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On the largest and least eigenvalues of eccentricity matrix of trees

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ABSTRACT

The eccentricity matrix $\varepsilon(G)$ of a graph G is constructed from the distance matrix of G by keeping only the largest distances for each row and each column. This matrix can be interpreted as the opposite of the adjacency matrix obtained from the distance matrix by keeping only the distances equal to 1 for each row and each column. The ε-eigenvalues of a graph G are those of its eccentricity matrix $\varepsilon(G)$. Wang et al. [24] proposed the problem of determining the maximum ε-spectral radius of trees with given order. In this paper, we consider the above problem of n-vertex trees with given diameter. The maximum ε-spectral radius of n-vertex trees with fixed odd diameter is obtained, and the corresponding extremal trees are also determined. Recently, Wei et al. [22] determined all connected graphs on n vertices of maximum degree less than $n-1$, whose least eccentricity eigenvalues are in $[-2\sqrt{2}, -2]$. Denote by S_n the star on n vertices. For tree T with order $n \geq 3$, it [22] was proved that $\varepsilon_n(T) \leq -2$ with equality if and only if $T \cong S_n$. According to the above results, the trees of order $n \geq 3$ with least ε-eigenvalues in $[-2\sqrt{2}, 0)$ are only S_n. Motivated by [22], we determine the trees with least ε-eigenvalues in $[-2-\sqrt{13}, -2\sqrt{2})$.

1. Introduction

In this paper, we only consider connected and simple graphs, and refer to Bondy and Murty [2] for notations and terminologies used but not defined here.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. $G-v$ (resp. $G-uv$) is the graph obtained from G by deleting vertex v together with incident edges (resp. edge $uv \in E(G)$). This notation is naturally extended if more than one vertex or edge is deleted. Similarly, $G+uv$ is obtained from G by adding an edge $uv \notin E(G)$. If $U \subseteq V(G)$, then we write $G[U]$ to denote the induced subgraph of G with vertex set U and two vertices being adjacent if and only if they are adjacent in G. A *pendant vertex* is the vertex of degree 1 and a *supporting vertex* is the neighbor of a pendant vertex. A *pendant edge* is an edge which is incident to a supporting vertex and a pendant vertex. Denote by P_n, C_n, S_n and K_n the path, cycle, star and complete graph on n vertices, respectively. An *acyclic* graph is one that contains no cycles. A connected acyclic graph is called a tree. If the tree is nontrivial, a vertex of degree one is called a leaf of the tree. A *caterpillar tree* is a tree with a single path containing at least one endpoint of every edge. For a real number x, denote by $\lfloor x \rfloor$ the greatest integer no more than x, and by $\lceil x \rceil$ the least integer no less than x. We may denote the $n \times n$ identity matrix by $\mathbf{I}_n$.

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We denote the *neighbors* of vertex u and the *degree* of vertex u in graph G by $N_G(u)$ and $d_G(u)$, respectively. The *distance* $d_G(u,v)$ between vertices u and v is the length of a shortest path between them in G and the *eccentricity* of vertex u is defined as $e_G(u) = \max\{d_G(u,v) | v \in V(G)\}$. Then the *diameter* of G, written as $diam(G)$, is $\max\{e_G(u) | u \in V(G)\}$. A *diametrical path* is a path whose length is equal to the diameter of G.

Let $M(G)$ be an $n \times n$ matrix closely related to the structural theory of a graph G. Then the *M-polynomial* of G is defined as $\varphi_M(G,\lambda) = \det(\lambda \mathbf{I}_n - M(G))$, and the roots of $\varphi_M(G,\lambda) = 0$ are the *M-eigenvalues*. The *M-spectrum* $Spec_M(G)$ of G is a multiset consisting of the distinct M-eigenvalues together with their multiplicities, in which the maximum modulus is called the *M-spectral radius* of G. It is well-known that there are several classical graph matrices, including adjacency matrix, distance matrix, Laplacian matrix, signless Laplacian matrix, resistance matrix and so on.

Let $D(G)$ be the *distance matrix* of G with (u,v)-entry $(D(G))_{uv} = d_G(u,v)$. The *eccentricity matrix* $\varepsilon(G)$ of G is constructed from the distance matrix $D(G)$ by only retaining the eccentricities in each row and each column and setting the rest elements in the corresponding row and column to be zero. To be more precise, the (u,v)-entry of eccentricity matrix is defined as

$$(\varepsilon(G))_{uv} = \begin{cases} (D(G))_{uv}, & \text{if } (D(G))_{uv} = \min\{e_G(u), e_G(v)\}; \\ 0, & \text{otherwise.} \end{cases}$$

It is obvious that $\varepsilon(G)$ is real and symmetric. Then the ε-eigenvalues of G are real, denoted by $\varepsilon_1(G) \geqslant \varepsilon_2(G) \geqslant \cdots \geqslant \varepsilon_n(G)$. Randić et al. [19,20] defined so-called D_{MAX} *matrix*, which was renamed as the eccentricity matrix by Wang et al. [23]. Furthermore, Dehmer and Shi [6] studied the uniqueness of D_{MAX}-matrix. Recently, Wang et al. [25] studied the graph energy based on the eccentricity matrix; Wang et al. [24] studied some spectral properties of the eccentricity matrix of graphs; Mahato et al. [16] studied the spectra of graphs based on the eccentricity matrix; Tura et al. [21] studied the eccentricity energy of complete multipartite graphs. Patel et al. [18] studied the irreducibility and the spectrum of the eccentricity matrix for particular classes of graphs, namely the windmill graphs, the coalescence of complete graphs and the coalescence of two cycles, and further estimated the eccentricity energy and inertia for the graphs of these classes. Lei et al. [11] characterized the graphs whose second least ε-eigenvalue is greater than $-\sqrt{15-\sqrt{193}}$; moreover it is shown that all these graphs are determined by their ε-spectrum. Wei et al. [22] determined the n-vertex trees with minimum ε-spectral radius. Furthermore, in [22], the authors identified all trees with given order and diameter having minimum ε-spectral.

Note that the adjacency matrix $A(G)$ can be regarded as constructed from the distance matrix $D(G)$ by selecting only the smallest distances for each row and each column, which correspond to adjacent vertices. From this point of view, the eccentricity matrix can be viewed as the opposite to the adjacency matrix [23] and these two matrices express two extremes of distance-like matrix.

The adjacency and distance matrices have been extensively studied and applied; see [1,3–5,7–10,12–14,17,26–28]. One of the most important facts is that the adjacency and distance matrices of connected graphs are irreducible, but it does not hold for all eccentricity matrices. Let T be a tree with at least two vertices. Recently, Wang et al. [23] proved that the eccentricity matrix of T is irreducible and they characterized the relationships between the A-eigenvalues and ε-eigenvalues of some graphs. Then ε-spectral radius $\varepsilon_1(T)$ is positive and there is an eigenvector corresponding to $\varepsilon_1(T)$, called *Perron eigenvector*, whose each coordinate is positive by Perron-Frobenius Theorem. Let M and N be two matrices with same order. If $(N)_{ij} \leqslant (M)_{ij}$ for each i, j, we let $N \leqslant M$.

In view of more novel properties of eccentricity matrix, further discussion is needed. In particular, Wang et al. [24] proposed the following problem.

Problem 1.1 *([24]). Which trees have the maximum ε-spectral radius?*

Recently, Wei et al. [22] determined all connected graphs on n vertices of maximum degree less than $n-1$, whose least eccentricity eigenvalues are in $[-2\sqrt{2}, -2]$. For tree T with order $n \geq 3$, it [22] was proved that $\varepsilon_n(T) \leq -2$ with equality if and only if $T \cong S_n$.

