Complete Solution to a Conjecture on the Fourth Maximal Energy Tree*

Bofeng Huo[1,2], Shengjin Ji[1], Xueliang Li[1], Yongtang Shi[1]

[1]Center for Combinatorics and LPMC-TJKLC
Nankai University, Tianjin 300071, China
E-mail: huobofeng@mail.nankai.edu.cn; jishengjin@mail.nankai.edu.cn;
lxl@nankai.edu.cn; shi@nankai.edu.cn
[2]Department of Mathematics and Information Science
Qinghai Normal University, Xining 810008, China

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Abstract

The energy of a simple graph G, denoted by $E(G)$, is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. Gutman et al. [Extremal energy trees, *MATCH Commun. Math. Comput. Chem.* **59** (2008), 315–320] conjectured that the fourth maximal energy tree should be $P_n(2, 6, n-9)$, which is the tree consisting of three internal disjoint pendent paths starting from the unique vertex of degree 3, the length of the paths are 2, 6 and $n-9$, respectively. Li and Li, Shan and Shao showed that the fourth maximal tree must be one of the two trees, $P_n(2, 6, n-9)$ and $T_n(2, 2|2, 2)$, and these two trees are incomparable in the so-called quasi-order, where $T_n(2, 2|2, 2)$ denotes the tree of order n obtained by attaching two pendent paths of length 2 to each end vertex of the path P_{n-8}, respectively. In this paper, by utilizing the Coulson integral formula and some knowledge of real analysis, especially by employing certain combinatorial techniques, we show that the energy of $P_n(2, 6, n-9)$ is greater than that of $T_n(2, 2|2, 2)$, and therefore completely confirm this conjecture.

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1 Introduction

Let G be a simple graph of order n, $A(G)$ the adjacency matrix of G. The characteristic polynomial of $A(G)$ is usually called the characteristic polynomial of G, denoted by

$$\phi(G,x) = \det(xI - A(G)) = x^n + a_1 x^{n-1} + \cdots + a_n \ .$$

It is well-known [3] that the characteristic polynomial of a bipartite graph G takes the form

$$\phi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} a_{2k}\, x^{n-2k} = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, b_{2k}\, x^{n-2k}$$

where $b_{2k} = (-1)^k a_{2k}$ and $b_{2k} \geq 0$ for all $k = 1, \ldots, \lfloor n/2 \rfloor$, especially $b_0 = a_0 = 1$. Moreover, the characteristic polynomial of a tree T can be expressed as

$$\phi(T,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, m(T,k)\, x^{n-2k}$$

where $m(T,k)$ is the number of k-matchings of T.

For a graph G, Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the eigenvalues of its characteristic polynomial. The energy of a graph G is defined as

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

This definition was proposed formally in the 1970s by Gutman [6]. However, certain facts and properties about graph energy were implicitly put forward before, see e. g. [1, 2, 21]. Within this early reasearch on graph energy, Gutman [4, 5] deduced the following formula

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log |x^n\, \phi(G, i/x)| \mathrm{d}x$$

where $i^2 = -1$. Furthermore, in the book of Gutman and Polansky [9], it was shown how the above equality can (easily) be converted into an explicit formula as follows:

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left[\left(\sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, a_{2k}\, x^{2k} \right)^2 + \left(\sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, a_{2k+1}\, x^{2k+1} \right)^2 \right] \mathrm{d}x \ .$$

In particular, the energy of a tree T can be expressed as

$$E(T) = \frac{2}{\pi} \int_{0}^{+\infty} x^{-2} \log \left[1 + \sum_{k=1}^{\lfloor n/2 \rfloor} m(T,k)\, x^{2k} \right] \mathrm{d}x \ .$$

For more results about graph energy, we refer the reader to the recent survey of Gutman, Li and Zhang [8].

