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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 $\Delta \geqslant 3$ and $t \geqslant 3$, 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 Li et al. (2009) [16] proved that among trees of order n with two vertices of maximum degree Δ, the maximal energy tree is either the graph T_a or the graph T_b, where $t = n + 4 - 4\Delta \geqslant 3$. 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 $\Delta \geqslant 7$ and any $t \geqslant 3$, while the maximal energy tree is T_a for $\Delta = 3$ and any $t \geqslant 3$. Moreover, for $\Delta = 4$, the maximal energy tree is T_a for all $t \geqslant 3$ but one exception that $t = 4$, for which T_b is the maximal energy tree. For $\Delta = 5$, the maximal energy tree is T_b for all $t \geqslant 3$ but 44 exceptions that t is both odd and $3 \leqslant t \leqslant 89$, for which T_a is the maximal energy tree. For $\Delta = 6$, the maximal energy tree is T_b for all $t \geqslant 3$ but three exceptions that $t = 3, 5, 7$, for which T_a is the maximal energy tree. One can see that for most cases of Δ, T_b is the maximal energy tree, $\Delta = 5$ is a turning point, and $\Delta = 3$ and 4 are exceptional cases, which means that for all chemical trees (whose maximum degrees are at most 4) with two vertices of maximum degree at least 3, T_a has maximal energy, with only one exception $T_a(4, 4)$.

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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 $\lambda_1, \lambda_2, \ldots, \lambda_n$ 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 [6]. If T is a tree of order n, then by Coulson integral formula [2,3,5,8], 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 of coefficients in the matching polynomial, this immediately motivates us to introduce a new graph polynomial

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

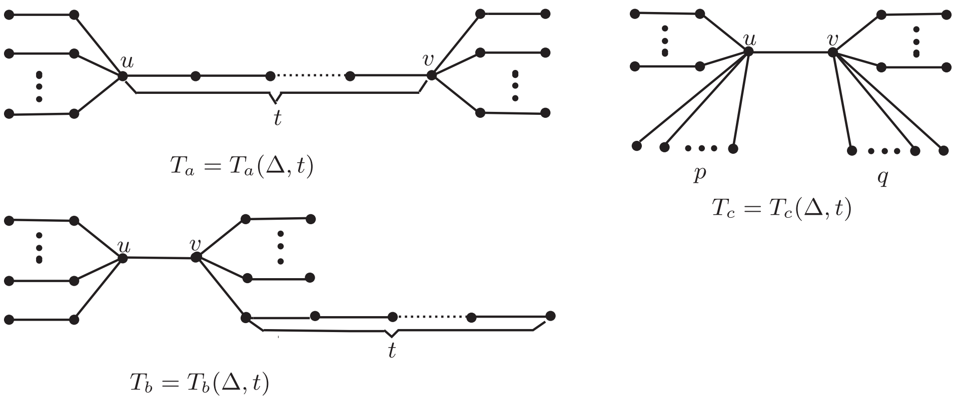
Then we have

$$E(T) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log m^+(T, x) dx. \tag{1}$$

Although $m^+(G, x)$ is nothing new but $m^+(G, x) = (ix)^n m(G, (ix)^{-1})$, 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 notations not defined here, we refer to the book of Bondy and Murty [1].

Graphs with extremal energies are interested in the 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 (Δ), the maximal energy tree has exactly one branching vertex (of degree Δ) 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 [18] 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 pendant vertex attached to a vertex of degree two is called a 2-*branch*.



$$d(u) = d(v) = \Delta, \ t = n - 4\Delta + 4, \ |p - q| \leq 1.$$

Fig. 1. The maximal energy trees with n vertices and two vertices u, v of maximum degree Δ.

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

(1) If $n \leqslant 4\Delta - 2$*, then the maximal energy tree is the graph* $T_c = T_c(\Delta, t)$*, depicted in Fig. 1, in which the numbers of pendant vertices attached to the two branching vertices* u *and* v *differ by at most 1.*

(2) If $n \geqslant 4\Delta - 1$*, 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 Fig. 1.*

From Theorem 1.1, one can see that for $n \geqslant 4\Delta - 1$, they could not determine which one of the trees 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 trees T_a and T_b has the maximal energy, solving this unsolved problem. It turns out 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 $n \geqslant 0$*, defining* $m^+(\overline{K_0}, x) = 1$*, where both* K_0 *and* $\overline{K_0}$ *are the null graph.*

Similar to the properties of a 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*

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

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,*

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

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 [19].

