MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **76** (2016) 615-633

ISSN 0340 - 6253

On the Maximal Energy of Integral Weighted Trees with Fixed Total Weight Sum

Shicai Gong[1,∗,†], Xueliang Li[2,‡], Ivan Gutman[3,4], Zhongmei Qin[2], Kang Yang[2]

[1]*School of Science, Zhejiang University of Science and Technology Hangzhou, 311300, P. R. China*
scgong@zafu.edu.cn

[2]*Center for Combinatorics and LPMC–TJKLC Nankai University, Tianjin 300071, P. R. China*
lxl@nankai.edu.cn, qinzhongmei90@163.com, yangkang@mail.nankai.edu.cn

[3]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*
gutman@kg.ac.rs

[4]*State University of Novi Pazar, Novi Pazar, Serbia*

(Received November 20, 2015)

Dedicated to Professor Fuji Zhang on the occasion of his 80th anniversary

Abstract

Let m be an integer and $W = \{w_1, w_2, \ldots, w_{n-1}\}$ be a positive sequence. Denote by $\mathcal{T}(n,m)$ the set of all weighted trees of order n with positive integral weights and fixed total weight sum m. Let further $\mathcal{T}(n,W)$ be the set of all weighted trees of order n with weight sequence W. We first introduce a new method to investigate the energy of weighted graphs, then using this method we determine the unique tree achieving maximal energy in $\mathcal{T}(n,W)$ for $w_1 \geq w_2 \geq w_3 \geq w_4 > w_5 = \cdots = w_{n-1}$, which supports a conjecture of the present authors in *MATCH Commun. Math. Comput. Chem.* **75** (2016) 267. Finally, we determine the unique tree having maximal energy in $\mathcal{T}(n,m)$ with $n \leq m \leq n+3$, which supports a conjecture by Brualdi et al., *Lin. Multilin. Algebra* **60** (2012) 1255.

∗Corresponding author

†Supported by the National Natural Science Foundation of China, (No. 11571315).

‡Supported by the National Natural Science Foundation of China, (No. 11371205).

1 Introduction

We consider graphs on n vertices in which to each edge a positive weight is assigned. The sequence of the weights of all edges of a weighted graph is referred to as the weight sequence of such a graph. Let $W = \{w_1, w_2, \ldots, w_{n-1}\}$ be a sequence, not necessarily integral, such that $w_i \geq 1$, $i = 1, 2, \ldots, n-1$. Denote by $\mathcal{T}(n, W)$ the set of all connected weighted trees of order n with weight sequence W. Let m be an integer such that $m \geq n-1$. Denote by $\mathcal{T}(n, m)$ the set of all weighted trees of order n with positive integral weights and fixed total weight sum m. A graph whose each edge has weight 1 is said to be un-weighted. Then, evidently, each element in $\mathcal{T}(n, n-1)$ is an un-weighted tree.

The energy of a (weighted) graph G of order n is defined as

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

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the (real) eigenvalues of the (nonnegative, symmetric) adjacency matrix $\mathbf{A}$ of G. More information on (weighted) graph energy can be found in [2–6, 11–13, 16, 18, 19, 21, 24, 28].

In [3], Brualdi et al. investigated the extremal energies in $\mathcal{T}(n, m)$. They showed that the path with weight sequence $\{2, 1, \ldots, 1\}$, where the weight of one of the pendent edges equals 2, is the unique integral weighted tree in $\mathcal{T}(n, n)$ $(n \geq 5)$ with maximal energy. For $m \geq n$, they conjectured the structure and distribution of weights of the unique maximum–energy tree in $\mathcal{T}(n, m)$ as follows:

Conjecture 1. [3, Conjecture 9] *Let $n \geq 5$ and $m \geq n$. The path with weight sequence $\{m-n+2, 1, \ldots, 1\}$, where the weight of one of the pendent edges equals $m-n+2$, is the unique integral weighted tree in $\mathcal{T}(n, m)$ with maximal energy.*

Let $\hat{\mathbb{E}}(n, W) = \max\{\mathcal{E}(T) : T \in \mathcal{T}(n, W)\}$ and $\hat{\mathbb{E}}(n, m) = \max\{\mathcal{E}(T) : T \in \mathcal{T}(n, m)\}$ be the maximal energies of trees in $\mathcal{T}(n, W)$ and $\mathcal{T}(n, m)$, respectively.

