MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **68** (2012) 703-720

ISSN 0340 - 6253

Proof of a Conjecture on Trees with Large Energy*

Hai-Ying Shan[a], Jia-Yu Shao[a†], Li Zhang[a], Chang-Xiang He[b]

[a] *Department of Mathematics, Tongji University, Shanghai, 200092, P. R. China*

[b] *College of Science, University of Shanghai for Science and Technology, Shanghai, 200093, China*

(Received December 13, 2011)

Abstract

The energy of a graph is defined as the sum of the absolute values of the eigenvalues of the graph. Based on a method of directly comparing the energies of the subdivision trees given in [1], together with using some computer-aided calculations and using some results provided by Andriantiana in [2], we prove that the conjecture proposed in [2] on the first $3n-84$ (when n is odd) and $3n-87$ (when n is even) largest energy trees is true.

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 [4, 5] 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 $\phi(G,x) = \sum_{i=0}^{n} a_i(G)x^{n-i}$.

Let $b_i(G) = |a_i(G)|$, and let $\widetilde{\phi}(G,x) = \sum_{i=0}^{n} b_i(G)x^{n-i}$. For the sake of simplicity, we sometime abbreviate $\phi(G,x)$ by $\phi(G)$, and $\widetilde{\phi}(G,x)$ by $\widetilde{\phi}(G)$.

* Supported by NSF of China No.10731040, No.11101088, No.11026147 and No.11101263. Supported by the Fundamental Research Funds for the Central Universities.

† Corresponding author.

‡ Email addresses: shan_haiying@tongji.edu.cn(Hai-Ying Shan), jyshao@tongji.edu.cn(Jia-Yu Shao), lizhang@tongji.edu.cn(Li Zhang), changxianghe@hotmail.com(Chang-Xiang He).

Now if G is a bipartite graph, then $\widetilde{\phi}(G,x)$ has the following form [1]:

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

The following integral formula by Gutman and Polansky ([6]) on the differences of the energies of two graphs of order n is the starting point of our discussions.

$$\mathbb{E}(G_1)-\mathbb{E}(G_2)=\frac{1}{\pi}\int_{-\infty}^{+\infty}\ln\left|\frac{\phi(G_1,ix)}{\phi(G_2,ix)}\right|\mathrm{d}x \qquad (i=\sqrt{-1}) \tag{1.2}$$

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

$$\phi(G,ix)=i^n\widetilde{\phi}(G,x) \qquad (G \text{ is bipartite, } i=\sqrt{-1}) \tag{1.3}$$

So we have the following another form of the integral formula (1.2) for the energy differences which does not involve the complex number i [1].

$$\mathbb{E}(G_1)-\mathbb{E}(G_2)=\frac{2}{\pi}\int_{0}^{+\infty}\ln\frac{\widetilde{\phi}(G_1,x)}{\widetilde{\phi}(G_2,x)}\mathrm{d}x \qquad (G_1,G_2 \text{ are bipartite graphs of order } n) \tag{1.4}$$

Definition 1.1. Let e be a cut edge of a graph G, and $G_e(k)$ 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 agree that $G(0)=G$.

The following recurrence relations for $\phi(G(k),x)$ and $\widetilde{\phi}(G(k),x)$ were obtained in [1].

Theorem 1.1. *[1] Let $G(k)$ be a k-subdivision graph of G on a cut edge e of G, then we have*

$$\phi(G(k+2),x)=x\phi(G(k+1),x)-\phi(G(k),x) \qquad (k\geq 0). \tag{1.5}$$

When G is a bipartite graph, then we further have

$$\widetilde{\phi}(G(k+2),x)=x\widetilde{\phi}(G(k+1),x)+\widetilde{\phi}(G(k),x) \qquad (k\geq 0). \tag{1.6}$$

The following Lemma 1.1 provides a new method to directly compare the energies of two k-subdivision bipartite graphs $G(k)$ and $H(k)$, which was first presented in [1].

Lemma 1.1. *[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 ($k \geq 0$). Let $g_k = \widetilde{\phi}(G(k), x)$, $h_k = \widetilde{\phi}(H(k), x)$, and $d_k = \dfrac{h_k}{g_k}$. Then for each fixed $x > 0$, we have*

(1). If $d_1 > d_0$, then we have:

$$d_m > d_k \qquad \text{for all even } m \text{ and } k \text{ with } m > k. \tag{1.7}$$

and

$$d_r > d_k \qquad \text{for all odd } r \text{ and even } k. \tag{1.8}$$

(2). If $d_1 < d_0$, then we have:

$$d_m > d_k \qquad \text{for all odd } m \text{ and } k \text{ with } m > k. \tag{1.9}$$

and

$$d_r > d_k \qquad \text{for all even } r \text{ and odd } k. \tag{1.10}$$

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

Proof. By the recurrence relation (1.6) in Theorem 1.1, 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 we see that if $d_1 > d_0$, then $d_{2j-1} > d_{2j+1} > d_{2j+2} > d_{2j}$, and thus (1.7) and (1.8) follow.

The proof of (2) is similar to that of (1), and the proof of (3) is obvious. □

Remark 1.1. Let $f_k = h_{k+1}g_k - h_k g_{k+1}$. Then by the recurrence relation (1.6) we have

$$f_k = h_{k+1}g_k - h_k g_{k+1} = \begin{vmatrix} h_{k+1} & h_k \\ g_{k+1} & g_k \end{vmatrix} = \begin{vmatrix} xh_k + h_{k-1} & h_k \\ xg_k + g_{k-1} & g_k \end{vmatrix} = \begin{vmatrix} h_{k-1} & h_k \\ g_{k-1} & g_k \end{vmatrix} = -f_{k-1}.$$

From this we can obtain that $f_k = (-1)^k f_0$. □

Let $T_n(a, b, c)$ (where $a + b + c = n - 1$) be the tree of order n consisting of three pendent paths of lengths a, b and c starting from its unique vertex of degree 3 (Sometimes we abbreviate $T_n(a, b, c)$ as $T(a, b, c)$).

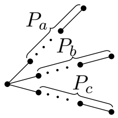

Fig. 1: The tree $T_n(a, b, c)$

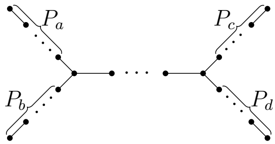

Fig. 2: The tree $T_n(a, b|c, d)$

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.2).

In the following, we also use $G > H$ to denote $\mathbb{E}(G) > \mathbb{E}(H)$.

Recently, Andriantiana [2] used some computer-aided calculations for the limits of the energy differences to obtain 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 as in the following theorem:

Theorem 1.2. *[2] The head of the list of all trees of order n ordered by decreasing energy is given as follows for large enough n:*

