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A New Method of Comparing the Energies of Subdivision Bipartite Graphs *

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Abstract

The energy of a graph is defined as the sum of the absolute values of the eigenvalues of the graph. A k-subdivision graph $G_e(k)$ is a graph obtained from a graph G by subdividing a cut edge e of G by k times. In this paper, we present a new method to compare the energies of two k-subdivision bipartite graphs of the same order. As an application of this method, we determine the first largest to the $\lfloor \frac{n-7}{2} \rfloor^{th}$ largest energy trees of order n for $n \geq 31$ (which is a partial result on a conjecture proposed by Andriantiana in [1]), and also give a simplified proof of the conjecture on the fourth maximal energy tree.

1 Introduction

Let G be a graph with n vertices and A be its adjacency matrix. Let $\lambda_1, \cdots, \lambda_n$ be the eigenvalues of A, then the *energy* of G, denoted by $\mathbb{E}(G)$, is defined [3, 4] as $\mathbb{E}(G) = \sum_{i=1}^{n} |\lambda_i|$.

The characteristic polynomial $\det(xI - A)$ of the adjacency matrix A of a graph G is also called the characteristic polynomial of G, written as $\phi(G, x) = \sum_{i=0}^{n} a_i(G) x^{n-i}$.

In this paper, we write $b_i(G) = |a_i(G)|$, and also write

$$\widetilde{\phi}(G, x) = \sum_{i=0}^{n} b_i(G) x^{n-i}.$$

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If G is a bipartite graph, then it is well known that $\phi(G,x)$ has the form

$$\phi(G,x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} a_{2i}(G)x^{n-2i} = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i b_{2i}(G)x^{n-2i} \tag{1.1}$$

and thus

$$\widetilde{\phi}(G,x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_{2i}(G)x^{n-2i}. \qquad (b_{2i}(G) = |a_{2i}(G)| = (-1)^i a_{2i}) \tag{1.2}$$

In case G is a forest, then $b_{2i}(G) = m(G,i)$, the number of i-matchings of G.

The following integral formula by Gutman and Polansky ([5]) on the difference of the energies of two graphs is the starting point of this paper.

$$\mathbb{E}(G_1) - \mathbb{E}(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\phi(G_1, ix)}{\phi(G_2, ix)} \right| \mathrm{d}x \qquad (i = \sqrt{-1}) \tag{1.3}$$

Now suppose again that G is a bipartite graph of order n. Then by (1.1) and (1.2) we have

$$\phi(G, ix) = i^n \widetilde{\phi}(G,x) \qquad (G \text{ is bipartite, } i = \sqrt{-1}) \tag{1.4}$$

Using (1.4) we can derive the following new formula from (1.3) which does not involve the complex number i.

Theorem 1.1. *If G_1, G_2 are both bipartite graphs of order n, then we have*

$$\mathbb{E}(G_1) - \mathbb{E}(G_2) = \frac{2}{\pi} \int_{0}^{+\infty} \ln \frac{\widetilde{\phi}(G_1, x)}{\widetilde{\phi}(G_2, x)} \mathrm{d}x \tag{1.5}$$

Proof. Since G_1, G_2 are both bipartite graphs of order n, it is easy to see that

$$\frac{\widetilde{\phi}(G_1,x)}{\widetilde{\phi}(G_2,x)} = \frac{\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(G_1)x^{n-2j}}{\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(G_2)x^{n-2j}} \text{ is an even function and } \frac{\widetilde{\phi}(G_1,x)}{\widetilde{\phi}(G_2,x)} > 0 \text{ for } x > 0.$$

So from (1.3) and (1.4) we have

$$\mathbb{E}(G_1) - \mathbb{E}(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\phi(G_1, ix)}{\phi(G_2, ix)} \right| \mathrm{d}x = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\widetilde{\phi}(G_1, x)}{\widetilde{\phi}(G_2, x)} \right| \mathrm{d}x = \frac{2}{\pi} \int_{0}^{+\infty} \ln \frac{\widetilde{\phi}(G_1, x)}{\widetilde{\phi}(G_2, x)} \mathrm{d}x.$$

$\square$

Definition 1.1. Let $f(x) = \sum_{i=0}^{n} a_i x^{n-i}$ and $g(x) = \sum_{i=0}^{n} b_i x^{n-i}$ be two monic polynomials of degree n with nonnegative coefficients.

(1). If $a_i \le b_i$ for all $0 \le i \le n$, then we write $f(x) \preccurlyeq g(x)$.

(2). If $f(x) \preccurlyeq g(x)$ and $f(x) \neq g(x)$, then we write $f(x) \prec g(x)$.

Now we define the following quasi-order for bipartite graphs (which is equivalent to the well known quasi-order defined by Gutman and Polansky in [5]).

Definition 1.2. Let G_1 and G_2 be two bipartite graphs of order n. Then we write $G_1 \preccurlyeq G_2$ if $\widetilde{\phi}(G_1, x) \preccurlyeq \widetilde{\phi}(G_2, x)$, write $G_1 \prec G_2$ if $\widetilde{\phi}(G_1, x) \prec \widetilde{\phi}(G_2, x)$ and write $G_1 \sim G_2$ if $\widetilde{\phi}(G_1, x) = \widetilde{\phi}(G_2, x)$.

According to the integral formula in Theorem 1.1, we can see that for two bipartite graphs G_1 and G_2 of order n,

$$G_1 \preccurlyeq G_2 \Longrightarrow \mathbb{E}(G_1) \leq \mathbb{E}(G_2); \qquad \textit{and} \qquad G_1 \prec G_2 \Longrightarrow \mathbb{E}(G_1) < \mathbb{E}(G_2).$$

The method of the quasi-order relation "$\preccurlyeq$" is an important tool in the study of graph energy.

Graphs with extremal energies are extensively studied in literature. Gutman [2] determined the first and second maximal energy trees of order n; N.Li, S.Li [9] determined the third maximal energy tree; Gutman et al. [6] conjectured that the fourth maximal energy tree is $P_n(2, 6, n-9)$ (see Fig.3 for this graph); B. Huo et al. [8] proved that this conjecture is true.

In this paper, we first consider in §2 a recurrence relation for the polynomial $\widetilde{\phi}(G(k), x)$ of a k-subdivision graph $G(k)$ which is obtained from a bipartite graph G) by subdividing some cut edge e of it k times. Then in §3 we present a new method of directly comparing the energies of two k-subdivision bipartite graphs $G(k)$ and $H(k)$ if they are quasi-order incomparable. Using this new method, we are able to provide a simplified proof of the above mentioned conjecture on the fourth maximal energy tree. By further using the new method in §4 and §5, we can determine the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees of order n for all $n \geq 31$.

Notice that recently Andriantiana [1] showed that, when n is sufficiently large, then the list of the first $3n-84$ (for odd n) and the first $3n-87$ (for even n) largest energy trees of order n can be determined. But from the proof in [1] it seems to be difficult to get a bound for how sufficiently large n should be, since the method used in [1] is to compare the limits of certain kinds of energy differences, and the integrand function in the integral formula for the energy difference may not be uniformly convergent to the limit function. In fact, it is also conjectured in [1] that the ordering in the list is true for all odd $n \geq 21777$ and for all even $n \geq 30866$. Now our ordering for the first $\lfloor \frac{n-7}{2} \rfloor$

largest energy trees of order n is true for all $n \geq 31$, so actually we have shown that the conjecture in [1] is true for the part of the first $\lfloor \frac{n-7}{2} \rfloor$ graphs in the list.

