Electronic Journal of Linear Algebra

Volume 17 *ELA Volume 17 (2008)* Article 29

2008

On minimal energies of trees with given diameter

Shuchao Li
lscmath@mail.ccnu.edu.cn

Nana Li

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

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

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

This concept was introduced by Gutman and is intensively studied in chemistry, since it can be used to approximate the total π-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]

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

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

$$G_1 \succeq G_2 \Leftrightarrow m(G_1,k) \geq m(G_2,k) \text{ for all } k = 0, 1, \ldots, \left\lfloor \tfrac{n}{2} \right\rfloor.$$

*Received by the editors January 7, 2008. Accepted for publication August 17, 2008. Handling Editor: Stephen J. Kirkland.

†Faculty of Mathematics and Statistics, Central China Normal University, Wuhan 430079, P.R. China (lscmath@mail.ccnu.edu.cn, Shuchao Li). The research was partially supported by National Science Foundation of China (Grant No. 10671081).

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

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 [2] determined trees with minimal, second-minimal, third-minimal and fourth-minimal energies, and the present authors [7] determined trees with fifth-, sixth- and seventh- minimal energies. More recent results in this direction can be found in [8]-[15] and the references therein.

Let $\mathscr{T}_{n,d}$ denote the set of n-vertex trees with diameter d, where $2 \leq d \leq n-1$. Obviously, $T \in \mathscr{T}_{n,2}$ is a star $K_{1,n-1}$, while $T \in \mathscr{T}_{n,n-1}$ 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 *pendent vertex* is a vertex of degree one, and a *pendent edge* is an edge incident with a pendent vertex. A *caterpillar* is a tree in which a removal of all pendent vertices makes a path. Let $T(n, d; n_1, \ldots, n_{d-1}) \in \mathscr{T}_{n,d}$ be a caterpillar obtained from a path $v_0 v_1 \ldots v_d$ by adding $n_i (n_i \geq 0)$ pendent 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 [9] proved that $T(n, d; n-d-1, 0, \ldots, 0)$ is the unique tree with minimal energy in $\mathscr{T}_{n,d}$. Zhou and Li [11] proved that the trees with the second-minimal energy in $\mathscr{T}_{n,d}$ 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 $d = 4$ $(n \geq 7)$, $T(n, 5; 1, 0, 0, n-7)$ 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 $\mathscr{T}_{n,d}$ having the minimal energy, which was obtained in [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 [7].

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

Lemma 1.2 ([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 ([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 ([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., $G \succ G'$).*

LEMMA 1.5 ([2]). *If we denote by $G \cup H$ the graph whose components are G and H, then*

$$P_l \succeq P_2 \cup P_{l-2} \succeq \ldots \succeq P_{2k} \cup P_{l-2k} \succeq P_{2k+1} \cup P_{l-2k-1} \succeq P_{2k-1} \cup P_{l-2k+1}$$
$$\succeq \ldots P_3 \cup P_{l-3} \succeq P_1 \cup P_{l-1},$$

where $l = 4k + r$, $0 \le r \le 3$.

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.