In [7], Gong et al. showed that the tree having maximal energy among $\mathcal{T}(n, W)$ is a path, they also conjectured the weight distribution of such a path as follows:

Conjecture 2. [7, Conjecture 11] Let $n \geq 3$ and $W = \{w_1, w_2, \ldots, w_{n-1}\}$ be a sequence of positive numbers with $w_1 \geq w_2 \geq \cdots \geq w_{n-1}$, and let $P = u_1e_1u_2e_2\ldots u_{n-1}e_{n-1}u_n$ be the path having energy $\hat{\mathbb{E}}(n, W)$. Suppose $w(e_1) \geq w(e_{n-1})$. Then for $i = 1, 2, \ldots, n-1$,

$$w(e_i) = \begin{cases} w_i & \text{if either } i \leq \lceil \frac{n-1}{2} \rceil \text{ and } i \text{ is odd, or } i > \lceil \frac{n-1}{2} \rceil \text{ and } n-i \text{ is even;} \\ w_{n+1-i}, & \text{otherwise.} \end{cases}$$

In this paper, we continue to investigate the trees with energies $\hat{\mathbb{E}}(n, W)$ and $\hat{\mathbb{E}}(n, m)$.

* * * * *

The paper is organized as follows. In Section 2, we introduce some notation and preliminary results. In Section 3, we first introduce a new method to investigate the energy of a weighted graph, then using this method we determine the weighted paths achieving the maximal energy in $\mathcal{T}(n, W)$ for $w_1 \geq w_2 \geq w_3 \geq w_4 > w_5 = \cdots = w_{n-1}$, which supports Conjecture 2. Then in Section 4 we determine the unique path having maximal energy in $\mathcal{T}(n, m)$ with $m \leq n+3$, which supports Conjecture 1.

2 Preliminary results

Let $G = (V(G), E(G))$ be a graph. For $V_1 = \{v_1, v_2, \ldots, v_s\} \subseteq V(G)$ and $E_1 = \{e_1, e_2, \ldots, e_k\} \subseteq E(G)$, denote by $G \backslash E_1$ the graph obtained from G by deleting all edges of E_1 and by $G \backslash V_1$ the graph obtained from G by removing all vertices of V_1 together with all incident edges. For convenience, we sometimes write $G \backslash e_1e_2\ldots e_k$ and $G \backslash v_1v_2\ldots v_s$ instead of $G \backslash E_1$ and $G \backslash V_1$, respectively. Denote by $P_n = u_1e_1u_2\ldots u_{n-1}e_{n-1}u_n$ the path on n vertices, where u_i and u_{i+1} are the two endvertices of the edge e_i. For a weighted path, we sometimes write P_n as $u_1w_1u_2w_2u_3\ldots u_{n-1}w_{n-1}u_n$ or $w_1w_2\ldots w_{n-1}$ briefly, where w_i denotes the weight of the edge e_i for $i = 1, 2, \ldots, n-1$. We refer to Cvetković et al. [5] for terminology and notation not defined here.

A graph is said to be *elementary* if it is isomorphic either to P_2 or to a cycle. The weight of P_2 is defined as the square of the weight of its unique edge. The weight of a cycle is the product of the weights of all its edges.

A graph $\mathscr{H}$ is called a *Sachs graph* if each component of $\mathscr{H}$ is an elementary graph [9, 10, 15, 17]. The weight of a Sachs graph $\mathscr{H}$, denoted by $\mathscr{W}(\mathscr{H})$, is the product of the weights of all elementary subgraphs contained in $\mathscr{H}$.

