

Ordering of Trees with a Given Bipartition by Their Energies and Hosoya Indices¹

Luzhen Ye

Department of Mathematics, Fuzhou University, Fuzhou , Fujian, P.R.China

Chen Rong Si²

College of Finance and Economics, Fuzhou University, Fuzhou, Fujian, P.R.China

(Received March 20, 2004)

Abstract

The energy of a graph G is defined as the sum of the absolute values of eigenvalues of G and the Hosoya index of a graph G is defined as the number of matchings of G . In this paper, for two given positive integers p and q ($q \geq p$) we characterize the trees with a given bipartition (p, q) which have the minimal and the second minimal energy of Hosoya index.

1. Introduction

Let T be a tree with n vertices and $V(T) = \{1, 2, \dots, n\}$ the set of vertices of T . The adjacency matrix $A(T)$ of T is the square matrix $A(T) = (a_{ij})$ of order n , where $a_{ij} = 1$ if vertices i and j are adjacent, and 0 otherwise. The characteristic polynomial of T ,

¹This work is supported by NSFC (10371102).

²Corresponding author, E-mail address: chenrongsi@fzu.edu.cn

denoted by $\phi(T)$, is defined as $\phi(T) = \det(xI - A(T))$, where I is the identity matrix of order n . It is well known [2] that for a tree T with n vertices

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

where $m(T, k)$ equals the number of k -matchings of T . The Hosoya index [5] of a graph G with n vertices, denoted by $Z(G)$, is defined as $Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G, k)$.

Chemists know that the experimental heats of formation of conjugated hydrocarbons are closely related to the total π -electron energy. The calculation of the total π -electron energy in a conjugated hydrocarbon can be reduced (within the framework of the HMO approximation) [5] to

$$E(T) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|,$$

where λ_i 's are the eigenvalues of the corresponding graph T . For a tree (acyclic graph) with n vertices, this energy is also expressible in terms of the Coulson integral [4,5] as

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

The fact that $E(T)$ is a strictly monotonously increasing function of all matching numbers $m(T, k)$, $k = 0, 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$, provides us a way of comparing the energies of a pair of trees. Gutman [4] introduced a quasi-ordering relation " \succeq " (i.e. reflexive and transitive relation) on the set of all forests (acyclic graphs) with n vertices: if T_1 and T_2 are two forests with n vertices and with characteristic polynomials in the form (1), then

$$T_1 \succeq T_2 \Leftrightarrow m(T_1, k) \geq m(T_2, k) \text{ for all } k = 0, 1, \dots, \lfloor \frac{n}{2} \rfloor.$$

If $T_1 \succeq T_2$ and there exists an integer j such that $m(T_1, j) > m(T_2, j)$, then we write $T_1 \succ T_2$.

Here, by (2) and the definition of Hosoya index, we have

$$T_1 \succeq T_2 \implies E(T_1) \geq E(T_2), \quad Z(T_1) \geq Z(T_2); \quad (3)$$

$$T_1 \succ T_2 \implies E(T_1) > E(T_2), \quad Z(T_1) > Z(T_2). \quad (4)$$

This increasing property of E has been successfully applied in the study of the extremal values of energy in different classes of graphs (see [3,4,6-15]). Gutman [4] determined the tree with the maximal energy, namely, the path. Furthermore, he got

$$\begin{cases} T \succ W_n \succ Z_n \succ Y_n \succ X_n, \\ E(T) > E(W_n) > E(Z_n) > E(Y_n) > E(X_n) \end{cases} \quad (5)$$

for any tree $T \neq X_n, Y_n, Z_n, W_n$ with n vertices, where X_n is the star $K_{1,n-1}$, Y_n is the graph obtained by attaching a pendent edge to a pendent vertex of $K_{1,n-2}$, Z_n is obtained by attaching two pendent edges to a pendent vertex of $K_{1,n-3}$, W_n is obtained by attaching

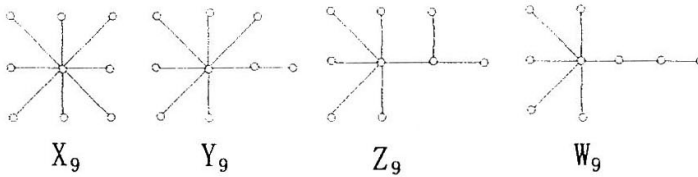


Fig. 1 The trees X_9 , Y_9 , Z_9 and W_9 .