Motivated by the above results, we now propose the following problem.

Problem 1.2. *For some given number $c < -2\sqrt{2}$, which trees with least eccentricity eigenvalues are in $[c, -2\sqrt{2})$?*

In this paper, we characterize the extremal trees having maximum ε-spectral radius with given order and odd diameter. On the other hand, we determine all the trees with least eccentricity eigenvalues in $[-2-\sqrt{13}, -2\sqrt{2})$.

Further on we need the following lemmas.

Lemma 1.3 *([15]). Let M be a Hermitian matrix of order s, and let N be a principle submatrix of M with order t. If $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_s$ list the eigenvalues of M and $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_t$ are the eigenvalues of N, then $\lambda_i \geqslant \mu_i \geqslant \lambda_{s-t+i}$ for $1 \leqslant i \leqslant t$.*

Lemma 1.4 *([15]). Let M and N be two nonnegative irreducible matrices with same order. If $(N)_{ij} \leqslant (M)_{ij}$ for each i, j, then $\rho(N) \leqslant \rho(M)$ with equality if and only if $M = N$, where $\rho(N)$ and $\rho(M)$ denote the spectral radius of N and M, respectively.*

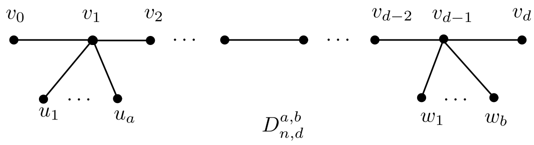

Fig. 1. Tree $D_{n,d}^{a,b}$.

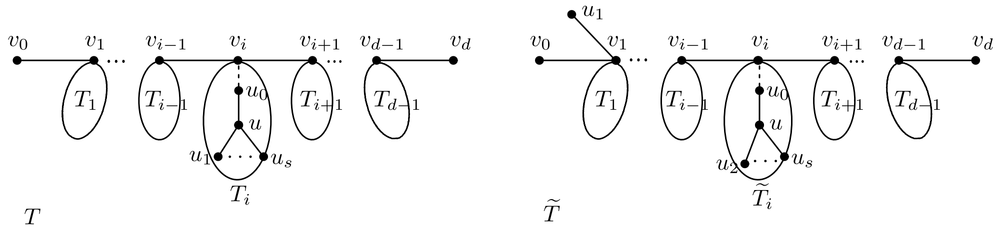

Fig. 2. Trees T and $\widetilde{T}$ in Lemma 2.3.

Lemma 1.5 *([23]). The eccentricity matrix $\varepsilon(T)$ of a tree T with at least two vertices is irreducible.*

Lemma 1.6 *([22]). Let G be an n-vertex connected graph with diameter d. Then $\varepsilon_1(G) \geqslant d$ and $\varepsilon_n(G) \leqslant -d$.*

Lemma 1.7 *([22]). Let T be a tree with order $n \geq 3$. Then $\varepsilon_n(T) \leqslant -2$ with equality if and only if $T \cong S_n$.*

2. The maximum ε-spectral radius of trees with fixed odd diameter

In this section, we characterize the extremal trees with fixed odd diameter having maximum ε-spectral radius. Firstly, we present a few technical lemmas aiming to provide some fundamental characterizations of extremal trees.

Denote by $\mathscr{T}_{n,d}$ the set of trees with order n and diameter d. It is easy to check that the tree with diameter 1 is K_2 and the tree with diameter 2 is a star with at least 3 vertices.

If $d \geqslant 3$ is odd, let $D_{n,d}^{a,b}$ be the tree obtained from $P_{d+1} = v_0v_1v_2\cdots v_d$ by attaching a pendant vertices to v_1 and b pendant vertices to v_{d-1}, where $a+b=n-d-1$ and $b \geqslant a \geqslant 0$, as depicted in Fig. 1.

Lemma 2.1 *([22]). Let $D_{n,3}^{a,b}$ be in $\mathscr{T}_{n,3}$ defined above, where $a+b=n-4$ and $b \geqslant a \geqslant 1$. Then $\varepsilon_1(D_{n,3}^{a-1,b+1}) < \varepsilon_1(D_{n,3}^{a,b})$.*

Our first main result in this section determines the unique tree among $\mathscr{T}_{n,3}$, having the maximum ε-spectral radius.

Theorem 2.2. *The maximum ε-spectral radius is achieved uniquely by tree $D_{n,3}^{\lfloor\frac{n-4}{2}\rfloor,\lceil\frac{n-4}{2}\rceil}$ among all the trees in $\mathscr{T}_{n,3}$.*

Proof. According to Lemma 2.1, it is easy to see that the maximum ε-spectral radius is achieved uniquely by tree $D_{n,3}^{a,b}$ satisfying $|b-a| \leq 1$ among all the trees in $\mathscr{T}_{n,3}$.

This completes the proof. $\square$

Lemma 2.3. *Let T be in $\mathscr{T}_{n,d}$ with a diametrical path $P_{d+1} = v_0v_1v_2\cdots v_d$ ($d \geqslant 5$ is odd), and let T_j be the connected component of $T - E(P_{d+1})$ containing v_j, $j \in \{0,1,\ldots,d\}$. Assume there exists a vertex $u_1 \in V(T_i)$ ($2 \leq i \leq \frac{d-1}{2}$) such that $d_{T_i}(v_i,u_1) = e_{T_i}(v_i) \geqslant 2$ (obviously, u_1 is a pendant vertex). Denote the unique neighbor of u_1 by u and all neighbors of u by $u_0,u_1,\ldots,u_s$ with $d_T(u_0) \geqslant 2$ and $d_T(u_j) = 1$ for $1 \leqslant j \leqslant s$ (see Fig. 2). Let*

$$\widetilde{T} = T - uu_1 + u_1v_1.$$

Then $\varepsilon_1(T) \leq \varepsilon_1(\widetilde{T})$, with equality if and only if $d_{T_i}(v_i,u_1) = e_{T_i}(v_i) = i$.

Proof. It is easy to check that $e_T(w) = e_{\widetilde{T}}(w)$ for each vertex $w \in V(T)\setminus\{u_1\}$, and $d_T(w,w') = d_{\widetilde{T}}(w,w')$ for $\{w,w'\} \subseteq V(T)\setminus\{u_1\}$. By the definition of eccentricity matrix, the (w,w')-entry of $\varepsilon(T)$ is equal to the (w,w')-entry of $\varepsilon(\widetilde{T})$ for each $\{w,w'\} \subseteq V(T)\setminus\{u_1\}$.

For $w \in \bigcup_{0 \leq j \leq \frac{d-1}{2}} V(T_j)$, note that

$$d_T(u_1,w) \leq d_T(u_1,v_{\frac{d-1}{2}}) + d_T(w,v_{\frac{d-1}{2}}) < \min\{e_T(w), e_T(u_1)\},$$

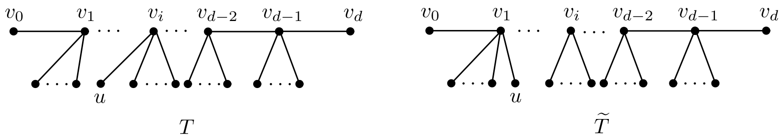

Fig. 3. Trees T and $\widetilde{T}$ in Lemma 2.4.

$$d_{\widetilde{T}}(u_1, w) \le d_{\widetilde{T}}(u_1, v_{\frac{d-1}{2}}) + d_{\widetilde{T}}(w, v_{\frac{d-1}{2}}) < \min\{e_{\widetilde{T}}(w), e_{\widetilde{T}}(u_1)\}.$$

Hence, $(\varepsilon(T))_{u_1 w} = 0 = (\varepsilon(\widetilde{T}))_{u_1 w}$ for $w \in \bigcup_{0 \le j \le \frac{d-1}{2}} V(T_j)$.