Denote by $\phi(G,\lambda)$ the *characteristic polynomial* of a graph G, defined as

$$\phi(G,\lambda) = \det\left[\lambda\,\mathbf{I}_n - \mathbf{A}(G)\right] = \sum_{k=0}^{n} a_k(G)\,\lambda^{n-k} \tag{1}$$

where $\mathbf{A}(G)$ is the adjacency matrix of G and $\mathbf{I}_n$ the identity matrix of order n. The following well known result determines all coefficients of the characteristic polynomial of a weighted graph in terms of its Sachs subgraphs [1, 5, 7, 8, 25, 26].

Theorem 3. *Let G be a weighted graph on n vertices with adjacency matrix $\mathbf{A}(G)$ and characteristic polynomial $\phi(G,\lambda) = \sum_{k=0}^{n} a_k(G)\,\lambda^{n-k}$. Then*

$$a_k(G) = \sum_{\mathscr{H}} (-1)^{p(\mathscr{H})}\, 2^{c(\mathscr{H})}\, \mathscr{W}(\mathscr{H})$$

where the summation is over all Sachs subgraphs $\mathscr{H}$ of G having k vertices, and where $p(\mathscr{H})$ and $c(\mathscr{H})$ are, respectively, the number of components and the number of cycles contained in $\mathscr{H}$.

In this paper, we write $b_k(G) = |a_k(G)|$ and

$$\tilde{\phi}(G,\lambda) = \sum_{k=0}^{n} b_k(G)\,\lambda^{n-k}\,. \tag{2}$$

Then we have the following recursions for the coefficient of the polynomial $\tilde{\phi}(G,\lambda)$ of a weighted graph G [7].

Lemma 4. *Let G be a weighted bipartite graph with a cut edge $e = uv$. Suppose that the weight of the edge e is w_e. Then*

$$b_k(G) = b_k(G\backslash e) + w_e^2\, b_{k-2}(G\backslash uv)\,.$$

From the Coulson integral formula for the energy (see [4, 16, 20, 21] and the references cited therein), it can be shown [11] that if G is a weighted bipartite graph with characteristic polynomial as in Eq. (1), then

$$\mathcal{E}(G) = \frac{1}{\pi}\int\limits_{-\infty}^{+\infty} \lambda^{-2} \ln\left(\sum_{k=0}^{\lfloor n/2\rfloor} b_{2k}\,\lambda^{2k}\right) d\lambda\,.$$

It follows that in the case of weighted trees, $\mathcal{E}(T)$ is a strict monotonically increasing function of the numbers b_{2k}, $k = 1, 2, \dots, \lfloor n/2 \rfloor$. Thus, in analogy to comparing the energies of two non-weighted trees [11, 29, 30], we introduce a quasi-ordering relation $\preceq$ for weighted trees (see also [14, 22]):

Definition 5. *Let T_1 and T_2 be two weighted trees of order n. If $b_{2k}(T_1) \le b_{2k}(T_2)$ for all k with $0 \le k \le \lfloor n/2 \rfloor$, then we write $T_1 \preceq T_2$. Furthermore, if $T_1 \preceq T_2$ and there exists at least one index k such that $b_{2k}(T_1) < b_{2k}(T_2)$, then we write $T_1 \prec T_2$. If $b_{2k}(T_1) = b_{2k}(T_2)$ for all k, then we call T_1 E-equivalent to T_2, denoted by $T_1 \sim T_2$.*

Note that there are non-isomorphic weighted graphs T_1 and T_2 with $T_1 \sim T_2$, which implies that in the general case $\preceq$ is a quasi-ordering, but not a partial ordering.

