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_a 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.

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

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

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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

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

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

$$E(T)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\log\left[\sum_{k=0}^{\lfloor n/2\rfloor}m(T,k)x^{2k}\right]dx.$$

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

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

Then we have

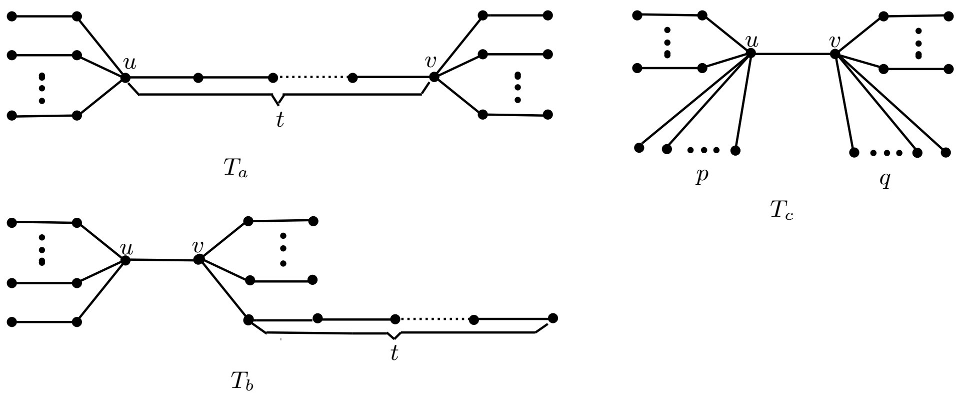
$$E(T)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\log m^+(T,x)dx. \tag{1}$$

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 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 the graph T_c depicted in Figure 1.1.



$d(u) = d_1$, $d(v) = d_2$, $t = n - 2d_1 - 2d_2 + 4$, $p \leq q$.

Figure 1.1 The maximal energy trees with n vertices and two vertices u and v of degree d_1 and d_2.

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*

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

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

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

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

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*

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

For convenience, we introduce the following notations:

$$\begin{aligned}
A_1 &= (x^2+1)(d_1x^6+d_2x^6+d_2x^4+d_1d_2x^4+d_1x^4+2x^4+2x^2+d_1x^2+d_2x^2+1),\\
A_2 &= x^2(x^2+1)(x^6+2x^4+d_1d_2x^4+d_1x^2+d_2x^2+x^2+1),\\
B_1 &= 2x^8+d_1x^8+6x^6+2d_1d_2x^6+d_1d_2x^4+2d_1x^4+4x^4+2d_2x^4+d_2x^2+d_1x^2\\
&\quad +3x^2+1,\\
B_2 &= x^2(x^2+1)(x^6+2x^4+d_1d_2x^4+d_1x^2+d_2x^2+x^2+1).
\end{aligned}$$

Using Lemmas 2.1 and 2.2 repeatedly, we can easily get the following two recursive formulas, where $t = n+4-2d_1-2d_2 \ge 3$:

$$m^+(T_a,x) = (1+x^2)^{d_1+d_2-5}(A_1m^+(P_{t-3},x)+A_2m^+(P_{t-4},x)), \tag{2}$$

and

$$m^+(T_b,x) = (1+x^2)^{d_1+d_2-5}(B_1m^+(P_{t-3},x)+B_2m^+(P_{t-4},x)), \tag{3}$$

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

$$m^+(T_a,x) - m^+(T_b,x) = (1+x^2)^{d_1+d_2-5}(d_2-2)x^6(x^2-(d_1-2))m^+(P_{t-3},x). \tag{4}$$

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 $t \ge 3$ and $d_1 > d_2 \ge 3$.

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 $1 \le k \le 3$, $d_2 \ge 7-k$ or $4 \le k \le 12$, $d_2 \ge 3$, the maximal energy tree is the graph T_b, where $t = n+4-2d_1-2d_2 \ge 3$.*

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

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

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

$$\begin{aligned} & E(T_a) - E(T_b) \\ \leq\ & \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2} \cdot \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_b, x)} dx \\ =\ & \frac{2}{\pi}\int_0^{+\infty} \frac{(d_2-2)x^4(x^2-(d_1-2))m^+(P_{t-3}, x)}{B_1 m^+(P_{t-3}, x) + B_2 m^+(P_{t-4}, x)} dx \\ \leq\ & \frac{2}{\pi}\int_{\sqrt{d_1-2}}^{+\infty} \frac{(d_2-2)x^4(x^2-(d_1-2))}{B_1 + B_2/(1+x^2)} dx + \frac{2}{\pi}\int_0^{\sqrt{d_1-2}} \frac{(d_2-2)x^4(x^2-(d_1-2))}{B_1+B_2} dx \\ <\ & \frac{2}{\pi}\int_{\sqrt{d_1-2}}^{+\infty} \frac{(d_2-2)x^4(x^2-(d_1-2))}{(d_1+3)x^8} dx + \frac{2}{\pi}\int_1^{\sqrt{d_1-2}} \frac{(d_2-2)x^4(x^2-(d_1-2))}{(5d_1d_2+6d_1+5d_2+26)x^{10}} dx \\ & + \frac{2}{\pi}\int_0^1 \frac{2(d_2-2)x^4(x^2-(d_1-2))}{(5d_1d_2+6d_1+5d_2+26)(x^2+1)} dx \\ =\ & \frac{2}{\pi} f(d_1, d_2). \end{aligned}$$

