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On a Conjecture on the Tree with Fourth Greatest Energy*

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Abstract

In [6], Ivan Gutman et al. conjectured that the tree $P_n(2,6,n-9)$ of order $n \geq 14$ has the fourth greatest energy among all trees of order n. By using the method of "quasi-order $\preccurlyeq$", two of the present authors [8] claimed to have proved this conjecture by showing that $T \prec P_n(2,6,n-9)$ for all trees T of order n with $T \notin \{P_n, P_n(2,2,n-5), P_n(2,4,n-7), P_n(2,6,n-9)\}$, where P_n, $P_n(2,2,n-5)$ and $P_n(2,4,n-7)$ are known to be the trees of order n with the first, second and third greatest energies. In this paper, we show that the trees $T_n(2,2|2,2)$ and $P_n(2,6,n-9)$ are quasi-order incomparable, thus the above result $T \prec P_n(2,6,n-9)$ is not true for $T = T_n(2,2|2,2)$. In this sense, the conjecture proposed in [6] has not been settled yet, and it cannot be settled by only using the quasi-order method.

1 Introduction

Let T be a tree of order n with a unique vertex v of degree at least 3. Then it can be easily seen that T must be a tree consisting of some internally disjoint pendent

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paths starting from v. Suppose that the lengths of these pendent paths are positive integers $a_1, \ldots, a_r$, then we denote this tree T by $P_n(a_1, a_2, \ldots, a_r)$ (or sometimes simply $P(a_1, a_2, \ldots, a_r)$), where $a_1 + a_2 + \cdots + a_r = n - 1$ (see Fig 1.1(a) for $P_n(2, 6, n-9)$).

Let $T_n(a, b|c, d)$ be the tree of order n obtained by attaching two pendent paths of lengths a and b to one end vertex of the path $P_{n-a-b-c-d}$ and attaching two pendent paths of lengths c and d to another end vertex of the path $P_{n-a-b-c-d}$, where a, b, c, d are all positive integers (see Fig. 1.1(b)).

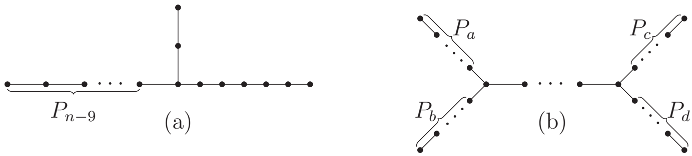

Fig. 1.1 $P_n(2, 6, n-9)$ and $T_n(a, b|c, d)$

Let G be a simple graph with n vertices and A be its adjacency matrix. The energy of G, denoted by $E(G)$, is defined [3, 4] to be the sum of the absolute values of all the n eigenvalues of A.

Let $m(G, k)$ be the number of k-matchings of G [1]. For a forest T with n vertices, its energy can be expressed by the following Coulson integral formula [5]:

$$E(T) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left(\sum_{k=0}^{\lfloor n/2 \rfloor} m(T, k) x^{2k} \right) dx \,. \tag{1.1}$$

The fact that $E(T)$ is a strictly monotonically increasing function of all the matching numbers $m(T, k)$ $(k = 0, 1, 2, \ldots, \lfloor n/2 \rfloor)$ is an obvious consequence of the formula (1.1). This in turn provides a way of comparing the energies of a pair of forests, and yields the following definition of the quasi-order relation $\preccurlyeq$ (Gutman [2]) on the set of all forests (acyclic graphs) with n vertices.

Definition 1.1. Let T_1 and T_2 be two forests of order n. If $m(T_1, k) \le m(T_2, k)$ for all $k = 0, 1, \ldots, \lfloor n/2 \rfloor$, then we write that $T_1 \preccurlyeq T_2$.

Furthermore, if $T_1 \preccurlyeq T_2$ and there exists at least one index j such that $m(T_1, j) < m(T_2, j)$, then we write that $T_1 \prec T_2$.

If $m(T_1, k) = m(T_2, k)$ for all k (i. e., if $T_1 \preccurlyeq T_2 \preccurlyeq T_1$), then we write $T_1 \sim T_2$.