According to the integral formula above, we have for two weighted trees T_1 and T_2 of order n that

$$T_1 \preceq T_2 \Longrightarrow \mathcal{E}(T_1) \le \mathcal{E}(T_2) \qquad \text{and} \qquad T_1 \prec T_2 \Longrightarrow \mathcal{E}(T_1) < \mathcal{E}(T_2)\,. \tag{3}$$

3 Tree(s) having energy $\hat{\mathbb{E}}(n, W)$

In [7], Gong et al. showed that the tree having maximal energy in $\mathcal{T}(n, W)$ is a path. For small order n (≤ 6), they determined the unique path having maximal energy in $\mathcal{T}(n, W)$; for larger order n, they gave a conjecture on the structure of the unique tree in $\mathcal{T}(n, W)$, and its weight distribution, see Conjecture 2.

In this section, we first introduce a method to compare the energies of two weighted graphs. Then, as an application, we determine the unique weighted paths having energy $\hat{\mathbb{E}}(n, W)$ for $w_1 \ge w_2 \ge w_3 \ge w_4 > w_5 = \cdots = w_{n-1}$.

In the following, we suppose that the weight of each edge of a graph is at least 1 and admit graphs having parallel edges. The *union* of the graphs $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$, denoted by $G_1 \cup G_2$, is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$. Then $G_1 \cup G_2$ may contain parallel edges if $V(G_1) \cap V(G_2) \ne \emptyset$.

Lemma 6. [23, Lemma 13] Let P_n be an un-weighted path of order n. If $n = 4k + i$, $i \in \{0, 1, 2, 3\}$, $k \geq 1$, then

$$\begin{aligned} P_n \succ P_2 \cup P_{n-2} &\succ P_4 \cup P_{n-4} \succ \cdots \succ P_{2k} \cup P_{n-2k} \succ P_{2k+1} \cup P_{n-2k-1} \\ &\succ P_{2k-1} \cup P_{n-2k+1} \succ \cdots \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1} \,. \end{aligned}$$

Definition 7. *Let G be a weighted graph and $e \in G$. The graph obtained from G by replacing the edge e with two parallel edges e' and e'', where the weight of each edge other than e' and e'' is preserved, is referred as a 2-split graph of G on the edge e, denote by $G_e(e', e'')$.*

Applying Lemma 4, we have

Lemma 8. *Let G be a weighted graph of order n and e a cut edge of G. Let also $G_e(e_1, e_2)$ be a weighted 2-split graph of G on the edge e. Then G is E-equivalent to $G_e(e_1, e_2)$ if*

$$(w(e_1))^2 + (w(e_2))^2 = (w(e))^2 \,.$$

Proof. Let $e = uv$ and $G^* = G_e(e_1, e_2)$. By Lemma 4, for each k,

$$b_k(G) = b_k(G \backslash e) + (w(e))^2 \, b_{k-2}(G \backslash uv) \,.$$

For G^*, we divide all its Sachs graphs having k vertices into three parts: those that contain the edge e_1, those that contain the edge e_2 and others. Then applying Theorem 3 we have

$$b_k(G^*) = b_k(G^* \backslash e_1 e_2) + \left[(w(e_1))^2 + (w(e_2))^2\right] b_{k-2}(G^* \backslash uv) \,.$$

Note that, strictly speaking, Theorem 3 applies to simple graphs, but it applies equally well to the above specified graphs if we replace $(w(e))^2$ by $(w(e_1))^2 + (w(e_2))^2$. Consequently, the result follows. □

As a consequence of Lemma 6, we have:

Lemma 9. *Let $P_n = u_1 e_1 u_2 \ldots u_{n-1} e_{n-1} u_n$ be an un-weighted path of order n, H_0 be a graph of order at least 1 and $v \in H_0$. Denote by H_n the graph obtained from the union of P_n and H_0 by adding an edge with weight at least 1 between u_n and v. If $n = 4p + i$, $i \in \{-1, 0, 1, 2\}$, $p \geq 1$, then $H_n \backslash u_1 u_2 \succ H_n \backslash u_s u_{s+1}$ for each $s = 2, 3, \ldots, n-1$.*

