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More Trees with Large Energy

Eric Ould Dadah Andriantiana
Department of Mathematical Sciences, Mathematics Division, Stellenbosch University
Private Bag X1, Matieland 7602, South Africa
ericoda@sun.ac.za

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Abstract

Let $\lambda_1, \lambda_2 \ldots, \lambda_n$ be the eigenvalues of an n-vertex graph G. The energy of G is defined as $\mathrm{En}(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$. The trees with largest, second, third and fourth-largest energy are known for any given number of vertices. For sufficiently large n, we extend this list until the first appearance of a tree with four leaves, which is the tree with $(3n-84)^{\text{th}}$ (resp. $(3n-87)^{\text{th}}$) largest energy for odd n (resp. for even n).

1 Introduction

Let G be a simple and undirected n-vertex graph with adjacency matrix $A(G)$. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the n roots of the polynomial $P(\lambda) = \det(\lambda I - A(G))$. The energy of G is defined as

$$\mathrm{En}(G) = \sum_{i=1}^{n} |\lambda_i|.$$

Apart from purely graph theoretical interest, the study of En is considerably motivated by applications in organic chemistry: for example, within the framework of Hückel molecular orbital approximation, the calculation of the theoretically computed total π-electron energy of a hydrocarbon molecule can be reduced to that of the energy of the corresponding molecular graph [6]. Moreover, the energy of graphs has certain relations to some well known topological indices such as the Merrifield-Simmons index, defined as the number of independent vertex subsets, and the Hosoya index which is the number of independent edge subsets: it often happens that in a given class of graphs there is an element which has the maximum energy, the maximum Hosoya index and the minimum Merrifield-Simmons index and/or an element with the minimum energy, the minimum Hosoya index and the maximum Merrifield-Simmons index; for instance, this is the case for the class of trees and some smaller classes as in [1, 8].

The characterisation of extremal graphs with respect to the energy for different types of graphs such as trees [3, 11, 13, 17], unicyclic [2, 10, 12], bicyclic [9, 16], tricyclic [15], tetracyclic graphs [14] and many others has been of interest to both graph theorists and chemists. A wider range of results can be found in the survey [5]. Let us denote by P_n the n-vertex path and by $T(i, j, n-i-j-1)$ the n-vertex tripod which has two branches of length i and j (see Figure 1), respectively. We can rearrange i, j and $n-i-j-1$ if needed and still have the same tripod. The four n-vertex trees with maximum energy, for

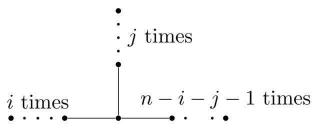


Figure 1: Tripod $T(i, j, n-i-j-1)$

$n \geq 15$, are $P_n, T(2, 2, n-5), T(2, 4, n-7)$ and $T(2, 6, n-9)$ ordered by decreasing energy [3, 11, 13]. In this paper our main result is an extension of this list, for large enough n, until the first appearance of a tree with four leaves, which is the tree with $(3n-84)^{\text{th}}$ (resp. $(3n-87)^{\text{th}}$) largest energy for odd n (resp. even n). To achieve this we extend an approach used in [7, 18, 20]: the technique consists of considering a graph obtained by attaching a subgraph G to the i^{th} vertex in a path, and then observing how the energy depends on the choice of the position i. Details for this are provided in Section 2, they are based on the formula [6]

$$\mathrm{En}(T) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log \mu(T, x) \tag{1}$$

for any tree T, where

$$\mu(T, x) = \sum_{k \geq 0} \mathrm{m}(G, k) x^{2k}, \tag{2}$$

and $\mathrm{m}(G, k)$ denotes the number of matchings of order k in G. Equation (1) is a particular case of the so-called Coulson integral formula for the energy of a graph, which has been used in most results on the energy of graphs. It follows from (1) that whenever we have two trees T_1 and T_2 which satisfy the inequality

$$\mu(T_1, x) > \mu(T_2, x)$$

for all real numbers $x > 0$, we can deduce that $\mathrm{En}(T_1) > \mathrm{En}(T_2)$. Therefore the study of En can be reduced to that of $\mu(., x)$ in appropriate situations. In Section 3 we show for all $n \geq 10$ that $H(2, 2, 2, 2, n)$, obtained by merging each end of P_{n-8} to the third vertex in a 5-vertex path, is the tree with maximum energy among all trees of order n and at least four leaves. Finally, Section 4 is devoted to ordering of all trees with energy greater than that of $H(2, 2, 2, 2, n)$.

2 "Sliding along a path" with respect to $\mu(., x)$

Let G be a connected graph with at least two vertices, and let v be a vertex of G. Let n and k be integers such that $n - 1 \geq k \geq 0$. We denote by $P(n, k, G, v)$ the graph which results from identifying v with the vertex v_{k+1} of a path $v_1, \cdots, v_n$ as in Figure 2. For a vertex v in a graph G we denote by $N_G(v)$ the set of vertices of G adjacent to v.

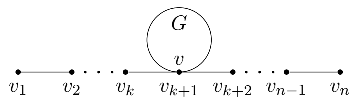


Figure 2: $P(n, k, G, v)$

In this section we aim to understand how $\mu(P(n, k, G, v), x)$ behaves as a function of k. The following lemma is an immediate consequence of the definition of $\mu(., x)$:

Lemma 1 ([6]). *Let G and G' be two disjoint graphs and let $x > 0$ be a real number. Then we have*

$$\mu(G \cup G', x) = \mu(G, x)\mu(G', x); \tag{3}$$

if $v \in V(G)$, then we have

$$\mu(G, x) = \mu(G - v, x) + x^2 \sum_{w \in N_G(v)} \mu(G - \{v, w\}, x). \tag{4}$$

The following ordering of the $P(n, k, G, v)$'s is well-known, see [7] and [18].

Lemma 2. *Let x be a positive real number and $n \geq 7$ an integer, then the following inequalities hold:*

$$\mu(P(n,0,G,v),x) > \mu(P(n,2,G,v),x) > \dots > \mu(P(n,2\lfloor(n-1)/4\rfloor,G,v),x)$$
$$> \mu(P(n,2\lfloor(n+1)/4\rfloor-1,G,v),x) > \dots > \mu(P(n,3,G,v),x) > \mu(P(n,1,G,v),x).$$

Note that $2\lfloor m/4\rfloor$ and $2\lfloor(m+2)/4\rfloor - 1$ are the two largest integers less or equal to $m/2$ for all positive integers m.

As k varies, G appears to be "sliding" along the path to which it is attached. This is the reason why lemmas of such a type are also called "Sliding along a path" [19].

