

On the Energy of Trees with Given Domination Number ¹

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Abstract

The energy of a graph is defined as the sum of the absolute values of all eigenvalues of the graph. In this paper, we present some sharp lower bounds on the energy of trees involving the domination number, and we also determine all extreme trees which attain these lower bounds.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set E . The *adjacency matrix* of G , $A = [a_{ij}]$, is an $n \times n$ matrix, where $a_{ij} = 1$ if v_i and v_j are adjacent and $a_{ij} = 0$, otherwise. Thus A is a real symmetric matrix with zeros on the diagonal, and all eigenvalues of A are real. The *characteristic polynomial* of G is just $\det(xI - A)$, denoted by $\Phi(G, x)$ or $\Phi(G)$. The *eigenvalues* of graph G , are the eigenvalues of A .

We denote the path on n vertices by P_n . A *pendent vertex* of G is a vertex of degree 1. A *pendent path* is a path whose inner vertices all have degree 2 and one of its endvertices is a pendent vertex. A *subdivision* of an edge uv is obtained by

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removing edge uv , and adding a new vertex w , and adding edges uw and vw . A *matching* of G is a set of mutually non-incident edges. k -*matching* is a matching of order k . For a graph $G = (V, E)$, we use $N(u)$ to denote the set of vertices adjacent to vertex u , and call a set $U \subseteq V$ a *vertex cover* of E if every edge of G is incident with a vertex in U . A *dominating set* of G is a set $U \subseteq V$ such that $U \cup N(U) = V$, where $N(U) = \cup_{u \in U} N(u)$. The *domination number* is the smallest cardinality among all dominating sets of G , denoted by $\gamma(G)$. If G has no isolate vertex, then $\gamma(G) \leq \frac{n}{2}$. A dominating set U of a graph G with $|U| = \gamma(G)$ is called a γ -*set*.

It is useful to partition the vertices of G into three sets according to how their removal affects $\gamma(G)$. Let $V(G) = V^+(G) \dot{\cup} V^0(G) \dot{\cup} V^-(G)$, for

$$V^+(G) = \{v \in V(G) : \gamma(G - v) > \gamma(G)\},$$

$$V^0(G) = \{v \in V(G) : \gamma(G - v) = \gamma(G)\},$$

$$V^-(G) = \{v \in V(G) : \gamma(G - v) < \gamma(G)\},$$

where $G - v$ is the graph obtained from G by deleting the vertex v and all the edges incident with v .

Note that removing a vertex can increase the domination number by more than one, but can decrease it by at most one. For example, removing the center vertex of the star $K_{1,n-1}$ increase the domination number by $n - 2$; and removing an endvertex of the path P_{3k+1} ($k \geq 1$) decrease the domination number by one.

Chemists have known that the experimental heats of formation of conjugated hydrocarbons are closely related to the total π -electron energy. And the calculation of the total energy of all π -electrons in a conjugated hydrocarbon can be reduced (within the framework of the HMO approximation [5]) to $E(G) = |\lambda_1(G)| + |\lambda_2(G)| + \dots + |\lambda_n(G)|$, where $\lambda_i(G)$ are the eigenvalues of the corresponding graph. For an acyclic graph (or a tree) T this energy is also expressible in terms of the Coulson integral formula (in [5]) as

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

where $m(T, k)$ is the number of k -matchings of T .

The fact that $E(T)$ is a strictly monotonically increasing function of all matching numbers $m(T, k)$, $k = 0, 1, \dots, \lceil n/2 \rceil$, provides us with a way of comparing the energies of trees.

There are numerous bounds on the energy of a graph [7]–[10]. Most of them only involve the number of vertices and edges of graphs. Very little is known about bounds for energy of a graph with domination number. However, the relationship between the domination number and adjacency spectral radius or Laplacian spectral radius are described in [11], [12].

