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

Luzhen Ye, Xinmei Yuan

2. School of Sciences, Jimei University, Xiamen 361021, China

3. Department of Mathematics, Yichun College, Yichun 336000, China

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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 $T_{n,p}$ 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 $T_{n,p}$.

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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2Corresponding author, E-mail address: lzye555@sina.com(L. Ye),
defined as \( \phi(T, x) = \text{det}(xI - A(T)) \), where \( I \) is the identity matrix of order \( n \). It is well known [3] that if \( T \) is a tree with \( n \) vertices then

\[
\phi(T, x) = \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} (-1)^k m(T, k)x^{n-2k},
\]

where \( m(T, k) \) equals the number of matchings with \( k \) edges in \( T \), and \( \left\lfloor \frac{n}{2} \right\rfloor \) 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

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

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

\[
Z(G) = \sum_{r=0}^{\left\lfloor \frac{n}{2} \right\rfloor} m(G, r),
\]

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 \( \pi \)-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

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

The fact that \( E(T) \) is a strictly monotonously increasing function of all matching numbers \( m(T, k), k = 0, 1, 2, \ldots, \left\lfloor \frac{n}{2} \right\rfloor \), 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

\[
T_1 \succeq T_2 \iff m(T_1, k) \geq m(T_2, k) \text{ for all } k = 0, 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor.
\]
If $T_1 \succeq T_2$ and there exists a $j$ such that $m(T_1, j) > m(T_2, j)$ then we write $T_1 \preceq T_2$.

Hence, by (2), we have

\[ T_1 \succeq T_2 \implies E(T_1) \geq E(T_2), \quad (3) \]

\[ T_1 \preceq T_2 \implies E(T_1) < E(T_2). \quad (4) \]

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

\[ E(X_n) < E(Y_n) < E(Z_n) < E(W_n) < E(T) \quad (5) \]

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 pendant edge to a pendant vertex of $K_{1,n-2}$, $Z_n$ by attaching two pendant edges to a pendant vertex of $K_{1,n-3}$, $W_n$ by attaching a $P_3$ (here $P_m$ denotes the path with $m$ vertices) to a pendant 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 pendant edge to each vertex of the star $K_{1,2^{n-1}}$, and $B_n$ is the tree obtained from $F_{n-2}$ by attaching a $P_2$ to the 2-degree vertex of a pendant 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 $T_{n,p}$ be the set of trees with $n$ vertices and with at most $p$ pendant vertices. Define the tree $T_{n,p}$ ($n > p \geq 2$) with $n$ vertices as follows:

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

$$T_1 = T - u, T_2 = T - u - v, T'_1 = T' - u' - v'$$

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 $T \succ T'$. 

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
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. $T > T'$).

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 $T > T_{n,p}$ 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:

\[
\begin{align*}
&\begin{cases}
T - v_0 \succeq T_{n-1,p} \\
T - v_0 - v_1 \succ T_{n-2,p}
\end{cases}, \text{ or} \\
&\begin{cases}
T - v_0 \succ T_{n-1,p} \\
T - v_0 - v_1 \succeq T_{n-2,p}
\end{cases}.
\end{align*}
\]

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:

\[
T - v_0 \succeq T_{n-1,p}, \ T - v_0 - v_1 \succeq T_{n-2,p}.
\]

\*

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

\[
\begin{cases}
T - v_0 \succeq T_{n-1,p-1}, \\
T - v_0 - v_1 \succ (p - 2)P_1 \cup P_{n-p}, \text{or} \\
T - v_0 \succ T_{n-1,p-1}, \\
T - v_0 - v_1 \geq (p - 2)P_1 \cup P_{n-p}.
\end{cases}
\]
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 $T_{n-t, p-t+2} \succeq (p-t)P_1 \cup P_{n-p}$. Thus, we have

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

that is,

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

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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References