We proceed to consider the following two possible cases.

Case 1. $e_{T_i}(v_i) < i$

In this case, for $w \in \bigcup_{\frac{d+1}{2} \le j \le d} V(T_j)$, we have

$$e_T(u_1) = d_T(u_1, v_d) \ge d_T(u_1, w),$$

$$e_T(w) = d_T(v_0, w) > d_T(u_1, w).$$

By the definition of eccentricity matrix, if $d_T(u_1, v_d) > d_T(u_1, w)$, then $(\varepsilon(T))_{u_1 w} = 0$. If $d_T(u_1, v_d) = d_T(u_1, w)$, then $(\varepsilon(T))_{u_1 w} = d_T(u_1, w)$. Hence, we have $(\varepsilon(T))_{u_1 w} \le d_T(u_1, w)$.

On the other hand, for $w \in \bigcup_{\frac{d+1}{2} \le j \le d} V(T_j)$, we have

$$e_{\widetilde{T}}(u_1) = d_{\widetilde{T}}(u_1, v_d) = d \ge d_{\widetilde{T}}(u_1, w),$$

$$e_{\widetilde{T}}(w) = d_{\widetilde{T}}(v_0, w) = d_{\widetilde{T}}(u_1, w).$$

By the definition of eccentricity matrix, we have $(\varepsilon(\widetilde{T}))_{u_1 w} = d_{\widetilde{T}}(u_1, w)$.

It is easy to see that $d_T(u_1, w) < d_{\widetilde{T}}(u_1, w)$. Hence, for $w \in \bigcup_{\frac{d+1}{2} \le j \le d} V(T_j)$, we have $(\varepsilon(T))_{u_1 w} < (\varepsilon(\widetilde{T}))_{u_1 w}$.

Case 2. $e_{T_i}(v_i) = i$.

In this case, for $w \in \bigcup_{\frac{d+1}{2} \le j \le d} V(T_j)$, we have $d_T(u_1, w) = e_T(w) = e_{\widetilde{T}}(w) = d_{\widetilde{T}}(u_1, w)$. Hence, $(\varepsilon(T))_{u_1 w} = (\varepsilon(\widetilde{T}))_{u_1 w}$.

Together with Cases 1 and 2, we have $\varepsilon(T) \leqslant \varepsilon(\widetilde{T})$, with equality if and only if $d_{T_i}(u_1, v_i) = i$. By Lemmas 1.4 and 1.5, we obtain $\varepsilon_1(T) \leqslant \varepsilon_1(\widetilde{T})$, with equality if and only if $d_{T_i}(u_1, v_i) = i$.

This completes the proof. $\square$

Lemma 2.4. *Given an n-vertex caterpillar tree T, $P_{d+1} = v_0 v_1 v_2 \cdots v_d$, ($d \geqslant 5$ is odd) is a diametrical path of T. Assume $d_T(v_i) \ge 3$ ($2 \le i \le \frac{d-1}{2}$). Moving a pendant edge, say $v_i u$ from v_i to v_1 yields the tree $\widetilde{T}$ (see Fig. 3). Then $\varepsilon_1(T) < \varepsilon_1(\widetilde{T})$.*

Proof. It is obvious that $d_T(w, w') = d_{\widetilde{T}}(w, w')$ for $\{w, w'\} \subseteq V(T) \setminus \{u\}$ and $e_T(w) = e_{\widetilde{T}}(w)$ for $w \in V(T) \setminus \{u\}$. By the definition of eccentricity matrix, we have $(\varepsilon(T))_{ww'} = (\varepsilon(\widetilde{T}))_{ww'}$ for any $\{w, w'\} \subseteq V(T) \setminus \{u\}$.

If w is a pendant neighbor of v_{d-1} (may be v_d), then $d_T(u, w) = d - i + 1 = e_T(u)$ and $d_{\widetilde{T}}(u, w) = d = e_{\widetilde{T}}(u)$. Hence, $(\varepsilon(T))_{uw} = d - i + 1 < d = (\varepsilon(\widetilde{T}))_{uw}$. If w is not a pendant neighbor of v_{d-1}, then we have $(\varepsilon(T))_{uw} < \min\{e_T(u), e_T(w)\}$. Thus, $(\varepsilon(T))_{uw} = 0 \leqslant (\varepsilon(\widetilde{T}))_{uw}$.

Clearly, $\varepsilon(T) \leqslant \varepsilon(\widetilde{T})$ and $\varepsilon(T) \neq \varepsilon(\widetilde{T})$. By Lemmas 1.4 and 1.5, we obtain $\varepsilon_1(T) < \varepsilon_1(\widetilde{T})$. $\square$

In the following, let $\Gamma(d) := (\frac{d+1}{2})^2 + (\frac{d+3}{2})^2 + \cdots + (d-1)^2 = \frac{d(d-1)(7d-5)}{24}$.

Lemma 2.5. *For odd $d \geqslant 5$, $\varepsilon_1(D_{n,d}^{a,b})$ is the largest root of equation $F_{a,b}(t) = 0$, where*

$$F_{a,b}(t) = t^4 - \Big[\Gamma(d)(n-d+1) + (a+1)(b+1)d^2\Big]t^2 + (a+1)(b+1)(\Gamma(d))^2.$$

Proof. Choose a diametrical path $P_{d+1} = v_0 v_1 v_2 \cdots v_d$ in $D_{n,d}^{a,b}$. Denote by $U = \{v_0, u_1, \cdots u_a\}$ the set of pendant neighbors of v_1 and let $W = \{v_d, w_1, \cdots w_b\}$ be the set of pendant neighbors of v_{d-1} in $D_{n,d}^{a,b}$. By definition, the eccentricity matrix $\varepsilon(D_{n,d}^{a,b})$ is equal to

$$
\begin{array}{c|c}
 & \begin{array}{cccccccccccccccc} v_0 & v_1 & \cdots & v_{\frac{d-3}{2}} & v_{\frac{d-1}{2}} & v_{\frac{d+1}{2}} & v_{\frac{d+3}{2}} & \cdots & v_{d-1} & v_d & u_1 & \cdots & u_a & w_1 & \cdots & w_b \end{array} \\
\begin{array}{c} v_0 \\ v_1 \\ \vdots \\ v_{\frac{d-3}{2}} \\ v_{\frac{d-1}{2}} \\ v_{\frac{d+1}{2}} \\ v_{\frac{d+3}{2}} \\ \vdots \\ v_{d-1} \\ v_d \\ u_1 \\ \vdots \\ u_a \\ w_1 \\ \vdots \\ w_b \end{array} &
\begin{pmatrix}
0 & 0 & \cdots & 0 & 0 & \frac{d+1}{2} & \frac{d+3}{2} & \cdots & d-1 & d & 0 & \cdots & 0 & d & \cdots & d \\
0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & d-1 & 0 & \cdots & 0 & d-1 & \cdots & d-1 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & \frac{d+3}{2} & 0 & \cdots & 0 & \frac{d+3}{2} & \cdots & \frac{d+3}{2} \\
0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & \frac{d+1}{2} & 0 & \cdots & 0 & \frac{d+1}{2} & \cdots & \frac{d+1}{2} \\
\frac{d+1}{2} & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \frac{d+1}{2} & \cdots & \frac{d+1}{2} & 0 & \cdots & 0 \\
\frac{d+3}{2} & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \frac{d+3}{2} & \cdots & \frac{d+3}{2} & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
d-1 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & d-1 & \cdots & d-1 & 0 & \cdots & 0 \\
d & d-1 & \cdots & \frac{d+3}{2} & \frac{d+1}{2} & 0 & 0 & \cdots & 0 & 0 & d & \cdots & d & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & 0 & \frac{d+1}{2} & \frac{d+3}{2} & \cdots & d-1 & d & 0 & \cdots & 0 & d & \cdots & d \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & 0 & \frac{d+1}{2} & \frac{d+3}{2} & \cdots & d-1 & d & 0 & \cdots & 0 & d & \cdots & d \\
d & d-1 & \cdots & \frac{d+3}{2} & \frac{d+1}{2} & 0 & 0 & \cdots & 0 & 0 & d & \cdots & d & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
d & d-1 & \cdots & \frac{d+3}{2} & \frac{d+1}{2} & 0 & 0 & \cdots & 0 & 0 & d & \cdots & d & 0 & \cdots & 0
\end{pmatrix}
\end{array}.
$$