For two trees T_1 and T_2 of the same order, if $m(T_1, k) \leq m(T_2, k)$ for all $k = 1, \ldots, \lfloor n/2 \rfloor$, it is clear that $E(T_1) \leq E(T_2)$. Therefore, one can introduce a quasi order $\preceq$ in the set of trees, that is, if $m(T_1, k) \leq m(T_2, k)$ holds for all $k \geq 0$, then define $T_1 \preceq T_2$, and so $T_1 \preceq T_2$ implies $E(T_1) \leq E(T_2)$ [5, 11, 24]. Similarly, one can generalize the quasi order to the cases of bipartite graphs [18] and unicyclic graphs [15]. The above quasi order method is commonly used to compare the energies of two trees, bipartite graphs or unicyclic graphs. However, for general graphs, it is hard to define such a quasi order. If, for two trees or bipartite graphs, the above quantities $m(T, k)$ or $|a_k(G)|$ cannot be compared uniformly, then the common comparing method is invalid, and this occasionally happened. Recently, for these quasi-order-incomparable problems, we found an efficient way to determine which one attains the extremal value of the energy, see [12–14].

Gutman [5] determined the first and second maximal-energy trees of order n. Li and Li [16] determined the third maximal energy tree. Gutman et al. [10] conjectured that the fourth maximal energy tree should be $P_n(2, 6, n-9)$, which is a tree of order n consisting of three internal disjoint pendent paths starting from the unique vertex of degree 3, the lengths of the paths are 2, 6 and $n - 9$, respectively. Li and Li [17], and, independently, Shan and Shao [22, 23] showed that the fourth maximal tree must be one of the two trees, $P_n(2, 6, n-9)$ and $T_n(2, 2|2, 2)$, and these two trees are incomparable in the above quasi-order, where $T_n(2, 2|2, 2)$ denotes the tree of order n obtained by attaching two pendent paths of length 2 to each end vertex of the path P_{n-8}, respectively (as shown in Figure 1). Actually, this problem was also mentioned in a lecture of Gutman, when he visited Nankai University in the fall of 2009, and later on. In this paper, we will employ the Coulson integral formula and some knowledge of real analysis, especially by using certain combinatorial techniques, to show that the conjecture is true, and hence get a complete solution to this open problem.

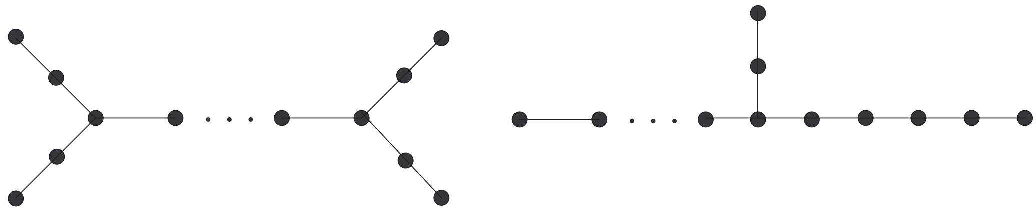

Figure 1. Trees $T_n(2,2|2,2)$ and $P_n(2,6,n-9)$.

2 Main results

In the following, we list some basic properties of the characteristic polynomial $\phi(G,x)$, which can be found in [3].

Lemma 2.1. *Let uv be an edge of G. Then*

$$\phi(G,x) = \phi(G-uv,x) - \phi(G-u-v,x) - 2\sum_{C\in\mathcal{C}(uv)} \phi(G-C,x)$$

where $\mathcal{C}(uv)$ is the set of cycles containing uv. In particular, if uv is a pendent edge with pendent vertex v, then $\phi(G,x) = x\,\phi(G-v,x) - \phi(G-u-v,x)$.

By Lemma 2.1, one easily obtains:

Lemma 2.2. *Let G be a forest and $e = uv$ be an edge of G. The characteristic polynomial of G satisfies $\phi(G,x) = \phi(G-e,x) - \phi(G-u-v,x)$.*

The following lemma is a well-known result due to Coulson and Jacobs [2], see also [7, 19, 20], which will be used in the sequel.

Lemma 2.3. *If G_1 and G_2 are two graphs with the same number of vertices, then*

$$E(G_1) - E(G_2) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \log\frac{\phi(G_1,ix)}{\phi(G_2,ix)}\,\mathrm{d}x\ .$$

In [10], Gutman et al. proposed the following conjecture on the fourth maximal energy tree of order n.