a P_3 (here P_m denotes the path with m vertices) to a pendent vertex of $K_{1,n-3}$ (Fig. 1 shows the trees X_9, Y_9, Z_9 and W_9). Zhang et al [13] characterized the trees with perfect matching having the minimal and the second minimal energies, which solved the conjectures proposed by Gutman [3], that is, they proved that $E(F_n) < E(B_n) < E(T)$ for any tree $T \neq F_n, B_n$ with n vertices having perfect matching, where F_n is the tree with n vertices obtained by adding a pendent edge to each vertex of the star $K_{1,\frac{n}{2}-1}$ (see Fig. 2), and B_n is the tree obtained from F_{n-2} by attaching a P_2 to the 2-degree vertex of a pendent edge (see Fig. 2). On the other hand, for a given positive integer d , Yan et al [12] characterized the tree with the minimal energy having diameter at least d . They proved that if T is a tree with n vertices having diameter at least d , then $E(T) \geq E(B_{n,d})$ with

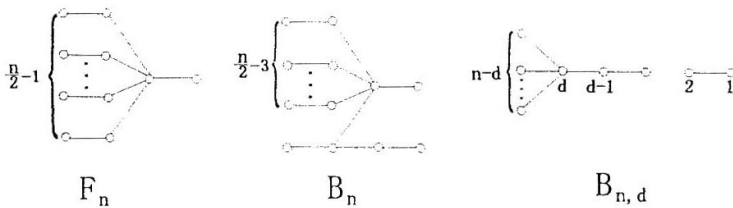


Fig.2 The trees F_n , B_n and $B_{n,d}$.

equality if and only if $T = B_{n,d}$, where $B_{n,d}$ is the tree with n vertices obtained from the path P_d by attaching $n - d$ pendent edges to an end vertex u of P_d (see Fig. 2).

In order to formulate our results, we need to introduce some notation in the following.

Let G be a connected bipartite graph with n vertices. Hence its vertex set can be uniquely partitioned into two subsets V_1 and V_2 such that each edge joins a vertex in V_1 with a vertex in V_2 . Suppose that V_1 has p vertices and V_2 has q vertices, where $p + q = n$. Then we say that G has a (p, q) -bipartition. Consider a star with $p + 1$ vertices. Attach $q - 1$

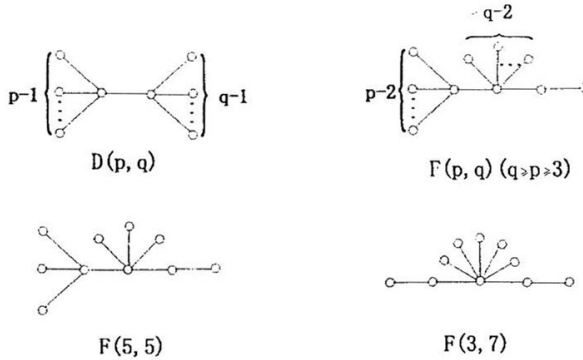


Fig.3 The trees $D_{p,q}$ and $F_{p,q}$.

pendent edges to a non-central vertex of the star. The resulting tree with $p + q$ vertices has a (p, q) -bipartition. Denote the resulting tree by $D(p, q)$ (see Fig. 3). We call $D(p, q)$ a double-star (see Brualdi et al [1]). If $q \geq p \geq 3$, we suppose that $F(p, q)$ is the tree obtained from $D(p - 1, q)$ by attaching a pendent edge to one of the vertices of degree one which join the vertex of degree q in $D(p - 1, q)$ (see Fig. 3). If $q \geq p = 2$, we suppose that $F(2, q)$ is the tree obtained from the path P_4 by attaching $q - 2$ pendent edges to an end vertex of P_4 (see Fig. 4).

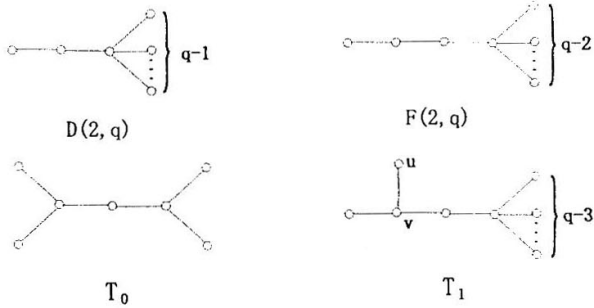


Fig.4 The trees $D(2, q)$, $F(2, q)$, T_0 and T_1 .

Now we are in the position to formulate our main results.

Theorem 1.1 Let T be a tree with a (p, q) -bipartition ($p, q \geq 1, p + q \geq 3$). Then

$$(1) \quad E(T) \geq \sqrt{2(p+q-1) + 2\sqrt{(p+q-1)^2 - 4(p-1)(q-1)}} + \sqrt{2(p+q-1) - 2\sqrt{(p+q-1)^2 - 4(p-1)(q-1)}};$$

$$(2) \quad Z(T) \geq pq + 1$$

with all equalities if and only if T is the double-star $D(p, q)$.

Theorem 1.2 Let p and q be two positive integers such that $q \geq p \geq 2$, and let T be a tree with a (p, q) -bipartition such that $T \neq D(p, q)$. Then

$$E(T) \geq E(F(p, q)) \quad \text{and} \quad Z(T) \geq Z(F(p, q)) = 2pq - p - 2q + 3$$

with all equalities if and only if $T = F(p, q)$.