Let $\mathbf{x}$ be a Perron eigenvector corresponding to $\rho := \varepsilon_1(D^{a,b}_{n,d})$, whose coordinate with respect to vertex v is $\mathbf{x}_v$. Since $\rho\mathbf{x}_u = \frac{d+1}{2}\mathbf{x}_{v_{\frac{d+1}{2}}} + \frac{d+3}{2}\mathbf{x}_{v_{\frac{d+3}{2}}} + \cdots + (d-1)\mathbf{x}_{v_{d-1}} + d\mathbf{x}_{v_d} + d\sum_{i=1}^{b}\mathbf{x}_{w_i}$ for each $u \in U$, we can get $\mathbf{x}_u = \mathbf{x}_{u'}$ for $\{u, u'\} \subseteq U$. Similarly, $\mathbf{x}_w = \mathbf{x}_{w'}$ for $\{w, w'\} \subseteq W$. Then we obtain

$$
\begin{aligned}
\rho\mathbf{x}_u &= \frac{d+1}{2}\mathbf{x}_{v_{\frac{d+1}{2}}} + \frac{d+3}{2}\mathbf{x}_{v_{\frac{d+3}{2}}} + \cdots + (d-1)\mathbf{x}_{v_{d-1}} + (b+1)d\mathbf{x}_w; \\
\rho\mathbf{x}_w &= (a+1)d\mathbf{x}_u + (d-1)\mathbf{x}_{v_1} + (d-2)\mathbf{x}_{v_2} + \cdots + \frac{d+1}{2}\mathbf{x}_{v_{\frac{d-1}{2}}}; \\
\rho\mathbf{x}_{v_1} &= (b+1)(d-1)\mathbf{x}_w; \\
&\vdots \\
\rho\mathbf{x}_{v_{\frac{d-1}{2}}} &= (b+1)\cdot\frac{d+1}{2}\mathbf{x}_w; \\
\rho\mathbf{x}_{v_{d-1}} &= (a+1)(d-1)\mathbf{x}_u; \\
&\vdots \\
\rho\mathbf{x}_{v_{\frac{d+1}{2}}} &= (a+1)\cdot\frac{d+1}{2}\mathbf{x}_u,
\end{aligned}
$$

for any $u \in U$, $w \in W$.

Hence,

$$
\begin{aligned}
\rho^2\mathbf{x}_u &= \rho\Big[\frac{d+1}{2}\mathbf{x}_{v_{\frac{d+1}{2}}} + \frac{d+3}{2}\mathbf{x}_{v_{\frac{d+3}{2}}} + \cdots + (d-1)\mathbf{x}_{v_{d-1}} + (b+1)d\mathbf{x}_w\Big] \\
&= (a+1)(\frac{d+1}{2})^2\mathbf{x}_u + (a+1)(\frac{d+3}{2})^2\mathbf{x}_u + \cdots + (a+1)(d-1)^2\mathbf{x}_u + (b+1)d\rho\mathbf{x}_w \\
&= (a+1)\Gamma(d)\mathbf{x}_u + (b+1)d\rho\mathbf{x}_w
\end{aligned}
$$

and

$$
\begin{aligned}
\rho^2\mathbf{x}_w &= \rho\Big[(a+1)d\mathbf{x}_u + (d-1)\mathbf{x}_{v_1} + (d-2)\mathbf{x}_{v_2} + \cdots + \frac{d+1}{2}\mathbf{x}_{v_{\frac{d-1}{2}}}\Big] \\
&= (a+1)d\rho\mathbf{x}_u + (b+1)(d-1)^2\mathbf{x}_w + (b+1)(d-2)^2\mathbf{x}_w + \cdots + (b+1)(\frac{d+1}{2})^2\mathbf{x}_w
\end{aligned}
$$

$$= (a+1)d\rho \mathbf{x}_u + (b+1)\Gamma(d)\mathbf{x}_w.$$

That is,

$$\rho^2\mathbf{x}_u - (a+1)\Gamma(d)\mathbf{x}_u - (b+1)d\rho\mathbf{x}_w = 0,$$
$$-(a+1)d\rho\mathbf{x}_u + \rho^2\mathbf{x}_w - (b+1)\Gamma(d)\mathbf{x}_w = 0.$$

Since $\mathbf{x}_u \neq 0$ and $\mathbf{x}_w \neq 0$, ρ is the largest root of

$$\begin{vmatrix} t^2-(a+1)\Gamma(d) & -(b+1)dt \\ -(a+1)dt & t^2-(b+1)\Gamma(d) \end{vmatrix} = 0.$$

By calculation and the fact $a+b = n-d-1$, we have

$$\begin{aligned} 0 &= \Big[t^2-(a+1)\Gamma(d)\Big]\Big[t^2-(b+1)\Gamma(d)\Big] - (a+1)(b+1)d^2t^2 \\ &= t^4 - \Big[(a+1)\Gamma(d)+(b+1)\Gamma(d)+(a+1)(b+1)d^2\Big]t^2 + (a+1)(b+1)(\Gamma(d))^2 \\ &= t^4 - \Big[\Gamma(d)(n-d+1)+(a+1)(b+1)d^2\Big]t^2 + (a+1)(b+1)(\Gamma(d))^2. \end{aligned}$$

For fixed odd $d \ge 5$, let $F_{a,b}(t) = t^4 - \Big[\Gamma(d)(n-d+1)+(a+1)(b+1)d^2\Big]t^2 + (a+1)(b+1)(\Gamma(d))^2$. Then ρ is the largest root of equation $F_{a,b}(t) = 0$. □

Lemma 2.6. *For odd $d \geqslant 5$, $\varepsilon_1(D_{n,d}^{0,n-d-1}) \neq \frac{\Gamma(d)}{d}$.*

Proof. Suppose to the contrary that there exist some n and odd d such that $\varepsilon_1(D_{n,d}^{0,n-d-1}) = \frac{\Gamma(d)}{d}$. Then by Lemma 2.5, we have

$$\begin{aligned} 0 &= F_{0,n-d-1}(\frac{\Gamma(d)}{d}) \\ &= (\frac{\Gamma(d)}{d})^4 - \big[\Gamma(d)(n-d+1)+(n-d)d^2\big](\frac{\Gamma(d)}{d})^2 + (n-d)(\Gamma(d))^2 \\ &= \frac{(\Gamma(d))^2}{d^4}\Big[(\Gamma(d))^2 - (\Gamma(d)(n-d+1)+(n-d)d^2)d^2 + (n-d)d^4\Big] \\ &= \frac{(\Gamma(d))^2}{d^4}\Big[(\Gamma(d))^2 - \Gamma(d)(n-d+1)d^2\Big] \\ &= \frac{(\Gamma(d))^3}{d^4}\Big[\Gamma(d) - (n-d+1)d^2\Big] \\ &= \frac{(\Gamma(d))^3}{d^4}\Big[\frac{d(d-1)(7d-5)}{24} - (n-d+1)d^2\Big] \\ &= (\frac{\Gamma(d)}{d})^3\Big[\frac{(d-1)(7d-5)}{24} - (n-d+1)d\Big]. \end{aligned}$$