P_n	$>$	$T(2,2,n-5)$	$>$	$\cdots$	$>$	$T(2,7,n-10)$	$>$
$T(4,4,n-9)$	$>$	$T(2,5,n-8)$	$>$	$T(4,6,n-11)$	$>$	$T(2,3,n-6)$	$>$
$T(4,8,n-13)$	$>$	$\cdots$	$>$	$T(4,18,n-23)$	$>$	$T(6,6,n-13)$	$>$
$T(4,20,n-25)$	$>$	$\cdots$	$>$	$T(4,15,n-20)$	$>$	$T(6,8,n-15)$	$>$
$T(4,13,n-18)$	$>$	$T(4,11,n-16)$	$>$	$T(6,10,n-17)$	$>$	$T(4,9,n-14)$	$>$
$T(6,12,n-19)$	$>$	$T(8,8,n-17)$	$>$	$T(6,14,n-21)$	$>$	$T(4,7,n-12)$	$>$
$T(6,16,n-23)$	$>$	$T(6,18,n-25)$	$>$	$\cdots$	$>$	$T(6,26,n-33)$	$>$
$T(8,10,n-19)$	$>$	$T(6,28,n-35)$	$>$	$\cdots$	$>$	$T(6,39,n-46)$	$>$
$T(8,12,n-21)$	$>$	$T(6,37,n-44)$	$>$	$\cdots$	$>$	$T(6,23,n-30)$	$>$
$T(8,14,n-23)$	$>$	$T(10,10,n-21)$	$>$	$T(6,21,n-28)$	$>$	$T(4,5,n-10)$	$>$
$T(6,19,n-26)$	$>$	$T(8,16,n-25)$	$>$	$T(8,18,n-27)$	$>$	$T(8,20,n-29)$	$>$
$T(10,12,n-23)$	$>$	$T(8,22,n-31)$	$>$	$\cdots$	$>$	$T(8,30,n-39)$	$>$
$T(10,14,n-25)$	$>$	$T(8,32,n-41)$	$>$	$\cdots$	$>$	$T(8,56,n-65)$	$>$
$T(12,12,n-25)$	$>$	$T(8,58,n-67)$	$>$	$\cdots$	$>$	$T(8,86,n-93)$	$>$
$T(10,16,n-27)$	$>$	$T(8,88,n-97)$	$>$	$\cdots$	$>$	$T(8,49,n-58)$	$>$
$T(10,18,n-29)$	$>$	$T(8,47,n-56)$	$>$	$\cdots$	$>$	$T(8,33,n-42)$	$>$
$T(12,14,n-27)$	$>$	$T(10,20,n-31)$	$>$	$T(8,31,n-40)$	$>$	$T(8,29,n-37)$	$>$
$T(8,27,n-36)$	$>$	$T(10,22,n-33)$	$>$	$T(8,25,n-34)$	$>$	$T(10,24,n-35)$	$>$
$T(8,23,n-32)$	$>$	$T(12,16,n-29)$	$>$	$T(10,26,n-37)$	$>$	$T(1,2,n-4)$	$>$
$T(8,21,n-30)$	$>$	$T(10,28,n-39)$	$>$	$T(10,30,n-41)$	$>$	$T(14,14,n-29)$	$>$
$T(10,32,n-43)$	$>$	$T(8,19,n-28)$	$>$	$T(10,34,n-45)$	$>$	$T(12,18,n-31)$	$>$
$T(10,36,n-47)$	$>$	$\cdots$	$>$	$T(10,44,n-55)$	$>$	$T(8,17,n-26)$	$>$
$T(10,46,n-57)$	$>$	$\cdots$	$>$	$T(10,52,n-63)$	$>$	$T(12,20,n-33)$	$>$

$$\begin{array}{lllllll}
T(10,54,n-65) & > & \cdots & > & T(10,70,n-81) & > & T(14,16,n-31) \ > \\
T(10,72,n-83) & > & \cdots & > & T(10,182,n-193) & > & T(12,22,n-35) \ > \\
T(10,184,n-195) & > & \cdots & > & T(10,175,n-186) & > & T(8,15,n-24) \ > \\
T(10,173,n-184) & > & \cdots & > & T(10,69,n-80) & > & T(12,24,n-37) \ > \\
T(10,67,n-78) & > & \cdots & > & T(10,53,n-64) & > & T(14,18,n-33) \ > \\
T(10,51,n-62) & > & T(10,49,n-60) & > & T(12,26,n-39) & > & T(10,47,n-58) \ > \\
\cdots & > & T(10,41,n-52) & > & T(16,16,n-33) & > & T(12,28,n-41) \ > \\
T(10,39,n-50) & > & T(10,37,n-49) & > & T(8,13,n-22) & > & T(12,30,n-43) \ > \\
T(10,35,n-46) & > & T(14,20,n-35) & > & T(10,33,n-44) & > & T(12,32,n-45) \ > \\
T(10,31,n-42) & > & T(12,34,n-47) & > & T(12,36,n-49) & > & T(10,29,n-40) \ > \\
T(12,38,n-51) & > & T(14,22,n-37) & > & T(16,18,n-35) & > & T(12,40,n-53) \ > \\
T(10,27,n-39) & > & T(12,42,n-55) & > & T(12,44,n-57) & > & T(12,46,n-59) \ > \\
T(10,25,n-36) & > & T(12,48,n-61) & > & T(14,24,n-39) & > & T(12,50,n-63) \ > \\
\cdots & > & T(12,64,n-77) & > & T(10,23,n-34) & > & T(12,66,n-79) \ > \\
\cdots & > & T(12,70,n-83) & > & T(14,26,n-41) & > & T(16,20,n-37) \ > \\
T(12,72,n-85) & > & \cdots & > & T(12,92,n-105) & > & T(8,11,n-20) \ > \\
T(12,94,n-107) & > & \cdots & > & T(12,130,n-143) & > & T(18,18,n-37) \ > \\
T(12,132,n-145) & > & \cdots & > & T(12,162,n-175) & > & T(14,28,n-43) \ > \\
T(12,164,n-177) & > & \cdots & > & T(12,224,n-237) & > & T(10,21,n-32) \ > \\
T(12,226,n-239) & > & \cdots & > & T(12,219,n-232) & > & T(3,4,n-8) \ > \\
T(12,217,n-230) & > & \cdots & > & T(12,111,n-124) & > & T(14,30,n-45) \ > \\
T(12,109,n-122) & > & \cdots & > & T(12,99,n-112) & > & T(16,22,n-39) \ > \\
T(12,97,n-110) & > & \cdots & > & T(12,85,n-98) & > & T_n(2,2|2,2)
\end{array}$$

It is also mentioned in [2] that computer check shows that Theorem 1.2 holds for all odd n from 21777 to 30001, and for all even n from 30866 to 40000. Based on these calculations, Andriantiana proposed the following conjecture in [2] (which gives certain bound for how sufficiently large n should be).

Conjecture 1. *Theorem 1.2 is true for all odd* $n \geq 21777$ *and all even* $n \geq 30866$.

Remark 1.2: Firstly, we notice that the following six graphs:

$$\begin{array}{lll}
T_n(6,17,n-24), & T_n(6,15,n-22), & T_n(6,13,n-20) \\
T_n(6,11,n-18), & T_n(6,9,n-16), & T_n(6,7,n-14)
\end{array} \tag{1.11}$$

were missing in the above list (It was pointed out in [2] that the energies of these six graphs are all greater than $\mathbb{E}(T_n(2,2|2,2))$ when n is sufficiently large). So we now add these 6 graphs to the list at the proper positions to obtain a new list, and we call this new list as the "Adjusted list".

For the convenience of our proof later, we would like to further add the following 9 graphs to the tail of the Adjusted list (after $T_n(2,2|2,2)$) at the proper positions:

$$\begin{array}{l}
T_n(1,4,n-6), T_n(3,6,n-10), T_n(5,6,n-12), T_n(8,9,n-18), T_n(10,19,n-30), \\
T_n(12,83,n-96), T_n(14,32,n-47), T_n(16,24,n-41), T_n(18,20,n-39).
\end{array} \tag{1.12}$$

For each fixed i, let

$$D_i = \{T_n(i,j,c) \mid i+j+c = n-1,\ i \le j \le c\} \quad (1.13).$$

Then it was shown in [2] that when n is sufficiently large, then each of the 9 graphs in (1.12) is the maximal energy graph in the suitable class D_i containing them whose energy is less than $\mathbb{E}(T_n(2,2|2,2))$.