The following remark is an immediate consequence of Lemma 2, it is particularly useful in practice to construct trees with larger energy than a given one (see [4] for instance).

Remark 1. *The graph transformation in Figure 3 reduces the number of leaves and increases the energy, for all integers $n > k > 1$. In general, the energy of a tree increases*

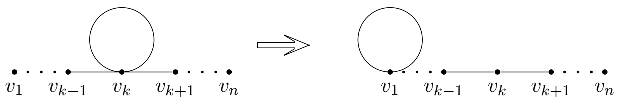


Figure 3:

if we replace a branch which is not a path by a path of the same order.

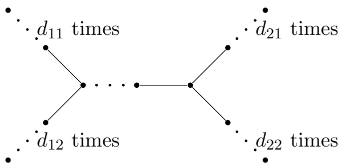
By considering one of the branches of a tripod as a sliding subgraph, the following theorem follows:

Theorem 1 ([3])**.** *For all positive integers i and n such that $n \geq 3i + 7$ we have*

$$\mathrm{En}(T(i,2\lceil i/2\rceil,n-i-2\lceil i/2\rceil-1)) > \mathrm{En}(T(i,2\lceil i/2\rceil+2,n-i-2\lceil i/2\rceil-3)) > \dots$$
$$> \mathrm{En}(T(i,2\lfloor(n-i-1)/4\rfloor,n-i-2\lfloor(n-i-1)/4\rfloor-1))$$
$$> \mathrm{En}(T(i,2\lfloor(n-i+1)/4\rfloor-1,n-i-2\lfloor(n-i+1)/4\rfloor)) >$$
$$\dots > \mathrm{En}(T(i,2\lfloor i/2\rfloor+3,n-i-2\lfloor i/2\rfloor-4)) > \mathrm{En}(T(i,2\lfloor i/2\rfloor+1,n-i-2\lfloor i/2\rfloor-2)).$$

3 Trees with at least four leaves and maximum energy

Throughout this section $d_{11}, d_{12}, d_{21}, d_{22}$ are always positive integers. For all integers n such that $d_{11} + d_{12} + d_{21} + d_{22} \leq n - 1$, we denote by $H(d_{11}, d_{12}, d_{21}, d_{22}, n)$ the n-vertex



$H(d_{11}, d_{12}, d_{21}, d_{22}, n)$

Figure 4:

quadripod as described in Figure 4. It is convenient to set

$$T(0, j, k) = P_{j+k+1},$$
$$T(-1, j, k) = P_j \cup P_k$$

and

$$\mu(T(-2, j, k), x) = \mu(P_j, x)\mu(P_{k-1}, x) + \mu(P_{j-1}, x)\mu(P_k, x)$$

for all positive integers j and k to have the well known relation

$$\mu(T(i, j, k+2), x) = \mu(T(i, j, k+1), x) + x^2\mu(T(i, j, k), x) \tag{5}$$

valid for $i \geq -2$ and $j, k \geq 1$. Note that for $n \geq d_{11} + d_{12} + d_{21} + d_{22} + 1$ we have

$$\begin{aligned}
&\mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n), x)\\
&\qquad = \mu(P_{d_{11}}, x)\mu(P_{d_{12}}, x)\mu(T(d_{21}, d_{22}, n - d_{11} - d_{12} - d_{21} - d_{22} - 2), x)\\
&\qquad + x^2\mu(P_{d_{11}-1}, x)\mu(P_{d_{12}}, x)\mu(T(d_{21}, d_{22}, n - d_{11} - d_{12} - d_{21} - d_{22} - 2), x)\\
&\qquad + x^2\mu(P_{d_{11}}, x)\mu(P_{d_{12}-1}, x)\mu(T(d_{21}, d_{22}, n - d_{11} - d_{12} - d_{21} - d_{22} - 2), x)\\
&\qquad + x^2\mu(P_{d_{11}}, x)\mu(P_{d_{12}}, x)\mu(T(d_{21}, d_{22}, n - d_{11} - d_{12} - d_{21} - d_{22} - 3), x)
\end{aligned}$$

which shows that (using (5))

$$\begin{aligned}
&\mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n+2), x)\\
&\qquad = \mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n+1), x) + x^2\mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n), x)
\end{aligned} \tag{6}$$

and

$$\begin{aligned}
&\mu(H(d_{11}, d_{12}, d_{21}, d_{22}+2, n+2), x)\\
&\qquad = \mu(H(d_{11}, d_{12}, d_{21}, d_{22}+1, n+1), x) + x^2\mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n), x).
\end{aligned} \tag{7}$$

Lemma 3. *The n-vertex tree with at least four leaves and maximum energy must be an element of*

$$\{H(1,1,1,1,n), H(1,1,2,d_{22},n), H(2,d_{12},2,d_{22},n) | d_{22} \geq d_{12} \geq 1\}.$$

Proof. Remark 1 reduces the set of candidates to be the set of quadripods. Using the Lemma of "Sliding along a path" we know that if $\max\{d_{11}, d_{12}\} \geq 3$ and $\min\{d_{11}, d_{12}\} \neq 2$, then for all positive x we have

$$\mu(H(d_{11}, d_{12}, d_{21}, d_{22}), x) < \mu(H(2, d_{12} + d_{11} - 2, d_{21}, d_{22}), x).$$

Similarly, if $\max\{d_{21}, d_{22}\} \geq 3$ and $\min\{d_{21}, d_{22}\} \neq 2$, then we have

$$\mu(H(d_{11}, d_{12}, d_{21}, d_{22}), x) < \mu(H(d_{11}, d_{12}, 2, d_{22} - d_{21} - 2), x).$$

□

Now we also have to use (4) in order to get the following relations:

$$\begin{aligned} \mu(H(1,1,1,1,n),x) &= \mu(T(1,1,n-4),x) + x^2\mu(T(1,1,n-6),x) \\ &< \mu(T(1,2,n-5),x) + x^2\mu(T(1,2,n-7),x) \text{ for all } n \geq 7 \\ &= \mu(H(1,2,1,1,n),x), \end{aligned} \tag{8}$$

$$\begin{aligned} \mu(H(1,2,1,1,n),x) &= \mu(H(1,1,1,1,n-1),x) + x^2\mu(T(1,1,n-5),x) \\ &< \mu(H(1,1,1,2,n-1),x) + x^2\mu(T(1,2,n-6),x) \text{ for all } n \geq 8 \\ &= \mu(H(1,2,1,2,n),x), \end{aligned} \tag{9}$$

$$\begin{aligned} \mu(H(1,1,2,2,n),x) &= \mu(H(1,1,1,2,n-1),x) + x^2\mu(T(1,1,n-5),x) \\ &< \mu(H(1,1,1,2,n-1),x) + x^2\mu(T(1,2,n-6),x) \text{ for all } n \geq 6 \\ &= \mu(H(1,2,1,2,n),x), \end{aligned} \tag{10}$$