Where

$$\begin{aligned} f(d_1, d_2) &= \frac{2(d_2-2)}{3(d_1+3)\sqrt{d_1-2}} - \frac{d_2-2}{15(26+6d_1+5d_1d_2+5d_2)}\left(3d_1 - 11 + \frac{2}{(d_1-2)^{3/2}}\right) \\ & \quad - \frac{28d_2 - 40d_1d_2 + 80d_1 - 30\pi d_1 + 30\pi + 15\pi d_2 d_1 - 56 - 15\pi d_2}{30(26+6d_1+5d_1d_2+5d_2)}. \end{aligned}$$

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

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

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 $m^+(P_{t-4},x) = m^+(P_{-1},x) = 0$. 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.

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

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

$$
\begin{aligned}
h_1 &= -\frac{2(d_2-2)}{3(d_2+k+3)^2\sqrt{d_2+k-2}}, \\
h_2 &= -\frac{d_2-2}{3(d_2+k+3)(d_2+k-2)^{3/2}}, \\
h_3 &= -\frac{-30\pi-40d_2+15d_2\pi+80}{780+330d_2+180k+150(d_2+k)d_2}, \\
h_4 &= \frac{108d_2-56-30\pi(d_2+k)-40(d_2+k)d_2+15d_2\pi(d_2+k)+30\pi-15d_2\pi+80k}{(780+330d_2+180k+150(d_2+k)d_2)^2} \\
& \quad \cdot(180+150d_2), \\
h_5 &= -\frac{\frac{d_2-2}{5}-\frac{d_2-2}{5(d_2+k-2)^{5/2}}}{26+11d_2+6k+5(d_2+k)d_2}, \\
h_6 &= \frac{\left(\frac{2}{15(d_2+k-2)^{3/2}}+\frac{3d_2+3k-11}{15}\right)(d_2-2)(5d_2+6)}{(26+11d_2+6k+5(d_2+k)d_2)^2}.
\end{aligned}
$$

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,

$$\begin{aligned}
\frac{h_5+h_6}{m} &= (2(d_2+k-2)+(3d_2+3k-11)(d_2+k-2)^{5/2})(5d_2+6) \\
&\quad -3(26+11d_2+6k+5(d_2+k)d_2)((d_2+k-2)^{5/2}-1) \\
&= (-70d_2^3-140d_2^2k+136d_2^2-70d_2k^2-8d_2k+296d_2-144k^2+576k-576) \\
&\quad \cdot\sqrt{d_2+k-2}+25d_2^2+25d_2+25d_2k+30k+54 \\
&< 0,
\end{aligned}$$

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 $m^+(P_{t-4},x)=m^+(P_{-1},x)=0$. 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 Θ' 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 Θ'' becomes a lower bound for $\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)}$. By numerical testing we can find the proper Θ' and Θ''.

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

$$\begin{aligned} E(T_a) - E(T_b) &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\log\left(1+\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_b,x)}\right)dx \\ &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\log\left(1+\frac{(d_2-2)x^6(x^2-(d_1-2))}{B_1+B_2\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)}}\right)dx. \end{aligned} \tag{8}$$

We first consider the case that t is odd and $t \geq 5$. By Eq. (8) and Lemma 3.6, we have

$$\begin{aligned} & E(T_a) - E(T_b) \\ > \ & \frac{2}{\pi}\int_{\sqrt{2}}^{+\infty} \frac{1}{x^2}\log\left(1+\frac{x^6(x^2-2)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx + \frac{2}{\pi}\int_0^{\sqrt{2}} \frac{1}{x^2}\log\left(1+\frac{x^6(x^2-2)}{B_1+B_2\frac{1}{1+x^2}}\right)dx \\ > \ & \frac{2}{\pi}\cdot 0.011179 > 0. \end{aligned}$$

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

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

It is equivalent to solve

$$\frac{\lambda_1^{t-3}-\lambda_2^{t-3}}{\lambda_1^{t-2}-\lambda_2^{t-2}} < -\frac{1}{\lambda_2} \qquad \text{i. e.,} \qquad \left(\frac{1+\sqrt{1+4x^2}}{2x}\right)^{2t-6} > \sqrt{1+4x^2}-1 \ .$$

