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ON MINIMAL ENERGIES OF TREES WITH GIVEN DIAMETER

SHUCHAO LI† AND NANA LI†

Abstract. The energy of $G$, denoted by $E(G)$, is defined as the sum of the absolute values of the eigenvalues of $G$. In this paper, the trees with a given diameter having the minimal energy are determined by three specific tree operations; using this method, together with previous work, a conjecture proposed by B. Zhou and F. Li [J. Math. Chem., 39:465–473, 2006] is completely solved.

Key words. Energy, Tree, Pendent vertex, Diameter.

AMS subject classifications. 05C50, 05C35.

1. Introduction. Let $G$ be a graph on $n$ vertices. The eigenvalues $\lambda_1, \ldots, \lambda_n$ of an adjacency matrix of $G$ are called the eigenvalues of $G$. The energy of $G$, denoted by $E(G)$, is defined as

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

This concept was introduced by Gutman and is intensively studied in chemistry, since it can be used to approximate the total $\pi$-electron energy of a molecule (see, e.g., [5, 6]). For more details on the chemical aspects and mathematical properties of $E(G)$, see [3]-[6].

For a graph $G$, let $m(G,k)$ be the number of $k$-matchings of $G$, $k \geq 1$, and define $m(G,0) = 1$, $m(G,k) = 0$ if $k < 0$. If $G$ is an acyclic graph on $n$ vertices, then the energy of $G$ can be expressed as the Coulson integral [6]

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} \ln \left( 1 + \sum_{k=1}^{\lfloor n/2 \rfloor} m(G,k)x^{2k} \right).$$

It is easy to see that $E(G)$ is a strictly increasing function of $m(G,k)$, $k = 1, \ldots, \lfloor n/2 \rfloor$. This observation led Gutman [2] to define a quasi-order over the set of all acyclic graphs: If $G_1, G_2$ are two acyclic graphs, then

$$G_1 \succeq G_2 \iff m(G_1,k) \geq m(G_2,k) \text{ for all } k = 0, 1, \ldots, \lfloor n/2 \rfloor.$$
If \( G_1 \succeq G_2 \), and there is a \( j \) such that \( m(G_1, j) > m(G_2, j) \), then we write \( G_1 \succ G_2 \). Therefore,

\[
G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2).
\]

This increasing property of \( E \) has been successfully applied in the study of the extremal values of energy over some significant classes of graphs. Gutman \cite{2} determined trees with minimal, second-minimal, third-minimal and fourth-minimal energies, and the present authors \cite{7} determined trees with fifth-, sixth- and seventh- minimal energies. More recent results in this direction can be found in \cite{8}-\cite{15} and the references therein.

Let \( \mathcal{T}_{n,d} \) denote the set of \( n \)-vertex trees with diameter \( d \), where \( 2 \leq d \leq n - 1 \). Obviously, \( T \in \mathcal{T}_{n,2} \) is a star \( K_{1,n-1} \), while \( T \in \mathcal{T}_{n,n-1} \) is a path \( P_n \). So we assume in the following that \( 3 \leq d \leq n - 2 \). Let \( N_G(v_i) \) denote the neighborhood of the vertex \( v_i \) in \( G \). A pendant vertex is a vertex of degree one, and a pendant edge is an edge incident with a pendant vertex. A caterpillar is a tree in which a removal of all pendant vertices makes a path. Let \( T(n,d;n_1,\ldots,n_{d-1}) \in \mathcal{T}_{n,d} \) be a caterpillar obtained from a path \( v_0v_1\ldots v_d \) by adding \( n_i (n_i \geq 0) \) pendant edges to \( v_i (i = 1,\ldots,d-1) \). And in this paper, if \( T_1 \) and \( T_2 \) are isomorphic, then we denote it by \( T_1 = T_2 \).

Yan and Ye \cite{9} proved that \( T(n,d;n-d-1,0,\ldots,0) \) is the unique tree with minimal energy in \( \mathcal{T}_{n,d} \). Zhou and Li \cite{11} proved that the trees with the second-minimal energy in \( \mathcal{T}_{n,d} \) are \( T(n,d;0,0,n-d-1,0,\ldots,0) \) if \( d \geq 6 \), \( T(n,3;1,n-5) \) if \( d = 3 \), \( T(n,4;1,0,n-6) \) or \( T(n,4;0,n-5,0) \) if \( d = 4 \) \((n \geq 7)\), \( T(n,5;1,0,n-7) \) or \( T(n,5;0,n-6,0,0) \) if \( d = 5 \) \((n \geq 8)\), and they also proposed the following conjecture.

