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On the minimal energy of trees with a given number of pendent vertices[1]

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Abstract

The energy $E(G)$ 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. Let $\mathcal{T}_{n,p}$ be the set of trees of order $n \geq p+1 \geq 3$ with at most p pendent vertices. We characterize the tree with the minimal energy or Hosoya index in $\mathcal{T}_{n,p}$.

1 Introduction

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

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defined as $\phi(T,x) = det(xI - A(T))$, where I is the identity matrix of order n. It is well known [3] that if T is a tree with n vertices then

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

where $m(T,k)$ equals the number of matchings with k edges in T, and $\lfloor \frac{n}{2} \rfloor$ denotes the largest integer not greater than $\frac{n}{2}$.

Gutman [4, 6] defined the energy of a graph G with n vertices, denoted by $E(G)$, as

$$E(G) = \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} |\lambda_i(G)|,$$

where $\lambda_i(G)$ are the eigenvalues of the adjacency matrix of G, and $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G)$. The Hosoya index of a graph G with n vertices, denoted by $Z(G)$, is defined as

$$Z(G) = \sum_{r=0}^{\lfloor \frac{n}{2} \rfloor} m(G,r),$$

where $m(G,r)$ denotes the number of matchings with r edges in G.

Historically chemists used the model in which the experimental heats of formation of conjugated hydrocarbons are closely related to the total $\pi-$electron energy. Today such a model is over simplistic, but nevertheless HMO has some value as it points to that part of the experimental heats of formation of conjugated hydrocarbons that can be viewed as due to molecular connectivity (molecular topology). The calculation of the total π-electron energy in a conjugated hydrocarbon can be reduced (within the framework of the HMO approximation [7]) to $E(G)$ of the corresponding graph G.

For a tree T with n vertices, this energy is also expressible in terms of the Coulson integral [7] as

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

The fact that $E(T)$ is a strictly monotonously increasing function of all matching numbers $m(T,k), k = 0, 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$, provides us a way of comparing the energies of a pair of trees. Gutman [5] 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

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

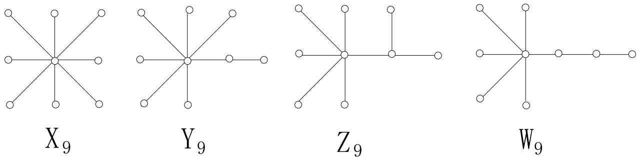

Fig. 1 The trees X_9, Y_9, Z_9 and W_9.

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

Hence, by (2), we have

$$T_1 \succeq T_2 \Longrightarrow E(T_1) \geq E(T_2), \tag{3}$$

$$T_1 \succ T_2 \Longrightarrow E(T_1) > E(T_2). \tag{4}$$

This increasing property of E has been successfully applied in the study of the extremal values of energy over a significant class of graphs (see [8-25]). In [6], Gutman determined the tree with the maximal energy, namely, the path. Furthermore, he proved that

$$E(X_n) < E(Y_n) < E(Z_n) < E(W_n) < E(T) \tag{5}$$

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 by attaching two pendent edges to a pendent vertex of $K_{1,n-3}$, W_n by attaching 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. On the other hand, Zhang et al [22] characterized the trees with a perfect matching having the minimal and the second minimal energies (which solved two conjectures proposed by Gutman [5], that is, they proved that $E(T) > E(B_n) > E(F_n)$ for any tree $T \neq F_n, B_n$ with n vertices having a perfect matching, where F_n is the tree with n vertices obtained by adding a pendent edge to each vertex of the star $K_{1,\frac{n}{2}-1}$, 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. Fig.2(a) and (b) show the two trees F_n and B_n. Some of recent results on the energy can be found in [2, 13, 15, 16, 18, 19, 20, 21, 25].