2. Lemmas

Let G be a graph and uv an edge of G . We denote by $G - uv$ (resp. $G - u$) the graph obtained from G by deleting the edge uv (resp. the vertex u and the edges adjacent to u).

Lemma 2.1[2] Let T be a tree with a pendent vertex u , and let v be the unique vertex of T adjacent to u . Then

$$\phi(T) = x\phi(T - u) - \phi(T - u - v).$$

Lemma 2.2[14,15] Let T_1 and T_2 be two acyclic graphs with n vertices and with characteristic polynomials

$$\phi(T_1) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_i x^{n-2i} \quad \text{and} \quad \phi(T_2) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b'_i x^{n-2i}$$

respectively. Then $T_1 \succeq T_2$ if and only if $b_0 - b'_0 = 0$ and $(-1)^i(b_i - b'_i) \geq 0$ for $i = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$; and $T_1 \succ T_2$ if and only if $T_1 \succeq T_2$ and there exists an integer $j \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor\}$ such that $(-1)^j(b_j - b'_j) > 0$.

Corollary 2.3 Let T and T' be two n -trees. Suppose that uv (resp. $u'v'$) is a pendent edge of T (resp. T') and u (resp. u') is a pendent vertex of T (resp. T'). Let $T_1 = T - u$, $T_2 = T - u - v$, $T'_1 = T' - u'$ and $T'_2 = T' - u' - v'$. If $T_1 \succeq T'_1$ and $T_2 \succ T'_2$; or $T_1 \succ T'_1$ and $T_2 \succeq T'_2$, then $T \succ T'$.

Proof By Lemma 2.1, we have

$$\phi(T) = x\phi(T_1) - \phi(T_2) \quad \text{and} \quad \phi(T') = x\phi(T'_1) - \phi(T'_2).$$

Hence

$$\phi(T) - \phi(T') = x(\phi(T_1) - \phi(T'_1)) - (\phi(T_2) - \phi(T'_2)).$$

Suppose that

$$x(\phi(T_1) - \phi(T'_1)) = \sum_{i \geq 0} a_i x^{n-2i} \quad \text{and} \quad \phi(T_2) - \phi(T'_2) = \sum_{i \geq 0} b_i x^{n-2i}.$$

Then if $T_1 \succ T'_1$ and $T_2 \succeq T'_2$, we have $a_0 = b_0 = 0$ and $(-1)^i a_i \geq 0$ and $(-1)^i b_i \geq 0$ for $i \geq 1$ and there exists at least a k such that $(-1)^k a_k > 0$. Hence, $(-1)^i(a_i - b_{i-1}) \geq 0$ for $i \geq 1$ and there exists at least a k such that $(-1)^k(a_k - b_{k-1}) > 0$. Note that

$$\phi(T) - \phi(T') = \sum_{i \geq 1} (a_i - b_{i-1}) x^{n-2i}.$$

Hence, by Lemma 2.2 we have $T \succ T'$. Similarly, if $T_1 \succeq T'_1$ and $T_2 \succ T'_2$ then $T \succ T'$. The corollary thus holds.

Lemma 2.4[2] Let $e = uv$ be an edge of graph G with n vertices. Then the number $m(G, i)$ of i -matchings of G is determined by:

$$m(G, i) = m(G - uv, i) + m(G - u - v, i - 1) \quad \text{for } i = 1, 2, \dots, \left\lfloor \frac{n}{2} \right\rfloor,$$

where $m(T, 0) = 1$.

By the above lemma, the following lemma is obvious.

Lemma 2.5 Let T be an acyclic graph with n vertices ($n > 1$) and T' a spanning subgraph (resp. a proper spanning subgraph) of T . Then $T \succeq T'$ (resp. $T \succ T'$).

Lemma 2.6 For a double-star $D(p, q)$, we have

$$(1) \quad \phi(D(p, q)) = x^{p+q-4}[x^4 - (p+q-1)x^2 + (p-1)(q-1)];$$

$$(2) \quad E(D(p, q)) = \sqrt{2(p+q-1) + 2\sqrt{(p+q-1)^2 - 4(p-1)(q-1)}} + \\ \sqrt{2(p+q-1) - 2\sqrt{(p+q-1)^2 - 4(p-1)(q-1)}};$$

$$(3) \quad Z(D(p, q)) = pq + 1.$$

Proof Let $D(p, q) = T$. It is easy to see that $m(T, 0) = 1$, $m(T, 1) = p + q - 1$, $m(T, 2) = (p-1)(q-1)$ and $m(T, i) = 0$ for $i = 3, 4, \dots, \left\lfloor \frac{p+q}{2} \right\rfloor$. Hence it is not difficult to see that the assertions (1)–(3) hold.