**Conjecture 1.1.** \( T(n,4;1,0,n-6) \) \((n \geq 7)\) and \( T(n,5;0,n-6,0,0) \) \((n \geq 9)\) achieve the second-minimal energy in the class of trees on \( n \) vertices and diameter \( d \) for \( d = 4 \) and \( d = 5 \), respectively.

In this paper, we use a new method to determine the trees in \( \mathcal{T}_{n,d} \) having the minimal energy, which was obtained in \cite{9} only by induction. Using this new method, we also show that Conjecture 1.1 is true for \( d = 5 \). We have showed that this conjecture is true for the case \( d = 4 \) in \cite{7}.

The following lemmas are needed for the proofs of our main results.

**Lemma 1.2** \cite{2}. Let \( G \) be a graph and \( uv \) be an edge of \( G \). Then \( m(G,k) = m(G-uv,k) + m(G-u-v,k-1) \) for all \( k \).

**Lemma 1.3** \cite{2}. For any tree \( T \neq K_{1,n-1} \), \( T(n,3;0,n-4) \) on \( n \) vertices, we have \( E(K_{1,n-1}) < E(T(n,3;0,n-4)) < E(T) \).

**Lemma 1.4** \cite{9}. Let \( G \) be a forest of order \( n(n > 1) \) and \( G' \) be a spanning subgraph (resp., a proper spanning subgraph) of \( G \). Then \( G \succeq G' \) (resp., \( G \succeq G' \)).
Lemma 1.5 ([2]). If we denote by \( G \cup H \) the graph whose components are \( G \) and \( H \), then
\[
P_1 \geq P_2 \cup P_{l-2} \geq \ldots \geq P_{2k} \cup P_{l-2k} \geq P_{2k+1} \cup P_{l-2k-1} \geq P_{2k-1} \cup P_{l-2k+1}
\]
where \( l = 4k + r \), \( 0 \leq r \leq 3 \).

2. Three specific tree operations. In this section, we introduce three specific tree operations and our technique is to employ these specific tree operations to transform tree with energy decreased after each application.

The following operation is introduced by Yu and Lv [10]. Let \( P = v_0v_1 \ldots v_k \) (\( k \geq 1 \)) be a path of a tree \( T \). If \( d_T(v_0) \geq 3 \), \( d_T(v_k) \geq 3 \) and \( d_T(v_i) = 2(0 < i < k) \), we call \( P \) an internal path of \( T \). If \( d_T(v_0) \geq 3 \), \( d_T(v_k) = 1 \) and \( d_T(v_i) = 2(0 < i < k) \), we call \( P \) a pendent path of \( T \) with root \( v_0 \), and particularly when \( k = 1 \), we call \( P \) a pendent edge. Let \( s(T) \) 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. We assume throughout this paper that \( T_{n,d} = T(n, d; n - d - 1, 0, \ldots, 0) \).

Let \( \mathcal{S}_{n,k} \) be the set of \( n \)-vertex trees with \( k \) pendent vertices. If \( T \in \mathcal{S}_{n,k} \) (\( 3 \leq k \leq n-2 \)), \( T \neq T_{n,n-k+1} \) and \( p(T) = 0 \), then we always can find two pendent vertices \( u_1 \) and \( v_1 \) of \( T \) such that \( d(u_1,v_1) = \max \{d(u,v) : u, v \in V(T)\} \). Let \( u_1u, v_1v \) be the edges in \( T \), then \( N_T(u) = \{u_1, u_2, \ldots, u_s, w\} (s \geq 2) \), \( N_T(v) = \{v_1, v_2, \ldots, v_t, w'\} (t \geq 2) \), where \( u_1, u_2, \ldots, u_s, v_1, v_2, \ldots, v_t \) are pendent vertices of \( T \), \( d_T(w) \geq 2 \) and \( d_T(w') \geq 2 \). Note that \( w = w' \), when \( d(u_1, v_1) = 3 \). If \( T' = T - \{uv_2, \ldots, vw_s\} + \{wu_2, \ldots, vu_s\} \) or \( T' = T - \{vu_2, \ldots, u_1v\} + \{wu_2, \ldots, w_t\} \), we say that \( T' \) is obtained from \( T \) by Operation I (see Figure 2.1). It is easy to see that \( T' \in \mathcal{S}_{n,k} \), \( p(T') = 1 \) and \( s(T') = s(T) - 1 \).

