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On minimal energies of trees of a prescribed diameter

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The energy of a graph is defined as the sum of the absolute values of all the eigenvalues of the graph. Let $\mathcal{T}_{n,d}$ denote the set of trees on n vertices and diameter d, $3 \leqslant d \leqslant n-2$. Yan and Ye [Appl. Math. Lett. 18 (2005) 1046–1052] have recently determined the unique tree in $\mathcal{T}_{n,d}$ with minimal energy. In this article, the trees in $\mathcal{T}_{n,d}$ with second-minimal energy are characterized.

KEY WORDS: diameter, eigenvalue, energy, tree

AMS subject classification: 05C50, 05C35

1. Introduction

Let G be a graph on n vertices. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of an adjacency matrix of G are called the eigenvalues of G. The energy of G, denoted by $E(G)$, is defined as

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

In chemistry, the energy of a given molecular graph is of interest since it is closely related to the total π-electron energy of the molecular represented by that graph [1,2]. For more details on the chemical aspects and mathematical properties of $E(G)$ see [1,3–5].

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

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left(\sum_{k=0}^{\lfloor n/2 \rfloor} m(G,k) x^{2k} \right) \mathrm{d}x.$$

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Thus $E(G)$ is a strictly monotonically increasing function of $m(G,k)$, $k = 1, \dots, \lfloor n/2 \rfloor$. This observation led Gutman [6] to define a quasi-order over the set of all acyclic graphs: if G_1 and G_2 are two acyclic graphs, then

$$G_1 \succeq G_2 \Leftrightarrow m(G_1,k) \geqslant m(G_2,k) \text{ for all } k \geqslant 1.$$

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,

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2). \tag{1}$$

This increasing property of energy has been used in the study of extremal values of energy over some significant classes of graphs. For instance, Gutman [6] determined trees with minimal, second-minimal, third-minimal and fourth-minimal energies, and Zhang and Li [7] determined trees of a perfect matching with minimal and second-minimal energies. More recent results in this direction can be found in [8–14].

Let $\mathcal{T}_{n,d}$ be the class of trees on n vertices and diameter d, where $2 \leqslant d \leqslant n-1$. 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 can assume in the following that $3 \leqslant d \leqslant n-2$.

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 $T(n,d;n_1,n_2,\dots,n_{d-1}) \in \mathcal{T}_{n,d}$ be a caterpillar obtained from a path $v_0, v_1, \dots, v_d$ by attaching n_i ($n_i \geqslant 0$) pendant edges to v_i ($i = 1, 2, \dots, d-1$). Clearly, $n = d + 1 + \sum_{i=1}^{d-1} n_i$.

Yan and Ye [15] proved that $T(n,d;n-d-1,0,\dots,0)$ is the unique tree with minimal energy in $\mathcal{T}_{n,d}$. In this paper, we prove that the trees with second-minimal energy in $\mathcal{T}_{n,d}$ are $T(n,d;0,0,n-d-1,0,\dots,0)$ if $d \geqslant 6$, $T(n,3;1,n-5)$ if $d = 3$, $T(n,4;1,0,n-6)$ or $T(n,4;0,n-5,0)$ if $d = 4$ ($n \geqslant 7$), $T(n,5;1,0,0,n-7)$ or $T(n,5;0,n-6,0,0)$ if $d = 5$ ($n \geqslant 8$).

2. Preliminaries

Let G be a graph and u a vertex of G, we denote by $G-u$ the graph formed from G by deleting the vertex u and the edges incident with u. For two graphs G and H, $G = H$ means G and H are isomorphic.

Lemma 1. Let G and G' be two acyclic graphs. Suppose that u (resp. u') is a pendant vertex of G (resp. G'), being adjacent to the vertex v (resp. v'). If $G-u \succeq G'-u'$ and $G-u-v \succ G'-u'-v'$; or $G-u \succ G'-u'$ and $G-u-v \succeq G'-u'-v'$, then $G \succ G'$.

Proof. Let k be a positive integer. Since u is a pendant vertex of G, being adjacent to v, we have

$$m(G,k) = m(G-u,k) + m(G-u-v,k-1). \tag{2}$$

Similarly,

$$m(G',k) = m(G'-u',k) + m(G'-u'-v',k-1). \tag{3}$$

If $G-u \succeq G'-u'$ and $G-u-v \succ G'-u'-v'$, i.e., $m(G-u,k) \geqslant m(G'-u',k)$, $m(G-u-v,k-1) \geqslant m(G'-u'-v',k-1)$ and there is at least one j such that $m(G-u-v,j-1) > m(G'-u'-v',j-1)$, then by (2) and (3), $m(G,k) \geqslant m(G',k)$ for all k and there is at least one j such that $m(G,j) > m(G',j)$, and so $G \succ G'$. Similarly, if $G-u \succ G'-u'$ and $G-u-v \succeq G'-u'-v'$, then $G \succ G'$. □

The following lemma follows easily from the definition of the quasi-order $\succeq$.

