On the Maximal Energy Trees with One Maximum and One Second Maximum Degree Vertex

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Abstract

For a simple graph $G$, the energy $E(G)$ is defined as the sum of the absolute values of all eigenvalues of its adjacent matrix. For $d_1 > d_2 \geq 3$ and $t \geq 3$, denote by $T_a$ the tree formed from a path $P_t$ on $t$ vertices by attaching $d_1 - 1$ $P_2$’s on one end and $d_2 - 1$ $P_2$’s on the other end of the path $P_t$, and $T_b$ the tree formed from $P_{t+2}$ by attaching $d_1 - 1$ $P_2$’s on an end of the $P_{t+2}$ and $d_2 - 2$ $P_2$’s on the vertex next to the end. In [14] Yao showed that among trees of order $n$ and two vertices of maximum degree $d_1$ and second maximum degree $d_2$ ($d_1 > d_2$), the maximal energy tree is either the graph $T_a$ or the graph $T_b$, where $t = n + 4 - 2d_1 - 2d_2 \geq 3$. However, she could not determine which one of $T_a$ and $T_b$ is the maximal energy tree. This is because the quasi-order method is invalid for comparing their energies. In this paper, we use a new method to determine the maximal energy tree. We prove that the maximal energy tree is $T_b$ if $d_1 \geq 7$, $d_2 \geq 3$ or $d_1 = 6, d_2 = 3$. Moreover, for $d_1 = 4$ and $d_2 = 3$, the maximal energy tree is the graph $T_b$ if $t = 4$, and the graph $T_a$ otherwise. For other cases, the maximal energy tree is the graph $T_b$ if (i) $d_1 = 5, d_2 = 4$, $t$ is odd and $3 \leq t \leq 45$, (ii) $d_1 = 5, d_2 = 3$, $t$ is odd and $3 \leq t \leq 29$, (iii) $d_1 = 6, d_2 = 5$, $t = 3, 5, 7$, (iv) $d_1 = 6, d_2 = 4$, $t = 5$; and for all the remaining cases, the maximal energy tree is the graph $T_b$.

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1 Introduction

Let $G$ be a simple graph of order $n$, and $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of $G$. Then the energy of $G$ is defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|,$$

which was introduced by Gutman in [9]. The match polynomial [6, 7] of $G$ is defined as

$$m(G, x) = \sum_{k=0}^{[n/2]} (-1)^k m(G, k) x^{n-2k},$$

where $m(G, k)$ denotes the number of $k$-matchings of $G$ and $m(G, 0) = 1$. If $G = T$ is a tree of order $n$, then the characteristic polynomial [5] of $G$ has the form

$$\varphi(T, x) = m(T, x) = \sum_{k=0}^{[n/2]} (-1)^k m(T, k) x^{n-2k}.$$

And, by Coulson integral formula [3, 4, 8, 11], we have for a tree $T$,

$$E(T) = \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \log \left[ \sum_{k=0}^{[n/2]} m(T, k) x^{2k} \right] dx.$$

As we did in [12], for convenience we use the so-called signless matching polynomial [1]

$$m^+(G, x) = \sum_{k=0}^{[n/2]} m(G, k) x^{2k}.$$

Then we have

$$E(T) = \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \log m^+(T, x) dx. \quad (1)$$

For basic properties of $m^+(G, x)$, we refer to our paper [12].

For more results on graph energy, we refer to the survey [10]. For terminology and notations not defined here, we refer to the book of Bondy and Murty [2].

Graphs with extremal energies are interested in literature. In 2009 Li et al. [13] showed that among trees of order $n$ with two vertices of maximum degree $\Delta (\geq 3)$, the maximal energy tree is either the graph $G_a$ or the graph $G_b$, where $t = n + 4 - 4\Delta \geq 3$ and $G_a$ is the tree formed from a path $P_t$ on $t$ vertices by attaching $\Delta - 1$ $P_2$’s on each end of the path $P_t$, $G_b$ is the tree formed from $P_{t+2}$ by attaching $\Delta - 1$ $P_2$’s on an end of the
Figure 1.1 The maximal energy trees with $n$ vertices and two vertices $u$ and $v$ of degree $d_1$ and $d_2$.

$P_{t+2}$ and $\Delta - 2$ $P_2$’s on the vertex next to the end. However, they could not determine which one of $G_a$ and $G_b$ is the maximal energy tree. In our recent paper [12], we used a new method to determine the maximal energy tree. In a similar way, Yao [14] gave the following Theorem 1.1 about the maximal energy tree with one maximum and one second maximum degree vertex.

