MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **64** (2010) 25-40

ISSN 0340 - 6253

Graph energy change due to edge grafting operations and its applications *

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(Received April 6, 2009)

Abstract

The energy of a graph is the sum of the absolute values of the eigenvalues of its adjacency matrix. The edge grafting operation on a graph is a kind of edge moving between the two pendent paths starting from the same vertex. In this paper we show how the graph energy change under the edge grafting operations. As the applications of this grafting method, we also obtain some new results on a conjecture about the tree of order n with the fourth maximal energy.

1 Introduction

Let G be a simple graph with n vertices and A be its adjacency matrix. Let $\lambda_1, \cdots, \lambda_n$ be the eigenvalues of A, then the energy of G, denoted by $E(G)$, is defined [5, 7] as $E(G) = \sum_{i=1}^{n} |\lambda_i|$.

In theoretical chemistry, the energy of a given molecular graph is related to the total π-electron energy of the molecule represented by that graph. So the graph energy has some specific chemical interests and has been extensively studied [1–21].

The characteristic polynomial $\det(xI - A)$ of the adjacent matrix A of a graph G is also called the characteristic polynomial of G, denoted by $\phi(G, x)$. Let $m(G, k)$ be the number of k-matchings of G. It is well known [2] that if G is a forest (acyclic graph), then we have: $\phi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k m(G,k) x^{n-2k}$.

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For a forest T with n vertices, its energy can be expressed by the following Coulson integral formula [10]:

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

The fact that $E(T)$ is a strictly monotonically increasing function of all the matching numbers $m(T,k)$ ($k = 0,1,2,\cdots,\lfloor \frac{n}{2} \rfloor$) is an obvious consequence of the formula (1.1). This in turn provides a way of comparing the energies of a pair of forests. That is, the method of the quasi-ordering relation "$\preceq$" defined by Gutman [10] on the set of all forests of order n as follows:

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 $k = 0,1,\cdots,\lfloor \frac{n}{2} \rfloor$, then we write that $T_1 \preceq T_2$.

Furthermore, if $T_1 \preceq T_2$ 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 $T_1 \preceq T_2 \preceq T_1$), we write $T_1 \sim T_2$.

The following lemma about the above defined quasi-ordering relation is frequently used.

Lemma 1.1. *Let u(respectively u') be a pendent vertex of a graph T (respectively,$T^{'}$), v (respectively, v') be the vertex adjacent to u(respectively u'). Suppose that $T - u \preceq T^{'} - u'$ and $T - u - v \preceq T^{'} - u' - v'$, then we have $T \preceq T^{'}$, with $T \sim T^{'}$ if and only if both the two relations $T-u \sim T^{'}-u'$ and $T-u-v \sim T^{'}-u'-v'$ hold.*

The proof of Lemma 1.1 can be seen from the following formula for the number of the k-matchings of T (and similarly of $T^{'}$):

$$m(T,k) = m(T-u,k) + m(T-u-v,k-1)$$

Since the number of the k-matchings of T which contains the edge uv is $m(T-u-v,k-1)$, and which does not contain the edge uv is $m(T-u,k)$.

According to the Coulson integral formula (1.1), we have for two forests T_1 and T_2 of order n that

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

In the present paper, we first define in §2 an operation on graphs called "edge grafting operation" which is a kind of edge moving between the two pendent paths starting from the same vertex (similar operations were considered for the number of matchings by Gutman [6]). Then we will consider the effect of this grafting operation on the quasi-ordering and the energy change of the trees. We will use the well-known quasi-ordering relation between $P_a \cup P_b$ and $P_c \cup P_d$ (when $a+b=c+d$) by Gutman [10] to show that if the lengths of the two pendent paths before (respectively, after) the grafting are a and b (respectively, c and d), and if $0 \leq a \leq b$, $0 \leq c \leq d$ and $a < c$, then the quasi-order between the two trees before and after the grafting is completely determined by the parity of the number a (see Theorem 2.3). As the applications of this grafting method, we are able to obtain some new results on a conjecture about the fourth maximal energy tree [11], as well as to provide simpler proofs on the determinations of the first three maximal energy trees of order n.

