, and S_n, denote, respectively, the complete graph, and the star on n vertices. Let $\mathrm{DS}(p, q)$ $(p + q = n,\ 2 \le p \le q)$ be a double star obtained by joining the centers of two stars S_p and S_q with an edge. The normalized Laplacian spectrum of $\mathrm{DS}(p,\, q)$ is

$$\mathrm{Spec}(\mathrm{DS}(p,q)) = \left\{ 2, 1 \pm \sqrt{\left(1 - \frac{1}{p}\right)\left(1 - \frac{1}{q}\right)}, \underbrace{1, \ldots, 1}_{n-4}, 0 \right\}. \tag{1.1}$$

For other undefined notations and terminology from graph theory, the readers are referred to [1].

Chung [6] gave an upper bound on ρ_{n-1} in the following:

$$\rho_{n-1}(G) \le 1 - 2\frac{\sqrt{\Delta_1 - 1}}{\Delta_1}\left(1 - \frac{2}{d}\right) + \frac{2}{d}, \quad (d \ge 4).$$

From the above, we can see that the upper bound for ρ_{n-1} of graphs is very close to 1. Li et al. [12] obtained the following result:

$$\rho_{n-1}(T) \le 1 - \sqrt{1 - \frac{n-1}{2(n-2)}}, \quad (T \ncong S_n,\ n \ge 5) \tag{1.2}$$

with equality holding if and only if $T \cong \mathrm{DS}(2,\, n-2)$. Li et al. [13] presented the following upper bound:

$$\rho_{n-1}(T) \le 1 - \frac{\sqrt{6}}{3}, \quad (n \ge 8,\ d \ge 5). \tag{1.3}$$

We give an upper bound on $\rho_{n-1}(T)$ in terms of Δ_1 and Δ_2, and we state the theorem as follows.

Theorem 1.1. *Let T be a tree of order $n \ge 3$. Then*

$$\rho_{n-1}(T) \le \begin{cases} 1 - \sqrt{\left(1 - \dfrac{1}{\Delta_1}\right)\left(1 - \dfrac{1}{\Delta_2}\right)}, & v_1 v_2 \in E(T); \\ 1 - \sqrt{1 - \dfrac{1}{\Delta_2}}, & v_1 v_2 \neq E(T), \end{cases} \tag{1.4}$$

where Δ_1 and Δ_2 are the maximum and the second maximum degrees of vertices v_1 and v_2 in T, respectively. Moreover, the equality holds in (1.4) *if and only if*

(i) *when* $v_1v_2 \in E(T)$, $T \cong S_n$ *or* $T \cong \mathrm{DS}(\Delta_2, \Delta_1)$, $\Delta_1 + \Delta_2 = n$.

(ii) *when* $v_1v_2 \neq E(T)$, $T \cong T(n, k, n_1, n_2, \ldots, n_k)$, $n_1 = n_2$.

The normalized Laplacian energy [4] (or Randić energy) of a graph G is

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\rho_i - 1|. \tag{1.5}$$

For several lower and upper bounds on normalized Laplacian energy, see [3, 4, 8–10]. In this paper, we obtain the following lower bound on $E_{\mathcal{L}}(T)$ in terms of Δ_1 and Δ_2 of trees T.

Theorem 1.2. *Let T be a tree of order $n \geq 3$. Then*

$$E_{\mathcal{L}}(T) \geq \begin{cases} 2 + 2\sqrt{\left(1 - \dfrac{1}{\Delta_1}\right)\left(1 - \dfrac{1}{\Delta_2}\right)}, & v_1v_2 \in E(T); \\ 2 + 2\sqrt{1 - \dfrac{1}{\Delta_2}}, & v_1v_2 \neq E(T), \end{cases} \tag{1.6}$$

where Δ_1 and Δ_2 are the maximum and the second maximum degrees of vertices v_1 and v_2 in T, respectively. Moreover, the equality holds in (1.6) *if and only if*

(i) *when* $v_1v_2 \in E(T)$, $T \cong S_n$ *or* $T \cong \mathrm{DS}(\Delta_2, \Delta_1)$, $\Delta_1 + \Delta_2 = n$.

(ii) *when* $v_1v_2 \neq E(T)$, $T \cong T(n, 2, \frac{n-1}{2}, \frac{n-1}{2})$.

2. Preliminaries

In this section, we shall list some previously known results that will be needed in the next two sections.

Lemma 2.1. [6] *Let G be a connected graph of order $n \geq 2$. Then $\rho_{n-1} \leq \frac{n}{n-1}$ with equality holding if and only if $G \cong K_n$. If G is not the complete graph K_n, then $\rho_{n-1} \leq 1$.*

Lemma 2.2. [6] *Let G be a graph and f be a harmonic eigenfunction of $\mathcal{L}$ associated with eigenvalue ρ. Then for any $v_i \in V(G)$, we have*

$$f(v_i) - \frac{1}{d_i} \sum_{v_iv_j \in E(G)} f(v_j) = \rho f(v_i). \tag{2.1}$$

Lemma 2.3. [5] *Let G be a graph, and let $H = G - e$, where e is an edge of G. If*

$$\rho_1(G) \geq \rho_2(G) \geq \cdots \geq \rho_n(G) \quad \text{and} \quad \rho_1(H) \geq \rho_2(H) \geq \cdots \geq \rho_n(H)$$

are the eigenvalues of $\mathcal{L}(G)$ and $\mathcal{L}(H)$, respectively, then

$$\rho_{i-1}(G) \geq \rho_i(H) \geq \rho_{i+1}(G) \quad \text{for } i = 1, 2, \ldots, n,$$

where $\rho_0(G) = 2$ and $\rho_{n+1}(G) = 0$.