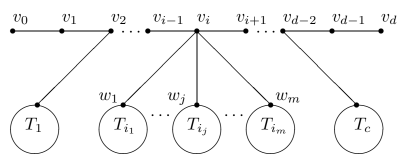
The following operation is introduced by Yu and Lv [10]. Let $P = v_0v_1 \ldots v_k$ $(k \ge 1)$ be a path of a tree T. If $d_T(v_0) \ge 3$, $d_T(v_k) \ge 3$ and $d_T(v_i) = 2(0 < i < k)$, we call P an internal path of T. If $d_T(v_0) \ge 3$, $d_T(v_k) = 1$ and $d_T(v_i) = 2(0 < i < k)$, we call P a 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 $\mathscr{S}_{n,k}$ be the set of n-vertex trees with k pendent vertices. If $T \in \mathscr{S}_{n,k}$ $(3 \le k \le n - 2)$, $T \ne T_{n,n-k+1}$ 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 $N_T(u) = \{u_1, u_2, \ldots, u_s, w\}(s \ge 2)$, $N_T(v) = \{v_1, v_2, \ldots, v_t, w'\}(t \ge 2)$, where $u_1, u_2, \ldots, u_s, v_1, v_2, \ldots, v_t$ are pendent vertices of T, $d_T(w) \ge 2$ and $d_T(w') \ge 2$. Note that $w = w'$, when $d(u_1, v_1) = 3$. If $T' = T - \{uu_2, \ldots, uu_s\} + \{vu_2, \ldots, vu_s\}$ or $T' = T - \{vv_2, \ldots, vv_t\} + \{uv_2, \ldots, uv_t\}$, we say that T' is obtained from T by **Operation I** (see Figure 2.1). It is easy to see that $T' \in \mathscr{S}_{n,k}$, $p(T') = 1$ and $s(T') = s(T) - 1$.

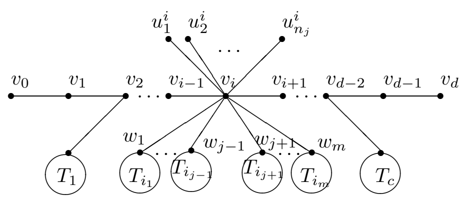
LEMMA 2.1 ([10]). *If T' is obtained from T by Operation* I, *then $E(T') < E(T)$.*

FIG. 2.1. *(a) $\Rightarrow$ (b) by Operation* I.

If $T \in \mathscr{T}_{n,d}$ $(3 \le d \le n-2)$, then we can always find two pendent vertices v_0 and v_d of T such that $d(v_0, v_d) = \max\{d(u, v) : u, v \in V(T)\}$. Let $P = v_0v_1 \ldots v_i \ldots v_d$ be one of the longest path in T, and $\mathscr{T} = \{T_1, \ldots, T_c\}$ be the set of connected components of $T - \{v_0, \ldots, v_d\}$. If $v_i \in V(P)$ $(1 \le i \le d-1)$, then $N_T(v_i) = \{v_{i-1}, v_{i+1}, w_1, \ldots, w_m\}$, where $w_j \in V(T_{i_j})$, $j = 1, 2, \ldots, m$ (e.g., see (a) in Figure 2.2). Choose a $T_{i_j} \in \mathscr{T}$ such that $|V(T_{i_j})| = n_j > 1$, if T' is obtained from T by replacing $T_{i_j} \cup v_i w_j$ with n_j pendent edges $u_1^i v_i, u_2^i v_i, \ldots, u_{n_j}^i v_i$, we say that T' is obtained from T by **Operation II** (see Figure 2.2). It is easy to see that $T' \in \mathscr{T}_{n,d}$. 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.



(a). T



(b). T'

FIG. 2.2. *(a) ⇒ (b) by Operation II.*

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 $w_j \in T_{i_j}$, $w_j v_i \in T$ and $F_j = T - V(T_{i_j})$. By Lemma 1.2, we have

$$\begin{aligned}
m(T', k) &= m(T' - u_1^i v_i, k) + m(T' - u_1^i - v_i, k-1) \\
&= m(T' - u_1^i v_i, k) + m(F_j - v_i, k-1) \\
&= m(T' - u_1^i v_i - u_2^i v_i, k) + 2m(F_j - v_i, k-1) \\
&\vdots \\
&= m(T' - u_1^i v_i - u_2^i v_i - \ldots - u_{n_j}^i v_i, k) + n_i m(F_j - v_i, k-1) \\
&= m(F_j, k) + n_j m(F_j - v_i, k-1). \qquad (2.1)
\end{aligned}$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

