On the Minimal Energy of Trees With a Given Number of Vertices of Odd Degree

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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 \(G\). In this paper, we characterize the tree with minimal energy among the trees of order \(n\) with at most \(k\) vertices of odd degree, where \(2 \leq k \leq n\).

1. INTRODUCTION

Apart from purely graph theoretical interest, the study of energy is considerably motivated by applications in organic chemistry: for example, within the framework of Hückel molecular orbital approximation. The calculation of the theoretically computed total \(\pi\)-electron energy of a hydrocarbon molecule can be reduced to that of the energy of the corresponding molecular graph [11]. Moreover, the energy of graphs has certain relations to some well known topological indices such the Merrifield-Simmons index, defined as the number of independent vertex subsets, and the Hosoya index.

Let \(T\) be a tree of order \(n\) and \(A(T)\) the adjacency matrix of \(T\). The characteristic polynomial of \(T\), denoted by \(\chi(T; x)\), is defined as \(\chi(T; x) = \det(xI_n - A(T))\). It is well known [3] that if \(T\) is a tree of order \(n\), then

\[
\chi(T; x) = \sum_{k=0}^{[n/2]} (-1)^k m(T, k)x^{n-2k},
\]  \(\text{(1)}\)
where \( m(T, k) \) equals the number of \( k \)-matchings of \( T \). The Hosoya index [11] of a graph \( G \) of order \( n \), denoted by \( Z(G) \), is defined as

\[
Z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G, k).
\]

Let \( G \) be a graph with \( n \) vertices, and \( d_G(u) \) the degree of vertex \( u \) of \( G \). Gutman [7] defined the energy of \( G \), denoted by \( E(G) \), as

\[
E(G) = \sum_{i=1}^{n} |\lambda_i(G)|,
\]

where \( \lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G) \) are the eigenvalues of the adjacency matrix of \( G \).

For a tree \( T \) (acyclic graph) of order \( n \), this energy is also expressible in terms of the Coulson integral [11] as

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

It is obvious that \( E(T) \) is a strictly monotonously increasing function of all matching numbers \( m(T, k), k = 2, 3, \ldots, \lfloor n/2 \rfloor \). It provides us a way to compare the energies of a pair of trees. Gutman [6] introduced a quasi-ordering relation "\( \geq \)" (i.e., reflective and transitive relation) on the set of all forests (acyclic graphs) of order \( n \); if \( T_1 \) and \( T_2 \) are two forests with \( n \) vertices and with characteristic polynomials in the form (1), then

\[
T_1 \succeq T_2 \iff m(T_1, k) \geq m(T_2, k) \text{ for all } k = 0, 1, \ldots, \lfloor n/2 \rfloor.
\]

If \( T_1 \succeq T_2 \) and there exists a \( j \) such that \( m(T_1, j) > m(T_2, j) \), then we write \( T_1 \succ T_2 \). Hence, by (2) and the definition of the Hosoya index, we have

\[
T_1 \succeq T_2 \implies E(T_1) \geq E(T_2), \ Z(T_1) \geq Z(T_2), \tag{3}
\]

\[
T_1 \succ T_2 \implies E(T_1) > E(T_2), \ Z(T_1) > Z(T_2). \tag{4}
\]

This increasing property of \( E(G) \) has been successfully applied in the study of the extremal values of energy over different classes of graphs (see for example papers [5,8,10, 13,20–24]). Most of results about the energy of graphs can be seen in the book [14] by Li, Shi, and Gutman and references therein.

Quite recently, Lin [15,16] determined the trees of order \( n \) with a given number of vertices of even degree which has the maximal Wiener index. Furthermore, Gutman,
and Lin [4] determined the first few trees whose all degrees are odd, having smallest and greatest Wiener indices. Gutman, Cruz, and Rada [9] characterized the Eulerian graphs with the smallest and greatest Wiener indices.

Let $T_n$ denote the set of trees of order $n$ and $T_{n,k}$ the set of trees of order $n$ with $k$ vertices of odd degree. Note that the number of vertices of odd degree is even. So $k$ is even. Obviously, $T_{n,k} \subset T_n$. If $k = 2$, the unique tree in $T_{n,2}$ is the path $P_n$. If $k = n$ and $n$ is even or $k = n - 1$ and $n$ is odd, the tree with minimal energy must be the star $K_{1,n-1}$. So, in the following, we just consider the case $4 \leq k \leq n-2$. In order to formulate our results, we need to define a tree $O_{n,k}$ with $n$ vertices as follows: $O_{n,k}$ is obtained by connecting the center of the star $K_{1,k-1}$ and one endpoint of the path $P_{n-k}$, see Figure 1, and we denote the set $\{O_{n,k} : 4 \leq k \leq n\}$ by $O_{n,k}$.

![Figure 1: The tree $O_{n,k}$.](image)

In this paper, we prove that if $T \in T_{n,k}$ ($4 \leq k \leq n-2$), then $E(T) \geq E(O_{n,k})$ and $Z(T) \geq Z(O_{n,k})$, with two equalities if and only if $T = O_{n,k}$. This result can be obtained from Theorem 27 in [2]. In this paper, we use different methods to prove it.