According to the Coulson integral formula (1.1), we can easily see the following relations between $\preccurlyeq$ and the energies for two forests T_1 and T_2 of order n:

$$T_1 \preceq T_2 \Rightarrow E(T_1) \leq E(T_2), \quad \text{and} \quad T_1 \prec T_2 \Rightarrow E(T_1) < E(T_2)$$

Many results on the maximal energy have been obtained for trees. For example, In [2], Gutman determined that the first and second maximal energy trees of order n are P_n and $P_n(2,2,n-5)$, respectively. N. Li and S. Li [7] determined that the third maximal energy tree is $P_n(2,4,n-7)$. Gutman et al. [6] also proposed the following conjecture about the fourth maximal energy tree of order n (Here we only quote the conjecture for the cases $n \geq 10$):

Conjecture 1. *For $n = 11$, the fourth maximal energy tree is $P_{11}(2,3,5)$; For $n = 13$, the fourth maximal energy tree is $P_{13}(4,4,4)$; For $n = 10, 12$ and $n \geq 14$, the fourth maximal energy tree is $P_n(2,6,n-9)$.*

The main result of [8] (Theorem 3.6 in [8]) is:

$(*)$ Let $\mathbf{T}$ be a tree of order $\mathbf{n \geq 14}$, which is not in $\{\mathbf{P_n}, \mathbf{P_n(2,2,n-5)}, \mathbf{P_n(2,4,n-7)}, \mathbf{P_n(2,6,n-9)}\}$. Then $\mathbf{T \prec P_n(2,6,n-9)}$.

It is obvious that an affirmative answer to Conjecture 1 for $n \geq 14$ would follow directly from the above assertion $(*)$.

In this paper, we will show that the trees $T_n(2,2|2,2)$ (which is not in $\{P_n, P_n(2,2,n-5), P_n(2,4,n-7), P_n(2,6,n-9)\}$) and $P_n(2,6,n-9)$ are quasi-order incomparable, thus the result $T \prec P_n(2,6,n-9)$ in assertion $(*)$ is not true for the tree $T = T_n(2,2|2,2)$. In this sense, we think that the Conjecture 1 for the case $n \geq 14$ has not been settled yet.

Up to now, the latest result about the Conjecture 1 is the following:

Theorem 1.1. [9] *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 $T_n(2,2|2,2)$.*

2 Incomparability of $\mathbf{T_n(2,2|2,2)}$ and $\mathbf{P_n(2,6,n-9)}$

In this section, we show that the two tress $T_n(2,2|2,2)$ and $P_n(2,6,n-9)$ of order n are quasi-order incomparable for all even n with $n \geq 10$, and all odd n with $n \geq 19$.

Let P_n be the path with n vertices and let $m(n,k) = m(P_n,k)$. Then the following special values and recurrence relation for $m(n,k)$ can be easily obtained:

$$m(n,0) = 1$$

$$m(n,1) = n-1$$

$$m(2k,k) = 1 \tag{2.1}$$

$$m(2k+1,k) = k+1 \tag{2.2}$$

$$m(n,k) = 0 \quad (\text{if } k < 0 \text{ or } 2k > n) \tag{2.3}$$

$$m(n,k) = m(n-1,k) + m(n-2,k-1) \qquad (n \geq 3)\ . \tag{2.4}$$

Here we assume that $m(G,k) = 0$ for all negative integers k.

Lemma 2.1. [5] *Let $e = uv$ be an edge of a graph G. Then:*

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

□

By taking $G = P_2 \cup P_r$ and e to be the edge in P_2, we can easily obtain from Lemma 2.1:

$$m(P_2 \cup P_r, k) = m(r,k) + m(r,k-1)\ . \tag{2.5}$$

Lemma 2.2. *Let $n \geq 8$, $G = P_n(2,2,n-5)$ and $G' = P_n(1,2,n-4)$. Then:*

$$m(G,k) - m(G',k) = m(n-7,k-3)\ .$$

Proof. Take an edge $e = uv$ in G and an edge $e' = u'v'$ in G' as in Fig. 2.1.