Proof. Because each edge of the path $P_n = u_1e_1u_2 \dots u_{n-1}e_{n-1}u_n$ is un-weighted and the new edge between u_n and v has weight at least 1, $H_n \backslash u_s u_{s+1}$ can be considered as the subgraph of $H_n \backslash u_1u_2$ obtained by deleting an edge. Hence, the result follows. $\square$

For a given weight sequence W, denote by $\mathcal{P}(n, W)$ the set of all weighted paths of order n with weight sequence W. Similarly, denote by $\mathcal{P}(n, m)$ the set of all integral weighted paths of order n with fixed total integer weight sum m. As a consequence of Lemma 9, we have

Theorem 10. *Let* $W = \{w_1, w_2, \dots, w_{n-1}\}$, $n \geq 3$, *be a weight sequence with* $w_1 > w_2 = \dots = w_{n-1} = 1$ *and* $P = u_1e_1u_2 \dots u_{n-1}e_{n-1}u_n \in \mathcal{P}(n, W)$. *Let also* G *be a given graph of order at least* 1 *and* $v \in G$. *Denote by* $\mathcal{P}(u_n, v)G$ *the set of all graphs obtained from the union of* P *and* G *by adding an edge between* u_n *and* v. *Then the graph having maximal energy among* $\mathcal{P}(u_n, v)G$ *satisfies*

$$w(e_1) = w_1 \quad and \quad w(e_i) = w_2 \quad for \ i = 2, 3, \dots, n-1 \, .$$

Proof. Let $\bar{P} = u_1e_1u_2 \dots u_{n-1}e_{n-1}u_n$ be the un-weighted path of order n and $\bar{H} = \bar{P}(u_n, v)G$, the graph obtained from the union of $\bar{P}$ and G by adding an edge between u_n and v. Denote by H^* the graph having maximal energy among $\mathcal{P}(u_n, v)G$. Note that for the induced path P_n of each graph in $\mathcal{P}(u_n, v)G$ there exists exactly one edge whose weight equals w_1. Then by Lemma 8, H^* is E-equivalent to the graph $\bar{H}_{e_i}(e_i, e')$ which is a weighted 2-split graph of H^* on the edge e_i whose weight equals w_1 for some i , $1 \leq i \leq n-1$, where $w(e_i) = 1$ and $w(e') = \sqrt{w_1^2 - 1}$. Applying Lemma 4 we have

$$b_k(H^*) = b_k(\bar{H}_{e_i}(e_i, e')) = b_k(\bar{H}) + (w_1^2 - 1) b_{k-2}(\bar{H} \backslash u_i u_{i+1}) \, .$$

Thus the result follows by Lemma 9. $\square$

For $n \leq 6$, Theorem 10 in [7] determines the unique path with $\hat{\mathbb{E}}(n, W)$ in $\mathcal{P}(n, W)$ for an arbitrarily given weight sequence W. For greater n, we can apply Theorem 10 to determine the weight distribution of the path having $\hat{\mathbb{E}}(n, W)$ in $\mathcal{P}(n, W)$ for some weight sequences W. The following two Lemmas can be considered as two corollaries of Theorem 10. Since the proofs are analogous to those of Theorem 14, we omit them.

Lemma 11. [7, Theorem 10] *Let* $n \geq 3$ *and* $W = \{x, \overbrace{y, \ldots, y}^{n-2}\}$ *be a sequence of positive numbers with* $x > y$*. Then, up to isomorphism,* $P = x \; \overbrace{y \; \ldots \; y}^{n-2}$ *is the unique path having energy* $\hat{\mathbb{E}}(n, W)$*.*

Lemma 12. [7, Theorem 11] *Let* $n \geq 3$ *and* $W = \{x, y, \overbrace{z, \ldots, z}^{n-3}\}$ *be a sequence of positive numbers with* $x \geq y > z$*. Then, up to isomorphism,* $P = x \; \overbrace{z \; \ldots \; z}^{n-3} \; y$ *is the unique path having energy* $\hat{\mathbb{E}}(n, W)$*.*

In order to prove Theorem 14, we first give the following Lemma.