Lemma 2. Let G be an acyclic graph and G' a spanning subgraph (resp. proper spanning subgraph) of G. Then $G \succeq G'$ (resp. $\succ G'$).

Recall that Hosoya's index of a graph G is given as $Z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G,k)$. If G_1 and G_2 are acyclic graphs, then $G_1 \succeq G_2$ and $Z(G_1) > Z(G_2)$ will imply that $G_1 \succ G_2$. Recall also that the Fibonacci numbers f_n, $n = 2, 3, \ldots$ are generated recursively from the relation $f_n = f_{n-1} + f_{n-2}$, using the initial conditions $f_0 = f_1 = 1$.

Lemma 3. For $2 \leqslant i \leqslant \lfloor n/2 \rfloor$, $i \neq 3$ and $n \geqslant 6$,

$$P_i \cup P_{n-i} \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1}.$$

Proof. Note that [1]

$$P_i \cup P_{n-i} \succeq P_3 \cup P_{n-3} \succeq P_1 \cup P_{n-1}$$

and $Z(P_s) = f_s$ for $s \geqslant 1$. So we only need to show that for $i = 2$ and $4 \leqslant i \leqslant \lfloor n/2 \rfloor$,

$$f_i f_{n-i} > f_3 f_{n-3} > f_1 f_{n-1}.$$

It is easy to see that $f_3 f_{n-3} - f_1 f_{n-1} = f_{n-5} > 0$ and $f_2 f_{n-2} - f_3 f_{n-3} = f_{n-6} > 0$. So $f_3 f_{n-3} > f_1 f_{n-1}$ and $f_2 f_{n-2} > f_3 f_{n-3}$.

Suppose that $4 \leqslant i \leqslant \lfloor n/2 \rfloor$. Define $f_{-1} = 0$. Then

$$\begin{aligned} f_i f_{n-i} - f_{i-1} f_{n-i+1} &= (f_{i-1} + f_{i-2}) f_{n-i} - f_{i-1}(f_{n-i} + f_{n-i-1}) \\ &= -(f_{i-1} f_{n-i-1} - f_{i-2} f_{n-i}) \\ &= (-1)^i (f_0 f_{n-2i} - f_{-1} f_{n-2i+1}) \\ &= (-1)^i f_{n-2i}, \end{aligned}$$

which implies that

$$f_i f_{n-i} - f_3 f_{n-3} = (f_{n-8} - f_{n-10}) + (f_{n-12} - f_{n-14}) + \cdots > 0,$$

i.e., $f_i f_{n-i} > f_3 f_{n-3}$. This proves the lemma. □

Lemma 4. Let $T \in \mathcal{T}_{n,n-2}$ with $n \geqslant 6$. Then $T \succ P_3 \cup P_{n-3}$.

Proof. Let $v_0, v_1, \ldots, v_{n-2}$ be a path of length $n-2$ in T. Then there is (exactly) one pendant vertex u outside this path. Suppose that u is adjacent to v_j $(1 \leqslant j \leqslant n-3)$. Now by lemmas 2 and 3, $T - u = P_{n-1} \succ P_2 \cup P_{n-3}$ and $P - u - v_j = P_j \cup P_{n-2-j} \succeq P_1 \cup P_{n-3}$. By lemma 1, the result follows. □

3. Main results

For $T \in \mathcal{T}_{n,d}$, assume in the following that $P(T) = v_0, v_1, \ldots, v_d$ is a diametrical path and that $V_1(T)$ is the set of pendant vertices of T lying outside $P(T)$. Since $d \leqslant n-2$, $V_1(T) \neq \emptyset$. To determine the trees in $\mathcal{T}_{n,d}$ with second-minimal energy, we have to consider the cases $d \geqslant 6$, $d = 3$, $d = 4$, and $d = 5$ separately.

