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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 $4 \le k \le n-2$, we determine, in the class of non-starlike trees with n vertices and k pendent vertices, the trees with minimal energy if $n \ge 6$ and the trees with second–minimal energy if $n \ge 8$.

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]

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \log \left[\sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} m(G,i) x^{2i} \right] dx$$

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 $i > \lfloor \frac{n}{2} \rfloor$. 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

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

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 $\mathbb{T}_{n,k}$ 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 $2 \leq r < s \leq$

$n-k+1$, $a,b \geq 1$ 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 $\mathbb{T}_{n,k}$ with minimal energy for $4 \leq k \leq n-2$ and trees in $\mathbb{T}_{n,k}$ with second–minimal energy for $4 \leq k \leq n-2$ and $n \geq 8$. More precisely, we show

- $A_{n,k}$ is the unique tree with minimal energy in $\mathbb{T}_{n,k}$ for $4 \leq k \leq n-2$;
- $S_n(n-5,3)$ is the unique tree with second–minimal energy in $\mathbb{T}_{n,n-2}$, $P_{n,n-3}^{2,3}(n-6,1)$ if $n=8$, $P_{n,n-3}^{2,4}(n-7,2)$ if $n \geq 9$ is the unique tree with second–minimal energy in $\mathbb{T}_{n,n-3}$, and $B_{n,k}$ is the unique tree with second–minimal energy in $\mathbb{T}_{n,k}$ for $4 \leq k \leq n-4$.

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 uv 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 $l \geq 3$. 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.

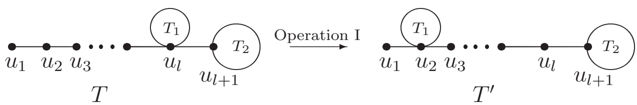

Fig. 1. Trees T and T' in Operation I.

Let T be a tree of 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 uu_i and adding edge vu_i for the pendent neighbor u_i of u with $i = 2, \ldots, l$. We say that T' is obtained from T by Operation II.

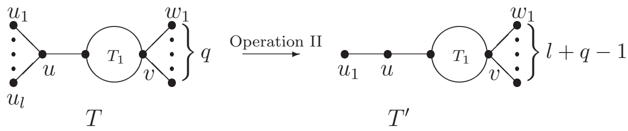

Fig. 2. Trees T and T' in Operation II.

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 $n \geq 9$, $E\left(P^{2,3}_{n,n-3}(n-6,1)\right) > E\left(P^{2,4}_{n,n-3}(n-7,2)\right)$.*

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

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

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,

$$\phi(T_1,x) = x^{n-6}\left[x^6 - (n-1)x^4 + (3n-13)x^2 - (n-5)\right],$$
$$\phi(T_2,x) = x^{n-4}\left[x^4 - (n-1)x^2 + (4n-21)\right].$$

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 $a_1 + a_2 + a_3 = b_1 + b_2 = n - 1$, $a_1 a_2 + a_2 a_3 + a_3 a_1 = 3n - 13$, $a_1 a_2 a_3 = n - 5$ and $b_1 b_2 = 4n - 21$. We have

$$
\begin{aligned}
\left[\frac{E(T_1)}{2}\right]^2 &= (\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3})^2 \\
&= a_1 + a_2 + a_3 + 2\left(\sqrt{a_1 a_2} + \sqrt{a_2 a_3} + \sqrt{a_3 a_1}\right) \\
&= n - 1 + 2\sqrt{a_1 a_2 + a_2 a_3 + a_3 a_1 + 2\sqrt{a_1 a_2 a_3}\left(\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3}\right)} \\
&= n - 1 + 2\sqrt{3n - 13 + \sqrt{n-5}\, E(T_1)}, \\
\left[\frac{E(T_2)}{2}\right]^2 &= \left(\sqrt{b_1} + \sqrt{b_2}\right)^2 \\
&= b_1 + b_2 + 2\sqrt{b_1 b_2} = n - 1 + 2\sqrt{4n - 21}.
\end{aligned}
$$

