MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **74** (2015) 285-306

ISSN 0340 - 6253

Maximum and Minimum Energy Trees with Two and Three Branched Vertices

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(Received October 20, 2014)

Abstract

The energy of a graph G is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. In this paper we find trees with minimal and maximal energy over the sets $\Omega(n,2)$ and $\Omega(n,3)$ of all trees with n vertices and exactly two and three branched vertices, respectively (see Figures 1 and 2). We show that $S(2,2;\mathbf{n-8};2,2)$ has maximal energy and $S(\underbrace{1,\ldots,1}_{n-4};\mathbf{2};1,1)$ has minimal energy over $\Omega(n,2)$. We also find the extremal values of the energy over the set $\Omega^t(n,2)$ of all trees in $\Omega(n,2)$ such that the distance between the two branched vertices is exactly t. Finally, we show that among all trees in $\Omega(n,3)$ the tree $S(1,1;\mathbf{1};1;\mathbf{1};\underbrace{1,\ldots,1}_{n-6})$ has minimal energy while the maximal energy is a attained in a tree of the form $S(2,2;\mathbf{p};2;\mathbf{q};2,2)$.

1 Introduction

Let G be a graph with n vertices. The energy of G, denoted by $\mathcal{E}(G)$, is defined by

$$\mathcal{E}(G)=\sum_{i=1}^{n}|\lambda_i|$$

where $\lambda_1,\ldots,\lambda_n$ are the eigenvalues of the graph G, i.e. the eigenvalues of the adjacency matrix of the graph G. This concept has a chemical motivation, it is related to the total

π-electron energy for graphs which in the Hückel molecular orbital theory represent the carbon-atom skeleton of a conjugated hydrocarbons [7]. However, it was in the 1970´s when this graph-spectrum-based invariant was recognized by Gutman as an interesting object of study from a mathematical point of view, independently from its possible chemical interpretation [6] . For further details on this theory we refer to [13] and the literature cited in.

One of the fundamental problems in the energy theory is to find the smallest and largest energy value in a significant class of graphs. For instance, it is well known that among the set $\mathcal{T}_n$ of all trees with n vertices, the star tree S_n has the minimal energy and the path tree P_n has the maximal energy [5]. Since then, many classes of trees have been investigated, among others, the set of trees with perfect matchings, chemical trees, Hückel trees, trees with a given diameter, trees with a number of pendent vertices, trees with a maximum degree vertex or trees with two maximum degree vertices ([1], [4], [10], [11], [12], [14]-[22], [23]).

The quasi-order method is of great value for comparing the energies of trees. Given two trees T_1 and T_2 with n vertices and characteristic polynomials

$$\Phi_{T_1}(x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(T_1,k)\, x^{n-2k} \quad \text{and} \quad \Phi_{T_2}(x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(T_2,k)\, x^{n-2k}$$

where $m(T_i,k)$ are the k-matching numbers of T_i, we write $T_1 \preceq T_2$ or $T_2 \succeq T_1$ if $m(T_1,k) \le m(T_2,k)$ for all $k \ge 0$. If, moreover, at least one of the inequalities is strict, then we write $T_1 \prec T_2$ or $T_2 \succ T_1$. As a consequence of Coulson´s integral formula [2]

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

it turns out that the energy is increasing with respect to the quasi-order order relation "$\preceq$", i.e. if $T_1 \prec T_2$ then $\mathcal{E}(T_1) < \mathcal{E}(T_2)$.

Our interest in this paper is to initiate the study of minimal and maximal energy for trees with a fixed number of branched vertices. Recall that a vertex u of a tree T is a branched vertex if the degree of u, denoted by $d_T(u)$, is greater than 2. The problem for trees with n vertices and exactly one branched vertex (i.e. starlike trees) was solved in [9]. It is natural then to consider the extremal value problem of the energy over the set of trees with few branched vertices.

Let us denote by $\Omega\,(n,2)$ the set of all trees with n vertices and exactly two branched vertices. The structure of a tree in $\Omega\,(n,2)$ is depicted in Figure 1.

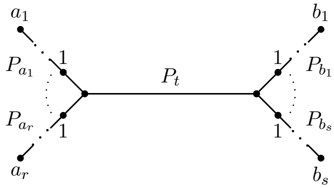


Figure 1: The tree $S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s)$ in $\Omega\,(n,2)$

We will find the trees in $\Omega\,(n,2)$ with maximal and minimal energy. More specifically, we show that $S\,(2,2;\mathbf{n-8};2,2)$ has maximal energy and $S(\underbrace{1,\ldots,1}_{n-4};\mathbf{2};1,1)$ has minimal energy over $\Omega\,(n,2)$. Later, we consider the subset $\Omega^t\,(n,2)$ of $\Omega\,(n,2)$ consisting of trees for which the two branched vertices are at a fixed distance t. Note that when $t=2$ we recover the set of two-starlike trees. Again, we find the trees in $\Omega^t\,(n,2)$ with maximal and minimal energy for arbitrary positive integer t.

We also study the energy over the set $\Omega\,(n,3)$ of all trees with n vertices and three branched vertices (see Figure 2).

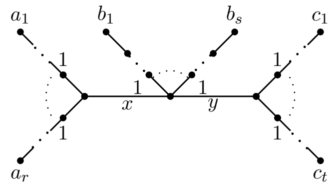


Figure 2: The tree $S\,(a_1,\ldots,a_r;\mathbf{x};b_1,\ldots,b_s;\mathbf{y};c_1,\ldots,c_t)$ in $\Omega(n,3)$

We show that the tree $S(1,1;\mathbf{1};1;\mathbf{1};\underbrace{1,\ldots,1}_{n-6})$ has minimal energy among all trees in $\Omega\,(n,3)$. A much more complicated problem is to determine the maximal energy over $\Omega\,(n,3)$. Mainly we show that the maximal energy tree belongs to the class of trees $\Omega^*\,(n,3)$ consisting of trees of the form $S\,(2,2;\mathbf{p};2;\mathbf{q};2,2)$, for positive integers p and q. This is possible using the increasing property of the energy with respect to the quasi-order relation defined above. However, inside the class $\Omega^*\,(n,3)$ we show through several examples that the trees are no longer comparable, and so finding the maximal energy tree is only possible by means of the Coulson's integral formula combined by methods of real analysis. In other words, finding the maximal energy tree in $\Omega(n,3)$ reduces to finding the maximal energy tree in $\Omega^*(n,3)$, which is now an open problem. For $16 \le n \le 200$ we computed the energy of all trees in $\Omega^*(n,3)$, which leads us to conjecture that the maximal energy over $\Omega(n,3)$ is attained when $p = 1$ and $q = n - 12$ if n is even, and $p = 4$ and $q = n - 15$ if n is odd.

