On the maximal energy tree with two maximum degree vertices

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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 $\Delta \geq 3$ and $t \geq 3$, denote by $T_a(\Delta, t)$ (or simply $T_a$) the tree formed from a path $P_t$ on $t$ vertices by attaching $\Delta - 1$ $P_2$’s on each end of the path $P_t$, and $T_b(\Delta, t)$ (or simply $T_b$) the tree formed from $P_{t+2}$ by attaching $\Delta - 1$ $P_2$’s on an end of the $P_{t+2}$ and $\Delta - 2$ $P_2$’s on the vertex next to the end. In [X. Li, X. Yao, J. Zhang and I. Gutman, Maximum energy trees with two maximum degree vertices, J. Math. Chem. 45(2009), 962–973], Li et al. proved that among trees of order $n$ with two vertices of maximum degree $\Delta$, the maximal energy tree is either the graph $T_a$ or the graph $T_b$, where $t = n + 4 - 4\Delta \geq 3$. However, they 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. It turns out that things are more complicated. We prove that the maximal energy tree is $T_b$ for $\Delta \geq 7$ and any $t \geq 3$, while the maximal energy tree is $T_a$ for $\Delta = 3$ and any $t \geq 3$. Moreover, for $\Delta = 4$, the maximal energy tree is $T_a$ for all $t \geq 3$ but $t = 4$, for which $T_b$ is the maximal energy tree. For $\Delta = 5$, the maximal energy tree is $T_b$ for all $t \geq 3$ but $t$ is odd and $3 \leq t \leq 89$, for which $T_a$ is the maximal energy tree. For $\Delta = 6$, the maximal energy tree is $T_b$ for all $t \geq 3$ but $t = 3, 5, 7$, for which $T_a$ is the maximal energy tree. One can see that for most $\Delta$, $T_b$ is the maximal energy tree, $\Delta = 5$ is a turning point, and $\Delta = 3$ and 4 are exceptional cases.

Keywords: graph energy, tree, Coulson integral formula.

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1 Introduction

Let $G$ be a simple graph of order $n$, it is well known [4] that the characteristic polynomial of $G$ has the form

$$\varphi(G, x) = \sum_{k=0}^{n} a_k x^{n-k}.$$ 

The match polynomial of $G$ is defined as

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

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

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

Let $\lambda_1, \lambda_2, \cdots, \lambda_n$ 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 [6]. If $T$ is a tree of order $n$, then by Coulson integral formula [5, 8], we have

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

In order to avoid the signs in the matching polynomial, this immediately motivates us to introduce a new graph polynomial

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

Then we have

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

Although $m^+(G, x)$ is nothing new but $m^+(G, x) = (ix)^nm(G, (ix)^{-1})$, we shall see later that this will bring us a lot of computational convenience. Some basic properties of $m^+(G, x)$ will be given in next section.

We refer to the survey [7] for more results on graph energy. For terminology and notation not defined here, we refer to the book of Bondy and Murty [1].
Graphs with extremal energies are interested in literature. Gutman [5] proved that the star and the path has the minimal and the maximal energy among all trees, respectively. Lin et al. [17] showed that among trees with a fixed number of vertices \( n \) and of maximum vertex degree \( \Delta \), the maximal energy tree has exactly one branching vertex (of degree \( \Delta \)) and as many as possible 2-branches. Li et al. [16] gave the following Theorem 1.1 about the maximal energy tree with two maximum degree vertices. In a similar way, Yao [19] studied the maximal energy tree with one maximum and one second maximum degree vertex. A branching vertex is a vertex whose degree is three or greater, and a pendent vertex attached to a vertex of degree two is called a 2-branch.

**Theorem 1.1** ([16]) Among trees with a fixed number of vertices \( n \) and two vertices of maximum degree \( \Delta \), the maximal energy tree has as many as possible 2-branches.

1. If \( n \leq 4\Delta - 2 \), then the maximal energy tree is the graph \( T_c = T_c(\Delta, t) \) depicted in Figure 1.1, in which the numbers of pendent vertices attached to the two branching vertices \( u \) and \( v \) differ by at most 1.
2. If \( n \geq 4\Delta - 1 \), then the maximal energy tree is either the graph \( T_a = T_a(\Delta, t) \) or the graph \( T_b = T_b(\Delta, t) \), depicted in Figure 1.1.

![Figure 1.1](image)

Figure 1.1 The maximal energy trees with \( n \) vertices and two vertices \( u, v \) of maximum degree \( \Delta \).