$$\begin{aligned} \mu(H(1,2,1,2,n),x) &= \mu(H(1,1,1,2,n-1),x) + x^2\mu(T(1,2,n-6),x) \\ &< \mu(H(1,2,1,2,n-1),x) + x^2\mu(T(1,2,n-6),x) \text{ for all } n \geq 9 \\ &= \mu(H(1,2,2,2,n),x), \end{aligned} \tag{11}$$

$$\mu(H(1,2,2,2,n),x) = \mu(H(1,2,1,2,n-1),x) + x^2\mu(T(1,2,n-6),x)$$

$$< \mu(H(1,2,2,2,n-1),x) + x^2\mu(T(2,2,n-7),x) \text{ for all } n \geq 10$$
$$= \mu(H(2,2,2,2,n),x), \quad (12)$$

$$\begin{aligned}
&\mu(H(2,2,2,n-7,n),x)\\
&= \mu(H(1,2,2,n-7,n-1),x) + x^2\mu(T(2,2,n-7),x)\\
&= x^2\mu^2(P_2,x)\mu(P_{n-7},x) + (1+x^2)\mu(T(2,2,n-7),x)\\
&< x^2\mu(P_2,x)\mu(T(2,2,n-10),x) + (1+x^2)\mu(T(2,2,n-7),x) \text{ for } n \geq 10\\
&= \mu(H(2,2,2,2,n),x) \qquad (13)
\end{aligned}$$

and for $3 \leq d_{22} \leq n-9$ (and hence $n \geq 12$)

$$\begin{aligned}
&\mu(H(2,2,2,d_{22},n),x)\\
&= (\mu(P_1,x) + x^2)\mu(T(2,d_{22},n-5-d_{22}),x)\\
&+ x^2\mu(P_1,x)\mu(P_2,x)\mu(T(2,d_{22},n-8-d_{22}),x)\\
&< (\mu(P_1,x)+x^2)\mu(T(2,2,n-7),x) + x^2\mu(P_1,x)\mu(P_2,x)\mu(T(2,2,n-10,x)\\
&= \mu(H(2,2,2,2,n),x). \qquad (14)
\end{aligned}$$

More inequalities are obtained by induction in the next two lemmas.

Lemma 4. *For all integers $n \geq 10$, $n-5 \geq d_{22} \geq 1$ and for all real numbers $x > 0$ we have*

$$\mu(H(1,1,2,d_{22},n),x) < \mu(H(2,2,2,2,n),x)$$

and

$$\mu(H(1,2,2,d_{22},n),x) < \mu(H(2,2,2,2,n),x). \quad (15)$$

Proof. Induction with respect to d_{22}: The initial cases corresponding to $d_{22} \in \{1,2\}$ were already obtained in (9), (10), (11) and (12), and the induction step follows from the relations in (6) and (7). □

Lemma 5. *Let $n \geq 10$, $d_{22} \geq d_{12}$ and $n-5 \geq d_{12}+d_{22}$. We have $\mu(H(2,d_{12},2,d_{22},n),x) < \mu(H(2,2,2,2,n),x)$ except if (d_{12},d_{22}) is in $\{(2,2),(2,n-8)\}$.*

Proof. For any given value of d_{22} we reason by induction with respect to d_{12}. The initial cases corresponding to $d_{12} \in \{1,2\}$ can be deduced from (13), (14), (15) using the relation $\mu(H(2,1,2,2,n),x) = \mu(H(2,2,2,1,n),x)$. Note that using Lemma 2 and (13) we have

$$\mu(H(2,3,2,n-8,n),x) < \mu(H(2,2,2,n-7,n),x) < \mu(H(2,2,2,2,n),x),$$

and in $H(2, d_{12}, 2, d_{22}, n), x)$ if $d_{12} \geq 4$, then $d_{22} < n-8$. The induction step follows from the recurrence relations for $\mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n), x)$. □

We are left to compare $\mathrm{En}(H(2,2,2,2,n))$ and $\mathrm{En}(H(2,2,2,n-8,n))$. As we will observe in the rest of this section the sign of $\mu(H(2,2,2,2,n),x) - \mu(H(2,2,2,n-8,n),x)$ depends on x. Therefore, we have to estimate each of $\mathrm{En}(H(2,2,2,2,n))$ and $\mathrm{En}(H(2,2,2,n-8,n))$ in order to be able to compare them. For this we need explicit expressions for $\mu(H(2,2,2,2,n),x)$ and $\mu(H(2,2,2,n-8,n),x)$. The characteristic polynomial $P(t) = t^2 - t - x^2$ of the recurrence relation

$$\mu(H(2,2,2,2,n+2),x) = \mu(H(2,2,2,2,n+1),x) + x^2\mu(H(2,2,2,2,n),x)$$

has two roots

$$t_1 = \frac{1+\sqrt{1+4x^2}}{2} = \frac{-1}{z^2-1} \qquad \text{and} \qquad t_2 = \frac{1-\sqrt{1+4x^2}}{2} = \frac{z^2}{z^2-1}$$

where $x = z/(1-z^2)$; to have x ranging in $(0,+\infty)$ we take $0 < z < 1$. This implies that

$$\mu(H(2,2,2,2,9+k),x) = A(z)\left(\frac{z^2}{z^2-1}\right)^k + B(z)\left(\frac{-1}{z^2-1}\right)^k \tag{16}$$

for some $A(z)$ and $B(z)$ which satisfy

$$\begin{cases} A(z) + B(z) = \mu(H(2,2,2,2,9),x) = \dfrac{(z^4-z^2+1)^3(z^4+3z^2+1)}{(z^2-1)^8} \\ A(z)\dfrac{z^2}{z^2-1} + B(z)\dfrac{-1}{z^2-1} = \mu(H(2,2,2,2,10),x) \\ \qquad\qquad = \dfrac{(z^4-z^2+1)^2(z^{12}+z^{10}-2z^8+z^6-2z^4+z^2+1)}{(z^2-1)^{10}}. \end{cases}$$

Solving the system of equations we get

$$A(z) = \frac{z^4(z^4-z^2+1)^2(z^4+z^2-1)^2}{(z^2-1)^9(z^2+1)} \qquad \text{and} \qquad B(z) = -\frac{(z^4-z^2-1)^2(z^4-z^2+1)^2}{(z^2-1)^9(z^2+1)}.$$