2 Two basic operations defined over trees

As we mentioned in the introduction, it is well known that if $T \in \mathcal{T}_n$ is different from S_n and P_n, then

$$\mathcal{E}(S_n) < \mathcal{E}(T) < \mathcal{E}(P_n)$$

We will show a stronger result, namely, that it is possible to construct sequences of trees

$$S_n = T_p \prec \cdots \prec T_1 \prec T_0 = T$$

and

$$T = U_0 \prec U_1 \prec \cdots \prec U_q = P_n$$

where T_i is obtained from T_{i-1} (resp. U_i is obtained from U_{i-1}) by an operation applied to T_{i-1} (resp. U_{i-1}). These operations will play an important role in the study of extremal values of the energy over the set of trees with two branched vertices.

In what follows we will need some results on the number of matchings [3].

Lemma 2.1 *Let G be a graph and e an edge connecting the vertices u and v. Then for all $k \ge 0$*

$$m(G,k) = m(G-e,k) + m(G-u-v,k-1).$$

Recall that the coalescence of the graphs G and H at the vertices u and v, respectively, denoted by $G(u,v)H$, is obtained by identifying the vertices u and v.

Lemma 2.2 *Let G and H be graphs with non-isolated vertices u and v, respectively. Then for every integer $k \ge 0$*

$$m(G(u,v)H,k) \le m(G \cup H,k)$$

and

$$m(G(u,v)H,2) < m(G \cup H,2).$$

Proof. For every $k \geq 0$ there exists a trivial injective function between the k-matchings of $G\,(u,v)\,H$ and the k-matchings of $G \cup H$. Moreover, an edge containing u in G and an edge containing v in H are independent in $G \cup H$ but not in $G\,(u,v)\,H$. ■

Consider the path P_n with n vertices and arbitrary trees A and X different from P_1, with vertices $a \in V\,(A)$ and $x \in V\,(X)$. For every $1 \leq i \leq n$ we define by coalescence the trees

$$X_{n,i} = P_n\,(i,x)\,X, \quad AX_{n,i} = A\,(a,n)\,X_{n,i} \quad \text{and } A_n = A\,(a,n)\,P_n$$

(see Figure 3).

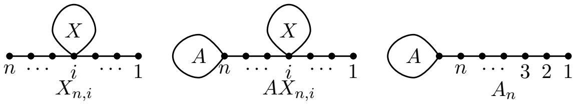


Figure 3: Some special trees.

The following result was shown by Gutman and Zhang ([8], see also [13]).

Lemma 2.3 *Let A and X be trees different from P_1. Then*

OP1 $AX_{n,i} \prec AX_{n,3}$ *for all* $2 \leq i \leq n-2$ *and* $i \neq 3$*;*

OP2 $AX_{n,2} \prec AX_{n,n-1}$ *for all* $n \geq 2$*,* $n \neq 3$*;*

OP3 $X_{n,2} \prec X_{n,4} \prec \cdots \prec X_{n,5} \prec X_{n,3} \prec X_{n,1}$.

We now prove the following result.

Theorem 2.4 $AX_{n,2} \prec AX_{n,1}$ *for every* $n \geq 2$.

Proof. Let $X' = X - x$. For every integer $k \geq 1$

$$m\,(AX_{n,2},k) = m\,(AX_{n-1,1},k) + m\,(A_{n-2} \cup X', k-1)$$

and

$$m\,(AX_{n,1},k) = m\,(A_{n-1} \cup X, k) + m\,(A_{n-2} \cup X', k-1)\,.$$

Since $AX_{n-1,1} = A_{n-1}\,(1,x)\,X$, it follows from Lemma 2.2 that

$$m\,(AX_{n-1,1},k) \leq m\,(A_{n-1} \cup X, k)$$

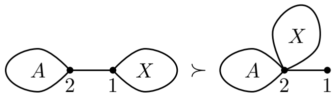


Figure 4: Case $n = 2$ in Theorem 2.4.

which implies $m\left(AX_{n,2},k\right) \leq m\left(AX_{n,1},k\right)$. Since $m\left(AX_{n-1,1},2\right) < m\left(A_{n-1} \cup X,2\right)$ then $AX_{n,2} \prec AX_{n,1}$ for every $n \geq 2$. ■

One important case of Theorem 2.4 is when $n = 2$ (see Figure 4).
This will be our first operation, which we call a $\mathcal{O}1$-type operation applied at vertex $a \in V\left(A\right)$.

Corollary 2.5 *Let $T \in \mathcal{T}_n$. Then there exists a sequence of trees $T_0, T_1, \ldots, T_p$ with n vertices such that*

$$S_n = T_p \prec \cdots \prec T_1 \prec T_0 = T.$$

Moreover, each T_i is obtained from T_{i-1} by a $\mathcal{O}1$-type operation, for every $i = 1, \ldots, p$.

Proof. Let u be a vertex of T of degree ≥ 2. If all neighbor vertices of u have degree 1 then $T = S_n$ and we are done. Otherwise u has a neighbor vertex of degree ≥ 2 which implies that there exists trees A and X (both different from P_1) such that $T = AX_{2,1}$. By Theorem 2.4

$$T_1 = AX_{2,2} \prec AX_{2,1} = T$$

and T_1 has one more pendent vertex than T. We can repeat this process until we reach the star S_n. ■

We now introduce a second operation applied to a tree, which we call a $\mathcal{O}2$-type operation. Let A be a tree. Denote by $A\left(n_1, n_2, \ldots, n_k\right)$ the tree which is obtained by joining the terminal vertices of $P_{n_1}, P_{n_2}, \ldots, P_{n_k}$ to a vertex u of A (see Figure 5).

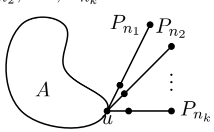


Figure 5: The tree $A\left(n_1, n_2, \ldots, n_k\right)$.