Hence, $\frac{(d-1)(7d-5)}{24} = (n-d+1)d$, i.e., $(d-1)(7d-5) = 24(n-d+1)d$. Note that $d-1$ and d are relatively prime. Therefore, we have $d|7d-5$. Clearly, $\frac{7d-5}{d} \le 6$. Combining $d \ge 5$ and d is odd, we have $d = 5$. Substituting $d = 5$ to $(d-1)(7d-5) = 24(n-d+1)d$, we have $n = 5$, which contradicts $n \ge d+1 = 6$. Thus for odd $d \geqslant 5$, $\varepsilon_1(D_{n,d}^{0,n-d-1}) \neq \frac{\Gamma(d)}{d}$. □

Our next main result in this section determines the unique tree among $\mathscr{T}_{n,d}$ with odd $d \geqslant 5$, having the maximum ε-spectral radius.

Theorem 2.7. *Let T be in $\mathscr{T}_{n,d}$ with odd $d \geqslant 5$. Then*

$$\varepsilon_1(T) \le \max\Big\{\varepsilon_1(D_{n,d}^{0,n-d-1}), \varepsilon_1(D_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil})\Big\}$$

with equality only if $T \cong D_{n,d}^{0,n-d-1}$ or $D_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}$. Especially, if $n-d-1 \ge 2$, we have $\varepsilon_1(D_{n,d}^{0,n-d-1}) \neq \varepsilon_1(D_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil})$. Hence, for odd $d \ge 5$, the extremal tree with maximum ε-spectral radius in $\mathscr{T}_{n,d}$ is unique.

Proof. Assume that T is the tree with maximum ε-spectral radius among $\mathscr{T}_{n,d}$ with odd $d \geqslant 5$. By making frequent use of Lemmas 2.3 and 2.4, we obtain that T is isomorphic to some $D_{n,d}^{a,b}$, where $b \geq a \geq 0$. For brevity, let $\rho := \varepsilon_1(T)$. If $\rho < \frac{\Gamma(d)}{d}$, then we have $T \cong D_{n,d}^{0,n-d-1}$. Otherwise, $1 \leq a \leq \left\lfloor \frac{n-d-1}{2} \right\rfloor \leq \left\lceil \frac{n-d-1}{2} \right\rceil \leq b$. By Lemma 2.5, we have

$$-F_{a-1,b+1}(\rho) = F_{a,b}(\rho) - F_{a-1,b+1}(\rho) = (b+1-a)[(\Gamma(d))^2 - d^2\rho^2] > 0.$$

Therefore, $F_{a-1,b+1}(\rho) < 0$ then $\rho = \varepsilon_1(D_{n,d}^{a,b}) = \varepsilon_1(T) < \varepsilon_1(D_{n,d}^{a-1,b+1})$, a contradiction. If $\rho = \frac{\Gamma(d)}{d}$, then by Lemma 2.6, we have $1 \leq a \leq \left\lfloor \frac{n-d-1}{2} \right\rfloor \leq \left\lceil \frac{n-d-1}{2} \right\rceil \leq b$. According to Lemma 2.5,

$$-F_{a-1,b+1}(\rho) = F_{a,b}(\rho) - F_{a-1,b+1}(\rho) = (b+1-a)[(\Gamma(d))^2 - d^2\rho^2] = 0.$$

Therefore, ρ is a root of $F_{a-1,b+1}(t)$. Clearly, $\varepsilon_1(D_{n,d}^{a-1,b+1}) = \rho = \frac{\Gamma(d)}{d}$. By similar discussion, we obtain $\varepsilon_1(D_{n,d}^{0,n-d-1}) = \rho = \frac{\Gamma(d)}{d}$, which contradicts Lemma 2.6. Thus, $\rho \neq \frac{\Gamma(d)}{d}$. If $\rho > \frac{\Gamma(d)}{d}$, we have $T \cong D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil}$. Otherwise, $0 \leq a \leq \left\lfloor \frac{n-d-1}{2} \right\rfloor - 1 < \left\lceil \frac{n-d-1}{2} \right\rceil + 1 \leq b$. According to Lemma 2.5,

$$-F_{a+1,b-1}(\rho) = F_{a,b}(\rho) - F_{a+1,b-1}(\rho) = (b-a-1)[d^2\rho^2 - (\Gamma(d))^2] > 0.$$

Therefore, $F_{a+1,b-1}(\rho) < 0$ then $\rho = \varepsilon_1(D_{n,d}^{a,b}) = \varepsilon_1(T) < \varepsilon_1(D_{n,d}^{a+1,b-1})$, a contradiction. Thus, we have

$$\rho \leq \max\left\{\varepsilon_1(D_{n,d}^{0,n-d-1}), \varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil})\right\}$$

with equality only if $T \cong D_{n,d}^{0,n-d-1}$ or $D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil}$.

Especially, if $a + b \geq 2$, we claim $\varepsilon_1(D_{n,d}^{0,n-d-1}) \neq \varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil})$. Otherwise, let $\alpha := \varepsilon_1(D_{n,d}^{0,n-d-1}) = \varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil})$. If $\alpha < \frac{\Gamma(d)}{d}$, as in the above proof, we have $\varepsilon_1(D_{n,d}^{0,n-d-1}) > \varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil})$, a contradiction. If $\alpha > \frac{\Gamma(d)}{d}$, similarly, we have $\varepsilon_1(D_{n,d}^{0,n-d-1}) < \varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil})$, a contradiction. Hence, for odd $d \geq 5$, the extremal tree with maximum ε-spectral radius in $\mathscr{T}_{n,d}$ is unique. $\square$

Remark 1. In Theorem 2.7, let $n = 25$ and $d = 21$. By a direct calculation, $\varepsilon_1(D_{25,21}^{0,3}) \approx 110.2597$ and $\varepsilon_1(D_{25,21}^{1,2}) \approx 109.4423$. Thus, $\varepsilon_1(D_{25,21}^{0,3}) > \varepsilon_1(D_{25,21}^{1,2})$. Note that, in this case, the values of $n(=25)$ and $d(=21)$ are very close. The following result shows that, when n is sufficiently large relative to d, $\varepsilon_1(D_{n,d}^{0,n-d-1}) < \varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil})$.

Corollary 2.8. *For fixed odd $d \geq 5$, if n is sufficiently large, the maximum ε-spectral radius is achieved uniquely by tree $D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil}$ among all the trees in $\mathscr{T}_{n,d}$.*

Proof. Let $\Delta(a,b) := \Big[\Gamma(d)(n-d+1) + (a+1)(b+1)d^2\Big]^2 - 4(a+1)(b+1)(\Gamma(d))^2$. According to Lemma 2.5, by a direct calculation, $(\varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil}))^2$ is equal to

$$\frac{1}{2}\Big[\Gamma(d)(n-d+1) + (\left\lfloor \frac{n-d-1}{2} \right\rfloor + 1)(\left\lceil \frac{n-d-1}{2} \right\rceil + 1)d^2\Big] + \frac{1}{2}\sqrt{\Delta(\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil)} \tag{2.1}$$

Hence, if n is sufficiently large, we have $\varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil}) > \frac{\Gamma(d)}{d}$. In view of the proof of Theorem 2.7, we have $T \cong D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil}$. $\square$

Similarly, we have the following corollary.