From Theorem 1.1 one can see that for \( n \geq 4\Delta - 1 \), they could not determine which one of the graphs \( T_a \) and \( T_b \) has the maximal energy. They gave small examples showing that both cases could happen. In fact, the quasi-order method they used before is invalid for the special case. Recently, for these quasi-order incomparable problems, Huo et al. found an efficient way to determine which one attains the extremal value of the energy,
we refer to [9–15] for details. In this paper, we will use this newly developed method to determine which one of the graphs $T_a$ and $T_b$ has the maximal energy, solving this unsolved problem. It turns that this problem is more complicated than those in [9–15].

2 Preliminaries

In this section, we will give some properties of the new polynomial $m^+(G, x)$, which will be used in what follows. The proofs are omitted, since they are the same as those for matching polynomial.

Lemma 2.1 Let $K_n$ be a complete graph with $n$ vertices and $\overline{K_n}$ the complement of $K_n$, then

$$m^+(\overline{K_n}, x) = 1,$$

for any $n \geq 0$, defining $m^+(\overline{K_0}, x) = 1$, where both $K_0$ and $\overline{K_0}$ are the null graph.

Similar to the properties of matching polynomial, we have

Lemma 2.2 Let $G_1$ and $G_2$ be two vertex disjoint graphs. Then

$$m^+(G_1 \cup G_2, x) = m^+(G_1, x) \cdot m^+(G_2, x).$$

Lemma 2.3 Let $e = uv$ be an edge of graph $G$. Then we have

$$m^+(G, x) = m^+(G - e, x) + x^2 m^+(G - u - v, x).$$

Lemma 2.4 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

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

The following recursive equations can be gotten from Lemma 2.3 immediately.

Lemma 2.5 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 $m^+(P_{-1}, x) = 0$. 

From Lemma 2.5, one can easily obtain

**Corollary 2.6** Let $P_t$ be a path on $t$ vertices. Then for any real number $x$,

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

Although $m^+(G, x)$ has many other properties, the above ones are enough for our use.

### 3 Main results

Before giving our main results, we state some knowledge on real analysis, for which we refer to [20].

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

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

To compare the energies of $T_a$ and $T_b$, or more precisely, $T_a(\Delta, t)$ and $T_b(\Delta, t)$, means to compare the values of two functions with the parameters $\Delta$ and $t$, which are denoted by $E(T_a(\Delta, t))$ and $E(T_b(\Delta, t))$. Since $E(T_a(2, t)) = E(T_b(2, t))$ for any $t \geq 2$ and $E(T_a(\Delta, 2)) = E(T_b(\Delta, 2))$ for any $\Delta \geq 2$, we always assume that $\Delta \geq 3$ and $t \geq 3$.

For notational convenience, we introduce the following things:

$$A_1 = (1 + x^2)(1 + \Delta x^2)(2x^4 + (\Delta + 2)x^2 + 1),$$
$$A_2 = x^2(1 + x^2)(x^6 + (\Delta^2 + 2)x^4 + (2\Delta + 1)x^2 + 1),$$
$$B_1 = (\Delta + 2)x^8 + (2\Delta^2 + 6)x^6 + (\Delta^2 + 4\Delta + 4)x^4 + (2\Delta + 3)x^2 + 1,$$
$$B_2 = x^2(1 + x^2)(x^6 + (\Delta^2 + 2)x^4 + (2\Delta + 1)x^2 + 1).$$

Using Lemmas 2.4 and 2.5 repeatedly, we can easily get the following two recursive formulas:

$$m^+(T_a, x) = (1 + x^2)^{2\Delta-5}(A_1m^+(P_{t-3}, x) + A_2m^+(P_{t-4}, x)), \quad (2)$$

and

$$m^+(T_b, x) = (1 + x^2)^{2\Delta-5}(B_1m^+(P_{t-3}, x) + B_2m^+(P_{t-4}, x)), \quad (3)$$

From Eqs. (2) and (3), by some elementary calculations we can obtain

$$m^+(T_a, x) - m^+(T_b, x) = (1 + x^2)^{2\Delta-5}(\Delta - 2)x^6(x^2 - (\Delta - 2))m^+(P_{t-3}, x). \quad (4)$$

Now we give one of our main results.
Theorem 3.2 Among trees with \( n \) vertices and two vertices of maximum degree \( \Delta \), the maximal energy tree has as many as possible 2-branches. If \( \Delta \geq 8 \) and \( t \geq 3 \), then the maximal energy tree is the graph \( T_b \), where \( t = n + 4 - 4\Delta \).