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, $E(T_1) > E(S_n) = 2\sqrt{n-1} > \frac{n-8}{\sqrt{n-5}}$. $\square$

Let T be a tree. Let $l(T)$ denote the number of vertices of degree at least 3 in T. If $v_0 v_1 \ldots v_t$ 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 $P^r_{n,k}$ 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 $\mathbb{T}_{n,k}$.*

Proof. Let $T \in \mathbb{T}_{n,k}$ with $T \ncong A_{n,k}$. 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 $T' \in \mathbb{T}_{n,k}$ 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

$$\begin{aligned} m\left(S_n(a,b), i\right) &= m\left(S_{n-1}(a, b-1), i\right) + m\left(P^2_{n-b-1,a+1}, i-1\right), \\ m\left(S_n(a+1,b-1), i\right) &= m\left(S_{n-1}(a, b-1), i\right) + m\left(P^2_{n-a-2,b}, i-1\right). \end{aligned}$$

Since $P^2_{n-a-2,b}$ is a proper subgraph of $P^2_{n-b-1,a+1}$ for $a \geq b$, we have

$$m\left(P^2_{n-b-1,a+1}, i-1\right) \geq m\left(P^2_{n-a-2,b}, i-1\right)$$

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

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

It is easily checked that $|\mathbb{T}_{n,k}| \geq 2$ if and only if either $4 \leq k \leq n-2$ and $n \geq 8$ or $n = 7$ and $k = 4$. Obviously, $\mathbb{T}_{7,4} = \{A_{7,4}, P^{2,3}_{7,4}(1,1)\}$, and $E\left(A_{7,4}\right) < E\left(P^{2,3}_{7,4}(1,1)\right)$. Thus, for the graphs with second–minimal energy in $\mathbb{T}_{n,k}$ 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 $\mathbb{T}_{n,n-2}$;

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

(iii) If $4 \leq k \leq n-4$, then $B_{n,k}$ is the unique tree with second–minimal energy in $\mathbb{T}_{n,k}$.

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 $T \ncong S_n(n-5,3), S_n(n-4,2)$, 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 $T \ncong A_{n,n-3}$, $P^{2,4}_{n,n-3}(n-7,2)$, $P^{2,3}_{n,n-3}(n-6,1)$. 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 pendent vertices to vertices v_2, v_3 and v_4, respectively, where $x+y+z = n-5$, $x \geq z$, $(x,y,z) \neq (n-6,0,1)$, $(n-7,0,2)$, $(n-6,1,0)$. If $y = 0$, then $n \geq 9$ and by the argument of Theorem 1, $T \succ P^{2,4}_{n,n-3}(n-7,2)$. If $y \geq 1$, then applying Operation II and by Lemma 2, we may easily have $T \succ P^{2,3}_{n,n-3}(n-6,1)$. By Lemma 5, we have the result in (ii).

In the following we prove (iii). Let $T \in \mathbb{T}_{n,k}$ with $T \ncong A_{n,k}$, $B_{n,k}$, 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, $T' \ncong A_{n,k}$. Assume that $l(T) = 2$ and $T \ncong A_{n,k}$. 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 $m(P_n,i) = \binom{n-i}{i}$, we have

$$\begin{aligned} m\left(S_n(3,3),i\right) &= 3\cdot 3\cdot \tbinom{d-2-i+2}{i-2} + 3\cdot \tbinom{d-1-i+1}{i-1} + 3\cdot \tbinom{d-1-i+1}{i-1} + \tbinom{d-i}{i} \\ &= 9\tbinom{d-i}{i-2} + 6\tbinom{d-i}{i-1} + \tbinom{d-i}{i}, \end{aligned}$$