Similarly, we can obtain the following.

Lemma 2.7 Let $F(p, q)$ be the tree defined as above and $q \geq p \geq 2$. Then

$$(1) \quad \phi(F(p, q)) = x^{p+q} - (p+q-1)x^{p+q-2} + (pq - q - 1)x^{p+q-4} - (p-2)(q-2)x^{p+q-6};$$

$$(2) \quad Z(F(p, q)) = 2pq - p - 2q + 3.$$

Lemma 2.8 Suppose that T is a tree with a $(2, c)$ -bipartition such that $T \neq D(2, q)$ and $T \neq F(2, q)$. Then $T \succ F(2, q)$.

Proof Note that, if $q = 2$, then there exists only one tree with a $(2, 2)$ -bipartition. If $q = 3$ then there exist exactly two trees $D(2, 3)$ and $F(2, 3) (= P_3)$ which have a $(2, 3)$ -bipartition. If $q = 4$ then there exist exactly two trees $D(2, 4)$ and $F(2, 4)$ which have a $(2, 4)$ -bipartition. Hence we may assume that $q \geq 5$. We proceed by induction on q . If $q = 5$ then there are exactly three trees $D(2, 5)$, $F(2, 5)$ and T_0 shown in Fig. 4, each of which has a $(2, 5)$ -bipartition. It is not difficult to see that $T_0 \succ F(2, 5) \succ D(2, 5)$. The lemma thus holds if $q \leq 5$. We assume inductively that the lemma holds if $|V_2| < q$. Now we assume that T is a tree with n vertices, which has a $(2, q)$ -bipartition, such that $T \neq D(p, q)$ and $T \neq F(2, q)$ ($q \geq 6$). Let V_1 and V_2 be the bipartition of vertex set of T with $|V_1| = 2$ and $|V_2| = q$. Let $T' = T - u$ and $T'' = T - u - v$. Then T' is a tree with $2 + q - 1 = q + 1$ vertices and T'' is a forest with q vertices. If $u \in V_1$, then T' is a tree with a $(1, q)$ -bipartition. This shows that $T = D(2, q)$, a contradiction. Hence $u \in V_2$ and T' is a tree with a $(2, q - 1)$ -bipartition. It is not difficult to see that $T' \neq D(2, q - 1)$ (otherwise T must be $D(2, q)$ or $F(2, q)$, also a contradiction). Note that, by Lemma 2.1,

$$\phi(T) = x\phi(T') - \phi(T''), \quad \phi(F(2, q)) = x\phi(F(2, q - 1)) - \phi((q - 3)P_1 \cup P_3).$$

We distinguish the following two cases.

Case 1 If $T' = F(2, q - 1)$, then T must be the tree T_1 shown in Fig. 4 since $T \neq D(2, q)$ and $T \neq F(2, q)$. Note that

$$\phi(T_1) = x^{q+2} - (q + 1)x^q + (3q - 7)x^{q-2},$$

and

$$\phi(F(2, q)) = x^{q+2} - (q + 1)x^q + (2q - 3)x^{q-2}.$$

It is obvious that if $q \geq 6$, then $T_1 \succ F(2, q)$.

Case 2 If $T' \neq D(2, q)$ and $T' \neq F(2, q)$, then by induction assumption we have

$$T' \succ F(2, q - 1). \quad (6)$$

Note that $u \in V_2$. Hence $v \in V_1$. Since $T' \neq D(2, q)$ and $T' \neq F(2, q)$, the degree $d_T(v)$ of vertex v in T is not larger than $q - 1$, that is, $d_T(v) \leq q - 1$. Hence T'' is a forest with q vertices having at least $q + 1 - (q - 1) = 2$ edges. Hence we have

$$T'' \succeq (q - 3)P_1 \cup P_3. \quad (7)$$

Hence, by Corollary 2.3, we have $T \succ F(2, q)$. The lemma thus follows.

Lemma 2.9 Suppose that T is a tree with a $(3, 3)$ -bipartition such that $T \neq D(3, 3)$ and $T \neq F(3, 3)$. Then $T \succ F(3, 3)$.

Proof Note that there exist exactly three trees $D(3, 3)$, $F(3, 3)$ and P_6 , each of which has a $(3, 3)$ -bipartition. It is not difficult to prove that $P_6 \succ F(3, 3) \succ D(3, 3)$. The lemma thus follows.

Lemma 2.10 Suppose that T is a tree with a $(3, 4)$ -bipartition such that $T \neq D(3, 4)$ and $T \neq F(3, 4)$. Then $T \succ F(3, 4)$.