Corollary 2.9. *If there exists T in $\mathscr{T}_{n,d}$ with odd $d \geqslant 5$ such that $\varepsilon_1(T) > \frac{\Gamma(d)}{d}$, then*

$$\varepsilon_1(T) \leq \varepsilon_1(D_{n,d}^{\left\lfloor \frac{n-d-1}{2} \right\rfloor, \left\lceil \frac{n-d-1}{2} \right\rceil})$$

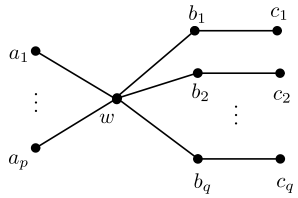

Fig. 4. $H_{p,q}$ with $p \geq 0$ and $q \geq 2$.

with equality if and only if $T \cong D_{n,d}^{\lfloor \frac{n-d-1}{2} \rfloor, \lceil \frac{n-d-1}{2} \rceil}$.

Together with Theorems 2.2 and 2.7, we obtain the following result.

Theorem 2.10. *Let T be an n-vertex tree with odd diameter d. Then*

$$\varepsilon_1(T) \leq \max\left\{\varepsilon_1(D_{n,d}^{0,n-d-1}), \varepsilon_1(D_{n,d}^{\lfloor \frac{n-d-1}{2} \rfloor, \lceil \frac{n-d-1}{2} \rceil})\right\}$$

with equality only if $T \cong D_{n,d}^{0,n-d-1}$ *or* $D_{n,d}^{\lfloor \frac{n-d-1}{2} \rfloor, \lceil \frac{n-d-1}{2} \rceil}$. *Especially,* $D_{n,3}^{\lfloor \frac{n-4}{2} \rfloor, \lceil \frac{n-4}{2} \rceil}$ *is the unique tree maximizing ε-spectral radius among all the trees in $\mathscr{T}_{n,3}$. In the case of odd $d \geq 5$, the extremal tree with maximum ε-spectral radius is also unique.*

3. Trees with least ε-eigenvalues in $[-2-\sqrt{13}, -2\sqrt{2})$

In this section, we investigate trees with least ε-eigenvalues in $[-2-\sqrt{13}, -2\sqrt{2})$. Let $\varepsilon_n(G)$ be the least ε-eigenvalue of a graph G with order n.

For $p \geq 0$ and $q \geq 2$, let $H_{p,q}$ be the graph obtained from the star S_{p+q+1} by attaching a pendant vertex to each of q chosen pendant vertices (see Fig. 4). Let $\mathbf{J}_{n\times m}$ and $\mathbf{0}_{n\times m}$ be respectively all-one and the all-zero $n \times m$ matrices. Let $\mathbf{J}_n = \mathbf{J}_{n\times n}$, $\mathbf{1}_n = \mathbf{J}_{n\times 1}$, and $\mathbf{0}_n = \mathbf{0}_{n\times 1}$.

The following is a key lemma that we will need in the proofs.

Lemma 3.1 *([4]). Let $\mathbf{M}$, $\mathbf{N}$, $\mathbf{P}$ and $\mathbf{Q}$ be respectively $p \times p$, $p \times q$, $q \times p$ and $q \times q$ matrices, where $\mathbf{Q}$ is invertible. Then*

$$\begin{vmatrix} \mathbf{M} & \mathbf{N} \\ \mathbf{P} & \mathbf{Q} \end{vmatrix} = |\mathbf{Q}| \cdot |\mathbf{M} - \mathbf{N}\mathbf{Q}^{-1}\mathbf{P}|.$$

Lemma 3.2. *For $p \geq 0$ and $q \geq 2$, the ε-polynomial of $H_{p,q}$ is*

$$\lambda^{p+1}(\lambda^2 + 4\lambda - 9)^{q-1}\left[\lambda^2 + (4-4q)\lambda - (9pq + 9q^2 + 9 - 14q)\right].$$

Proof. Let $n = p + 2q + 1$. Let w be the center of S_{p+q+1}, A be the set of pendant neighbors of w, B be the set of non-pendant neighbors of w, and C be the set of pendant vertices that are not neighbors of w. Then $\{w\} \bigcup A \bigcup B \bigcup C$ is a partition of $V(H_{p,q})$ (see Fig. 4), and with respect to this partition, we have

$$\varepsilon(H_{p,q}) - \lambda\mathbf{I}_n = \begin{pmatrix} -\lambda & \mathbf{0}_p^\top & \mathbf{0}_q^\top & 2\mathbf{1}_q^\top \\ \mathbf{0}_p & -\lambda\mathbf{I}_p & \mathbf{0}_{p\times q} & 3\mathbf{J}_{p\times q} \\ \mathbf{0}_q & \mathbf{0}_{q\times p} & -\lambda\mathbf{I}_q & 3\mathbf{J}_q - 3\mathbf{I}_q \\ 2\mathbf{1}_q & 3\mathbf{J}_{q\times p} & 3\mathbf{J}_q - 3\mathbf{I}_q & 4\mathbf{J}_q - (\lambda+4)\mathbf{I}_q \end{pmatrix}.$$

Let

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & -2 & -3\mathbf{1}_p^\top & (\frac{12}{\lambda+4} - 3)\mathbf{1}_q^\top \\ 0 & 1 & 0 & \mathbf{0}_p^\top & (\frac{9}{\lambda+4})\mathbf{1}_q^\top \\ 0 & 0 & -\lambda & \mathbf{0}_p^\top & (-\frac{6}{\lambda+4})\mathbf{1}_q^\top \\ \mathbf{0}_p & \mathbf{1}_p & \mathbf{0}_p & -\lambda\mathbf{I}_p & \mathbf{0}_{p\times q} \\ \mathbf{0}_q & \mathbf{1}_q & \mathbf{0}_q & \mathbf{0}_{qp} & (-\lambda + \frac{9}{\lambda+4})\mathbf{I}_q \end{pmatrix}, \mathbf{B} = \begin{pmatrix} -4\mathbf{1}_q^\top \\ -3\mathbf{1}_q^\top \\ 2\mathbf{1}_q^\top \\ \mathbf{0}_{p\times q} \\ -3\mathbf{I}_q \end{pmatrix}$$

and

$$\mathbf{C} = \begin{pmatrix} \mathbf{1}_q & \mathbf{0}_q & \mathbf{0}_q & \mathbf{0}_{q\times p} & \mathbf{0}_{q\times q} \end{pmatrix}.$$