Lemma 2.4. *Let T be a tree of order n. Also let T^* be a tree obtained by removing k pendant vertices from T. Then*

$$\rho_{n-1}(T) \leq \rho_{n-k-1}(T^*).$$

Proof. Denote by T^i the tree obtained by removing one pendant vertex from T^{i-1}, $1 \leq i \leq k$, where $T^0 \cong T$. Then we have $T^k \cong T^*$. By Lemma 2.3, we have

$$\rho_{n-1}(T) \leq \rho_{n-2}(T^1) \leq \rho_{n-3}(T^2) \leq \cdots \leq \rho_{n-k-1}(T^k) = \rho_{n-k-1}(T^*). \qquad \square$$

Let $e = uv$ be an edge of a graph G. Let G' be the graph obtained from G by contracting the edge e into a new vertex u_e and adding a new pendant edge $u_e v_e$, where v_e is a new pendant vertex. We say that G' is obtained from G by separating an edge uv. In [12], Li et al. study how the second smallest normalized Laplacian eigenvalue behaves when the graph is perturbed by separating an edge.

Lemma 2.5. [12] *Let $e = uv$ be a cut edge of a connected graph G and suppose that $G - uv = G_1 \cup G_2$ ($|V(G_1)|, |V(G_2)| \geq 2$), where G_1 and G_2 are two components of $G - uv$, $u \in V(G_1)$ and $v \in V(G_2)$. Let G' be the graph obtained from G by separating the edge uv. Then $\rho_{n-1}(G) \leq \rho_{n-1}(G')$, and the inequality is strict if $f(v_e) \neq 0$, where f is a harmonic eigenfunction associated with $\rho_{n-1}(G')$.*

The following result is obtained by Chung [6].

Lemma 2.6. *Let G be a bipartite graph of order n. Then $\rho_i(G) + \rho_{n-i+1}(G) = 2$, $1 \leq i \leq \lceil \frac{n}{2} \rceil$.*

Lemma 2.7. [12] *Let G be a connected graph with a cut vertex v. Then $\rho_{n-1} \leq 1$. Moreover, if $\rho_{n-1} = 1$, then v is adjacent to every vertex of G and $\delta(G) = 1$, where $\delta(G)$ is the minimum degree of graph G.*

The following result is very similar to the result in [7], so we omit the proof.

Lemma 2.8. *Let $G = (V, E)$ be a graph with vertex subset $V' = \{v_1, v_2, \ldots, v_k\}$ having the same set of neighbors $\{v_{k+1}, v_{k+2}, \ldots, v_s\}$, where $V = \{v_1, \ldots, v_k, \ldots, v_s, \ldots, v_n\}$. Then this graph G has at least $k-1$ equal normalized Laplacian eigenvalues 1.*

3. Bounds on the second smallest normalized Laplacian eigenvalue of trees

Let $e = uv$ be an edge of graph G, and define two sets $N_u(e)$ and $N_v(e)$ as follows:

$$N_u(e) = \{w \in V(G) \mid d_G(w, u) < d_G(w, v)\},$$
$$N_v(e) = \{w \in V(G) \mid d_G(w, v) < d_G(w, u)\}.$$

The number of elements of $N_u(e)$ and $N_v(e)$ are denoted by $n_u(e)$ and $n_v(e)$, respectively. Thus, $n_u(e)$ counts the vertices of G lying closer to the vertex u than to vertex v. The meaning of $n_v(e)$ is analogous. Vertices equidistant from both ends of the edge uv belong neither to $N_u(e)$ nor to $N_v(e)$. Note that for any edge e of G, $n_u(e) \geq 1$ and $n_v(e) \geq 1$, because $u \in N_u(e)$ and $v \in N_v(e)$. We now give some upper bounds on the second smallest normalized Laplacian eigenvalue of trees.

Theorem 3.1. *Let T be a tree of order n. Then*

$$\rho_{n-1}(T) \leq 1 - \max_{wz \in E(T)} \left\{ \sqrt{\left(1 - \frac{1}{n_w(e)}\right)\left(1 - \frac{1}{n_z(e)}\right)} \right\}, \tag{3.1}$$

where $n_w(e)$ counts the number of vertices of T lying closer to the vertex w than to vertex z, where $e = wz \in E(T)$. Moreover, the equality holds in (3.1) *if and only if $T \cong S_n$ or $T \cong \mathrm{DS}(p,q)$, $p+q=n$.*

Proof. Let d be the diameter of tree T. For $d=2$, we have $T \cong S_n$ and hence $\rho_{n-1}(T) = 1$, the equality holds in (3.1). For $d=3$, we have $T \cong \mathrm{DS}(p,q)$, $p+q=n$, $p \leq q$. By (1.1), we get the equality in (3.1).

Now we assume that $d \geq 4$. Suppose we consider an edge $e = wz \in E(T)$ such that $n_z \geq n_w \geq 2$. Let T^1 be the tree obtained from T by separating an edge uv such that $e = wz \neq uv$ and $d_u, d_v \geq 2$. By Lemma 2.5, we have $\rho_{n-1}(T) \leq \rho_{n-1}(T^1)$. Repeating the above process by at most $n - d_w - d_z$ times, we can obtain a sequence of trees:

$$T, T^1, T^2, \ldots, T^{k-1}, T^k = \mathrm{DS}(n_w, n_z) \quad (n_w + n_z = n,\ n_z \geq n_w)$$

with $\rho_{n-1}(T) \leq \rho_{n-1}(T^1) \leq \rho_{n-1}(T^2) \leq \cdots \leq \rho_{n-1}(T^{k-1}) \leq \rho_{n-1}(T^k) = \rho_{n-1}(\mathrm{DS}(n_w, n_z))$. By Lemma 2.5, we get $\rho_{n-1}(T^{k-1}) < \rho_{n-1}(T^k) = \rho_{n-1}(\mathrm{DS}(n_w, n_z))$ (otherwise, the harmonic eigenfunction f associated with $\rho_{n-1}(T^k) = \rho_{n-1}(\mathrm{DS}(n_w, n_z))$ must be equal to zero, a contradiction). By (1.1), we get the required result. □

We now obtain a lower bound on $\rho_2(T)$ of tree T.