Theorem 2.6 *Let A be a tree. Then*

$$A\left(n_1, n_2, \ldots, n_k, x, y\right) \prec A\left(n_1, n_2, \ldots, n_k, x+y\right).$$

Proof. Let $X = A(n_1, n_2, \ldots, n_k)$. Then

$$A(n_1, n_2, \ldots, n_k, x, y) = X_{x+y+1,y+1}$$

and

$$A(n_1, n_2, \ldots, n_k, x+y) = X_{x+y+1,1}.$$

The result follows from **OP3** in Lemma 2.3. ■

Corollary 2.7 *Let $U \in \mathcal{T}_n$. Then there exists a sequence of trees $U_0, U_1, \ldots, U_q$ with n vertices such that*

$$U = U_0 \prec U_1 \prec \cdots \prec U_q = P_n.$$

Moreover, each U_i is obtained from U_{i-1} by a $\mathcal{O}2$-type operation, for every $i = 1, \ldots, q$.

Proof. If U has a vertex u of degree ≥ 3 then there exists a tree A such that

$$U = A(n_1, n_2, \ldots, n_k, x, y).$$

By Theorem 2.6

$$U \prec U_1 = A(n_1, n_2, \ldots, n_k, x+y)$$

Moreover, this operation decreases in one the degree of u in U. Eventually, repeating this process a finite number of times will end in a tree with no vertex of degree ≥ 3. This is the tree P_n. ■

3 Extremal values of the energy of trees with 2 branched vertices

Let T be a tree. Recall that a vertex u of T is a branched vertex if $d_T(u) \geq 3$. We denote by $\Omega(n,2)$ the set of all trees with n vertices and two branched vertices. The tree depicted in Figure 1 will be denoted by $S(a_1, \ldots, a_r; \mathbf{t}; b_1, \ldots, b_s)$. We begin considering the problem of maximal energy in $\Omega(n,2)$.

Lemma 3.1 *Let $n \geq 10$. Then*

1. $S(2,2;\mathbf{n-7};1,2) \prec S(2,2;\mathbf{n-8};2,2)$.

2. $S(2,2;\mathbf{n-6};1,1) \prec S(2,2;\mathbf{n-8};2,2)$.

3. $S(1,1;\mathbf{n-5};1,2) \prec S(2,2;\mathbf{n-8};2,2)$.

4. $S(1,1;\mathbf{n-4};1,1) \prec S(2,2;\mathbf{n-8};2,2)$.

5. $S(1,2;\mathbf{n-6};1,2) \prec S(2,2;\mathbf{n-8};2,2)$.

Proof. This can be easily shown using **OP1** in Lemma 2.3. ■

Theorem 3.2 *Let* $n \geq 10$ *and* $T = S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s) \in \Omega(n,2)$ *where* $t \geq 3$. *Then*

$$T \preceq S(2,2;\mathbf{n-8};2,2).$$

Proof. By Theorem 2.6 we can construct a tree $T_1 \in \Omega(n,2)$ of the form $T_1 = S(p,q;\mathbf{t};r,s)$ such that $T \preceq T_1$. Assume first that $p+q \geq 4$. Then by **OP3** in Lemma 2.3 there exists a tree $T_2 = S(2,p+q-2;\mathbf{t};r,s) \in \Omega(n,2)$ such that $T_1 \preceq T_2$. Since $t \geq 3$, we can apply **OP1** in Lemma 2.3 to construct a tree $T_3 = S(2,2;\mathbf{t+p+q-4};r,s) \in \Omega(n,2)$ such that $T_2 \preceq T_3$. Now if $r+s \geq 4$ then a similar argument ends the proof. Otherwise $r+s \leq 3$ which implies that $T_3 = S(2,2;\mathbf{n-7};1,2)$ or $T_3 = S(2,2;\mathbf{n-6};1,1)$, and the result follows from parts 1 and 2 of Lemma 3.1. The only case left to consider is when $p+q \leq 3$ and $r+s \leq 3$, but in this situation the result follows from parts 3-5 of Lemma 3.1. ■

The condition $t \geq 3$ in the hypothesis of Theorem 3.2 is necessary, as we can see in our next example.

Example 3.3 *The trees* $A = S(2,2;\mathbf{2};2,3)$ *and* $B = S(2,2;\mathbf{3};2,2)$ *belonging to* $\Omega(11,2)$ *are not comparable. In fact,*

$$\begin{aligned}\Phi_A(x) &= X^{11} - 10X^9 + 34X^7 - 49X^5 + 29X^3 - 5X \\ \Phi_B(x) &= X^{11} - 10X^9 + 34X^7 - 48X^5 + 29X^3 - 6X\end{aligned}$$

When $t = 2$ we can prove the following result.

Theorem 3.4 *Let* $n \geq 10$ *and* $U = S(a_1,\ldots,a_r;\mathbf{2};b_1,\ldots,b_s) \in \Omega(n,2)$. *Then*

$$U \preceq S(2,2;\mathbf{2};2,n-8).$$

Proof. By Theorem 2.6 we can construct a tree $U_1 \in \Omega(n,2)$ of the form $U_1 = S(p,q;\mathbf{2};r,s)$ such that $U \preceq U_1$. Note that $p+q+r+s \geq 8$. We may assume without loosing generality that $p+q \geq 4$. Hence by **OP3** in Lemma 2.3 there exists a tree $U_2 = S\,(2,p+q-2;\mathbf{2};r,s) \in \Omega(n,2)$ such that $U_1 \preceq U_2$. If $r+s \geq 4$ then by **OP3** in Lemma 2.3 and [13, Lemma 7.18]

$$\begin{aligned} U_2 &\preceq S\,(2,p+q-2;\mathbf{2};2,r+s-2) \\ &\preceq S\,(2,2;\mathbf{2};2,n-8)\,. \end{aligned}$$

Otherwise $r+s \leq 3$. If $U_2 = S\,(2,n-7;\mathbf{2};2,1)$ then again by [13, Lemma 7.18]

$$U_2 \preceq S\,(2,n-8;\mathbf{2};2,2)$$

and we are done. If $U_2 = S\,(2,n-6;\mathbf{2};1,1)$ then by [13, Lemma 7.19] and the argument above

$$\begin{aligned} U_2 &\preceq S\,(2,n-7;\mathbf{2};1,2) \\ &\preceq S\,(2,n-8;\mathbf{2};2,2)\,. \end{aligned}$$

■

Corollary 3.5 *For every $n \geq 11$, $S\,(2,2;\mathbf{n-8};2,2)$ is the tree with maximal energy in $\Omega(n,2)$.*

Proof. Using Coulson's integral formula it was shown in [14] that for every $n \geq 11$,

$$\mathcal{E}\,(S\,(2,2;\mathbf{n-8};2,2)) > \mathcal{E}\,(S\,(2,2;\mathbf{2};2,n-8))\,.$$

The result follows from Theorems 3.2 and 3.4. ■

In order to find the minimal tree in $\Omega(n,2)$ we prove the following result. Recall that $A_n = A\,(a,n)\,P_n$ for a given tree A (Figure 3).