**Theorem 1.1 ([14])** Among trees with a fixed number of vertices $(n)$ and two vertices of maximum degree $d_1$ and second maximum degree $d_2$ ($d_1 > d_2$), the maximal energy tree has as many as possible 2-branches.

1. If $n \geq 2d_1 + 2d_2 - 1$, then the maximal energy tree is either the graph $T_a$ or the graph $T_b$, depicted in Figure 1.1.
2. If $n \leq 2d_1 + 2d_2 - 2$, then the maximal energy tree is among the graph $T_c$ depicted in Figure 1.1.

From Theorem 1.1, one can also see that for $n \geq 2d_1 + 2d_2 - 1$, she could not determine which one of the trees $T_a$ and $T_b$ has the maximal energy. In fact, the quasi-order method they used before is invalid for the special case. In this paper, we will use the Coulson integral formula method to determine which one of the trees $T_a$ and $T_b$ has the maximal energy. One must notice that since $d_1 \neq d_2$ here, the energy is a function in two variables $d_1$ and $d_2$, and this makes our discussion much more complicated.
2 Preliminaries

In this section, we list some useful properties of the signless matching polynomial $m^+(G, x)$, which will be used in the sequel, and already appeared in [12].

Lemma 2.1 Let $v$ be a vertex of $G$ and $N(v) = \{v_1, v_2, \ldots, v_r\}$ the set of all neighbors of $v$ in $G$. Then

$$m^+(G, x) = m^+(G - v, x) + x^2 \sum_{v_i \in N(v)} m^+(G - v - v_i, x).$$

Lemma 2.2 Let $P_t$ denote a path on $t$ vertices. Then

1. $m^+(P_t, x) = m^+(P_{t-1}, x) + x^2 m^+(P_{t-2}, x)$, for any $t \geq 1$,
2. $m^+(P_t, x) = (1 + x^2) m^+(P_{t-2}, x) + x^2 m^+(P_{t-3}, x)$, for any $t \geq 2$.

The initials are $m^+(P_0, x) = m^+(P_1, x) = 1$, and we define $m^+(P_{-1}, x) = 0$.

Corollary 2.3 Let $P_t$ be a path on $t$ vertices. Then for any real number $x$,

$$m^+(P_{t-1}, x) \leq m^+(P_t, x) \leq (1 + x^2)m^+(P_{t-1}, x), \text{ for any } t \geq 1.$$ 

3 Main results

Before giving our main results, we state some knowledge on real analysis, for which we refer to [15].

Lemma 3.1 For any real number $X > -1$, we have

$$\frac{X}{1+X} \leq \log(1 + X) \leq X.$$ 

For convenience, we introduce the following notations:

$$A_1 = (x^2 + 1)(d_1x^6 + d_2x^6 + d_2x^4 + d_1d_2x^4 + d_1x^4 + 2x^4 + 2x^2 + d_1x^2 + d_2x^2 + 1),$$

$$A_2 = x^2(x^2 + 1)(x^6 + 2x^4 + d_1d_2x^4 + d_1x^2 + d_2x^2 + x^2 + 1).$$
\[ B_1 = 2x^8 + d_1 x^8 + 6x^6 + 2d_1 d_2 x^6 + d_1 d_2 x^4 + 2d_1 x^4 + 4x^4 + 2d_2 x^4 + d_2 x^2 + d_1 x^2 + 3x^2 + 1, \]
\[ B_2 = x^2(x^2 + 1)(x^6 + 2x^4 + d_1 d_2 x^4 + d_1 x^2 + d_2 x^2 + x^2 + 1). \]

Using Lemmas 2.1 and 2.2 repeatedly, we can easily get the following two recursive formulas, where \( t = n + 4 - 2d_1 - 2d_2 \geq 3: \)
\[ m^+(T_a, x) = (1 + x^2)^{d_1 + d_2 - 5}(A_1 m^+(P_{t-3}, x) + A_2 m^+(P_{t-4}, x)), \quad (2) \]
and
\[ m^+(T_b, x) = (1 + x^2)^{d_1 + d_2 - 5}(B_1 m^+(P_{t-3}, x) + B_2 m^+(P_{t-4}, x)), \quad (3) \]

From Eqs. (2) and (3), by some elementary calculations we can obtain
\[ m^+(T_a, x) - m^+(T_b, x) = (1 + x^2)^{d_1 + d_2 - 5}(d_2 - 2)x^6(x^2 - (d_1 - 2))m^+(P_{t-3}, x). \quad (4) \]

We know directly from Figure 1.1 that if \( t = 2 \) or \( d_2 = 2, T_a \cong T_b \), then \( E(T_a) = E(T_b) \), so we only consider the cases \( t \geq 3 \) and \( d_1 > d_2 \geq 3. \)

Now we give a useful lemma.