As for the ordering of the trees with larger energies, Gutman [4] determined the first and second maximal energy trees of order n. Li and Li [14] determined the third maximal energy tree. Gutman et al [11] 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 $P_n(2,6,n-9)$.*

(Where the notation $P_n(a,b,c)$ will be defined in §2.)

In this paper, we will apply our grafting operation method obtained in §2 to show that the Conjecture 1 for $n = 10, 11, 12, 13$ is true. For $n \geq 14$, we will show that the fourth maximal energy tree must be one of the two trees $P_n(2,6,n-9)$ and $T_n(2,2|2,2)$ (see Theorem 3.2), and these two trees are quasi-order incomparable.

2 The grafting operation and its effect on the energy of graphs

In this section, we will introduce the operation of edge grafting, and will show the effect of this operation on the graph energy change. We will also give some applications of this grafting method on the ordering of the energy of trees which will be used in the study of Conjecture 1.

The following well-known result obtained by Gutman [10] will be the base of our grafting method.

Theorem 2.1. *[10] Let $n = 4k$ or $4k+1$ or $4k+2$ or $4k+3$. Then*

$$P_n \succ P_2 \cup P_{n-2} \succ P_4 \cup P_{n-4} \succ \cdots \succ P_{2k} \cup P_{n-2k} \succeq$$
$$P_{2k+1} \cup P_{n-2k-1} \succeq P_{2k-1} \cup P_{n-2k+1} \succ \cdots \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1}$$

(Note that in the middle of the above relation, some of the "$\succeq$" may become "$=$" according to the residue of n module 4.)

Firstly, we restate the above Theorem 2.1 in the following equivalent form.

Theorem 2.2. *Let $a+b = c+d = n$ with $0 \le a \le b$ and $0 \le c \le d$. Assume that $a < c$, then we have:*

(1) If a is even, then $P_a \cup P_b \succ P_c \cup P_d$.

(2) If a is odd, then $P_a \cup P_b \prec P_c \cup P_d$.

Now we describe what is the edge grafting operation.

Definition 2.1 (the grafting operation)**.** Let u be a vertex of a graph H, and a, b be non-negative integers. Let $H_u(a, b)$ be the graph obtained by attaching to H two (new) pendent paths of lengths a and b at u (see Figure 1). If $a+b = c+d$, then we say that $H_u(c, d)$ is obtained from $H_u(a, b)$ by grafting edges on these two pendent paths at u.

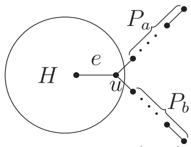

Fig. 1. The graph $H_u(a, b)$

Theorem 2.3 (the grafting theorem)**.** *Let a, b, c, d be nonnegative integers with $a+b = c+d$. Assume that $0 \le a \le b$, $0 \le c \le d$ and $a < c$. Let u be a non-isolated vertex of a graph H. Then the following statements are true:*

(1). If a is even, then $H_u(a,b) \succ H_u(c,d)$

(2). If a is odd, then $H_u(a,b) \prec H_u(c,d)$

Proof. Let $e = uv$ be an edge incident with u in H. Let $H^{'} = H - e$ and $H^* = H - u - v$. Notice that the number of the k-matchings of $H_u(a,b)$ which contains e is $m(H^* \cup P_a \cup P_b, k-1)$, and the number of the k-matchings of $H_u(a,b)$ which does not contain e is $m(H_u^{'}(a,b), k)$. So we have

$$m(H_u(a,b), k) = m(H_u^{'}(a,b), k) + m(H^* \cup P_a \cup P_b, k-1) \tag{2.1}$$

Similar formula holds for $m(H_u(c,d), k)$.

(1) If a is even. By using induction on the number of edges of H, we have $H_u^{'}(a,b) \succeq H_u^{'}(c,d)$ (equality holds when u is a pendent vertex of H). So we have

$$m(H_u^{'}(a,b), k) \geq m(H_u^{'}(c,d), k).$$

On the other hand, by Theorem 2.2 we have $H^* \cup P_a \cup P_b \succ H^* \cup P_c \cup P_d$. So we also have

$$m(H^* \cup P_a \cup P_b, k-1) \geq m(H^* \cup P_c \cup P_d, k-1),$$

with the strict inequality holding for at least one k. From these two inequalities and the formula (2.1) we obtain that $H_u(a,b) \succ H_u(c,d)$.