Hence, (16) becomes

$$\begin{aligned} &\mu(H(2,2,2,2,n),x) \\ &\quad = \frac{(z^4-z^2+1)^2}{z^2+1}\left(z^{-14}(z^4+z^2-1)^2\left(\frac{z^2}{z^2-1}\right)^n + (z^4-z^2-1)^2\left(\frac{-1}{z^2-1}\right)^n\right) \qquad (17) \\ &\quad = \frac{(z^4-z^2+1)^2}{(z^2+1)(1-z^2)^n}\left(z^{-14}(z^4+z^2-1)^2(-1)^n z^{2n} + (z^4-z^2-1)^2\right). \qquad (18) \end{aligned}$$

In a similar way one can also obtain

$$\mu(H(2,2,2,n-8,n),x) = \frac{z^4-z^2+1}{(z^2+1)(1-z^2)^n}\left[(-1)^n z^{2n-12}(z^{10}+z^8-2z^6 \right.$$
$$\left. +2z^4-2z^2+1)+z^{10}-2z^8+2z^6-2z^4+z^2+1\right].$$

It is convenient to use the following abbreviations

$$\begin{aligned} Q_1(z) &= (z^4-z^2+1)(z^4+z^2-1)^2 \\ Q_2(z) &= z^{12}+z^{10}-2z^8+2z^6-2z^4+z^2 \\ &= z^{12}+(z^5-z^3)^2+(z^3-z)^2 \\ R_1(z) &= (z^4-z^2+1)(z^4-z^2-1)^2 \\ R_2(z) &= z^{10}-2z^8+2z^6-2z^4+z^2+1\ . \end{aligned}$$

Note that

$$\begin{aligned} R_1(z)-R_2(z) &= -z^6(Q_1(z)-Q_2(z)) \\ &= (z^2-1)z^6(z^2-z-1)\left(z-\frac{\sqrt{5}-1}{2}\right)\left(z+\frac{\sqrt{5}+1}{2}\right). \end{aligned} \tag{19}$$

Equation (1) can be rewritten in terms of z as

$$\mathrm{En}(T) = \frac{2}{\pi}\int_0^1 \frac{dz}{z^2}(1+z^2)\log\mu(T,x).$$

For even n we have

$$\begin{aligned} \frac{\mu(H(2,2,2,2,n),x)}{\mu(H(2,2,2,n-8,n),x)} &= \frac{z^{2n-14}Q_1(z)+R_1(z)}{z^{2n-14}Q_2(z)+R_2(z)} \\ &= 1+\frac{z^{2n-14}(Q_1(z)-Q_2(z))+R_1(z)-R_2(z)}{z^{2n-14}Q_2(z)+R_2(z)} \\ &= 1+\frac{(R_1(z)-R_2(z))(1-z^{2n-20})}{z^{2n-14}Q_2(z)+R_2(z)} \\ &= 1+\frac{(z^2-1)(z^2-z-1)\left(z-\frac{\sqrt{5}-1}{2}\right)\left(z+\frac{\sqrt{5}+1}{2}\right)(1-z^{2n-20})z^6}{z^{2n-14}Q_2(z)+R_2(z)}\ . \end{aligned}$$

Let

$$I_-(n) = \frac{2}{\pi}\int_0^{\frac{\sqrt{5}-1}{2}} \frac{dz}{z^2}(1+z^2)\log\frac{\mu(H(2,2,2,2,n),x)}{\mu(H(2,2,2,n-8,n),x)}$$

$$\geq \frac{2}{\pi}\int_0^{\frac{\sqrt{5}-1}{2}} \frac{dz}{z^2}(1+z^2)\log\left(1+\frac{(z^2-1)\left(z-\frac{\sqrt{5}-1}{2}\right)\left(z+\frac{\sqrt{5}+1}{2}\right)(z^2-z-1)z^6}{R_2(z)}\right)$$

$$> -0.003$$

and for $n \geq 12$ let

$$I_+(n)$$
$$= \frac{2}{\pi}\int_{\frac{\sqrt{5}-1}{2}}^{1} \frac{dz}{z^2}(1+z^2)\log\frac{\mu(H(2,2,2,2,n),x)}{\mu(H(2,2,2,n-8,n),x)}$$

$$\geq \frac{2}{\pi}\int_{\frac{\sqrt{5}-1}{2}}^{1} \frac{dz}{z^2}(1+z^2)\log\left(1+\frac{(z^2-1)\left(z-\frac{\sqrt{5}-1}{2}\right)\left(z+\frac{\sqrt{5}+1}{2}\right)(z^2-z-1)(1-z^{2\cdot 12-20})z^6}{z^{2\cdot 12-14}Q_2(z)+R_2(z)}\right)$$

$$> 0.009$$

to have

$$\mathrm{En}(H(2,2,2,2,n)) - \mathrm{En}(H(2,2,2,n-8,n)) = I_-(n) + I_+(n) > 0 \tag{20}$$

whenever n is even and at least 12.

For odd n we have

$$\frac{\mu(H(2,2,2,2,n),x)}{\mu(H(2,2,2,n-8,n),x)} = \frac{R_1(z)-z^{2n-14}Q_1(z)}{R_2(z)-z^{2n-14}Q_2(z)}$$
$$= 1+\frac{(z^2-1)z^6(z^2-z-1)\left(z-\frac{\sqrt{5}-1}{2}\right)\left(z+\frac{\sqrt{5}+1}{2}\right)(1+z^{2n-20})}{R_2(z)-z^{2n-14}Q_2(z)}.$$

Let

$$J_-(n)$$
$$= \frac{2}{\pi}\int_0^{\frac{\sqrt{5}-1}{2}} \frac{dz}{z^2}(1+z^2)\frac{\mu(H(2,2,2,2,n),x)}{\mu(H(2,2,2,n-8,n),x)}$$

$$\geq \frac{2}{\pi}\int_0^{\frac{\sqrt{5}-1}{2}} \frac{dz}{z^2}(1+z^2)\log\left(1+\frac{(z^2-1)(z^2-z-1)\left(z-\frac{\sqrt{5}-1}{2}\right)\left(z+\frac{\sqrt{5}+1}{2}\right)(1+z^{2\cdot 11-20})z^6}{R_2(z)-z^{2\cdot 11-14}Q_2(z)}\right)$$

$$> -0.004$$

and

$$J_+(n) = \frac{2}{\pi} \int\limits_{\frac{\sqrt{5}-1}{2}}^{1} \frac{dz}{z^2}(1+z^2) \frac{\mu(H(2,2,2,2,n),x)}{\mu(H(2,2,2,n-8,n),x)}$$

$$\geq \frac{2}{\pi} \int\limits_{\frac{\sqrt{5}-1}{2}}^{1} \frac{dz}{z^2}(1+z^2) \log \left(1 + \frac{(z^2-1)(z^2-z-1)\left(z-\frac{\sqrt{5}-1}{2}\right)\left(z+\frac{\sqrt{5}-1}{2}\right)z^6}{R_2(z)} \right)$$

$$> 0.021.$$

Again this leads to

$$\mathrm{En}(H(2,2,2,2,n)) - \mathrm{En}(H(2,2,2,n-8,n)) = J_-(n) + J_+(n) > 0 \text{ for odd } n \geq 11.$$