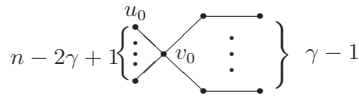


Fig. 1. $T(n, \gamma)$

Motivated by all these works, in the present paper, we are devoted to find some sharp lower bounds for the energy of trees involving the domination number. In order to formulate our main results, we need to define a tree $T(n, \gamma)$ (where $n \geq 2\gamma$) which was named (in [4]) wounded spider. $T(n, \gamma)$ is the tree obtained by subdividing exactly $\gamma - 1$ edges of the edges of the star $K_{1, n-\gamma}$ (as shown in Fig. 1.). We now consider the following set of trees:

$$\mathcal{T}_{n, \gamma} = \{T : |V(T)| = n, \gamma(T) = \gamma\}.$$

It is easy to see that the following are equivalent:

- (1) $\mathcal{T}_{n, \gamma} \neq \emptyset$,
- (2) $n \geq 2\gamma$,
- (3) $T(n, \gamma)$ is definable.

A natural question to ask is : How do we determine the trees in $\mathcal{T}_{n, \gamma}$ that have the minimal energy? In Section 2, we mainly discuss this question and give the following result.

Theorem 1.1 For any $T \in \mathcal{T}_{n, \gamma}$,

$$E(T) \geq E(T(n, \gamma)).$$

Equality holds if and only if $T = T(n, \gamma)$.

In Section 3, we calculate the value of the energy of $T(n, \gamma)$. Consequently, we describe a sharp lower bound of the energy of a tree as a function of its order and domination number as follows.

Theorem 1.2 *Let T be a tree of order n , and γ be the domination number of T , then*

$$E(T) \geq 2\gamma - 4 + 2\sqrt{n - \gamma + 1 + 2\sqrt{n - 2\gamma + 1}}.$$

Equality holds if and only if $T = T(n, \gamma)$.

In Section 4, we give a more general form of Theorem 1.1.

2 The tree with minimum energy among all trees in $\mathcal{T}_{n,\gamma}$

We start this section with a quasi-ordering relation " \succeq " which was introduced by Gutman in [6].

Definition 2.1 [6] *Let G and G' be two forests of order n , $G \succeq G'$, if and only if $m(G, k) \geq m(G', k)$ for $k = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$; $G \succ G'$ if and only if $G \succeq G'$ and there is a $k(1 \leq k \leq \lfloor \frac{n}{2} \rfloor)$ such that $m(G, k) > m(G', k)$.*

Observation 2.1 *Let G and G' be two forests of order n , if $G \succeq G'$, then $E(G) \geq E(G')$; if $G \succ G'$, then $E(G) > E(G')$.*

This observation follows from the Coulson integer formula definition for energy of forests, and provides us with a way of comparing the energies of trees.

Lemma 2.1 [1] *The maximum cardinality of a matching in a bipartite graph is equal to the minimum cardinality of a vertex cover.*

As a simple application of the above lemma, the assertion of the following lemma holds.

Lemma 2.2 *Let G be a bipartite graph without isolate vertex, and γ be the domination number of G , then G has a γ - matching.*

Lemma 2.3 [2] *Let G be a forest of order n ($n > 1$) and G' be a spanning subgraph (respectively a proper spanning subgraph) of G . Then $G' \preceq G$ (respectively $G' \prec G$).*

Lemma 2.4 [2] *Let T and T' be two trees. Suppose that uv (respectively $u'v'$) is a pendent edge of T (respectively T') and u (respectively u') is a pendent vertex of T (respectively T'). Let $T_1 = T - u$, $T_2 = T - \{u, v\}$, $T'_1 = T' - u'$ and $T'_2 = T' - \{u', v'\}$. If $T'_1 \preceq T_1$ and $T'_2 \prec T_2$, or $T'_1 \prec T_1$ and $T'_2 \preceq T_2$, then $T' \prec T$.*

Lemma 2.5 [3] *Let $e = uv$ be an edge of graph G of order n . The number $m(G, k)$ of k - matchings of G is determined by*

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

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

Lemma 2.6 [4] *A vertex $v \in V^+(G)$ if and only if*

- (a) v is not an isolate vertex and is in every γ - set of G ,
- (b) no subset $S \subseteq V - (N(v) \cup \{v\})$ with cardinality $\gamma(G)$ dominates $G - v$.

We use $\mathcal{P}(G)$ to denote the set of all pendent vertices of G . The following is a simple application of the above lemma.

Lemma 2.7 *Let G be a connected graph, then $\mathcal{P}(G) \subseteq V^0(G) \cup V^-(G)$.*

Proof. Since $V(G) = V^+(G) \dot{\cup} V^0(G) \dot{\cup} V^-(G)$, we only need to show that for any $u \in \mathcal{P}(G)$, $u \notin V^+(G)$. By Lemma 2.6, it suffices to find a γ - set which does not contain u .