Lemma 3.6 *Let $p,q \geq 2$ be integers such that $p \leq q$. Then*

$$S(\underbrace{1,\ldots,1}_{p};\mathbf{t};\underbrace{1,\ldots,1}_{q}) \succ S(\underbrace{1,\ldots,1}_{p-1};\mathbf{t};\underbrace{1,\ldots,1}_{q+1}).$$

Proof. Let $U = S(\underbrace{1,\ldots,1}_{p};\mathbf{t};\underbrace{1,\ldots,1}_{q})$ and $V = S(\underbrace{1,\ldots,1}_{p-1};\mathbf{t};\underbrace{1,\ldots,1}_{q+1})$. Consider the star trees $A = S_{q+1}$ and $B = S_p$. Applying Lemma 2.1 to the tree U we obtain

$$m(U,k) = m(S(\underbrace{1,\ldots,1}_{p-1};\mathbf{t};\underbrace{1,\ldots,1}_{q}),k) + m(A_{t-1},k-1);$$

for every $k \geq 1$. Similarly,

$$m(V,k) = m(S(\underbrace{1,\ldots,1}_{p-1};\mathbf{t};\underbrace{1,\ldots,1}_{q}),k) + m(B_{t-1},k-1);$$

for every $k \geq 1$. Since $q > p-1$, then B_{t-1} is a (proper) subgraph of A_{t-1} and consecuently $m(B_{t-1},k-1) \leq m(A_{t-1},k-1)$ (the inequality is strict for $k=2$). Hence $V \prec U$. ■

For $n \geq 6$ let $S_2 = S(\underbrace{1,\ldots,1}_{n-4};\mathbf{2};1,1)$.

Theorem 3.7 *Let $n \geq 6$ and $T \in \Omega(n,2)$, $T \neq S_2$. Then $T \succ S_2$.*

Proof. By Theorem 2.6 there exists a tree $Q_1 = S(\underbrace{1,\ldots 1}_{r};\mathbf{t};\underbrace{1,\ldots 1}_{s}) \in \Omega(n,2)$ such that $Q_1 \prec T$. Now by a repeated application of Theorem 2.4 we construct a tree $Q_2 = S(\underbrace{1,\ldots,1}_{p};\mathbf{2};\underbrace{1,\ldots,1}_{q}) \in \Omega(n,2)$ such that $Q_2 \prec Q_1$, where we can assume without loosing generality that $p \leq q$. Now by Lemma 3.6 we deduce that $S_2 \prec Q_2$. ■

4 Extremal values of the energy of trees with 2 branched vertices at a fixed distance

Consider the set $\Omega^t(n,2)$ of all trees in $\Omega(n,2)$ such that the distance between the two branched vertices is t. We next find the trees with maximal and minimal energy in $\Omega^t(n,2)$. Consider the tree $R_1 = S(1,1;\mathbf{t};\underbrace{1,\ldots,1}_{n-t-2})$, where $n \geq t+4$.

Theorem 4.1 *Let $n \geq t+4$ and $T \in \Omega^t(n,2)$, $T \neq R_1$. Then $R_1 \prec T$.*

Proof. By Theorem 2.6 there exists a tree $T_1 = S(\underbrace{1,\ldots,1}_{p};\mathbf{t};\underbrace{1,\ldots,1}_{q}) \in \Omega^t(n,2)$ such that $T_1 \prec T$. We may assume that $p \leq q$. Now a repeated application of Lemma 3.6 gives that $R_1 \prec T_1$. ■

Let $G_{uv}(P_a,P_b)$ be the tree obtained from G by joining the path P_a to the vertex u and joining the path P_b to the vertex v (see Figure 6).

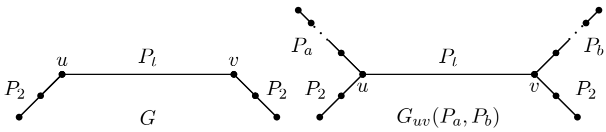


Figure 6: Trees in Lemma 4.2.

Lemma 4.2 *Let $l \geq 2$ be an integer. Then $G_{uv}(P_l, P_2) \succ G_{uv}(P_{l+1}, P_1)$.*

Proof. Let $A = G_{uv}(P_l, P_2)$ and $B = G_{uv}(P_{l+1}, P_1)$. By Lemma 2.1

$$m(A, k) = m(G_{uv}(P_l, P_1), k) + m(G_{uv}(P_l, P_0), k-1);$$

for every integer $k \geq 1$; in analogous manner

$$m(B, k) = m(G_{uv}(P_l, P_1), k) + m(G_{uv}(P_{l-1}, P_1), k-1).$$

Hence $m(A, k) - m(B, k) = m(A', k-1) - m(B', k-1)$ where A' and B' are the trees shown in Figure 7. Now by a repeated application of Lemma 2.1 to A' and B' we deduce

$$m(A', k-1) = m(A' - wz, k-1) + m(A' - w - z, k-2),$$

and

$$m(B', k-1) = m(B' - xy, k-1) + m(B' - x - y, k-2).$$

Note that $A' - w - z$ is the lineal tree, consequently $m(A' - w - z, k-2) > m(B' - x - y, k-2)$. Hence in order to obtain the desire result we compare $A'' = A' - wz$ and $B'' = B' - xy$ (see Figure 7).

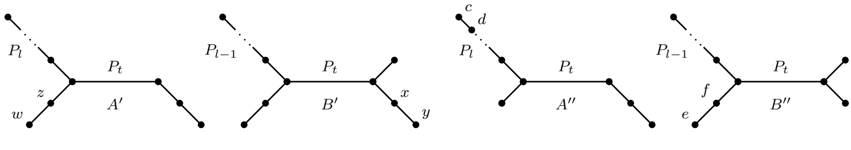


Figure 7: Trees in the proof of Lemma 4.2.