Lemma 2.1 ([10]). If \( T' \) is obtained from \( T \) by Operation I, then \( E(T') < E(T) \).

![Fig. 2.1. (a) ⇒ (b) by Operation I.](image)
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where \( w_j \in V(T_i), j = 1, 2, \ldots, m \) (e.g., see (a) in Figure 2.2). Choose a \( T_i \in \mathcal{T} \) such that \( |V(T_i)| = n_j > 1 \), if \( T' \) is obtained from \( T \) by replacing \( T_i \cup v_iw_j \) with \( n_j \) pendant edges \( u_1^iw_i, u_2^iw_i, \ldots, u_{n_j}^iw_i \), we say that \( T' \) is obtained from \( T \) by Operation II (see Figure 2.2). It is easy to see that \( T' \in \mathcal{T}_{n,d} \). Now we show that Operation II makes the energy of a tree decrease strictly. In the following proof, we use the same notations as above.

**Lemma 2.2.** If \( T' \) is obtained from \( T \) by Operation II (e.g., see Figure 2.2), then \( E(T') < E(T) \).

**Proof.** Let \( w_j \in T_i, w_jv_i \in T \) and \( F_j = T - V(T_i) \). By Lemma 1.2, we have

\[
m(T', k) = m(T' - u_1^iv_i, k) + m(T' - u_1^iv_i, k - 1) \\
= m(T' - u_1^iv_i, k) + m(F_j - v_i, k - 1) \\
= m(T' - u_1^iv_i - u_2^iv_i, k) + 2m(F_j - v_i, k - 1) \\
\vdots \\
= m(T' - u_1^iv_i - u_2^iv_i - \ldots - u_{n_j}^iv_i, k) + n_jm(F_j - v_i, k - 1) \\
= m(F_j, k) + n_jm(F_j - v_i, k - 1).
\] (2.1)
By Lemmas 1.2, 1.3 and 1.4, we have
\[
m(T, k) = m(T - v_i w_j, k) + m(T - v_i w_j, k - 1) \\
= m(F_j \cup T_{ij}, k) + m((F_j - v_i) \cup (T_{ij} - w_j), k - 1) \\
= \sum_{l=0}^{k} m(F_j, k-l) m(T_{ij}, l) + \sum_{l=0}^{k-1} m(F_j - v_i, k-1-l) m(T_{ij} - w_j, l) \\
> \sum_{l=0}^{k} m(F_j, k-l) m(T_{ij}, l) + m(F_j - v_i, k-1) \\
\geq \sum_{l=0}^{k} m(F_j, k-l) m(K_1, n_j, 1, l) + m(F_j - v_i, k-1) \\
\geq m(F_j, k) + (n_j - 1) m(F_j - v_i, k-1) + m(F_j - v_i, k-1) \\
= m(T', k).
\]

The last equality holds by Eq. (2.1).

It is easy to see that \( m(T, 1) = m(T', 1) \). So, \( T \succ T' \) and \( E(T) > E(T') \). \( \square \)

By Lemma 2.2, we immediately get the following result.

**Lemma 2.3.** Let \( T \in \mathcal{T}_{n,d} \) (3 \( \leq d \leq n - 2 \)), if \( T \) is not a caterpillar, then repeated using Operation II we can finally get a caterpillar \( T' \) with \( E(T') < E(T) \).