After adding these 9 graphs in (1.12) to the Adjusted list (at the proper positions after $T_n(2,2|2,2)$), we obtain a new list, which will be called the "Extended adjusted list" as the following:

List 1: **The Extended adjusted list**

P_n	$> T_n(2,2,n-5)$	$>\quad\cdots$	$> T_n(2,7,n-10)$	$>$
$T_n(4,4,n-9)$	$> T_n(2,5,n-8)$	$> T_n(4,6,n-11)$	$> T_n(2,3,n-6)$	$>$
$T_n(4,8,n-13)$	$>\quad\cdots$	$> T_n(4,18,n-23)$	$> T_n(6,6,n-13)$	$>$
$T_n(4,20,n-25)$	$>\quad\cdots$	$> T_n(4,15,n-20)$	$> T_n(6,8,n-15)$	$>$
$T_n(4,13,n-18)$	$> T_n(4,11,n-16)$	$> T_n(6,10,n-17)$	$> T_n(4,9,n-14)$	$>$
$T_n(6,12,n-19)$	$> T_n(8,8,n-17)$	$> T_n(6,14,n-21)$	$> T_n(4,7,n-12)$	$>$
$T_n(6,16,n-23)$	$> T_n(6,18,n-25)$	$>\quad\cdots$	$> T_n(6,26,n-33)$	$>$
$T_n(8,10,n-19)$	$> T_n(6,28,n-35)$	$>\quad\cdots$	$> T_n(6,39,n-46)$	$>$
$T_n(8,12,n-21)$	$> T_n(6,37,n-44)$	$>\quad\cdots$	$> T_n(6,23,n-30)$	$>$
$T_n(8,14,n-23)$	$> T_n(10,10,n-21)$	$> T_n(6,21,n-28)$	$> T_n(4,5,n-10)$	$>$
$T_n(6,19,n-26)$	$> T_n(8,16,n-25)$	$> \mathbf{T_n(6,17,n-24)}$	$> \mathbf{T_n(6,15,n-22)}$	$>$
$T_n(8,18,n-27)$	$> T_n(8,20,n-29)$	$> T_n(10,12,n-23)$	$> T_n(8,22,n-31)$	$>$
$\mathbf{T_n(6,13,n-20)}$	$> T_n(8,24,n-33)$	$>\quad\cdots$	$> T_n(8,30,n-39)$	$>$
$T_n(10,14,n-25)$	$> T_n(8,32,n-41)$	$> T_n(8,34,n-43)$	$> T_n(8,36,n-45)$	$>$
$\mathbf{T_n(6,11,n-18)}$	$> T_n(8,38,n-47)$	$>\quad\cdots$	$> T_n(8,56,n-65)$	$>$
$T_n(12,12,n-25)$	$> T_n(8,58,n-67)$	$>\quad\cdots$	$> T_n(8,86,n-93)$	$>$
$T_n(10,16,n-27)$	$> T_n(8,88,n-97)$	$>\quad\cdots$	$> T_n(8,49,n-58)$	$>$
$T_n(10,18,n-29)$	$> T_n(8,47,n-56)$	$>\quad\cdots$	$> T_n(8,33,n-42)$	$>$
$T_n(12,14,n-27)$	$> T_n(10,20,n-31)$	$> \mathbf{T_n(6,9,n-16)}$	$> T_n(8,31,n-40)$	$>$
$T_n(8,29,n-37)$	$> T_n(8,27,n-36)$	$> T_n(10,22,n-33)$	$> T_n(8,25,n-34)$	$>$
$T_n(10,24,n-35)$	$> T_n(8,23,n-32)$	$> T_n(12,16,n-29)$	$> T_n(10,26,n-37)$	$>$
$T_n(1,2,n-4)$	$> T_n(8,21,n-30)$	$> T_n(10,28,n-39)$	$> T_n(10,30,n-41)$	$>$
$T_n(14,14,n-29)$	$> T_n(10,32,n-43)$	$> T_n(8,19,n-28)$	$> T_n(10,34,n-45)$	$>$
$T_n(12,18,n-31)$	$> T_n(10,36,n-47)$	$>\quad\cdots$	$> T_n(10,44,n-55)$	$>$
$T_n(8,17,n-26)$	$> T_n(10,46,n-57)$	$>\quad\cdots$	$> T_n(10,52,n-63)$	$>$
$T_n(12,20,n-33)$	$> T_n(10,54,n-65)$	$>\quad\cdots$	$> T_n(10,70,n-81)$	$>$
$T_n(14,16,n-31)$	$> T_n(10,72,n-83)$	$>\quad\cdots$	$> T_n(10,182,n-193)$	$>$
$T_n(12,22,n-35)$	$> T_n(10,184,n-195)$	$>\quad\cdots$	$> T_n(10,175,n-186)$	$>$
$T_n(8,15,n-24)$	$> T_n(10,173,n-184)$	$>\quad\cdots$	$> T_n(10,69,n-80)$	$>$
$\mathbf{T_n(6,7,n-14)}$	$> T_n(12,24,n-37)$	$> T_n(10,67,n-78)$	$>\quad\cdots$	$>$
$T_n(10,53,n-64)$	$> T_n(14,18,n-33)$	$> T_n(10,51,n-62)$	$> T_n(10,49,n-60)$	$>$
$T_n(12,26,n-39)$	$> T_n(10,47,n-58)$	$>\quad\cdots$	$> T_n(10,41,n-52)$	$>$
$T_n(16,16,n-33)$	$> T_n(12,28,n-41)$	$> T_n(10,39,n-50)$	$> T_n(10,37,n-49)$	$>$

$$T_n(8,13,n-22) > T_n(12,30,n-43) > T_n(10,35,n-46) > T_n(14,20,n-35) >$$
$$T_n(10,33,n-44) > T_n(12,32,n-45) > T_n(10,31,n-42) > T_n(12,34,n-47) >$$
$$T_n(12,36,n-49) > T_n(10,29,n-40) > T_n(12,38,n-51) > T_n(14,22,n-37) >$$
$$T_n(16,18,n-35) > T_n(12,40,n-53) > T_n(10,27,n-39) > T_n(12,42,n-55) >$$
$$T_n(12,44,n-57) > T_n(12,46,n-59) > T_n(10,25,n-36) > T_n(12,48,n-61) >$$
$$T_n(14,24,n-39) > T_n(12,50,n-63) > \cdots > T_n(12,64,n-77) >$$
$$T_n(10,23,n-34) > T_n(12,66,n-79) > \cdots > T_n(12,70,n-83) >$$
$$T_n(14,26,n-41) > T_n(16,20,n-37) > T_n(12,72,n-85) > \cdots >$$
$$T_n(12,92,n-105) > T_n(8,11,n-20) > T_n(12,94,n-107) > \cdots >$$
$$T_n(12,130,n-143) > T_n(18,18,n-37) > T_n(12,132,n-145) > \cdots >$$
$$T_n(12,162,n-175) > T_n(14,28,n-43) > T_n(12,164,n-177) > \cdots >$$
$$T_n(12,224,n-237) > T_n(10,21,n-32) > T_n(12,226,n-239) > \cdots >$$
$$T_n(12,219,n-232) > T_n(3,4,n-8) > T_n(12,217,n-230) > \cdots >$$
$$T_n(12,111,n-124) > T_n(14,30,n-45) > T_n(12,109,n-122) > \cdots >$$
$$T_n(12,99,n-112) > T_n(16,22,n-39) > T_n(12,97,n-110) > \cdots >$$
$$T_n(12,85,n-98) > T_n(2,2|2,2) > T_n(12,83,n-96) > T_n(14,32,n-47) >$$
$$T_n(10,19,n-30) > T_n(18,20,n-39) > T_n(16,24,n-41) > T_n(8,9,n-18) >$$
$$T_n(5,6,n-12) > T_n(3,6,n-10) > T_n(1,4,n-6)$$

In this paper, we will prove that Conjecture 1 is true for all $n \geq 7526$ by using our new method of directly comparing the energies of two k-subdivision trees $G(k)$ and $H(k)$ given in the above Lemma 1.1, together with some computer-aided calculations to obtain the results in Theorem 2.1 and Theorem 2.2 of Section 2, and also by using some known results given by Andriantiana in [2]. We also show that 7526 is the smallest number such that Conjecture 1 is true.

2 The proof of Conjecture 1

In [11] and [12], Shan et al. studied how graph energies change under edge grafting operations on unicyclic or bipartite graphs and proved the following result in the comparison of the quasi-order on unicyclic or bipartite graphs:

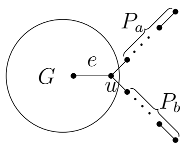

Fig. 3: The graph $G_u(a,b)$

Lemma 2.1. *([11], 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*

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 $G_u(a,b) \prec G_u(c,d)$. □

In this paper, we use $< n >$ to denote the set $\{1, 2, \cdots, n\}$.