Proof. From Eq. (1), we have

\[
E(T_a) - E(T_b) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \frac{m^+(T_a, x)}{m^+(T_b, x)} dx
= \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)}\right) dx.
\]

(5)

We express \( g(\Delta, t, x) \) as

\[
g(\Delta, t, x) = \frac{1}{x^2} \log \left(1 + \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)}\right).
\]

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, by Lemma 3.1 we have

\[
\frac{1}{x^2} \cdot \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_a, x)} \leq g(\Delta, t, x) \leq \frac{1}{x^2} \cdot \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)}.
\]

(6)

Substituting the recursive formulas (2), (3) and (4) to Eq. (6), we get that

\[
g(\Delta, t, x) \leq \frac{1}{x^2} \cdot \frac{(1 + x^2)^{2\Delta-5}(\Delta - 2)x^6(x^2 - (\Delta - 2))m^+(P_{t-3}, x)}{(1 + x^2)^{2\Delta-5}(B_1m^+(P_{t-3}, x) + B_2m^+(P_{t-4}, x))}
= \frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))m^+(P_{t-3}, x)}{B_1m^+(P_{t-3}, x) + B_2m^+(P_{t-4}, x)},
\]

and

\[
g(\Delta, t, x) \geq \frac{1}{x^2} \cdot \frac{(1 + x^2)^{2\Delta-5}(\Delta - 2)x^6(x^2 - (\Delta - 2))m^+(P_{t-3}, x)}{(1 + x^2)^{2\Delta-5}(A_1m^+(P_{t-3}, x) + A_2m^+(P_{t-4}, x))}
= \frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))m^+(P_{t-3}, x)}{A_1m^+(P_{t-3}, x) + A_2m^+(P_{t-4}, x)}.
\]

By Corollary 2.6 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 \( \Delta \geq 3 \) and \( t \geq 4 \). Then if \( x \geq \sqrt{\Delta - 2} \),

\[
|g(\Delta, t, x)| \leq \frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))}{B_1 + B_2/(1 + x^2)}
= \frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))}{(\Delta + 3)x^8 + (3\Delta^2 + 8)x^6 + (\Delta^2 + 6\Delta + 5)x^4 + (2\Delta + 4)x^2 + 1}.
\]
and if $x \leq \sqrt{\Delta - 2}$,

$$|g(\Delta, t, x)| \leq \frac{(\Delta - 2)x^4(\Delta - 2 - x^2)}{A_1 + A_2/(1 + x^2)} = \frac{(\Delta - 2)x^4(\Delta - 2 - x^2)}{(2\Delta + 1)x^8 + (2\Delta^2 + 4\Delta + 4)x^6 + (\Delta^2 + 6\Delta + 5)x^4 + (2\Delta + 4)x^2 + 1}.$$ 

Since for $\Delta \geq 3$ and any $x \geq 0$, we always have

$$(\Delta - 2)x^4(x^2 - (\Delta - 2))(1 + x^2) \leq (\Delta + 3)x^8 + (3\Delta^2 + 8)x^6 + (\Delta^2 + 6\Delta + 5)x^4 + (2\Delta + 4)x^2 + 1,$$

and

$$(\Delta - 2)x^4(\Delta - 2 - x^2)(1 + x^2) \leq (2\Delta + 1)x^8 + (2\Delta^2 + 4\Delta + 4)x^6 + (\Delta^2 + 6\Delta + 5)x^4 + (2\Delta + 4)x^2 + 1,$$

we can get that for $\Delta \geq 3$ and any $x \geq 0$,

$$|g(\Delta, t, x)| \leq \frac{1}{1 + x^2},$$

while $\int_0^{+\infty} \frac{2}{1 + x^2} dx = \frac{\pi}{2}$ is convergent. From the well-known Weierstrass’s criterion (for example, see [20]), we can get that $E(T_a) - E(T_b) = \frac{2}{\pi} \int_0^{+\infty} g(\Delta, t, x)dx$ is uniformly convergent. Then

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

Thus, for $t \geq 4$, we have

$$E(T_a) - E(T_b)\leq \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)} dx = \frac{2}{\pi} \int_0^{+\infty} \frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))}{B_1m^+(P, x) + B_2m^+(P, x)} dx = \frac{2}{\pi} \int_{\sqrt{\Delta - 2}}^{+\infty} \frac{(\Delta - 2)x^4(\Delta - 2 - x^2)}{B_1 + B_2} dx.$$ 