By using Lemma 2.1 we obtain

$$m(A'', k-1) = m(A'' - cd, k-1) + m(A'' - c - d, k-2);$$

and

$$m(B'', k-1) = m(B''-ef, k-1) + m(B''-e-f, k-2).$$

Note that $A''-cd = X_{3,1} \cup P_1$ and $B''-ef = X_{3,2} \cup P_1$ where X is shown in Figure 8. Therefore by **OP3** given in Lemma 2.3, $A''-cd \succ B''-ef$. Similary, $A''-c-d = X'_{l+t,j}$ and $B''-e-f = X'_{l+t,2}$ where $X' = P_2$. Again by **OP3** in Lemma 2.3, $A''-c-d \succ B''-e-f$. It follows that $m(A'', k-1) > m(B'', k-1)$ and the result follows. ■

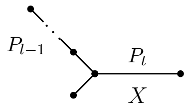


Figure 8: Tree in the proof of Lemma 4.2.

Lemma 4.3 *Let a, b be integers such that $a \geq b \geq 2$. If b is odd then $G_{uv}(P_a, P_b) \prec G_{uv}(P_{a+1}, P_{b-1})$. If b is even then $G_{uv}(P_a, P_b) \succ G_{uv}(P_{a+1}, P_{b-1})$.*

Proof. Let $R = G_{uv}(P_a, P_b)$ and $S = G_{uv}(P_{a+1}, P_{b-1})$. For every integer $k \geq 1$

$$m(R, k) = m(G_{uv}(P_a, P_{b-1}), k) + m(G_{uv}(P_a, P_{b-2}), k-1)$$

and

$$m(S, k) = m(G_{uv}(P_a, P_{b-1}), k) + m(G_{uv}(P_{a-1}, P_{b-1}), k-1).$$

Hence

$$m(R, k) - m(S, k) = (-1)\left[m(G_{uv}(P_{a-1}, P_{b-1}), k-1) - m(G_{uv}(P_a, P_{b-2}), k-1)\right]$$

Repeating this argument $b-2$ times we deduce

$$m(R, k) - m(S, k) = (-1)^{b-2}\left[m(G_{uv}(P_{a-b+2}, P_2), k-b+2) - m(G_{uv}(P_{a-b+3}, P_1), k-b+2)\right].$$

By Lemma 4.2, $G_{uv}(P_{a-b+2}, P_2) \succ G_{uv}(P_{a-b+3}, P_1)$ and the result follows. ■

Theorem 4.4 *Let $M = 4k + i$, where $i \in \{0, 1, 2, 3\}$. Then*

$$\begin{aligned} G_{uv}(P_{n-2}, P_2) &\succ G_{uv}(P_{n-4}, P_4) \succ \cdots \succ G_{uv}(P_{M-2k}, P_{2k}) \succ G_{uv}\left(P_{M-(2k+1)}, P_{2k+1}\right) \\ &\succ G_{uv}\left(P_{M-(2k-1)}, P_{2k-1}\right) \succ \cdots \succ G_{uv}(P_{M-3}, P_3) \succ G_{uv}(P_{M-1}, P_1). \end{aligned}$$

Proof. Let $A = G_{uv}(P_a, P_b)$ and $B = G_{uv}(P_{a-2}, P_{b+2})$, where $2 \leq b \leq a-4$. Then for every integer $k \geq 1$

$$m(A,k) = m(G_{uv}(P_{a-1}, P_b), k) + m(G_{uv}(P_{a-2}, P_b), k-1)$$

and

$$m(B,k) = m(G_{uv}(P_{a-2}, P_{b+1}), k) + m(G_{uv}(P_{a-2}, P_b), k-1).$$

Consequently

$$m(A,k) - m(B,k) = (-1)\left[m(G_{uv}(P_{a-2}, P_{b+1}), k) - m(G_{uv}(P_{a-1}, P_b), k)\right]$$

and so

$$\begin{aligned} m(A,k) - m(B,k) &= \\ &(-1)^b \left[m(G_{uv}(P_{a-b-1}, P_2), k-b+1) - m(G_{uv}(P_{a-b}, P_1), k-b+1)\right]. \end{aligned}$$

By Lemma 4.2, if b is even then $A \succ B$ and if b is odd then $A \prec B$. Only remains to prove that $G_{uv}(P_{M-2k}, P_{2k}) \succ G_{uv}(P_{M-(2k+1)}, P_{2k+1})$, but this is a direct consequence of Lemma 4.3. ■

Let $n \geq t+7$ and consider the tree $R_2 = S(2,2;\mathbf{t};2,n-t-6) \in \Omega^t(n,2)$.

Corollary 4.5 *Let $n \geq t+7$ and $T \in \Omega^t(n,2)$, $T \neq R_2$. Then $T \prec R_2$.*

Proof. Let $T = S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s) \in \Omega^t(n,2)$. As in the proof of Theorem 3.2, there exists a tree $T_1 \in \Omega^t(n,2)$ of the form $T_1 = S(2,r;\mathbf{t};2,s)$ such that $T \prec T_1$, where $r+s = n-t-4$. Note that $T_1 = G_{uv}(P_r, P_s)$, therefore the result follows from Theorem 4.4. ■

5 Extremal values for the energy of trees with three branched vertices

Let $\Omega(n,3)$ denote the set of all trees with n vertices and exactly three branched vertices. The tree depicted in Figure 2 will be denoted by $S(a_1,\ldots,a_r;\mathbf{x};b_1,\ldots,b_s;\mathbf{y};c_1,\ldots,c_t)$ where $\mathbf{x}$ and $\mathbf{y}$ denote the distances between the branched vertices.

One particular tree of major importance is the tree $V_1 = S(1,1;\mathbf{1};1;\mathbf{1};\underbrace{1,\ldots,1}_{n-6}) \in \Omega(n,3)$. In fact, we will show that the minimal energy over the set $\Omega(n,3)$ is attained in V_1 (see Figure 9.)

First we need some preliminary results.

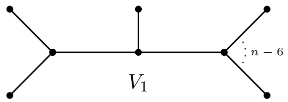


Figure 9: The tree V_1 where the minimal energy is attained in $\Omega(n,3)$

Lemma 5.1 *Let p', q' and r' be positive integers where $2 \le p' \le r'+1$ and let S', T' be the following trees in $\Omega(n,3)$:*

$$S' = S(\underbrace{1,\dots,1}_{p'};\mathbf{1};\underbrace{1,\dots,1}_{q'};\mathbf{1};\underbrace{1,\dots,1}_{r'}) \quad \text{and} \quad T' = S(\underbrace{1,\dots,1}_{p'-1};\mathbf{1};\underbrace{1,\dots,1}_{q'};\mathbf{1};\underbrace{1,\dots,1}_{r'+1}).$$

Then $S' \succ T'$.

