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 Δ, 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 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 $t \geq 3$ but 44 exceptions that t is both 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 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

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

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 [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

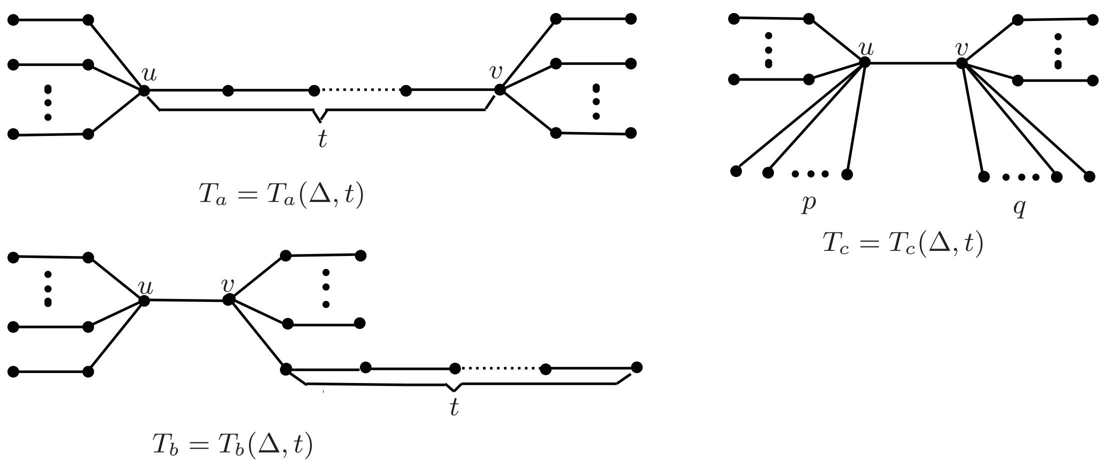
$$E(T)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\log m^+(T,x)dx. \tag{1}$$

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 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*.

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 $n \leq 4\Delta - 2$, *then the maximal energy tree is the graph* $T_c = T_c(\Delta, t)$, *depicted in Figure 1.1, in which the numbers of pendant 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.*



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

Figure 1.1 The maximal energy trees with n vertices and two vertices u, v of maximum degree Δ.

From Theorem 1.1, one can see that for $n \geq 4\Delta - 1$, 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 $n \geq 0$, defining $m^+(\overline{K_0},x)=1$, where both K_0 and $\overline{K_0}$ are the null graph.

Similar to the properties of 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*

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

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*

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

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,*

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

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*

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

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

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:

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

and

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

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

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

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 $\Delta \geq 8$ 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

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

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

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

So,

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

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 $t \geq 4$. So, we have

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

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 $\Delta\geq 65$ we get that

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

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 $\Delta\geq 24$.

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 get that

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

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 $3\leq\Delta\leq 7$. 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.*

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

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

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

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

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

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 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

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

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

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

∎

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

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

$$\begin{aligned} E(T_a) - E(T_b) &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\log\left(1+\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_b,x)}\right)dx \\ &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\log\left(1+\frac{(\Delta-2)x^6(x^2-(\Delta-2))}{B_1+B_2\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)}}\right)dx. \end{aligned} \tag{7}$$

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

$$\begin{aligned} &E(T_a) - E(T_b) \\ > \ & \frac{2}{\pi}\int_{\sqrt{2}}^{+\infty} \frac{1}{x^2}\log\left(1+\frac{2x^6(x^2-2)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx + \frac{2}{\pi}\int_0^{\sqrt{2}} \frac{1}{x^2}\log\left(1+\frac{2x^6(x^2-2)}{B_1+B_2\frac{1}{1+x^2}}\right)dx \\ > \ & \frac{2}{\pi}\cdot 0.02088 > 0. \end{aligned}$$

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,

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

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

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

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

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

For $t = 3$ and any even t with $4 \le t \le 14$, 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 $t = n - 4\Delta + 4 \ge 3$. Then*
(i) for $\Delta = 5$, the maximal energy tree is the graph T_a if t is odd and $3 \le t \le 89$, 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 $t \ge 3$.

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

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

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

$$\begin{aligned} E(T_a)-E(T_b) &< \frac{2}{\pi}\int_{\sqrt{3}}^{+\infty}\frac{1}{x^2}\log\left(1+\frac{3x^6(x^2-3)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx \\ &\quad +\frac{2}{\pi}\int_0^{\sqrt{3}}\frac{1}{x^2}\log\left(1+\frac{3x^6(x^2-3)}{B_1+B_2\frac{2.1}{1+\sqrt{1+4x^2}}}\right)dx \\ &< \frac{2}{\pi}\cdot(-4.43\times 10^{-4}) < 0. \end{aligned}$$

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 $t \geq 2339$, 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

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

For any even t with $4 \leq t \leq 8$ and any odd t with $3 \leq t \leq 2337$, 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 $3 \leq t \leq 89$, 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

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

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

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

For any odd t with $3 \leq t \leq 25$, 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 $t \geq 4$, 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

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

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. ∎

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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