By Lemmas 1.2, 1.3 and 1.4, we have

$$\begin{aligned}
m(T,k) &= m(T-v_iw_j,k)+m(T-v_i-w_j,k-1)\\
&= m(F_j\cup T_{i_j},k)+m((F_j-v_i)\cup(T_{i_j}-w_j),k-1)\\
&= \sum_{l=0}^{k} m(F_j,k-l)m(T_{i_j},l)+\sum_{l=0}^{k-1} m(F_j-v_i,k-1-l)m(T_{i_j}-w_j,l)\\
&> \sum_{l=0}^{k} m(F_j,k-l)m(T_{i_j},l)+m(F_j-v_i,k-1)\\
&\geq \sum_{l=0}^{k} m(F_j,k-l)m(K_{1,n_j-1},l)+m(F_j-v_i,k-1)\\
&\geq m(F_j,k)+(n_j-1)m(F_j-v_i,k-1)+m(F_j-v_i,k-1)\\
&= m(T',k).
\end{aligned}$$

The last equality holds by Eq. (2.1).

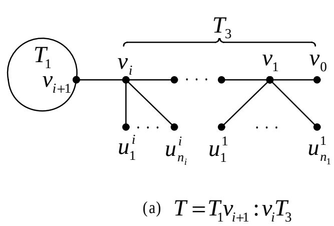
It is easy to see that $m(T,1)=m(T',1)$. So, $T \succ T'$ and $E(T)>E(T')$. ☐

By Lemma 2.2, we immediately get the following result.

LEMMA 2.3. *Let $T\in\mathscr{T}_{n,d}$ $(3\leq d\leq n-2)$, 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 $\mathscr{T}_{n,d}$ and $P=v_0v_1\ldots v_i\ldots v_d$ 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 $i=\min\{i|v_i\in V(P),d_T(v_i)>2 \text{ and } 2\leq i\leq d-1\}$. 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 $u_1^i,u_2^i,\ldots,u_{n_i}^i$. If $T'=T-\{u_1^iv_i,\ldots,u_{n_i}^iv_i\}+\{u_1^iv_1,\ldots,u_{n_i}^iv_1\}$, we say that T' is obtained from T by **Operation Ⅲ** (see Figure 2.3). It is easy to see that $T'\in\mathscr{T}_{n,d}$.

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.



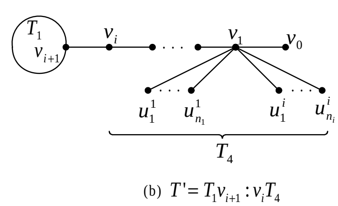


FIG. 2.3. *(a) ⇒ (b) by Operation* Ⅲ.

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

ELA
http://math.technion.ac.il/iic/ela

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

$$\begin{aligned} m(T,k) &= m(T - v_iv_{i+1}, k) + m(T - v_i - v_{i+1}, k-1) \\ &= m(T_1 \cup T_3, k) + m((T_1 - v_{i+1}) \cup (T_3 - v_i), k-1) \\ &= \sum_{j=0}^{k} m(T_1, k-j)m(T_3, j) + \sum_{j=0}^{k-1} m(T_1 - v_{i+1}, k-1-j)m(T_3 - v_i, j), \end{aligned}$$

and

$$\begin{aligned} m(T',k) &= m(T' - v_iv_{i+1}, k) + m(T' - v_i - v_{i+1}, k-1) \\ &= m(T_1 \cup T_4, k) + m((T_1 - v_{i+1}) \cup (T_4 - v_i), k-1) \\ &= \sum_{j=0}^{k} m(T_1, k-j)m(T_4, j) + \sum_{j=0}^{k-1} m(T_1 - v_{i+1}, k-1-j)m(T_4 - v_i, j). \end{aligned}$$

So,

$$\begin{aligned} m(T,k) - m(T',k) = &\sum_{j=0}^{k} m(T_1, k-j)(m(T_3, j) - m(T_4, j)) \\ &+ \sum_{j=0}^{k-1} m(T_1 - v_{i+1}, k-1-j)(m(T_3 - v_i, j) - m(T_4 - v_i, j)). \end{aligned}$$