So, in what follows, we may assume that \( T \) is a caterpillar in \( \mathcal{T}_{n,d} \) and \( P = v_0 v_1 \ldots v_i \ldots v_d \) is one of the longest path in \( T \). Without loss of generality, let \( T = T(n, d; n_1, n_2, \ldots, n_{d-1}) \) and \( i = \min\{i \mid v_i \in V(P), d_T(v_i) > 2 \text{ and } 2 \leq i \leq d - 1\} \). Obviously, if \( i = d - 1 \), then \( T = T(n,d; n - d - 1,0, \ldots, 0) \), so we assume that \( 2 \leq i \leq d - 2 \). Let the \( n_i \) vertices which are adjacent to \( v_i \) are \( u_{i,1}^1, u_{i,2}^1, \ldots, u_{i,n_i}^1 \). If \( T' = T - \{u_{i,1}^1, v_i, u_{i,2}^1, \ldots, u_{i,n_i}^1\} + \{u_{i,1}^1, v_i, u_{i,2}^1, \ldots, u_{i,n_i}^1\} \), we say that \( T' \) is obtained from \( T \) by Operation III (see Figure 2.3). It is easy to see that \( T' \in \mathcal{T}_{n,d} \).

Now we show that Operation III makes the energy of a tree decrease strictly. In the following proof, we use the same notations as above.

\[\text{Fig. 2.3. (a) } T = T_{ij} : v_i T_j, \quad \text{(b) } T = T_{ij} : v_i T_j.\]
Lemma 2.4. If $T'$ is obtained from $T$ by Operation III (e.g., see Figure 2.3), then $E(T') < E(T)$.

Proof. By Lemma 1.2, we have

$$m(T, k) = m(T - v_i, v_{i+1}, k) + m(T - v_i, v_{i+1}, k - 1)$$

$$= m(T_1 ∪ T_3, k) + m((T_1 - v_i) ∪ (T_3 - v_i), k - 1)$$

$$= \sum_{j=0}^k m(T_1, k-j)m(T_3, j) + \sum_{j=0}^{k-1} m(T_1 - v_i, k - 1 - j)m(T_3 - v_i, j),$$

and

$$m(T', k) = m(T' - v_i, v_{i+1}, k) + m(T' - v_i, v_{i+1}, k - 1)$$

$$= m(T_1 ∪ T_3, k) + m((T_1 - v_i) ∪ (T_3 - v_i), k - 1)$$

$$= \sum_{j=0}^k m(T_1, k-j)m(T_3, j) + \sum_{j=0}^{k-1} m(T_1 - v_i, k - 1 - j)m(T_3 - v_i, j).$$

So,

$$m(T, k) - m(T', k) = \sum_{j=0}^k m(T_1, k-j)(m(T_3, j) - m(T_4, j))$$

$$+ \sum_{j=0}^{k-1} m(T_1 - v_i, k - 1 - j)(m(T_3 - v_i, j) - m(T_4 - v_i, j)).$$

We have $m(T_3, j) = m(T_3 - \{u_1^i v_i, \ldots, u_{n_i}^i v_i\}, j) + n_i m(T_3 - \{v_i, u_1^i, \ldots, u_{n_i}^i\}, j - 1)$ (resp., $m(T_4, j) = m(T_4 - \{u_1^i v_1, \ldots, u_{n_i}^i v_1\}, j) + n_i m(P_{i-1}, j - 1)$), according to the vertices $u_1^i, \ldots, u_{n_i}^i$ are saturated or not in the $j$-matchings of $T_3$ (resp., $T_4$). And also, $m(T_3 - \{u_1^i, \ldots, u_{n_i}^i\}, v_i, j - 1) = m(P_{i-1}, j - 1) + n_i m(P_{i-2}, j - 2)$ according to the vertices $u_1^i, \ldots, u_{n_i}^i$ are saturated or not in the $(j - 1)$-matchings of $T_3 - \{v_i, u_1^i, \ldots, u_{n_i}^i\}$. Note that $T_3 - \{u_1^i v_i, \ldots, u_{n_i}^i v_i\} = T_4 - \{u_1^i v_1, \ldots, u_{n_i}^i v_1\}$. Define $m(P_0, 0) = 1$ and $m(P_0, k) = 0$ for $k > 0$, and hence,

$$m(T_3, j) - m(T_4, j) = n_i[m(P_i, j - 1) + n_i m(P_{i-2}, j - 2) - m(P_{i-1}, j - 1)]$$