Proof. We compute directly the characteristic polynomials of S' and T' :

$$\Phi_{S'} = x^n - (n-1)\,x^{n-2} + \left[p'\left(q'+r'+1\right) + \left(q'+1\right)r'\right]x^{n-4} - p'q'r'x^{n-6}$$

and

$$\Phi_{T'} = x^n - (n-1)\,x^{n-2} + \left[(p'-1)\left(q'+r'+2\right) + \left(q'+1\right)\left(r'+1\right)\right]x^{n-4} - (p'-1)\,q'\left(r'+1\right)x^{n-6}.$$

Note that

$$p'q'r' - (p'-1)\,q'\left(r'+1\right) = q'\left(r'-p'+1\right) \ge 0$$

and

$$\begin{aligned} & \left[p'\left(q'+r'+1\right) + \left(q'+1\right)r'\right] - \left[(p'-1)\left(q'+r'+2\right) + \left(q'+1\right)\left(r'+1\right)\right] \\ = \; & r'-p'+1 \ge 0. \end{aligned}$$

Consequently, $S' \succ T'$. ■

Lemma 5.2 *Let q' and h' be positive integers and $U' = S(1,1;\mathbf{1};\underbrace{1,\dots,1}_{q'};\mathbf{1};\underbrace{1,\dots,1}_{h'}) \in \Omega(n,3)$.*

1. *If $2 \le q' \le h'$ then*

$$U' \succ V' = S(1,1;\mathbf{1};\underbrace{1,\dots,1}_{q'-1};\mathbf{1};\underbrace{1,\dots,1}_{h'+1}).$$

2. *If $q' > h' \ge 2$ then*

$$U' \succ W' = S(1,1;\mathbf{1};\underbrace{1,\dots,1}_{q'+1};\mathbf{1};\underbrace{1,\dots,1}_{h'-1}).$$

Proof. 1. We compute the characteristic polynomials of U' and V' :

$$\Phi_{U'} = x^n - (n-1)\,x^{n-2} + [2\,(q'+h'+1) + (q'+1)\,h']\,x^{n-4} - 2q'h'x^{n-6}$$

and

$$\Phi_{V'} = x^n - (n-1)\,x^{n-2} + [2\,(q'+h'+1) + q'\,(h'+1)]\,x^{n-4} - 2\,(q'-1)\,(h'+1)\,x^{n-6}.$$

Since $2 \leq q' \leq h'$ then

$$2q'h' - 2\,(q'-1)\,(h'+1) = 2\,(h'-q'+1) \geq 0$$

and

$$(q'+1)\,h' - q'\,(h'+1) = h' - q' \geq 0.$$

Consequently $U' \succ V'$.

2. The characteristic polynomial of W' is

$$\Phi_{W'} = x^n - (n-1)\,x^{n-2} + [2\,(q'+h'+1) + (q'+2)\,(h'-1)]\,x^{n-4} - 2\,(q'+1)\,(h'-1)\,x^{n-6}.$$

Furthermore,

$$(q'+1)\,h' - (q'+2)\,(h'-1) = q' - h' + 2 > 0$$

and

$$2q'h' - 2\,(q'+1)\,(h'-1) = 2\,(q'-h'+1) > 0$$

implies that $U' \succ W'$. ■

Theorem 5.3 *Let $n \geq 8$ and $S \in \Omega\,(n,3)$, $S \neq V_1$. Then $V_1 \prec S$.*

Proof. By Theorem 2.4 there exists a tree $S' \in \Omega\,(n,3)$ of the form

$$S' = S(\underbrace{1,\ldots,1}_{p'};\mathbf{1};\underbrace{1,\ldots,1}_{q'};\mathbf{1};\underbrace{1,\ldots,1}_{r'})$$

where $2 \leq p' \leq r'+1$, such that $S \succ S'$. By Lemma 5.1 we construct a tree $U' \in \Omega\,(n,3)$ of the form

$$U' = S(1,1;\mathbf{1};\underbrace{1,\ldots,1}_{q'};\mathbf{1};\underbrace{1,\ldots,1}_{h'})$$

such that $S' \succ U'$. If $q' \leq h'$ then by part 1 of Lemma 5.2, $U' \succ V_1$. If $q' > h'$ then by part 2 of Lemma 5.2 there exists a tree $W' \in \Omega\,(n,3)$ of the form

$$W' = S(1,1;\mathbf{1};\underbrace{1,\ldots,1}_{n-7};\mathbf{1};1,1)$$

such that $U' \succ W'$. Finally note that

$$\Phi_{V_1} = x^n - (n-1)\, x^{n-2} + 4\,(n-5)\, x^{n-4} - 2\,(n-6)\, x^{n-6}$$

and

$$\Phi_{W'} = x^n - (n-1)\, x^{n-2} + 4\,(n-5)\, x^{n-4} - 4\,(n-7)\, x^{n-6}.$$

Since for $n \geq 8$

$$4\,(n-7) - 2\,(n-6) = 2n - 16 \geq 0$$

it follows that $W' \succ V_1$ and consequently, $S \succ V_1$. ■

The maximal value for the energy over $\Omega\,(n,3)$ is more complicated as we shall see next. We will rely on **OP1-OP3** given in Lemma 2.3 and one more operation **OP4** which compares the two trees shown in Figure 10.

Lemma 5.4 *[**OP4**] Let S and T be the trees depicted in Figure 10. For the fragment A being an arbitrary tree and $n \geq 4$ we have $S \prec T$.*

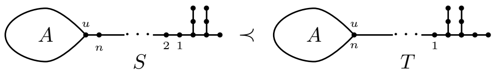


Figure 10: Trees involved in operation **OP4**

Proof. The characteristic polynomials of S and T are given by

$$\Phi_S(x) = \Phi_A(x)\Phi_{W_1}(x) - \Phi_{A-u}(x)\Phi_{W_2}(x)$$

and

$$\Phi_T(x) = \Phi_A(x)\Phi_{Z_1}(x) - \Phi_{A-u}(x)\Phi_{Z_2}(x)$$

where W_1, W_2, Z_1 and Z_2 are shown in Figure 11.