We calculate the two parts respectively. The first part is

$$\frac{2}{\pi} \int_{\sqrt{\Delta - 2}}^{+\infty} \frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))}{B_1 + B_2(1 + x^2)} dx = \frac{2}{\pi} \int_{\sqrt{\Delta - 2}}^{+\infty} \frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))}{(\Delta + 3)x^8 + (3\Delta^2 + 8)x^6 + (\Delta^2 + 6\Delta + 5)x^4 + (2\Delta + 4)x^2 + 1} dx < \frac{2}{\pi} \int_{\sqrt{\Delta - 2}}^{+\infty} \frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))}{(\Delta + 3)x^8} dx = \frac{2}{\pi} \cdot \frac{2\sqrt{\Delta - 2}}{3(\Delta + 3)}.$$
The second part is
\[
\frac{2}{\pi} \int_0^{\sqrt{\Delta-2}} \frac{(\Delta - 2)x^4(\Delta - 2 - x^2)}{B_1 + B_2} \, dx
\]
\[
= \frac{2}{\pi} \int_0^{\sqrt{\Delta-2}} \frac{(\Delta - 2)x^4(\Delta - 2 - x^2)}{h(\Delta, x)} \, dx
\]
\[
> \frac{2}{\pi} \int_0^1 \frac{(\Delta - 2)x^4(\Delta - 2 - x^2)}{\frac{5\Delta^2 + 11\Delta + 26}{2}(x^2 + 1)} \, dx + \frac{2}{\pi} \int_1^{\sqrt{\Delta-2}} \frac{(\Delta - 2)x^4(\Delta - 2 - x^2)}{(5\Delta^2 + 11\Delta + 26)x^{10}} \, dx
\]
\[
= \frac{2}{\pi} \left( \frac{-45\pi \Delta - 34\Delta^2 + 74\Delta + 30\pi - 12 + 15\pi \Delta^2 + \frac{4}{\sqrt{\Delta-2}}}{30(26 + 11\Delta + 5\Delta^2)} \right),
\]
where \( h(\Delta, x) = x^{10} + (\Delta^2 + \Delta + 5)x^8 + (3\Delta^2 + 2\Delta + 9)x^6 + (\Delta^2 + 6\Delta + 6)x^4 + (2\Delta + 4)x^2 + 1 \).

Now, when \( \Delta \geq 65 \), we have that
\[
E(T_a) - E(T_b) < \frac{2}{\pi} \cdot f(\Delta, x) < 0.
\]
For \( t = 3 \), we have \( m^+(P_{t-4}, x) = m^+(P_{t-1}, x) = 0 \). By a similar method as above, we can get that \( E(T_a) - E(T_b) < 0 \) when \( \Delta \geq 24 \).

Therefore, for \( \Delta \geq 65 \) and \( t \geq 3 \), we have \( E(T_a) < E(T_b) \).

For \( 8 \leq \Delta \leq 64 \), we can calculate
\[
E(T_a) - E(T_b) \leq \frac{2}{\pi} \cdot f(\Delta, x) < 0
\]
directly by computer programm, as shown in Table I

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

The proof is thus complete.

Now we are left with the cases \( 3 \leq \Delta \leq 7 \). At first, we consider the case of \( \Delta = 3 \) and \( t \geq 3 \). In this case, we have \( n = 4\Delta - 4 + t \geq 11 \).

**Theorem 3.3** Among trees with \( n \) vertices and two vertices of maximum degree \( \Delta = 3 \), the maximal energy tree has as many as possible 2-branches. If \( n \geq 11 \), then the maximal energy tree is the graph \( T_a \).
\[ f(\Delta, x) \]