Theorem 3.2. *Let T be a tree of order n. Then*

$$\rho_2(T) \geq 1 + \max_{wz \in E(T)} \left\{ \sqrt{\left(1 - \frac{1}{n_w(e)}\right)\left(1 - \frac{1}{n_z(e)}\right)} \right\}, \tag{3.2}$$

where $n_w(e)$ counts the number of vertices of T lying closer to the vertex w than to vertex z, where $e = wz \in E(T)$. Moreover, the equality holds in (3.2) *if and only if $T \cong S_n$ or $T \cong \mathrm{DS}(p,q)$, $p+q=n$.*

Proof. By Lemma 2.6, we have $\rho_2(T) = 2 - \rho_{n-1}(T)$. By (3.1), we get the required result in (3.2). Moreover, the equality holds in (3.2) if and only if $T \cong S_n$ or $T \cong \mathrm{DS}(p,q)$, $(p+q=n,\, p \le q)$, by Theorem 3.1. □

Denote by $T(n,k,n_1,n_2,\ldots,n_k)$ the tree of order n formed by joining the center v_i of star S_{n_i} to a new vertex v for $i = 1,2,\ldots,k$; that is,

$$T(n,k,n_1,n_2,\ldots,n_k) - \{v\} = S_{n_1} \cup S_{n_2} \cup \cdots \cup S_{n_k}.$$

Therefore this tree $T(n,k,n_1,n_2,\ldots,n_k)$ has $n_1+n_2+\cdots+n_k+1 = n$ vertices and assume that $n_1 \ge n_2 \ge \cdots \ge n_k \ge 1$. In particular, $T(n,k,n_1,n_2,\ldots,n_k) \cong S_n$ for $n_1 = 1$. Let $T \cong T(n,k,n_1,n_2,\ldots,n_k)$ and

$$\mathrm{SN}(v) = \{v_i \in V(T) : \text{there exists a vertex } v_j \in N_T(v) \text{ with } n_i = n_j, 1 \le i \ne j \le k\}.$$

Lemma 3.3. *Let $T \cong T(n,k,n_1,n_2,\ldots,n_k)$ be a tree of order n with $n_1 \ge n_2 \ge \cdots \ge n_k$. If any $v_i \in \mathrm{SN}(v) \ne \emptyset$, then*

$$\rho_{n-1}(T) \le 1 - \sqrt{1 - \frac{1}{n_i}}.$$

Proof. We only have to prove $1 - \sqrt{1 - \frac{1}{n_i}}$ is an eigenvalue of T. If $n_i = 1$, then there exist two vertices v_i and v_k in T such that $n_i = n_k = 1$ with $v_i v \in E(T)$, $v_k v \in E(T)$ (from the given condition). By Lemma 2.8, $\rho = 1 = 1 - \sqrt{1 - \frac{1}{n_i}}$ is an eigenvalue of T. Otherwise, $n_i \ge 2$. Then we have to prove that $\rho = 1 - \sqrt{1 - \frac{1}{n_i}}$ (< 1) is an eigenvalue of T. Let $r = \max\{j \mid n_j > 1, 1 \le j \le k\}$. Then $n_{r+1} = n_{r+2} = \cdots = n_k = 1$. In T, $d(v) = k$ and $vv_j \in E(T)$, $1 \le j \le k$. Since $d(v_j) = n_j$, we can assume that $v_{j,1}, v_{j,2}, \ldots, v_{j,n_j-1}$ are the remaining vertices adjacent to vertex v_j, $j = 1,2,\ldots,r$. Again since $n_2 \ge 2$, we can assume that ρ $(\ne 1,2)$ is a non-zero eigenvalue of T. From (2.1), we can easily get

$$f(v_{j,1}) = f(v_{j,2}) = \cdots = f(v_{j,n_j-1}), \quad 1 \le j \le r,$$
$$f(v_{r+1}) = f(v_{r+2}) = \cdots = f(v_k).$$

We denote $f(v_{j,1})$ by x_j for $1 \le j \le r$, $f(v_j)$ by y_j for $1 \le j \le k$ $(y_{r+1} = y_{r+2} = \cdots = y_k)$. For $1 \le j \le r$, from (2.1), we have

$$\rho x_j = x_j - y_j, \tag{3.3}$$

$$\rho y_j = y_j - \frac{n_j - 1}{n_j} x_j - \frac{1}{n_j} f(v), \tag{3.4}$$

and

$$\rho y_{r+1} = y_{r+1} - f(v), \tag{3.5}$$

$$\rho f(v) = f(v) - \frac{1}{k} \sum_{j=1}^{k} y_j. \tag{3.6}$$

From (3.3) and (3.4), we get

$$(1-\rho)f(v) = (n_j\rho^2 - 2n_j\rho + 1)y_j \quad \text{for } 1 \le j \le r. \tag{3.7}$$

Note that (3.7) is also true for $r+1 \le j \le k$ by (3.5) (since $n_j = 1$, $r+1 \le j \le k$). Then we have

$$(1-\rho)f(v) = (n_j\rho^2 - 2n_j\rho + 1)y_j \quad \text{for } 1 \le j \le k, \tag{3.8}$$

$$k(1-\rho)f(v) = \sum_{j=1}^{k} y_j. \tag{3.9}$$

Let

$$a_j = n_j\rho^2 - 2n_j\rho + 1, \quad j = 1, 2, \ldots, k.$$

Also let

$$A_j = \prod_{t=1, t\neq j}^{r+1} a_t \quad \text{for} \quad j = 1, 2, \ldots, r+1;\ A_{r+1} = A_{r+2} = \cdots = A_k.$$