Note that

$$\Phi_T(x) - \Phi_S(x) = \Phi_A(x)\left(\Phi_{Z_1}(x) - \Phi_{W_1}(x)\right) - \Phi_{A-u}(x)\left(\Phi_{Z_2}(x) - \Phi_{W_2}(x)\right).$$

Since $W_1 \prec Z_1$ and $W_2 \prec Z_2$ [13, Lemma 7.19], polynomials $\Phi_{Z_1}(x) - \Phi_{W_1}(x)$ and $\Phi_{Z_2}(x) - \Phi_{W_2}(x)$ are alternating which implies that the polynomial $\Phi_T(x) - \Phi_S(x)$ is alternating. This clearly implies that $S \prec T$. ■

Let $T = S(a_1,\ldots,a_r;\mathbf{x};b_1,\ldots,b_s;\mathbf{y};c_1,\ldots,c_t) \in \Omega(n,3)$. By Theorem 2.6 we can construct a tree $X_1 \in \Omega(n,3)$ of the form $X_1 = S(a,b;\mathbf{c};d;\mathbf{e};f,g)$ such that $T \prec X_1$.

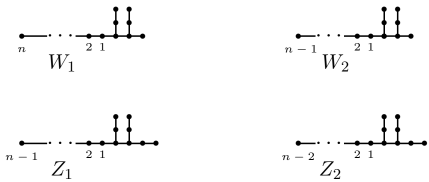


Figure 11: Trees W_1, W_2, Z_1, Z_2 involved in the proof Lemma 5.4

Therefore in order to consider the problem of maximal energy in $\Omega(n, 3)$ we can assume without loosing generality that our initial tree has the form $S(a, b; \mathbf{c}; d; \mathbf{e}; f, g)$ as is shown in Figure 12.

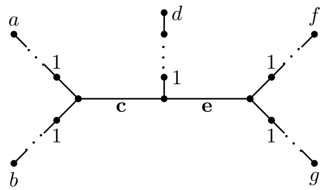


Figure 12: The tree $S(a, b; \mathbf{c}; d; \mathbf{e}; f, g)$

From now on we consider the condition $\mathbf{c} \geq 2$ and $\mathbf{e} \geq 2$. In our next result we show that we can reduce the problem to the case $d = 2$.

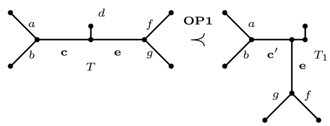
Lemma 5.5 *Let $n \geq 15$ and $T = S(a, b; \mathbf{c}; d; \mathbf{e}; f, g) \in \Omega(n, 3)$ where $\mathbf{c} \geq 2$ and $\mathbf{e} \geq 2$. Then*

$$T \prec S(a', b'; \mathbf{c}'; 2; \mathbf{e}'; f', g'),$$

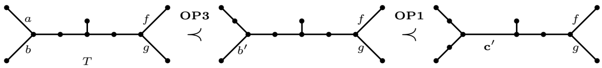
where $\mathbf{c}' \geq 2$ and $\mathbf{e}' \geq 2$.

Proof. We divide the proof in two cases, when $d = 1$ and $d > 2$.

1. Assume that $d = 1$. If $\mathbf{c} \geq 3$ then by **OP1** given in Lemma 2.3

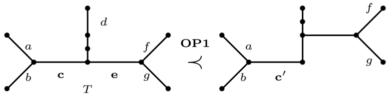


where $\mathbf{c}' = \mathbf{c} - 1 \geq 2$ and we are done. Similarly occurs if $\mathbf{e} \geq 3$ so we next assume that $\mathbf{c} = \mathbf{e} = 2$. Since $n \geq 15$ then $a + b \geq 5$. Therefore by **OP1** and **OP3** in Lemma 2.3



where $b' = a + b - 2 \geq 3$ and $\mathbf{c}' = b' \geq 3$. The result follows now from the previous case since $\mathbf{c}' \geq 3$.

2. Assume that $d > 2$. This is a direct consequence of **OP1** in Lemma 2.3 bearing in mind that $\mathbf{c} \geq 2$ gives



where $\mathbf{c}' = \mathbf{c} + d - 2 \geq 2$.

■

Now we are ready to address the main result of this section.

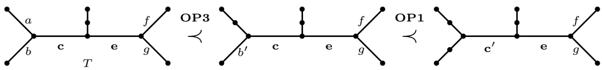
Theorem 5.6 *Let* $n \geq 15$ *and* $T = S(a, b; \mathbf{c}; d; \mathbf{e}; f, g) \in \Omega(n, 3)$ *where* $\mathbf{c} \geq 2$ *and* $\mathbf{e} \geq 2$. *Then there exists positive integers* $\mathbf{p}$ *and* $\mathbf{q}$ *such that*

$$T \prec S(2, 2; \mathbf{p}; 2; \mathbf{q}; 2, 2)$$

Proof. By Lemma 5.5 we may assume that $d = 2$. We divide the proof in two parts, we first show:

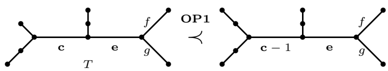
1. If $a + b + \mathbf{c} \geq 5$ then $T \prec S(2, 2; \mathbf{c}'; 2; \mathbf{e}; f, g)$. In fact, we consider three cases:

a) $a + b \geq 4$. Then we apply operations **OP1** and **OP3** in Lemma 2.3 to obtain

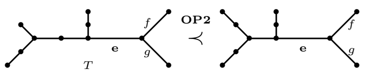


where $b' = a + b - 2 \geq 2$ and $\mathbf{c}' = a + b + \mathbf{c} - 4 \geq 2$.

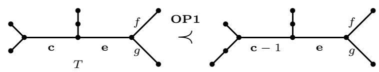
b) $a + b = 3$. If $\mathbf{c} \geq 3$ then by **OP1** in Lemma 2.3



Otherwise $\mathbf{c} = 2$, so by **OP2** in Lemma 2.3

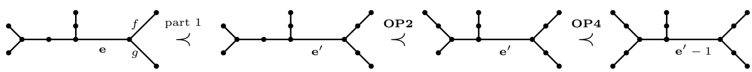


c) $a+b=2$. Then $\mathbf{c} \geq 3$ and so by **OP1** in Lemma 2.3



where $\mathbf{c}-1 \geq 2$. Now the result follows from case b).

