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

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Abstract

The energy $\mathcal{E}(G)$ 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 π-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

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

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 $\mathcal{Z}(G)$, is defined as

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

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 $\mathcal{E}(G)$, as

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

where $\lambda_1(G), \lambda_2(G), \cdots, \lambda_n(G)$ 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

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

It is obvious that $\mathcal{E}(T)$ is a strictly monotonously increasing function of all matching numbers $m(T,k)$, $k = 2, 3, \cdots, \lfloor n/2 \rfloor$. It provides us a way to compare the energies of a pair of trees. Gutman [6] introduced a quasi-ordering relation "$\succeq$" (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

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

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

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

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

This increasing property of $\mathcal{E}(G)$ 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 $\mathcal{T}_n$ denote the set of trees of order n and $\mathcal{T}_{n,k}$ 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, $\mathcal{T}_{n,k} \subset \mathcal{T}_n$. If $k = 2$, the unique tree in $\mathcal{T}_{n,2}$ 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 $\mathcal{O}_{n,k}$.

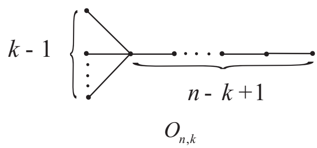

Figure 1: The tree $O_{n,k}$.

In this paper, we prove that if $T \in \mathcal{T}_{n,k}$ $(4 \leq k \leq n-2)$, then $\mathcal{E}(T) \geq \mathcal{E}(O_{n,k})$ and $\mathcal{Z}(T) \geq \mathcal{Z}(O_{n,k})$, 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 $\mathcal{T}_n$ $(n \geq 4)$. 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 $T_0 \in \mathcal{T}_{n,k}$.

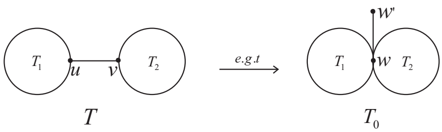

Figure 2: The tree T and T_0.

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 $\mathcal{E}(T) > \mathcal{E}(T_0)$.

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 $d_T(v_k) = 1$, $d_T(v_i) = 2$ $(0 < i < k)$, 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 $p(T) = 2$.

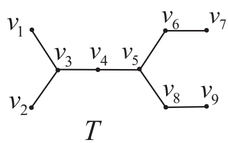

Figure 3: The tree T.

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 $T' \in \mathcal{T}_{n,k}$.

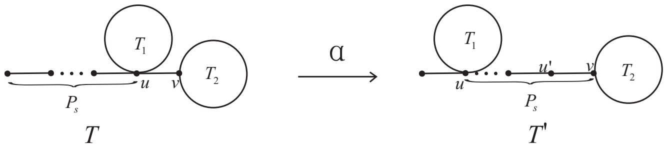

Figure 4: The $\alpha-transformation$ of the tree T.

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 $T^{'} = T - \{uu_2, ..., uu_s\} + \{vu_2, ..., vu_s\}$ or $T^{'} = T - \{vv_2, ..., vv_t\} + \{uv_2, ..., uv_t\}$, we say that $T^{'}$ is obtained from T by $\beta-transformation$. It is easy to see that $p(T^{'}) = 1$ and $s(T^{'}) = s(T) - 1$.

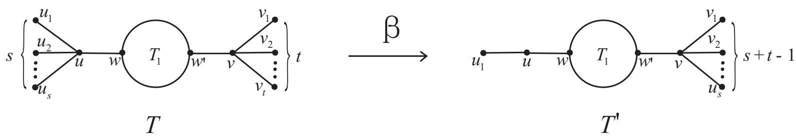

Figure 5: The $\beta-transformation$ of the tree T.

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 $T^{'} \in \mathcal{T}_{n,k}$ with $s(T^{'}) = s - 1$. 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 $\mathcal{O}_{n,k}$ $(4 \leq k \leq n)$, 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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