2 Some recurrence relations of $\phi(G,x)$ and $\widetilde{\phi}(G,x)$ for k-subdivision bipartite graphs

The following lemma is an alternative form of Heilbronner's recurrence formula [7].

Lemma 2.1. *[7] Let uv be a cut edge of a graph G, then $\phi(G,x) = \phi(G-uv,x) - \phi(G-u-v,x)$.*

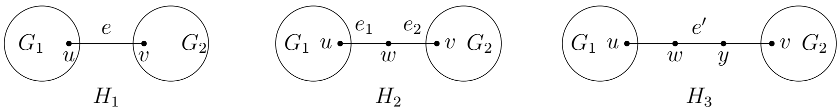

Fig. 1: The graphs H_1, H_2 and H_3

For the sake of simplicity, we sometimes abbreviate $\phi(G,x)$ by $\phi(G)$.

The following relation can be derived from Lemma 2.1.

Lemma 2.2. *Let H_1, H_2, H_3 be graphs as shown in Fig.1. Then we have*

$$\phi(H_3,x) = x\phi(H_2,x) - \phi(H_1,x)$$

Proof. Let G_1' be the graph obtained from G_1 by attaching a new pendent edge uw to G_1 at u, and G_2' be the graph obtained from G_2 by attaching a new pendent edge vy to G_2 at v. Then by using Lemma 2.1 we have

$$\phi(G_1') = x\phi(G_1) - \phi(G_1-u), \quad \text{and} \quad \phi(G_2') = x\phi(G_2) - \phi(G_2-v).$$

Now using Lemma 2.1 for H_3 and its cut edge $e' = wy$, we have

$$\phi(H_3) = \phi(H_3-e') - \phi(H_3-w-y) = \phi(G_1')\phi(G_2') - \phi(G_1)\phi(G_2)$$
$$=(x\phi(G_1) - \phi(G_1-u))(x\phi(G_2) - \phi(G_2-v)) - \phi(G_1)\phi(G_2)$$
$$=(x^2-1)\phi(G_1)\phi(G_2) - x\phi(G_1)\phi(G_2-v) - x\phi(G_2)\phi(G_1-u) + \phi(G_1-u)\phi(G_2-v)$$

Also using Lemma 2.1 for H_2 and $H_2 - e_1$ we have

$$\phi(H_2) = \phi(H_2-e_1) - \phi(H_2-u-w) = \phi(H_2-e_1-e_2) - \phi(H_2-e_1-w-v)$$
$$-\phi((G_1-u)\cup G_2) = x\phi(G_1)\phi(G_2) - \phi(G_1)\phi(G_2-v) - \phi(G_1-u)\phi(G_2)$$

Using Lemma 2.1 for H_1 we also have

$$\phi(H_1) = \phi(H_1-e) - \phi(H_1-u-v) = \phi(G_1)\phi(G_2) - \phi(G_1-u)\phi(G_2-v)$$

Now it is easy to verify from the above three equations that $\phi(H_3) = x\phi(H_2) - \phi(H_1)$. $\square$

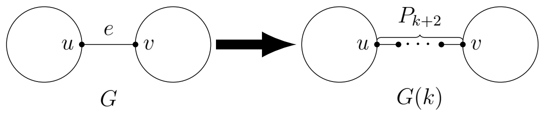

Fig. 2: Graph G and its k-subdivision graph

Definition 2.1. Let e be a cut edge of a graph G, and let $G_e(k)$ denote the graph obtained by replacing e with a path of length $k+1$ (for simplicity of notations, we usually abbreviate $G_e(k)$ by $G(k)$). We say that $G(k)$ is a k-subdivision graph of G on the cut edge e. We also set $G(0) = G$.

From Lemma 2.2, we have the following recurrence relation for $\phi(G(k), x)$.

Theorem 2.1. *Let $G(k)$ be a k-subdivision graph of G on the cut edge e of G, then we have*

$$\phi(G(k+2), x) = x\phi(G(k+1), x) - \phi(G(k), x) \qquad (k \geq 0)$$

Proof. Take $H_1 = G(k)$ in Lemma 2.2 and let e be an edge in H_1 on the path of length $k+1$ obtained by k-subdividing the edge e. Then $H_2 = G(k+1)$ and $H_3 = G(k+2)$. The result now follows from Lemma 2.2. □

Theorem 2.2. *Let G be a bipartite graph of order n and let $G(k)$ be a k-subdivision graph (of order $n+k$) of G on some cut edge e. Then we have*

$$\widetilde{\phi}(G(k+2), x) = x\widetilde{\phi}(G(k+1), x) + \widetilde{\phi}(G(k), x) \qquad (k \geq 0) \qquad (2.1)$$

Proof. By Theorem 2.1, we have

$$\phi(G(k+2), x) = x\phi(G(k+1), x) - \phi(G(k), x)$$

replace x by ix, we get

$$\phi(G(k+2), ix) = ix\phi(G(k+1), ix) - \phi(G(k), ix).$$

Now using (1.4) for $G(k+2), G(k+1)$ and $G(k)$ (since they are all bipartite) we have

$$i^{n+k+2}\widetilde{\phi}(G(k+2), x) = i^{n+k+1}ix\widetilde{\phi}(G(k+1), x) - i^{n+k}\widetilde{\phi}(G(k), x)$$

Dividing both sides by i^{n+k+2} we get (2.1). □

Theorem 2.3. *Let e, e' be cut edges of bipartite graphs G and H of order n , respectively. If $G(0) \preccurlyeq H(0)$ and $G(1) \preccurlyeq H(1)$, then we have $G(k) \preccurlyeq H(k)$ for all $k \geq 2$, with $G(k) \sim H(k)$ if and only if both the two relations $H(0) \sim G(0)$ and $H(1) \sim G(1)$ hold.*

Proof. The result follows directly from Theorem 2.2 and induction on k. □

Theorem 2.4. *Let G, H be bipartite graphs of order n, e_1, e_2 be two cut edges of G and e'_1, e'_2 be two cut edges of H. Let $G(a, b)$ denote the graph obtained from G by subdividing e_1, e_2 a and b times, respectively and $H(c, d)$ denote the graph obtained from H by subdividing e'_1, e'_2 c and d times, respectively. If*

$$G(0,0) \preccurlyeq H(0,0) \qquad \text{and} \qquad G(0,1) \preccurlyeq H(0,1), \tag{2.2}$$

$$G(1,0) \preccurlyeq H(1,0) \qquad \text{and} \qquad G(1,1) \preccurlyeq H(1,1) \tag{2.3}$$

then we have $G(l, k) \preccurlyeq H(l, k)$ for all $l \geq 0$ and $k \geq 0$. Moreover, if one of l and k is at least 2, then $G(l, k) \prec H(l, k)$ if each of (2.2) and (2.3) contains at least one strict relation.