Lemma 13. *Let* $n \geq 5$ *and* $P^* = u_1e_1u_2e_2\ldots u_{n-1}e_{n-1}u_n \in \mathcal{P}(n, W)$*. Let the weight of the edge* e_i *be denoted by* w_i *for* $i = 1, 2, \ldots, n-1$*. If* $\mathcal{E}(P^*) = \hat{\mathbb{E}}(n, W)$*, then*

(**a**) $w_1 \geq w_4$ *and* $w_2 \leq w_3$*;*

(**b**) $w_{n-1} \geq w_{n-4}$ *and* $w_{n-2} \leq w_{n-3}$ *.*

Proof. (**a**) By contradiction. Supposing that the result does not hold, we have $w_1 < w_4$ or $w_2 < w_3$. Now we divide the proof into three cases and get the contradiction.

Case (1): $w_1 < w_4$ and $w_2 \leq w_3$.

Let P^{**} be the weighted path obtained from P^* by exchanging the edges e_1 and e_4, that is, $P^{**} = u_1e_4u_2e_2u_3e_3u_4e_1u_5\ldots u_{n-1}e_{n-1}u_n$. Then by the hypothesis that $\mathcal{E}(P^*) = \hat{\mathbb{E}}(n, W)$, we have

$$\mathcal{E}(P^{**}) \leq \mathcal{E}(P^*) \,. \tag{4}$$

Applying Lemma 4, we have

$$\begin{aligned} b_k(P^*) &= b_k(P^*\backslash e_1) + w_1^2\, b_{k-2}(P^*\backslash u_1u_2) \\ &= b_k(P^*\backslash e_1e_4) + w_4^2\, b_{k-2}(P^*\backslash e_1u_4u_5) \\ &+ w_1^2\, b_{k-2}(P^*\backslash u_1u_2e_4) + w_1^2w_4^2\, b_{k-4}(P^*\backslash u_1u_2u_4u_5) \end{aligned}$$

and

$$\begin{aligned} b_k(P^{**}) &= b_k(P^{**}\backslash e_4) + w_4^2\, b_{k-2}(P^{**}\backslash u_1 u_2) \\ &= b_k(P^{**}\backslash e_1 e_4) + w_1^2\, b_{k-2}(P^{**}\backslash e_4 u_4 u_5) \\ &+ w_4^2\, b_{k-2}(P^{**}\backslash u_1 u_2 e_1) + w_1^2 w_4^2\, b_{k-4}(P^{**}\backslash u_1 u_2 u_4 u_5)\,. \end{aligned}$$

Note that

$$P^*\backslash e_1 u_4 u_5 = P^{**}\backslash e_4 u_4 u_5 \ , \ \ P^*\backslash e_1 e_4 = P^{**}\backslash e_1 e_4 \ , \ \ P^*\backslash u_1 u_2 e_1 = P^{**}\backslash u_1 u_2 e_4\,.$$

Then

$$\begin{aligned} b_k(P^{**}) - b_k(P^*) &= (w_1^2 - w_4^2)\big[b_{k-2}(P^*\backslash e_1 u_4 u_5) - b_{k-2}(P^*\backslash u_1 u_2 e_4)\big] \\ &= (w_1^2 - w_4^2)\big[b_{k-2}(P^*\backslash e_1 e_2 u_4 u_5) + w_2^2 b_{k-4}(P^*\backslash e_1 u_2 u_3 u_4 u_5) \\ &- b_{k-2}(P^*\backslash u_1 u_2 e_3 e_4) - w_3^2 b_{k-4}(P^*\backslash u_1 u_2 u_3 u_4)\big] \geq 0 \end{aligned}$$

and there exists at least one index k such that $b_k(P^{**}) - b_k(P^*) > 0$ as $P^*\backslash e_1 u_2 u_3 u_4 u_5$ is a proper subgraph of $P^*\backslash u_1 u_2 u_3 u_4$. Thus $P^* \prec P^{**}$, a contradiction to conditions (3) and (4).