Let $T_n(i)$ be the i^{th} graph in the Extended adjusted list (except those graphs in each piece of "$\cdots$" in the list). That is : $T_n(1) = P_n$, $T_n(164) = T_n(2,2|2,2)$, and

$$T_n(i) = T_n(a_i, b_i, n-1-a_i-b_i) \qquad (i \in < 173 > \backslash \{1, 164\}),$$

where

$$(a_2, b_2) = (2,2), \quad (a_3, b_3) = (2,7), \quad (a_4, b_4) = (4,4), \cdots, (a_{173}, b_{173}) = (1,4)$$

as in the following table (also see Appendix of [2]).

Table 1: **The table for (a_i, b_i) with $i \in < 173 > \backslash \{1, 164\}$**

$(a_2,b_2)=(2,2)$	$(a_3,b_3)=(2,7)$	$(a_4,b_4)=(4,4)$	$(a_5,b_5)=(2,5)$
$(a_6,b_6)=(4,6)$	$(a_7,b_7)=(2,3)$	$(a_8,b_8)=(4,8)$	$(a_9,b_9)=(4,18)$
$(a_{10},b_{10})=(6,6)$	$(a_{11},b_{11})=(4,20)$	$(a_{12},b_{12})=(4,15)$	$(a_{13},b_{13})=(6,8)$
$(a_{14},b_{14})=(4,13)$	$(a_{15},b_{15})=(4,11)$	$(a_{16},b_{16})=(6,10)$	$(a_{17},b_{17})=(4,9)$
$(a_{18},b_{18})=(6,12)$	$(a_{19},b_{19})=(8,8)$	$(a_{20},b_{20})=(6,14)$	$(a_{21},b_{21})=(4,7)$
$(a_{22},b_{22})=(6,16)$	$(a_{23},b_{23})=(6,18)$	$(a_{24},b_{24})=(6,26)$	$(a_{25},b_{25})=(8,10)$
$(a_{26},b_{26})=(6,28)$	$(a_{27},b_{27})=(6,39)$	$(a_{28},b_{28})=(8,12)$	$(a_{29},b_{29})=(6,37)$
$(a_{30},b_{30})=(6,23)$	$(a_{31},b_{31})=(8,14)$	$(a_{32},b_{32})=(10,10)$	$(a_{33},b_{33})=(6,21)$
$(a_{34},b_{34})=(4,5)$	$(a_{35},b_{35})=(6,19)$	$(a_{36},b_{36})=(8,16)$	$(a_{37},b_{37})=(6,17)$
$(a_{38},b_{38})=(6,15)$	$(a_{39},b_{39})=(8,18)$	$(a_{40},b_{40})=(8,20)$	$(a_{41},b_{41})=(10,12)$
$(a_{42},b_{42})=(8,22)$	$(a_{43},b_{43})=(6,13)$	$(a_{44},b_{44})=(8,24)$	$(a_{45},b_{45})=(8,30)$
$(a_{46},b_{46})=(10,14)$	$(a_{47},b_{47})=(8,32)$	$(a_{48},b_{48})=(8,36)$	$(a_{49},b_{49})=(6,11)$
$(a_{50},b_{50})=(8,38)$	$(a_{51},b_{51})=(8,56)$	$(a_{52},b_{52})=(12,12)$	$(a_{53},b_{53})=(8,58)$
$(a_{54},b_{54})=(8,86)$	$(a_{55},b_{55})=(10,16)$	$(a_{56},b_{56})=(8,88)$	$(a_{57},b_{57})=(8,49)$
$(a_{58},b_{58})=(10,18)$	$(a_{59},b_{59})=(8,47)$	$(a_{60},b_{60})=(8,33)$	$(a_{61},b_{61})=(12,14)$
$(a_{62},b_{62})=(10,20)$	$(a_{63},b_{63})=(6,9)$	$(a_{64},b_{64})=(8,31)$	$(a_{65},b_{65})=(8,29)$
$(a_{66},b_{66})=(8,27)$	$(a_{67},b_{67})=(10,22)$	$(a_{68},b_{68})=(8,25)$	$(a_{69},b_{69})=(10,24)$
$(a_{70},b_{70})=(8,23)$	$(a_{71},b_{71})=(12,16)$	$(a_{72},b_{72})=(10,26)$	$(a_{73},b_{73})=(1,2)$
$(a_{74},b_{74})=(8,21)$	$(a_{75},b_{75})=(10,28)$	$(a_{76},b_{76})=(10,30)$	$(a_{77},b_{77})=(14,14)$
$(a_{78},b_{78})=(10,32)$	$(a_{79},b_{79})=(8,19)$	$(a_{80},b_{80})=(10,34)$	$(a_{81},b_{81})=(12,18)$
$(a_{82},b_{82})=(10,36)$	$(a_{83},b_{83})=(10,44)$	$(a_{84},b_{84})=(8,17)$	$(a_{85},b_{85})=(10,46)$
$(a_{86},b_{86})=(10,52)$	$(a_{87},b_{87})=(12,20)$	$(a_{88},b_{88})=(10,54)$	$(a_{89},b_{89})=(10,70)$

$(a_{90}, b_{90}) = (14, 16)$	$(a_{91}, b_{91}) = (10, 72)$	$(a_{92}, b_{92}) = (10, 182)$	$(a_{93}, b_{93}) = (12, 22)$
$(a_{94}, b_{94}) = (10, 184)$	$(a_{95}, b_{95}) = (10, 175)$	$(a_{96}, b_{96}) = (8, 15)$	$(a_{97}, b_{97}) = (10, 173)$
$(a_{98}, b_{98}) = (10, 69)$	$(a_{99}, b_{99}) = (6, 7)$	$(a_{100}, b_{100}) = (12, 24)$	$(a_{101}, b_{101}) = (10, 67)$
$(a_{102}, b_{102}) = (10, 53)$	$(a_{103}, b_{103}) = (14, 18)$	$(a_{104}, b_{104}) = (10, 51)$	$(a_{105}, b_{105}) = (10, 49)$
$(a_{106}, b_{106}) = (12, 26)$	$(a_{107}, b_{107}) = (10, 47)$	$(a_{108}, b_{108}) = (10, 41)$	$(a_{109}, b_{109}) = (16, 16)$
$(a_{110}, b_{110}) = (12, 28)$	$(a_{111}, b_{111}) = (10, 39)$	$(a_{112}, b_{112}) = (10, 37)$	$(a_{113}, b_{113}) = (8, 13)$
$(a_{114}, b_{114}) = (12, 30)$	$(a_{115}, b_{115}) = (10, 35)$	$(a_{116}, b_{116}) = (14, 20)$	$(a_{117}, b_{117}) = (10, 33)$
$(a_{118}, b_{118}) = (12, 32)$	$(a_{119}, b_{119}) = (10, 31)$	$(a_{120}, b_{120}) = (12, 34)$	$(a_{121}, b_{121}) = (12, 36)$
$(a_{122}, b_{122}) = (10, 29)$	$(a_{123}, b_{123}) = (12, 38)$	$(a_{124}, b_{124}) = (14, 22)$	$(a_{125}, b_{125}) = (16, 18)$
$(a_{126}, b_{126}) = (12, 40)$	$(a_{127}, b_{127}) = (10, 27)$	$(a_{128}, b_{128}) = (12, 42)$	$(a_{129}, b_{129}) = (12, 44)$
$(a_{130}, b_{130}) = (12, 46)$	$(a_{131}, b_{131}) = (10, 25)$	$(a_{132}, b_{132}) = (12, 48)$	$(a_{133}, b_{133}) = (14, 24)$
$(a_{134}, b_{134}) = (12, 50)$	$(a_{135}, b_{135}) = (12, 64)$	$(a_{136}, b_{136}) = (10, 23)$	$(a_{137}, b_{137}) = (12, 66)$
$(a_{138}, b_{138}) = (12, 70)$	$(a_{139}, b_{139}) = (14, 26)$	$(a_{140}, b_{140}) = (16, 20)$	$(a_{141}, b_{141}) = (12, 72)$
$(a_{142}, b_{142}) = (12, 92)$	$(a_{143}, b_{143}) = (8, 11)$	$(a_{144}, b_{144}) = (12, 94)$	$(a_{145}, b_{145}) = (12, 130)$
$(a_{146}, b_{146}) = (18, 18)$	$(a_{147}, b_{147}) = (12, 132)$	$(a_{148}, b_{148}) = (12, 162)$	$(a_{149}, b_{149}) = (14, 28)$
$(a_{150}, b_{150}) = (12, 164)$	$(a_{151}, b_{151}) = (12, 224)$	$(a_{152}, b_{152}) = (10, 21)$	$(a_{153}, b_{153}) = (12, 226)$
$(a_{154}, b_{154}) = (12, 219)$	$(a_{155}, b_{155}) = (3, 4)$	$(a_{156}, b_{156}) = (12, 217)$	$(a_{157}, b_{157}) = (12, 111)$
$(a_{158}, b_{158}) = (14, 30)$	$(a_{159}, b_{159}) = (12, 109)$	$(a_{160}, b_{160}) = (12, 99)$	$(a_{161}, b_{161}) = (16, 22)$
$(a_{162}, b_{162}) = (12, 97)$	$(a_{163}, b_{163}) = (12, 85)$	$(a_{165}, b_{165}) = (12, 83)$	$(a_{166}, b_{166}) = (14, 32)$
$(a_{167}, b_{167}) = (10, 19)$	$(a_{168}, b_{168}) = (18, 20)$	$(a_{169}, b_{169}) = (16, 24)$	$(a_{170}, b_{170}) = (8, 9)$
$(a_{171}, b_{171}) = (5, 6)$	$(a_{172}, b_{172}) = (3, 6)$	$(a_{173}, b_{173}) = (1, 4)$	