2. If $a+b=2$ and $\mathbf{c}=2$ then $T \prec S\,(2,2;\mathbf{1};2;\mathbf{e}';2,2)$. To see this note that $n \geq 15$ implies $\mathbf{e}+f+g \geq 8$. Hence applying part 1. of this theorem, **OP2** and **OP4** we deduce



where $\mathbf{e}' = \mathbf{e}+f+g-4 \geq 4$.

■

In view of Theorem 5.6 it would be interesting to find the maximal value of the energy among all trees of the form $S(2,2;\mathbf{p};2;\mathbf{q};2,2)$, where $\mathbf{p}$ and $\mathbf{q}$ are positive integers. Unfortunately, this will not be possible through quasi-ordering relations, as we can see in the following examples.

Example 5.7 *Note that given a tree* $T = S\,(2,2;\mathbf{p};2;\mathbf{q};2,2) \in \Omega(n,3)$*,* $\mathbf{q}$ *is determined by the value of* $\mathbf{p}$ *via the relation* $\mathbf{q} = n-11-\mathbf{p}$*.*

1. Consider the case $n=20$

$\mathbf{p}$	*Energy*	*Characteristic polynomial*
1	*24.5488*	$x^{20}-19x^{18}+150x^{16}-642x^{14}+1633x^{12}-2548x^{10}+2427x^{8}-1352x^{6}+396x^{4}-47x^{2}+1$
4	*24.5447*	$x^{20}-19x^{18}+150x^{16}-641x^{14}+1624x^{12}-2520x^{10}+2389x^{8}-1331x^{6}+395x^{4}-49x^{2}+1$
2	*24.5443*	$x^{20}-19x^{18}+150x^{16}-641x^{14}+1623x^{12}-2513x^{10}+2375x^{8}-1321x^{6}+394x^{4}-50x^{2}+1$
3	*24.5441*	$x^{20}-19x^{18}+150x^{16}-641x^{14}+1624x^{12}-2521x^{10}+2395x^{8}-1339x^{6}+397x^{4}-48x^{2}+1$

As we can see the maximal energy is attained in the value $\mathbf{p}=1$*. We note that none of the trees with* $2 \leq \mathbf{p} \leq 4$ *are comparable with this tree.*

2. Consider the case $n = 21$

$\mathbf{p}$	*Energy*	*Characteristic polynomial*
4	*25.748*	$x^{21} - 20x^{19} + 168x^{17} - 774x^{15} + 2148x^{13} - 3722x^{11} + 4041x^9 - 2676x^7 + 1007x^5 - 184x^3 + 11x$
2	*25.7467*	$x^{21} - 20x^{19} + 168x^{17} - 774x^{15} + 2147x^{13} - 3714x^{11} + 4021x^9 - 2658x^7 + 1004x^5 - 186x^3 + 11x$
1	*25.7419*	$x^{21} - 20x^{19} + 168x^{17} - 775x^{15} + 2158x^{13} - 3758x^{11} + 4100x^9 - 2721x^7 + 1019x^5 - 182x^3 + 10x$
3	*25.7365*	$x^{21} - 20x^{19} + 168x^{17} - 774x^{15} + 2148x^{13} - 3723x^{11} + 4048x^9 - 2690x^7 + 1017x^5 - 185x^3 + 10x$
5	*25.7362*	$x^{21} - 20x^{19} + 168x^{17} - 774x^{15} + 2148x^{13} - 3722x^{11} + 4042x^9 - 2682x^7 + 1015x^5 - 186x^3 + 10x$

In this case the maximal energy is attained in the value $\mathbf{p} = 4$. *Again none of the trees for* $2 \leq \mathbf{p} \leq 5$ *are comparable with this tree.*

Let $\Omega^*(n,3) \subset \Omega(n,3)$ denotes the set of all trees of the form $S(2,2;\mathbf{p};2;\mathbf{q};2,2)$. Actually, we computed for all $15 \leq n \leq 200$ the energy of the trees in $\Omega^*(n,3)$ and the behavior is exactly the same as in the previous example. In other words, when n is even the maximal energy is attained in the value $\mathbf{p} = 1$ and when n is odd the maximal energy is attained at $\mathbf{p} = 4$. Consequently we conjecture:

Conjecture 5.8 *For every* $n \geq 16$, *the maximal value of the energy over* $\Omega^*(n,3)$ *is attained in* $S(2,2;\mathbf{1};2;\mathbf{n-12};2,2)$ *when* n *is even and in* $S(2,2;\mathbf{4};2;\mathbf{n-15};2,2)$ *when* n *is odd.*

On the other hand, the conditions $\mathbf{c} \geq 2$ and $\mathbf{e} \geq 2$ in the hypothesis of Theorem 5.6 are necessary, as we can see in our next example.

Example 5.9 *The trees* $T = S(2,2;\mathbf{1};2;\mathbf{1};2,4)$, $A = S(2,2;\mathbf{1};2;\mathbf{3};2,2)$ *and* $B = S(2,2;\mathbf{2};2;\mathbf{2};2,2)$ *belonging to* $\Omega(15,3)$ *are not comparable. In fact,*

$$\begin{aligned}
\Phi_T(x) &= X^{15} - 14X^{13} + 75X^{11} - 198X^9 + 275X^7 - 197X^5 + 65x^3 - 7x \\
\Phi_A(x) &= X^{15} - 14X^{13} + 75X^{11} - 197X^9 + 273X^7 - 198X^5 + 67x^3 - 7x \\
\Phi_B(x) &= X^{15} - 14X^{13} + 75X^{11} - 196X^9 + 267X^7 - 190X^5 + 65x^3 - 8x
\end{aligned}$$

However note that $\mathcal{E}(T) = 18.0779 < \mathcal{E}(A) = 18.0805 < \mathcal{E}(B) = 18.0889$.

This leads to the following conjecture:

Conjecture 5.10 *For every* $n \geq 16$, *the maximal value of the energy over* $\Omega(n,3)$ *is attained in* $S(2,2;\mathbf{1};2;\mathbf{n-12};2,2)$ *when* n *is even and in* $S(2,2;\mathbf{4};2;\mathbf{n-15};2,2)$ *when* n *is odd.*

In conclusion, the general problem of the maximal value of the energy over $\Omega(n,3)$ is still an open problem. In this section we showed that using quasi-order relations, Theorem 5.6 is as far as we can get. From this point on, it seems that any progress is possible only by means of the Coulson's integral formula combined by methods of real analysis (see [13]).

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