**Lemma 3.2** Among trees with \( n \) vertices and two vertices of maximum and second maximum degree \( d_1 \) and \( d_2 \), let \( k = d_1 - d_2 \), if \( 1 \leq k \leq 3, d_2 \geq 7 - k \) or \( 4 \leq k \leq 12, d_2 \geq 3 \), the maximal energy tree is the graph \( T_b \), where \( t = n + 4 - 2d_1 - 2d_2 \geq 3. \)

**Proof.** Since \( m^+(T_a, x) > 0 \) and \( m^+(T_b, x) > 0 \), we have
\[ \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)} = \frac{m^+(T_a, x)}{m^+(T_b, x)} - 1 > -1. \]

Therefore, from Eq. (1) and Lemma 3.1, we get that
\[ E(T_a) - E(T_b) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \frac{m^+(T_a, x)}{m^+(T_b, x)} dx \]
\[ = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \left( 1 + \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)} \right) dx \]
\[ \leq \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \cdot \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)} dx. \quad (5) \]
By Corollary 2.3, we have \( m^+(P_{t-4}, x) \leq m^+(P_{t-3}, x) \) and \( m^+(P_{t-4}, x) \geq \frac{m^+(P_{t-3}, x)}{1+x^2} \) for \( t \geq 4 \). So, we have

\[
E(T_a) - E(T_b) \leq \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \cdot \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)} dx
\]

\[
= \frac{2}{\pi} \int_0^{+\infty} \frac{(d_2 - 2)x^4(x^2 - (d_1 - 2))m^+(P_{t-3}, x)}{B_1m^+(P_{t-3}, x) + B_2m^+(P_{t-4}, x)} dx
\]

\[
\leq \frac{2}{\pi} \int_0^{+\infty} \frac{(d_2 - 2)x^4(x^2 - (d_1 - 2))}{\sqrt{d_1 - 2}} \frac{B_1 + B_2/(1 + x^2)}{B_1 + B_2} dx + \frac{2}{\pi} \int_0^{\sqrt{d_1 - 2}} \frac{(d_2 - 2)x^4(x^2 - (d_1 - 2))}{B_1 + B_2} dx
\]

\[
+ \frac{2}{\pi} \int_0^1 \frac{2(d_2 - 2)x^4(x^2 - (d_1 - 2))}{(5d_1d_2 + 6d_1 + 5d_2 + 26)(x^2 + 1)} dx = \frac{2}{\pi} f(d_1, d_2).
\]

Where

\[
f(d_1, d_2) = \frac{2(d_2 - 2)}{3(d_1 + 3)\sqrt{d_1 - 2}} - \frac{d_2 - 2}{15(26 + 6d_1 + 5d_1d_2 + 5d_2)} \left( 3d_1 - 11 + \frac{2}{(d_1 - 2)^{3/2}} \right)
\]

- \[
= \frac{28d_2 - 40d_1d_2 + 80d_1 - 30\pi d_1 + 30\pi + 15\pi d_2d_1 - 56 - 15\pi d_2}{30(26 + 6d_1 + 5d_1d_2 + 5d_2)}.
\]

Now, for \( k = d_1 - d_2 \), we have that

1. if \( k = 1 \), when \( d_2 \geq 62 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
2. if \( k = 2 \), when \( d_2 \geq 60 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
3. if \( k = 3 \), when \( d_2 \geq 57 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
4. if \( k = 4 \), when \( d_2 \geq 54 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
5. if \( k = 5 \), when \( d_2 \geq 50 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
6. if \( k = 6 \), when \( d_2 \geq 47 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
7. if \( k = 7 \), when \( d_2 \geq 43 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
8. if \( k = 8 \), when \( d_2 \geq 40 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
9. if \( k = 9 \), when \( d_2 \geq 35 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
10. if \( k = 10 \), when \( d_2 \geq 31 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).
(11) if \( k = 11 \), when \( d_2 \geq 24 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).