Theorem 1. Let $T \in \mathcal{T}_{n,d}$ with $d \geqslant 6$. If $T \neq T(n, d; n-d-1, 0, \ldots, 0)$, $T(n, d; 0, 0, n-d-1, 0, \ldots, 0)$, then $T \succ T(n, d; 0, 0, n-d-1, 0, \ldots, 0)$.

Proof. Let $T_{n,d,1} = T(n, d; n-d-1, 0, \ldots, 0)$ and $T_{n,d,2} = T(n, d; 0, 0, n-d-1, 0, \ldots, 0)$.

Let u' be a pendant vertex of $T_{n,d,2}$ adjacent to the vertex v' of maximal degree (in fact, of degree $n-d+1$). Then $T_{n,d,2} - u' = T_{n-1,d,2}$ and $T_{n,d,2} - u' - v' = (n-d-2)P_1 \cup P_3 \cup P_{d-3}$.

For fixed d, we prove the result by induction on n.

If $n = d+2$, then there is a unique $u \in V_1(T)$ adjacent to some vertex v_j in $P(T)$. Since $T \neq T_{n,d,1}, T_{n,d,2}$, we have $2 \leqslant j \leqslant d-2$, and $j \neq 3, d-3$. Then $T - u = P(T) = P_{d+1} = T_{n,d,2} - u'$ and by lemma 3, $T - u - v_j = P_j \cup P_{d-j} \succ P_3 \cup P_{d-3} = T_{n,d,2} - u' - v'$. It follows from lemma 1 that $T \succ T_{n,d,2}$. Thus the result holds if $n = d+2$.

Suppose that $n \geqslant d+3$ and the result holds for trees in $\mathcal{T}_{n-1,d}$ with $d \geqslant 6$. Let $T \in \mathcal{T}_{n,d}$ with $d \geqslant 6$, and $T \neq T_{n,d,1}, T_{n,d,2}$.

Suppose that there is a pendant vertex $u \in V_1(T)$ such that its neighbor v lies outside $P(T)$. Obviously $T-u \neq T_{n,d,1}$. By the induction hypothesis,

$$T-u \succeq T_{n-1,d,2}.$$

Since $T-u-v$ contains a proper spanning subgraph $(n-d-2)P_1 \cup P_3 \cup P_{d-3}$. By lemma 2,

$$T-u-v \succ (n-d-2)P_1 \cup P_3 \cup P_{d-3}.$$

By lemma 1, $T \succ T_{n,d,2}$.

Now suppose that for any pendant vertex in $V_1(T)$, its neighbor lies on P, i.e., T is a caterpillar, say $T = T(n,d;n_1,\dots,n_{d-1})$, where v_i has degree n_i+2, $i = 1,2,\dots,d-1$.

Case 1. $n_j \geqslant 1$ for some j with $2 \leqslant j \leqslant d-2$. Let $u \in V_1(T)$ such that u is adjacent to v_j.

Subcase 1.1. $T-u = T_{n-1,d,1}$. Then one of v_1 and v_{d-1}, say v_1, has degree $(n-d-2)+2$. Let $u_1 \in V_1(T)$ such that u_1 is adjacent to v_1. Then $T-u_1 \neq T_{n-1,d,1}$. By the induction hypothesis,

$$T-u_1 \succeq T_{n-1,d,2}.$$

Note also that $T-u_1-v_1 = (n-d-2)P_1 \cup T_1$ where $T_1 = P_d$ or $T_1 \in \mathcal{T}_{d,d-2}$. By lemma 2 or 4, $T_1 \succ P_3 \cup P_{d-3}$. So

$$T-u_1-v_1 \succ (n-d-2)P_1 \cup P_3 \cup P_{d-3}.$$

Now by lemma 1, $T \succ T_{n,d,2}$.

Subcase 1.2. $T-u = T_{n-1,d,2}$. Then one of v_3 and v_{d-3}, say v_3, has degree $(n-d-2)+2$. Let $u_3 \in V_1(T)$ such that u_3 is adjacent to v_3. Obviously, $T-u_3 \neq T_{n-1,d,1}$. By the induction hypothesis,

$$T-u_3 \succeq T_{n-1,d,2}.$$

Note that $T-u_3-v_3$ contains a proper spanning subgraph $(n-d-2)P_1 \cup P_3 \cup P_{d-3}$. By lemma 2,

$$T-u_3-v_3 \succ (n-d-2)P_1 \cup P_3 \cup P_{d-3}.$$

By lemma 1, $T \succ T_{n,d,2}$.