If u is not in any γ - set, then we are done. If u is in some γ - set of G , write S . Let v be the unique vertex adjacent to u in G , then $(S - \{u\}) \cup \{v\}$ is the γ - set as required. □

Lemma 2.8 *Let T be a tree, and $\mathcal{P}(T) \subseteq V^-(T)$, then T has a pendent path of order 3.*

Proof. Let $P = uvw \dots s$ be a longest path of T , where $u, s \in \mathcal{P}(T)$. For $\mathcal{P}(T) \subseteq V^-(T)$, $\gamma(T - u) = \gamma - 1$, and u is the unique pendent vertex in $N(v)$.

We now shall show that $d(v) = 2$. Otherwise, let $x \notin \{u, w\}$ be a neighbor of v , by the preceding argument, $x \notin \mathcal{P}(T)$. Thus, x has a neighbor different from v , say y . Note that T is a tree, y is not in the path P . Thus $yxvPw$ is a path with longer length, which contradicts the choice of P .

Therefore uvw is a pendent path of order 3. □

Now we are ready to prove the key lemma of this section.

Lemma 2.9 *For any $T \in \mathcal{T}_{n,\gamma}$ (where $n \geq 2\gamma$), we have $T \succeq T(n, \gamma)$, and equality holds if and only if $T = T(n, \gamma)$.*

Proof. The proof is induction on n , the order of T .

When $n = 2$, then for $\gamma \leq \frac{n}{2} = 1$, the assertion is trivial. We now assume that $n \geq 3$ and the assertion holds for smaller values of n and all $\gamma \leq \frac{n}{2}$.

For $|T| = n$, when $\gamma = 1$, there is nothing to prove since T is a star $K_{1,n-1}$. Now we assume our result holds for trees with order n and domination number less than γ .

According to Lemma 2.7, we distinguish between the following two cases.

Case 1. If $\mathcal{P}(T) \cap V^0(T) \neq \emptyset$.

Let $u \in \mathcal{P}(T) \cap V^0(T)$. Since $\gamma(T - u) = \gamma$, $T - u \in \mathcal{T}_{n-1,\gamma}$, and $\mathcal{T}_{n-1,\gamma} \neq \emptyset$. By induction hypothesis,

$$T - u \succeq T(n - 1, \gamma) = T(n, \gamma) - u_0 \quad (1),$$

where u_0 is a pendent vertex of $T(n, \gamma)$ as shown in Fig. 1.

Let v be the unique vertex adjacent to u in T . By Lemma 2.2, T has a γ - matching, thus T has a $(\gamma - 1)$ - matching which does not contain v . Therefore, it follows that $T - u - v$ has a $(\gamma - 1)$ - matching, which implies $T(n, \gamma) - u_0 - v_0 = (\gamma - 1)K_2 \cup (n - 2\gamma)K_1$ is a spanning subgraph of $T - u - v$. By Lemma 2.3, $T - u - v \succeq T(n, \gamma) - u_0 - v_0$.

Combining the above with Lemma 2.4, we can get our result $T \succeq T(n, \gamma)$. If the equality holds, then in (1), $T - u = T(n - 1, \gamma)$. Suppose $T \neq T(n, \gamma)$, then $T(n, \gamma) - u_0 - v_0 = (\gamma - 1)K_2 \cup (n - 2\gamma)K_1$ is a proper spanning subgraph of $T - u - v$, which implies that $T \succ T(n, \gamma)$, a contradiction. Hence $T = T(n, \gamma)$.

Case 2. If $\mathcal{P}(T) \cap V^0(T) = \emptyset$, i.e., $\mathcal{P}(T) \subseteq V^-(T)$.

By Lemma 2.8, T has a pendent path of order 3, write xyz , where x is a pendent vertex. Then $T - x - y$ is a tree, and for obvious reasons $\gamma(T - x - y) = \gamma - 1$. So $\mathcal{T}_{n-1, \gamma-1} \neq \emptyset$ and $\mathcal{T}_{n-2, \gamma-1} \neq \emptyset$.