Let $I = \{i \in <173> \setminus \{1, 163, 164\} \mid a_i = a_{i+1}\}$. Then from this table (for (a_i, b_i)) we see that

$I = \{2, 8, 11, 14, 22, 23, 26, 29, 37, 39, 44, 47, 50, 53, 56, 59, 64, 65, 75, 82, 85, 88, 91, 94, 97, 101, 104, 107, 111, 120, 128, 129, 134, 137, 141, 144, 147, 150, 153, 156, 159, 162\}$.

For proving the Conjecture 1, we need to further introduce some notations. First we take $n = 300$, and denote

$$T_{300}(i) = G_i \qquad (i \in <173>).$$

Then for $i \neq 1, 164$, $T_n(i)$ is a subdivision graph of G_i when $n \geq 300$ (for some cut edge on the pendent path of length $299 - a_i - b_i$ of G_i). Also, it is easy to see that $T_n(1) = P_n$ is a subdivision graph of $G_1 = P_{300}$, and $T_n(164) = T_n(2, 2|2, 2)$ is a subdivision graph of $G_{164} = T_{300}(2, 2|2, 2)$. Thus all these graphs $T_n(i)$ $(i \in <173>)$ in the Extended adjusted list can be written as:

$$T_n(i) = G_i(n - 300) \qquad (n \geq 300), \qquad \text{or equivalently} \quad G_i(k) = T_{k+300}(i) \qquad (k \geq 0).$$

Let $d_0^i(x) = \dfrac{\widetilde{\phi}(G_i)}{\widetilde{\phi}(G_{i+1})}$. In general, let

$$d_k^i(x) = \frac{\widetilde{\phi}(G_i(k))}{\widetilde{\phi}(G_{i+1}(k))} \qquad (i \in <172>,\ k \geq 0).$$

Then we have

$$d_1^i(x) - d_0^i(x) = \frac{\widetilde{\phi}(G_i(1))\widetilde{\phi}(G_{i+1}) - \widetilde{\phi}(G_i)\widetilde{\phi}(G_{i+1}(1))}{\widetilde{\phi}(G_{i+1})\widetilde{\phi}(G_{i+1}(1))}. \tag{2.1}$$

Remark 2.1. Let $f_k^i(x) = \widetilde{\phi}(G_i(k+1))\widetilde{\phi}(G_{i+1}(k)) - \widetilde{\phi}(G_i(k))\widetilde{\phi}(G_{i+1}(k+1))$ (where $f_0^i(x)$ is just the numerator of the right hand side of (2.1)). Then from Remark 1.1 we can see that

$$f_k^i(x) = (-1)^k f_0^i(x). \qquad \square$$

Using computer, we have calculated all these polynomials $f_0^i(x) = \widetilde{\phi}(G_i(1))\widetilde{\phi}(G_{i+1}) - \widetilde{\phi}(G_i)\widetilde{\phi}(G_{i+1}(1))$ ($i \in <173> \backslash I$). These calculations are not difficult since all these G_j and $G_j(1)$ are trees of order 300 and 301, respectively. From these computer-aided calculations we find the following important fact.

Theorem 2.1. *For each $i \in <173> \backslash I$, either all the coefficients of $\widetilde{\phi}(G_i(1))\widetilde{\phi}(G_{i+1}) - \widetilde{\phi}(G_i)\widetilde{\phi}(G_{i+1}(1))$ (the numerator of the right hand side of (2.1)) are nonnegative, or all the coefficients of $\widetilde{\phi}(G_i(1))\widetilde{\phi}(G_{i+1}) - \widetilde{\phi}(G_i)\widetilde{\phi}(G_{i+1}(1))$ are nonpositive.*

Proof. For each $i \in <173> \backslash I$, let m_i and M_i be, respectively, the minimal value and the maximal value of all the nonzero coefficients of the polynomial $\widetilde{\phi}(G_i(1))\widetilde{\phi}(G_{i+1}) - \widetilde{\phi}(G_i)\widetilde{\phi}(G_{i+1}(1))$. Then by using computer we have calculated one of the m_i and M_i for each $i \in <173> \backslash I$ as in the following Table 2.

From Table 2 we can see that for each $i \in <173> \backslash I$, either $m_i > 0$ or $M_i < 0$. If $m_i > 0$, then all the coefficients of $\widetilde{\phi}(G_i(1))\widetilde{\phi}(G_{i+1}) - \widetilde{\phi}(G_i)\widetilde{\phi}(G_{i+1}(1))$ are nonnegative. If $M_i < 0$, then all the coefficients of $\widetilde{\phi}(G_i(1))\widetilde{\phi}(G_{i+1}) - \widetilde{\phi}(G_i)\widetilde{\phi}(G_{i+1}(1))$ are nonpositive. This proves the theorem. $\square$

Table 2: The value m_i or M_i of the polynomial $\widetilde{\phi}(G_i(1))\widetilde{\phi}(G_{i+1}) - \widetilde{\phi}(G_i)\widetilde{\phi}(G_{i+1}(1))$ for $i \in <173> \backslash I$

i	M_i	m_i	i	M_i	m_i	i	M_i	m_i	i	M_i	m_i	i	M_i	m_i	i	M_i	m_i
3	-1		4		1	5	-1		6		1	7	-1		9		1
10	-1		12	-1		13		1	15	-1		16		1	17	-1	
18		1	19	-1		20		1	21	-1		24		1	25	-1	
27	-1		28		1	30	-1		31		1	32		1	33	-1	
34		1	35	-1		36		1	38	-1		40		1	41	-1	
42		1	43	-1		45		1	46	-1		48		1	49	-1	
51		1	52	-1		54		1	55	-1		57	-1		58		1
60	-1		61	-1		62		1	63		1	66	-1		67		1

68	-1		69		1	70	-1		71	-1		72		1	73		1
74	-1		76		1	77	-1		78		1	79	-1		80		1
81	-1		83		1	84	-1		86		1	87	-1		89		1
90	-1		92		1	93	-1		95	-1		96		1	98	-1	
99	-1		100		1	102	-1		103		1	105	-1		106		1
108	-1		109	-1		110		1	112	-1		113	-1		114		1
115	-1		116		1	117	-1		118		1	119	-1		121		1
122	-1		123		1	124		1	125	-1		126		1	127	-1	
130		1	131	-1		132		1	133	-1		135		1	136	-1	
138		1	139		1	140	-1		142		1	143	-1		145		1
146	-1		148		1	149	-1		151		1	152	-1		154	-1	
155		1	157	-1		158		1	160	-1		161		1	163	-1	
164	1		165	-1		166		1	167	-1		168	-1		169		1
170	-1		171	-1		172	-1										

Using more computer-aided calculations, we further obtain the following important result.