Denote by

$$A = \prod_{j=1}^{r+1} a_j = a_j A_j, \quad 1 \le j \le k.$$

If $y_j = 0$, $1 \le j \le k$, then by (2.1), we have $x_j = 0$, $1 \le j \le r$ and $f(v) = 0$, a contradiction. Thus all the y_j's can not be zero. Then there exist two vertices $v_p, v_q \in V(T)$ $(1 \le p, q \le r)$ such that $y_p \neq 0$ and $y_q \neq 0$. (Otherwise, from (3.3), (3.4), (3.5) and (3.6), we get that all the eigencomponents are zero, a contradiction.) If $f(v) = 0$, then from (3.7), we get $a_p = a_q = 0$. Then we have $A_j = 0$ for $j = 1, 2, \ldots, k$ and hence

$$\sum_{j=1}^{k} n_j A_j = 0. \tag{3.10}$$

Otherwise, $f(v) \neq 0$. By (3.8), $a_j \neq 0$, $j = 1, 2, \ldots, k$. Then $A_j \neq 0$, $j = 1, 2, \ldots, k$. Multiply by A_j to each side of (3.8), we have $(1-\rho)A_j f(v) = a_j A_j y_j = A y_j$, $1 \le j \le k$. Using this result with (3.9), we get

$$(1-\rho)f(v)\sum_{j=1}^{k} A_j = \sum_{j=1}^{k}(1-\rho)A_j f(v) = \sum_{j=1}^{k} A y_j = A\sum_{j=1}^{k} y_j = (1-\rho)kAf(v).$$

Thus we have

$$\begin{aligned} 0 &= kA - \sum_{j=1}^{k} A_j \\ &= \sum_{j=1}^{k} (A - A_j) \\ &= \sum_{j=1}^{k} A_j(n_j\rho^2 - 2n_j\rho) \qquad \text{as } a_j = n_j\rho^2 - 2n_j\rho + 1 \\ &= \sum_{j=1}^{k} n_jA_j\rho(\rho - 2), \end{aligned}$$

that is,

$$\sum_{j=1}^{k} n_jA_j = 0, \quad \text{as } \rho \neq 0, 2,$$

again satisfies (3.10).

Now we have to check whether $1 - \sqrt{1 - \frac{1}{n_i}}$ is a solution of (3.10) or not. For this we assume that $\rho = 1 - \sqrt{1 - \frac{1}{n_i}}$. Then there exists a vertex v_p in $\mathrm{SN}(v)$ such that $n_i = n_p$. Since $a_j = n_j\rho^2 - 2n_j\rho + 1$, we have $a_i = a_p = 0$. Thus $A_j = 0$ for all $j = 1, 2, \dots, k$, which satisfies (3.10). Therefore

$$\rho = 1 - \sqrt{1 - \frac{1}{n_i}}, \quad v_i \in \mathrm{SN}(v),$$

is a solution of (3.10), that is, ρ is an eigenvalue of tree T. This completes the proof. □

Lemma 3.4. *Let $T \cong T(n, k, n_1, n_2, \dots, n_k)$ be a tree of order n. Then $1 - \sqrt{1 - \frac{1}{n_i}}$ ($n_i > 1$) is an eigenvalue of T if and only if $v_i \in \mathrm{SN}(v) \neq \emptyset$.*

Proof. Suppose that $v_i \in \mathrm{SN}(v) \neq \emptyset$. Then by the proof of Lemma 3.3, we have that $1 - \sqrt{1 - \frac{1}{n_i}}$ is an eigenvalue of T.

Conversely, let $\rho = 1 - \sqrt{1 - \frac{1}{n_i}}$ ($n_i > 1$) be an eigenvalue of T. By contradiction we will prove that $v_i \in \mathrm{SN}(v) \neq \emptyset$ for $n_i > 1$. For this we assume that $v_i \notin \mathrm{SN}(v)$. Then there is no vertex v_j such that $n_i = n_j$, $j = 1, 2, \dots, k$ ($j \neq i$). From the proof of Lemma 3.3, we have $a_t = n_t\rho^2 - 2n_t\rho + 1$, $t = 1, 2, \dots, k$. Moreover, $A_s = \prod_{t=1, t\neq s}^{r+1} a_t$ for $s = 1, 2, \dots, r+1$. Since $\rho = 1 - \sqrt{1 - \frac{1}{n_i}}$ ($n_i > 1$) is an eigenvalue of T, we have $a_i = 0$ and $a_t \neq 0$ as $n_i \neq n_t$, $t = 1, 2, \dots, k$ ($t \neq i$). Therefore $A_i \neq 0$ and $A_t = 0$, $t = 1, 2, \dots, k$ ($t \neq i$), that is, $\sum_{j=1}^{k} n_jA_j \neq 0$, a contradiction by (3.10). This completes the proof. □