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

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

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 Δ 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 $t \geqslant 2$ and $E(T_a(\Delta, 2)) = E(T_b(\Delta, 2))$ for any $\Delta \geqslant 2$, we always assume that $\Delta \geqslant 3$ and $t \geqslant 3$.

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:

$$m^+(T_a, x) = (1 + x^2)^{2\Delta - 5}(A_1 m^+(P_{t-3}, x) + A_2 m^+(P_{t-4}, x)) \quad (2)$$

and

$$m^+(T_b, x) = (1 + x^2)^{2\Delta-5}(B_1 m^+(P_{t-3}, x) + B_2 m^+(P_{t-4}, x)). \quad (3)$$

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

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

Now we give one of our main results.

Theorem 3.2. *Among trees with n vertices and two vertices of maximum degree Δ, the maximal energy tree has as many as possible 2-branches. If $\Delta \geqslant 8$ and $t \geqslant 3$, then the maximal energy tree is the graph T_b, where $t = n + 4 - 4\Delta$.*

Proof. From Eq. (1), we have

$$\begin{aligned} E(T_a) - E(T_b) &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\log\frac{m^+(T_a, x)}{m^+(T_b, x)}dx \\ &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\log\left(1 + \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)}\right)dx. \end{aligned} \quad (5)$$

We use $g(\Delta, t, x)$ to express

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

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

$$\frac{1}{x^2}\cdot\frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_a, x)} \leqslant g(\Delta, t, x) \leqslant \frac{1}{x^2}\cdot\frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)}. \quad (6)$$

So,

$$\begin{aligned} &\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\cdot\frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_a, x)}dx \leqslant E(T_a) - E(T_b) \\ &\quad\leqslant \frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\cdot\frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)}dx. \end{aligned}$$

By Corollary 2.6, we have $m^+(P_{t-4}, x) \leqslant m^+(P_{t-3}, x)$ and $m^+(P_{t-4}, x) \geqslant \frac{m^+(P_{t-3},x)}{1+x^2}$ for $\Delta \geqslant 3$ and $t \geqslant 4$. So, we have

$$\begin{aligned} &E(T_a) - E(T_b) \\ &\quad\leqslant \frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\cdot\frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)}dx \\ &\quad= \frac{2}{\pi}\int_0^{+\infty}\frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))m^+(P_{t-3}, x)}{B_1 m^+(P_{t-3}, x) + B_2 m^+(P_{t-4}, x)}dx \\ &\quad\leqslant \frac{2}{\pi}\int_{\sqrt{\Delta-2}}^{+\infty}\frac{(\Delta - 2)x^4(x^2 - (\Delta - 2))}{B_1 + B_2/(1 + x^2)}dx - \frac{2}{\pi}\int_0^{\sqrt{\Delta-2}}\frac{(\Delta - 2)x^4(\Delta - 2 - x^2)}{B_1 + B_2}dx. \end{aligned}$$

We look at the last two parts separately. The first part is

$$\begin{aligned}
&\frac{2}{\pi}\int_{\sqrt{\Delta-2}}^{+\infty}\frac{(\Delta-2)x^4(x^2-(\Delta-2))}{B_1+B_2/(1+x^2)}dx\\
&=\frac{2}{\pi}\int_{\sqrt{\Delta-2}}^{+\infty}\frac{(\Delta-2)x^4(x^2-(\Delta-2))}{(\Delta+3)x^8+(3\Delta^2+8)x^6+(\Delta^2+6\Delta+5)x^4+(2\Delta+4)x^2+1}dx\\
&<\frac{2}{\pi}\int_{\sqrt{\Delta-2}}^{+\infty}\frac{(\Delta-2)x^4(x^2-(\Delta-2))}{(\Delta+3)x^8}dx=\frac{2}{\pi}\cdot\frac{2\sqrt{\Delta-2}}{3(\Delta+3)}.
\end{aligned}$$

The second part is

$$\begin{aligned}
&\frac{2}{\pi}\int_0^{\sqrt{\Delta-2}}\frac{(\Delta-2)x^4(\Delta-2-x^2)}{B_1+B_2}dx\\
&=\frac{2}{\pi}\int_0^{\sqrt{\Delta-2}}\frac{(\Delta-2)x^4(\Delta-2-x^2)}{h(\Delta,x)}dx\\
&>\frac{2}{\pi}\int_0^{1}\frac{(\Delta-2)x^4(\Delta-2-x^2)}{\frac{5\Delta^2+11\Delta+26}{2}(x^2+1)}dx+\frac{2}{\pi}\int_1^{\sqrt{\Delta-2}}\frac{(\Delta-2)x^4(\Delta-2-x^2)}{(5\Delta^2+11\Delta+26)x^{10}}dx\\
&=\frac{2}{\pi}\left(\frac{-45\pi\Delta-34\Delta^2+74\Delta+30\pi-12+15\pi\Delta^2+\frac{4}{\sqrt{\Delta-2}}}{30(26+11\Delta+5\Delta^2)}\right),
\end{aligned}$$