Proof. Using Theorem 2.3 for e_2 and e'_2 we have

$$(2.2) \Longrightarrow G(0, k) \preccurlyeq H(0, k) \quad (k \geq 0), \tag{2.4}$$

$$(2.3) \Longrightarrow G(1, k) \preccurlyeq H(1, k) \quad (k \geq 0). \tag{2.5}$$

Now using Theorem 2.3 for e_1 and e'_1 we also have

$$(2.4) \text{ and } (2.5) \Longrightarrow G(l, k) \preccurlyeq H(l, k) \qquad (l \geq 0).$$

When (2.2) and (2.3) both contain strict relations, we have both strict relations in (2.4) and (2.5) for $k \geq 2$. Thus $G(l, k) \prec H(l, k)$ for all $k \geq 2$ by Theorem 2.3. Similar arguments apply to the case $l \geq 2$. □

3 A new method of directly comparing the energies of k-subdivision bipartite graphs

Notice that if the conditions in Theorem 2.3 do not hold, then $G(k)$ and $H(k)$ might be quasi-order incomparable. In this section, we present a new method to directly compare the energies of two k-subdivision bipartite graphs $G(k)$ and $H(k)$ when they are quasi-order incomparable. Using this method, we give a simplified proof of the conjecture on the fourth maximal energy tree.

In the following, we always write $g_k = \widetilde{\phi}(G(k), x)$, $h_k = \widetilde{\phi}(H(k), x)$, and $d_k = \dfrac{h_k}{g_k}$.

Lemma 3.1. *Let $G(k)$, $H(k)$ be k-subdivision graphs on some cut edges of the bipartite graphs G and H of order n, respectively ($k \geq 0$), g_k, h_k and d_k be defined as above. Then for each fixed $x > 0$, we have*

(1). If $d_1 > d_0$, then $d_0 < d_k < d_1$ for all $k \geq 2$;

(2). If $d_1 < d_0$, then $d_1 < d_k < d_0$ for all $k \geq 2$;

(3). If $d_1 = d_0$, then $d_k = d_0$ for all k.

(So in any case we have $d_k \geq \min\{d_0, d_1\}$.)

Proof. By the recurrence relations in Theorem 2.2, we have

$$\begin{aligned} d_k =& \frac{h_k}{g_k} = \frac{xh_{k-1} + h_{k-2}}{xg_{k-1} + g_{k-2}} = \frac{xd_{k-1}g_{k-1} + d_{k-2}g_{k-2}}{xg_{k-1} + g_{k-2}} \\ =& \left(\frac{xg_{k-1}}{xg_{k-1} + g_{k-2}}\right) d_{k-1} + \left(\frac{g_{k-2}}{xg_{k-1} + g_{k-2}}\right) d_{k-2} \end{aligned}$$

This tells us that d_k is a convex combination of d_{k-1} and d_{k-2} with positive coefficients, which implies that d_k lies in the open interval (d_{k-1}, d_{k-2}) or (d_{k-2}, d_{k-1}) if $d_{k-1} \neq d_{k-2}$. Using this fact and the induction on k we obtain that d_k always lies in the open interval (d_0, d_1) or (d_1, d_0) when $d_0 \neq d_1$, and $d_k = d_0$ when $d_1 = d_0$. □

The following theorem can be derived from Lemma 3.1:

Theorem 3.1. *(1). If $h_1g_0 - h_0g_1 = \widetilde{\phi}(H(1), x)\widetilde{\phi}(G(0), x) - \widetilde{\phi}(H(0), x)\widetilde{\phi}(G(1), x) > 0$ (which is equivalent to $d_1(x) > d_0(x)$) for all $x > 0$, then we have*

$$\mathbb{E}(H(k)) - \mathbb{E}(G(k)) > \mathbb{E}(H(0)) - \mathbb{E}(G(0)) \quad \textit{(for all } k > 0.\textit{)}$$

(2). If $h_1g_0 - h_0g_1 = \widetilde{\phi}(H(1), x)\widetilde{\phi}(G(0), x) - \widetilde{\phi}(H(0), x)\widetilde{\phi}(G(1), x) < 0$(which is equivalent to $d_1(x) < d_0(x)$) for all $x > 0$, then we have

$$\mathbb{E}(H(k)) - \mathbb{E}(G(k)) > \mathbb{E}(H(1)) - \mathbb{E}(G(1)) \quad \textit{for all } k \neq 1.$$

Proof. (1). Since $d_1(x) > d_0(x)$ for all $x > 0$, by (1) of Lemma 3.1 we have $d_k(x) > d_0(x)$ for all $x > 0$ and $k > 0$. So by (1.5) we have

$$\begin{aligned} &\mathbb{E}(H(k)) - \mathbb{E}(G(k)) = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{\widetilde{\phi}(H(k), x)}{\widetilde{\phi}(G(k), x)} \mathrm{d}x = \frac{2}{\pi} \int_0^{+\infty} \ln d_k(x) \mathrm{d}x \\ &> \frac{2}{\pi} \int_0^{+\infty} \ln d_0(x) \mathrm{d}x = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{\widetilde{\phi}(H(0), x)}{\widetilde{\phi}(G(0), x)} \mathrm{d}x = \mathbb{E}(H(0)) - \mathbb{E}(G(0)) \quad (k > 0). \end{aligned}$$

The proof of (2) is similar to that of (1). □

In [10], Shan et al. show that the fourth largest energy tree is either $P_n(2,6,n-9)$ or $T_n(2,2|2,2)$ (see Fig.3 and Fig.4 in §4 for the definitions of these two graphs). B. Huo et al.[8] proved that the conjecture on the fourth maximal energy tree is true by showing that $\mathbb{E}(P_n(2,6,n-9)) > \mathbb{E}(T_n(2,2|2,2))$. Now by using Theorem 3.1, we are able to give a simplified proof of the conjecture on the fourth maximal energy tree.

Theorem 3.2. *If* $n \geq 10$*, then*

$$\mathbb{E}(P_n(2,6,n-9)) > \mathbb{E}(T_n(2,2|2,2))$$

Proof. Let $H = P_{10}(2,6,1)$ and $G = T_{10}(2,2|2,2)$, e be the pendent edge on the pendent path of length 1 in H, and e' be the edge between the two vertices of degree 3 in G. Then we have $P_n(2,6,n-9) = H(n-10)$ and $T_n(2,2|2,2) = G(n-10)$. By direct calculations, we have

$$\widetilde{\phi}(H(0),x) = \widetilde{\phi}(P_{10}(2,6,1),x) = x^{10} + 9\,x^8 + 27\,x^6 + 31\,x^4 + 12\,x^2 + 1,$$
$$\widetilde{\phi}(G(0),x) = \widetilde{\phi}(T_{10}(2,2|2,2),x) = x^{10} + 9\,x^8 + 26\,x^6 + 30\,x^4 + 13\,x^2 + 1,$$
$$\widetilde{\phi}(H(1),x) = \widetilde{\phi}(P_{11}(2,6,2),x) = x^{11} + 10\,x^9 + 35\,x^7 + 52\,x^5 + 32\,x^3 + 6\,x,$$
$$\widetilde{\phi}(G(1),x) = \widetilde{\phi}(T_{11}(2,2|2,2),x) = x^{11} + 10\,x^9 + 34\,x^7 + 48\,x^5 + 29\,x^3 + 6\,x.$$

So we have

$\widetilde{\phi}(H(1),x)\widetilde{\phi}(G(0),x) - \widetilde{\phi}(H(0),x)\widetilde{\phi}(G(1),x) = 2x^{15} + 22x^{13} + 89x^{11} + 168x^9 + 156x^7 + 66x^5 + 9x^3 > 0$ $(x > 0)$.