Lemma 3.5. [2] *Let $T \cong T(n,k,n_1,n_1,\dots,n_1)$ be a tree of order n. Then the distinct normalized Laplacian eigenvalues of T are:*

$$2,\ 1+\sqrt{1-\frac{1}{n_1}},\ 1,\ 1-\sqrt{1-\frac{1}{n_1}},\ 0.$$

Corollary 3.6. *Let $T \cong T(n,k,n_1,n_2,\dots,n_k)$ be a tree of order n with $n_1 = n_2$. Then*

$$\rho_{n-1}(T) = 1-\sqrt{1-\frac{1}{n_1}}.$$

Proof. Since $v_1 \in \mathrm{SN}(v)$, by Lemma 3.3, we have

$$\rho_{n-1}(T) \le 1-\sqrt{1-\frac{1}{n_1}}.$$

Let T^* be a tree obtained from T by adding s_i (≥ 0 pendent edges to v_i ($i = 3,4,\dots,k$) such that $T^* \cong T(n^*,k,n_1,n_1,\dots,n_1)$, where $n^* = n+\sum_{i=3}^{k} s_i = kn_1+1$. Then by Lemmas 2.4 and 3.5, we have

$$\rho_{n-1}(T) \ge \rho_{n^*-1}(T^*) = 1-\sqrt{1-\frac{1}{n_1}}.$$

Hence

$$\rho_{n-1}(T) = 1-\sqrt{1-\frac{1}{n_1}}.$$ □

Theorem 3.7. *Let $T = T(n,k,n_1,n_2,\dots,n_k)$ be a tree of order n with $n_1 \ge n_2 \ge \cdots \ge n_k$. Then*

$$\rho_{n-1}(T) \ge 1-\sqrt{1-\frac{1}{n_1}} \tag{3.11}$$

with equality holding if and only if $n_1 = n_2$.

Proof. By Lemma 2.4 and Corollary 3.6, we can get the required result in (3.11).

If $T \cong T(n,k,n_1,n_2,\dots,n_k)$, $n_1 = n_2$, then by Corollary 3.6, the equality holds in (3.11). Conversely, let

$$\rho_{n-1}(T) = 1-\sqrt{1-\frac{1}{n_1}}.$$

If $n_1 = 1$, then $T \cong T(n,n-1,1,\dots,1)$. Otherwise, by Lemma 3.4, we have $T \cong T(n,k,n_1,n_2,\dots,n_k)$, $n_1 = n_2$. □

Theorem 3.8. *Let $T = T(n,k,n_1,n_2,\dots,n_k)$ be a tree of order n with $n_1 \ge n_2 \ge \cdots \ge n_k$. Then*

$$\rho_{n-1}(T) \le 1-\sqrt{1-\frac{1}{n_2}} \tag{3.12}$$

with equality holding if and only if $n_1 = n_2$.

Proof. The first part of the proof is similar to the proof of Theorem 3.7.

If $T \cong T(k, n_1, n_2, \ldots, n_k)$, $n_1 = n_2$, then by Corollary 3.6, the equality holds in (3.12). Conversely, let $\rho_{n-1}(T) = 1 - \sqrt{1 - \frac{1}{n_2}}$. By contradiction we will prove $T \cong T(n, k, n_1, n_2, \ldots, n_k)$ with $n_1 = n_2$. For this we assume that $T \cong T(n, k, n_1, n_2, \ldots, n_k)$ with $n_1 > n_2$. If $n_2 = 1$, then $T \cong \mathrm{DS}(p, q)$ $(p \leq q,\ p + q = n)$. By (1.1),

$$\rho_{n-1}(T) = 1 - \sqrt{\left(1 - \frac{1}{p}\right)\left(1 - \frac{1}{q}\right)} < 1,$$

a contradiction. Otherwise, $n_2 > 1$. We denote by T^{**}, a tree obtained from T such that $T^{**} = T - \{v_3, v_4, \ldots, v_k\}$. Therefore $T^{**} \cong T(n_1 + n_2 + 1, 2, n_1, n_2)$. Since $n_1 > n_2$, $v_2 \notin \mathrm{SN}(v)$ and hence by Lemma 3.4, $1 - \sqrt{1 - \frac{1}{n_2}}$ is not an eigenvalue of T^{**}. By (3.12), we have

$$\rho_{n-1}(T) \leq \rho_{n_1+n_2}(T^{**}) < 1 - \sqrt{1 - \frac{1}{n_2}},$$

a contradiction. This completes the proof. $\square$

Denote by $T_i(n^*, k, n_1, n_2, \ldots, n_k, h)$ (see, Figure 3.1), a tree of order n^* $(= n + h)$ obtained from $T(n, k, n_1, n_2, \ldots, n_k)$ $(n_k \geq 2)$ by adding h pendant edges to a pendant vertex, neighbor of v_i $(1 \leq i \leq k)$, that is,

$$\begin{aligned} &T_i(n^*, k, n_1, n_2, \ldots, n_k, h) - v \\ &= \mathrm{DS}(h + 1, n_i - 1) \cup S_{n_1} \cup S_{n_2} \cup \cdots \cup S_{n_{i-1}} \cup S_{n_{i+1}} \cup \cdots \cup S_{n_k}. \end{aligned}$$

Therefore this tree $T_i(n^*, k, n_1, n_2, \ldots, n_k, h)$ has $\sum_{j=1}^{k} n_j + h + 1 = n^*$ vertices. Moreover, the tree $T_i(n^*, k, n_1, n_2, \ldots, n_k, h)$ has diameter 5.

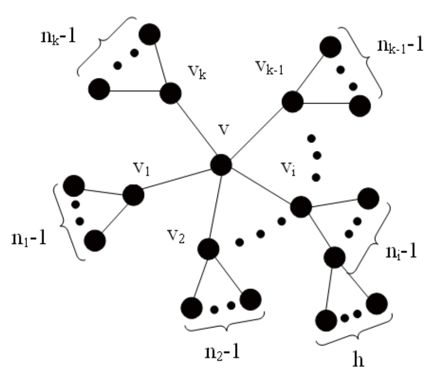

Figure 3.1: Tree $T_i(n^*, k, n_1, n_2, \ldots, n_k, h)$.