Case (2): $w_1 \geq w_4$ and $w_2 > w_3$.

Let P^{**} be the weighted path obtained from P^* by exchanging the edges e_2 and e_3, that is, $P^{**} = u_1 e_1 u_2 e_3 u_3 e_2 u_4 e_4 u_5 \ldots u_{n-1} e_{n-1} u_n$. Then by the hypothesis that $\mathcal{E}(P^*) = \hat{\mathbb{E}}(n, W)$, we have

$$\mathcal{E}(P^{**}) \leq \mathcal{E}(P^*)\,. \tag{5}$$

Using the same argument in the Case (1), we also can derive a contradiction.

Case (3): $w_1 < w_4$ and $w_2 > w_3$.

Let P^{**} be the weighted path obtained from P^* by exchanging the edges e_2 and e_3, e_1 and e_4, that is, $P^{**} = u_1 e_4 u_2 e_3 u_3 e_2 u_4 e_1 u_5 \ldots u_{n-1} e_{n-1} u_n$. Then by the hypothesis that $\mathcal{E}(P^*) = \hat{\mathbb{E}}(n, W)$, we have

$$\mathcal{E}(P^{**}) \leq \mathcal{E}(P^*)\,. \tag{6}$$

Applying Lemma 4, we have

$$\begin{aligned} b_k(P^*) &= b_k(P^*\backslash e_1 e_2 e_3 e_4) + w_4^2\, b_{k-2}(P^*\backslash u_1 u_2 u_3 u_4 u_5) + w_3^2\, b_{k-2}(P^*\backslash u_1 u_2 u_3 u_4) \\ &+ w_2^2\, b_{k-2}(P^*\backslash u_2 u_3 u_4) + w_2^2\, w_4^2\, b_{k-4}(P^*\backslash u_2 u_3 u_4 u_5) + w_1^2\, b_{k-2}(P^*\backslash u_1 u_2 u_3 u_4) \\ &+ w_1^2\, w_4^2\, b_{k-4}(P^*\backslash u_1 u_2 u_3 u_4 u_5) + w_1^2\, w_3^2\, b_{k-4}(P^*\backslash u_1 u_2 u_3 u_4) \end{aligned}$$

and

$$\begin{aligned} b_k(P^{**}) &= b_k(P^{**}\backslash e_1e_2e_3e_4) + w_1^2\, b_{k-2}(P^{**}\backslash u_1u_2u_3u_4u_5) + w_2^2\, b_{k-2}(P^{**}\backslash u_1u_2u_3u_4) \\ &+ w_3^2\, b_{k-2}(P^{**}\backslash u_2u_3u_4) + w_1^2 w_3^2\, b_{k-4}(P^{**}\backslash u_2u_3u_4u_5) + w_4^2\, b_{k-2}(P^{**}\backslash u_1u_2u_3u_4) \\ &+ w_1^2\, w_4^2\, b_{k-4}(P^{**}\backslash u_1u_2u_3u_4u_5) + w_2^2\, w_4^2\, b_{k-4}(P^{**}\backslash u_1u_2u_3u_4)\,. \end{aligned}$$

Then

$$\begin{aligned} b_k(P^{**}) - b_k(P^*) &= (w_1^2 - w_4^2)\big[b_{k-2}(P^*\backslash u_1u_2u_3u_4u_5) - b_{k-2}(P^*\backslash u_1u_2u_3u_4)\big] \\ &+ (w_1^2\, w_3^2 - w_2^2\, w_4^2)\big[b_{k-4}(P^*\backslash u_1u_2u_3u_4u_5) - b_{k-4}(P^*\backslash u_1u_2u_3u_4)\big] \geq 0 \end{aligned}$$

and there exists at least one index k such that $b_k(P^{**}) - b_k(P^*) > 0$ as $P^*\backslash u_1u_2u_3u_4u_5$ is a proper subgraph of $P^*\backslash u_1u_2u_3u_4$. Thus $P^* \prec P^{**}$, a contradiction to conditions (3) and (6). Consequently, the result (**a**) follows.