$$= n_i(n_1 + 1)m(P_{i-2}, j - 2).$$

We denote $T_3 - v_i$ (resp., $T_4 - v_i$) by $T_2$ (resp., $T_3$). If $i \geq 3$, we have

$$m(T_2, j) = m(T_2 - v_1, v_2, j) + m(T_2 - v_i, v_{i-1}, j - 1)$$

$$= m(P_{i-2} ∪ K_{1,n_1+1}, j) + m(P_{i-3}, j - 1)$$

$$= m(P_{i-2}, j) + (n_1 + 1)m(P_{i-2}, j - 1) + m(P_{i-3}, j - 1),$$
and similarly, \( m(T_5, j) = m(P_{i-2}, j) + (n_i + n_1 + 1)m(P_{i-2}, j - 1) + m(P_{i-3}, j - 1) \).

So,
\[
m(T_3 - v_i, j) - m(T_4 - v_i, j) = -n_i m(P_{i-2}, j - 1).
\]

And if \( i = 2 \), then
\[
m(T_2, j) - m(T_5, j) = m(K_{1,n_1+1}, j) - m(K_{1,n_1+n_1+1}, j)
= -n_i m(P_0, j - 1) = \begin{cases} -n_i, & \text{if } j = 1; \\ 0, & \text{otherwise.} \end{cases}
\]

Therefore,
\[
m(T, k) - m(T', k) = n_i \sum_{j=0}^{k} m(T_1, k - j)(n_1 + 1)m(P_{i-2}, j - 2)
\quad - n_i \sum_{j=0}^{k-1} m(T_1 - v_{i+1}, k - 1 - j)m(P_{i-2}, j - 1)
\quad + n_i \sum_{j=0}^{k-2} m(T_1, j)(n_1 + 1)m(P_{i-2}, k - 2 - j)
\quad - n_i \sum_{j=0}^{k-1} m(T_1 - v_{i+1}, j)m(P_{i-2}, k - 2 - j)
\quad = n_i \sum_{j=0}^{k-2} m(P_{i-2}, k - 2 - j)((n_1 + 1)m(T_1, j) - m(T_1 - v_{i+1}, j))
\quad \geq n_i \sum_{j=0}^{k-2} m(P_{i-2}, k - 2 - j)(m(T_1, j) - m(T_1 - v_{i+1}, j)) \geq 0.
\]

If \( i \neq d - 1 \), then
\[
m(T, 3) - m(T', 3) \geq n_i \sum_{j=0}^{1} m(P_{i-2}, 1 - j)(m(T_1, j) - m(T_1 - v_{i+1}, j))
\geq n_i m(P_{i-2}, 0)(m(T_1, 1) - m(T_1 - v_{i+1}, 1)) > 0.
\]

So, \( T \succ T' \) and \( E(T) > E(T') \) in this case.

If \( i = d - 1 \), then Operation III is a special case of Operation I, and in this case, Lemma 2.1 yields \( E(T') < E(T) \). Therefore, our result holds. \( \square \)

3. Main results. In this section, we determine the tree with minimum energy among \( \mathcal{T}_{n,d} \) by a new method. Furthermore, we determine the trees with the second minimal energy among \( \mathcal{T}_{n,d} \) for \( 3 \leq d \leq 5 \).
From Lemma 2.4, we immediately get the following result.

**Lemma 3.1.** Let \( T \in \mathcal{T}_{n,d} \) \((3 \leq d \leq n - 2)\) and \( T \) be a caterpillar. Then by repeating Operation I, we can finally get the tree \( T_{n,d} \) with \( E(T_{n,d}) < E(T) \).

So we get the following result.

**Theorem 3.2** ([9]). Let \( T \in \mathcal{T}_{n,d} \) and \( T \neq T_{n,d} \). Then \( E(T) > E(T_{n,d}) \), i.e., \( T_{n,d} \) is the unique tree with the minimum energy among trees in \( \mathcal{T}_{n,d} \).