Proof Since $T \neq D(3, 4)$ and $T \neq F(3, 4)$, T must be the one of the five trees T_i 's ($i = 2, 3, 4, 5, 6$) shown in Fig. 5. Note that

$$\phi(T_2) = x^7 - 6x^5 + 8x^3 - 2x, \quad \phi(T_3) = x^7 - 6x^5 + 9x^3 - 2x;$$

$$\phi(T_4) = x^7 - 6x^5 + 9x^3 - 3x, \quad \phi(T_5) = x^7 - 6x^5 + 9x^3 - 4x;$$

$$\phi(T_6) = x^7 - 6x^5 + 10x^3 - 4x, \quad \phi(F(3, 4)) = x^7 - 6x^5 + 7x^3 - 2x.$$

It is obvious that $T_i \succ F(3, 4)$ for $i = 2, 3, 4, 5, 6$. The lemma thus holds.

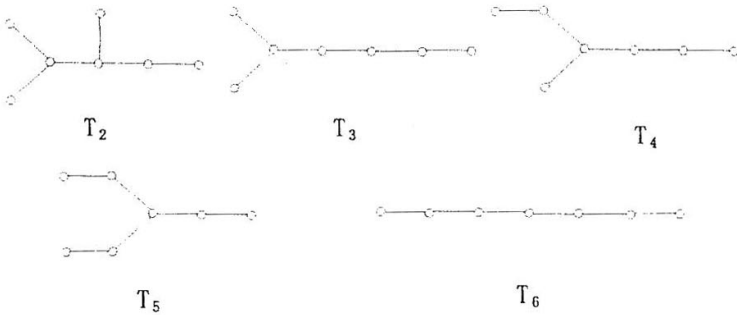


Fig.5 The trees T_2, T_3, T_4, T_5 and T_6 .

3. The proof of main results

The proof of Theorem 1.1. By Lemma 2.5 and (3) and (4), it suffices to prove that $T \succeq D(p, q)$ with equality if and only if T is the double-star $D(p, q)$. If $p = 1$, then $T = D(1, q)$ and the theorem holds. The theorem also holds when $q = 1$. Hence we may now assume that $p \geq 2$ and $q \geq 2$. We proceed by induction on $n = p + q$. If $p = q = 2$, that is $p + q = 4$, there exists only one tree $P_4 = D(2, 2)$ which has a $(2, 2)$ -bipartition. Hence the theorem holds if $p + q = 4$. We assume inductively that the theorem holds if the number of vertices of a tree T^* is less than $p + q$. Let V_1 and V_2 be the bipartition of vertex set of T with $|V_1| = p$ and $|V_2| = q$. Let u be a pendent vertex and uv a pendent edge in T , where we may assume that $u \in V_1$ and $v \in V_2$. Let $T' = T - u$ and $T'' = T - u - v$. Then T' is a tree with a $(p - 1, q)$ -bipartition and T'' a forest with $p + q - 2$ vertices. By Lemma 2.1, we have

$$\phi(D(p, q)) = x\phi(D(p - 1, q)) - \phi((p - 2)P_1 \cup K_{1, q-1}),$$

and

$$\phi(T) = x\phi(T') - \phi(T'').$$

Hence, by Corollary 2.3, it suffices to prove that $T' \succeq D(p - 1, q)$ and $T'' \succ (p - 2)P_1 \cup K_{1, q-1}$; or $T' \succ D(p - 1, q)$ and $T'' \succeq (p - 2)P_1 \cup K_{1, q-1}$.

We denote the degree of v in T by $d_T(v)$. Since $v \in V_2$ and T has a (p, q) -bipartition, $d_T(v) \leq p$. Hence T'' is a forest with at least $p + q - 1 - p = q - 1$ edges. This shows that $m(T'', 1) \geq q - 1$. Hence $T'' \succeq (p - 2)P_1 \cup K_{1, q-1}$ with the equality if and only if $T'' = (p - 2)P_1 \cup K_{1, q-1}$. It is not difficult to see that $T'' = (p - 2)P_1 \cup K_{1, q-1}$ if and only if $T = D(p, q)$. Hence if $T \neq D(p, q)$, then $T'' \succ (p - 2)P_1 \cup K_{1, q-1}$. On the other hand, since T' is a tree with a $(p - 1, q)$ -bipartition with $p + q - 1$ ($< p + q$) vertices, by induction assumption, we have $T' \succeq D(p - 1, q)$. Hence, by Corollary 2.3, $T \succ D(p, q)$ if $T \neq D(p, q)$. The theorem is thus proved.

Proof of Theorem 1.2. By (3), (4) and Theorem 1.1, it suffices to prove that if T is a tree with a (p, q) -bipartition ($q \geq p \geq 2$) such that $T \neq D(p, q)$ and $T \neq F(p, q)$, then $T \succ F(p, q)$.

By Lemma 2.8, $T \succ F(2, q)$ if $p = 2$. Hence we may assume that $q \geq p \geq 3$ and proceed by induction on $p + q$.

