ON MINIMAL ENERGIES OF NON–STARLIKE TREES WITH GIVEN NUMBER OF PENDENT VERTICES

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Abstract

The energy of a graph is defined as the sum of the absolute values of its eigenvalues. A tree is non-starlike if it has at least two vertices of degree greater than two. For \(4 \leq k \leq n - 2\), we determine, in the class of non-starlike trees with \(n\) vertices and \(k\) pendent vertices, the trees with minimal energy if \(n \geq 6\) and the trees with second–minimal energy if \(n \geq 8\).

1. INTRODUCTION

Let \(G\) be a graph with \(n\) vertices, and and let \(\lambda_1, \lambda_2, \ldots, \lambda_n\) be its eigenvalues [1]. Then the energy of \(G\) is defined as [2, 3]

\[
E(G) = \sum_{i=1}^{n} |\lambda_i|.
\]

For a survey of the mathematical properties and chemical applications of \(E(G)\), see the recent reviews [4, 5].

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Gutman [6] determined the $n$-vertex trees with minimal, second-minimal, third-minimal, and fourth-minimal energy, as well as the $n$-vertex trees with maximal and second-maximal energy. Recently, these results were extended in [7, 8]. Minimal or maximal energies have been determined within various subclasses of trees, see [9–15]. Related results on the energy of trees may be found in [16, 17].

Let $G$ be an acyclic graph with $n$ vertices. Then $E(G)$ can be expressed as the Coulson integral formula [3]

$$E(G) = \frac{2}{\pi} \int_{0}^{\infty} \log \left[ \sum_{i=0}^{[n/2]} m(G, i) x^{2i} \right] dx$$

where $m(G, i)$ denotes the number of $i$-matchings in $G$, and in convention, $m(G, 0) = 1$, and it is obvious that $m(G, i) = 0$ for $i > [n/2]$. This formula led Gutman [6] to introduce a quasi-order relation over the class of all acyclic graphs: if $G_1$ and $G_2$ are two acyclic graphs, then

$$G_1 \succeq G_2 \iff m(G_1, i) \geq m(G_2, i) \text{ for } i \geq 1.$$

If $G_1 \succeq G_2$ and there exists a $j$ such that $m(G_1, j) > m(G_2, j)$, then we write $G_1 \succ G_2$.

For acyclic graphs $G_1$ and $G_2$,

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2).$$

A tree in which exactly one vertex has degree (i.e., number of first neighbors) greater than two is said to be starlike. Otherwise, it is non-starlike.

The starlike trees (with a given number of vertices), extremal with respect to the relation “$\succeq$”, have been characterized in [18], from which properties on the ordering of starlike trees respect to their energies can be deduced.

A pendent vertex is a vertex of degree one. Obviously, the number of pendent vertices in a non-starlike tree with $n$ vertices is at least 4 and at most $n - 2$. Let $T_{n,k}$ be the class of non-starlike trees in with $n$ vertices and $k$ pendent vertices, where $4 \leq k \leq n - 2$.

For integers $n$ and $k$ with $4 \leq k \leq n - 2$, let $P_{n,k}^{r,s}(a, b)$ be the tree formed from the path $P_{n-k+2}$ whose vertices are labelled consecutively as $v_1, \ldots, v_{n-k+2}$ by attaching $a$ pendent vertices to vertex $v_r$ and $b$ pendent vertices to $v_s$, where $2 \leq r < s \leq n - k - 2$. 
\(n-k+1\), \(a, b \ge 1\) and \(a+b = k-2\). Let \(S_n(a+1, b+1) = P_{n,k}^{2,n-k+1}(a, b)\), i.e., \(S_n(a+1, b+1)\) is the tree obtained from the path with \(n-a-b-2\) vertices by attaching \(a+1\) and \(b+1\) pendent vertices to its two end vertices respectively. Let \(A_{n,k} = P_{n,k}^{2,n-k+1}(k-3, 1) = S_n(k-2, 2)\) and \(B_{n,k} = P_{n,k}^{2.4}(k-3, 1)\).