Let \( a(T) \) be the number of vertices in the path \( P = v_0 v_1 \ldots v_d \) with degree more than 2. Let \( T \in \mathcal{T}_{n,d} \) and \( T \neq T_{n,d} \). If \( a(T) = 1 \), we can finally get \( T' = T(n, d; 0, \ldots, 0, n_i, 0, \ldots, 0) \) by a series of Operation II, where \( n_i = n - (d + 1) \) for \( i \neq 1, d - 1 \). If \( a(T) \geq 2 \), we can finally get a caterpillar \( T' \) and \( a(T') = a(T) \) by a series of Operation II. Therefore, if we denote the series of Operations II or III from \( T \) to \( T_{n,d} \) as follows:

\[
T = T_0 \Rightarrow T_1 \Rightarrow T_2 \Rightarrow \cdots \Rightarrow T_{m-1} \Rightarrow T_m = T_{n,d},
\]

then \( T_m \) is obtained from \( T_{m-1} \) by only one time of Operation III. Let \( \mathcal{T}_1 = \{ T | T \neq T_{n,d} \text{ and } T_{n,d} \text{ can be obtained from } T \text{ through Operation III once} \} \), then the tree in \( \mathcal{T}_{n,d} \) of the second minimal energy lies in \( \mathcal{T}_1 \). In fact, it is the tree in \( \mathcal{T}_1 \) of the minimum energy.

If \( a(T) = 1 \), then \( \mathcal{T}_1 = \{ T(n, d; 0, \ldots, 0, n_i = n - (d + 1), 0, \ldots, 0) | 2 \leq i \leq d - 2 \} \), we will show that the tree with the minimum energy among \( \mathcal{T}_1 \) is \( T(n, d; 0, 0, n - (d + 1), 0, \ldots, 0) \). If \( a(T) \geq 2 \), then

\[
\mathcal{T}_1 = \{ T(n, d; 0, \ldots, 0, n, 0, \ldots, 0, n_{d-1}) | n_i + n_{d-1} = n - (d + 1), n_i \geq 1 \},
\]

we will show that via this case the tree with the minimum energy in \( \mathcal{T}_1 \) is \( T(n, d; 1, 0, \ldots, 0, n - d - 2) \). And at last, we compare the energy between \( T(n, d; 0, 0, n - (d + 1), 0, \ldots, 0) \) and \( T(n, d; 1, 0, \ldots, 0, n - d - 2) \).

**Lemma 3.3.** If \( a(T) = 1 \), then the tree with the minimum energy in \( \mathcal{T}_1 \) is \( T(n, d; 0, 0, n - (d + 1), 0, \ldots, 0) \) for \( 4 \leq d \leq n - 2 \).

**Proof.** Since \( a(T) = 1 \) and Operation II does not change the number of vertices in \( v_0 v_1 \ldots v_d \) with degree more than 2, we can finally get a caterpillar \( T' \) and \( a(T') = a(T) = 1 \) by a series of Operation II. Then we can get \( T_{n,d} \) from \( T' \) by applying Operation III once. Hence,

\[
\mathcal{T}_1 = \{ T(n, d; 0, \ldots, 0, n_i, 0, \ldots, 0) | n_i = n - (d + 1), i \neq 1, d - 1 \}.
\]

Let \( T_i \in \mathcal{T}_1 \), and suppose that the \( n_i \) vertices which are adjacent to \( v_i \) are \( u_1, \ldots, u_{n_i} \). Then

\[
m(T_i, k) = m(P_{d+1}, k) + (n - (d + 1))m(P_i \cup P_{d-1}, k - 1) \text{ for all } k,
\]
according to the vertices $u_1, \ldots, u_n$, are saturated or not in the $k$-matchings of $T_i$. Note that $i \neq 1, d - 1$. Then we have $m(P_i \cup P_{d-i}, k - 1) \geq m(P_1 \cup P_{d-1}, k - 1)$ by Lemma 1.5. Therefore, the result follows. \(\square\)

**Lemma 3.4.** If $a(T) \geq 2$, then the tree with the minimum energy in $T_i$ is $T(n, d; 1, 0, \ldots, n - d - 2)$ for $3 \leq d \leq n - 2$.