We have $m(T_3, j) = m(T_3 - \{u_1^i v_i, \dots, u_{n_i}^i v_i\}, j) + n_i m(T_3 - \{v_i, u_1^i, \dots, u_{n_i}^i\}, j-1)$ (resp., $m(T_4, j) = m(T_4 - \{u_1^i v_1, \dots, u_{n_1}^i v_1\}, j) + n_i m(P_{i-1}, j-1)$), according to the vertices $u_1^i, \dots, u_{n_i}^i$ are saturated or not in the j-matchings of T_3 (resp., T_4). And also, $m(T_3 - \{u_1^i, \dots, u_{n_i}^i, v_i\}, j-1) = m(P_i, j-1) + n_1 m(P_{i-2}, j-2)$ according to the vertices $u_1^1, \dots, u_{n_1}^1$ are saturated or not in the $(j-1)$-matchings of $T_3 - \{v_i, u_1^i, \dots, u_{n_i}^i\}$. Note that $T_3 - \{u_1^i v_i, \dots, u_{n_i}^i v_i\} = T_4 - \{u_1^i v_1, \dots, u_{n_i}^i v_1\}$. Define $m(P_0, 0) = 1$ and $m(P_0, k) = 0$ for $k > 0$, and hence,

$$\begin{aligned} m(T_3, j) - m(T_4, j) &= n_i[m(P_i, j-1) + n_1 m(P_{i-2}, j-2) - m(P_{i-1}, j-1)] \\ &= n_i(n_1+1)m(P_{i-2}, j-2). \end{aligned}$$

We denote $T_3 - v_i$ (resp., $T_4 - v_i$) by T_2 (resp., T_5). If $i \geq 3$, we have

$$\begin{aligned} m(T_2, j) &= m(T_2 - v_1v_2, j) + m(T_2 - v_1 - v_2, j-1) \\ &= m(P_{i-2} \cup K_{1,n_1+1}, j) + m(P_{i-3}, j-1) \\ &= m(P_{i-2}, j) + (n_1+1)m(P_{i-2}, j-1) + m(P_{i-3}, j-1), \end{aligned}$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

ELA
http://math.technion.ac.il/iic/ela

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

$$\begin{aligned} m(T_2, j) - m(T_5, j) &= m(K_{1,n_1+1}, j) - m(K_{1,n_i+n_1+1}, j) \\ &= -n_i m(P_0, j-1) = \begin{cases} -n_i, & \text{if } j = 1; \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

Therefore,

$$\begin{aligned} m(T,k) - m(T',k) &= n_i \sum_{j=0}^{k} m(T_1, k-j)(n_1+1)m(P_{i-2}, j-2) \\ &\quad - n_i \sum_{j=0}^{k-1} m(T_1 - v_{i+1}, k-1-j)m(P_{i-2}, j-1) \\ &= n_i \sum_{j=0}^{k-2} m(T_1, j)(n_1+1)m(P_{i-2}, k-2-j) \\ &\quad - n_i \sum_{j=0}^{k-1} m(T_1 - v_{i+1}, j)m(P_{i-2}, k-2-j) \\ &= n_i \sum_{j=0}^{k-2} m(P_{i-2}, k-2-j)((n_1+1)m(T_1, j) - m(T_1 - v_{i+1}, j)) \\ &\geq n_i \sum_{j=0}^{k-2} m(P_{i-2}, k-2-j)(m(T_1, j) - m(T_1 - v_{i+1}, j)) \geq 0. \end{aligned}$$

If $i \neq d-1$, then

$$\begin{aligned} m(T,3) - m(T',3) &\geq n_i \sum_{j=0}^{1} m(P_{i-2}, 1-j)(m(T_1, j) - m(T_1 - v_{i+1}, j)) \\ &\geq n_i m(P_{i-2}, 0)(m(T_1, 1) - m(T_1 - v_{i+1}, 1)) > 0. \end{aligned}$$

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. □

3. Main results. In this section, we determine the tree with minimum energy among $\mathscr{T}_{n,d}$ by a new method. Furthermore, we determine the trees with the second minimal energy among $\mathscr{T}_{n,d}$ for $3 \leq d \leq 5$.