Conjecture 2.4. *For $n \geq 14$, the fourth maximal-energy tree is $P_n(2,6,n-9)$.*

Recently, Shan and Shao [22] showed:

Theorem 2.5. *If $n \geq 14$, then the fourth maximal-energy tree of order n is one of the two trees $P_n(2,6,n-9)$ and $T_n(2,2|2,2)$.*

We completely settle this problem by showing:

Theorem 2.6. *For $n \geq 14$, the fourth maximal energy tree is $P_n(2,6,n-9)$.*

Before showing our main result, we give some useful lemmas. For brevity, we introduce some notations. We use $T_A(n)$ and $T_B(n)$ to denote $P_n(2,6,n-9)$ and $T_n(2,2|2,2)$, respectively. One can obtain the characteristic polynomials of $T_A(n)$ and $T_B(n)$ for $n = 10, 11$ as follows:

$$\phi(T_A(10),x) = x^{10} - 9x^8 + 27x^6 - 31x^4 + 12x^2 - 1$$

$$\phi(T_A(11),x) = x^{11} - 10x^9 + 35x^7 - 52x^5 + 32x^3 - 6x$$

$$\phi(T_B(10),x) = x^{10} - 9x^8 + 26x^6 - 30x^4 + 13x^2 - 1$$

$$\phi(T_B(11),x) = x^{11} - 10x^9 + 34x^7 - 48x^5 + 29x^3 - 6x \ .$$

Define

$$Y_1(x) = \frac{x + \sqrt{x^2-4}}{2}$$

$$Y_2(x) = \frac{x - \sqrt{x^2-4}}{2}$$

$$A_1(x) = \frac{Y_1(x)\phi(T_A(11),x) - \phi(T_A(10),x)}{(Y_1(x))^{12} - (Y_1(x))^{10}}$$

$$A_2(x) = \frac{Y_2(x)\phi(T_A(11),x) - \phi(T_A(10),x)}{(Y_2(x))^{12} - (Y_2(x))^{10}}$$

$$B_1(x) = \frac{Y_1(x)\phi(T_B(11),x) - \phi(T_B(10),x)}{(Y_1(x))^{12} - (Y_1(x))^{10}}$$

$$B_2(x) = \frac{Y_2(x)\phi(T_B(11),x) - \phi(T_B(10),x)}{(Y_2(x))^{12} - (Y_2(x))^{10}} \ .$$

It is easy to verify that $Y_1(x) + Y_2(x) = x$ and $Y_1(x)\,Y_2(x) = 1$.

By Lemmas 2.1 and 2.2, we can easily obtain

Lemma 2.7. $\phi(T_A(n),x) = x\,\phi(T_A(n-1),x) - \phi(T_A(n-2),x)$ *and* $\phi(T_B(n),x) = x\phi(T_B(n-1),x) - \phi(T_B(n-2),x)$.

Lemma 2.8. *For $n \geq 10$ and $x \neq \pm 2$, the characteristic polynomials of $T_A(n)$ and $T_B(n)$ have the following form*

$$\phi(T_A(n),x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n$$

and

$$\phi(T_B(n),x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n\,.$$

Proof. By Lemma 2.7, we notice that both $\phi(T_A(n),x)$ and $\phi(T_B(n),x)$ satisfy the recursive formula $f(n,x) = xf(n-1,x) - f(n-2,x)$. Therefore, the general solution of this linear homogeneous recurrence relation is $f(n,x) = C_1(x)(Y_1(x))^n + C_2(x)(Y_2(x))^n$. By some elementary calculations, we can easily obtain that $C_i(x) = A_i(x)$ for $\phi(T_A(n),x)$, and $C_i(x) = B_i(x)$ for $\phi(T_B(n),x)$, $i = 1,2$, from the corresponding initial values $\phi(T_A(10),x)$, $\phi(T_A(11),x)$; $\phi(T_B(10),x)$, $\phi(T_B(11),x)$. $\square$

We recall some knowledge from real analysis, for which we refer to [26].