$$\begin{aligned} m\left(B_{n,3+3},i\right) &= 4\cdot 2\cdot \tbinom{d-2-i+2}{i-2} + 4\cdot \tbinom{d-1-i+1}{i-1} + \tbinom{d+1-i}{i} + \tbinom{d-2-i+1}{i-1} \\ &\quad + \tbinom{d-2-i+2}{i-2} \\ &= 9\tbinom{d-i}{i-2} + 4\tbinom{d-i}{i-1} + \tbinom{d-i+1}{i} + \tbinom{d-i-1}{i-1}, \end{aligned}$$

and thus

$$m\left(S_n(3,3),i\right) - m\left(B_{n,3+3},i\right) = \tbinom{d-i}{i-1} - \tbinom{d-i-1}{i-1}.$$

It follows that $m\left(S_n(3,3),i\right) \geq m\left(B_{n,3+3},i\right)$ 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

$$\begin{aligned} m\left(S_n(a,3),i\right) &= m\left(S_{n-1}(a-1,3),i\right) + m\left(P^2_{d+2,4}, i-1\right), \\ m\left(B_{n,a+3},i\right) &= m\left(B_{n-1,a+2},i\right) + m\left(P^2_{d+1,3}, i-1\right). \end{aligned}$$

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

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 $T' \ncong B_{n,k}$. Then we have either $T' \cong P^{2,s}_{n,k}(k-3,1)$ with $3 \leq s \leq n-k$ and $s \neq 4$, or $k \geq 4$ and $T' \cong P^{2,s}_{n,k}(1,k-3)$ 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, $P^{2,s}_{c+4,4}(1,1) \succ P^{2,4}_{c+4,4}(1,1) \cong B_{c+4,4}$. 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 $P^{(s-2)}_{c+1,3} \succ P^2_{c+1,3}$, and thus $P^{2,s}_{c+4,4}(1,1) \succ P^{2,4}_{c+4,4}(1,1) \cong B_{c+4,4}$. We have shown that $P^{2,s}_{c+4,4}(1,1) \succ B_{c+4,4}$ for $3 \leq s \leq c$ and $s \neq 4$, which will be the starting point of Claims 2 and 3.

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

$$\begin{aligned} m\left(P^{2,s}_{c+x+3,x+3}(x,1),i\right) &= m\left(P^{2,s}_{c+x+2,x+2}(x-1,1),i\right) \\ &\quad + m\left(P^{2,s}_{c+x+3,x+3}(x,1) - v_1 - v_2, i-1\right), \\ m\left(B_{c+x+3,x+3},i\right) &= m\left(B_{c+x+2,x+2},i\right) + m\left(xP_1 \cup P^2_{c+1,3}, i-1\right). \end{aligned}$$

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

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

If $x = 1$ and $s \neq 4$, then $P^{2,s}_{c+x+3,x+3}(1,x) \succ B_{c+x+3,x+3}$. If $x = 1$ and $s = 4$, then

$P^{2,s}_{c+x+3,x+3}(1,x) \cong B_{c+x+3,x+3}$. Suppose that $x \geq 2$. By Lemma 1, we have

$$\begin{aligned} m\left(P^{2,s}_{c+x+3,x+3}(1,x), i\right) &= m\left(P^{2,s}_{c+x+2,x+2}(1,x-1), i\right) \\ &\quad + m\left((x-1)P_1 \cup P^2_{s,3} \cup P_{c+2-s}, i-1\right), \\ m\left(B_{c+x+3,x+3}, i\right) &= m\left(B_{c+x+2,x+2}, i\right) + m\left(xP_1 \cup P^2_{c+1,3}, i-1\right). \end{aligned}$$

Obviously, $m\left((x-1)P_1 \cup P^2_{s,3} \cup P_{c+2-s}, i-1\right) \geq m\left(xP_1 \cup P^2_{c+1,3}, i-1\right)$ and then $m\left(P^{2,s}_{c+x+3,x+3}(1,x), i\right) \geq m\left(B_{c+x+3,x+3}, i\right)$ 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 $T \succ T' \succ B_{n,k}$. $\square$

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