The conclusion for this section is summarized in the following theorem (the case of $n = 9$ can be checked easily):

Theorem 2. *Among all trees with at least four leaves and order* n *at least* 9, $H(2,2,2,2,n)$ *is the unique tree with maximum energy.*

4 Comparison of $\mathrm{En}(H(2,2,2,2,n))$ with the energy of tripods

It will be convenient to use the following abbreviation:

$$g_{a,n,r}(i) := a^i + (-1)^r a^{n-i}.$$

It is easy to see that for all non-negative integers n, r and $a \in (0,1)$, the function $g_{a,n,r}$ is positive and decreasing for $i \in [0, n/2)$.

For the tripod $T(i,j,k)$ of order n, we can assume $1 \leq i \leq j \leq k = n-i-j-1$ without loss of generality. We know that

$$\mu(T(i,j,k),x) = \mu(P_{i+j+1},x)\mu(P_{k-1},x) + x^2(\mu(P_{i+j+1},x)\mu(P_{k-2},x) + \mu(P_i,x)\mu(P_j,x)\mu(P_{k-1},x)).$$

In a similar way as to get (18) we also obtain

$$\mu(P_n,x) = \frac{z^2}{z^2+1}\left(\frac{z^2}{z^2-1}\right)^n + \frac{1}{z^2+1}\left(\frac{-1}{z^2-1}\right)^n \tag{21}$$

which leads to (remember that $i+j+k=n-1$)

$$\mu(P_i,x)\mu(P_j,x)\mu(P_{k-1},x) = \frac{1}{(z^2+1)^3(1-z^2)^{n-2}}\big((-1)^{n-2}z^{2(n+1)}+(-1)^{k-1}z^{2k}+(-1)^{j+k-1}z^{2(j+k+1)} +(-1)^{i+k-1}z^{2(i+k+1)}+(-1)^{i+j}z^{2(i+j+2)}+1+(-1)^j z^{2(j+1)}+(-1)^i z^{2(i+1)}\big),$$

$$\mu(P_{i+j+1},x)\mu(P_{k-1},x) = \frac{1}{(z^2+1)^2(1-z^2)^{n-1}}\big((-1)^{n-1}z^{2(n+1)}+1-(-1)^{i+j}z^{2(n-k+1)}+(-1)^{k+1}z^{2k}\big),$$

$$\mu(P_{i+j+1},x)\mu(P_{k-2},x) = \frac{1}{(z^2+1)^2(1-z^2)^{n-2}}\big((-1)^n z^{2n}+1-(-1)^{i+j}z^{2(n-k+1)}+(-1)^k z^{2(k-1)}\big)$$

and

$$\mu(P_{i+j+1},x)\mu(P_{k-1},x)+x^2\mu(P_{i+j+1},x)\mu(P_{k-2},x) = \frac{1}{(z^2+1)^2(1-z^2)^n}\big((-1)^n z^{2(n+2)}+1-(-1)^{i+j}z^{2(n-k+1)}+(-1)^k z^{2(k+1)}\big).$$

Consequently we have

$$\mu(T(i,j,n-i-j-1),x) = \frac{1}{(z^2+1)^3(1-z^2)^n}\big((-1)^n z^{2(n+2)}(2+z^2)+1+2z^2 +(-1)^i g_{z^2,n+3,n}(i+2)+(-1)^j g_{z^2,n+3,n}(j+2)-(-1)^{i+j}g_{z^2,n+3,n}(i+j+2)\big). \quad (22)$$

Using the expressions in (18) and (22) we get

$$\begin{aligned} D(i,j,n,z) &:= \frac{\mu(T(i,j,n-1-i-j),x)}{\mu(H(2,2,2,2,n),x)} \\ &= \frac{(-1)^n z^{2(n+2)}(2+z^2)+1+2z^2+(-1)^i g_{z^2,n+3,n}(i+2)}{(1+z^2)^2(z^4-z^2+1)^2\left(z^{-14}(z^4+z^2-1)^2(-1)^n z^{2n}+(z^4-z^2-1)^2\right)} \\ &+ \frac{(-1)^j g_{z^2,n+3,n}(j+2)-(-1)^{i+j}g_{z^2,n+3,n}(i+j+2)}{(1+z^2)^2(z^4-z^2+1)^2\left(z^{-14}(z^4+z^2-1)^2(-1)^n z^{2n}+(z^4-z^2-1)^2\right)} \end{aligned}$$

and

$$\begin{aligned} D(i,j,\infty,z) &:= \lim_{n\to\infty} D(i,j,n,z) \\ &= \frac{1+2z^2+(-1)^i z^{2i+4}+(-1)^j z^{2j+4}-(-1)^{i+j}z^{2i+2j+4}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2}. \end{aligned} \quad (23)$$

Note that under the assumptions on i,j,k,n if i tends to infinity, then necessarily $i,j,k,n-i,n-j,n-k$ also tend to infinity, hence we have

$$\lim_{i\to\infty} D(i,j,n,z) = \frac{1+2z^2}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2}$$

$$= \frac{1+2z^2}{(1+z^2)^2((z^4-z^2)^2-1)^2}$$

which implies (remember the relation $x = z/(1-z^2)$)

$$\lim_{i\to\infty} \mathrm{En}(T(i,j,n-i-j-1)) - \mathrm{En}(H(2,2,2,2,n))$$

$$= \lim_{i\to\infty} \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log \frac{\mu(T(i,j,n-1-i-j),x)}{\mu(H(2,2,2,2,n),x)} \tag{24}$$

$$= \frac{2}{\pi} \int_0^1 \frac{dz}{z^2}(1+z^2) \log \frac{1+2z^2}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2}$$

$$< -0.014. \tag{25}$$

This shows that there are only finitely many values of i for which the energy of $T(i,j,n-i-j-1)$ is greater than that of $H(2,2,2,2,n)$. Next we determine such values of i.

Lemma 6. *For n large enough, if* $\mathrm{En}(T(i,j,n-i-j-1)) > \mathrm{En}(H(2,2,2,2,n))$, *then* $i \in I = \{1,2,3,4,5,6,8,10,12,14,\ 16,18\}$.