Lemma 3.9. *Let $T = T_i(n^*, k, \underbrace{n_1, n_1, \ldots, n_1}_{k-1}, n_k, h)$ be a tree of order n^* $(= (k-1)n_1 + n_k + h + 1)$ with $n_1 \geq n_k \geq 2$, $k \geq 3$. Then*

$$\rho_{n^*-1}(T) < 1 - \sqrt{1 - \frac{1}{n_1}}.$$

Proof. Let $H_1 \cong T(n^*, k, n_1+h, \underbrace{n_1, \ldots, n_1}_{k-2}, n_k)$, $H_2 \cong T(n^*, k, n_k+h, \underbrace{n_1, n_1, \ldots, n_1}_{k-1})$ $(n_1 < n_k + h)$ and $H_3 \cong T(n^*, k, \underbrace{n_1, n_1, \ldots, n_1}_{k-1}, n_k + h)$ $(n_1 \geq n_k + h)$. By Lemma 2.5, one can see easily that

$$\rho_{n^*-1}(T_i(n^*, k, \underbrace{n_1, n_1, \ldots, n_1}_{k-1}, n_k, h)) \leq \rho_{n^*-1}(H_t), \quad t = 1, 2, 3 \tag{3.13}$$

and the inequality is strict if $f(v_e) \neq 0$, where f is a harmonic eigenfunction associated with $\rho_{n^*-1}(H_t)$ and v_e is a pendant vertex adjacent to vertex v_i in H_t, $t = 1, 2, 3$. By Theorem 3.8,

$$\rho_{n^*-1}(H_t) < 1 - \sqrt{1 - \frac{1}{n_1}} \quad (t = 1, 2)$$

and

$$\rho_{n^*-1}(H_3) \leq 1 - \sqrt{1 - \frac{1}{n_1}}. \tag{3.14}$$

Now we have to prove that the inequality in (3.13) is strict for H_3 (for this tree $i = k$). We prove this by contradiction. For this we assume that $f(v_e) = 0$. Then by (2.1), we must have $f(v_k) = 0$ and $f(v_{k,r}) = 0$, $v_{k,r}$ is a pendant vertex with $v_k v_{k,r} \in E(H_3)$. Again by (2.1) at v_k, we have $f(v) = 0$. At v, we have

$$(1 - \rho_{n^*-1}) f(v) = \frac{1}{k} \sum_{j=1}^{k-1} f(v_j).$$

By symmetry and from the above, we get $f(v_1) = f(v_2) = \cdots = f(v_{k-1}) = 0$. Similarly, one can see easily that $f(v_{j,r}) = 0$, $v_{j,r}$ is a pendant vertex with $v_j v_{j,r} \in E(H_3)$, $j = 1, 2, \ldots, k-1$. Therefore all the eigencomponents corresponding to $\rho_{n^*-1}(H_3)$ are zero, a contradiction. Hence the inequality in (3.13) is strict. From (3.13) and (3.14), we get the required result. $\square$

Theorem 3.10. *Let $T_i(n^*, k, n_1, n_2, \ldots, n_k, h)$ be a tree of order n^* $(= \sum_{i=1}^{k} n_i + h + 1)$ with $n_k \geq 2$, $k \geq 3$. Then*

$$\rho_{n^*-1}(T_i(n^*, k, n_1, n_2, \ldots, n_k, h)) < 1 - \sqrt{1 - \frac{1}{n_2}}.$$

Proof. For $i = 1$ or 2, by Lemma 2.5 and Theorem 3.8, we get

$$\begin{aligned}\rho_{n^*-1}(T_i(n^*, k, n_1, n_2, \ldots, n_k, h)) &\leq \rho_{n^*-1}(T(n^*, k, n_1', n_2', n_3, \ldots, n_k)) \\ &< 1 - \sqrt{1 - \frac{1}{n_2}},\end{aligned}$$

where $(n_1', n_2') = (n_1 + h, n_2)$ or $(n_1, n_2 + h)$. Otherwise, $3 \leq i \leq k$. By removing pendant vertices associated with vertices $v_3, v_4, \ldots, v_{i-1}, v_{i+1}, \ldots, v_k$ and $n_1 - n_2$ number of pendant vertices adjacent to v_1 from $T_i(n^*, k, n_1, n_2, \ldots, n_k, h)$, we obtain a new tree $T_3(n^{**}, 3, n_2, n_2, n_i, h)$, where $n^{**} = 2n_2 + n_i + h + 1$. For $3 \leq i \leq k$, by Lemmas 2.4 and 3.9, we get

$$\begin{aligned}\rho_{n^*-1}(T_i(n^*, k, n_1, n_2, \ldots, n_k, h)) &\leq \rho_{n^{**}-1}(T_3(n^{**}, 3, n_2, n_2, n_i, h)) \\ &< 1 - \sqrt{1 - \frac{1}{n_2}}.\end{aligned}$$ □

We are now ready to give our proof of Theorem 1.1:

Proof of Theorem 1.1. Let d be the diameter of tree T. For $d = 2$, then $T \cong S_n$ and the equality holds in (1.4). For $d = 3$, then $T \cong \mathrm{DS}(\Delta_2, \Delta_1)$, $\Delta_1 + \Delta_2 = n$ and the equality holds in (1.4), by (1.1). Otherwise, $d \geq 4$.

First we assume that $e = v_1v_2 \in E(T)$. By Theorem 3.1, we have

$$\rho_{n-1}(T) \leq 1 - \sqrt{\left(1 - \frac{1}{n_{v_1}(e)}\right)\left(1 - \frac{1}{n_{v_2}(e)}\right)} < 1 - \sqrt{\left(1 - \frac{1}{\Delta_1}\right)\left(1 - \frac{1}{\Delta_2}\right)}$$

as $n_{v_1}(e) \geq \Delta_1$ and $n_{v_2}(e) \geq \Delta_2$ with at least one of them must be strict.