In order to formulate our results, we need to introduce some notation as follows. Suppose n and p are two positive integers and $n \geq p+1 \geq 3$. Let $\mathcal{T}_{n,p}$ be the set of trees with n vertices and with at most p pendent vertices. Define the tree $T_{n,p}$ $(n > p \geq 2)$ with n vertices as follows:

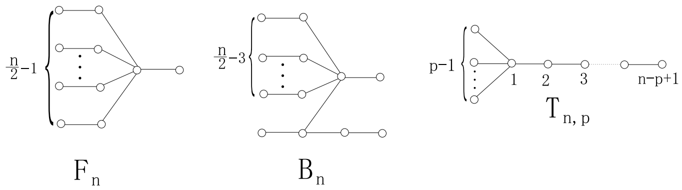

Fig.2 (a) The tree F_n; (b) the tree B_n; (c) the broom $T_{n,p}$.

$T_{n,p}$ is obtained from the path P_{n-p+1} with $n-p+1$ vertices by attaching $p-1$ pendent edges to an end vertex of P_{n-p+1}. $T_{n,p}$ is called a broom (see Brualdi et al [1]). Fig.2(c) shows the broom $T_{n,p}$. Obviously, $T_{n,p}$ is a tree with n vertices and with exactly p pendent vertices.

In this paper, we prove the following

Theorem 1.1 Let n and p be two positive integers, $n \geq p+1 \geq 3$, and let T be a tree with n vertices and with at most p pendent vertices. Then

$$E(T) \geq E(T_{n,p})$$

with equality if and only if T is the broom $T_{n,p}$.

Corollary 1.2 Let n and p be two positive integers, $n \geq p+1 \geq 3$, and let T be a tree with n vertices and with at most p pendent vertices. Then

$$Z(T) \geq Z(T_{n,p})$$

with equality if and only if T is the broom $T_{n,p}$, where $Z(T)$ denotes the Hosoya index of T.

2. Proofs of the main results

Given a graph G and an edge st, we denote by $G-st$ (resp. $G-s$) the graph obtained from G by deleting the edge st (resp. the vertex s and the edges adjacent to it).

Lemma 2.1 [21] Let T and T' be two trees of order n. 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 $T \succ T'$.

The following lemma is obvious but useful.

Lemma 2.2 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. $T \succ T'$).

Now we are in the position to prove the main results.

Proof of Theorem 1.1 If $n = p + 1$, then $T_{n,p} = K_{1,n-1}$. By Gutman [6], then $T \succeq K_{1,n-1}$ with equality if and only if $T = T_{n,p} = K_{1,n-1}$.

If $n = p+2$, then $T_{n,p} = Y_n$, where Y_n is the tree with n vertices obtained from a star $K_{1,n-2}$ by attaching one pendent edge to one of pendent vertices of $K_{1,n-2}$. Since T is a tree with $p + 2$ vertices and with at most p pendent vertices, we have $T \neq K_{1,n-1}$. By Gutman [6], then $T \succeq T_{n,p}$ with equality if and only if $T = T_{n,p} = Y_n$.

Hence in the following we may assume that $n \geq p + 3$. We prove the theorem by induction on n. By (3) and (4), it suffices to prove that $T \succ T_{n,p}$ for any tree $T(T \neq T_{n,p})$ with n vertices and with at most p pendent vertices.

Suppose the diameter of T is d. Note that $n \geq p+3$. Hence $d \geq 3$. Let $v_0 - v_1 - \ldots - v_d$ be a path in T. Then both v_0 and v_d are pendent vertices in T. We consider the following two cases:

Case (i) The degree of v_1 in T equals two, i.e., $d_T(v_1) = 2$.

Then $T - v_0$ is a tree with $n - 1$ vertices and with at most p pendent vertices. By Lemma 2.1, we only need to prove the following:

$$\begin{cases} T - v_0 \succeq T_{n-1,p} \\ T - v_0 - v_1 \succ T_{n-2,p} \end{cases}, \text{or}$$

$$\begin{cases} T - v_0 \succ T_{n-1,p} \\ T - v_0 - v_1 \succeq T_{n-2,p} \end{cases}.$$

Note that both $T - v_0$ and $T_{n-1,p}$ are trees with $n-1$ vertices and with at most p pendent vertices, and both $T - v_0 - v_1$ and $T_{n-2,p}$ are trees with $n - 2$ vertices and with at most p pendent vertices. By induction, we have the following:

$$T - v_0 \succeq T_{n-1,p}, \ T - v_0 - v_1 \succeq T_{n-2,p}. \tag{6}$$

Subcase 1 $T - v_0 = T_{n-1,p}$.