In this paper, we determine the trees in \(T_{n,k}\) with minimal energy for \(4 \le k \le n-2\) and trees in \(T_{n,k}\) with second–minimal energy for \(4 \le k \le n-2\) and \(n \ge 8\). More precisely, we show

- \(A_{n,k}\) is the unique tree with minimal energy in \(T_{n,k}\) for \(4 \le k \le n-2\);
- \(S_n(n-5, 3)\) is the unique tree with second–minimal energy in \(T_{n,n-2}\), \(P_{n,n-3}^{2.3}(n-6, 1)\) if \(n = 8\), \(P_{n,n-3}^{2.4}(n-7, 2)\) if \(n \ge 9\) is the unique tree with second–minimal energy in \(T_{n,n-3}\), and \(B_{n,k}\) is the unique tree with second–minimal energy in \(T_{n,k}\) for \(4 \le k \le n-4\).

2. PRELIMINARIES

For convenience, let \(m(G, i) = 0\) for a graph \(G\) if \(i < 0\). Let \(T\) be a tree with vertex set \(V(T)\). For \(u \in V(T)\), \(d_u\) denotes the degree of \(u\) in \(T\).

Lemma 1. [3] Let \(T\) be a tree, and let \(uw\) be an edge of \(T\). Then

\[m(T, i) = m(T - uv, i) + m(T - u - v, i - 1).\]

Moreover, if \(u\) is a pendent vertex, then

\[m(T, i) = m(T - u, i) + m(T - u - v, i - 1).\]

Let \(T\) be a tree of the form in Fig. 1, where \(T_1\) and \(T_2\) are subtrees of \(T\) with at least two vertices, \(u_l \in V(T_1)\), \(u_{l+1} \in V(T_2)\) and \(l \ge 3\). Let \(T'\) be the tree formed from \(T\) by deleting edge \(u_l u\) and adding edge \(u_2 u\) for every neighbor \(u\) of \(u_l\) in \(V(T_1)\).

We say that \(T'\) is obtained from \(T\) by Operation I.

Fig. 1. Trees \(T\) and \(T'\) in Operation I.
Let $T$ be a tree of diameter at least 3 which is of the form in Fig. 2, where $u_1$ and $w_1$ are end vertices of a diametrical path, $l, q \geq 2$, $T_1$ is a tree with $v \in V(T_1)$. Let $T'$ be the tree formed from $T$ by deleting edge $u_1 w_1$ and adding edge $vu_1$ for the pendent neighbor $u_i$ of $u$ with $i = 2, \ldots, l$. We say that $T'$ is obtained from $T$ by Operation II.

![Diagram of trees T and T']

**Fig. 2.** Trees $T$ and $T'$ in Operation II.

**Lemma 2.** [14] If $T'$ is obtained from $T$ by Operation I or II, then $T \succ T'$.

**Lemma 3.** [13] For integers $i$ and $l$ with $2 \leq i \leq \lfloor \frac{l}{2} \rfloor$, $i \neq 3$, and $l \geq 6$, $P_i \cup P_{l-i} \succ P_3 \cup P_{l-3} \succ P_1 \cup P_{l-1}$.

**Lemma 4.** [6] Let $T$ be a tree on $n$ vertices. If $T$ is different from the path $P_n$ and the star $S_n$, then $P_n \succ T \succ S_n$.

**Lemma 5.** For $n \geq 9$, $E(P_{n,n-3}^{2,3}(n-6,1)) > E(P_{n,n-3}^{2,4}(n-7,2))$.

**Proof.** Let $T_1 = P_{n,n-3}^{2,3}(n-6,1)$ and $T_2 = P_{n,n-3}^{2,4}(n-7,2)$. It can be easily seen that

- $m(T_1, 2) = 3n - 13$, $m(T_1, 3) = n - 5$, $m(T_1, i) = 0$ for $i \geq 4$,
- $m(T_2, 2) = 4n - 21$, $m(T_2, i) = 0$ for $i \geq 3$.