The proof of (2) is similar to that of (1). $\square$

If we take $a = 0$ in Theorem 2.3, then we obtain the following corollary.

Corollary 2.1 (the "total grafting operation"). *Let u be a non-isolated vertex of a graph H, and a, b be positive integers. Then we always have $H_u(0, a+b) \succ H_u(a,b)$.*

In the following, we use $N_3(G)$ to denote the number of vertices in G with degree at least 3, and $\Delta(G)$ be the maximal degree of G.

Let T be a tree of order n with $N_3(T) = 1$. Then it can be easily seen that T must be a tree consisting of some internally disjoint pendent paths starting from its unique vertex with degree at least 3. Suppose that the lengths of these pendent paths are positive integers $a_1, \cdots, a_r$. Then we denote this tree T by $P_n(a_1, a_2, \cdots, a_r)$, where $a_1 + a_2 + \cdots + a_r = n - 1$. Sometimes we also denote $P_n(a_1, a_2, \cdots, a_r)$

by $P_n(a_1, a_2, \cdots, a_{r-1}, x)$ or even simply by $P_n(a_1, a_2, \cdots, a_{r-1}, *)$, since x (or $*$) is uniquely determined by n and $a_1, a_2, \cdots, a_{r-1}$.

Now we show some applications of the grafting Theorem 2.3 (These applications will be further used in the study of the Conjecture 1 in §3).

Theorem 2.4. *Let T be tree of order n with $N_3(T) \geq 1$, then there exists a tree T' of order n with $N_3(T') = N_3(T) - 1$ such that $T \prec T'$.*

Proof. Let v be a vertex of T, let u be a vertex with degree at least 3 which is furthest to v. Then there are $(d(u) - 1)$ many pendent paths starting from u. By using $(d(u) - 2)$ many "total grafting" operations at these pendent paths, we finally obtain a tree T' of order n with $N_3(T') = N_3(T) - 1$ (since the vertex u has degree 2 in the new tree T'), and $T \prec T'$ follows directly from Corollary 2.1.

□

Note: If $N_3(T) \geq 2$ in Theorem 2.4, then by taking v to be a vertex with the maximal degree $\Delta(T)$, the tree T' in Theorem 2.4 can further satisfies $\Delta(T') = \Delta(T)$.

Now we show that the determinations of the first and second maximal energy tree of order n can be easily obtained by using the grafting method.

Corollary 2.2. *Suppose T is a tree of order $n \geq 6$ with $T \neq P_n, P_n(2, 2, x)$. Then*

$$T \prec P_n(2, 2, x) \prec P_n.$$

Proof. The relation $P_n(2, 2, x) \prec P_n$ follows easily from Theorem 2.4.

Now since $T \neq P_n$, we have $N_3(T) \geq 1$. By using Theorem 2.4 several times we can obtain a tree T_1 of order n with $N_3(T_1) = 1$. Thus $T_1 = P_n(a_1, \cdots, a_r)$ for some $r \geq 3$. By using $(r - 3)$ many "total grafting" operations on T_1 we further obtain a tree $T_2 = P_n(a, b, c)$ of order n for some positive integers a, b, c. Finally, by further using grafting Theorem 2.3 at most twice on T_2, we can obtain $P_n(2, 2, x)$. Thus we have:

$$T \preceq T_1 \preceq T_2 = P_n(a, b, c) \preceq P_n(2, b, c + a - 2) \preceq P_n(2, 2, x)$$

Since $T \neq P_n(2, 2, x)$, the total number of the grafting operations used here is at least 1. Thus we have $T \prec P_n(2, 2, x)$.