Next we assume that $v_1v_2 \notin E(T)$. We now consider two cases:

Case (i). $d = 4$. In this case $T \cong T(n, k, n_1, n_2, \ldots, n_k)$. Therefore $n_1 = \Delta_1$ and $n_2 = \Delta_2$. These results with Theorem 3.8, we get

$$\rho_{n-1}(T) \leq 1 - \sqrt{1 - \frac{1}{n_2}} = 1 - \sqrt{1 - \frac{1}{\Delta_2}}$$

with equality holding if and only if $T \cong T(k, n_1, n_2, \ldots, n_k)$, $n_1 = n_2$.

Case (ii). $d \geq 5$. Since $v_1v_2 \notin E(T)$, then there exists a vertex v of degree k (≥ 2) such that $e_p = vv_p \in E(T)$ and $e_q = vv_q \in E(T)$, where $n_{v_p}(e_p) \geq \Delta_1$ and $n_{v_q}(e_q) \geq \Delta_2$. Without loss of generality, we can assume that $n_{v_p}(e_p) \geq n_{v_q}(e_q)$. Let T' be a tree obtained from T by separating an edge wz such that $e = wz \notin \{e_p, e_q\}$ and $d_w, d_z \geq 2$. By Lemma 2.5, we have $\rho_{n-1}(T) \leq \rho_{n-1}(T')$. Since $d \geq 5$, repeating the above process, we can obtain a sequence of trees:

$$T, T', T'', \ldots, T^{n'-1}, T^{n'} = T_i(n^*, k, n_1, n_2, \ldots, n_k, h)$$

with $\rho_{n-1}(T) \le \rho_{n-1}(T') \le \rho_{n-1}(T'') \le \cdots \le \rho_{n-1}(T^{n'-1}) \le \rho_{n-1}(T^{n'})$. By Theorem 3.10, one can get easily that

$$\rho_{n-1}(T) \le \rho_{n-1}(T^{n'}) < 1 - \sqrt{1 - \frac{1}{n_2}} \le 1 - \sqrt{1 - \frac{1}{\Delta_2}} \quad \text{as } n_2 \ge \Delta_2.$$

This completes the proof of the theorem. □

Corollary 3.11. *Let T be a tree of order $n \ge 3$. Then*

$$\rho_{n-1}(T) \le \frac{1}{\Delta_2} \tag{3.15}$$

with equality holding if and only if $T \cong S_n$ or $T \cong \mathrm{DS}(n/2, n/2)$ (n is even).

Proof. For $v_1v_2 \notin E(T)$, we have $\Delta_2 \ge 2$ and hence

$$1 - \sqrt{1 - \frac{1}{\Delta_2}} < 1 - \sqrt{\left(1 - \frac{1}{\Delta_1}\right)\left(1 - \frac{1}{\Delta_2}\right)}.$$

Since $\Delta_1 \ge \Delta_2$, one can see easily that

$$1 - \sqrt{\left(1 - \frac{1}{\Delta_1}\right)\left(1 - \frac{1}{\Delta_2}\right)} \le \frac{1}{\Delta_2}$$

with equality holding if and only if $\Delta_2 = 1$ or $\Delta_1 = \Delta_2$. By Theorem 1.1, we get the required result in (3.15). Moreover, the equality holds in (3.15) if and only if $T \cong S_n$ or $T \cong \mathrm{DS}(n/2, n/2)$ (n is even). □

Remark 3.12. For $\Delta_2 \ge 2$, one can see easily that

$$1 - \sqrt{1 - \frac{1}{\Delta_2}} < 1 - \sqrt{1 - \frac{n-1}{2(n-2)}}.$$

Therefore our result in (1.4) is always better than the result in (1.2) when $v_1v_2 \notin E(T)$.

Remark 3.13. For $\Delta_2 \ge 3$ with $v_1v_2 \notin E(T)$, our result is better than the result in (1.3).

Remark 3.14. For $d \ge 5$, one can easily check that the upper bound in (1.3) is always better than the upper bound in (1.2). For $v_1v_2 \in E(T)$, the upper bound in (1.4) is better than the upper bound in (1.3) when $\Delta_2 \ge 6$ because

$$1 - \sqrt{\left(1 - \frac{1}{\Delta_1}\right)\left(1 - \frac{1}{\Delta_2}\right)} < 1 - \frac{\sqrt{6}}{3},$$

that is,

$$(\Delta_1 - 3)(\Delta_2 - 3) > 6.$$

But for the graph H_1 (see, Figure 3.2), the upper bound in (1.3) is better than the upper bound in (1.4).

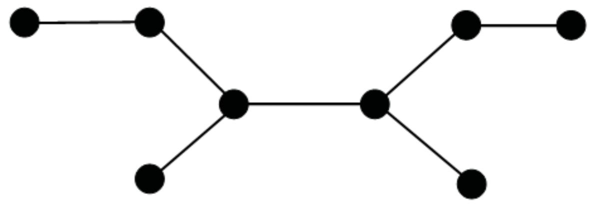

Figure 3.2: Tree H_1.

Remark 3.15. For any given n, we can always make a tree $T(n,k,n_1,n_2,\ldots,n_k)$ $(n_1=n_2)$ such that the equality holding in (1.4).

4. Normalized Laplacian energy of trees

In this section we give some lower bounds on the normalized Laplacian energy of trees. In the literature several lower bounds were established [9,11], but all the lower bounds are in terms of several graph invariants, not easy to compute. Here we give some lower bounds on normalized Laplacian energy of trees.

Theorem 4.1. *Let T be a tree of order n. Then*

$$E_{\mathcal{L}}(T) \geq 2 + 2 \max_{uv\in E(T)} \left\{ \sqrt{\left(1-\frac{1}{n_u(e)}\right)\left(1-\frac{1}{n_v(e)}\right)} \right\} \tag{4.1}$$

with equality holding if and only if $T \cong S_n$ or $T \cong \mathrm{DS}(p,q)$ $(2 \leq p \leq q,\ p+q=n)$.

