More Trees with Large Energy

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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 \( E_n(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n| \). 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

\[
E_n(G) = \sum_{i=1}^{n} |\lambda_i|.
\]

Apart from purely graph theoretical interest, the study of \( E_n \) 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 \( \pi \)-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 $n \geq 15$, 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 $(3n - 84)^{th}$ (resp. $(3n - 87)^{th}$) 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]

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

for any tree $T$, where

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

and $m(G, k)$ 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 $\text{En}(T_1) > \text{En}(T_2)$. 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 $v$.

$$\begin{array}{c}
P(n, k, G, v) \\
\begin{array}{c}
\bigcirc \\
v \\
v_1 \quad \cdots \quad v_k \quad v_{k+1} \quad \cdots \quad v_{n-1} \quad v_n
\end{array}
\end{array}$$

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

$$\mu(G \cup G', x) = \mu(G, x)\mu(G', x); \quad (3)$$

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

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

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:

$$
\mu(P(n,0,G,v),x) > \mu(P(n,2,G,v),x) > \cdots > \mu(P(n,2[(n-1)/4],G,v),x)
$$

$$
> \mu(P(n,2[(n+1)/4] - 1,G,v),x) > \cdots > \mu(P(n,3,G,v),x) > \mu(P(n,1,G,v),x).
$$

Note that $2[m/4]$ and $2[(m+2)/4] - 1$ 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](image)

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

$$
\text{En}(T(i,2[i/2], n - i - 2[i/2] - 1)) > \text{En}(T(i,2[i/2] + 2, n - i - 2[i/2] - 3)) > \cdots > \text{En}(T(i,2[(n-i-1)/4], n - i - 2[(n-i-1)/4] - 1)) > \text{En}(T(i,2[(n-i+1)/4] - 1, n - i - 2[(n-i+1)/4] - 1)) > \cdots > \text{En}(T(i,2[i/2] + 3, n - i - 2[i/2] - 4)) > \text{En}(T(i,2[i/2] + 1, n - i - 2[i/2] - 2)).
$$

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
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

\[ \mu(T(i, j, k + 2), x) = \mu(T(i, j, k + 1), x) + x^2 \mu(T(i, j, k), x) \quad (5) \]

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

\[ \mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n), x) \]
\[ = \mu(P_{d_{11}}, x)\mu(P_{d_{12}}, x)\mu(T(d_{21}, d_{22}, n - d_{11} - d_{12} - d_{21} - d_{22} - 2), x) \]
\[ + x^2 \mu(P_{d_{11}-1}, x)\mu(P_{d_{12}}, x)\mu(T(d_{21}, d_{22}, n - d_{11} - d_{12} - d_{21} - d_{22} - 2), x) \]
\[ + x^2 \mu(P_{d_{11}}, x)\mu(P_{d_{12}-1}, x)\mu(T(d_{21}, d_{22}, n - d_{11} - d_{12} - d_{21} - d_{22} - 2), x) \]
\[ + x^2 \mu(P_{d_{11}}, x)\mu(P_{d_{12}}, x)\mu(T(d_{21}, d_{22}, n - d_{11} - d_{12} - d_{21} - d_{22} - 3), x) \]

which shows that (using (5))

\[ \mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n + 2), x) \]
\[ = \mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n + 1), x) + x^2 \mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n), x) \quad (6) \]