| \( \Delta \) | \( f(\Delta, x) \) | \( \Delta \) | \( f(\Delta, x) \) | \( \Delta \) | \( f(\Delta, x) \) |
|-------------|-----------------|-------------|-----------------|-------------|-----------------|
| 8           | -0.00377        | 23          | -0.20792        | 38          | -0.29961        |
| 9           | -0.02418        | 24          | -0.21611        | 39          | -0.30403        |
| 10          | -0.04352        | 25          | -0.22390        | 40          | -0.30830        |
| 11          | -0.06168        | 26          | -0.23132        | 41          | -0.31244        |
| 12          | -0.07866        | 27          | -0.23841        | 42          | -0.31644        |
| 13          | -0.10933        | 28          | -0.24518        | 43          | -0.32032        |
| 14          | -0.13613        | 29          | -0.25165        | 44          | -0.32409        |
| 15          | -0.15972        | 30          | -0.25786        | 45          | -0.32774        |
| 16          | -0.17048        | 31          | -0.26381        | 46          | -0.33129        |
| 17          | -0.18063        | 32          | -0.26953        | 47          | -0.33473        |
| 18          | -0.19022        | 33          | -0.27502        | 48          | -0.33808        |
| 19          | -0.19931        | 34          | -0.28031        | 49          | -0.34134        |
| 20          | -0.20792        | 35          | -0.28540        | 50          | -0.34451        |
| 21          | -0.20957        | 36          | -0.29031        | 51          | -0.34759        |
| 22          | -0.20317        | 37          | -0.29504        | 52          | -0.35060        |
| 23          | -0.20475        | 38          | -0.29839        | 53          | -0.35353        |
| 24          | -0.20792        | 39          | -0.29961        | 54          | -0.35638        |
| 25          | -0.20894        | 40          | -0.30163        | 55          | -0.35917        |
| 26          | -0.21095        | 41          | -0.30364        | 56          | -0.36188        |
| 27          | -0.21296        | 42          | -0.30566        | 57          | -0.36454        |
| 28          | -0.21497        | 43          | -0.30768        | 58          | -0.36713        |
| 29          | -0.21698        | 44          | -0.30970        | 59          | -0.36965        |
| 30          | -0.21899        | 45          | -0.31172        | 60          | -0.37213        |
| 31          | -0.22099        | 46          | -0.31374        | 61          | -0.37454        |
| 32          | -0.22290        | 47          | -0.31576        | 62          | -0.37791        |
| 33          | -0.22491        | 48          | -0.31778        | 63          | -0.38022        |
| 34          | -0.22692        | 49          | -0.31980        | 64          | -0.38255        |
| 35          | -0.22893        | 50          | -0.32182        | 65          | -0.38488        |
| 36          | -0.23094        | 51          | -0.32384        | 66          | -0.38721        |
| 37          | -0.23295        | 52          | -0.32586        | 67          | -0.38954        |

Table 1 The values of \( f(\Delta, x) \) for \( 8 \leq \Delta \leq 67 \).

Proof. For \( \Delta = 3 \) and \( t \geq 4 \), by Eqs. (1), (6) and Corollary 2.6, we have

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

\[
= \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \cdot \frac{x^6(x^2 - 1)m^+(P_{t-3}, x)}{A_1 m^+(P_{t-3}, x) + A_2 m^+(P_{t-4}, x)} \, dx
\]

\[
\geq \frac{2}{\pi} \int_1^{+\infty} \frac{x^4(x^2 - 1)}{A_1 + A_2} \, dx - \frac{2}{\pi} \int_0^1 \frac{x^4(1 - x^2)}{A_1 + \frac{A_2}{1 + x^2}} \, dx
\]

\[
= \frac{2}{\pi} \int_1^{+\infty} \frac{x^4(x^2 - 1)}{x^{10} + 18x^8 + 41x^6 + 33x^4 + 10x^2 + 1} \, dx
\]

\[
- \frac{2}{\pi} \int_0^1 \frac{x^4(1 - x^2)}{7x^8 + 34x^6 + 32x^4 + 10x^2 + 1} \, dx
\]

\[
> \frac{2}{\pi} \cdot 0.00996 > 0.
\]

For \( \Delta = 3 \) and \( t = 3 \), we can compare the energies of the two graphs directly and get that \( E(T_a) > E(T_b) \).

Therefore, for \( \Delta = 3 \) and \( t \geq 3 \), we have \( E(T_a) > E(T_b) \).

Now we give two lemmas about the properties of the new polynomial \( m^+(P_t, x) \).
Lemma 3.4 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 $\lambda_2 = \frac{1-\sqrt{1+4x^2}}{2}$.