Theorem 2.2. *For each fixed* $i \in< 173 > \backslash I$, *there exist some odd number* $n_i \leq 7527$ *and some even number* $m_i \leq 7526$ *such that* $T_{n_i}(i) > T_{n_i}(i+1)$ *and* $T_{m_i}(i) > T_{m_i}(i+1)$.

Proof. See Appendix A in Section 3 for those values of n_i and m_i for each $i \in< 173 > \backslash I$. □

The following Theorem 2.3 (together with using the edge grafting Lemma 2.1 for those $i \in I$) determines the inner order of all graphs in the Extended adjusted list in the energy decreasing order when $n \geq 7527$.

Theorem 2.3. *For each* $i \in< 173 > \backslash I$, *and each* $n \geq 7526$, *we have*

$$T_n(i) > T_n(i+1)$$

Proof. Take any fixed $i \in< 173 > \backslash I$. For the sake of simplicity of notations, we abbreviate $d_k^i(x)$ as $d_k(x)$ for this fixed i. Thus from the integral formula (1.4) for the energy differences we have:

$$\mathbb{E}(G_i(k)) - \mathbb{E}(G_{i+1}(k)) = \frac{2}{\pi}\int_0^{+\infty} \ln \frac{\widetilde{\phi}(G_i(k),x)}{\widetilde{\phi}(G_{i+1}(k),x)}\mathrm{d}x = \frac{2}{\pi}\int_0^{+\infty} \ln d_k(x)\mathrm{d}x. \qquad (2.2)$$

From Theorem 2.1 and equation (2.1), we can also see that if $i \in< 173 > \backslash I$, then

$$\text{either} \quad d_1(x) \geq d_0(x) \quad (\text{for all } x > 0) \quad \text{or} \quad d_1(x) \leq d_0(x) \quad (\text{for all } x > 0). \qquad (2.3)$$

So it suffices for us to consider the following two cases.

Case 1. $d_1(x) \geq d_0(x)$ for all $x > 0$.

Then by Lemma 1.1, we have

$$d_m(x) \geq d_k(x) \qquad \text{for all even m and k with } m \geq k, \text{ and all } x > 0$$

and

$$d_r(x) \geq d_k(x) \qquad \text{for all odd r and even k , and all } x > 0.$$

From this and the integral formula (2.2) we have

$$\mathbb{E}(G_i(m)) - \mathbb{E}(G_{i+1}(m)) \geq \mathbb{E}(G_i(k)) - \mathbb{E}(G_{i+1}(k)) \quad (m, k \text{ even and } m \geq k) \tag{2.4}$$

and

$$\mathbb{E}(G_i(r)) - \mathbb{E}(G_{i+1}(r)) \geq \mathbb{E}(G_i(k)) - \mathbb{E}(G_{i+1}(k)) \quad (r \text{ odd and } k \text{ even}). \tag{2.5}$$

Now take m_i as in Theorem 2.2, and take $k = m_i - 300$, take $m = n - 300$ with even $n \geq 7526$ in (2.4), and $r = n - 300$ with odd $n \geq 301$ in (2.5). By Theorem 2.2 and $G_i(k) = T_{k+300}(i) = T_{m_i}(i)$, we see that the right hand sides of (2.4) and (2.5) are $\mathbb{E}(T_{m_i}(i)) - \mathbb{E}(T_{m_i}(i+1)) > 0$, so the left hand sides of (2.4) and (2.5) are also positive, which implies that

$$T_n(i) > T_n(i+1) \qquad \text{for all even } n \geq 7526$$

and

$$T_n(i) > T_n(i+1) \qquad \text{for all odd } n \geq 301$$

as desired.

Case 2. $d_1(x) \leq d_0(x)$ for all $x > 0$.

Similarly we can have equations (2.4') and (2.5'), where (2.4') and (2.5') are obtained from (2.4) and (2.5) by replacing all "even" by "odd", and all "odd" by "even".

Now take n_i as in Theorem 2.2, and take $k = n_i - 300$, take $m = n - 300$ with odd $n \geq 7526$, and $r = n - 300$ with even $n \geq 300$, we can also obtain the desired results by using similar arguments as in Case 1. □

The following result in [2] will be used in the proof of Theorem 2.5.

Theorem 2.4. *[2] Among all trees of order $n \geq 10$ with at least 4 pendent vertices, $T_n(2,2|2,2)$ is the unique tree with maximal energy.* □

Theorem 2.5. *Let $n \geq 7526$ and T be a tree of order n, $T \neq T_n(2,2|2,2)$ and T is not one of the trees in the Extended adjusted list before $T_n(2,2|2,2)$. Then $T < T_n(2,2|2,2)$.*

Proof. If T contains at least 4 pendent vertices. Then by Theorem 2.4 we have $T < T_n(2,2|2,2)$.

If T contains at most 3 pendent vertices, then T contains exactly 3 pendent vertices since $T \neq P_n$. So T must be of the form $T_n(i,j,c)$, where $i+j+c = n-1$. Without loss of generality, we assume $i \leq j \leq c$.

By the hypothesis that T is not one of the trees in the Extended adjusted list before $T_n(2,2|2,2)$, we can see that $i \notin \{2,4,6\}$. We now consider the following cases.

Case 1. $i \geq 20$. Then by Lemma 2.1 and Theorem 2.3 for the inner order of the Extended adjusted list, we have

$$T_n(i,j,c) \leq T_n(20,20,n-41) < T_n(18,20,n-39) < T_n(2,2|2,2).$$

All the following cases (Case 2 to Case 17) will follow from the hypothesis (that T is not one of the trees in the Extended adjusted list before $T_n(2,2|2,2)$), Lemma 2.1 and Theorem 2.3 for the inner order of the Extended adjusted list.

Case 2. $i = 1$. Then we have $T_n(1,j,c) \leq T_n(1,4,n-6) < T_n(2,2|2,2)$.

Case 3. $i = 3$. Then we have $T_n(3,j,c) \leq T_n(3,6,n-10) < T_n(2,2|2,2)$.

Case 4. $i = 5$. Then we have $T_n(5,j,c) \leq T_n(5,6,n-12) < T_n(2,2|2,2)$.

Case 5. $i = 7$. Then we have $T_n(7,j,c) \leq T_n(7,8,n-16) < T_n(8,9,n-18) < T_n(2,2|2,2)$.

Case 6. $i = 8$. Then we have $T_n(8,j,c) \leq T_n(8,9,n-18) < T_n(2,2|2,2)$.

Case 7. $i = 9$. Then we have $T_n(9,j,c) \leq T_n(9,10,n-20) < T_n(8,9,n-18) < T_n(2,2|2,2)$.

Case 8. $i = 10$. Then we have $T_n(10,j,c) \leq T_n(10,19,n-30) < T_n(2,2|2,2)$.

Case 9. $i = 11$. Then we have $T_n(11,j,c) \leq T_n(11,12,n-24) < T_n(12,83,n-96) < T_n(2,2|2,2)$.

Case 10. $i = 12$. Then we have $T_n(12,j,c) \leq T_n(12,83,n-96) < T_n(2,2|2,2)$.

Case 11. $i = 13$. Then we have $T_n(13, j, c) \leq T_n(13, 14, n-28) < T_n(14, 32, n-47) < T_n(2, 2|2, 2)$.

Case 12. $i = 14$. Then we have $T_n(14, j, c) \leq T_n(14, 32, n-47) < T_n(2, 2|2, 2)$.