Then we have

$$
\begin{aligned}
&|\mathbf{A}-\mathbf{B}[-(\lambda+4)\mathbf{I}_q]^{-1}\mathbf{C}| \\
=&\begin{vmatrix}
1-\frac{4q}{\lambda+4} & 0 & -2 & -3\mathbf{1}_p^\top & (\frac{12}{\lambda+4}-3)\mathbf{1}_q^\top \\
-\frac{3q}{\lambda+4} & 1 & 0 & \mathbf{0}_p^\top & (\frac{9}{\lambda+4})\mathbf{1}_q^\top \\
\frac{2q}{\lambda+4} & 0 & -\lambda & \mathbf{0}_p^\top & (-\frac{6}{\lambda+4})\mathbf{1}_q^\top \\
\mathbf{0}_p & \mathbf{1}_p & \mathbf{0}_p & -\lambda\mathbf{I}_p & \mathbf{0}_{p\times q} \\
\frac{-3}{\lambda+4}\mathbf{1}_q & \mathbf{1}_q & \mathbf{0}_q & \mathbf{0}_{q\times p} & (-\lambda+\frac{9}{\lambda+4})\mathbf{I}_q
\end{vmatrix} \\
=&\begin{vmatrix}
1-\frac{4q}{\lambda+4} & -\frac{3p}{\lambda} & -2 & -3\mathbf{1}_p^\top & (\frac{12}{\lambda+4}-3)\mathbf{1}_q^\top \\
-\frac{3q}{\lambda+4} & 1 & 0 & \mathbf{0}_p^\top & (\frac{9}{\lambda+4})\mathbf{1}_q^\top \\
\frac{2q}{\lambda+4} & 0 & -\lambda & \mathbf{0}_p^\top & (-\frac{6}{\lambda+4})\mathbf{1}_q^\top \\
\mathbf{0}_p & \mathbf{0}_p & \mathbf{0}_p & -\lambda\mathbf{I}_p & \mathbf{0}_{p\times q} \\
\frac{-3}{\lambda+4}\mathbf{1}_q & \mathbf{1}_q & \mathbf{0}_q & \mathbf{0}_{q\times p} & (-\lambda+\frac{9}{\lambda+4})\mathbf{I}_q
\end{vmatrix} \\
=&(-\lambda)^p\begin{vmatrix}
1-\frac{4q}{\lambda+4} & -\frac{3p}{\lambda} & -2 & (\frac{12}{\lambda+4}-3)\mathbf{1}_q^\top \\
-\frac{3q}{\lambda+4} & 1 & 0 & (\frac{9}{\lambda+4})\mathbf{1}_q^\top \\
\frac{2q}{\lambda+4} & 0 & -\lambda & (-\frac{6}{\lambda+4})\mathbf{1}_q^\top \\
-\frac{3}{\lambda+4}\mathbf{1}_q & \mathbf{1}_q & \mathbf{0}_q & (-\lambda+\frac{9}{\lambda+4})\mathbf{I}_q
\end{vmatrix} \\
=&(-\lambda)^p\begin{vmatrix}
1-\frac{4q}{\lambda+4}-(\frac{12}{\lambda+4}-3)\frac{3q}{\lambda^2+4\lambda-9} & -\frac{3p}{\lambda}+(\frac{12}{\lambda+4}-3)(\frac{\lambda+4}{\lambda^2+4\lambda-9})q & -2 & (\frac{12}{\lambda+4}-3)\mathbf{1}_q^\top \\
-\frac{3q}{\lambda+4}-\frac{9}{\lambda+4}\cdot\frac{3q}{\lambda^2+4\lambda-9} & 1+\frac{9q}{\lambda^2+4\lambda-9} & 0 & (\frac{9}{\lambda+4})\mathbf{1}_q^\top \\
\frac{2q}{\lambda+4}+\frac{6}{\lambda+4}\cdot\frac{3q}{\lambda^2+4\lambda-9} & -\frac{6q}{\lambda^2+4\lambda-9} & -\lambda & (-\frac{6}{\lambda+4})\mathbf{1}_q^\top \\
\mathbf{0}_q & \mathbf{0}_q & \mathbf{0}_q & (-\lambda+\frac{9}{\lambda+4})\mathbf{1}_q
\end{vmatrix} \\
=&(-\lambda)^p(\frac{\lambda^2+4\lambda-9}{\lambda+4})^q(-1)^q\begin{vmatrix}
1-\frac{4q}{\lambda+4}+\frac{3\lambda}{\lambda+4}\cdot\frac{3q}{\lambda^2+4\lambda-9} & -\frac{3p}{\lambda}-\frac{3q\lambda}{\lambda^2+4\lambda-9} & -2 \\
-\frac{3q}{\lambda+4}-\frac{27q}{(\lambda+4)(\lambda^2+4\lambda-9)} & 1+\frac{9q}{\lambda^2+4\lambda-9} & 0 \\
\frac{2q}{\lambda+4}+\frac{18q}{(\lambda+4)(\lambda^2+4\lambda-9)} & -\frac{6q}{\lambda^2+4\lambda-9} & -\lambda
\end{vmatrix} \\
=&(-1)^{p+q+1}\lambda^{p+1}(\lambda^2+4\lambda-9)^{q-1}(\lambda+4)^{-q}\cdot\left[\lambda^2+(4-4q)\lambda-(9pq+9q^2+9-14q)\right].
\end{aligned}
$$

Thus

$$
\begin{aligned}
&|\varepsilon(H_{p,q})-\lambda\mathbf{I}_n| \\
=&\begin{vmatrix}
1 & 0 & -2 & -3\mathbf{1}_p^\top & -3\mathbf{1}_q^\top & -4\mathbf{1}_q^\top \\
0 & 1 & 0 & \mathbf{0}_p^\top & \mathbf{0}_q^\top & -3\mathbf{1}_q^\top \\
0 & 0 & -\lambda & \mathbf{0}_p^\top & \mathbf{0}_q^\top & 2\mathbf{1}_q^\top \\
\mathbf{0}_p & \mathbf{0}_p & \mathbf{0}_p & -\lambda\mathbf{I}_p & \mathbf{0}_{p\times q} & 3\mathbf{J}_{p\times q} \\
\mathbf{0}_q & \mathbf{0}_q & \mathbf{0}_q & \mathbf{0}_{q\times p} & -\lambda\mathbf{I}_q & 3\mathbf{J}_q-3\mathbf{I}_q \\
\mathbf{0}_q & \mathbf{0}_q & 2\mathbf{1}_q & 3\mathbf{J}_{q\times p} & 3\mathbf{J}_q-3\mathbf{I}_q & 4\mathbf{J}_q-(\lambda+4)\mathbf{I}_q
\end{vmatrix} \\
=&\begin{vmatrix}
1 & 0 & -2 & -3\mathbf{1}_p^\top & -3\mathbf{1}_q^\top & -4\mathbf{1}_q^\top \\
0 & 1 & 0 & \mathbf{0}_p^\top & \mathbf{0}_q^\top & -3\mathbf{1}_q^\top \\
0 & 0 & -\lambda & \mathbf{0}_p^\top & \mathbf{0}_q^\top & 2\mathbf{1}_q^\top \\
\mathbf{0}_p & \mathbf{1}_p & \mathbf{0}_p & -\lambda\mathbf{I}_p & \mathbf{0}_{p\times q} & \mathbf{0}_{p\times q} \\
\mathbf{0}_q & \mathbf{1}_q & \mathbf{0}_q & \mathbf{0}_{q\times p} & -\lambda\mathbf{I}_q & -3\mathbf{I}_q \\
\mathbf{1}_q & \mathbf{0}_q & \mathbf{0}_q & \mathbf{0}_{q\times p} & -3\mathbf{I}_q & -(\lambda+4)\mathbf{I}_q
\end{vmatrix}
\end{aligned}
$$

$$
\begin{aligned}
&=\begin{vmatrix}
1 & 0 & -2 & -3\mathbf{1}_p^\top & (\frac{12}{\lambda+4}-3)\mathbf{1}_q^\top & -4\mathbf{1}_q^\top \\
0 & 1 & 0 & \mathbf{0}_p^\top & \frac{9}{\lambda+4}\mathbf{1}_q^\top & -3\mathbf{1}_q^\top \\
0 & 0 & -\lambda & \mathbf{0}_p^\top & -\frac{6}{\lambda+4}\mathbf{1}_q^\top & 2\mathbf{1}_q^\top \\
\mathbf{0}_p & \mathbf{1}_p & \mathbf{0}_p & -\lambda\mathbf{I}_p & \mathbf{0}_{p\times q} & \mathbf{0}_{p\times q} \\
\mathbf{0}_q & \mathbf{1}_q & \mathbf{0}_q & \mathbf{0}_{q\times p} & (-\lambda+\frac{9}{\lambda+4})\mathbf{I}_q & -3\mathbf{I}_q \\
\mathbf{1}_q & \mathbf{0}_q & \mathbf{0}_q & \mathbf{0}_{q\times p} & \mathbf{0}_{q\times q} & -(\lambda+4)\mathbf{I}_q
\end{vmatrix} \\
&=\begin{vmatrix}
\mathbf{A} & \mathbf{B} \\
\mathbf{C} & -(\lambda+4)\mathbf{I}_q
\end{vmatrix} \\
&=|-(\lambda+4)\mathbf{I}_q|\cdot|\mathbf{A}-\mathbf{B}[-(\lambda+4)\mathbf{I}_q]^{-1}\mathbf{C}| \qquad \text{(by Lemma 3.1)} \\
&=(-1)^{p+1}\lambda^{p+1}(\lambda^2+4\lambda-9)^{q-1}\big[\lambda^2+(4-4q)\lambda-(9pq+9q^2+9-14q)\big].
\end{aligned}
$$