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

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

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

$$\begin{aligned}
& E(T_a) - E(T_b) \\
> \; & \frac{2}{\pi}\int_5^{+\infty} \frac{1}{x^2}\log\left(1+\frac{x^6(x^2-2)}{B_1+B_2}\right)dx + \frac{2}{\pi}\int_{\sqrt{2}}^{5} \frac{1}{x^2}\log\left(1+\frac{x^6(x^2-2)}{B_1+B_2\frac{2}{-1+\sqrt{1+4x^2}}}\right)dx \\
& +\frac{2}{\pi}\int_0^{\sqrt{2}} \frac{1}{x^2}\log\left(1+\frac{x^6(x^2-2)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right)dx \\
> \; & \frac{2}{\pi}\cdot 0.001634 > 0.
\end{aligned}$$

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 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 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

$$\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} < \frac{2.1}{1 + \sqrt{1 + 4x^2}}. \tag{10}$$

It is equivalent to solve

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

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

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

Therefore, when $t \ge 10$, i.e., $2t - 6 > 13$, we have that Ineq. (10) holds for $x \in [1, \sqrt{3}]$. Then, if t is even and $t \ge 10$, from Eq. (8) and Lemma 3.6 we have

$$\begin{aligned}
E(T_a) - E(T_b) &< \frac{2}{\pi} \int_{\sqrt{3}}^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1+\sqrt{1+4x^2}}} \right) dx \\
&\quad + \frac{2}{\pi} \int_{1}^{\sqrt{3}} \frac{1}{x^2} \log \left(1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{2.1}{1+\sqrt{1+4x^2}}} \right) dx \\
&\quad + \frac{2}{\pi} \int_{0}^{1} \frac{1}{x^2} \log \left(1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2} \right) dx \\
&< \frac{2}{\pi} \cdot (-0.000231) < 0.
\end{aligned}$$

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

$$\frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} > \frac{1.9}{1 + \sqrt{1 + 4x^2}}, \tag{11}$$

that is

$$2t - 6 > \log_{\frac{1+\sqrt{1+4x^2}}{2x}} \left(39 - \frac{38}{\sqrt{1 + 4x^2} + 1} \right).$$

Then we get that when $t \ge 699$, and $x \in [\sqrt{3}, 190]$, the Ineq. (11) holds. Thus, if t is odd and $t \ge 699$, from Eq. (8) and Lemma 3.6 we have

$$\begin{aligned}
&E(T_a) - E(T_b) \\
&< \frac{2}{\pi} \int_{190}^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{1}{1+x^2}} \right) dx + \frac{2}{\pi} \int_{\sqrt{3}}^{190} \frac{1}{x^2} \log \left(1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{1.9}{1+\sqrt{1+4x^2}}} \right) dx \\
&\quad + \frac{2}{\pi} \int_{0}^{\sqrt{3}} \frac{1}{x^2} \log \left(1 + \frac{2x^6(x^2 - 3)}{B_1 + B_2 \frac{2}{1+\sqrt{1+4x^2}}} \right) dx \\
&< \frac{2}{\pi} \cdot (-1.41 \times 10^{-5}) < 0.
\end{aligned}$$

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 programm, 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

$$\begin{aligned} E(T_a) - E(T_b) &< \frac{2}{\pi} \int_{\sqrt{3}}^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{x^6(x^2-3)}{B_1 + B_2 \frac{2}{1+\sqrt{1+4x^2}}} \right) dx \\ &\quad + \frac{2}{\pi} \int_0^{\sqrt{3}} \frac{1}{x^2} \log \left(1 + \frac{x^6(x^2-3)}{B_1 + B_2} \right) dx \\ &< \frac{2}{\pi} \cdot (-1.224 \times 10^{-4}) < 0. \end{aligned}$$

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 programm, 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

$$\begin{aligned} &E(T_a) - E(T_b) \\ &< \frac{2}{\pi} \int_{22}^{+\infty} \frac{1}{x^2} \log \left(1 + \frac{3x^6(x^2-4)}{B_1 + B_2 \frac{1}{1+x^2}} \right) dx + \frac{2}{\pi} \int_2^{22} \frac{1}{x^2} \log \left(1 + \frac{3x^6(x^2-4)}{B_1 + B_2 \frac{1}{1+\sqrt{1+4x^2}}} \right) dx \\ &\quad + \frac{2}{\pi} \int_0^2 \frac{1}{x^2} \log \left(1 + \frac{3x^6(x^2-4)}{B_1 + B_2 \frac{2}{1+\sqrt{1+4x^2}}} \right) dx \\ &< \frac{2}{\pi} \cdot (-0.002914) < 0. \end{aligned}$$

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 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. ∎

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