Proof. We use the notation in (23).

a) For even $i = 2k$ and even $j = 2(k+l)$ we obtain:

$$\begin{aligned} D(i,j,\infty,z) = ee(i,j,z) &:= \frac{1+2z^2+z^{2i+4}+z^{2j+4}-z^{2i+2j+4}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \\ &\le ee(i,i,z) = \frac{1+2z^2+2z^{2i+4}-z^{4i+4}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \\ &\le ee(20,20,z) \text{ for all } i \ge 20, \end{aligned}$$

where

$$\frac{2}{\pi}\int_0^1 \frac{dz}{z^2}(1+z^2)\log ee(20,20,z) < -0.001.$$

This shows that for n large enough, $k \ge 10$ and $l \ge 0$ we have $\mathrm{En}(T(2k,2(k+l),n-4k-2l-1)) < \mathrm{En}(H(2,2,2,2,n))$.

b) For even $i = 2k$ and odd $j = 2k+1$ we obtain:

$$\begin{aligned} D(i,j,\infty,z) = eo(i,j,z) &:= \frac{1+2z^2+z^{2i+4}-z^{2j+4}+z^{2i+2j+4}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \\ &\le eo(i,\infty,z) = \frac{1+2z^2+z^{2i+4}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \end{aligned}$$

$$\leq eo(14, \infty, z) \text{ for all } i \geq 14,$$

and

$$\frac{2}{\pi}\int_0^1 \frac{dz}{z^2}(1+z^2)\log eo(14,\infty,z) < -0.001.$$

This means that (for n large enough) the energy of a tripod $T(2k, 2(k+l)+1, n-4k-2l-2)$ can only be greater than that of $H(2,2,2,2,n)$ if $k \leq 6$.

c) For odd $i = 2k+1$ and even $j = 2(k+l+1)$ we obtain:

$$\begin{aligned} D(i,j,\infty,z) &= \frac{1+2z^2 - z^{2i+4} + z^{2j+4} + z^{2i+2j+4}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \\ &\leq \frac{1+2z^2 - z^{2i+4} + z^{2i+6} + z^{4i+6}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \\ &\leq oe(i,z) := \frac{1+2z^2+z^{4i+6}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \\ &\leq oe(7,z) \text{ for all } i \geq 7 \end{aligned}$$

and

$$\frac{2}{\pi}\int_0^1 \frac{dz}{z^2}(1+z^2)\log oe(7,z) < -0.002.$$

Hence (for n large enough) for all integers $l \geq 0$ a tripod $T(2k+1, 2(k+l+1), n-4k-2l-2)$ that can possibly have greater energy than that of $H(2,2,2,2,n)$ must satisfy $k \in \{0,1,2\}$.

d) For odd i and odd j we obtain:

$$\begin{aligned} D(i,j,\infty,z) = oo(i,j,z) &:= \frac{1+2z^2 - z^{2i+4} - z^{2j+4} - z^{2i+2j+4}}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \\ &\leq oo(\infty,\infty,z) = \frac{1+2z^2}{(1+z^2)^2(z^4-z^2+1)^2(z^4-z^2-1)^2} \end{aligned}$$

where as we have seen in (25)

$$\frac{2}{\pi}\int_0^1 \frac{dz}{z^2}(1+z^2)\log oo(\infty,\infty,z) < -0.014.$$

□

For any given value of i, Theorem 1 allows us to obtain the complete list of all tripods of order n and with shortest branch of length i, ordered by their energies. In the following we determine the place of $H(2,2,2,2,n)$ in each list corresponding to a value in I. For $i=1$ we have

$$\frac{2}{\pi}\int_0^1 \frac{dz}{z^2}(1+z^2)\log D(1,2,\infty,z) > 0.004$$

and

$$\frac{2}{\pi}\int_0^1 \frac{dz}{z^2}(1+z^2)\log D(1,4,\infty,z) < -0.034,$$

thus $\mathrm{En}(T(1,2,n-4)) > \mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(1,4,n-6)) > \cdots > \mathrm{En}(T(1,1,n-3))$, if n is large enough. Since

$$\frac{2}{\pi}\int_0^1 \frac{dz}{z^2}(1+z^2)\log D(2,3,\infty,z) > 0.030$$

we deduce that for $i=2$ and n large enough we have

$$\mathrm{En}(T(2,2,n-5)) > \cdots > \mathrm{En}(T(2,3,n-6)) > \mathrm{En}(H(2,2,2,2,n)).$$

By similar arguments, for large enough n we also have:

$\mathrm{En}(T(3,4,n-8)) > \mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(3,6,n-10)) > \cdots > \mathrm{En}(T(3,3,n-7))$,

$\mathrm{En}(T(4,4,n-9)) > \cdots > \mathrm{En}(T(4,5,n-10)) > \mathrm{En}(H(2,2,2,2,n))$,

$\mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(5,6,n-12)) > \cdots > \mathrm{En}(T(5,5,n-11))$,

$\mathrm{En}(T(6,6,n-13)) > \cdots > \mathrm{En}(T(6,7,n-14)) > \mathrm{En}(H(2,2,2,2,n))$,

$\mathrm{En}(T(8,8,n-17)) > \cdots > \mathrm{En}(T(8,11,n-20)) > \mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(8,9,n-18))$,

$\mathrm{En}(T(10,10,n-21)) > \cdots > \mathrm{En}(T(10,21,n-32)) > \mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(10,19,n-30)) > \cdots > \mathrm{En}(T(10,11,n-22))$,

$\mathrm{En}(T(12,12,n-25)) > \cdots > \mathrm{En}(T(12,85,n-98)) > \mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(12,83,n-96)) > \cdots > \mathrm{En}(T(12,13,n-26))$,

$\mathrm{En}(T(14,14,n-29)) > \cdots > \mathrm{En}(T(14,30,n-45)) > \mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(14,32,n-47)) > \cdots > \mathrm{En}(T(14,15,n-30))$,

$\mathrm{En}(T(16,16,n-33)) > \cdots > \mathrm{En}(T(16,22,n-49)) > \mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(16,24,n-41)) > \cdots > \mathrm{En}(T(16,17,n-34))$,

$\mathrm{En}(T(18,18,n-37)) > \mathrm{En}(H(2,2,2,2,n)) > \mathrm{En}(T(18,20,n-39)) > \cdots > \mathrm{En}(T(18,19,n-38))$.