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

ELA
http://math.technion.ac.il/iic/ela

From Lemma 2.4, we immediately get the following result.

LEMMA 3.1. *Let $T \in \mathscr{T}_{n,d}$ $(3 \leq d \leq n-2)$ 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 $T \in \mathscr{T}_{n,d}$ 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 $\mathscr{T}_{n,d}$.*

Let $a(T)$ be the number of vertices in the path $P = v_0v_1 \dots v_d$ with degree more than 2. Let $T \in \mathscr{T}_{n,d}$ and $T \neq T_{n,d}$. If $a(T) = 1$, we can finally get $T' = T(n, d; 0, \dots, 0, n_i, 0, \dots, 0)$ 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

$$\mathscr{T}_1 = \{T | T \neq T_{n,d} \text{ and } T_{n,d} \text{ can be obtained from } T \text{ through Operation Ⅲ once}\},$$

then the tree in $\mathscr{T}_{n,d}$ of the second minimal energy lies in $\mathscr{T}_1$. In fact, it is the tree in $\mathscr{T}_1$ of the minimum energy.

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

$$\mathscr{T}_1 = \{T(n, d; 0, \dots, n_i, 0, \dots, 0, n_{d-1}) | n_i + n_{d-1} = n-(d+1), n_i \geq 1\},$$

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

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

Proof. Since $a(T) = 1$ and Operation Ⅱ does not change the number of vertices in $v_0v_1 \dots v_d$ 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,

$$\mathscr{T}_1 = \{T(n, d; 0, \dots, 0, n_i, 0, \dots, 0) | n_i = n-(d+1), i \neq 1, d-1\}.$$

Let $T_i \in \mathscr{T}_1$, and suppose that the n_i vertices which are adjacent to v_i are $u_1, \dots, u_{n_i}$. Then

$$m(T_i, k) = m(P_{d+1}, k) + (n-(d+1))m(P_i \cup P_{d-i}, k-1) \text{ for all } k,$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

ELA
http://math.technion.ac.il/iic/ela

according to the vertices $u_1, \ldots, u_{n_i}$ are saturated or not in the k-matchings of T_i. Note that $i \neq 1, d-1$. Then we have $m(P_i \cup P_{d-i}, k-1) \geq m(P_3 \cup P_{d-3}, k-1)$ by Lemma 1.5. Therefore, the result follows. □

Lemma 3.4. *If $a(T) \geq 2$, then the tree with the minimum energy in $\mathscr{T}_1$ 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,

$$\mathscr{T}_1 = \{T(n, d; 0, \ldots, 0, n_i, 0, \ldots, 0, n_{d-1}) | n_i + n_{d-1} = n - (d+1), \\ n_i \geq 1, \text{and } i \neq d-1\}.$$

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

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

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

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

In the following, we shall show that

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

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

$$T_0 = T(n, d; s, 0, \ldots, 0, t) \text{ and } T_0' = T(n, d; 1, 0, \ldots, 0, s+t-1).$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

ELA
http://math.technion.ac.il/iic/ela

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 $u'_1, \ldots, u'_s, w'_1, \ldots, w'_{t-1}$ that are adjacent to v_{d-1} in T'_0. For all k, we have

$$\begin{aligned} m(T_0, k) &= m(T(n-s+1, d; 1, 0, \ldots, 0, t), k) \\ &\quad + (s-1)m(T(n-s-2, d-2; 0, \ldots, 0, t), k-1), \end{aligned}$$