Note that the eigenvalues of a tree $T$ with $n$ vertices are the $n$ roots of its characteristic polynomial, which may be written as [3]

$$
\phi(T, x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i m(T, i) x^{n-2i}.
$$

Thus,

- $\phi(T_1, x) = x^{n-6} [x^6 - (n-1)x^4 + (3n-13)x^2 - (n-5)]$,
- $\phi(T_2, x) = x^{n-4} [x^4 - (n-1)x^2 + (4n-21)]$.
Let $\sqrt{a_1}, \sqrt{a_2}, \sqrt{a_3}$ be the positive eigenvalues of $T_1$, and $\sqrt{b_1}, \sqrt{b_2}$ be the positive eigenvalues of $T_2$. Then $a_1 + a_2 + a_3 = b_1 + b_2 = n - 1$, $a_1a_2 + a_2a_3 + a_3a_1 = 3n - 13$, $a_1a_2a_3 = n - 5$ and $b_1b_2 = 4n - 21$. We have

$$\left[ \frac{E(T_1)}{2} \right]^2 = (\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3})^2$$

$$= a_1 + a_2 + a_3 + 2(\sqrt{a_1a_2} + \sqrt{a_2a_3} + \sqrt{a_3a_1})$$

$$= n - 1 + 2\sqrt{a_1a_2 + a_2a_3 + a_3a_1} + 2\sqrt{a_1a_2a_3} (\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3})$$

$$= n - 1 + 2\sqrt{3n - 13} + \sqrt{n - 5} E(T_1),$$

$$\left[ \frac{E(T_2)}{2} \right]^2 = (\sqrt{b_1} + \sqrt{b_2})^2$$

$$= b_1 + b_2 + 2\sqrt{b_1b_2} = n - 1 + 2\sqrt{4n - 21}.$$ 

Now it is easily seen that $E(T_1) > E(T_2)$ is equivalent to $n - 8 < \sqrt{n - 5} E(T_1)$, i.e., $E(T_1) > \frac{n - 8}{\sqrt{n - 5}}$, which is obviously true, because by Lemma 4, $E(T_1) > E(S_n) = 2\sqrt{n - 1} > \frac{n - 8}{\sqrt{n - 5}}$. \hfill \Box

Let $T$ be a tree. Let $l(T)$ denote the number of vertices of degree at least 3 in $T$. If $v_0v_1\ldots v_t$ is a path (of length $t$) in $T$ such that $d_{v_0} \geq 3$, $d_{v_t} = 1$ and $d_{v_i} = 2$ for $i = 2, \ldots, t - 1$, where $t \geq 1$, then it is called a pendent path of $T$. If $t = 1$, then it is a pendent edge. Let $p(T)$ be the number of pendent paths of length at least 2 in $T$.

For integers $n$ and $k$ with $3 \leq k \leq n - 2$, let $P_{n,k}^r$ be the tree formed from the path $P_{n-k+2}$ labelled as $v_1, \ldots, v_{n-k+2}$ by attaching $k - 2$ pendent vertices to vertex $v_r$, where $2 \leq r \leq \lfloor \frac{n-k+2}{2} \rfloor$.

3. RESULTS

Note that Operations I and II do not change the number of pendent paths and hence the number of pendent vertices, and that Operation II reduces the number of vertices of degree at least 3 by one. For a tree $T$ of diameter at least 3, if Operation I can not be applied to $T$ then Operation II may be applied to get a tree $T'$ and when the diameter is at least 4 and $l(T') \geq 2$, Operation II may be applied to $T'$.

Now we are ready to prove our results.
Theorem 1. For integer \( n \) and \( k \) with \( 4 \leq k \leq n - 2 \), \( A_{n,k} \) is the unique tree with minimal energy in \( T_{n,k} \).

Proof. Let \( T \in T_{n,k} \) with \( T \not\sim A_{n,k} \). We will prove that \( T \succ A_{n,k} \).