□

The following Lemmas 2.1-2.3 show that the first, second and third maximal energy trees among all the trees of order n with $N_3(T) = 1$ are $P_n(2,2,*)$, $P_n(2,4,*)$ and $P_n(2,6,*)$ (These trees are mutually distinct when $n \geq 14$). Lemma 2.1 deals with the case where $N_3(T) = 1$ and $\Delta(T) = 3$.

Lemma 2.1. *Let $T = P_n(a,b,c)$ be a tree of order $n \geq 10$, $T \neq P_n(2,2,x)$, $P_n(2,4,y), P_n(2,6,z)$, and $T \neq P_{10}(3,3,3)$. Then $T \prec P_n(2,6,z)$*

Proof. Without loss of generality, we may assume that $a \leq b \leq c$. Now we consider the following cases:

Case 1: $a = 1$. Using the grafting Theorem 2.3, we can derive easily that $T = P_n(a,b,c) = P_n(b,1,c) \preceq P_n(2,1,*) \preceq P_n(2,6,z)$. Also, $T \neq P_n(2,6,z)$ implies that the strict quasi-ordering holds.

Case 2: $a = 2$. Then none of b, c is 2,4 or 6 by our assumption. So it follows from the grafting Theorem 2.3 that $T = P_n(2,b,c) \prec P_n(2,6,z)$.

Case 3: $a = 3$. Since $T \neq P_{10}(3,3,3)$, we have $n \geq 11$. By the grafting Theorem 2.3 we have $T = P_n(3,b,c) = P_n(b,3,c) \prec P_n(2,3,b+c-2) \preceq P_n(2,6,z)$ (Since $n \geq 11$ implies $z \neq 1$).

Case 4: $a \geq 4$. We consider the following two subcases:

Subcase 4.1. $a = b = 4$. Then by the grafting Theorem 2.3 we have $P_n(a,b,c) = P_n(4,4,c) \prec P_n(2,6,c)$.

Subcase 4.2. $b \geq 5$. Then $P_n(a,b,c) \prec P_n(2,b,c+a-2) \preceq P_n(2,6,z)$ since none of b and $c+a-2$ is in $\{2,4\}$.

□

The following Lemmas 2.2 and 2.3 deal with the case where $N_3(T) = 1$ and $\Delta(T) \geq 4$.

Lemma 2.2. *Let $T = P_n(a_1, \cdots, a_r)$ with $r \geq 4$ and $T \neq P_n(2,2,2,x)$. Then*

$$T \prec P_n(2,2,2,x)$$

Proof. By using $(r-4)$ many total grafting operations on T, we can have $T \preceq P_n(a_1,a_2,a_3,*)$.

By further using grafting theorem at most 3 times on $P_n(a_1,a_2,a_3,*)$, we will finally obtain $P_n(2,2,2,x)$ with $P_n(a_1,a_2,a_3,*) \preceq P_n(2,2,2,x)$.

Since $T \neq P_n(2,2,2,x)$, the total number of the grafting operations used here is at least 1. Thus we have $T \prec P_n(2,2,2,x)$.

□

By using Lemma 1.1 together with the grafting theorem and mathematical induction, we can also deduce the following result.

Lemma 2.3. *Let $n \geq 10$, then*

$$P_n(2,2,2,x) \prec P_n(2,6,y)$$

Proof. We will prove this lemma by using induction on n.

If $n = 10$, then $x = 3$ and $y = 1$. By direct calculation we have:

$$\phi(P_n(2,2,2,3),x) = x^{10} - 9x^8 + 25x^6 - 28x^4 + 12x^2 - 1$$

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

By comparing the coefficients of these two characteristic polynomials we can easily see that $P_n(2,2,2,3) \prec P_n(2,6,1)$.

If $n = 11$, then $y = 2$. The result now follows from the fact that $P_n(2,6,2) = P_n(2,2,6)$ is the tree of order 11 having the second maximal energy (see Corollary 2.2).

Now we assume that $n \geq 12$.

Fig. 2. The graphs $P_n(2,2,2,x)$ and $P_n(2,6,y)$

As shown in Figure 2, Let $T = P_n(2,2,2,x)$, and $T' = P_n(2,6,y)$. Let u (respectively u') be a pendent vertex on the pendent path of length x (respectively y) in T (respectively T'), and v (respectively v') be the vertex incident with u (respectively u').