Proof. Let d be the diameter of tree T. For $d=2$, $T\cong S_n$ and hence the equality holds in (4.1). For $d=3$, $T\cong \mathrm{DS}(p,q)$ $(2\leq p\leq q,\ p+q=n)$. Using (1.1) in (1.5), one can see easily that the equality holds in (4.1). Otherwise, $d\geq 4$.

Let ν $(1\leq \nu\leq n-1)$ be the largest positive integer such that

$$\rho_\nu > 1.$$

Also let $S_k(T)$ be the sum of the largest k normalized Laplacian eigenvalues of tree T. Then

$$S_k(T) = \sum_{i=1}^{k} \rho_i.$$

One can easily see that

$$S_\nu(T) - S_k(T) = \sum_{i=k+1}^{\nu} \rho_i \geq \nu - k \quad \text{for } \nu > k,$$

$$S_k(T) - S_\nu(T) = \sum_{i=\nu+1}^{k} \rho_i \leq k - \nu \quad \text{for } k > \nu$$

and

$$S_\nu(T) = S_k(T) \quad \text{for } k = \nu.$$

From the above, we conclude that for any k, $1 \leq k \leq n-1$,

$$S_\nu(T) - S_k(T) \geq \nu - k,$$

that is,

$$2S_\nu(T) - 2\nu \geq 2S_k(T) - 2k.$$

Using the above result in (1.5), we have

$$\begin{aligned} E_{\mathcal{L}}(T) &= \sum_{i=1}^{\nu}(\rho_i - 1) + \sum_{i=\nu+1}^{n}(1-\rho_i) \\ &= 2S_\nu(T) - 2\nu \qquad\qquad \text{as } \sum_{i=1}^{n-1}\rho_i = n \\ &\geq 2S_{n-2}(T) - 2(n-2). \end{aligned}$$

Since $S_{n-2}(T) = n - \rho_{n-1}$, we get

$$E_{\mathcal{L}}(T) \geq 4 - 2\rho_{n-1}.$$

Since $d \geq 4$, by Theorem 3.1,

$$E_{\mathcal{L}}(T) > 2 + 2 \max_{uv \in E(T)} \left\{ \sqrt{\left(1 - \frac{1}{n_u(e)}\right)\left(1 - \frac{1}{n_v(e)}\right)} \right\}.$$

This completes the proof. □

Lemma 4.2. *Let $T \cong T(n, k, n_1, n_2, \ldots, n_k)$ with $n_1 = n_2 \geq n_3 \geq \cdots \geq n_k$ $(n_1 \geq 2)$ be a tree of order n. Then $\rho_3 = \rho_4 = \cdots = \rho_{n-2} = 1$ if and only if $T \cong T(n, 2, \frac{n-1}{2}, \frac{n-1}{2})$.*

Proof. If $T \cong T(n, 2, \frac{n-1}{2}, \frac{n-1}{2})$, then the normalized Laplacian spectrum of tree T is the following:

$$\left(2, 1 \pm \sqrt{\frac{n-3}{n-1}}, \underbrace{1, 1, \ldots, 1}_{n-4}, 0\right).$$

Thus we have $\rho_3 = \rho_4 = \cdots = \rho_{n-2} = 1$. Otherwise, $k \geq 3$ and hence $T \supseteq T(n^*, 3, n_1, n_1, 1)$ $(n \geq n^*)$. The normalized Laplacian spectrum of tree $T(n^*, 3, n_1, n_1, 1)$ is the following:

$$\left(2, 1 \pm \sqrt{\frac{n_1 - 1}{n_1}}, 1 \pm \sqrt{\frac{n_1 - 1}{3n_1}}, \underbrace{1, 1, \ldots, 1}_{n^*-6}, 0\right).$$

By Lemma 2.3, we have

$$\rho_{n-2}(T(n,k,n_1,n_1,n_3,\ldots,n_k)) \leq \rho_{n^*-2}(T(n^*,3,n_1,n_1,1)) < 1 \quad (n \geq n^*).$$

This completes the proof of the lemma. □

We are now giving our proof of Theorem 1.2.

Proof of Theorem 1.2. For $T \cong S_n$ or $T \cong \mathrm{DS}(\Delta_2,\Delta_1)$, $\Delta_1+\Delta_2 = n$, $v_1v_2 \in E(T)$, one can see easily that the equality holds in (1.6). Otherwise, $d \geq 4$.

Similarly, from the proof of Theorem 4.1, we get

$$E_{\mathcal{L}}(T) = 2S_\nu(T) - 2\nu \geq 2S_2(T) - 4 = 2\rho_2 \quad \text{as } \rho_1 = 2.$$

By Lemma 2.6 with Theorem 1.1, we get the required result in (1.6). The first part of the proof is done.

For $d \geq 4$, the equality holds in (1.6) if and only if $\nu = 2$ and $T \cong T(n,k,n_1,n_2,\ldots,n_k)$, $n_1 = n_2 \geq 2$, $v_1v_2 \notin E(T)$, by Theorem 1.1. Since $\nu = 2$, $\rho_i \leq 1$, $i = 3,4,\ldots,n-1$. By Lemma 2.6, $\rho_2 + \rho_{n-1} = 2$. Thus we have $\sum_{i=3}^{n-2}\rho_i = n-4$, this implies that $\rho_3 = \rho_4 = \cdots = \rho_{n-2} = 1$. Hence the equality holds in (1.6) if and only if $T \cong T(n,2,\frac{n-1}{2},\frac{n-1}{2})$ with $v_1v_2 \notin E(T)$, by Lemma 4.2. □

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