Proof. By Lemma 2.5, $m^+(P_t, x) = m^+(P_{t-1}, x) + x^2m^+(P_{t-2}, x)$ for any $t \geq 1$. Thus, it satisfies the recursive formula $h(t, x) = h(t-1, x) + x^2h(t-2, x)$, and the general solution of this linear homogeneous recurrence relation is $h(t, x) = P(x)\lambda_1^t + Q(x)\lambda_2^t$, where $\lambda_1 = \frac{1+\sqrt{1+4x^2}}{2}$ and $\lambda_2 = \frac{1-\sqrt{1+4x^2}}{2}$. Considering the initial values $m^+(P_1, x) = 1$ and $m^+(P_2, x) = 1 + x^2$, by some elementary calculations, we can easily obtain that

$$P(x) = \frac{1+\sqrt{1+4x^2}}{2\sqrt{1+4x^2}}; \quad Q(x) = \frac{-1+\sqrt{1+4x^2}}{2\sqrt{1+4x^2}}.$$

Thus,

$$m^+(P_t, x) = P(x)\lambda_1^t + Q(x)\lambda_2^t = \frac{1}{\sqrt{1+4x^2}}(\lambda_1^{t+1} - \lambda_2^{t+1}).$$

As we have defined, the initials are $m^+(P_{-1}, x) = 0$ and $m^+(P_0, x) = 1$, from which we can get the result for all $t \geq -1$. 

Lemma 3.5 Suppose $t \geq 4$. If $t$ is even, then

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

If $t$ is odd, then

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

Proof. From Corollary 2.6 we know that

$$\frac{1}{1 + x^2} \leq \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} \leq 1.$$

By the definitions of $\lambda_1$ and $\lambda_2$, we conclude that $\lambda_1 > 0$ and $\lambda_2 < 0$ for any $x$. By Lemma 3.4 if $t$ is even, then

$$\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} - \frac{2}{1 + \sqrt{1 + 4x^2}} = \frac{\lambda_1^{t-3} - \lambda_2^{t-3}}{\lambda_1^{t-2} - \lambda_2^{t-2}} - \frac{1}{\lambda_1} = -\frac{\lambda_2^{t-3}(\lambda_1 - \lambda_2)}{\lambda_1(\lambda_1^{t-2} - \lambda_2^{t-2})} > 0.$$

Thus,

$$\frac{2}{1 + \sqrt{1 + 4x^2}} < \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} \leq 1.$$
If $t$ is odd, then obviously
\[ \frac{1}{1 + x^2} \leq \frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} < \frac{2}{1 + \sqrt{1 + 4x^2}}. \]

Now we deal with the case $\Delta = 4$ and $t \geq 3$.

**Theorem 3.6** Among trees with $n$ vertices and two vertices of maximum degree $\Delta = 4$, the maximal energy tree has as many as possible 2-branches. The maximal energy tree is the graph $T_b$ if $t = 4$, and the graph $T_a$ otherwise, where $t = n + 4 - 4\Delta$.

**Proof.** By Eqs. (2), (3), (4) and (5), we have
\[
E(T_a) - E(T_b) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{m^+(T_a,x) - m^+(T_b,x)}{m^+(T_b,x)}\right) dx
\]
\[= \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{(\Delta - 2)x^6(x^2 - (\Delta - 2))}{B_1 + B_2 \frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)}}\right) dx. \tag{7}\]

We first consider the case that $t$ is odd and $t \geq 5$. In the proof of Theorem 3.2, we know that the function $\frac{1}{x^2} \log \left(1 + \frac{m^+(T_a,x) - m^+(T_b,x)}{m^+(T_b,x)}\right)$ is uniformly convergent. Therefore, by Eq. (7) and Lemma 3.5, we have
\[
E(T_a) - E(T_b) > \frac{2}{\pi} \int_{\sqrt{2}}^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{2x^6(x^2 - 2)}{B_1 + B_2 \frac{m^+(P_{t-4},x)}{1 + \sqrt{1 + 4x^2}}}ight) dx
\]
\[> \frac{2}{\pi} \cdot 0.02088 > 0. \]

If $t$ is even, we want to find $t$ and $x$ satisfying that
\[
\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} < \frac{2}{-1 + \sqrt{1 + 4x^2}}. \tag{8}\]

It is equivalent to solve
\[
\frac{\lambda_1^{t-3} - \lambda_2^{t-3}}{\lambda_1^{t-2} - \lambda_2^{t-2}} < -\frac{1}{\lambda_2},
\]
which means to solve
\[
\left(\frac{\lambda_1}{-\lambda_2}\right)^{t-3} > -2\lambda_2,
\]
that is
\[
\left(\frac{1 + \sqrt{1 + 4x^2}}{2x}\right)^{2t-6} > \sqrt{1 + 4x^2} - 1.
\]
Thus,
\[ 2t - 6 > \log_{1 + \sqrt{1 + 4x^2}}(\sqrt{1 + 4x^2} - 1). \]