Also by using a computer we can obtain

$\mathbb{E}(H(0)) \doteq 11.937511$, $\quad\mathbb{E}(G(0)) \doteq 11.924777$, $\quad$ So $\mathbb{E}(H(0)) - \mathbb{E}(G(0)) \doteq 0.012734 > 0$.

So by Theorem 3.1 we have for $n \geq 10$,

$\mathbb{E}(P_n(2,6,n-9)) - \mathbb{E}(T_n(2,2|2,2)) = \mathbb{E}(H(n-10)) - \mathbb{E}(G(n-10)) \geq \mathbb{E}(H(0)) - \mathbb{E}(G(0)) > 0$. □

Combining Theorem 3.2 with the result that the fourth largest energy tree is either $P_n(2,6,n-9)$ or $T_n(2,2|2,2)$ ([10]), we conclude that the fourth maximal energy tree is $P_n(2,6,n-9)$.

Remark: Here we would like to mention that, the main points of the simplification in the proof of Theorem 3.2 are:

1. We use the integral formula (1.5) (instead of (1.3)) which uses the real polynomial $\widetilde{\phi}(G_j, x)$ instead of the complex polynomial $\phi(G_j, ix)$ for $j = 1, 2$.

2. The recurrence relation (2.1) for $\widetilde{\phi}(G(k), x)$ allows us to use Lemma 3.1 to directly compare $d_k(x)$ and $d_0(x)$ (namely directly compare the integrands $\ln d_k(x)$ and $\ln d_0(x)$ in the formula (1.5) for $\mathbb{E}(H(k)) - \mathbb{E}(G(k))$ and $\mathbb{E}(H(0)) - \mathbb{E}(G(0))$), without the need of solving the recurrence relation (2.1) to obtain explicit expressions for $h_k = \widetilde{\phi}(H(k), x)$ and $g_k = \widetilde{\phi}(G(k), x)$. □

Notice that in Theorem 3.1, we need either $d_1(x) > d_0(x)$ for all $x > 0$ or $d_0(x) > d_1(x)$ for all $x > 0$. Now if neither of these two conditions holds, then neither $d_0(x)$ nor $d_1(x)$ is a lower bound for $d_k(x)$ $(k \geq 2)$. Although in this case we cannot use Theorem 3.1, but by Lemma 3.1 we still have $\min\{d_0(x), d_1(x)\}$ as a lower bound for $d_k(x)$ (for all $x > 0$). Thus we can still obtain the following lower bound (which is independent of k) for $\mathbb{E}(H(k)) - \mathbb{E}(G(k))$.

Theorem 3.3. *Let $G(k)$, $H(k)$ be k-subdivision graphs of bipartite graphs G and H on some cut edges. Let $d_k(x) = \dfrac{\widetilde{\phi}(H(k), x)}{\widetilde{\phi}(G(k), x)}$ and let $D = \{x > 0 | d_0(x) > d_1(x)\}$, Let D^C be the complement of D in $(0, \infty)$. Then :*

$$\mathbb{E}(H(k)) - \mathbb{E}(G(k)) \geq \frac{2}{\pi} \int_0^{+\infty} \ln \min\{d_0(x), d_1(x)\} dx = \frac{2}{\pi} \int_D \ln d_1(x) dx + \frac{2}{\pi} \int_{D^C} \ln d_0(x) dx \tag{3.1}$$

where the right hand side of (3.1) can also be written as:

$$\frac{2}{\pi} \int_D \ln d_1(x) dx + \frac{2}{\pi} \int_{D^C} \ln d_0(x) dx = \frac{2}{\pi} \int_0^{+\infty} \ln d_1(x) dx - \frac{2}{\pi} \int_{D^C} \ln d_1(x) dx \tag{3.2}$$
$$+\frac{2}{\pi} \int_{D_C} \ln d_0(x) dx = \mathbb{E}(H(1)) - \mathbb{E}(G(1)) - \frac{2}{\pi} \int_{D^C} \ln \frac{d_1(x)}{d_0(x)} dx$$

or equivalently,

$$\frac{2}{\pi} \int_D \ln d_1(x) dx + \frac{2}{\pi} \int_{D^C} \ln d_0(x) dx = \mathbb{E}(H(0)) - \mathbb{E}(G(0)) + \frac{2}{\pi} \int_D \ln \frac{d_1(x)}{d_0(x)} dx \tag{3.3}$$

Theorem 3.3 will be used several times in §4 and §5 in the proof of our main results.

4 Some upper bounds for the energies of non-starlike trees

In the following discussions, we will divide the trees into two classes. One is called the starlike trees, and the other one is the non-starlike trees. In this section, we will give some upper bounds for the energies of the non-starlike trees. We will show that the energy of a non-starlike tree is bounded above either by the energy of $P_n(1, 2, n-4)$, or by the energy of $T_n(2, 2|2, 2)$ (see Fig.3 and Fig.4).

Let $N_3(G)$ be the number of vertices in G with degree at least 3, and $\Delta(G)$ be the maximal degree of G. A tree T is called starlike if $N_3(T) \leq 1$, and is called non-starlike if $N_3(T) \geq 2$.

It is easy to see that if $N_3(T) = 0$, then T is the path P_n. Now if $N_3(T) = 1$, then T consists of some internally disjoint pendent paths starting from its unique vertex with degree at least 3. Suppose that the lengths of these pendent paths are positive integers $a_1, a_2, \cdots, a_k$. Then we denote this tree T by $P_n(a_1, a_2, \cdots, a_k)$, where $a_1 + a_2 + \cdots + a_k = n - 1$ and $k = \Delta(T)$ (see Fig.3). Sometimes we also denote $P_n(a_1, a_2, \cdots, a_k)$ by $P_n(a_1, a_2, \cdots, a_{k-1}, *)$, since $*$ is uniquely determined by n and $a_1, a_2, \cdots, a_{k-1}$.

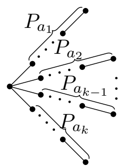

Fig. 3: The starlike tree $P_n(a_1, a_2, \cdots, a_k)$

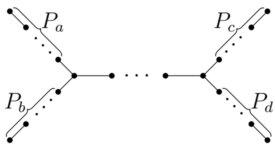

Fig. 4: The tree $T_n(a, b|c, d)$

Let a, b, c, d be positive integers with $a+b+c+d \leq n-2$. Let $T_n(a, b|c, d)$ be the tree of order n obtained by attaching two pendent paths of lengths a and b to one end vertex of the path $P_{n-a-b-c-d}$, and attaching two pendent paths of lengths c and d to another end vertex of the path $P_{n-a-b-c-d}$ (see Fig.4).