Note that \( l(T) \geq 2 \). If \( l(T) \geq 3 \), or \( l(T) = 2 \) and \( p(T) \geq 1 \), then applying Operations I and II to \( T \), and by Lemma 2, we get a tree \( T' \in T_{n,k} \) such that \( l(T') = 2 \), \( p(T') = 0 \) and \( T \succ T' \). Assume that \( l(T) = 2 \) and \( p(T) = 0 \). Then \( T \) is a tree \( S_n(a, b) \) with \( a \geq b \geq 3 \) and \( a + b = k \).

Claim. \( S_n(a, b) \succ S_n(a + 1, b - 1) \) for \( a \geq b \geq 3 \).

If \( a + b = n - 2 \), then this follows easily. Suppose that \( a + b \leq n - 3 \). By Lemma 1, we have

\[
m(S_n(a, b), i) = m(S_{n-1}(a, b - 1), i) + m(P_{n-b-1,a+1}^2, i - 1),
\]

\[
m(S_n(a + 1, b - 1), i) = m(S_{n-1}(a, b - 1), i) + m(P_{n-a-2,b}^2, i - 1).
\]

Since \( P_{n-a-2,b}^2 \) is a proper subgraph of \( P_{n-b-1,a+1}^2 \) for \( a \geq b \), we have

\[
m(P_{n-b-1,a+1}^2, i - 1) \geq m(P_{n-a-2,b}^2, i - 1)
\]

and then \( m(S_n(a, b), i) \geq m(S_n(a + 1, b - 1), i) \) for all \( i \geq 0 \) and it is strict for \( i = 2 \). This proves the Claim.

By the Claim, \( T \succ S_n(k - 2, 2) \approx A_{n,k} \). \( \square \)

It is easily checked that \( |T_{n,k}| \geq 2 \) if and only if either \( 4 \leq k \leq n - 2 \) and \( n \geq 8 \) or \( n = 7 \) and \( k = 4 \). Obviously, \( T_{7,4} = \{A_{7,4}, P_{7,4}^{2,3}(1, 1)\} \), and \( E(A_{7,4}) < E(P_{7,4}^{2,3}(1, 1)) \). Thus, for the graphs with second–minimal energy in \( T_{n,k} \) with \( 4 \leq k \leq n - 2 \), we may assume that \( n \geq 8 \).

Theorem 2. For integers \( n \) and \( k \) with \( 4 \leq k \leq n - 2 \) and \( n \geq 8 \), we have

(i) \( S_n(n - 5, 3) \) is the unique tree with the second–minimal energy in \( T_{n,n-2} \);

(ii) \( P_{n,n-3}^{2,3}(n - 6, 1) \) if \( n = 8 \), \( P_{n,n-3}^{2,4}(n - 7, 2) \) if \( n \geq 9 \) is the unique tree with second–minimal energy in \( T_{n,n-3} \);

(iii) If \( 4 \leq k \leq n - 4 \), then \( B_{n,k} \) is the unique tree with second–minimal energy in \( T_{n,k} \).
Proof. Any tree $T \in \mathbb{T}_{n,n-2}$ is of the form $S_n(n-2-c, c)$ with $2 \leq c \leq \frac{n-2}{2}$. By direct check or by the Claim in the proof of Theorem 1, if $T \not\cong S_n(n-5, 3), S_n(n-4, 2)$, then $T \succ S_n(n-5, 3) \succ S_n(n-4, 2)$. Thus $S_n(n-5, 3)$ is the unique tree with the second-minimal energy in $\mathbb{T}_{n,n-2}$. This proves (i).

Let $T \in \mathbb{T}_{n,n-3}$ with $T \not\cong A_{n,n-3}, P_{n,n-3}^2(n-7, 2), P_{n,n-3}^2(n-6, 1)$. Then $l(T) \geq 2$ and $T$ must be of the form obtained from the path $P_5 = v_1v_2v_3v_4v_5$ by attaching $x, y$ and $z$ pendant vertices to vertices $v_2, v_3$ and $v_4$, respectively, where $x+y+z = n-5$, $x \geq z$, $(x, y, z) \not= (n-6, 0, 1), (n-7, 0, 2), (n-6, 1, 0)$. If $y = 0$, then $n \geq 9$ and by the argument of Theorem 1, $T \succ P_{n,n-3}^2(n-7, 2)$. If $y \geq 1$, then applying Operation II and by Lemma 2, we may easily have $T \succ P_{n,n-3}^2(n-6, 1)$. By Lemma 5, we have the result in (ii).