Lemma 2.9. *For any real number $X > -1$, we have*

$$\frac{X}{1+X} \leq \log(1+X) \leq X\,.$$

Proof of Theorem 2.6: By Lemma 2.3, the difference between the energies of these two trees is

$$E(T_B(n)) - E(T_A(n)) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \log\frac{\phi(T_B(n),ix)}{\phi(T_A(n),ix)}\,\mathrm{d}x$$

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty} \log\frac{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}\,\mathrm{d}x\,. \qquad (1)$$

By the definition of $Y_1(x)$ and $Y_2(x)$, $Y_1(ix) = \frac{x+\sqrt{x^2+4}}{2}i$, $Y_2(ix) = \frac{x-\sqrt{x^2+4}}{2}i$. For convenience, we define $Z_1(x) = -iY_1(ix) = \frac{x+\sqrt{x^2+4}}{2}$, $Z_2(x) = -iY_2(ix) = \frac{x-\sqrt{x^2+4}}{2}$, and

$$f_{10} = -\phi(T_A(10), ix) = x^{10} + 9x^8 + 27x^6 + 31x^4 + 12x^2 + 1$$

$$f_{11} = i\phi(T_A(11), ix) = x^{11} + 10x^9 + 35x^7 + 52x^5 + 32x^3 + 6x$$

$$g_{10} = -\phi(T_B(10), ix) = x^{10} + 9x^8 + 26x^6 + 30x^4 + 13x^2 + 1$$

$$g_{11} = i\phi(T_B(11), x) = x^{11} + 10x^9 + 34x^7 + 48x^5 + 29x^3 + 6x \ .$$

Thus, it follows that

$$A_1(ix) = \frac{Z_1(x)f_{11} + f_{10}}{(Z_1(x))^{10}((Z_1(x))^2+1)} \quad , \quad A_2(ix) = \frac{Z_2(x)f_{11} + f_{10}}{(Z_2(x))^{10}((Z_2(x))^2+1)}$$

$$B_1(ix) = \frac{Z_1(x)g_{11} + g_{10}}{(Z_1(x))^{10}((Z_1(x))^2+1)} \quad , \quad B_2(ix) = \frac{Z_2(x)g_{11} + g_{10}}{(Z_2(x))^{10}((Z_2(x))^2+1)} \ .$$

When $n \to \infty$,

$$\frac{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n} \to \begin{cases} \dfrac{B_1(ix)}{A_1(ix)} & \text{if } x > 0 \\[2ex] \dfrac{B_2(ix)}{A_2(ix)} & \text{if } x < 0 \ . \end{cases}$$

When n is even, since $Y_1(ix) \cdot Y_2(ix) = 1$, we have

$$\log \frac{B_1(ix)(Y_1(ix))^{n+2} + B_2(ix)(Y_2(ix))^{n+2}}{A_1(ix)(Y_1(ix))^{n+2} + A_2(ix)(Y_2(ix))^{n+2}} - \log \frac{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}$$

$$= \log\left(1 + \frac{K_0(x)}{H_0(n,x)}\right)$$

where $K_0(x) = (A_1(ix)B_2(ix) - A_2(ix)B_1(ix))\left((Y_2(ix))^2 - (Y_1(ix))^2\right)$ and $H_0(n,x) = \phi(T_A(n+2), ix) \cdot \phi(T_B(n), ix)$. Then, by some calculations,

$$K_0(x) = \frac{(f_{11}g_{10} - f_{10}g_{11})(x^2+4)x}{((Z_1(x))^2+1)((Z_2(x))^2+1)} = (f_{11}g_{10} - f_{10}g_{11})x$$

$$= 2x^{16} + 22x^{14} + 89x^{12} + 168x^{10} + 156x^8 + 66x^6 + 9x^4 > 0$$

no matter whether x is positive or negative. According to the expression of the characteristic polynomial of trees, it is easy to observe that $H_0(n,x)$ is a polynomial such that each term is of even degree of x and all coefficients are negative. Obviously, $\log\left(1+\frac{K_0(x)}{H_0(n,x)}\right) \leq 0$ for all x and even n. So, the integrand of Eq.(1) is monotonically decreasing on n when n is even. Therefore,

$$\int_{-\infty}^{+\infty} \log\frac{\phi(T_B(n),ix)}{\phi(T_A(n),ix)}\,\mathrm{d}x \leq \int_{-\infty}^{+\infty} \log\frac{\phi(T_B(14),ix)}{\phi(T_A(14),ix)}\,\mathrm{d}x\ .$$