We can count the tripods whose energy are greater than $\mathrm{En}(H(2,2,2,2,n))$ and obtain the following theorem:

Theorem 3. *For large enough n the quadripod $H(2,2,2,2,n)$ is the $(3n-84)^{th}$ (resp. $(3n-87)^{th}$) tree with largest energy for odd n (resp. for even n).*

Proof. Use the fact that there are $\lfloor (n-i-1)/2 \rfloor - i + 1$ tripods of order n for which the length of the shortest branch is i. Including the path we have

$$-61 + \sum_{i=1}^{6} \left\lfloor \frac{n-2i-1}{2} \right\rfloor = 6 \left\lfloor \frac{n-1}{2} \right\rfloor - 82 = \begin{cases} 3n-85 \text{ if } n \text{ is odd} \\ 3n-88 \text{ if } n \text{ is even} \end{cases}$$

trees with greater energy than $H(2,2,2,2,n)$, for large enough n. □

For a tree T, let $\mathrm{diam}(T)$ denote the diameter of T, defined as the length of a longest path in T. The following theorem is a simple consequence of the results obtained so far:

Theorem 4. *For all i in $I' = \{1,2,3,4,6,8,10,12,14, 16,18\}$ and n large enough, the n-vertex tree with diameter $n-i-1$ and maximum energy is $T(i, 2\lceil i/2 \rceil, n-2\lceil i/2 \rceil - i - 1)$.*

Proof. Let i be an element of I' and T_i be a tree of diameter $n-i-1$ which is maximal with respect to the energy. We know that $\mathrm{diam}(P_n) = n-1 > n-i-1$ for all $n \geq i+1$, hence $T_i \neq P_n$. As we have seen above for large enough n (in particular we assume $n \geq 3i+1$), there exists a tripod $T(i, j_0, n-j_0-i-1)$ which has diameter $n-i-1$ such that $\mathrm{En}(T(i, j_0, n-j_0-i-1)) > \mathrm{En}(H(2,2,2,2,n))$. Using Theorem 2 this implies that T_i is a tripod. More precisely $T_i = T(i, j, n-j-i-1)$ for some $j \geq i$, in order to satisfy $\mathrm{diam}(T_i) = n-i-1$. From Theorem 1, if $j \neq 2\lceil i/2 \rceil$, then we have

$$\mathrm{En}(T(i, j, n-j-i-1)) < \mathrm{En}(T(i, 2\lceil i/2 \rceil, n-2\lceil i/2 \rceil - i - 1)).$$

Therefore, we conclude that $T_i = T(i, 2\lceil i/2 \rceil, n-2\lceil i/2 \rceil - i - 1)$. □

5 Main result

For simplicity we write $G > G'$ instead of $\mathrm{En}(G) > \mathrm{En}(G')$. By ordering all the tripods with larger energy than that of $H(2,2,2,2,n)$ we obtain the head of the list of trees ordered by decreasing energy, until the first appearance of a non-tripod. Each "..." in the list refers to the chain obtained for a fixed shortest branch by using Theorem 1. For any inequality that cannot be obtained from Theorem 1, see the values in the appendix:

Theorem 5. *The head of the list of all trees ordered by decreasing energy is given as follows for large enough n:*

$$
\begin{array}{llllllll}
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) & > \\
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) & > & H(2,2,2,2,n). &
\end{array}
$$

Computer check shows that Theorem 5 holds for all odd n starting from 21777 to

30001 and for all even n starting from 30866 to 40000. Our final conjecture is based on this observation.

Conjecture 1. *Theorem 5 holds for all odd* $n \geq 21777$ *and for all even* $n \geq 30866$.

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Appendix

Let us denote by $\mathfrak{d}(i,j)$ the limit

$$\lim_{n\to\infty} \mathrm{En}(T(i,j,n-i-j-1)) - \mathrm{En}(H(2,2,2,2,n))$$

for all integers $i \leq j$. Then we have the following values rounded to six decimal places:

$\mathfrak{d}(2,2)$	≈ 0.065993	$\mathfrak{d}(2,7)$	≈ 0.040329	$\mathfrak{d}(4,4)$	≈ 0.037612
$\mathfrak{d}(2,5)$	≈ 0.037493	$\mathfrak{d}(4,6)$	≈ 0.031345	$\mathfrak{d}(2,3)$	≈ 0.030513
$\mathfrak{d}(4,8)$	≈ 0.028282	$\mathfrak{d}(4,18)$	≈ 0.023946	$\mathfrak{d}(6,6)$	≈ 0.023909
$\mathfrak{d}(4,20)$	≈ 0.023683	$\mathfrak{d}(4,15)$	≈ 0.020244	$\mathfrak{d}(6,8)$	≈ 0.020135
$\mathfrak{d}(4,13)$	≈ 0.019647	$\mathfrak{d}(4,11)$	≈ 0.018763	$\mathfrak{d}(6,10)$	≈ 0.017948
$\mathfrak{d}(4,9)$	≈ 0.017378	$\mathfrak{d}(6,12)$	≈ 0.016566	$\mathfrak{d}(8,8)$	≈ 0.015891
$\mathfrak{d}(6,14)$	≈ 0.015637	$\mathfrak{d}(4,7)$	≈ 0.015026	$\mathfrak{d}(6,16)$	≈ 0.014983
$\mathfrak{d}(6,18)$	≈ 0.014504	$\mathfrak{d}(6,26)$	≈ 0.013472	$\mathfrak{d}(8,10)$	≈ 0.013381
$\mathfrak{d}(6,28)$	≈ 0.013329	$\mathfrak{d}(6,39)$	≈ 0.011775	$\mathfrak{d}(8,12)$	≈ 0.011767
$\mathfrak{d}(6,37)$	≈ 0.011718	$\mathfrak{d}(6,23)$	≈ 0.010881	$\mathfrak{d}(8,14)$	≈ 0.010667
$\mathfrak{d}(10,10)$	≈ 0.010636	$\mathfrak{d}(6,21)$	≈ 0.010629	$\mathfrak{d}(4,5)$	≈ 0.010537
$\mathfrak{d}(6,19)$	≈ 0.010306	$\mathfrak{d}(8,16)$	≈ 0.009883	$\mathfrak{d}(8,18)$	≈ 0.009304
$\mathfrak{d}(8,20)$	≈ 0.008864	$\mathfrak{d}(10,12)$	≈ 0.008849	$\mathfrak{d}(8,22)$	≈ 0.008523
$\mathfrak{d}(8,30)$	≈ 0.007708	$\mathfrak{d}(10,14)$	≈ 0.007616	$\mathfrak{d}(8,32)$	≈ 0.007584
$\mathfrak{d}(8,56)$	≈ 0.006934	$\mathfrak{d}(12,12)$	≈ 0.006928	$\mathfrak{d}(8,58)$	≈ 0.006911
$\mathfrak{d}(8,86)$	≈ 0.006732	$\mathfrak{d}(10,16)$	≈ 0.006729	$\mathfrak{d}(8,88)$	≈ 0.006725
$\mathfrak{d}(8,49)$	≈ 0.006104	$\mathfrak{d}(10,18)$	≈ 0.006069	$\mathfrak{d}(8,47)$	≈ 0.006066
$\mathfrak{d}(8,33)$	≈ 0.005602	$\mathfrak{d}(12,14)$	≈ 0.005592	$\mathfrak{d}(10,20)$	≈ 0.005564
$\mathfrak{d}(8,31)$	≈ 0.005486	$\mathfrak{d}(8,29)$	≈ 0.005347	$\mathfrak{d}(8,27)$	≈ 0.005181
$\mathfrak{d}(10,22)$	≈ 0.005169	$\mathfrak{d}(8,25)$	≈ 0.004979	$\mathfrak{d}(10,24)$	≈ 0.004855
$\mathfrak{d}(8,23)$	≈ 0.00473	$\mathfrak{d}(12,16)$	≈ 0.004622	$\mathfrak{d}(10,26)$	≈ 0.0046
$\mathfrak{d}(1,2)$	≈ 0.004585	$\mathfrak{d}(8,21)$	≈ 0.004418	$\mathfrak{d}(10,28)$	≈ 0.004391
$\mathfrak{d}(10,30)$	≈ 0.004217	$\mathfrak{d}(14,14)$	≈ 0.004172	$\mathfrak{d}(10,32)$	≈ 0.004071
$\mathfrak{d}(8,19)$	≈ 0.004018	$\mathfrak{d}(10,34)$	≈ 0.003947	$\mathfrak{d}(12,18)$	≈ 0.003895
$\mathfrak{d}(10,36)$	≈ 0.003841	$\mathfrak{d}(10,44)$	≈ 0.00354	$\mathfrak{d}(8,17)$	≈ 0.003497
$\mathfrak{d}(10,46)$	≈ 0.003486	$\mathfrak{d}(10,52)$	≈ 0.003358	$\mathfrak{d}(12,20)$	≈ 0.003336
$\mathfrak{d}(10,54)$	≈ 0.003324	$\mathfrak{d}(10,70)$	≈ 0.003141	$\mathfrak{d}(14,16)$	≈ 0.003135
$\mathfrak{d}(10,72)$	≈ 0.003126	$\mathfrak{d}(10,182)$	≈ 0.002896	$\mathfrak{d}(12,22)$	≈ 0.002896
$\mathfrak{d}(10,184)$	≈ 0.002895	$\mathfrak{d}(10,175)$	≈ 0.0028	$\mathfrak{d}(8,15)$	≈ 0.002799
$\mathfrak{d}(10,173)$	≈ 0.002799	$\mathfrak{d}(10,69)$	≈ 0.002548	$\mathfrak{d}(12,24)$	≈ 0.002544
$\mathfrak{d}(10,67)$	≈ 0.002531	$\mathfrak{d}(10,53)$	≈ 0.002355	$\mathfrak{d}(14,18)$	≈ 0.002354
$\mathfrak{d}(10,51)$	≈ 0.002318	$\mathfrak{d}(10,49)$	≈ 0.002277	$\mathfrak{d}(12,26)$	≈ 0.002258
$\mathfrak{d}(10,47)$	≈ 0.002231	$\mathfrak{d}(10,41)$	≈ 0.002055	$\mathfrak{d}(16,16)$	≈ 0.002043
$\mathfrak{d}(12,28)$	≈ 0.002022	$\mathfrak{d}(10,39)$	≈ 0.001979	$\mathfrak{d}(10,37)$	≈ 0.001892
$\mathfrak{d}(8,13)$	≈ 0.001834	$\mathfrak{d}(12,30)$	≈ 0.001825	$\mathfrak{d}(10,35)$	≈ 0.001792
$\mathfrak{d}(14,20)$	≈ 0.001749	$\mathfrak{d}(10,33)$	≈ 0.001674	$\mathfrak{d}(12,32)$	≈ 0.001659
$\mathfrak{d}(10,31)$	≈ 0.001536	$\mathfrak{d}(12,34)$	≈ 0.001518	$\mathfrak{d}(12,36)$	≈ 0.001397
$\mathfrak{d}(10,29)$	≈ 0.001373	$\mathfrak{d}(12,38)$	≈ 0.001292	$\mathfrak{d}(14,22)$	≈ 0.001271
$\mathfrak{d}(16,18)$	≈ 0.001216	$\mathfrak{d}(12,40)$	≈ 0.001201	$\mathfrak{d}(10,27)$	≈ 0.001176
$\mathfrak{d}(12,42)$	≈ 0.001122	$\mathfrak{d}(12,44)$	≈ 0.001052	$\mathfrak{d}(12,46)$	≈ 0.00099
$\mathfrak{d}(10,25)$	≈ 0.000938	$\mathfrak{d}(12,48)$	≈ 0.000934	$\mathfrak{d}(14,24)$	≈ 0.000887

$\mathfrak{d}(12,50) \approx 0.000885$	$\mathfrak{d}(12,64) \approx 0.000651$	$\mathfrak{d}(10,23) \approx 0.000646$
$\mathfrak{d}(12,66) \approx 0.000629$	$\mathfrak{d}(12,70) \approx 0.000589$	$\mathfrak{d}(14,26) \approx 0.000573$
$\mathfrak{d}(16,20) \approx 0.000573$	$\mathfrak{d}(12,72) \approx 0.000571$	$\mathfrak{d}(12,92) \approx 0.00045$
$\mathfrak{d}(8,11) \approx 0.000443$	$\mathfrak{d}(12,94) \approx 0.000442$	$\mathfrak{d}(12,130) \approx 0.000351$
$\mathfrak{d}(18,18) \approx 0.00035$	$\mathfrak{d}(12,132) \approx 0.000348$	$\mathfrak{d}(12,162) \approx 0.000314$
$\mathfrak{d}(14,28) \approx 0.000314$	$\mathfrak{d}(12,164) \approx 0.000312$	$\mathfrak{d}(12,224) \approx 0.000282$
$\mathfrak{d}(10,21) \approx 0.000281$	$\mathfrak{d}(12,226) \approx 0.000281$	$\mathfrak{d}(12,219) \approx 0.000207$
$\mathfrak{d}(3,4) \approx 0.000206$	$\mathfrak{d}(12,217) \approx 0.000206$	$\mathfrak{d}(12,111) \approx 0.000101$
$\mathfrak{d}(14,30) \approx 0.000097$	$\mathfrak{d}(12,109) \approx 0.000096$	$\mathfrak{d}(12,99) \approx 0.000065$
$\mathfrak{d}(16,22) \approx 0.000063$	$\mathfrak{d}(12,97) \approx 0.000058$	$\mathfrak{d}(12,85) \approx 0.000005.$