Subcase 1.3. $T-u \neq T_{n-1,d,1}, T_{n-1,d,2}$. By the induction hypothesis,

$$T-u \succ T_{n-1,d,2}$$

and since $T - u - v_j$ contains a spanning subgraph $(n-d-2)P_1 \cup P_j \cup P_{d-j}$, it follows from lemmas 2 and 3 that

$$T - u - v_j \succeq (n-d-2)P_1 \cup P_3 \cup P_{d-3}.$$

Therefore, by lemma 1, $T \succ T_{n,d,2}$.

Case 2. $n_2 = \cdots = n_{d-2} = 0$. Then $n_1, n_{d-1} \geqslant 1$ and $n_1 + n_d = n - d - 1$. Suppose without loss of generality that $n_1 \leqslant n_{d-1}$. Let $u \in V_1(T)$ such that u is adjacent to $v = v_{d-1}$. Since $n_{d-1} > 1$, we have $T - u \neq T_{n-1,d,1}, T_{n-1,d,2}$. By the induction hypothesis,

$$T - u \succ T_{n-1,d,2}.$$

Observe that $T - u - v = n_{d-1}P_1 \cup T_2 = (n-d-1-n_1)P_1 \cup T_2$, where $T_2 = T(d-1+n_1, d-2; n_1, 0, \ldots, 0)$. By lemmas 2 and 4, $T_2 \succeq (n_1-1)$ $P_1 \cup T(d, d-2; 1, 0, \ldots, 0) \succ (n_1-1)P_1 \cup P_3 \cup P_{d-3}$ and then

$$T - u - v \succ (n-d-2)P_1 \cup P_3 \cup P_{d-3}.$$

By lemma 1, $T \succ T_{n,d,2}$.

Combining Cases 1 and 2, we conclude that result holds for $T \in \mathcal{T}_{n,d}$ when $d \geqslant 6$. The theorem is thus proved. □

Note that any $T \in \mathcal{T}_{n,3}$ is of the form $T(n, 3; a, b)$ with $a, b \geqslant 0$ and $a+b = n-4$, and that $m(T(n, 3; a, b), 2) = (a+1)(b+1)$ and $m(T(n, 3; a, b), k) = 0$ for $k \geqslant 3$. We can easily have the following.

Theorem 2. Let $T(n, 3; a, b) \in \mathcal{T}_{n,3}$ with $1 \leqslant a \leqslant b$. Then

$$T(n, 3; a, b) \succ T(n, 3; a-1, b+1).$$

If $T \in \mathcal{T}_{6,4}$, then either $T = T(6, 4; 1, 0, 0)$ or $T = T(6, 4; 0, 1, 0)$. Obviously $T(6, 4; 0, 1, 0) \succ T(6, 4; 1, 0, 0)$.

Theorem 3. Let $T \in \mathcal{T}_{n,4}$ with $n \geqslant 7$. If $T \neq T(n, 4; n-5, 0, 0)$, $T(n, 4; 1, 0, n-6)$, $T(n, 4; 0, n-5, 0)$, then $T \succ T(n, 4; 1, 0, \ n-6)$.

Proof. If $n = 7$, then $T = T(7, 4; 1, 1, 0)$ and the result follows readily.

Suppose that $n \geqslant 8$ and the result holds for trees in $\mathcal{T}_{n-1,4}$. Let $T \in \mathcal{T}_{n,4}$, and $T \neq T(n, 4; n-5, 0, 0)$, $T(n, 4; 1, 0, n-6)$, $T(n, 4; 0, n-5, 0)$.

Let u' be a pendant vertex adjacent to the vertex v' of degree $n-4$ in $T(n, 4; 1, 0, n-6)$. Then $T(n, 4; 1, 0, n-6) - u' =$ T(n,4;1,0, n-7), $T(n, 4; 1, 0, n-6) - u' - v' = (n-6)P_1 \cup K_{1,3}$.

Suppose first that for some $u \in V_1(T)$ such that u and v_2 have a common neighbor v outside $P(T)$. Obviously, $T - u \neq T(n-1, 4; n-6, 0, 0), T(n-1, 4; 1, 0, n-7)$.

If $T - u = T(n-1, 4; 0, n-6, 0)$, then T is the tree formed from $T(n-1, 4; 0, n-6, 0)$ by adding to one pendant vertex outside the path $P(T)$ a pendant edge. Note that $m(T, 2) = 3n - 12$, $m(T(n, 4; 1, 0, n-6), 2) = 3n - 13$, and $m(T(n, 4; 1, 0, n-6), k) = 0$ for $k \geqslant 3$. Thus $T \succ T(n, 4; 1, 0, n-6)$.