Since for \( x \in (0, +\infty) \), \( \frac{1 + \sqrt{1 + 4x^2}}{2x} \) 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
\[
\log_{1 + \sqrt{1 + 4x^2}}(\sqrt{1 + 4x^2} - 1) \leq \log_{10}(\sqrt{101} - 1) < 23.
\]

Therefore, when \( t \geq 15 \), i.e., \( 2t - 6 > 23 \), we have that Ineq. (8) 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. (7), we have
\[
E(T_a) - E(T_b) > \frac{2}{\pi} \int_{\sqrt{2}}^{+\infty} \frac{1}{x^2} \log \left( 1 + \frac{2x^6(x^2 - 2)}{B_1 + B_2} \right) dx + \frac{2}{\pi} \int_{5}^{\sqrt{2}} \frac{1}{x^2} \log \left( 1 + \frac{2x^6(x^2 - 2)}{B_1 + B_2 - \frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx
\]
\[
+ \frac{2}{\pi} \int_{0}^{\sqrt{2}} \frac{1}{x^2} \log \left( 1 + \frac{2x^6(x^2 - 2)}{B_1 + B_2 - 1 + \sqrt{1 + 4x^2}} \right) dx
\]
\[
> \frac{2}{\pi} \cdot 0.003099 > 0.
\]

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

The proof is thus complete.

The following theorem gives the result for the cases of \( \Delta = 5, 6, 7 \).

**Theorem 3.7** For trees with \( n \) vertices and two vertices of maximum degree \( \Delta \), let \( t = n - 4\Delta + 4 \geq 3 \). Then

(i) for \( \Delta = 5 \), the maximal energy tree is the graph \( T_a \) if \( t \) is odd and \( 3 \leq t \leq 89 \), and the graph \( T_b \) otherwise.

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

(iii) for \( \Delta = 7 \), the maximal energy tree is the graph \( T_b \) for any \( t \geq 3 \).

*Proof.* In the proof of Theorem 3.2, we know that the function \( \frac{1}{x^2} \log \left( 1 + \frac{m(T_a,x) - m(T_b,x)}{m(T_b,x)} \right) \) is uniformly convergent. We consider the following cases separately:

(i) \( \Delta = 5 \).
If $t$ is even, we want to find $t$ and $x$ satisfying that

$$\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} < \frac{2.1}{1 + \sqrt{1 + 4x^2}}. \tag{9}$$

It is equivalent to solve

$$\frac{\lambda_1^{t-3} - \lambda_2^{t-3}}{\lambda_1^{t-2} - \lambda_2^{t-2}} < \frac{2.1}{2\lambda_1},$$

which means to solve

$$\left(\frac{\lambda_1}{-\lambda_2}\right)^{t-3} > -\frac{2.1\lambda_2 + 2\lambda_1}{0.1\lambda_1},$$

that is,

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

Thus,

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

Since for $x \in (0, +\infty)$, $\frac{1 + \sqrt{1 + 4x^2}}{2x}$ is decreasing and $-\frac{42}{\sqrt{1 + 4x^2} + 1}$ is increasing, we have that $\log_{\frac{1 + \sqrt{1 + 4x^2}}{2x}}\left(41 - \frac{42}{\sqrt{1 + 4x^2} + 1}\right)$ is increasing. Thus, if $x \in (0, \sqrt{3})$, we have

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

Therefore, when $t \geq 10$, i.e., $2t - 6 > 13$, we have that Ineq. (9) holds for $x \in (0, \sqrt{3}]$. Thus, if $t$ is even and $t \geq 10$, from Eq. (7) and Lemma 3.5, we have

$$E(T_a) - E(T_b) < \frac{2}{\pi} \int_{\sqrt{3}}^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{3x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}}\right) dx$$
$$+ \frac{2}{\pi} \int_{0}^{\sqrt{3}} \frac{1}{x^2} \log \left(1 + \frac{3x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}}\right) dx$$
$$< \frac{2}{\pi} \cdot (-4.43 \times 10^{-4}) < 0.$$

If $t$ is odd, we want to find $t$ and $x$ satisfying that

$$\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} > 1.99 \frac{1 + \sqrt{1 + 4x^2}}{1 + x^2}, \tag{10}$$

that is

$$2t - 6 > \log_{\frac{1 + \sqrt{1 + 4x^2}}{2x}}\left(399 - \frac{398}{\sqrt{1 + 4x^2} + 1}\right).$$