Case 13. $i = 15$. Then we have $T_n(15, j, c) \leq T_n(15, 16, n-28) < T_n(16, 24, n-41) < T_n(2, 2|2, 2)$.

Case 14.$i = 16$. Then we have $T_n(16, j, c) \leq T_n(16, 24, n-41) < T_n(2, 2|2, 2)$.

Case 15. $i = 17$. Then we have $T_n(17, j, c) \leq T_n(17, 18, n-28) < T_n(18, 20, n-39) < T_n(2, 2|2, 2)$.

Case 16. $i = 18$. Then we have $T_n(18, j, c) \leq T_n(18, 20, n-39) < T_n(2, 2|2, 2)$.

Case 17. $i = 19$. Then we have $T_n(19, j, c) \leq T_n(19, 20, n-40) < T_n(18, 20, n-39) < T_n(2, 2|2, 2)$.

□

For the counting of the number of graphs in the Extended adjusted list before $T_n(2, 2|2, 2)$, recalling that the class $D_i = \{T_n(i, j, c) \mid i + j + c = n - 1,\ i \leq j \leq c\}$ was defined in (1.13) (for fixed i), it is not difficult to see that

$$|D_i| = \left\lfloor \frac{n-1-i}{2} \right\rfloor - (i-1). \tag{2.6}$$

Let N_i be the number of graphs in the class D_i which are also in the Extended adjusted list before $T_n(2, 2|2, 2)$. In [2, Theorem 3], Andriantiana showed that the total number of trees of order n whose energy is greater than the energy of $T_n(2, 2|2, 2)$ (including P_n) is

$$\sum_{i=1}^{19} N_i + 1 = \sum_{i=1}^{6} |D_{2i}| - 25 = 6\left\lfloor \frac{n-1}{2} \right\rfloor - 82 = \begin{cases} 3n - 85 & \text{if } n \text{ is odd;} \\ 3n - 88 & \text{if } n \text{ is even,} \end{cases} \tag{2.7}$$

which is the same as the total number of graphs in the Extended adjusted list before $T_n(2, 2|2, 2)$ by Theorem 2.5. Thus when n is odd, $T_n(2, 2|2, 2)$ is the $(3n-84)^{th}$ graph in the Extended adjusted list, and when n is even, $T_n(2, 2|2, 2)$ is the $(3n-87)^{th}$ graph in the Extended adjusted list.

Combining this counting with the results in Theorem 2.5 (for exclusion) and Theorem 2.3 (for the inner order of the graphs in the Extended adjusted list), we finally obtain the following result (which is stronger than Conjecture 1).

Theorem 2.6. *Conjecture 1 is true for all* $n \geq 7526$.

Remark 2.2. Finally, we would like to point out that: if $n = 7525$, then computer calculations show that

$$\mathbb{E}(T_{7525}(154)) \doteq 9580.268894388544 \qquad \text{and} \qquad \mathbb{E}(T_{7525}(155)) \doteq 9580.268894388575.$$

From this we see that $T_{7525}(154) < T_{7525}(155)$. This shows that 7526 is the smallest number such that Conjecture 1 is true.

3 Appendix

Appendix A: Computer calculations for Theorem 2.2

i	n_i	$\mathbb{E}(T_{n_i}(i))$	$\mathbb{E}(T_{n_i}(i+1))$	m_i	$\mathbb{E}(T_{m_i}(i))$	$\mathbb{E}(T_{m_i}(i+1))$
3	31	38.61692304744	38.61674190434	12	14.52548002281	14.48527570942
4	11	13.1191889021	13.06926754747	96	121.41525808957	121.41525466141
5	23	28.41531320271	28.41474078655	12	14.51104883982	14.44570221615
6	13	15.67513125975	15.63497136197	40	50.11484661552	50.11478821044
7	35	43.70432133869	43.70417158023	14	17.03843761804	16.98079923363
9	25	30.98614432296	30.95760664991	78	98.48446442957	98.48446230519
10	57	71.72181052007	71.7217970614	26	32.28746363957	32.23409007027
12	199	252.5308229199	252.5308215789	22	27.22908053265	27.18970061991
13	21	25.85963102863	25.82073610508	72	90.8417812226	90.84176790207
15	77	97.185289635	97.185252909	18	22.14060071309	22.04685015995
16	19	23.33136385353	23.27573495334	68	85.74703029557	85.74699652254
17	77	97.18391080531	97.18388305485	20	24.66009705112	24.58774151975
18	21	25.88221856132	25.863592507	32	39.91525352594	39.91522303148
19	47	58.97786352988	58.97783296543	22	27.17962573807	27.12999286265
20	23	28.43243978762	28.38671120574	66	83.19841528621	83.1984149156
21	315	400.22337892145	400.22337875204	24	29.74018502018	29.67315798161
24	35	43.72547582392	43.69051940165	86	108.6592338027	108.65922518356
25	103	130.28825237429	130.28825107753	36	45.00413176635	44.94124063005
27	891	1133.608280437	1133.608280424	48	60.31726706078	60.27873350237
28	47	58.97403352883	58.94335566932	262	332.74377124426	332.74377112798
30	177	224.50944115225	224.5094390335	32	39.95053296336	39.90585025643
31	25	30.98046897108	30.96112466203	68	85.7396645528	85.73966162072
32	31	38.59428407108	38.55601529599	690	877.68793272315	877.6879327231
33	161	204.1367311966	204.13672880549	30	37.40504598841	37.36860671488
34	29	36.03514334958	36.00611147786	84	106.11037942676	106.11036713871
35	129	163.39100436768	163.39099443398	28	34.85968675292	34.79263446388
36	27	33.52965703795	33.45556470305	1252	1593.247463590	1593.247463587
38	1637	2083.44305226516	2083.4430522644	28	34.83298968574	34.75177066157
40	31	38.62710408758	38.59525531356	108	136.66475657604	136.66475607346
41	63	79.34805250911	79.34802971439	32	39.90370656171	39.8406821419
42	33	41.17545509554	41.1269206075	410	521.17926294879	521.17926281488
43	165	209.22773460119	209.22773113621	34	42.45971562601	42.38559360236
45	41	51.36713439516	51.32902118085	96	121.38522113854	121.38522108056
46	131	165.935329438	165.93532780493	42	52.63524173076	52.56704610687
48	47	59.00965828216	58.96562394347	246	312.36768819287	312.36768777045
49	569	723.62003112613	723.62003102519	48	60.27649071691	60.20428525697
51	67	84.48083562314	84.4400595336	260	330.19246811009	330.19246805264
52	211	267.79678731201	267.79678723518	68	85.73586594232	85.66488032599