(resp.,

$$\begin{aligned} m(T'_0, k) &= m(T(n-s+1, d; 1, 0, \ldots, 0, t), k) \\ &\quad + (s-1)m(T(n-s-t, d-2; 1, 0, \ldots, 0), k-1)), \end{aligned}$$

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 $T(n-s-2, d-2; 0, \ldots, t)$, hence by Lemma 1.3, $T(n-s-2, d-2; 0, \ldots, t) \succ T(n-s-t, d-2; 1, 0, \ldots, 0)$. 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. □

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

$$f'(y) = \frac{-2x^{12} - 6x^{10} - 10x^8 - 6x^6 - x^4}{[1 + (y-1)x^2 + (4y-19)x^4 + (2y-12)x^6]^2} < 0.$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

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* $\mathscr{T}_{n,d}$,

(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) ([7])$T(n, 4; 1, 0, n-6)(n \geq 7)$ *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 $\mathscr{T}_1 = \emptyset$; otherwise, by Lemma 3.4, the tree with the minimum energy in $\mathscr{T}_1$ 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 $\mathscr{T}_{9,5}$ and when $n = 10$, $T(10, 5; 0, 4, 0, 0)$ has the second-minimal energy among $\mathscr{T}_{10,5}$, which are examples that confirm our results.

Acknowledgments. The authors are grateful to the referee for his or her valuable comments, corrections and suggestions, which led to an improved version of the original manuscript.

REFERENCES

[1] D. Cvetković, M. Doob, and H. Sachs. *Spectra of Graphs–Theory and Applications*. Academic Press, New York, 1980.
[2] I. Gutman. Acyclic systems with extremal Hückel π-electron energy. *Theoret. Chem. Acta (Berl.)*, 45:79–87, 1977.
[3] I. Gutman. Topology and stability of conjugated hydrocarbons. The dependence of total π-electron energy on molecular topology. *Journal of the Serbian Chemical Society*, 70:441–456, 2005.
[4] I. Gutman. The energy of graph. *Ber. Math.-Statist. Sekt. Forsch. Graz*, 103:1–22, 1978.
[5] I. Gutman. The energy of a graph: old and new results, in: A. Betten, A. Kohnert, R. Laue, A.

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 17, pp. 414-425, August 2008

ELA
http://math.technion.ac.il/iic/ela

Wassermann (Eds.), *Algebraic Combinatorics and Applications*. Springer, Berlin, 196–211, 2001.

[6] I. Gutman and O.E. Polansky. *Mathematical Concepts in Organic Chemistry*. Springer, Berlin, 1986.

[7] N. Li and S. Li. On the Extremal Energies of Trees. *MATCH Commun. Math. Comput. Chem.*, 59:291–314, 2008.

[8] I. Shparlinski. On the energy of some circulant graphs. *Linear Algebra Appl.*, 414:378–382, 2006.

[9] W. Yan and L. Ye. On the minimal energy of trees with a given diameter. *Appl. Math. Lett.*, 18:1046–1052, 2005.

[10] A. Yu and X. Lv. Minimum energy on trees with k pendent vertices. *Linear Algebra Appl.*, 418:625–633, 2006.

[11] B. Zhou and F. Li. On minimal energies of trees of a prescribled diameter. *J. Math. Chem.*, 39:465–473, 2006.

[12] Y. Hou. On trees with the least energy and a given size of matching, *J. Syst. Sci. Math. Sci.*, 23:491-494, 2003 (in Chinese).

[13] J. Koolen and V. Moulton. Maximal energy bipartite graphs. *Graphs Combin.*, 19:131–135, 2003.

[14] X. Wang and X. Guo. On the minimal energy of trees with a given number of non-pendent edges. *Journal of Mathematical Study*, 39:109–116, 2006.

[15] F. Zhang and H. Li. On acyclic conjugated molecules with minimal energies. *Discr. Appl. Math.*, 92:71–84, 1999.