and

\[ \mu(H(d_{11}, d_{12}, d_{21}, d_{22} + 2, n + 2), x) \]
\[ = \mu(H(d_{11}, d_{12}, d_{21}, d_{22} + 1, n + 1), x) + x^2 \mu(H(d_{11}, d_{12}, d_{21}, d_{22}, n), x). \quad (7) \]
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:
\[
\mu(H(1, 1, 1, 1, n), x) = \mu(T(1, 1, n - 4), x) + x^2 \mu(T(1, 1, n - 6), x)
< \mu(T(1, 2, n - 5), x) + x^2 \mu(T(1, 2, n - 7), x) \text{ for all } n \geq 7
= \mu(H(1, 2, 1, 1, n), x),
\]
(8)
\[
\mu(H(1, 2, 1, 1, n), x) = \mu(H(1, 1, 1, 1, n - 1), x) + x^2 \mu(T(1, 1, n - 5), x)
< \mu(H(1, 1, 1, 2, n - 1), x) + x^2 \mu(T(1, 2, n - 6), x) \text{ for all } n \geq 8
= \mu(H(1, 2, 1, 2, n), x),
\]
(9)
\[
\mu(H(1, 1, 2, n), x) = \mu(H(1, 1, 1, 2, n - 1), x) + x^2 \mu(T(1, 1, n - 5), x)
< \mu(H(1, 1, 1, 2, n - 1), x) + x^2 \mu(T(1, 2, n - 6), x) \text{ for all } n \geq 6
= \mu(H(1, 2, 1, 2, n), x),
\]
(10)
\[
\mu(H(1, 2, 1, 2, n), x) = \mu(H(1, 1, 1, 2, n - 1), x) + x^2 \mu(T(1, 2, n - 6), x)
< \mu(H(1, 2, 1, 2, n - 1), x) + x^2 \mu(T(1, 2, n - 6), x) \text{ for all } n \geq 9
= \mu(H(1, 2, 2, n), x),
\]
(11)
\[
\mu(H(1, 2, 2, n), x) = \mu(H(1, 2, 1, 2, n - 1), x) + x^2 \mu(T(1, 2, n - 6), x)
\]
< μ(\(H(1,2,2,2,n-1), x\)) + x^2 \mu(\(T(2,2,n-7), x\))$ for all \(n \geq 10$

\begin{equation}
\mu(\(H(2,2,2,n), x\)) = \mu(\(H(2,2,2,n-7), x\))
\end{equation}

\[
\mu(\(H(2,2,2,n), x\)) = \mu(\(H(1,2,2,n-7,n-1), x\)) + x^2 \mu(\(T(2,2,n-7), x\))
\]
\[
x^2 \mu(\(P_2, x\)) \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(\(T(2,2,n-7), x\))$ for \(n \geq 10$

\begin{equation}
\mu(\(H(2,2,2,2,n), x\)) = \mu(\(H(2,2,2,n), x\))
\end{equation}

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

\begin{equation}
\mu(\(H(2,2,2,d_{22}, n), x\)) = (\(\mu(P_1, x) + x^2\)) \mu(\(T(2,d_{22}, n - 5 - d_{22}), x\))
\end{equation}

\[
+ 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(\(H(2,2,2,2,n), x\)).
\end{equation}

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(\(H(2,2,2,2,n), x\)).
\end{equation}

**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 $\text{En}(H(2, 2, 2, 2, n))$ and $\text{En}(H(2, 2, 2, n - 8, n))$. 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 $\text{En}(H(2, 2, 2, 2, n))$ and $\text{En}(H(2, 2, 2, n - 8, n))$ 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

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

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

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

(16)

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

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

Solving the system of equations we get

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

Hence, (16) becomes

$$
\mu(H(2, 2, 2, 2, n), x) = \frac{(z^4 - z^2 + 1)^2}{z^2 + 1} \left(z^{-14}(z^4 + z^2 - 1)^2 \left(\frac{z^2}{z^2 - 1}\right)^n + (z^4 - z^2 - 1)^2 \left(\frac{-1}{z^2 - 1}\right)^n\right) \quad (17)
$$

$$
= \frac{(z^4 - z^2 + 1)^2}{(z^2 + 1)(1 - z^2)^n} \left(z^{-14}(z^4 + z^2 - 1)^2(-1)^nz^{2n} + (z^4 - z^2 - 1)^2\right). \quad (18)
$$
In a similar way one can also obtain
\[
\mu(H(2, 2, 2, n - 8, n), x) = \frac{z^4 - z^2 + 1}{(z^2 + 1)(1 - z^2)^n} \left[ (-1)^n z^{2n-12} (z^{10} + z^8 - 2z^6 + 2z^4 - 2z^2 + 1) \right] .
\]

It is convenient to use the following abbreviations
\[
Q_1(z) = (z^4 - z^2 + 1)(z^4 + z^2 - 1)^2
\]
\[
Q_2(z) = z^{12} + z^{10} - 2z^8 + 2z^6 - 2z^4 + z^2
\]
\[
= z^{12} + (z^5 - z^3)^2 + (z^3 - z)^2
\]
\[
R_1(z) = (z^4 - z^2 + 1)(z^4 - z^2 - 1)^2
\]
\[
R_2(z) = z^{10} - 2z^8 + 2z^6 - 2z^4 + z^2 + 1
\]