(12) if \( k = 12 \), when \( d_2 \geq 3 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) < 0 \).

For smaller \( d_2 \), we consider the following inequality

\[ E(T_a) - E(T_b) \leq \frac{2}{\pi} \cdot g(d_1, d_2, x) < 0 \]

where

\[
g(d_1, d_2, x) = \int_0^{\sqrt{d_1 - 2}} \frac{1}{x^2} \log \left( 1 + \frac{(d_2 - 2)x^6(x^2 - (d_1 - 2))}{B_1 + B_2} \right) dx + \int_{\sqrt{d_1 - 2}}^{+\infty} \frac{1}{x^2} \log \left( 1 + \frac{(d_2 - 2)x^6(x^2 - (d_1 - 2))}{B_1 + \frac{B_2}{1+x^2}} \right) dx.
\]

By direct calculations, using a computer with the Maple programm, we can get that

1. if \( k = 1 \), when \( 6 \leq d_2 \leq 61 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} g(d_1, d_2, x) < 0 \).
2. if \( k = 2 \), when \( 5 \leq d_2 \leq 59 \), \( E(T_a) - E(T_b) < 0 \).
3. if \( k = 3 \), when \( 4 \leq d_2 \leq 56 \), \( E(T_a) - E(T_b) < 0 \).
4. if \( 4 \leq k \leq 11 \), when \( 3 \leq d_2 \leq 53 \), \( E(T_a) - E(T_b) < 0 \).

Then, from all the above results, we get the following conclusion: for all \( t \geq 4 \),

1. if \( k = 1 \), when \( d_2 \geq 6 \), \( E(T_a) - E(T_b) < 0 \).
2. if \( k = 2 \), when \( d_2 \geq 5 \), \( E(T_a) - E(T_b) < 0 \).
3. if \( k = 3 \), when \( d_2 \geq 4 \), \( E(T_a) - E(T_b) < 0 \).
4. if \( 4 \leq k \leq 12 \), when \( d_2 \geq 3 \), \( E(T_a) - E(T_b) < 0 \).

If \( t = 3 \), we have \( m^+(P_{t-4}, x) = m^+(P_{t-1}, x) = 0 \). By a similar method as above, we can get the same result.

The proof is now complete.

Next we consider the case \( k \geq 13 \).

**Lemma 3.3** Among trees with \( n \) vertices and two vertices of maximum and second maximum degree \( d_1 \) and \( d_2 \), let \( k = d_1 - d_2 \), if \( k \geq 13 \), \( d_2 \geq 3 \), then the maximal energy tree is the graph \( T_b \), where \( t = n + 4 - 2d_1 - 2d_2 \geq 3 \).
Proof. In Lemma 3.2 we proved that if \( t \geq 4, d_2 \geq 3 \), \( E(T_a) - E(T_b) < \frac{2}{\pi} f(d_1, d_2) \). Let \( d_1 = d_2 + k \), then \( f(d_1, d_2) = h(d_2, k) \). We first want to show that \( h(d_2, k) \) is monotonically decreasing in \( k \).

\[
h(d_2, k) = \frac{2(d_2 - 2)}{3(d_2 + k + 3)\sqrt{d_2 + k - 2}} - \frac{d_2 - 2}{15(26 + 6(d_2 + k) + 5(d_2 + k)d_2 + 5d_2)} \left( 3(d_2 + k) - 11 + \frac{2}{(d_2 + k - 2)^{3/2}} \right) = \frac{28d_2 - 40(d_2 + k)d_2 + 80(d_2 + k) - 30\pi(d_2 + k)}{30(26 + 6(d_2 + k) + 5(d_2 + k)d_2 + 5d_2)} + \frac{30\pi + 15\pi d_2(d_2 + k) - 56 - 15\pi d_2}{30(26 + 6(d_2 + k) + 5(d_2 + k)d_2 + 5d_2)}.
\]