Since for $x \in (0, +\infty)$, $\log_{\frac{1 + \sqrt{1 + 4x^2}}{2x}}\left(399 - \frac{398}{\sqrt{1 + 4x^2} + 1}\right)$ is increasing, we have that if $x \in [\sqrt{3}, 390]$,

$$\log_{\frac{1 + \sqrt{1 + 4x^2}}{2x}}\left(399 - \frac{398}{\sqrt{1 + 4x^2} + 1}\right) < 4671.$$
Therefore, for $t \geq 2339$, i.e., $2t - 6 \geq 4671$, we have that Ineq. (10) holds for $x \in [\sqrt{3}, 390]$. Thus, if $t$ is odd and $t \geq 2339$, from Eq. (7) and Lemma 3.5, we have

$$E(T_a) - E(T_b) < \frac{2}{\pi} \int_{\sqrt{3}}^{\infty} \frac{1}{x^2} \log \left(1 + \frac{3x^6(x^2 - 3)}{B_1 + B_2 \frac{1.99}{1 + \sqrt{1 + 4x^2}}} \right) dx$$

$$+ \frac{2}{\pi} \int_{0}^{\sqrt{3}} \frac{1}{x^2} \log \left(1 + \frac{3x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx$$

$$+ \frac{2}{\pi} \int_{0}^{390} \frac{1}{x^2} \log \left(1 + \frac{3x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx$$

$$< \frac{2}{\pi} \cdot (-6.66 \times 10^{-6}) < 0.$$ 

For any even $t$ satisfying that $4 \leq t \leq 8$ and any odd $t$ satisfying that $3 \leq t \leq 2337$, by comparing the energies of the two graphs directly by matlab program, we get that $E(T_a) > E(T_b)$ for any odd $t$ satisfying $3 \leq t \leq 89$, and $E(T_a) < E(T_b)$ for the other cases.

(ii) $\Delta = 6.$

If $t$ is even and $t \geq 4$, from Eq. (7) and Lemma 3.5, we have

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

$$+ \frac{2}{\pi} \int_{0}^{2} \frac{1}{x^2} \log \left(1 + \frac{4x^6(x^2 - 4)}{B_1 + B_2} \right) dx$$

$$< \frac{2}{\pi} \cdot (-0.02027) < 0.$$ 

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

$$E(T_a) - E(T_b) < \frac{2}{\pi} \int_{22}^{\infty} \frac{1}{x^2} \log \left(1 + \frac{4x^6(x^2 - 4)}{B_1 + B_2 \frac{1}{1 + \sqrt{1 + 4x^2}}} \right) dx$$

$$+ \frac{2}{\pi} \int_{0}^{22} \frac{1}{x^2} \log \left(1 + \frac{4x^6(x^2 - 4)}{B_1 + B_2 \frac{2}{1 + \sqrt{1 + 4x^2}}} \right) dx$$

$$< \frac{2}{\pi} \cdot (-2.56 \times 10^{-4}) < 0.$$
For any odd \( t \) satisfying that \( 3 \leq t \leq 25 \), by comparing the energies of the two graphs directly by matlab programm, we get that \( E(T_a) > E(T_b) \) for \( t = 3, 5, 7 \), and \( E(T_a) < E(T_b) \) for the other cases.

(iii) \( \Delta = 7 \).

If \( t \) is even and \( t \geq 4 \), by the same method as used in (ii), we get that \( E(T_a) - E(T_b) < \frac{2}{\pi} \cdot (-0.04445) < 0 \).

If \( t \) is odd and \( t \geq 5 \), we have that

\[
E(T_a) - E(T_b) < \frac{2}{\pi} \int_0^{\frac{5}{\sqrt{5}}} \frac{dx}{x^2} \log \left( 1 + \frac{5x^6(x^2 - 5)}{B_1 + B_2 \frac{1}{1+x^2}} \right)
\]

\[
+ \frac{2}{\pi} \int_{\frac{5}{\sqrt{5}}}^{+\infty} \frac{dx}{x^2} \log \left( 1 + \frac{5x^6(x^2 - 5)}{B_1 + B_2 \frac{2}{1+\sqrt{1+4x^2}}} \right)
\]

\[
< \frac{2}{\pi} \cdot (-0.01031) < 0.
\]

For \( t = 3 \), we can compare the energies of the two graphs directly by matlab programm and get that \( E(T_a) < E(T_b) \).

The proof is now complete.

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