Note that
\[
R_1(z) - R_2(z) = -z^6 (Q_1(z) - Q_2(z))
\]
\[
= (z^2 - 1) z^6 (z^2 - z - 1) \left( z - \frac{\sqrt{5} - 1}{2} \right) \left( z + \frac{\sqrt{5} + 1}{2} \right) . \tag{19}
\]

Equation (1) can be rewritten in terms of \( z \) as
\[
E_n(T) = \frac{2}{\pi} \int_0^1 \frac{dz}{z^2} (1 + z^2) \log \mu(T, x).
\]

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

Let
\[
I_-(n) = \frac{2}{\pi} \int_0^{\frac{\sqrt{5} - 1}{2}} \frac{dz}{z^2} (1 + z^2) \log \frac{\mu(H(2, 2, 2, 2, n), x)}{\mu(H(2, 2, 2, n - 8, n), x)}
\]
\[ \geq \frac{2}{\pi} \int_0^{\sqrt{\frac{\pi}{2}}} \frac{dz}{z^2} \frac{(z^2-1) \left( z - \frac{\sqrt{5} - 1}{2} \right) \left( z + \frac{\sqrt{5} + 1}{2} \right) (z^2 - z - 1)z^6}{R_2(z)} \]

> \text{−0.003}

and for \( n \geq 12 \) let

\[ I_+(n) = \frac{2}{\pi} \int_0^{\sqrt{\frac{\pi}{2}}} \frac{dz}{z^2} (1 + z^2) \log \left( 1 + \frac{(z^2 - 1) \left( z - \frac{\sqrt{5} - 1}{2} \right) \left( z + \frac{\sqrt{5} + 1}{2} \right) (z^2 - z - 1)z^6}{R_2(z)} \right) \]

\[ > 0.009 \]

to have

\[ \text{En}(H(2, 2, 2, 2, n)) - \text{En}(H(2, 2, 2, n - 8, n)) = I_-(n) + I_+(n) > 0 \quad (20) \]

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

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

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

> \text{−0.004}
and

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

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

\[ > 0.021. \]

Again this leads to

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

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 \( \text{En}(H(2, 2, 2, 2, n)) \) 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

\[ \mu(P_n, x) = \frac{z^2}{z^2 + 1} \left( \frac{z^2}{z^2 - 1} \right)^n + \frac{1}{z^2 + 1} \left( \frac{-1}{z^2 - 1} \right)^n \quad (21) \]
which leads to (remember that $i + j + k = n - 1$)

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

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

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

and

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

$$
+ (-1)^{i+j}g_{z,n+3,n}(i + 2) + (-1)^{j}g_{z,n+3,n}(j + 2) - (-1)^{i+j}g_{z,n+3,n}(i + j + 2) \right). \quad (22)
$$

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

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

$$
+ \frac{(-1)^{j}g_{z,n+3,n}(j + 2) - (-1)^{i+j}g_{z,n+3,n}(i + j + 2)}{(1 + z^2)^2(z^4 - z^2 + 1)^2(z^{-14}(z^4 + z^2 - 1)^2(-1)^{n}z^{2n} + (z^4 - z^2 - 1)^2)}
$$

and

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

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 \( x = z/(1 - z^2) \))

\[
\lim_{i \to \infty} \text{En}(T(i, j, n - i - j - 1)) - \text{En}(H(2, 2, 2, n))
\]

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

\[
= \frac{2}{\pi} \int_0^1 \frac{dz}{z^2} \log \frac{1 + 2z^2}{(1 + z^2)^2(z^4 - z^2 + 1)^2(z^4 - z^2 - 1)^2} < -0.014.
\]

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 \( H(2, 2, 2, n) \). Next we determine such values of \( i \).