The derivative of \( h(d_2, k) \) on \( k \) is

\[
h'(d_2, k) = h_1 + h_2 + h_3 + h_4 + h_5 + h_6,
\]

where

\[
h_1 = -\frac{2(d_2 - 2)}{3(d_2 + k + 3)^2\sqrt{d_2 + k - 2}},
\]

\[
h_2 = -\frac{d_2 - 2}{3(d_2 + k + 3)(d_2 + k - 2)^{3/2}},
\]

\[
h_3 = -\frac{30\pi - 40d_2 + 15d_2\pi + 80}{780 + 330d_2 + 180k + 150(d_2 + k)d_2},
\]

\[
h_4 = \frac{108d_2 - 56 - 30\pi(d_2 + k) - 40(d_2 + k)d_2 + 15d_2\pi(d_2 + k) + 30\pi - 15d_2\pi + 80k}{(780 + 330d_2 + 180k + 150(d_2 + k)d_2)^2} \cdot (180 + 150d_2),
\]

\[
h_5 = -\frac{\frac{d_2 - 2}{5} - \frac{d_2 - 2}{5(d_2 + k - 2)^{3/2}}}{26 + 11d_2 + 6k + 5(d_2 + k)d_2},
\]

\[
h_6 = \left( \frac{\frac{2}{15(d_2 + k - 2)^{3/2}} + \frac{3d_2 + 15}{15}}{26 + 11d_2 + 6k + 5(d_2 + k)d_2} \right) (d_2 - 2)(5d_2 + 6)
\]

Clearly, \( h_1, h_2 \leq 0 \),

\[
h_3 + h_4 = -\frac{264d_2 - 170d_2^2 + 90d_2\pi + 75d_2^2\pi + 1208 - 480\pi}{15(5d_2^2 + 5d_2k + 11d_2 + 6k + 26)^2} < 0.
\]
Moreover,  
\[
\frac{h_5 + h_6}{m} = (2(d_2 + k - 2) + (3d_2 + 3k - 11)(d_2 + k - 2)^{5/2})(5d_2 + 6) \\
- 3(26 + 11d_2 + 6k + 5(d_2 + k)d_2)((d_2 + k - 2)^{5/2} - 1) \\
= (-70d_2^3 - 140d_2^2k + 136d_2^2 - 70d_2k^2 - 8d_2k + 296d_2 - 144k^2 + 576k - 576) \\
\cdot \sqrt{d_2 + k - 2 + 25d_2^2 + 25d_2 + 25d_2k + 30k + 54} < 0 ,
\]
where  
\[
m = \frac{d_2 - 2}{15(d_2 + k - 2)^{5/2}(26 + 11d_2 + 6k + 5(d_2 + k)d_2)^2} > 0 .
\]
Thus,  
\[
h_5 + h_6 < 0 .
\]
Therefore,  
\[
h'(d_2, k) < 0 ,
\]
and hence  
\[
h(d_2, k)
\]
is monotonically decreasing in  
\[
k.
\]
Then, for any  
\[
d_2 \geq 3 , k \geq 13 ,
\]
\[
f(d_1, d_2) = h(d_2, k) < h(d_2, 12) < 0 .
\]
Thus  
\[
E(T_a) - E(T_b) < 0 .
\]

If  
\[
t = 3 ,
\]
we have  
\[
m^+(P_{t-4}, x) = m^+(P_{t-1}, x) = 0 .
\]
By a similar method as above, we can get the same result.

From Lemmas 3.2 and 3.3, we can get the following result immediately.

**Theorem 3.4** Among trees with  
\[
n
\]
vertices and two vertices of maximum and second maximum degree  
\[
d_1
\]
and  
\[
d_2
\], if  
\[
d_1 \geq 7
\]
and  
\[
d_2 \geq 3
\], then the maximal energy tree is the graph  
\[
T_b .
\]

Now we have proved that for most cases,  
\[
T_b
\]
has the maximal energy among trees with  
\[
n
\]
vertices and two vertices of maximum and second maximum degree. Only the following six special cases are left undetermined:  
\[
(d_1, d_2) = (4, 3) , (5, 4) , (5, 3) , (6, 5) , (6, 4) , (6, 3) .
\]
Before solving them, we give two lemmas [12] about the properties of the signless matching polynomial  
\[
m^+(P_t, x)
\]
for our later use.