54	97	122.68272908538	122.64158969649	380	482.98038325788	482.9803832392
55	373	474.0635325853	474.06353253391	98	123.93069762262	123.85923488339
57	497	631.94527320407	631.94527296118	60	75.59212049365	75.54973193161
58	59	74.25164960121	74.21752375519	1200	1527.035211593	1527.035211590
60	921	1171.799329451	1171.799329449	44	55.22330661566	55.17891484985
61	97	122.64045498347	122.64045273735	32	39.88978803772	39.83466859389
62	33	41.17451516988	41.12529980356	324	411.67804012123	411.67803990173
63	43	53.86823852213	53.83668630597	174	220.69356566884	220.69356444742
66	833	1059.753707433	1059.753707424	38	47.58562051202	47.52568217406
67	37	46.25052799352	46.1913608749	162	205.414430398	205.41442536761
68	267	339.09716195517	339.09716044795	36	45.03984533344	44.92420995422
69	37	46.27060789683	46.20455839278	194	246.15725872225	246.15725821845
70	285	362.01548564656	362.01548452695	34	42.49414550779	42.43375449496
71	125	158.2925328742	158.29253208621	38	47.53508019103	47.46933848051
72	39	48.81843118925	48.77461504176	278	353.10832153579	353.10832135254
73	33	41.13000476692	41.09293320995	146	185.04242228271	185.04242043053
74	565	718.52413655172	718.52413646042	40	50.09621611332	50.01464305718
76	43	53.91372425528	53.87449124175	118	149.39206458922	149.39206147298
77	105	132.8257530381	132.82575075287	44	55.17662420199	55.10565817507
78	45	56.46122283434	56.41149788851	292	370.93305610508	370.93305603494
79	349	443.50281022485	443.50281015293	46	57.7292786462	57.6513243676
80	47	59.00863839855	58.96846530649	122	154.4846011531	154.48459853777
81	129	163.38502176493	163.38501849303	48	60.26891168499	60.19707442498
83	57	71.74476207657	71.6980088559	326	414.2224838473	414.22248354732
84	877	1115.77462741012	1115.77462739327	58	73.00327500763	72.9267210021
86	65	81.93285564498	81.88998194412	192	243.60928978789	243.60928888023
87	229	290.71189481518	290.71189444945	66	83.18562706848	83.11113467538
89	83	104.85455749969	104.8109928652	304	386.21092589633	386.21092588268
90	291	369.65351058799	369.65351044918	84	106.10250916495	106.0272393354
92	195	247.46450470576	247.42052473359	2168	2759.52772369383	2759.5277236938
93	803	1021.55420126842	1021.55420126698	196	248.70175185942	248.62588563186
95	1629	2073.25062514444	2073.25062514363	188	238.55994074831	238.51598135221
96	187	237.23402745926	237.1999323843	1962	2497.24030698757	2497.24030698723
98	1081	1375.51477232155	1375.51477231009	82	103.60008190683	103.55625028161
99	3793	4828.54111441289	4828.5411144128	38	47.54304071185	47.46502493941
100	81	102.26378737146	102.2278732969	644	819.11087577983	819.11087571588
102	3215	4092.60841735	4092.6084173492	66	83.22974800416	83.18461615334
103	65	81.88903290539	81.85187496547	396	503.34778493594	503.34778471441
105	749	952.79853372871	952.79853370269	62	78.13728217971	78.09111324016
106	61	76.79604498436	76.75747303169	454	577.1954147291	577.19541452831
108	965	1227.81837311383	1227.81837308352	54	67.95256167362	67.90600091439
109	135	171.02296426934	171.02296353989	42	52.62324086316	52.5554558524
110	53	66.61114364065	66.56787619031	362	460.05743175776	460.05743159197
112	213	270.33802603534	270.33802549918	50	62.8603388244	62.81764979316
113	979	1245.643523798	1245.643523778	44	55.18053579977	55.10090330377
114	49	61.52591781013	61.47252064775	406	516.0796191466	516.07961902556
115	503	639.58041544044	639.58041537113	48	60.31427107382	60.26456609566
116	47	58.96888167689	58.92465148367	276	350.55900497905	350.55900459991

117	843	1072.4826076824	1072.48260761188	46	57.76823707836	57.64646963128
118	47	59.00804034973	58.93871437589	222	281.80443202229	281.8044308631
119	767	975.716138414	975.71613832169	48	60.28517238407	60.19213535194
121	51	64.10265128424	64.04685776788	474	602.65929607023	602.65929588766
122	371	471.51160322882	471.51160271664	52	65.36796386996	65.28370627328
123	53	66.64986705067	66.60825007682	162	205.41052707807	205.41052614236
124	39	48.81754655225	48.79664447631	82	103.55414725595	103.55414108842
125	191	242.32577626141	242.32577578966	54	67.90461766924	67.82958902175
126	55	69.19703121134	69.14511593817	468	595.01967719933	595.01967714437
127	447	568.27811472151	568.27811443051	56	70.45715730224	70.37552501824
130	61	76.83826247828	76.78848576276	336	426.95228077789	426.95228020209
131	1609	2047.78396439252	2047.78396438707	62	78.09387833773	78.01358950398
132	63	79.38526575446	79.34149054824	158	200.31726118176	200.31725978728
133	343	435.86026078058	435.86026073742	64	80.63612815577	80.55968028702
135	79	99.76035558625	99.71260108371	1006	1280.021406276	1280.021406261
136	787	1001.18007475522	1001.18007469514	80	101.00865403019	100.92921852467
138	85	107.40070352579	107.35544209372	254	322.54672100152	322.5467206966
139	43	53.91278633319	53.88276574049	278	353.10429420224	353.10429419875
140	443	563.18458603456	563.18458601713	86	108.6461723969	108.5680481322
142	107	135.41444945501	135.36784378701	796	1012.6410375646	1012.64103753169
143	2587	3293.01199263552	3293.01199262884	108	136.65676119441	136.57773372059
145	145	183.80007379648	183.75419589944	726	923.51423269228	923.514232685
146	575	731.25252331572	731.25252329392	146	185.03811136195	184.95931655827
148	177	224.54502821686	224.49910301413	1516	1929.37306196582	1929.37306196554
149	703	894.22747952079	894.22747951702	178	225.78111403414	225.70223870067
151	239	303.48739953776	303.4412306802	3790	4824.71954734348	4824.71954734334
152	6297	8016.73078097378	8016.73078097372	240	304.72129325556	304.64224155064
154	7527	9582.81537351517	9582.81537351497	234	297.12779300591	297.08177963631
155	233	295.80172032711	295.76533856832	2790	3551.47997715734	3551.479977157
157	1811	2304.97758749491	2304.97758749392	126	159.61981572456	159.57356947899
158	125	158.28808115106	158.2509977438	2236	2846.10520599038	2846.10520598925
160	2241	2852.47066844866	2852.47066844706	114	144.34137074054	144.29508561283
161	113	143.00830442669	142.97104183846	1176	1496.47146523763	1496.47146523687
163	1669	2124.17742608899	2124.17742608395	100	126.51664684462	126.47039133233
164	97	122.63480349274	122.55452231649	990	1259.64893062728	1259.64893060524
165	413	524.98656988214	524.98656968916	98	123.97027219795	123.92361576384
166	49	61.55500194201	61.5017856981	248	314.90667086684	314.90667001447
167	279	354.37102470569	354.3710228515	40	50.09307851979	50.00460516523
168	105	132.82135005714	132.8213487806	42	52.59369440793	52.55035236396
169	43	53.91257566319	53.85934436887	80	101.00597298491	101.0059466448
170	51	64.05079616858	64.05067168147	20	24.67739980341	24.641039012
172	17	20.68050389273	20.67690659018	12	14.50026296409	14.44570221615

References

[1] H. Y. Shan, J. Y. Shao, L. Zhang, C. X. He, A new method of comparing the energies of subdivision bipartite graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 721–740.

[2] E. O. D. Andriantiana, More trees with large energy, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 675–695.

[3] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

[4] I. Gutman, The energy of a graph, *Ber. Math.-Statist. Sekt. Forsch. Graz* **103** (1978) 1–22.

[5] I. Gutman, The energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer–Verlag, Berlin, 2001, pp. 196–211.

[6] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[7] I. Gutman, S. Radenković, N. Li, S. Li, Extremal energy trees, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 315–320.

[8] E. Heilbronner, Das Kompositions–Prinzip: Eine anschauliche Methode zur elektronen–theoretischen Behandlung nicht oder niedrig symmetrischer Molekeln im Rahmen der MO–Theorie, *Helv. Chim. Acta* **36** (1953) 170–188.

[9] B. Huo, S. Ji, X. Li, Y. Shi, Complete solution to a conjecture on the fourth maximal energy tree, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 903–912.

[10] N. Li, S. Li, On the extremal energies of trees, *MATCH Commun. Math. Comput. Chem* **59** (2008) 291–314.

[11] H. Y. Shan, J. Y. Shao, Graph energy change due to edge grafting operations and its applications, *MATCH Commun. Math. Comput. Chem* **64** (2010) 25–40.

[12] H. Y. Shan, J. Y. Shao, F. Gong, Y. Liu, An edge grafting theorem on the energy of unicyclic and bipartite graphs, *Lin. Algebra Appl.* **433** (2010) 547–556.