If $p + q = 6$ or 7 , then $p = q = 3$ or $p = 3$ and $q = 4$. Hence the theorem is immediate from Lemma 2.9 and Lemma 2.10 if $p + q = 6$ or 7 .

We now suppose that $p + q \geq 8$ and $q \geq p \geq 3$. We assume inductively that the result holds if the number of vertices of a tree T^* is less than $p + q$. Let u be a pendent vertex of T and uv a pendent edge of T . Let $T' = T - u$ and $T'' = T - u - v$. Then T' is a tree with $p + q - 1$ vertices and T'' is a forest with $p + q - 2$ vertices. We distinguish the following two cases.

Case 1 If $u \in V_1$, then T' is a tree with a $(p - 1, q)$ -bipartition. It is obvious that $T' \neq D(p - 1, q)$ (otherwise T must be $D(p, q)$ or $F(p, q)$, a contradiction). By Lemma 2.1, we have

$$\begin{aligned}\phi(T) &= x\phi(T') - \phi(T''), \\ \phi(F(p, q)) &= x\phi(F(p - 1, q)) - \phi((p - 3)P_1 \cup D(2, q - 1)).\end{aligned}$$

We distinguish the following two subcases.

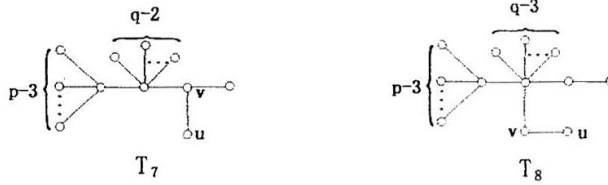


Fig.6 The trees T_7 and T_8 .

Subcase 1 If $T' = F(p - 1, q)$, then T must be one of the trees T_7 and T_8 depicted in Fig.6 since $T \neq D(p, q)$ and $T \neq F(p, q)$. It is not difficult to find that

$$\begin{aligned}\phi(T_7) &= x^{p+q} - (p + q - 1)x^{p+q-2} + (pq + p - q - 5)x^{p+q-4} - 2(p - 3)(q - 2)x^{p+q-6}, \\ \phi(T_8) &= x^{p+q} - (p + q - 1)x^{p+q-2} + (pq + p - q - 4)x^{p+q-4} - \\ &\quad (2pq - 3p - 5q + 7)x^{p+q-6} + (p - 3)(q - 3)x^{p+q-8}, \\ \phi(F(p, q)) &= x^{p+q} - (p + q - 1)x^{p+q-2} + (pq - q - 1)x^{p+q-4} - (p - 2)(q - 2)x^{p+q-6}.\end{aligned}$$

It is obvious that $T_7 \succ F(p, q)$ and $T_8 \succ F(p, q)$. Hence $T \succ F(p, q)$ if $T' = F(p - 1, q)$.

Subcase 2 If $T' \neq F(p-1, q)$, then the degree $d_T(v)$ of vertex v in T is not larger than p since T has a (p, q) -bipartition. Hence $d_T(v) = p$ or $d_T(v) \leq p-1$.

First, we suppose that $d_T(v) \leq p-1$. Then $T'' = T - u - v$ has at least $p+q-1-(p-1) = q$ edges, that is, T'' is a forest with $p+q-2$ vertices having at least q edges. We now prove the following:

claim 1

$$T'' \succeq (p-3)P_1 \cup D(2, q-1). \quad (8)$$

In fact, $m(T'', 0) = 1$ and $m(T'', 1) \geq q$. Hence, in order to prove the claim we need to show that $m(T'', 2) \geq m((p-3)P_1 \cup D(2, q-1), 2) = q-2$. If T'' has a unique connected component which is not an isolated vertex, denoted by T''_1 , then $T''_1 \neq K_{1,j}$ for $j \in \{q, q+1, \dots, p+q-3\}$ since T has a (p, q) -bipartition and $T'' = T - u - v$. Hence T''_1 is a tree with at least q edges which is not a star. By (5) we have $m(T'', 2) = m(T''_1, 2) \geq m(Y_{q+1}, 2) = q-2$, where Y_{q+1} is the tree obtained by attaching an edge to a pendent vertex of $K_{1,q-1}$. If there exist at least s ($s > 1$) connected components in T'' each of which is not an isolated vertex, denoted by $T''_1, T''_2, \dots, T''_s$, then $\sum_{i=1}^s e_i \geq q$ and $e_i \geq 1$, where e_i denotes the number of edges in T''_i for $i = 1, 2, \dots, s$. Hence it is not difficult to see that $m(T'', 2) \geq q-2$. The claim thus follows.

Note that T' is a tree with $p+q-1$ vertices and with a $(p-1, q)$ -bipartition such that $T' \neq D(p-1, q)$ and $T' \neq F(p-1, q)$. Then, by induction assumption, we have

$$T' \succ F(p-1, q). \quad (9)$$

By (8), (9) and Corollary 2.3, we have $T \succ F(p, q)$.