**Lemma 3.5** For  
\[
t \geq -1
\], the polynomial  
\[
m^+(P_t, x)
\]
has the following form  
\[
m^+(P_t, x) = \frac{1}{\sqrt{1 + 4x^2}}(\lambda_1^{t+1} - \lambda_2^{t+1}) ,
\]
where  
\[
\lambda_1 = \frac{1 + \sqrt{1 + 4x^2}}{2}
\]
and  
\[
\lambda_2 = \frac{1 - \sqrt{1 + 4x^2}}{2} .
\]
Lemma 3.6 Suppose \( t \geq 4 \). If \( t \) is even, then
\[
\frac{2}{1 + \sqrt{1 + 4x^2}} < \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} \leq 1. \tag{6}
\]
If \( t \) is odd, then
\[
\frac{1}{1 + x^2} \leq \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} < \frac{2}{1 + \sqrt{1 + 4x^2}}. \tag{7}
\]
Note that
\[
\lim_{t \to \infty} \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} = \frac{2}{1 + \sqrt{1 + 4x^2}}.
\]
Therefore, in view of Ineq. (6), if \( t \) is even and sufficiently large, then for some \( x \), there exists some \( \frac{2}{1 + \sqrt{1 + 4x^2}} < \Theta' < 1 \), such that \( \Theta' \) becomes an upper bound for \( \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} \).

Analogously, in view of Ineq. (7), if \( t \) is odd and sufficiently large, then for some \( x \) there exists some \( \frac{1}{1 + x^2} < \Theta'' < \frac{2}{1 + \sqrt{1 + 4x^2}} \), such that \( \Theta'' \) becomes a lower bound for \( \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} \).

By numerical testing we can find the proper \( \Theta' \) and \( \Theta'' \).

Now we are ready to deal with the case \( d_1 = 4, d_2 = 3 \).

Theorem 3.7 Among trees with \( n \) vertices and two vertices of maximum and second maximum degree \( d_1 = 4 \) and \( d_2 = 3 \), letting \( t = n + 4 - 2d_1 - 2d_2 \geq 3 \), the maximal energy tree is the graph \( T_b \) if \( t = 4 \), and the graph \( T_a \) otherwise.

Proof. By Eqs. (2), (3), (4) and (5), we have
\[
E(T_a) - E(T_b) = \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \log \left( 1 + \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)} \right) dx
\]
\[
= \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \log \left( 1 + \frac{(d_2 - 2)x^6(x^2 - (d_1 - 2))}{B_1 + B_2\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)}} \right) dx. \tag{8}
\]

We first consider the case that \( t \) is odd and \( t \geq 5 \). By Eq. (8) and Lemma 3.6, we have
\[
E(T_a) - E(T_b)
> \frac{2}{\pi} \int_{\sqrt{2}}^{+\infty} \frac{1}{x^2} \log \left( 1 + \frac{x^6(x^2 - 2)}{B_1 + B_2\frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx + \frac{2}{\pi} \int_{0}^{\sqrt{2}} \frac{1}{x^2} \log \left( 1 + \frac{x^6(x^2 - 2)}{B_1 + B_2\frac{1}{1 + 2x^2}} \right) dx
> \frac{2}{\pi} \cdot 0.011179 > 0.
\]
If $t$ is even, we want to find $t$ and $x$ satisfying that
\[
\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} < \frac{2}{1 + \sqrt{1 + 4x^2}}.
\] (9)

It is equivalent to solve
\[
\frac{\lambda_1^{t-3} - \lambda_2^{t-3}}{\lambda_1^{t-2} - \lambda_2^{t-2}} < -\frac{1}{\lambda_2} \quad \text{i.e.,} \quad \left(1 + \frac{\sqrt{1 + 4x^2}}{2x}\right)^{2t-6} > \sqrt{1 + 4x^2} - 1.
\]

Thus,
\[
2t - 6 > \log_{1 + \sqrt{1 + 4x^2}}(\sqrt{1 + 4x^2} - 1).
\]

Since for $x \in (0, +\infty)$, $1 + \sqrt{1 + 4x^2}$ is decreasing and $\sqrt{1 + 4x^2} - 1$ is increasing, we have that $\log_{1 + \sqrt{1 + 4x^2}}(\sqrt{1 + 4x^2} - 1)$ is increasing. Thus, if $x \in [\sqrt{2}, 5]$, then
\[
\log_{1 + \sqrt{1 + 4x^2}}(\sqrt{1 + 4x^2} - 1) \leq \log_{\sqrt{101} - 1}(1) < 23.
\]

Therefore, when $t \geq 15$, i.e., $2t - 6 > 23$, we have that Ineq. (9) holds for $x \in [\sqrt{2}, 5]$.