Now we use Lemma 2.5 by taking $G = T$, $uv = xy$, then

$$\begin{aligned} m(T, k) &= m(T - xy, k) + m(T - x - y, k - 1) \\ &= m(T - x, k) + m(T - x - y, k - 1) \\ &\geq m(T(n - 1, \gamma - 1), k) + m(T(n - 2, \gamma - 1), k - 1) \quad (2) \\ &= m(T(n, \gamma), k). \end{aligned}$$

Hence $T \succeq T(n, \gamma)$ as desired. Equality attained if and only if the equality in (2) holds for every integer k , that is $T - x = T(n - 1, \gamma - 1)$, $T - x - y = T(n - 2, \gamma - 1)$. Thus $T = T(n, \gamma)$. \square

Now we come to our main result in this section.

Theorem 2.1 For any $T \in \mathcal{T}_{n, \gamma}$,

$$E(T) \geq E(T(n, \gamma)).$$

Equality holds if and only if $T = T(n, \gamma)$.

Lemma 2.10 $E(T(n, \gamma)) > E(T(n - 1, \gamma))$.

Proof. $T(n - 1, \gamma) \cup K_1$ is a proper spanning subgraph of $T(n, \gamma)$, by Lemma 2.3, $E(T(n, \gamma)) > E(T(n - 1, \gamma) \cup K_1) = E(T(n - 1, \gamma))$. \square

That is to say, $E(T(n, \gamma))$ is a strictly monotonically increasing function in the variable n . Let \mathcal{T}_γ be the set of trees with given domination number γ . Then for any $T \in \mathcal{T}_\gamma$, the number of the vertices of T is at least 2γ . These facts suggest us to obtain the following result.

Corollary 2.1 Let $T \in \mathcal{T}_\gamma$, then $E(T) \geq E(T(2\gamma, \gamma))$, and equality holds if and only if $T = T(2\gamma, \gamma)$.

3 Some sharp lower bounds of energy of trees based on the domination number

In this section, we give some sharp lower bounds for energy of trees based on the domination number.

Lemma 3.1 [3] *Let v be a pendent vertex of G and u be the vertex adjacent to v . Then $\Phi(G, x) = x\Phi(G - v, x) - \Phi(G - u - v, x)$.*

Lemma 3.2

$$E(T(n, \gamma)) = 2\gamma - 4 + 2\sqrt{n - \gamma + 1 + 2\sqrt{n - 2\gamma + 1}}.$$

Proof. By Lemma 3.1, the characteristic polynomial of $T(n, \gamma)$ is

$$\Phi(T(n, \gamma)) = x^{n-2\gamma}(x^2 - 1)^{\gamma-2}[x^4 - (n - \gamma + 1)x^2 + n - 2\gamma + 1].$$

Let $x_1 > 0$, $x_2 > 0$, $-x_1$, $-x_2$ be the roots of the equation of

$$x^4 - (n - \gamma + 1)x^2 + n - 2\gamma + 1 = 0.$$

By the relation between the roots and equation,

$$\begin{aligned} (x_1 + x_2)^2 &= n - \gamma + 1 + 2\sqrt{n - 2\gamma + 1} \\ \Rightarrow x_1 + x_2 &= \sqrt{n - \gamma + 1 + 2\sqrt{n - 2\gamma + 1}}. \end{aligned}$$

So we have $E(T(n, \gamma)) = 2\gamma - 4 + 2\sqrt{n - \gamma + 1 + 2\sqrt{n - 2\gamma + 1}}$. □

Combining Theorem 2.1 and Lemma 3.2, we can get a lower bound for the energy of a tree according to its domination number and order.

Theorem 3.1 *Let T be a tree of order n , and γ be the domination number of T , then*

$$E(T) \geq 2\gamma - 4 + 2\sqrt{n - \gamma + 1 + 2\sqrt{n - 2\gamma + 1}}.$$

Equality holds if and only if $T = T(n, \gamma)$.

Observation 3.1 *From the formula for the energy of $T(n, \gamma)$, we can get the following results:*

- (1). $E(T(n, \gamma)) > E(T(n, \gamma - 1))$, for all $\gamma \geq 2$.
- (2). $E(T(n_1, \gamma_1)) > E(T(n_2, \gamma_2))$, if $n_1 \geq n_2$ and $\gamma_1 > \gamma_2$ (or $n_1 > n_2$ and $\gamma_1 \geq \gamma_2$).
- (3). Let T be a tree of order n , then

$$E(T) \geq 2\sqrt{n-1}.$$

Equality holds if and only if $T = T(n, 1)$, i.e., $T = K_{1, n-1}$.