**Proof.** It is easy to see that we can finally get a caterpillar $T'$ and $a(T') = a(T) \geq 2$ by a series of Operation II. Then we can get $T_{n,d}$ from $T'$ by one or more times of Operation III. Hence,

$$\mathcal{G}_1 = \{T(n, d; 0, \ldots, 0, i, 0, \ldots, 0, n_{d-1}) \mid n_i + n_{d-1} = n - (d + 1),$$

$$n_i \geq 1, \text{and } i \neq d - 1\}.$$ 

Let $n_i = s$ and $n_{d-1} = t$ be fixed. We shall show that

$$T(n, d; 0, \ldots, n_i = s, 0, \ldots, n_{d-1} = t) \succ T(n, d; s, 0, \ldots, 0, t), \text{ if } i \neq 1.$$ 

Let $T(n, d; 0, \ldots, n_i = s, 0, \ldots, n_{d-1} = t) = T_1$ and $T(n, d; s, 0, \ldots, 0, t) = T_2$. Then

$$m(T_1, k) = tm(T(n - (t + 2), d - 2; 0, \ldots, 0, n_i, 0, \ldots, 0), k - 1)$$

$$+ m(T(n - t, d; 0, \ldots, 0, n_i, 0, \ldots, 0), k),$$

and

$$m(T_2, k) = tm(T(n - (t + 2), d - 2; s, 0, \ldots, 0), k - 1) + m(T(n - t, d; s, 0, \ldots, 0), k).$$

Then by Theorem 3.2,

$$T(n - (t + 2), d - 2; s, 0, \ldots, 0) \prec T(n - (t + 2), d - 2; 0, \ldots, 0, n_i, 0, \ldots, 0)$$

and $T(n - t, d; s, 0, \ldots, 0) \prec T(n - t, d; 0, \ldots, 0, n_i, 0, \ldots, 0)$ if $i \neq 1$. So we have $m(T_1, k) \geq m(T_2, k)$ and $m(T_1, k) = m(T_2, k)$ for all $k$ if and only if $i = 1$. Hence, $T_1 \succ T_2$ and

$$E(T(n, d; 0, \ldots, 0, n_i = s, 0, \ldots, t)) > E(T(n, d; n_1 = s, 0, \ldots, 0, t)), \text{ if } i \neq 1.$$ 

In the following, we shall show that

$$T(n, d; s, 0, \ldots, t) \succ T(n, d; 1, 0, \ldots, 0, s + t - 1), \text{ if } s > 1.$$ 

Without loss of generality, we may assume that $s \leq t$. Let

$$T_0 = T(n, d; s, 0, \ldots, 0, t) \text{ and } T_0' = T(n, d; 1, 0, \ldots, 0, s + t - 1).$$
Let the \( s \) vertices which are adjacent to \( v_1 \) in \( T_0 \) be \( u_1, \ldots, u_s \), and suppose that there are \( s + t - 1 \) vertices \( u_1', \ldots, u_s', u_1'', \ldots, u_{s-1}' \) that are adjacent to \( v_{d-1} \) in \( T'_0 \). For all \( k \), we have
\[
m(T_0, k) = m(T(n - s + 1, d; 1, 0, \ldots, 0), k) \\
+ (s - 1)m(T(n - s - 2, d - 2; 0, \ldots, 0), k - 1),
\]
(resp.,
\[
m(T'_0, k) = m(T(n - s + 1, d; 1, 0, \ldots, 0), k) \\
+ (s - 1)m(T(n - s - t, d - 2; 1, 0, \ldots, 0), k - 1)),
\]
according to the vertices \( u_1, \ldots, u_{s-1} \) are saturated or not in the \( k \)-matchings of \( T_0 \) (resp., \( u_1', \ldots, u_{s-1}' \) are saturated or not in the \( k \)-matchings of \( T'_0 \)). Note that \( t \geq s > 1 \). Then \( T(n - s - t, d - 2; 1, 0, \ldots, 0) \) is a proper subgraph of \( T(n - s - 2, d - 2; 0, \ldots, 0) \), hence by Lemma 1.3, \( T(n - s - 2, d - 2; 0, \ldots, 0) \) is greater than \( T(n - s - t, d - 2; 1, 0, \ldots, 0) \).

Therefore, \( m(T_0, k) \geq m(T'_0, k) \) and there exists a \( j \), such that \( m(T_0, j) > m(T'_0, j) \).