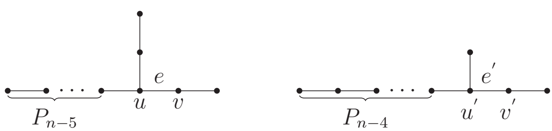

Fig. 2.1 $G = P_n(2,2,n-5)$ and $G' = P_n(1,2,n-4)$

Then we have $G-e=G^{'}-e^{'}$. Thus by Lemma 2.1 and the recurrence relation (2.4), we have:

$$\begin{aligned} m(G,k)-m(G^{'},k) &= m(G-u-v,k-1)-m(G^{'}-u^{'}-v^{'},k-1) \\ &= m(P_2\cup P_{n-5},k-1)-m(n-4,k-1) \\ &= m(n-5,k-2)+m(n-5,k-1)-m(n-4,k-1) \\ &= m(n-5,k-2)-m(n-6,k-2)=m(n-7,k-3)\ . \end{aligned}$$

□

Lemma 2.3. *Let* $n\geq 12$*,* $G=P_n(2,2,n-5)$ *and* $G^{'}=P_n(2,4,n-7)$ *. Then:*

$$m(G,k)-m(G^{'},k)=m(n-10,k-4)\ .$$

Proof. Take an edge $e=uv$ in G and an edge $e^{'}=u^{'}v^{'}$ in $G^{'}$ as in Fig 2.2.

Fig. 2.2 $G=P_n(2,2,n-5)$ and $G^{'}=P_n(2,4,n-7)$

Then we have $G-e=G^{'}-e^{'}$. Thus by Lemma 2.1 and Lemma 2.2,

$$\begin{aligned} m(G,k)-m(G^{'},k) &= m(G-u-v,k-1)-m(G^{'}-u^{'}-v^{'},k-1) \\ &= m(P_{n-3}(2,2,n-8),k-1)-m(P_{n-3}(1,2,n-7),k-1) \\ &= m(n-10,k-4)\ . \end{aligned}$$

Here the last equation follows from Lemma 2.2. □

Lemma 2.4. *Let* $n\geq 14$ *,* $T=T_n(2,2|2,2)$ *and* $P=P_n(2,6,n-9)$ *. Then:*

$$m(T,k)-m(P,k)=m(n-12,k-4)+2m(n-12,k-5)-m(P_{n-6}(2,2,n-11),k-2)\ . \quad (2.6)$$

Proof. Take an edge $e=uv$ in T and $e^{'}=u^{'}v^{'}$ in P as in Fig. 2.3.

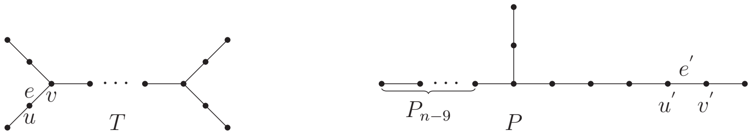

Fig. 2.3 The edges e in T and $e^{'}$ in P

Then we have

$T - e = P_2 \cup P_{n-2}(2, 2, n-7)$ $\quad$ $P - e^{'} = P_2 \cup P_{n-2}(2, 4, n-9)$

$T - u - v = P_1 \cup P_2 \cup P_{n-5}(2, 2, n-10)$ $\quad$ $P - u^{'} - v^{'} = P_1 \cup P_{n-3}(2, 3, n-9)$.