2. Main results

Let $G$ be a graph and $uv$ an edge of $G$. Denote $G - uv$ (resp. $G - u$) the graph obtained from $G$ by deleting the edge $uv$ (resp. the vertex $u$ and edges incident to $u$). In order to prove the main results, we introduce some lemmas as follows.

**Definition 2.1.** Let $T$ be a tree in $T_n$ ($n \geq 4$). Let $e = uv$ be a nonpendant edge of $T$, and let $T_1$ and $T_2$ be the two components of $T - e$, $u \in T_1$, $v \in T_2$. $T_0$ is obtained from $T$ in the following ways.

1) Contract the edge $e = uv$, denote the new vertex by $w$;

2) Attach a pendent vertex $w'$ to the vertex $w$.

The procedures 1) and 2) are called the edge-growing transformation of $T$ [18] (on edge $e=uv$), or e.g.t of $T$ (on edge $e = uv$) for short, see Figure 2.
Remark: It is easy to check that if $T \in \mathcal{T}_{n,k}$, $d_T(u)$, $d_T(v)$ are both odd, then by the e.g.t of $T$ (on edge $e = uv$), $d_{T_0}(w)$ is odd, and $T_0 \in \mathcal{T}_{n,k}$. Similarly, if $d_T(u)$ is odd, $d_T(v)$ is even (resp. $d_T(u)$ is even, $d_T(v)$ is odd), then by the e.g.t of $T$ (on edge $e = uv$), $d_{T_0}(w)$ is even, and $T_0 \in \mathcal{T}_{n,k}$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{tree.png}
\caption{The tree $T$ and $T_0$.}
\end{figure}

\textbf{Lemma 2.2.} [17] Let $T \in \mathcal{T}_n$ ($n \geq 4$) with at least a nonpendent edge. If $T_0$ can be obtained from $T$ by one step of e.g.t (on edge $e = uv$), then $T \succ T_0$, and $E(T) > E(T_0)$.

Let $P = v_0v_1...v_k$ be a path of a tree $T$. If $d_T(v_0) \geq 3$, $d_T(v_k) \geq 3$, we call $P$ an internal path of $T$. If $d_T(v_0) \geq 3$ and $d_T(v_i) = 1$, $d_T(v_i) = 2$ ($0 < i < k$), we call $P$ a pendent path of $T$ with root $v_0$, particularly, when $k = 1$, we call $P$ a pendent edge. Let $s(T)$ the be the number of vertices in $T$ with degree more than 2 and $p(T)$ the number of pendent paths in $T$ with length more than 1. For example, we consider the tree $T$ as shown in Figure 3. $v_3v_4v_5$ is an internal path of $T$, while $v_5v_6v_7$, $v_5v_8v_9$, $v_3v_1$, and $v_3v_2$ are all pendent paths of $T$; $s(T) = 2$ and $p(T) = 2$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{tree1.png}
\caption{The tree $T$.}
\end{figure}

If $T \in \mathcal{T}_{n,k}$ ($4 \leq k \leq n - 2$), $T \neq O_{n,k}$, and $p(T) \neq 0$, then $T$ can be seen as the tree as shown in Figure 4, where $P_s$ ($s \geq 3$) is the pendent path of $T$ with $s$ vertices and root $u$, $T_1$ and $T_2$ are two subtrees of $T$ with vertices $u$ and $v$ as roots, respectively, and $T_1, T_2 \neq P_1$. If $T'$ is obtained from $T$ by replacing $P_s$ with a pendent edge and replacing the edge $uv$ with a path $P_s$, we say that $T'$ is obtained from $T$ by $\alpha$-transformation (as shown in Figure 4). It is easy to see that $T' \in \mathcal{T}_{n,k}$. 

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{tree2.png}
\caption{The tree $T$.}
\end{figure}
Lemma 2.3. [19] Let $T \in \mathcal{T}_n$ ($n \geq 6$), if $T'$ is obtained from $T$ by $\alpha$–transformation, then $T' \prec T$, $\mathcal{E}(T') < \mathcal{E}(T)$.

If $T \in \mathcal{T}_{n,k}$ ($4 \leq k \leq n-2$), $T \neq O_{n,k}$ and $p(T) = 0$, then there exists at least a longest path $P$ of the tree $T$, we assume that the vertices $u_1$ and $v_1$ are two endpoints of the path $P$. Let $u_1u, v_1v \in E(T)$, then $N_T(u) = \{u_1, u_2, ..., u_s, w\}$ ($s \geq 2$), $N_T(v) = \{v_1, v_2, ..., v_t, w'\}$ ($t \geq 2$), where $u_1, u_2, ..., u_s, v_1, v_2, ..., v_t$ are pendent vertices of $T$, $d_T(w) \geq 2$ and $d_T(w') \geq 2$. Note that $w = v$ (resp. $u = w'$) when the length of the path $P$ equals 3. If $T' = T - \{uw_2, ..., uw_s\} + \{vw_2, ..., vw_t\}$ or $T' = T - \{vv_2, ..., vv_s\} + \{uw_2, ..., uw_t\}$, we say that $T'$ is obtained from $T$ by $\beta$–transformation. It is easy to see that $p(T') = 1$ and $s(T') = s(T) - 1$.