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 $\Delta\geqslant 65$ we get that

$$\begin{aligned}
&E(T_a)-E(T_b)\\
&<\frac{2}{\pi}\cdot\frac{2\sqrt{\Delta-2}}{3(\Delta+3)}-\frac{2}{\pi}\left(\frac{-45\pi\Delta-34\Delta^2+74\Delta+30\pi-12+15\pi\Delta^2+\frac{4}{\sqrt{\Delta-2}}}{30(26+11\Delta+5\Delta^2)}\right)\leqslant 0.
\end{aligned}$$

For $t=3$, we have $m^+(P_{t-4},x)=m^+(P_{-1},x)=0$. By a similar method as above, we can get that $E(T_a)-E(T_b)<0$ when $\Delta\geqslant 24$.

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

For $8\leqslant\Delta\leqslant 64$, we can get that

$$E(T_a)-E(T_b)\leqslant\frac{2}{\pi}\cdot f(\Delta,x)<0$$

by direct calculations, using a computer with the Maple programm, as shown in Table 1, where

$$f(\Delta,x)=\int_{\sqrt{\Delta-2}}^{+\infty}\frac{(\Delta-2)x^4(x^2-(\Delta-2))}{B_1+\frac{B_2}{1+x^2}}dx-\int_0^{\sqrt{\Delta-2}}\frac{(\Delta-2)x^4(\Delta-2-x^2)}{B_1+B_2}dx.$$

The proof is thus complete. □

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

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 $n\geqslant 11$, then the maximal energy tree is the graph T_a.*

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

Δ	$f(\Delta, x)$	Δ	$f(\Delta, x)$	Δ	$f(\Delta, x)$	Δ	$f(\Delta, x)$
8	−0.00377	23	−0.20792	38	−0.29961	53	−0.35353
9	−0.02418	24	−0.21611	39	−0.30403	54	−0.35638
10	−0.04352	25	−0.22390	40	−0.30830	55	−0.35917
11	−0.06168	26	−0.23132	41	−0.31244	56	−0.36188
12	−0.07866	27	−0.23841	42	−0.31644	57	−0.36454
13	−0.09452	28	−0.24518	43	−0.32032	58	−0.36713
14	−0.10933	29	−0.25165	44	−0.32409	59	−0.36965
15	−0.12317	30	−0.25786	45	−0.32774	60	−0.37213
16	−0.13613	31	−0.26381	46	−0.33129	61	−0.37454
17	−0.14829	32	−0.26953	47	−0.33473	62	−0.37691
18	−0.15972	33	−0.27502	48	−0.33808	63	−0.37922
19	−0.17048	34	−0.28031	49	−0.34134	64	−0.38148
20	−0.18063	35	−0.28540	50	−0.34451	65	−0.38369
21	−0.19022	36	−0.29031	51	−0.34759	66	−0.38586
22	−0.19931	37	−0.29504	52	−0.35060	67	−0.38798

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

$$\begin{aligned} E(T_a) - E(T_b) &\geqslant \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2} \cdot \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_a, x)} dx \\ &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2} \cdot \frac{x^6(x^2-1)m^+(P_{t-3}, x)}{A_1 m^+(P_{t-3}, x) + A_2 m^+(P_{t-4}, x)} dx \\ &\geqslant \frac{2}{\pi}\int_1^{+\infty} \frac{x^4(x^2-1)}{A_1 + A_2} dx - \frac{2}{\pi}\int_0^1 \frac{x^4(1-x^2)}{A_1 + \frac{A_2}{1+x^2}} dx \\ &= \frac{2}{\pi}\int_1^{+\infty} \frac{x^4(x^2-1)}{x^{10} + 18x^8 + 41x^6 + 33x^4 + 10x^2 + 1} dx \\ &\quad - \frac{2}{\pi}\int_0^1 \frac{x^4(1-x^2)}{7x^8 + 34x^6 + 32x^4 + 10x^2 + 1} dx \\ &> \frac{2}{\pi} \cdot 0.00996 > 0. \end{aligned}$$

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

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

We now we give two lemmas about the properties of the new polynomial $m^+(P_t, x)$ for our later use.