**Lemma 6.** For \( n \) large enough, if \( \text{En}(T(i, j, n - i - j - 1)) > \text{En}(H(2, 2, 2, 2, n)) \), 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:

\[
D(i, j, \infty, z) = ee(i, j, z) := \frac{1 + 2z^2 + z^{2i+4} + z^{2j+4} - z^{2i+2j+4}}{(1 + z^2)^2(z^4 - z^2 + 1)^2(z^4 - z^2 - 1)^2} 
\]

\[
\leq ee(i, i, z) = \frac{1 + 2z^2 + 2z^{2i+4} - z^{4i+4}}{(1 + z^2)^2(z^4 - z^2 + 1)^2(z^4 - z^2 - 1)^2} 
\]

\[
\leq ee(20, 20, z) \text{ for all } i \geq 20,
\]

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, \( k \geq 10 \) and \( l \geq 0 \) we have \( \text{En}(T(2k, 2(k + l), n - 4k - 2l - 1)) < \text{En}(H(2, 2, 2, 2, n)) \).

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

\[
D(i, j, \infty, z) = eo(i, j, z) := \frac{1 + 2z^2 + z^{2i+4} - z^{2j+4} + z^{2i+2j+4}}{(1 + z^2)^2(z^4 - z^2 + 1)^2(z^4 - z^2 - 1)^2} 
\]

\[
\leq eo(i, \infty, z) = \frac{1 + 2z^2 + z^{2i+4}}{(1 + z^2)^2(z^4 - z^2 + 1)^2(z^4 - z^2 - 1)^2} 
\]
\[ \leq eo(14, \infty, z) \text{ for all } i \geq 14, \]

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:

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

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:

\[
D(i, j, \infty, z) = oo(i, j, z) := \frac{1 + 2z^2 - z^{2i+4} - z^{2j+4} - z^{2i+2j+4}}{(1 + z^2)^2(z^4 - z^2 + 1)^2(z^4 - z^2 - 1)^2}
\leq oo(\infty, \infty, z) = \frac{1 + 2z^2}{(1 + z^2)^2(z^4 - z^2 + 1)^2(z^4 - z^2 - 1)^2}
\]

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

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

and

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

We can count the tripods whose energy are greater than $\text{En}(H(2, 2, 2, 2, n))$ 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 \( n \). \( \square \)

For a tree \( T \), let \( \text{diam}(T) \) 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 \( \text{diam}(P_n) = n - 1 > n - i - 1 \) 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 \( \text{En}(T(i, j_0, n - j_0 - i - 1)) > \text{En}(H(2, 2, 2, 2, n)) \). 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 \( \text{diam}(T_i) = n - i - 1 \). From Theorem 1, if \( j \neq 2\lceil i/2 \rceil \), then we have

\[
\text{En}(T(i, j, n - j - i - 1)) < \text{En}(T(i, 2\lceil i/2 \rceil, n - 2\lceil i/2 \rceil - i - 1)).
\]

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

5 Main result

For simplicity we write \( G > G' \) instead of \( \text{En}(G) > \text{En}(G') \). 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 \( n \):
\[
\]

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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**References**


Appendix

Let us denote by $d(i, j)$ the limit

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

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

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\[ \begin{array}{c|c|c|c|c}
\varv(12, 50) \approx 0.000885 & \varv(12, 64) \approx 0.000651 & \varv(10, 23) \approx 0.000646 \\
\varv(12, 66) \approx 0.000629 & \varv(12, 70) \approx 0.000589 & \varv(14, 26) \approx 0.000573 \\
\varv(16, 20) \approx 0.000573 & \varv(12, 72) \approx 0.000571 & \varv(12, 92) \approx 0.000445 \\
\varv(8, 11) \approx 0.000443 & \varv(12, 94) \approx 0.000442 & \varv(12, 130) \approx 0.000351 \\
\varv(18, 18) \approx 0.00035 & \varv(12, 132) \approx 0.000348 & \varv(12, 162) \approx 0.000314 \\
\varv(14, 28) \approx 0.000314 & \varv(12, 164) \approx 0.000312 & \varv(12, 224) \approx 0.000282 \\
\varv(10, 21) \approx 0.000281 & \varv(12, 226) \approx 0.000281 & \varv(12, 219) \approx 0.000207 \\
\varv(3, 4) \approx 0.000206 & \varv(12, 217) \approx 0.000206 & \varv(12, 111) \approx 0.000101 \\
\varv(14, 30) \approx 0.000097 & \varv(12, 109) \approx 0.000096 & \varv(12, 99) \approx 0.000065 \\
\varv(16, 22) \approx 0.000063 & \varv(12, 97) \approx 0.000058 & \varv(12, 85) \approx 0.00005.
\end{array} \]