Now we calculate the difference of $E(T_a)$ and $E(T_b)$. When $t$ is even and $t \geq 15$, from Eq. (8) we have
\[
E(T_a) - E(T_b)
\]
\[
> \frac{2}{\pi} \int_5^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{x^6(x^2 - 2)}{B_1 + B_2}\right) dx + \frac{2}{\pi} \int_{\sqrt{2}}^{5} \frac{1}{x^2} \log \left(1 + \frac{x^6(x^2 - 2)}{B_1 + B_2 - \frac{2}{1 + \sqrt{1 + 4x^2}}}\right) dx
\]
\[
+ \frac{2}{\pi} \int_0^{\sqrt{2}} \frac{1}{x^2} \log \left(1 + \frac{x^6(x^2 - 2)}{B_1 + B_2 - \frac{2}{1 + \sqrt{1 + 4x^2}}}\right) dx > \frac{2}{\pi} \cdot 0.001634 > 0.
\]

For $t = 3$ and any even $t$ with $4 \leq t \leq 14$, by computing the energies of the two graphs directly by a computer with Maple program, we can get that $E(T_a) < E(T_b)$ for $t = 4$, and $E(T_a) > E(T_b)$ for the other cases.

The proof is thus complete.\[\]

The following theorem gives the result for the cases: $(d_1, d_2) = (5, 4), (5, 3), (6, 5), (6, 4), (6, 3)$.

**Theorem 3.8** Among trees with $n$ vertices and two vertices of maximum and second maximum degree $d_1$ and $d_2$, letting $t = n + 4 - 2d_1 - 2d_2 \geq 3,$
(i) for \( d_1 = 5, d_2 = 4 \), the maximal energy tree is the graph \( T_a \) if \( t \) is odd and \( 3 \leq t \leq 45 \), and the graph \( T_b \) otherwise.

(ii) for \( d_1 = 5, d_2 = 3 \), the maximal energy tree is the graph \( T_a \) if \( t \) is odd and \( 3 \leq t \leq 29 \), and the graph \( T_b \) otherwise.

(iii) for \( d_1 = 6, d_2 = 5 \), the maximal energy tree is the graph \( T_a \) if \( t = 3, 5, 7 \), and the graph \( T_b \) otherwise.

(iv) for \( d_1 = 6, d_2 = 4 \), the maximal energy tree is the graph \( T_a \) if \( t = 5 \), and the graph \( T_b \) otherwise.

(v) for \( d_1 = 6, d_2 = 3 \), the maximal energy tree is the graph \( T_b \) for any \( t \geq 3 \).

Proof. We consider the following cases separately:

(i) \( d_1 = 5, d_2 = 4 \).

If \( t \) is even, we want to find \( t \) and \( x \) satisfying that

\[
\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} < \frac{2.1}{1 + \sqrt{1 + 4x^2}}.
\]

(10)

It is equivalent to solve

\[2t - 6 > \log_{\frac{1 + \sqrt{1 + 4x^2}}{42}} \left( 41 - \frac{42}{\sqrt{1 + 4x^2} + 1} \right).\]

If \( x \in [1, \sqrt{3}] \),

\[\log_{\frac{1 + \sqrt{1 + 4x^2}}{42}} \left( 41 - \frac{42}{\sqrt{1 + 4x^2} + 1} \right) \leq \log_{\frac{1 + \sqrt{13}}{42}} \left( 41 - \frac{42}{1 + \sqrt{13}} \right) < 13.\]

Therefore, when \( t \geq 10 \), i.e., \( 2t - 6 > 13 \), we have that Ineq. (10) holds for \( x \in [1, \sqrt{3}] \).

Then, if \( t \) is even and \( t \geq 10 \), from Eq. (8) and Lemma 3.6 we have

\[
E(T_a) - E(T_b) < \frac{2}{\pi} \int_{\sqrt{3}}^{1+\infty} \frac{1}{x^2} \log \left( 1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx
\]

\[
+ \frac{2}{\pi} \int_{1}^{\sqrt{3}} \frac{1}{x^2} \log \left( 1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx
\]

\[
+ \frac{2}{\pi} \int_{0}^{1} \frac{1}{x^2} \log \left( 1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2} \right) dx < \frac{2}{\pi} \cdot (-0.000231) < 0.
\]
If \( t \) is odd, we want to find \( t \) and \( x \) satisfying that
\[
\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} > \frac{1.9}{1 + \sqrt{1 + 4x^2}}
\]  
(11)
that is
\[
2t - 6 > \log_{1 + \sqrt{1 + 4x^2}} \left( 39 - \frac{38}{\sqrt{1 + 4x^2} + 1} \right).
\]
Then we get that when \( t \geq 699 \), and \( x \in [\sqrt{3}, 190] \), the Ineq. (11) holds. Thus, if \( t \) is odd and \( t \geq 699 \), from Eq. (8) and Lemma 3.6 we have
\[
E(T_a) - E(T_b) < \frac{2}{\pi} \int_{\sqrt{3}}^{+\infty} \frac{1}{x^2} \log \left( 1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{1}{1 + \sqrt{1 + 4x^2}}} \right) dx + \frac{2}{\pi} \int_{\sqrt{3}}^{\sqrt{3}} \frac{1}{x^2} \log \left( 1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx < \frac{2}{\pi} \cdot (-1.41 \times 10^{-5}) < 0.
\]