Now we assume that $d_T(v) = p$. Since T has a (p, q) -bipartition and $T \neq D(p, q)$, $T \neq F(p, q)$; T is obtained from the star $K_{1,p}$ by attaching some pendent edges to each pendent vertex of $K_{1,p}$. Without loss of generality, we may assume that the pendent vertices of $K_{1,p}$ are $u, v_1, v_2, \dots, v_{p-1}$ and T is obtained from $K_{1,p}$ by attaching s_i pendent edges to the pendent vertex v_i of $K_{1,p}$ for $i = 1, 2, \dots, p'$ ($p' \leq p-1$), where $s_i > 0$. Note that $T \neq D(p, q)$. Then $p' > 1$. It is obvious that $\sum_{i=1}^{p'} s_i = p+q-1-p = q-1$. Note that if s_1 and s_2 are two positive integers, then $s_1 s_2 \geq s_1 + s_2 - 1$. Hence $\sum_{1 \leq i < j \leq p'} s_i s_j \geq$

$s_1 + s_2 - 1 + s_3 + \cdots + s_{p'} = q - 2$. It is not difficult to show that

$$\begin{aligned}
 m(T, 2) &= (p-1) \sum_{i=1}^{p'} s_i + \sum_{1 \leq i < j \leq p'} s_i s_j = (p-1)(q-1) + \sum_{1 \leq i < j \leq p'} s_i s_j \\
 &\geq (p-1)(q-1) + (q-2) = pq - p - 1; \\
 m(T, 3) &\geq (p-p') \sum_{1 \leq l < m \leq p'} s_l s_m + (p'-2) \sum_{1 \leq l < m \leq p'} s_l s_m \\
 &= (p-2) \sum_{1 \leq l < m \leq p'} s_l s_m \geq (p-2)(q-2).
 \end{aligned}$$

Note that $\sum_{1 \leq i < j \leq p'} s_i s_j = s_1 + s_2 - 1 + s_3 + \cdots + s_{p'} = q - 2$ if and only if $p' = 2$ (without loss of generality, we may assume that $s_1 \neq 0$ and $s_2 \neq 0$) and $s_1 = 1, s_2 = q - 2$; or $p' = 2$ and $s_1 = q - 1, s_2 = 1$. Hence if $p = q$, then since $T \neq F(p, q)$ we have

$$m(T, 3) \geq (p-2) \sum_{1 \leq l < m \leq p'-1} s_l s_m > (p-2)(q-2).$$

Note that

$$\phi(F(p, q)) = x^{p+q} - (p+q-1)x^{p+q-2} + (pq-q-1)x^{p+q-4} - (p-2)(q-2)x^{p+q-6}.$$

Hence if $q \geq p \geq 3$, we have $T \succ F(p, q)$.

Case 2 If $u \in V_2$, then T' is a tree with a $(p, q-1)$ -bipartition. If $p = q$, we may assume that $p' = q$ and $q' = p$. Then T is a tree with a (p', q') -bipartition and T' is a tree with $(p'-1, q')$ -bipartition ($p'-1 < q'$). By a similar reasoning as that in the proof of case 1, we can prove that $T \succ F(p, q)$. When $q > p$, then T' is a tree with a $(p, q-1)$ -bipartition and $p \leq q-1$. We distinguish the following three subcases.

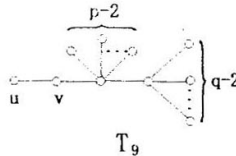


Fig.7 The tree T_9 .

Subcase 1 If $T' = D(p, q-1)$, then T must be the tree T_9 shown in Fig.7 since $T \neq D(p, q)$ and $T \neq F(p, q)$. Note that

$$\phi(T_9) = x^{p+q} - (p+q-1)x^{p+q-2} + (pq-p-1)x^{p+q-4} - (p-2)(q-2)x^{p+q-6} \quad \text{and}$$

$$\phi(F(p, q)) = x^{p+q} - (p+q-1)x^{p+q-2} + (pq-q-1)x^{p+q-4} - (p-2)(q-2)x^{p+q-6}.$$

It is obvious that $T_9 \succ F(p, q)$ when $q > p \geq 3$.

Subcase 2 If $T' = F(p, q-1)$, then T must be one of the trees T_{10} and T_{11} depicted in Fig.8 since $T \neq D(p, q)$ and $T \neq F(p, q)$.