Obviously, we have

$$T - u = P_{n-1}(2,2,2,x-1), \text{and } \; T' - u' = P_{n-1}(2,6,y-1)$$

$$T - u - v = P_{n-2}(2,2,2,x-2), \text{and } \; T^{'} - u' - v' = P_{n-2}(2,6,y-2)$$

By the inductive hypothesis, we have $T - u \prec T^{'} - u'$ and $T - u - v \prec T^{'} - u' - v'$. Thus by using Lemma 1.1 we have $P_n(2,2,2,x) \prec P_n(2,6,y)$. The lemma is proved. $\square$

Combining Lemmas 2.2 and 2.3, we obtain (for any integer $r \geq 4$, $n \geq 10$ and any positive integers $a_1, \cdots, a_r$ with $a_1 + \cdots + a_r = n-1$) that

$$P_n(a_1, \cdots, a_r) \prec P_n(2,6,*) \quad (r \geq 4 \text{ and } n \geq 10) \tag{2.2}$$

3 Applications on the conjecture about the fourth maximal energy tree

In this section, we further apply the grafting method given in §2 to study the Conjecture 1 about the fourth maximal energy tree. We will show that the Conjecture 1 for $n = 10, 11, 12, 13$ is true; While for $n \geq 14$, we will show that the fourth maximal energy tree must be one of the two trees $P_n(2,6,n-9)$ and $T_n(2,2|2,2)$, but these two trees are quasi-order incomparable when $n \geq 19$.

As a by-product of the study of Conjecture 1, we are also able to give a simpler proof for the determination of the third maximal energy tree.

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.3). It is not difficult to see that if T is a tree of order n with $\Delta(T) = 3$ and $N_3(T) = 2$, then T must be of the form $T_n(a,b|c,d)$.

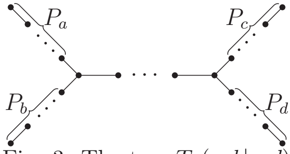

Fig. 3. The tree $T_n(a,b|c,d)$

The following Lemma 3.1 shows that all trees of order $n \geq 10$ with $\Delta(T) = 3$ and $N_3(T) = 2$, except $T_n(2,2|2,2)$, satisfies $T \prec P_n(2,6,*)$.

Lemma 3.1. *Let $T = T_n(a, b|c, d)$ be a tree of order $n \geq 10$ and $T \neq T_n(2, 2|2, 2)$, then $T \prec P_n(2, 6, *)$.*

Proof. Let k be the distance between the two vertices with degree 3 in T, then $k = n - 1 - a - b - c - d \geq 1$. Without lose of generality, we may assume that $a \leq b$, $c \leq d$, and $a \leq c$. We consider the following cases.

Case 1: $a = 1$. Then by using the grafting Theorem 2.3 we have

$$T = T(1, b|c, d) \prec P_n(1, b, c + d + k) \preceq P_n(1, 2, n - 4) \preceq P_n(2, 6, *)$$

Case 2: $a \geq 2$. Then $T \neq T_n(2, 2|2, 2)$ implies that $n \geq 11$. We further divide this case into the following two subcases.

Subcase 2.1: There is an integer among a, b, c, d (say d) which is not in $\{2, 4\}$. Then by using the total grafting operation Corollary 2.1 we have $T_n(a, b|c, d) \prec P_n(a + b + k, c, d)$ with $a + b + k \geq 5$. Note that none of $a + b + k$ and d is in $\{2, 4\}$, so $P_n(a + b + k, c, d)$ is not $P_n(2, 2, *)$ or $P_n(2, 4, *)$. Thus by $n \geq 11$ and Lemma 2.1 we have $P_n(a + b + k, c, d) \preceq P_n(2, 6, *)$. So $T = T_n(a, b|c, d) \prec P_n(2, 6, *)$.

Subcase 2.2 If a, b, c, d are all in $\{2, 4\}$. We consider the following two situations.