So, \( T_0 \succ T'_0 \) and \( E(T_0) > E(T'_0) \). The lemma thus follows. \( \square \)

**Lemma 3.5.** \( E(T(n, 5; 0, 0, n - 6, 0)) > E(T(n, 5; 1, 0, 0, n - 7)) \) for \( n \geq 9 \).

**Proof.** Let \( T_n := T(n, 5; 0, 0, n - 6, 0) \) and \( T'_n := T(n, 5; 1, 0, 0, n - 7) \). It is easy to see that for all \( k \),
\[
m(T_n, k) = m(P_6, k) + (n - 6)m(P_2 \cup P_3, k - 1)
\]
and
\[
m(T'_n, k) = m(P_6, k) + (n - 7)(m(P_4, k - 1) + m(P_2, k - 2)).
\]

So, \( m(T_n, 0) = m(T'_n, 0) = 1, m(T_n, 1) = m(T'_n, 1) = n - 1, m(T_n, 2) = 3n - 12, m(T'_n, 2) = 4n - 19, m(T_n, 3) = 2n - 11, m(T'_n, 3) = 2n - 12, m(T_n, k) = 0 \) if \( k \geq 4 \), and \( m(T'_n, k) = 0 \) if \( k \geq 4 \).

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

Hence,
\[
E(T_n) - E(T'_n) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \frac{1 + (n - 1)x^2 + (3n - 12)x^4 + (2n - 11)x^6}{1 + (n - 1)x^2 + (4n - 19)x^4 + (2n - 12)x^6}.
\]

For a fixed \( x > 0 \), let \( f(y) := \frac{1 + (y - 1)x^2 + (3y - 12)x^4 + (2y - 11)x^6}{1 + (y - 1)x^2 + (4y - 19)x^4 + (2y - 12)x^6} \). Then we have that
\[
f'(y) = -\frac{2x^{12} - 6x^{10} - 10x^8 - 6x^6 - x^4}{[1 + (y - 1)x^2 + (4y - 19)x^4 + (2y - 12)x^6]^2} < 0.
\]
So, $f(n)$ is a strictly decrease function of $n$. Therefore, for all $n \geq 9$, we have that $E(T_n) - E(T'_n) \leq E(T_9) - E(T'_9) < 0$. The result thus follows.

**Theorem 3.6.** Among the trees in $\mathcal{T}_{n,d}$,

(i) $T(n, 3; 1, n-5)$ is the unique tree achieving the second-minimal energy in the class of trees on $n$ vertices and diameter $d$ for $d = 3$.

(ii) $T(n, 4; 1, 0, n-6)(n \geq 7)$ is the unique tree achieving the second-minimal energy in the class of trees on $n$ vertices and diameter $d$ for $d = 4$.

(iii) $T(n, 5; 0, n-6, 0, 0)$ ($n \geq 9$) is the unique tree achieving the second-minimal energy in the class of trees on $n$ vertices and diameter $d$ for $d = 5$.

**Proof.** Here we should only prove (i) and (iii). For the proof of (ii), see [7].

(i) When $d(T) = 3$, it is easy to see that if $a(T) = 1$, then we have $\mathcal{T}_1 = \emptyset$; otherwise, by Lemma 3.4, the tree with the minimum energy in $\mathcal{T}_1$ is $T(n, 3; 1, 0, n-5)$. Therefore, $T(n, 3; 1, 0, n-5)$ is the unique tree achieving the second-minimal energy in the class of trees on $n$ vertices and diameter $d$ for $d = 3$.

(iii) Combining Lemmas 1.5, 3.4 and 3.5 implies that $T(n, 5; 0, n-6, 0, 0)$ ($n \geq 9$) is the unique tree achieving the second-minimal energy in the class of trees on $n$ vertices and diameter $d$ for $d = 5$.

**Remark.** (1) By (ii) and (iii) of Theorem 3.6, Conjecture 1.1 is completely solved by us.

(2) For $n \leq 10$, by Appendix of tables of graph spectra in the book: Spectra of Graphs [1], when $n = 9$, $T(9, 5; 0, 3, 0, 0)$ has the second-minimal energy among $\mathcal{T}_{9,5}$ and when $n = 10$, $T(10, 5; 0, 4, 0, 0)$ has the second-minimal energy among $\mathcal{T}_{10,5}$, which are examples that confirm our results.

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**REFERENCES**


Minimal Energies of Trees with Given Diameter