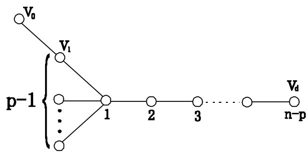

Fig. 3 The tree T.

Since $T \neq T_{n,p}$, T has the form of the tree illustrated in Fig. 3. Hence $T - v_0 - v_1 = T_{n-2,p-1}$. By induction, we have

$$T - v_0 - v_1 = T_{n-2,p-1} \succ T_{n-2,p}.$$

Hence we have $T - v_0 = T_{n-1,p}$ and $T - v_0 - v_1 \succ T_{n-2,p}$, which implies that $T \succ T_{n,p}$.

Subcase 2 $T - v_0 \neq T_{n-1,p}$.

By induction, we have the following:

$$T - v_0 \succ T_{n-1,p}.$$

By (6) we have $T \succ T_{n,p}$.

By Subcases 1 and 2, we have proved that if $d_T(v_1) = 2$ then $T \succ T_{n,p}$.

Case (*ii*) The degree of v_1 in T is more than two, i.e., $d_T(v_1) > 2$.

Suppose $d_T(v_1) = t \geq 3$. Since $v_0 - v_1 - \ldots - v_d$ is one of the longest paths in T, $T - v_1$ has a unique component T_0 with at least two vertices. Hence T has the form of the tree showed in Fig. 4. Obviously, T_0 is a tree with $n - t$ vertices and the number of pendent vertices of T_0 is no more than $p - (t-1) + 1 = p - t + 2$ (otherwise, T has a path of length more than d, a contradiction). Particularly, $t \leq p$, since if $t > p$ then T has at least t $(> p)$ pendent vertices, a contradiction. Furthermore, $t \neq p$ (since if $t = p$ then $T = T_{n,p}$, a contradiction with $T \neq T_{n,p}$). By Lemma 2.1, we only need to prove the following:

$$\begin{cases} T - v_0 \succeq T_{n-1,p-1} \\ T - v_0 - v_1 \succ (p-2)P_1 \cup P_{n-p} \end{cases}, \text{or}$$

$$\begin{cases} T - v_0 \succ T_{n-1,p-1} \\ T - v_0 - v_1 \succeq (p-2)P_1 \cup P_{n-p} \end{cases}.$$

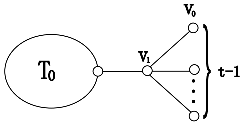

Fig. 4 The tree T.

Note that both $T - v_0$ and $T_{n-1,p-1}$ are trees with $n-1$ vertices and with at most $p-1$ pendent vertices, and T_0 is a tree with $n-t$ vertices and with at most $p-t+2$ pendent vertices. By induction, we have $T - v_0 \succeq T_{n-1,p}$ and $T_0 \succeq T_{n-t,p-t+2}$. Again note that $(p-t)P_1 \cup P_{n-p}$ is a proper subgraph of $T_{n-t,p-t+2}$. Hence, by Lemma 2.2. we have $T_{n-t,p-t+2} \succ (p-t)P_1 \cup P_{n-p}$. Thus, we have

$$(t-2)P_1 \cup T_0 \succeq (t-2)P_1 \cup T_{n-t,p-t+2} \succ (t-2)P_1 \cup (p-t)P_1 \cup P_{n-p} = (p-2)P_1 \cup P_{n-p},$$

that is,

$$T - v_0 - v_1 = (p-2)P_1 \cup T_0 \succ (p-2)P_1 \cup P_{n-p}.$$

Hence we have proved that if $d_T(v_1) > 2$ then $T \succ T_{n,p}$.

The theorem follows immediately from Cases (i) and (ii). ■

Proof of Corollary 1.2 Note that, for any tree T with n vertices, the Hosoya index $Z(T) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} m(T,i)$. Hence, if T_1 and T_2 are two trees with n vertices such that $T_1 \succ T_2$ then $Z(T_1) > Z(T_2)$. It is obvious that the corollary follows from Theorem 1.1. ■

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