(1). If $c = 4$. Then $d = 4$ since $c \leq d \leq 4$. By using the total grafting Corollary 2.1 and Lemma 2.1 we have:

$$T_n(a, b|4, 4) \prec P_n(a + b + k, 4, 4) \prec P_n(2, 6, *)$$

(2). If $c = 2$. Then $a = c = 2$ since $2 \leq a \leq c$. It follows that one of b and d is 4 (say, $b = 4$) since $T_n(a, b|c, d) \neq T_n(2, 2|2, 2)$.

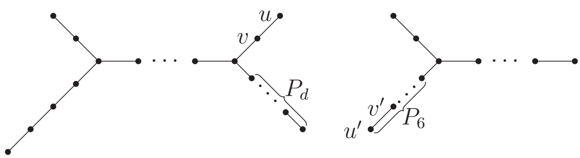

Fig. 4. $T = T_n(2, 4|2, d)$ and $T' = P_n(2, 6, *)$

Now let $T' = P_n(2, 6, *)$. Let u (respectively u') be the pendent vertex on the pendent path of length $c = 2$ (respectively length 6) in T (respectively T'), and

v (respectively v') be the vertex incident with u (respectively u') (see Figure 4). Then by using the grafting operations several times we have

$$T - u = T_n(2,4|2,d) - u = T_{n-1}(2,4|1,d) \prec P_{n-1}(6+k,1,d)$$
$$\prec P_{n-1}(2+k,5,d) \preceq P_{n-1}(2,5,*) = P_n(2,6,*) - u' = T' - u'.$$
$$T - u - v = T_n(2,4|2,d) - u - v = P_{n-2}(2,4,*) = P_n(2,6,*) - u' - v' = T' - u' - v'.$$

Therefore the result $T \prec T'$ follows immediately from Lemma 1.1 □

Using Lemma 3.1 and the results obtained in §2, we can obtain the following Lemma 3.2 which asserts that the third (and the fourth, if $P_n(2,2,x)$, $P_n(2,4,y)$ and $P_n(2,6,z)$ are distinct) maximal energy tree must be among the trees listed in the following lemma.

Lemma 3.2. *Let T be a tree of order $n \geq 10$. If $T \neq P_n, P_n(2,2,x)$, $P_n(2,4,y)$,$P_n(2,6,z), T_n(2,2|2,2)$ and $P_{10}(3,3,3)$, then $T \prec P_n(2,6,z)$.*

Proof. Since $T \neq P_n$, we have $\Delta(T) \geq 3$. We divide the proof into the following cases.

Case 1: $\Delta(T) = 3$.

Subcase 1.1: $N_3(T) = 1$. Then $T = P_n(a,b,c)$. The result follows directly from Lemma 2.1.

Subcase 1.2: $N_3(T) = 2$. Then we have $T = T_n(a,b|c,d)$, and the result follows directly from Lemma 3.1.

Subcase 1.3: $N_3(T) \geq 3$. Then by using Theorem 2.4 several times we can obtain a tree T_1 with $\Delta(T_1) = 3$, $N_3(T_1) = 2$, and $T_1 \neq T_n(2,2|2,2)$. Thus from Subcase 1.2 we have $T \prec T_1 \prec P_n(2,6,z)$.

Case 2: $\Delta(T) \geq 4$.

Subcase 2.1: $N_3(T) = 1$. Then we have $T = P_n(a_1, \cdots, a_r)$ with $r = \Delta(T) \geq 4$, and the result follows directly from Eq.(2.2).

Subcase 2.2: $N_3(T) \geq 2$. Then by using Theorem 2.4 several times we can obtain a tree T_1 with $\Delta(T_1) = \Delta(T) \geq 4$, $N_3(T_1) = 1$, and $T \prec T_1$. The result now follows from Subcase 2.1.

□

The following Lemma 3.3 further asserts that the tree $T_n(2,2|2,2)$ mentioned in Lemma 3.2 could not be the third maximal energy tree. (the original proof for the third maximal energy tree will be complete if this $T_n(2,2|2,2)$ is excluded.)