It is not difficult to see that if T is a tree of order n with $\Delta(T) = 3$ and $N_3(T) = 2$, then T must be of the form $T_n(a, b|c, d)$, where $a + b + c + d \leq n - 2$.

In [10] and [11], Shan et al. studied how graph energies change under edge grafting operations on unicyclic or bipartite graphs and proved the following result on the quasi-order on unicyclic or bipartite graphs:

Lemma 4.1. *([10], The edge grafting operation) Let u be a vertex of a graph G. Denote $G_u(a, b)$ the graph obtained by attaching to G two (new) pendent paths of lengths a and b*

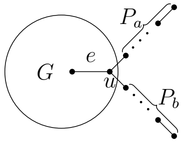

Fig. 5: The graph $G_u(a, b)$

at u. Let a, b, c, d be nonnegative integers with $a + b = c + d$. Assume that $0 \leq a \leq b$, $0 \leq c \leq d$ and $a < c$. If u is a non-isolated vertex of a unicyclic or bipartite graph G, then the following statements are true:

(1). If a is even, then $G_u(a, b) \succ G_u(c, d)$.

(2). If a is odd, then $G_u(a, b) \prec G_u(c, d)$.

If $a = 0$, then we say that $G_u(0, b)$ is obtained from $G_u(c, d)$ by a *total edge grafting* operation.

The following result in [10] was obtained directly by using the edge grafting operation.

Theorem 4.1. *[10] Let T be a tree of order n with $N_3(T) \geq 2$. Then there exists a tree T' of order n with $N_3(T') = N_3(T) - 1$ and $\Delta(T') = \Delta(T)$ such that $T \prec T'$.*

In the following, we will give some upper bounds for the energies of trees of the form $T_n(a, b|c, d)$. First we consider the case $1 \in \{a, b, c, d\}$ in the following Theorem 4.2. The other case where $min\{a, b, c, d\} \geq 2$ will be considered in Lemma 4.3, 4.4 and Theorem 4.3.

Theorem 4.2. *[10] Let $T = T_n(1, b|c, d)$. Then $T \prec P_n(1, 2, n - 4)$.*

Proof. By using total edge grafting on the two pendent paths of lengths c and d, we have $T \prec P_n(1, b, n-2-b)$. Using the edge grafting operation again, we have $P_n(1, b, n-2-b) \preceq P_n(1, 2, n - 4)$. Thus the result follows. □

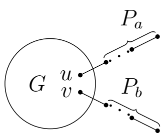

Fig. 6: $G_{u,v}(a, b)$

The following Lemma generalizes Lemma 4.1, and is called "edge grafting operation at different vertices".

Lemma 4.2. *[11] Let u, v be two vertices of a unicyclic or bipartite graph G. Let $G_{u,v}(a, b)$ be the graph obtained from G by attaching a pendent path of length a to u and attaching a pendent path of length b to v (as shown in Fig.6). Suppose that G satisfies:*

(i). $G_{u,v}(0, 2) \succ G_{u,v}(1, 1)$.

(ii). For any nonnegative integers p, q, $G_{u,v}(p, q) = G_{u,v}(q, p)$.

Let a, b, c, d be nonnegative integers with $a \leq b,\ c \leq d,\ a + b = c + d$, and $a < c$, then we have

(1) If a is even, then $G_{u,v}(a, b) \succ G_{u,v}(c, d)$.

(2) If a is odd, then $G_{u,v}(a, b) \prec G_{u,v}(c, d)$.

Fig. 7: $T_{12}(3, 2|2, 2)$ and $T_{12}(2, 2|2, 2)$

Now we use the methods given in §3 to prove the following two lemmas, which consider the tree $T_n(a, 2|2, 2)$ in two cases $3 \leq a \leq n - 9$ and $a = n - 8$. These two lemmas will only be used in the proof of Theorem 4.3 later.

Lemma 4.3. *Let $3 \leq a \leq n - 9$. Then $T_n(a, 2|2, 2) \prec T_n(2, 2|2, 2)$.*

Proof. Let e_1, e_2 be the cut edges of $G = T_{12}(3, 2|2, 2)$ and e'_1, e'_2 be the cut edges of $H = T_{12}(2, 2|2, 2)$ as shown in Fig.7. respectively. Then we have $T_n(a, 2|2, 2) = G(a-3, n-9-a)$ and $T_n(2, 2|2, 2) = H(a - 3, n - 9 - a)$.

By direct calculations, we have

$$\begin{aligned}
\widetilde{\phi}(H(0,0), x) =&\widetilde{\phi}(T_{12}(2,2|2,2), x) = x^{12} + 11\,x^{10} + 43\,x^8 + 74\,x^6 + 59\,x^4 + 19\,x^2 + 1,\\
\widetilde{\phi}(G(0,0), x) =&\widetilde{\phi}(T_{12}(3,2|2,2), x) = x^{12} + 11\,x^{10} + 43\,x^8 + 74\,x^6 + 57\,x^4 + 17\,x^2,\\
\widetilde{\phi}(H(1,0), x) =&\widetilde{\phi}(H(0,1), x) = \widetilde{\phi}(T_{13}(2,2|2,2), x) = x^{13} + 12\,x^{11} + 53\,x^9 + 108\,x^7 +\\
&107\,x^5 + 48\,x^3 + 7\,x,\\
\widetilde{\phi}(G(1,0), x) =&\widetilde{\phi}(T_{13}(4,2|2,2), x) = x^{13} + 12\,x^{11} + 53\,x^9 + 108\,x^7 + 105\,x^5 + 46\,x^3 + 7\,x,\\
\widetilde{\phi}(G(0,1), x) =&\widetilde{\phi}(T_{13}(3,2|2,2), x) = x^{13} + 12\,x^{11} + 53\,x^9 + 108\,x^7 + 106\,x^5 + 46\,x^3 + 6\,x,\\
\widetilde{\phi}(H(1,1), x) =&\widetilde{\phi}(T_{14}(2,2|2,2), x) = x^{14} + 13\,x^{12} + 64\,x^{10} + 151\,x^8 + 181\,x^6 + 107\,x^4\\
&+26\,x^2 + 1,\\
\widetilde{\phi}(G(1,1), x) =&\widetilde{\phi}(T_{14}(4,2|2,2), x) = x^{14} + 13\,x^{12} + 64\,x^{10} + 151\,x^8 + 180\,x^6 + 105\,x^4\\
&+25\,x^2 + 1.
\end{aligned}$$

By comparing the coefficients of the polynomials above, we find that

$$G(0,0) \prec H(0,0),\ G(0,1) \prec H(0,1),\ G(1,0) \prec H(1,0),\ G(1,1) \prec H(1,1).$$

So by Theorem 2.4 we have $T_n(a,2|2,2) = G(a-3, n-9-a) \prec H(a-3, n-9-a) = T_n(2,2|2,2)$. □

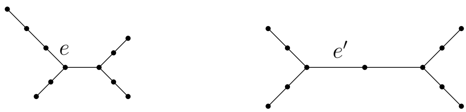

Fig. 8: $G = T_{11}(3,2|2,2)$ and $H = T_{11}(2,2|2,2)$

Now we consider the remaining case $a = n-8$ for the trees of the form $T_n(a,2|2,2)$.