By computer-aided calculations, $E(T_B(14)) \doteq 17.00079$, $E(T_B(14)) \doteq 17.04710$, and then

$$\int_{-\infty}^{+\infty} \log\frac{\phi(T_B(14),ix)}{\phi(T_A(14),ix)}\,\mathrm{d}x = \pi(E(T_B(14)) - E(T_A(14))) \doteq -0.14549 < 0\ .$$

Suppose now that n is odd and $x > 0$. Then we have

$$\log\frac{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n} - \log\frac{B_1(ix)}{A_1(ix)} = \log\left(1+\frac{K_1(n,x)}{H_1(n,x)}\right)$$

where $K_1(n,x) = (A_1(ix)B_2(ix) - A_2(ix)B_1(ix))\cdot(Y_2(ix))^n$ and $H_1(n,x) = \phi(T_A(n),ix)\cdot B_1(ix)$. Notice that $K_1(n,x) = \frac{(f_{11}g_{10}-f_{10}g_{11})(Z_2(x))^n}{\sqrt{x^2+4}}\cdot i^n$ and $H_1(n,x)/i^n$ is a polynomial such that each term is of odd degree of x and all coefficients are positive. Then $\frac{K_1(n,x)}{H_1(n,x)} < 0$ for all $x > 0$ and odd n, since at this time $(Z_2(x))^n = \left(\frac{x-\sqrt{x^2+4}}{2}\right)^n < 0$ and $f_{11}g_{10}-f_{10}g_{11} = 2x^{15} + 22x^{13} + 89x^{11} + 168x^9 + 156x^7 + 66x^5 + 9x^3 > 0$. Similarly, we can show that

$$\log\frac{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n} - \log\frac{B_2(ix)}{A_2(ix)} < 0$$

for all $x < 0$ and odd n. Therefore, we have proved that the integrand of Eq. (1) is not greater than the corresponding limit function when n is odd.

Since $1 + \frac{B_1(ix)-A_1(ix)}{A_1(ix)} = \frac{B_1(ix)}{A_1(ix)} > 0$ for $x > 0$ and $1 + \frac{B_2(ix)-A_2(ix)}{A_2(ix)} = \frac{B_2(ix)}{A_2(ix)} > 0$ for $x < 0$, $\frac{B_1(ix)-A_1(ix)}{A_1(ix)} > -1$ and $\frac{B_2(ix)-A_2(ix)}{A_2(ix)} > -1$. In terms of Lemma 2.9 and by some computer-aided calculations, we obtain that

$$\int_{0}^{+\infty} \log\frac{B_1(ix)}{A_1(ix)}\,\mathrm{d}x < \int_{0}^{+\infty} \frac{B_1(ix)-A_1(ix)}{A_1(ix)}\,\mathrm{d}x \doteq -0.07713$$

and

$$\int_{-\infty}^{0} \log\frac{B_2(ix)}{A_2(ix)}\,\mathrm{d}x < \int_{0}^{+\infty} \frac{B_2(ix)-A_2(ix)}{A_2(ix)}\,\mathrm{d}x \doteq -0.07713\ .$$

Therefore, when n is odd,

$$\int\limits_{-\infty}^{+\infty} \log \frac{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}\, \mathrm{d}x$$

$$\leq \int\limits_{0}^{+\infty} \log \frac{B_1(ix)}{A_1(ix)}\, \mathrm{d}x + \int\limits_{-\infty}^{0} \log \frac{B_2(ix)}{A_2(ix)}\, \mathrm{d}x < -0.15426 < 0 \ .$$

The proof is thus complete. $\square$

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