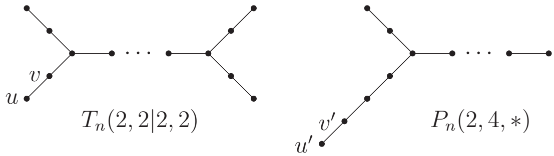

Fig. 5. $T = T_n(2,2|2,2)$ and $T' = P_n(2,4,*)$

Lemma 3.3. *If $n \geq 10$, then $T_n(2,2|2,2) \prec P_n(2,4,*)$*

Proof. Let $T = T_n(2,2|2,2)$ and $T' = P_n(2,4,*)$. Let u (respectively u') be the pendent vertex on a pendent path of length 2 (respectively length 4) in T (respectively T'), and v (respectively v') be the vertex incident with u (respectively u') (see Figure 5). Then by using the grafting operations several times we have

$$T - u = T_n(2,2|2,2) - u = T_{n-1}(1,2|2,2) \prec P_{n-1}(1,2,n-5)$$

$$\prec P_{n-1}(2,3,n-7) = P_n(2,4,*) - u' = T' - u'.$$

$$T - u - v = T_n(2,2|2,2) - u - v = P_{n-2}(2,2,*) = P_n(2,4,*) - u' - v' = T' - u' - v'.$$

Therefore the result $T \prec T'$ follows immediately from Lemma 1.1 □

Combining the above Lemmas 2.1, 3.2 and 3.3, we can immediately obtain the following two theorems about the third and fourth maximal energy trees.

Theorem 3.1. *If $n \geq 10$, then the third maximal energy tree of order n is $P_n(2,4,n-7)$.*

Theorem 3.2. *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 $T_n(2,2|2,2)$.*

Proof. Since $n \geq 14$, the trees $P_n(2,2,x)$, $P_n(2,4,y)$ and $P_n(2,6,z)$ are mutually distinct. Thus the result follows directly from Lemma 3.2 and Theorem 3.1.

□

Remark 3.1. For $n \geq 19$, the two trees $P_n(2,6,n-9)$ and $T_n(2,2|2,2)$ are quasi-order incomparable. This can be verified by the following computations.

$$m(T_n(2,2|2,2),2) - m(P_n(2,6,n-9),2) = -1$$

$$m(T_n(2,2|2,2),[n/2]-1) - m(P_n(2,6,n-9),[n/2]-1) = \begin{cases} 1 & \text{if } n \text{ is even;} \\ \frac{n-17}{2} & \text{if } n \text{ is odd.} \end{cases}$$

It seems to be difficult to prove which one of the two trees $P_n(2,6,n-9)$ and $T_n(2,2|2,2)$ has the larger energy.

Finally, we point out that the Conjecture 1 for $n = 10, 11, 12, 13$ is true.

Theorem 3.3. *(1) For $n = 10$, the fourth maximal energy tree is $P_{10}(2,6,1)$;*

(2) For $n = 11$, the fourth maximal energy tree is $P_{11}(2,3,5)$;

(3) For $n = 12$, the fourth maximal energy tree is $P_{12}(2,6,3)$;

(4) For $n = 13$, the fourth maximal energy tree is $P_{13}(4,4,4)$;

Proof. (1) For $n = 10$. By using computer we find that

$$E(P_{10}(2,6,1)) \doteq 11.937, E(T_{10}(2,2|2,2)) \doteq 11.924, E(P_{10}(3,3,3)) \doteq 11.475.$$

So using Lemma 3.2 we obtain that the fourth maximal energy tree is $P_{10}(2,6,1)$.

(2) For $n = 11$. In this case the two trees $P_{11}(2,2,x)$ and $P_{11}(2,6,z)$ in Lemma 3.2 are the same. Firstly, by using computer we find that

$$E(P_{11}(2,3,5)) \doteq 13.069, \quad E(T_{11}(2,2|2,2)) \doteq 13.059, \quad E(P_{11}(2,2,2,4)) \doteq 13.020 \tag{3.1}$$

Let T be a tree of order 11 with $T \neq P_{11}, P_{11}(2,2,6), P_{11}(2,4,4)$ and $P_{11}(2,3,5)$. Then we can show that one of the following three relations hold

$$T \prec P_{11}(2,3,5), \quad \text{or} \quad T \preceq T_{11}(2,2|2,2), \quad \text{or} \quad T \preceq P_{11}(2,2,2,4) \tag{3.2}$$

by considering the cases (and subcases) similar to that in the proof of Lemma 3.2.