Lemma 3.4. *For $t \geqslant -1$, the polynomial $m^+(P_t, x)$ has the following form:*

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

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, $m^+(P_t, x) = m^+(P_{t-1}, x) + x^2 m^+(P_{t-2}, x)$ for any $t \geqslant 1$. Thus, it satisfies the recursive formula $h(t, x) = h(t-1, x) + x^2 h(t-2, x)$, 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,

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

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 $t \geqslant -1$. □

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

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

If t is odd, then

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

Proof. From Corollary 2.6, we know that

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

By the definitions of λ_1 and λ_2, we conclude that $\lambda_1 > 0$ and $\lambda_2 < 0$ for any x. By Lemma 3.4, if t is even, then

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

Thus,

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

If t is odd, then obviously

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

Now we are ready to deal with the case $\Delta = 4$ and $t \geqslant 3$.

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)–(5), we have

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

$$= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\log\left(1 + \frac{(\Delta-2)x^6(x^2-(\Delta-2))}{B_1 + B_2\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)}}\right)dx. \quad (7)$$

We first consider the case that t is odd and $t \geqslant 5$. By Eq. (7) and Lemma 3.5, we have

$$E(T_a) - E(T_b)$$

$$> \frac{2}{\pi}\int_{\sqrt{2}}^{+\infty} \frac{1}{x^2}\log\left(1 + \frac{2x^6(x^2-2)}{B_1 + B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx + \frac{2}{\pi}\int_0^{\sqrt{2}} \frac{1}{x^2}\log\left(1+\frac{2x^6(x^2-2)}{B_1+B_2\frac{1}{1+x^2}}\right)dx$$

$$> \frac{2}{\pi}\cdot 0.02088 > 0.$$

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

$$\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} < \frac{2}{-1+\sqrt{1+4x^2}}. \quad (8)$$

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,

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

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 $\log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(\sqrt{1+4x^2} - 1\right)$ is increasing. Thus, if $x \in [\sqrt{2}, 5]$, then

$$\log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(\sqrt{1+4x^2} - 1\right) \leqslant \log_{\frac{1+\sqrt{101}}{10}}\left(\sqrt{101} - 1\right) < 23.$$

Therefore, when $t \geqslant 15$, 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 $t \geqslant 15$, from Eq. (7) we have

$$\begin{aligned}
&E(T_a) - E(T_b) \\
&\quad > \frac{2}{\pi}\int_5^{+\infty} \frac{1}{x^2}\log\left(1 + \frac{2x^6(x^2-2)}{B_1 + B_2}\right)dx + \frac{2}{\pi}\int_{\sqrt{2}}^{5} \frac{1}{x^2}\log\left(1 + \frac{2x^6(x^2-2)}{B_1 + B_2\frac{2}{-1+\sqrt{1+4x^2}}}\right)dx \\
&\quad + \frac{2}{\pi}\int_0^{\sqrt{2}} \frac{1}{x^2}\log\left(1 + \frac{2x^6(x^2-2)}{B_1 + B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx \\
&\quad > \frac{2}{\pi}\cdot 0.003099 > 0.
\end{aligned}$$

For $t = 3$ and any even t with $4 \leqslant t \leqslant 14$, by computing the energies of the two graphs directly by a computer with the Maple programm, 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 now 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 Δ, let $t = n - 4\Delta + 4 \geqslant 3$. Then*

(i) for $\Delta = 5$, the maximal energy tree is the graph T_a if t is odd and $3 \leqslant t \leqslant 89$, 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 $t \geqslant 3$.

Proof. 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 $x \in (0, \sqrt{3}]$,

$$\log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(41 - \frac{42}{\sqrt{1+4x^2}+1}\right) \leqslant \log_{\frac{1+\sqrt{13}}{2\sqrt{3}}}\left(41 - \frac{42}{1+\sqrt{13}}\right) < 13.$$

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

$$\begin{aligned} &E(T_a) - E(T_b) \\ &\quad < \frac{2}{\pi}\int_{\sqrt{3}}^{+\infty} \frac{1}{x^2} \log\left(1 + \frac{3x^6(x^2-3)}{B_1 + B_2\frac{2}{1+\sqrt{1+4x^2}}}\right) dx \\ &\quad + \frac{2}{\pi}\int_{0}^{\sqrt{3}} \frac{1}{x^2} \log\left(1 + \frac{3x^6(x^2-3)}{B_1 + B_2\frac{2.1}{1+\sqrt{1+4x^2}}}\right) dx \\ &\quad < \frac{2}{\pi}\cdot(-4.43 \times 10^{-4}) < 0. \end{aligned}$$