In the following we prove (iii). Let $T \in \mathbb{T}_{n,k}$ with $T \not\cong A_{n,k}, B_{n,k}$, where $4 \leq k \leq n-4$.

Note that $l(T) \geq 2$. If $l(T) \geq 3$, then by making use of Operation II and if necessary Operation I to $T$, and by Lemma 2, we get a tree $T' \in \mathbb{T}_{n,k}$ such that $l(T') = 2$ and $T \succ T'$. By the definition of Operation II, $T' \not\cong A_{n,k}$. Assume that $l(T) = 2$ and $T \not\cong A_{n,k}$. Let $u, v$ be the two vertices in $T$ with $d_u \geq d_v \geq 3$.

Suppose that $d_u \geq d_v \geq 4$. Applying Operation I, and by Lemma 2, we find $T \succeq S_n(d_u+1, d_v-1)$. By the proof of Theorem 1, we have $T \succeq S_n(k-3, 3)$.

Claim 1. $S_n(a, 3) \succ B_{n,a+3}$, where $a \geq 3$.

Let $d = n-a-3$. Since $m(P_n, i) = \binom{n-i-1}{i}$, we have

\[
m(S_n(3, 3), i) = 3 \cdot 3 \cdot \binom{d-2-i+2}{i-2} + 3 \cdot \binom{d-1-i+1}{i-1} + 3 \cdot \binom{d-1-i+1}{i-1} + \binom{d-i}{i} = 9(d-i) + 6(d-i) + \binom{d-i}{i},
\]

\[
m(B_{n,3+3}, i) = 4 \cdot 2 \cdot \binom{d-2-i+2}{i-2} + 4 \cdot \binom{d-1-i+1}{i-1} + \binom{d+1-i}{i} + \binom{d-2-i+1}{i-1}
+ \binom{d-2-i+2}{i-2}
= 9(d-i) + 4(d-i) + \binom{d-i+1}{i} + \binom{d-i-1}{i-1},
\]

and thus

\[m(S_n(3, 3), i) - m(B_{n,3+3}, i) = \binom{d-i}{i-1} - \binom{d-i-1}{i-1}.\]

It follows that $m(S_n(3, 3), i) \geq m(B_{n,3+3}, i)$ for all $i \geq 0$ and it is strict for $i = 2$. 

Thus the claim is true for $a = 3$. Suppose that $a \geq 4$ and it is true for $a - 1$. By Lemma 1 we have
\[
m(S_n(a, 3), i) = m(S_{n-1}(a - 1, 3), i) + m(P^2_{d+2, 4}, i - 1),
\]
\[
m(B_{n,a+3}, i) = m(B_{n-1,a+2}, i) + m(P^2_{d+1,3}, i - 1).
\]

Since $P^2_{d+1,3}$ is a proper subgraph of $P^2_{d+2,4}$, we have $m(S_n(a, 3), i) \geq m(B_{n,a+3}, i)$ for all $i \geq 1$ and it is strict for $i = 2$. Now Claim 1 follows. By Claim 1, $T \geq S_n(k - 3, 3) \succ B_{n,k}$.

Now suppose that $d_u \geq d_v = 3$. If $p(T) \geq 2$, then applying Operation I to $T$ we may get a tree $T'$ such that $T'$ with $p(T') = 1$, and by Lemma 2, $T \succ T'$. Suppose that $T' \not\succ B_{n,k}$. Then we have either $T' \cong P^2_{n,k}(k - 3, 1)$ with $3 \leq s \leq n - k$ and $s \neq 4$, or $k \geq 4$ and $T' \cong P^2_{n,k}(1, k - 3)$ with $3 \leq s \leq n - k$.