For subcase 1.1, $T = P_{11}(a,b,c)$. Then by the assumption at least one of (and thus two of) a, b, c is odd. Then it is easy to show that $T \prec P_{11}(2,3,5)$ by our grafting method;

For subcase 1.2, $T = T_{11}(a, b|c, d)$. Then either $T = T_{11}(2, 2|2, 2)$, or at least one of a, b, c, d is odd since $n = 11$. In the latter case we can easily show that $T \prec P_{11}(2, 3, 5)$ by using the grafting method and subcase 1.1;

For subcase 1.3, we can use Theorem 2.4 to show that $T \prec T_{11}(a, b|c, d)$ for some positive integers a, b, c, d, and then use subcase 1.2.

For subcases 2.1 and 2.2, we can either use Lemma 2.2 or use Theorem 2.4 to show that $T \preceq P_{11}(2, 2, 2, 4)$.

Combining (3.1) and (3.2), we obtain that the fourth maximal energy tree of order 11 is $P_{11}(2, 3, 5)$.

(3) For $n = 12$. By using computer we find that

$$E(P_{12}(2, 6, 3)) \doteq 14.500, \quad E(T_{12}(2, 2|2, 2)) \doteq 14.459.$$

So using Lemma 3.2 we obtain that the fourth maximal energy tree is $P_{12}(2, 6, 3)$.

(4) For $n = 13$. In this case the two trees $P_{13}(2, 4, y)$ and $P_{13}(2, 6, z)$ in Lemma 3.2 are the same. Firstly, by using computer we find that

$$\begin{aligned} &E(P_{13}(4, 4, 4)) \doteq 15.664, \quad E(P_{13}(2, 5, 5)) \doteq 15.639, \quad E(T_{13}(2, 2|2, 2)) \doteq 15.619, \\ &E(T_{13}(2, 2|2, 4)) \doteq 15.606, \quad E(P_{13}(2, 2, 2, 6)) \doteq 15.575. \end{aligned} \tag{3.3}$$

Let T be a tree of order 13 with $T \neq P_{13}, P_{13}(2, 2, 8), P_{13}(2, 4, 6)$ and $P_{13}(4, 4, 4)$. Then we can use the grafting method to show that one of the following five relations hold

$$\begin{aligned} &T \prec P_{13}(4, 4, 4), \quad T \preceq P_{13}(2, 5, 5), \quad T \preceq P_{13}(2, 2, 2, 6) \\ &T \preceq T_{13}(2, 2|2, 2), \quad T \preceq T_{13}(2, 2|2, 4) \end{aligned} \tag{3.4}$$

by considering the cases (and subcases) similar to that in the proof of Lemma 3.2.

For subcase 1.1, $T = P_{13}(a, b, c)$. Then by the assumption at least one of (and thus two of) a, b, c is odd. Then it is easy to show that $T \preceq P_{13}(2, 5, 5)$ by using our grafting method;

For subcase 1.2, $T = T_{13}(a, b|c, d)$. Then either $T = T_{13}(2, 2|2, 2)$, or $T = T_{13}(2, 2|2, 4)$, or at least one of a, b, c, d is odd since $n = 13$. In the latter case we can easily show that $T \prec P_{13}(2, 5, 5)$ by using the grafting method and subcase 1.1;

For subcase 1.3, we can use Theorem 2.4 to show that $T \prec T_{13}(a, b|c, d)$ for some positive integers a, b, c, d, and then use subcase 1.2.

For subcases 2.1 and 2.2, we can either use Lemma 2.2 or use Theorem 2.4 to show that $T \preceq P_{13}(2,2,2,6)$.

Combining (3.3) and (3.4), we obtain that the fourth maximal energy tree of order 13 is $P_{13}(4,4,4)$.

$\square$

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