If $T - u \neq T(n-1, 4; 0, n-6, 0)$, then by the induction hypothesis,

$$T - u \succ T(n-1, 4; 1, 0, n-7).$$

Observe that $T - u - v$ contains a proper spanning subgraph $(n-7)P_1 \cup P_5$. By lemma 2,

$$T - u - v \succ (n-6)P_1 \cup K_{1,3}.$$

Now by lemma 1, $T \succ T(n, 4; 1, 0, n-6)$.

Now suppose that T is a caterpillar $T(n, 4; n_1, n_2, n_3)$ with $n_1 + n_2 + n_3 = n - 5$. It is easy to see that $m(T, 2) = 2n - 7 + n_1n_2 + n_2n_3 + n_1n_3$. If $n_2 = 0$, then since $T \neq T(n, 4; n-5, 0, 0)$, $T(n, 4; 1, 0, n-6)$, we have $1 < n_1 < n-6$ and $m(T, 2) = 2n - 7 + n_1(n - 5 - n_1) > 3n - 13$. If $n_2 \neq 0$, then since $T \neq T(n, 4; 0, n-5, 0)$, we have $1 \leqslant n_2 \leqslant n-6$ and so $m(T, 2) = 2n - 7 + n_2(n - 5 - n_2) + n_1n_3 \geqslant 3n - 13$ and $m(T, 3) = n_1n_2n_3 + n_2(n - 4 - n_2) > 0$. Note that $m(T(n, 4; 1, 0, n-6), 2) = 3n - 13$, $m(T(n, 4; 1, 0, n-6), k) = 0$ for $k \geqslant 3$. It follows that $T \succ T(n, 4; 1, 0, n-6)$. This completes the proof. □

If $T \in \mathcal{T}_{7,5}$, then either $T = T(7, 5; 1, 0, 0, 0)$ or $T = T(7, 5; 0, 1, 0, 0)$. Obviously $T(7, 5; 0, 1, 0, 0) \succ T(7, 5; 1, 0, 0, 0)$.

Theorem 4. Let $T \in \mathcal{T}_{n,5}$ with $n \geqslant 8$. If $T \neq T(n, 5; n-6, 0, 0, 0)$, $T(n, 5; 1, 0, 0, n-7)$, $T(n, 5; 0, n-6, 0, 0)$, then $T \succ T(n, 5; 1, 0, 0, n-7)$.

Proof. If $n = 8$, then T is one of $T_1 = T(8, 5; 1, 1, 0, 0)$, $T_2 = T(8, 5; 1, 0, 1, 0)$, $T_3 = T(8, 5; 0, 1, 1, 0)$, or T_4, where T_4 is a tree obtained by joining a central vertex of P_6 to a vertex of P_2. Let $T^* = T(8, 5; 1, 0, 0, 1)$. It can be easily checked from the following table that the result holds.

T	$m(T,2)$	$m(T,3)$	$m(T,4)$
T_1	13	6	0
T_2	13	5	0
T_3	13	7	1
T_4	14	7	1
T^*	13	4	0

Suppose that $n \geqslant 9$ and the result holds for trees in $\mathcal{T}_{n-1,5}$. Let $T \in \mathcal{T}_{n,5}$, and $T \neq T(n, 5; n-6, 0, 0, 0)$, $T(n, 5; 1, 0, 0, n-7)$, $T(n, 5; 0, n-6, 0, 0)$.

Let u' be a pendant vertex adjacent to the vertex v' of degree $n-5$ in $T(n, 5; 1, 0, 0, n-7)$. Then $T(n, 5; 1, 0, 0, n-7) - u' = T(n-1, 5; 1, 0, 0, n-8)$, $T(n, 5; 1, 0, 0, n-7) - u' - v' = (n-7)P_1 \cup T(5, 3; 1, 0)$.

Suppose first that for some $u \in V_1(T)$ such that u and one of v_2 or v_3, say v_2, have a common neighbor v outside $P(T)$. Obviously, $T-u \neq T(n-1, 5; n-7, 0, 0, 0)$, $T(n-1, 5; 1, 0, 0, n-8)$.