Lemma 2.4. [19] Let $T \in \mathcal{T}_n$ ($n \geq 6$). If $T'$ is obtained from $T$ by $\beta$–transformation, then $T' \prec T$, $\mathcal{E}(T') < \mathcal{E}(T)$, and $s(T') = s(T) - 1$, $p(T') = 1$.

Theorem 2.5. For $T \in \mathcal{T}_{n,k}$, and $4 \leq k \leq n-2$, then

$$\mathcal{E}(T) \geq \mathcal{E}(O_{n,k}),$$

with equality if and only if $T = O_{n,k}$.

Proof. For $T \in \mathcal{T}_{n,k}$, $T \neq O_{n,k}$, denote $T_a$ is obtained from $T$ by continually using the e.g.t of $T$ (on $e = uv$) as shown in the previous Remark until all degrees of the nonpendent vertices of the tree $T_a$ are even. Obviously, $T_a \in \mathcal{T}_{n,k}$, if all degrees of the nonpendent...
vertices of $T$ are even, we let $T = T_a$. Then, by Lemma 2.2, we have $\mathcal{E}(T) \geq \mathcal{E}(T_a)$, with equality if and only if $T = T_a$. In this case, if $T_a = O_{n,k}$, then $\mathcal{E}(T) > \mathcal{E}(O_{n,k})$. In the following, we just deal with the case when $T_a \neq O_{n,k}$.

We shall show $\mathcal{E}(T_a) > \mathcal{E}(O_{n,k})$ by induction on $s(T_a)$. When $s(T_a) = 1$, note $T_a \neq K_{1,n-1}, P_n, O_{n,k}$, then $p(T_a) \geq 2$, we can finally get the tree $O_{n,k}$ from $T_a$ by $\alpha$–transformation, by Lemma 2.3, we have $\mathcal{E}(T_a) > \mathcal{E}(O_{n,k})$. We suppose the result holds for any tree $T'_a \in \mathcal{T}_{n,k}$ with $s(T'_a) = s - 1$. Let $s(T_a) = s \geq 2$. If $p(T_a) \neq 0$, we can finally get a tree $T_b \in \mathcal{T}_{n,k}$ from $T_a$ by $\alpha$–transformation such that $p(T_b) = 0$, $s(T_b) = s$ and $\mathcal{E}(T_a) > \mathcal{E}(T_b)$. If $p(T_a) = 0$, we let $T_a = T_b$. By Lemma 2.4, we can get a tree $T_c \in \mathcal{T}_{n,k}$ from $T_b$ by one step of $\beta$–transformation such that $p(T_c) = 1$, $s(T_c) = s - 1$, and $\mathcal{E}(T_b) > \mathcal{E}(T_c)$. Hence $\mathcal{E}(T_a) \geq \mathcal{E}(T_b) > \mathcal{E}(T_c)$. By the hypothesis of the induction, we have

$$\mathcal{E}(T) \geq \mathcal{E}(T_a) \geq \mathcal{E}(T_b) > \mathcal{E}(T_c) > \mathcal{E}(O_{n,k}).$$

Therefore, if $T \in \mathcal{T}_{n,k}$, and $4 \leq k \leq n - 2$, then $\mathcal{E}(T) \geq \mathcal{E}(O_{n,k})$, and the equality holds if and only if $T = O_{n,k}$. ■

By using the e.g.t of $O_{n,k}$ and Lemma 2.2, the following result is immediate.

**Lemma 2.6.** For the trees of $O_{n,k}$ ($4 \leq k \leq n$), we have

$$\mathcal{E}(K_{1,n-1}) \leq \mathcal{E}(O_{n,k}) < \mathcal{E}(O_{n,k-1}) < \cdots < \mathcal{E}(O_{n,4}) < \mathcal{E}(O_{n,3}) < \mathcal{E}(P_n),$$

with the equality holds if and only if $K_{1,n-1} = O_{n,k}$.

Lemma 2.6 can be obtained from the so called “Sliding along a path” [1,12].

**Theorem 2.7.** Let $T$ be a tree of order $n$ with at most $k$ ($4 \leq k \leq n$) vertices of odd degree. Then

$$\mathcal{E}(T) \geq \mathcal{E}(O_{n,k}),$$

with equality if and only if $T = O_{n,k}$.

By the same way as used in proving Theorem 2.5, for $T \in \mathcal{T}_{n,k}$, we have $T \succeq O_{n,k}$, with equality if and only if $T = O_{n,k}$. By (3) and (4), the following result is immediate.

**Corollary 2.8.** For $T \in \mathcal{T}_{n,k}$, and $4 \leq k \leq n - 2$, then

$$\mathcal{Z}(T) \geq \mathcal{Z}(O_{n,k}),$$
with equality if and only if $T = O_{n,k}$.

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References