Suppose that $3 \leq s \leq c$ and $s \neq 4$. We have by Lemma 3 that $P_{s-1} \cup P_{c+2-s} \succ P_3 \cup P_{c-2}$, and thus by Lemma 1, $P^s_{c+3,3} \succ P^4_{c+3,3}$. If $s = 3$, then by Lemmas 1 and 4, $P^2_{c+4,4}(1, 1) \succ P^2_{c+4,4}(1, 1) \cong B_{c+4,4}$. If $5 \leq s \leq c$, then by Lemma 3, we have $P_{s-3} \cup P_{c+2-s} \succ P_1 \cup P_{c-2}$, and by Lemma 1, we have $P_{c+1,3}^{(s-2)} \succ P^2_{c+1,3}$, and thus $P^2_{c+4,4}(1, 1) \succ P^2_{c+4,4}(1, 1) \cong B_{c+4,4}$. We have shown that $P^2_{c+4,4}(1, 1) \succ B_{c+4,4}$ for $3 \leq s \leq c$ and $s \neq 4$, which will be the starting point of Claims 2 and 3.

Claim 2. $P^2_{c+3,x+3}(x, 1) \succ B_{c+x+3,x+3}$, where $x \geq 1$, $3 \leq s \leq c$, $s \neq 4$.

If $x = 1$, then the claim follows. Suppose that $x \geq 2$ and it is true for $x - 1$. By Lemma 1,
\[
m(P^2_{c+3,x+3}(x, 1), i) = m(P^2_{c+x+2,x+2}(x - 1, 1), i)
\]
\[+ m(P^2_{c+x+3,x+3}(x, 1) - v_1 - v_2, i - 1),
\]
\[
m(B_{c+x+3,x+3}, i) = m(B_{c+x+2,x+2}, i) + m(xP_1 \cup P^2_{c+1,3}, i - 1).
\]

If $s \neq 3$, then $c \geq 5$, $P^s_{c+1,3} \succ P^2_{c+1,3}$, and thus $P^2_{c+x+3,x+3}(x, 1) - v_1 - v_2 = xP_1 \cup P^2_{c+1,3} \succ xP_1 \cup P^2_{c+1,3}$. If $s = 3$, then $c \geq 3$, $P_{c+1} \succ P^2_{c+1,3}$; and thus $P^2_{c+x+3,x+3}(x, 1) - v_1 - v_2 = xP_1 \cup P^2_{c+1,3} \succ xP_1 \cup P^2_{c+1,3}$. Thus Claim 2 follows.

Claim 3. $P^2_{c+x+3,x+3}(1, x) \succ B_{c+x+3,x+3}$, where $x \geq 2$ and $3 \leq s \leq c$.

If $x = 1$ and $s \neq 4$, then $P^2_{c+x+3,x+3}(1, x) \succ B_{c+x+3,x+3}$. If $x = 1$ and $s = 4$, then
Suppose that $x \geq 2$. By Lemma 1, we have

$$m(P_{c+x+3,x+3}^{2,s}(1,x), i) = m(P_{c+x+2,x+2}^{2,s}(1,x-1), i) + m((x-1)P_1 \cup P_{s,3}^{2} \cup P_{c+2-s}^{2}, i-1),$$

$$m(B_{c+x+3,x+3}, i) = m(B_{c+x+2,x+2}, i) + m(xP_1 \cup P_{c+1,3}^{2}, i-1).$$

Obviously, $m((x-1)P_1 \cup P_{s,3}^{2} \cup P_{c+2-s}^{2}, i-1) \geq m(xP_1 \cup P_{c+1,3}^{2}, i-1)$ and then $m(P_{c+x+3,x+3}^{2,s}(1,x), i) \geq m(B_{c+x+3,x+3}, i)$ for all $i \geq 1$ and it is strict for $i = 2$. Thus Claim 3 follows.

Setting $x = k - 3$ and $c = n - k$ in Claims 2 and 3, we have $T \succ T' \succ B_{n,k}$. □

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**References**