- (4). Let T be a non-star tree of order n , then

$$E(T) \geq 2\sqrt{n-1+2\sqrt{n-3}}.$$

Equality holds if and only if $T = T(n, 2)$.

- (5). Let T be a tree with domination number γ , then

$$E(T) \geq 2\gamma - 4 + 2\sqrt{\gamma + 3}.$$

Equality holds if and only if $T = T(2\gamma, \gamma)$.

4 A more general form of Theorem 2.1

In this section, we turn to a general form of Theorem 2.1.

Definition 4.1 *We define a tree $H_T(w)$ which consists of two trees H and T , where H and T have a unique common vertex w .*

Lemma 4.1 *Let H be a tree with at least one edge, $w \in V(H)$, and T be a tree of order n . $H_n(w)$ be the tree obtained from H by attaching $n - 1$ distinct pendent edges (not in H) to w . Then $H_T(w) \succeq H_n(w)$, and equality holds if and only if $H_T(w) = H_n(w)$.*

Proof. We proceed by induction on n , the order of T .

If $n = 1$, there is nothing to prove. Now we assume our result holds for smaller values of n .

Let $u \notin V(H)$ be a pendent vertex attached to w in $H_n(w)$, x be a pendent vertex of T , and y be the unique vertex adjacent to x in T . By induction hypothesis,

$$H_T(w) - x \succeq H_{n-1}(w) = H_n(w) - u. \quad (3)$$

Since $H_n(w) - u - w = (H - w) \cup (n-2)K_1$ is a spanning subgraph of $H_T(w) - x - y$, by Lemma 2.3, $H_T(w) - x - y \succeq H_n(w) - u - w$. Thus $H_T(w) \succeq H_n(w)$ follows from Lemma 2.4.

If the equality of the result holds, in (3), $H_T(w) - x = H_{n-1}(w)$. Suppose $H_T(w) \neq H_n(w)$, then $y \neq w$. Since H has at least one edge, $H_n(w) - u - w$ is a proper spanning subgraph of $H_T(w) - x - y$, and $H_T(w) \succ H_n(w)$, which yields a contradiction. Thus $H_T(w) = H_n(w)$. \square

Lemma 4.2 *Let $T \in \mathcal{T}_{n,\gamma}$ (where $n \geq 2\gamma$), and H be a tree with at least one edge. $H_{n,\gamma}(w)$ be the tree formed from H by attaching $n - 2\gamma + 1$ distinct pendent edges and $\gamma - 1$ new pendent paths of length 2 to the vertex w of the tree H . Then $H_T(w) \succeq H_{n,\gamma}(w)$, and equality holds if and only if $H_T(w) = H_{n,\gamma}(w)$.*

The proof of the above lemma is similar to that of Lemma 2.9. Only one step is different: For $|T| = n$, when $\gamma = 1$, the result of the above lemma is not obvious, but it could follow from Lemma 4.1.

Theorem 4.1 *Let $T \in \mathcal{T}_{n,\gamma}$ (where $n \geq 2\gamma$), and H be a tree with at least one edge. $H_{n,\gamma}(w)$ be the tree formed from H by attaching $n - 2\gamma + 1$ distinct pendent edges and $\gamma - 1$ new pendent paths of length 2 to the vertex w of the tree H . Then*

$$E(H_T(w)) \geq E(H_{n,\gamma}(w)),$$

and equality holds if and only if $H_T(w) = H_{n,\gamma}(w)$.

By Theorem 4.1, we can get a simple proof of Theorem 2.1, the details are left to the reader. The following is a general form of Corollary 2.1.

Corollary 4.1 *Let $T \in \mathcal{T}_\gamma$, and H be a tree with at least one edge. $H_{2\gamma,\gamma}(w)$ be the tree formed from H by attaching one pendent edge and $\gamma - 1$ new pendent paths of length 2 to the vertex w of the tree H . Then*

$$E(H_T(w)) \geq E(H_{2\gamma,\gamma}(w)),$$

and equality holds if and only if $H_T(w) = H_{2\gamma,\gamma}(w)$.

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