Note that the ε-polynomial of $H_{p,q}$ is $|\lambda\mathbf{I}_n-\varepsilon(H_{p,q})|=|-[\varepsilon(H_{p,q})-\lambda\mathbf{I}_n]|=(-1)^n|\varepsilon(H_{p,q})-\lambda\mathbf{I}_n|$. The result follows easily. □

Lemma 3.3. *Let ε_n be the least ε-eigenvalue of $H_{p,q}$, where $n=p+2q+1$. Then we have $\varepsilon_n\le -2-\sqrt{13}$, with equality if and only if one of the following conditions holds:*

(i) $p=0$ *and* $2\le q\le 4$;
(ii) $p=1$ *and* $q=2$ *or* 3;
(iii) $p=2$ *and* $q=2$.

Proof. In view of Lemma 3.2, it is easy to see that the distinct ε-eigenvalues of $H_{p,q}$ are $0,-2\pm\sqrt{13}$ and $\frac{1}{2}\Big[(4q-4)\pm\sqrt{(4-4q)^2+4(9pq+9q^2+9-14q)}\Big]$. It follows that $\varepsilon_n\le -2-\sqrt{13}$. And we have

$$\varepsilon_n\in\Big\{-2-\sqrt{13},\ \frac{1}{2}\Big[(4q-4)-\sqrt{(4-4q)^2+4(9pq+9q^2+9-14q)}\Big]\Big\}.$$

By simplifying the following inequality

$$\frac{1}{2}\Big[(4q-4)-\sqrt{(4-4q)^2+4(9pq+9q^2+9-14q)}\ge -2-\sqrt{13},$$

we obtain

$$4q(9p+9q-4\sqrt{13}-22)\le 0. \tag{3.2}$$

Since $q\ge 2$, we have $9p+9q-4\sqrt{13}-22\le 0$ if and only if $\varepsilon_n=-2-\sqrt{13}$. Note that $p\ge 0$ and $q\ge 2$, then $9p+9q-4\sqrt{13}-22\le 0$ implies $2\le q\le 4$. We distinguish the following four cases.

Case 1. $p=0$.

In this case, it is easy to see that $9p+9q-4\sqrt{13}-22\le 0$ for $2\le q\le 4$.

Case 2. $p=1$.

In this case, we have $9p+9q-4\sqrt{13}-22\le 0$ if and only if $q=2$ or 3.

Case 3. $p=2$.

In this case, it is easy to see that $9p+9q-4\sqrt{13}-22\le 0$ if and only if $q=2$.

Case 4. $p\ge 3$.

In this case, by calculation, we have $9p+9q-4\sqrt{13}-22>0$ for $q\ge 2$.
This completes the proof. □

Theorem 3.4. *Let T be a tree with $n\ge 3$ vertices. Then $\varepsilon_n(T)\in[-2-\sqrt{13},-2\sqrt{2})$ if and only if one of the following conditions holds:*

(i) $T = P_4$;
(ii) $T = D^{0,1}_{n,3}$;
(iii) $T = H_{p,q}$ *for* $p = 0$ *and* $2 \le q \le 4$;
(iv) $T = H_{p,q}$ *for* $p = 1$ *and* $q = 2$ *or* 3;
(v) $T = H_{p,q}$ *for* $p = 2$ *and* $q = 2$.

Proof. Suppose $\varepsilon_n(T) \in [-2-\sqrt{13}, -2\sqrt{2})$. Let d be the diameter of T. If $d = 2$, then $T = S_n$, by Lemma 2.5, $\varepsilon_n(T) = -2$, a contradiction. If $d = 5$, then $\varepsilon(P_6)$ is a principle submatrix of $\varepsilon(T)$. By a direct calculation and Lemma 1.3, we have $\varepsilon_n(T) \le \varepsilon_6(P_6) \approx -8.0902 < -2-\sqrt{13}$, a contradiction. If $d \ge 6$, then by Lemma 1.6, we have $\varepsilon_n(T) \le -6 < -2-\sqrt{13}$, a contradiction. Thus $d = 3$ or 4.

First suppose that $d = 3$. Then T is some $D^{a,b}_{n,3}$ with $b \ge a \ge 0$. If $a = b = 0$, then $T = D^{a,b}_{n,3} = P_4$. By calculating, we have $\varepsilon_4(P_4) = -4 \in [-2-\sqrt{13}, -2\sqrt{2})$. This is (i). If $a = 0, b = 1$, then $T = D^{0,1}_{n,3}$. By calculating, we have $\varepsilon_5(D^{0,1}_{n,3}) \approx -5.3752 \in [-2-\sqrt{13}, -2\sqrt{2})$. This is (ii). Otherwise, $D^{1,1}_{n,3}$ or $D^{0,2}_{n,3}$ is an induced subgraph of T. Note that $\varepsilon(D^{1,1}_{n,3})$ or $\varepsilon(D^{0,2}_{n,3})$ is a principle submatrix of $\varepsilon(T)$. By a direct calculation, we obtain $\varepsilon_6(D^{1,1}_{n,3}) \approx -7.1231$ and $\varepsilon_6(D^{0,2}_{n,3}) \approx -6.4694$, and by Lemma 1.3, we have $\varepsilon_n(T) \le \varepsilon_6(D^{1,1}_{n,3}) < -2-\sqrt{13}$ or $\varepsilon_n(T) \le \varepsilon_6(D^{0,2}_{n,3}) < -2-\sqrt{13}$, a contradiction.

Next suppose that $d = 4$. Then $D^{0,1}_{n,4}$ is an induced subgraph of T or $T = H_{p,q}$ for some $p \ge 0$ and $q \ge 2$. In the former case, $\varepsilon(D^{0,1}_{n,4})$ is a principle submatrix of $\varepsilon(T)$. By a direct calculation and Lemma 1.3, we have $\varepsilon_n(T) \le \varepsilon_6(D^{0,1}_{n,4}) \approx -7.5621 < -2-\sqrt{13}$, a contradiction. In the latter case, (iii), (iv) and (v) follow from Lemma 3.3.

This completes the proof. $\square$

4. Concluding remarks

Remark 1. Theorem 2.10 characterizes trees with maximum ε-spectral radius among n-vertex trees with fixed odd diameter. For trees with maximum ε-spectral radius among n-vertex trees with fixed even diameter, it seems that it can not be determined similarly as the proof of Theorem 2.10 and an interesting research problem is put forward as follows.

Problem 4.1. *Characterize the trees with maximum ε-spectral radius among n-vertex trees with fixed even diameter.*

Declaration of competing interest

The authors declare that they have no conflicts of interest.

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