For any even \( t \) with \( 4 \leq t \leq 8 \) and any odd \( t \) with \( 3 \leq t \leq 697 \), by computing the energies of the two graphs directly by a computer with Matlab program, we get that \( E(T_a) > E(T_b) \) for any odd \( t \) with \( 3 \leq t \leq 45 \), and \( E(T_a) < E(T_b) \) for the other cases.

(ii) \( d_1 = 5, d_2 = 3 \).

If \( t \) is even and \( t \geq 4 \), from Eq. (8) and Lemma 3.6, we have
\[
E(T_a) - E(T_b) < \frac{2}{\pi} \int_{\sqrt{3}}^{+\infty} \frac{1}{x^2} \log \left( 1 + \frac{x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx + \frac{2}{\pi} \int_{\sqrt{3}}^{\sqrt{3}} \frac{1}{x^2} \log \left( 1 + \frac{x^6(x^2 - 3)}{B_1 + B_2} \right) dx < \frac{2}{\pi} \cdot (-1.224 \times 10^{-4}) < 0.
\]

If \( t \) is odd and \( t \geq 699 \), by the similar proof in (i), we get that \( E(T_a) - E(T_b) < \frac{2}{\pi} \cdot (-9.90 \times 10^{-4}) < 0 \).

For any odd \( t \) with \( 3 \leq t \leq 697 \), by computing the energies of the two graphs directly with Matlab program, we get that \( E(T_a) > E(T_b) \) for any odd \( t \) with \( 3 \leq t \leq 29 \), and \( E(T_a) < E(T_b) \) for the other cases.

(iii) \( d_1 = 6, d_2 = 5 \).
If \( t \) is even, by the similar method as used in (ii), we get that \( E(T_a) - E(T_b) < \frac{2}{\pi} \cdot (-0.018405) < 0 \).

If \( t \) is odd, similar to the proof in (i), we can show that when \( t \geq 27 \) and \( x \in [2, 22] \), the following inequality holds:

\[
\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} > \frac{1}{1 + \sqrt{1 + 4x^2}}.
\]

Hence, if \( t \) is odd and \( t \geq 27 \), we have

\[
E(T_a) - E(T_b) < 2\pi \cdot (-0.002914) < 0.
\]

For any odd \( t \) with \( 3 \leq t \leq 25 \), by computing the energies of the two graphs directly, we can get that \( E(T_a) > E(T_b) \) for \( t = 3, 5, 7 \), and \( E(T_a) < E(T_b) \) for the other cases.

(iv) \( d_1 = 6, d_2 = 4 \).

If \( t \) is even, by the similar method as used in (ii), we get that \( E(T_a) - E(T_b) < \frac{2}{\pi} \cdot (-0.015171) < 0 \).

If \( t \) is odd and \( t \geq 27 \), by the similar proof as used in (iii), we get that \( E(T_a) - E(T_b) < \frac{2}{\pi} \cdot (-0.004557) < 0 \).

For any odd \( t \) with \( 3 \leq t \leq 25 \), by computing the energies of the two graphs directly, we get that \( E(T_a) > E(T_b) \) for \( t = 5 \), and \( E(T_a) < E(T_b) \) for the other cases.

(v) \( d_1 = 6, d_2 = 3 \).

If \( t \) is even, by the similar method as used in (ii), we get that \( E(T_a) - E(T_b) < \frac{2}{\pi} \cdot (-0.009652) < 0 \).

If \( t \) is odd and \( t \geq 27 \), by the similar proof as used in (iii), we get that \( E(T_a) - E(T_b) < \frac{2}{\pi} \cdot (-0.004244) < 0 \).

For any odd \( t \) with \( 3 \leq t \leq 25 \), by computing the energies of the two graphs directly, we get that \( E(T_a) < E(T_b) \) for all \( t \geq 3 \).

The proof is now complete.
References