Lemma 4.4. $\mathbb{E}(T_n(n-8,2|2,2)) < \mathbb{E}(T_n(2,2|2,2))$ *for all* $n \geq 11$.

Proof. Consider the cut edges e of $G = T_{11}(3,2|2,2)$ and e' of $H = T_{11}(2,2|2,2)$ as shown in Fig.8. Let $G(k)$, $H(k)$ be graphs obtained by subdividing the cut edges e of G and e' of H respectively k times. Then we have $T_n(n-8,2|2,2) = G(n-11)$ and $T_n(2,2,2,2) = H(n-11)$. Denote $g_k = \widetilde{\phi}(G(k),x)$ and $h_k = \widetilde{\phi}(H(k),x)$.

By direct calculations, we have

$$\begin{aligned}
h_0 =& \widetilde{\phi}(T_{11}(2,2|2,2),x) = x^{11} + 10\,x^9 + 34\,x^7 + 48\,x^5 + 29\,x^3 + 6\,x,\\
g_0 =& \widetilde{\phi}(T_{11}(3,2|2,2),x) = x^{11} + 10\,x^9 + 34\,x^7 + 49\,x^5 + 29\,x^3 + 5\,x,\\
h_1 =& \widetilde{\phi}(T_{12}(2,2|2,2),x) = x^{12} + 11\,x^{10} + 43\,x^8 + 74\,x^6 + 59\,x^4 + 19\,x^2 + 1,\\
g_1 =& \widetilde{\phi}(T_{12}(4,2|2,2),x) = x^{12} + 11\,x^{10} + 43\,x^8 + 75\,x^6 + 59\,x^4 + 18\,x^2 + 1.
\end{aligned}$$

So we have

$$h_1 g_0 - h_0 g_1 = x(x-1)(x+1)(x^6 + 7\,x^4 + 11\,x^2 + 1)(x^2+1)^3.$$

Thus

$$D = \{x | h_1 g_0 - h_0 g_1 < 0, x > 0\} = (0,1).$$

Also by using a computer we can find:

$$\mathbb{E}(H(0)) \doteq 13.059967, \qquad \mathbb{E}(G(0)) \doteq 13.015698$$

and by using computer to calculate the integral we can further obtain

$$\mathbb{E}(H(0)) - \mathbb{E}(G(0)) + \frac{2}{\pi}\int_D \ln\frac{d_1(x)}{d_0(x)}\mathrm{d}x = \mathbb{E}(H) - \mathbb{E}(G) + \frac{2}{\pi}\int_0^1 \ln\frac{h_1 g_0}{h_0 g_1}\mathrm{d}x \doteq 0.005951 > 0.$$

So using Theorem 3.3, we obtain $\mathbb{E}(H(k)) - \mathbb{E}(G(k)) > 0$ for all $k \geq 0$. Thus $\mathbb{E}(T_n(n-8, 2|2, 2)) < \mathbb{E}(T_n(2, 2|2, 2))$. □

Theorem 4.3. *Let $n \geq 11$, and assume that $a, b, c, d \geq 2$ and a, b, c, d are not all equal to 2. Then we have*

$$\mathbb{E}(T_n(a, b|c, d)) < \mathbb{E}(T_n(2, 2|2, 2)).$$

Proof. By using the edge grafting operation in Lemma 4.1, we have

$$T_n(a, b|c, d) \preccurlyeq T_n(a + b - 2, 2|2, c + d - 2).$$

By using Lemma 4.2 (edge grafting on different vertices), we also have

$$T_n(a + b - 2, 2|2, c + d - 2) \preccurlyeq T_n(a + b + c + d - 6, 2|2, 2).$$

Write $x = a + b + c + d - 6$, then we have $3 \leq x \leq n - 8$ since at least one of a, b, c, d is greater than 2.

Now If $3 \leq x \leq n - 9$, then by Lemma 4.3 we have $T_n(x, 2|2, 2) \prec T_n(2, 2|2, 2)$. So $\mathbb{E}(T_n(a, b|c, d)) \leq \mathbb{E}(T_n(x, 2|2, 2)) < \mathbb{E}(T_n(2, 2|2, 2))$.

If $x = n - 8$, then by Lemma 4.4 we have $\mathbb{E}(T_n(a, b|c, d)) \leq \mathbb{E}(T_n(x, 2|2, 2)) < \mathbb{E}(T_n(2, 2|2, 2))$. □

5 The trees of order n with the first $\lfloor \frac{n-7}{2} \rfloor$ largest energies

In this section, we will determine the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees of order $n \geq 31$ by using the method of directly comparing energies given in §3.

First, we divide the class of starlike trees into the following four subclasses:

(C1). The path P_n.

(C2). The class $S_n = \{P_n(2, a, b) \mid a + b = n - 3,\ 1 \leq a \leq b\}$.

(C3). The starlike trees T of order n with $\Delta(T) = 3$ and $T \notin S_n$.

(C4). The starlike trees T of order n with $\Delta(T) \geq 4$.

For convenience, we also define the following class (C5):

(C5). The class of non-starlike trees of order n (i.e., $N_3(T) \geq 2$).

It is obvious that the union of the classes (C1)-(C5) is the class of all the trees of order n.

Now, our strategy of proving the main result is as follows. Firstly, using the quasi-order defined by Gutman and Polansky in [5], we can obtain (in Theorem 5.1) a total ordering of all the $\lfloor \frac{n-3}{2} \rfloor$ trees in S_n. Secondly, we can show (in Theorem 5.2) that the maximal tree (under the quasi-order) in the class (C3) is $P_n(4,4,*)$, and the maximal tree in the class (C4) is $P_n(2,2,2,*)$. Next, by directly comparing the energies of the largest energy trees in the classes (C3) and (C4) with some smaller energy graphs in S_n, and comparing the energies of the tree $T_n(2,2|2,2)$ in the class (C5) with the smallest energy tree $P_n(2,1,n-4)$ in S_n, we obtain that the first $\lfloor \frac{n-9}{2} \rfloor$ largest energy trees in S_n together with P_n are the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees in the class of all trees of order n.

Theorem 5.1. *[5] Let* $S_n = \{P_n(2,a,b) \mid a+b = n-3,\ 1 \le a \le b\}$*. Let* $k = \lfloor \frac{n-3}{2} \rfloor$, $t = \lfloor \frac{k}{2} \rfloor$ *and* $l = \lfloor \frac{k-1}{2} \rfloor$*. Then we have the following total order for the trees in* S_n*:*

$$\begin{aligned} &P_n(2,2,*) \succ P_n(2,4,*) \succ \cdots \succ P_n(2,2t,*) \succ P_n(2,2l+1,*) \succ \cdots \\ &\succ P_n(2,3,*) \succ P_n(2,1,*)\ . \end{aligned} \tag{5.1}$$

Proof. The result follows directly from Lemma 4.1 by using the edge grafting operation. □

Theorem 5.2. *Let* $n \ge 11$*. Then we have*
(1). If $T \in$*(C3) and* $T \ne P_n(4,4,n-9)$*, then* $T \prec P_n(4,4,n-9)$ *.*
(2). If $T \in$*(C4) and* $T \ne P_n(2,2,2,n-7)$*, then* $T \prec P_n(2,2,2,n-7)$ *.*

Proof. (1) Since $T \in$(C3), T must be of the form $P_n(a,b,c)$ with $2 \notin \{a,b,c\}$. Without loss of generality, we may assume that $a \le b \le c$. Then $b+c \ge 7$ since $n \ge 11$. So by Lemma 4.1 we have $T = P_n(a,b,c) \preccurlyeq P_n(a,4,b+c-4)$ and $P_n(a,4,b+c-4) \preccurlyeq P_n(4,4,n-9)$ since $b+c-4 \ne 2$. Also $T \ne P_n(4,4,n-9)$ implies that at least one of the above two relations is strict. Thus we have $T = P_n(a,b,c) \prec P_n(4,4,n-9)$.