Now by (2.5) and Lemma 2.3,

$$\begin{aligned} & m(T-e,k) - m(P-e^{'},k) \\ =& \sum_{i=k-1}^{k} [m(P_{n-2}(2,2,n-7),i) - m(P_{n-2}(2,4,n-9),i)] \\ =& \sum_{i=k-1}^{k} m(n-12,i-4) = m(n-12,k-4) + m(n-12,k-5) \ . \end{aligned} \tag{2.7}$$

By taking the pendant edge in a pendant path of length 3 in $P_{n-3}(2, 3, n-9)$ and using Lemma 2.1, we obtain

$$m(P_{n-3}(2,3,n-9),k-1) = m(P_{n-4}(2,2,n-9),k-1) + m(P_{n-5}(1,2,n-9)) \ . \tag{2.8}$$

By (2.5), (2.8), Lemma 2.2, and Lemma 2.1 we also have

$$\begin{aligned} & m(T-u-v,k-1) - m(P-u^{'}-v^{'},k-1) \\ =& m(P_2 \cup P_{n-5}(2,2,n-10),k-1) - m(P_{n-3}(2,3,n-9),k-1) \\ =& [m(P_{n-5}(2,2,n-10),k-1) + m(P_{n-5}(2,2,n-10),k-2)] \\ -& [m(P_{n-4}(2,2,n-9),k-1) + m(P_{n-5}(1,2,n-9),k-2)] \\ =& [m(P_{n-5}(2,2,n-10),k-1) - m(P_{n-4}(2,2,n-9),k-1)] \\ +& [m(P_{n-5}(2,2,n-10),k-2) - m(P_{n-5}(1,2,n-9),k-2)] \\ =& -m(P_{n-6}(2,2,n-11),k-2) + m(n-12,k-5) \ . \end{aligned} \tag{2.9}$$

Now adding (2.7), (2.9) and using Lemma 2.1 we obtain (2.6). □

Theorem 2.1. *Let $n \geq 14$, $T = T_n(2,2|2,2)$ and $P = P_n(2,6,n-9)$, as before. Then*

(1). $m(T,2) - m(P,2) = -1$.

(2). If n is even with $n = 2k+2$, then $m(T,k) - m(P,k) = 1$.

(3). If n is odd with $n = 2k+3$, then $m(T,k) - m(P,k) = \frac{n-17}{2}$.

Proof. (1). Take $k = 2$ in (2.6) and using (2.3), we obtain (1).

(2). Since $n = 2k+2$ and $P_{n-6}(2,2,n-11)$ has a (unique) perfect matching when n is even, we have

$$m(P_{n-6}(2,2,n-11), k-2) = m(P_{2k-4}(2,2,2k-9), k-2) = 1 \ .$$

Thus by (2.6), (2.1) and (2.3),

$$m(T,k) - m(P,k) = m(2k-10, k-4) + 2m(2k-10, k-5) - 1 = 0 + 2 - 1 = 1 \ .$$

(3). First note that when r is even, then $P_r(1,2,r-4)$ has a perfect matching and thus $m(P_r(1,2,r-4), r/2) = 1$.

Now $n = 2k+3$. Take the pendent edge in a pendent path of length 2 in $P_{n-6}(2,2,n-11)$ and use Lemma 2.1 , we have by the above note and (2.2) that

$$\begin{aligned} &m(P_{n-6}(2,2,n-11), k-2) = m(P_{n-7}(1,2,n-11), k-2) + m(n-8, k-3) \\ =&1 + m(2k-5, k-3) = 1 + k - 2 = k - 1 \ . \end{aligned}$$

So by (2.6), (2.3), and (2.2) we have:

$$\begin{aligned} &m(T,k) - m(P,k) = m(2k-9, k-4) + 2m(2k-9, k-5) - (k-1) \\ =&0 + 2(k-4) - (k-1) = k - 7 = \frac{n-17}{2} \ . \end{aligned}$$

$\square$

Remark: From results (1) and (2) we can see that T and P are quasi-order incomparable when n is even with $n \geq 14$;

From results (1) and (3) we can see that T and P are quasi-order incomparable when n is odd with $n \geq 19$.

Finally, we propose the following conjecture:

Conjecture 2. $E(P_n(2,6,n-9)) > E(T_n)(2,2|2,2)$ *for all* $n \geq 14$

By Theorem 1.1 ([9]), we see that if this Conjecture 2 is true, then Conjecture 1 (on the tree with the fourth greatest energy), proposed in [6] would also be true.

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