If $T-u = T(n-1, 5; 0, n-7, 0, 0)$, then T is the tree formed from $T(n-1, 5; 0, n-7, 0, 0)$ by adding to one pendant vertex outside the path $P(T)$ a pendant edge. Thus $m(T, 2) = 4n - 18$, $m(T, 3) = 5n - 31$, $m(T, 4) = 2n - 15$. Note that $m(T(n, 5; 1, 0, 0, n-7), 2) = 4n - 19$, $m(T(n, 5; 1, 0, 0, n-7), 3) = 2(n-6)$, and $m(T(n, 5; 1, 0, 0, n-7), k) = 0$ for $k \geqslant 4$. So $T \succ T(n, 5; 1, 0, 0, n-7)$.

If $T-u \neq T(n-1, 5; 0, n-7, 0, 0)$, then by the induction hypothesis,

$$T - u \succeq T(n-1, 5; 1, 0, 0, n-8).$$

Observe that $T - u - v$ contains a proper spanning subgraph $(n-8)P_1 \cup P_6$. By lemma 2,

$$T - u - v \succ (n-7)P_1 \cup T(5, 3; 1, 0).$$

Now by lemma 1, $T \succ T(n, 5; 1, 0, 0, n-7)$.

Now suppose that T is a caterpillar $T(n, 5; n_1, n_2, n_3, n_4)$, where $n_1 + n_2 + n_3 + n_4 = n - 6$ and the degree of v_i is $n_i + 2$ ($i = 1, 2, 3, 4$).

If $n_2 > 1$ or $n_3 > 1$, say $n_2 > 1$, then choose a pendant vertex u that is adjacent to the vertex $v = v_2$. If $\max\{n_2, n_3\} = 1$, say $n_2 = 1$, then one of n_1 and n_4 is at least 1, we may choose a pendant vertex u that is adjacent to the vertex $v \in \{v_1, v_4\}$ (of degree at least 3). In either case, $T - u \neq T(n-1, 5; n-7, 0, 0, 0)$, $T(n-1, 5; 1, 0, 0, n-8)$, $T(n-1, 5; 0, n-7, 0, 0)$. By the induction hypothesis,

$$T - u \succ T(n-1, 5; 0, n-7, 0, 0).$$

On the other hand, $T - u - v$ contains a spanning subgraph $(n-8)P_1 \cup P_2 \cup P_4$, $(n-8)P_1 \cup P_2 \cup K_{1,3}$, $(n-8)P_1 \cup P_3 \cup P_3$, $(n-7)P_1 \cup P_5$, or $(n-7)P_1 \cup T(5, 3; 1, 0)$. By lemma 2,

$$T - u - v \succeq (n-7)P_1 \cup T(5, 3; 1, 0).$$

By lemma 1, $T \succ T(n, 5; 1, 0, 0, n-7)$.

We are left with the case $n_2 = n_3 = 0$. Since $T \neq T(n, 5; 1, 0, 0, n-7)$, we have $1 < n_1 < n-7$, and so $m(T, 2) = 3n - 12 + n_1(n - 6 - n_1) > 4n - 19$ and $m(T, 3) = n - 5 + n_1(n - 6 - n_1) > 2n - 12$. Therefore, $T \succ T(n, 5; 1, 0, 0, n-7)$. This completes the proof. $\square$

By theorems 1–4 and using the increasing property (1) of energy, we conclude that the trees $T(n, d; 0, 0, n-d-1, 0, \ldots, 0)$ if $d \geqslant 6$, $T(n, 3; 1, n-5)$ if $d = 3$ ($n \geqslant 6$), $T(n, 4; 1, 0, n-6)$ or $T(n, 4; 0, n-5, 0)$ if $d = 4$ ($n \geqslant 7$), $T(n, 5; 1, 0, 0, n-7)$ or $T(n, 5; 0, n-6, 0, 0)$ if $d = 5$ ($n \geqslant 8$) achieve second-minimal energy in the class of trees on n vertices and diameter d.

By direct calculation (rounded to three decimal places), we have

$$E(T(7,4;1,0,1)) = 6.828\,,\ E(T(7,4;0,2,0)) = 7.596,$$

$$E(T(8,5;1,0,0,1)) = 8.472\,,\ E(T(8,5;0,2,0,0)) = 8.520,$$

$$E(T(9,5;1,0,0,2)) = 9.060\,,\ E(T(9,5;0,3,0,0)) = 9.050.$$

We are then led to conjecture that $T(n, 4; 1, 0, n-6)$ ($n \geqslant 7$) and $T(n, 5; 0, n-6, 0, 0)$ ($n \geqslant 9$) achieve second-minimal energy in the class of trees on n vertices and diameter d for $d = 4$ and $d = 5$, respectively.

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