(2) Since $\Delta(T) \ge 4$ for $T \in$(C4), by using Lemma 4.1 we can derive that $T \preccurlyeq P_n(a,b,c,d)$ for some tree $P_n(a,b,c,d)$. By further using the edge grafting operations at most 3 times on $P_n(a,b,c,d)$, we will finally obtain $P_n(a,b,c,d) \preccurlyeq P_n(2,2,2,n-7)$. Also $T \ne P_n(2,2,2,n-7)$ implies that at least one of the above relations is strict. Thus we have $T \prec P_n(2,2,2,n-7)$. □

By using the method of directly comparing energies given in §3, the following Theorem 5.3 and Theorem 5.4 will exclude out $P_n(2,2,2,*)$ (the maximal energy tree in the class (C4)) and $T_n(2,2|2,2)$ (in the class (C5)) from the list of the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees by the smallest energy tree $P_n(2,1,n-4)$ in S_n.

Fig. 9: $P_9(2,2,2,2)$ and $P_9(2,1,5)$

Theorem 5.3. *Let $n \geq 10$. Then we have $\mathbb{E}(P_n(2,2,2,n-7)) < \mathbb{E}(P_n(2,1,n-4))$*

Proof. Consider the cut edges e of $G = P_9(2,2,2,2)$ and e' of $H = P_9(2,1,5)$ as shown in Fig.9.

Let $G(k)$, $H(k)$ be graphs obtained by subdividing the cut edges e of G and e' of H respectively k times. Then we have $P_n(2,2,2,n-7) = G(n-9)$ and $P_n(2,1,n-4) = H(n-9)$. Denote $g_k = \widetilde{\phi}(G(k),x)$ and $h_k = \widetilde{\phi}(H(k),x)$.

By direct calculations, we have

$$\begin{aligned} h_0 =& \widetilde{\phi}(P_9(2,1,5),x) = x^9 + 8x^7 + 20x^5 + 17x^3 + 4x, \\ g_0 =& \widetilde{\phi}(P_9(2,2,2,2),x) = x^9 + 8\,x^7 + 18\,x^5 + 16\,x^3 + 5\,x, \\ h_1 =& \widetilde{\phi}(P_{10}(2,1,6),x) = x^{10} + 9\,x^8 + 27\,x^6 + 31\,x^4 + 12\,x^2 + 1, \\ g_1 =& \widetilde{\phi}(P_{10}(2,2,2,3),x) = x^{10} + 9\,x^8 + 25\,x^6 + 28\,x^4 + 12\,x^2 + 1. \end{aligned}$$

So we have $\quad h_1 g_0 - h_0 g_1 = (2\,x^4 + 8\,x^2 + 1)(x^2+1)^3 > 0$ for all $x > 0$.

Also we can compute that $\mathbb{E}(H(0)) = \mathbb{E}(G(0)) = 6 + 2\sqrt{5}$. So using Theorem 3.1, we have

$\mathbb{E}(P_n(2,1,n-4)) - \mathbb{E}(P_n(2,2,2,n-7)) = \mathbb{E}(H(n-9)) - \mathbb{E}(G(n-9)) > \mathbb{E}(H(0)) - \mathbb{E}(G(0)) = 0.$ □

Notice that $P_n(2,2,2,n-7)$ and $P_n(2,1,n-4)$ are quasi-order incomparable when $n \geq 11$. So Theorem 5.3 can not be proven by only using the quasi-order method.

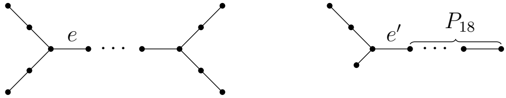

Fig. 10: $T_{22}(2,2|2,2)$ and $P_{22}(2,1,18)$

Theorem 5.4. *Let $n \geq 22$. Then we have $\mathbb{E}(T_n(2,2|2,2)) < \mathbb{E}(P_n(2,1,n-4))$.*

Proof. Consider the cut edges e of $G = T_{22}(2,2|2,2)$ and e' of $H = P_{22}(2,1,18)$ as shown in Fig.10.

Let $G(k)$, $H(k)$ be graphs obtained by subdividing the cut edges e of G and e' of H respectively k times. Then we have $T_n(2,2|2,2) = G(n-22)$ and $P_n(2,1,n-4) = H(n-22)$. Denote $g_k = \widetilde{\phi}(G(k),x)$ and $h_k = \widetilde{\phi}(H(k),x)$.

By direct calculations, we have

$$\begin{aligned}
h_0 =& x^{22} + 21\,x^{20} + 189\,x^{18} + 953\,x^{16} + 2955\,x^{14} + 5824\,x^{12} + 7293\,x^{10} + 5643\,x^{8} + \\
& 2541\,x^{6} + 595\,x^{4} + 57\,x^{2} + 1, \\
g_0 =& x^{22} + 21\,x^{20} + 188\,x^{18} + 939\,x^{16} + 2879\,x^{14} + 5625\,x^{12} + 7046\,x^{10} + 5546\,x^{8} + \\
& 2598\,x^{6} + 644\,x^{4} + 64\,x^{2} + 1, \\
h_1 =& x^{23} + 22\,x^{21} + 209\,x^{19} + 1123\,x^{17} + 3756\,x^{15} + 8113\,x^{13} + 11375\,x^{11} + 10153\,x^{9} + \\
& 5511\,x^{7} + 1672\,x^{5} + 241\,x^{3} + 11\,x, \\
g_1 =& x^{23} + 22\,x^{21} + 208\,x^{19} + 1108\,x^{17} + 3667\,x^{15} + 7850\,x^{13} + 10982\,x^{11} + 9912\,x^{9} + \\
& 5546\,x^{7} + 1768\,x^{5} + 268\,x^{3} + 12\,x.
\end{aligned}$$

So we have

$$h_1 g_0 - h_0 g_1 = x(x^8 + 7\,x^6 + 11\,x^4 - 4\,x^2 - 1)(x^2+1)^3$$

$$D = \{x | h_1 g_0 - h_0 g_1 < 0, x > 0\} \doteq (0, 0.663073).$$

By using a computer we can also find

$\mathbb{E}(H(0)) \doteq 27.182092$, $\quad \mathbb{E}(G(0)) \doteq 27.175139$, and

$$\mathbb{E}(H(0)) - \mathbb{E}(G(0)) + \frac{2}{\pi} \int\limits_{D} \ln \frac{h_1 g_0}{h_0 g_1} \mathrm{d}x \doteq 0.000425 > 0\ .$$

So by using Theorem 3.3, we have $\mathbb{E}(P_n(2,1,n-4)) - \mathbb{E}(T_n(2,2|2,2)) = \mathbb{E}(H(n-22)) - \mathbb{E}(G(n-22) > 0$. □

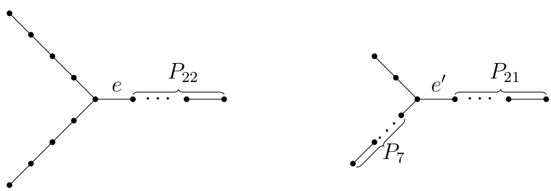

Fig. 11: $P_{31}(4,4,22)$ and $P_{31}(2,7,21)$

The following Theorem 5.5 will exclude out the maximal energy tree in the class (C3) by the fourth smallest energy tree in S_n.