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

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

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 $x \in [\sqrt{3}, 390]$, then

$$\log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(399 - \frac{398}{\sqrt{1+4x^2}+1}\right) < 4671.$$

Therefore, for $t \geqslant 2339$, i.e., $2t - 6 \geqslant 4671$, we have that Ineq. (10) holds for $x \in [\sqrt{3}, 390]$. Thus, if t is odd and $t \geqslant 2339$, from Eq. (7) and Lemma 3.5 we have

$$\begin{aligned} &E(T_a) - E(T_b) \\ &\quad < \frac{2}{\pi}\int_{390}^{+\infty} \frac{1}{x^2} \log\left(1 + \frac{3x^6(x^2-3)}{B_1+B_2\frac{1}{1+x^2}}\right) dx + \frac{2}{\pi}\int_{\sqrt{3}}^{390} \frac{1}{x^2} \log\left(1 + \frac{3x^6(x^2-3)}{B_1 + B_2\frac{1.99}{1+\sqrt{1+4x^2}}}\right) dx \\ &\quad + \frac{2}{\pi}\int_{0}^{\sqrt{3}} \frac{1}{x^2} \log\left(1 + \frac{3x^6(x^2-3)}{B_1 + B_2\frac{2}{1+\sqrt{1+4x^2}}}\right) dx \\ &\quad < \frac{2}{\pi}\cdot(-6.66 \times 10^{-6}) < 0. \end{aligned}$$

For any even t with $4 \leqslant t \leqslant 8$ and any odd t with $3 \leqslant t \leqslant 2337$, by computing the energies of the two graphs directly by a computer with the Matlab programm, we get that $E(T_a) > E(T_b)$ for any odd t with $3 \leqslant t \leqslant 89$, and $E(T_a) < E(T_b)$ for the other cases.

(ii) $\Delta = 6$.

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

$$\begin{aligned} E(T_a) - E(T_b) &< \frac{2}{\pi}\int_2^{+\infty} \frac{1}{x^2}\log\left(1+\frac{4x^6(x^2-4)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx \\ &+\frac{2}{\pi}\int_0^2 \frac{1}{x^2}\log\left(1+\frac{4x^6(x^2-4)}{B_1+B_2}\right)dx \\ &< \frac{2}{\pi}\cdot(-0.02027) < 0. \end{aligned}$$

If t is odd, similar to the proof in (i), we can show that when $t \geqslant 27$ 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 $t \geqslant 27$, we have

$$\begin{aligned} &E(T_a) - E(T_b) \\ &< \frac{2}{\pi}\int_{22}^{+\infty} \frac{1}{x^2}\log\left(1+\frac{4x^6(x^2-4)}{B_1+B_2\frac{1}{1+x^2}}\right)dx + \frac{2}{\pi}\int_2^{22} \frac{1}{x^2}\log\left(1+\frac{4x^6(x^2-4)}{B_1+B_2\frac{1}{1+\sqrt{1+4x^2}}}\right)dx \\ &+\frac{2}{\pi}\int_0^2 \frac{1}{x^2}\log\left(1+\frac{4x^6(x^2-4)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx \\ &< \frac{2}{\pi}\cdot(-2.56\times 10^{-4}) < 0. \end{aligned}$$

For any odd t with $3 \leqslant t \leqslant 25$, by computing the energies of the two graphs directly by a computer with the Matlab programm, 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.

(iii) $\Delta = 7$.

If t is even and $t \geqslant 4$, 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 $t \geqslant 5$, we have that

$$\begin{aligned} E(T_a) - E(T_b) &< \frac{2}{\pi}\int_{\sqrt{5}}^{+\infty} \frac{1}{x^2}\log\left(1+\frac{5x^6(x^2-5)}{B_1+B_2\frac{1}{1+x^2}}\right)dx \\ &+\frac{2}{\pi}\int_0^{\sqrt{5}} \frac{1}{x^2}\log\left(1+\frac{5x^6(x^2-5)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx \\ &< \frac{2}{\pi}\cdot(-0.01031) < 0. \end{aligned}$$

For $t = 3$, we can compute the energies of the two graphs directly by a computer with the Matlab programm and get that $E(T_a) < E(T_b)$.

The proof is now complete. $\square$

Chemical trees are interested in chemical literature. A chemical tree is a tree whose maximum degree is at most 4. From the above theorems, one can observe the following interesting result:

Corollary 3.8. *For all chemical trees of order n with two vertices of maximum degree at least 3, the graph T_a has maximal energy, with only one exception that $\Delta = 4$ and $t = 4$, for which $T_b(4, 4)$ has larger energy than $T_a(4, 4)$.*

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