Bear in mind the following equations:

$$\phi(T_{10}) = x\phi(F(p, q-1)) - \phi(D(p-1, q-1));$$

$$\phi(T_{11}) = x\phi(F(p, q-1)) - \phi(F(p-1, q-1));$$

$$\phi(F(p, q)) = x\phi(F(p, q-1)) - \phi((q-3)K_1 \cup P_2 \cup K_{1,p-2});$$

$$\phi(D(p-1, q-1)) = x^{p+q-2} - (p+q-3)x^{p+q-4} + (p-2)(q-2)x^{p+q-6};$$

$$\phi(F(p-1, q-1)) = x^{p+q-2} - (p+q-3)x^{p+q-4} + (pq-p-2q+1)x^{p+q-6} + (p-3)(q-3)x^{p+q-8};$$

$$\phi((q-3)P_1 \cup P_2 \cup K_{1,p-2}) = x^{p+q-2} - (p-1)x^{p+q-4} + (p-2)x^{p+q-6}$$

It is obvious that if $q > p \geq 3$, we have

$$D(p-1, q-1) \succ (q-3)P_1 \cup P_2 \cup K_{1,p-2} \quad \text{and} \quad F(p-1, q-1) \succ (q-3)P_1 \cup P_2 \cup K_{1,p-2}.$$

By Corollary 2.3, we have

$$T_{10} \succ F(p, q), \quad \text{and} \quad T_{11} \succ F(p, q).$$

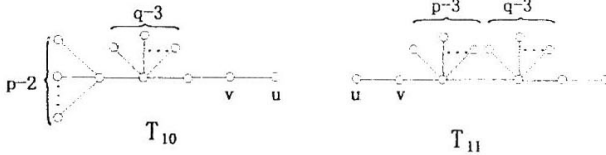


Fig.8 The trees T_{10} and T_{11} .

Subcase 3 If $T' \neq D(p, q-1)$ and $T' \neq F(p, q-1)$, then by induction assumption we have

$$T' \succ F(p, q-1). \quad (10)$$

Note that the degree $d_T(v)$ of v in T is not larger than q since T has a (p, q) -bipartition and $T \neq D(p, q)$, $T \neq F(p, q)$, that is, $d_T(v) = q$ or $d_T(v) \leq q-1$.

First we suppose that $d_T(v) \leq q-1$. Hence T'' is a forest with a $(p-1, q-1)$ -bipartition having at least $p+q-1-(q-1) = p$ edges. By a similar reasoning as that in the proof of Claim 1, we can prove that

$$T'' \succeq (q-3)P_1 \cup P_2 \cup K_{1,p-2}. \quad (11)$$

Note that

$$\phi(T) - \phi(F(p, q)) = x[\phi(T') - \phi(F(p, q-1))] - [\phi(T'') - \phi((q-3)P_1 \cup P_2 \cup K_{1,p-2})].$$

Hence by (10) and (11), we have $T \succ F(p, q)$.

Now we assume that $d_T(v) = q$. By a similar reasoning as that in the proof of Subcase 2, we can prove that $T \succ F(p, q)$.

The theorem has thus been proved.

References

- [1] E.A. Brualdi, J.L. Goldwasser. Permanent of the Laplacian matrix of trees and bipartite graphs, *Discrete Math.*, 48(1984), 1-21.
- [2] D.M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs*, Academic Press, New York, 1980.
- [3] I. Gutman, Acyclic conjugated molecules, trees and their energies, *J. Math. Chem.*, 1(1987), 123-143.
- [4] I. Gutman, Acyclic systems with extremal Hückel π -electron energy, *Theoret. Chim. Acta (Berlin)*, 45(1977), 79-87.
- [5] I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
- [6] I. Gutman, Y. Hou, Bipartite unicyclic graphs with greatest energy, *MATCH Commun. Math. Comput. Chem.*, 43(2001), 17-28.

- [7] Y. Hou, Unicyclic graphs with minimal energy, *J. Math. Chem.*, 29(2001), 163-168.
- [8] Y. Hou, Bicyclic graphs with minimal energy, *Linear Multilinear Algebra*, 49(2002), 347-354.
- [9] Y. Hou, I. Gutman, C.-W. Wou, Unicyclic graphs with maximal energy, *Linear Algebra Appl.*, 356(2002), 27-36.
- [10] H. Li, On minimal energy ordering of acyclic conjugated molecules, *J. Math. Chem.*, 25(1999), 145-169.
- [11] J. Rada, A. Tineo, Polygonal chains with minimal energy, *Linear Algebra Appl.*, 372(2003), 333-344.
- [12] W.G. Yan, Y.N. Ye, On the minimal energy of trees with a given diameter, submitted.
- [13] F. Zhang, H. Li, On acyclic conjugated molecules with minimal energies, *Discrete Appl. Math.*, 92(1999), 71-84.
- [14] F. Zhang, Z. Li, L. Wang, Hexagonal chains with minimal total π -energy, *Chem. Phys. Lett.*, 337(2001), 125-130.
- [15] F. Zhang, Z. Li, L. Wang, Hexagonal chains with maximal total π -energy, *Chem. Phys. Lett.*, 337(2001), 131-137.