Theorem 5.5. *Let $n \geq 31$. Then we have $\mathbb{E}(P_n(4,4,n-9)) < \mathbb{E}(P_n(2,7,n-10))$.*

Proof. Consider the cut edges e of $G = P_{31}(4,4,22)$ and e' of $H = P_{31}(2,7,21)$ as shown in Fig.11.

Let $G(k)$, $H(k)$ be graphs obtained by subdividing the cut edges e of G and e' of H respectively k times. Then we have $P_n(4,4,n-9) = G(n-31)$ and $P_n(2,7,n-10) = H(n-31)$. Denote $g_k = \widetilde{\phi}(G(k),x)$ and $h_k = \widetilde{\phi}(H(k),x)$.

By direct calculations, we have

$$\begin{aligned} h_0 =& \widetilde{\phi}(P_{31}(2,7,21),x) = x^{31} + 30\,x^{29} + 405\,x^{27} + 3252\,x^{25} + 17296\,x^{23} + 64220\,x^{21} + \\ & 170943\,x^{19} + 329768\,x^{17} + 460696\,x^{15} + 460851\,x^{13} + 322620\,x^{11} + 152131\,x^{9} + \\ & 45426\,x^{7} + 7738\,x^{5} + 619\,x^{3} + 15\,x, \\ g_0 =& \widetilde{\phi}(P_{31}(4,4,22),x) = x^{31} + 30\,x^{29} + 405\,x^{27} + 3252\,x^{25} + 17295\,x^{23} + 64200\,x^{21} + \\ & 170772\,x^{19} + 328952\,x^{17} + 458317\,x^{15} + 456496\,x^{13} + 317681\,x^{11} + 148864\,x^{9} + \\ & 44349\,x^{7} + 7644\,x^{5} + 636\,x^{3} + 16\,x, \\ h_1 =& \widetilde{\phi}(P_{32}(2,7,22),x) = x^{32} + 31\,x^{30} + 434\,x^{28} + 3629\,x^{26} + 20198\,x^{24} + 78938\,x^{22} + \\ & 222724\,x^{20} + 459365\,x^{18} + 693530\,x^{16} + 760145\,x^{14} + 593801\,x^{12} + 320464\,x^{10} + \\ & 113705\,x^{8} + 24470\,x^{6} + 2774\,x^{4} + 125\,x^{2} + 1, \\ g_1 =& \widetilde{\phi}(P_{32}(4,4,23),x) = x^{32} + 31\,x^{30} + 434\,x^{28} + 3629\,x^{26} + 20197\,x^{24} + 78917\,x^{22} + \\ & 222534\,x^{20} + 458396\,x^{18} + 690471\,x^{16} + 753971\,x^{14} + 585871\,x^{12} + 314249\,x^{10} + \\ & 111032\,x^{8} + 24007\,x^{6} + 2792\,x^{4} + 132\,x^{2} + 1. \end{aligned}$$

So we have

$$h_1 g_0 - h_0 g_1 = x\,(x^4 + 3\,x^2 + 1)\,(x^{12} + 12\,x^{10} + 53\,x^8 + 107\,x^6 + 99\,x^4 + 34\,x^2 + 1) > 0$$

for all $x > 0$.

By using a computer we can also find

$$\mathbb{E}(H(0)) \doteq 38.616923, \qquad \mathbb{E}(G(0)) \doteq 38.616742$$

So using Theorem 3.1, we have $\mathbb{E}(P_n(2,7,n-10)) - \mathbb{E}(P_n(4,4,n-9)) = \mathbb{E}(H(n-31)) - \mathbb{E}(G(n-31)) \geq \mathbb{E}(H(0)) - \mathbb{E}(G(0)) \doteq 0.000181 > 0$. □

Theorem 5.6. *Let $n \geq 31$. Let $S'_n = S_n \backslash \{P_n(2,5,n-8), P_n(2,3,n-6), P_n(2,1,n-4)\}$ be the first $\lfloor \frac{n-9}{2} \rfloor$ trees in the quasi-order list (5.1) of S_n. Then P_n and the $\lfloor \frac{n-9}{2} \rfloor$ trees in S'_n are the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees in the class of all trees of order n.*

Proof. It is obvious by the quasi-order list (5.1) that the smallest energy tree in the set $\{P_n\} \cup S'_n$ is $P_n(2,7,n-10)$. Now take any tree $T \notin \{P_n\} \cup S'_n$ of order n, we consider the following four cases:

Case 1: $T \in$(C2). Then $T \in S_n \backslash S'_n$. By the quasi-order list (5.1) we have $T \prec P_n(2,7,n-10)$.

Case 2: $T \in$(C3). Then by Theorem 5.2 and Theorem 5.5 we have

$$\mathbb{E}(T) \leq \mathbb{E}(P_n(4,4,n-9)) < \mathbb{E}(P_n(2,7,n-10)).$$

Case 3: $T \in$(C4). Then by Theorem 5.2, 5.3 and the list (5.1) we have

$$\mathbb{E}(T) \leq \mathbb{E}(P_n(2,2,2,n-7)) < \mathbb{E}(P_n(2,1,n-4)) < \mathbb{E}(P_n(2,7,n-10)).$$

Case 4: $T \in$(C5).

Subcase 4.1: $N_3(T) = 2$ and $\Delta(T) = 3$. Then T is of the form $T_n(a,b|c,d)$. So by Theorem 4.2, 4.3, 5.4 and the list (5.1) we have

$$\mathbb{E}(T) < \mathbb{E}(P_n(2,1,n-4)) < \mathbb{E}(P_n(2,7,n-10)).$$

Subcase 4.2: $N_3(T) = 2$ and $\Delta(T) \geq 4$. Then a tree T' with $N_3(T') = 2$ and $\Delta(T') = 3$ can be obtained from T by using total edge grafting several times. So $T \prec T'$, and thus by Subcase 4.1 we have $\mathbb{E}(T) < \mathbb{E}(T') < \mathbb{E}(P_n(2,7,n-10))$.

Subcase 4.3: $N_3(T) \geq 3$. Using Theorem 4.1 several times we can obtain a tree T' with $N_3(T') = 2$ and $T \prec T'$. So by Subcases 4.1 and 4.2 we have $\mathbb{E}(T) < \mathbb{E}(T') < \mathbb{E}(P_n(2,7,n-10))$. □

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