The proof of (**b**) is analogous. □

Theorem 14. *Let $n \geq 7$ and $W = \{x, y, z, s, \overbrace{t, \ldots, t}^{n-5}\}$ be a positive number sequence with $x \geq y \geq z \geq s \geq t$. Then, up to isomorphism, $P^* = x\ t\ z\ \overbrace{t\ \ldots\ t}^{n-7}\ s\ t\ y$ is the unique path achieving energy $\hat{\mathbb{E}}(n, W)$.*

Proof. Let $P^* = u_1e_1u_2e_2u_3 \ldots u_{n-1}e_{n-1}u_n$. Without loss of generality, suppose that $s > t = 1$. Let $w_i = w(e_i)$ for $i = 1, 2, \ldots, n-1$. We divide our proof into three assertions.

Assertion 1. $w_1 > 1$ and $w_{n-1} > 1$.

We first claim that $w_1 > 1$. Otherwise, assume to the contrary that i $(i \geq 2)$ is the least index such that $w_i > 1$. Note that P^* can be considered as the graph obtained from the union of the weighted paths P_{i+1} and P_{n-i-1} by adding an edge with weight at least 1. Then applying Theorem 10, a contradiction will be encountered. Similarly, $w_{n-1} > 1$.

Assertion 2. $w_3 > 1$ and $w_{n-3} > 1$.

Suppose now that i and j $(2 \leq i < j \leq n-2)$ are two other indices of P^* such that $w_i > 1$ and $w_j > 1$. We have the following Claim.

Claim 15. $i \geq 3,\ j \leq n-3$. *Moreover, if* $n \geq 8,\ i \leq j-2$.

Proof of Claim 15. We first show that $i \geq 3$. Otherwise we have $i = 2$. By Lemma 13, we have $w_3 \geq w_2 > 1$, and $w_h = 1$, for $h = 4, \ldots, n-2$. Let P^{**} be the weighted path obtained from P^* by exchanging the edges e_2 and e_{n-3}, that is, $P^{**} = u_1e_1u_2e_{n-3}u_3e_3u_4 \ldots u_{n-3}e_2u_{n-2}e_{n-2}u_{n-1}e_{n-1}u_n$. Then by the hypothesis that $\mathcal{E}(P^*) = \hat{\mathbb{E}}(n, W)$, we have $\mathcal{E}(P^{**}) \leq \mathcal{E}(P^*)$.

Applying Lemma 4, we have

$$\begin{aligned} b_k(P^*) &= b_k(P^*\backslash e_2) + w_2^2\, b_{k-2}(P^*\backslash u_2u_3) \\ &= b_k(P^*\backslash e_2e_{n-3}) + b_{k-2}(P^*\backslash e_2u_{n-3}u_{n-2}) \\ &+ w_2^2\, b_{k-2}(P^*\backslash u_2u_3e_{n-3}) + w_2^2\, b_{k-4}(P^*\backslash u_2u_3u_{n-3}u_{n-4}) \end{aligned}$$

and

$$\begin{aligned} b_k(P^{**}) &= b_k(P^{**}\backslash e_{n-3}) + b_{k-2}(P^{**}\backslash u_2u_3) \\ &= b_k(P^{**}\backslash e_2e_{n-3}) + w_2^2\, b_{k-2}(P^{**}\backslash e_{n-3}u_{n-3}u_{n-2}) \\ &+ b_{k-2}(P^{**}\backslash u_2u_3e_2) + w_2^2\, b_{k-4}(P^{**}\backslash u_2u_3u_{n-3}u_{n-4})\,. \end{aligned}$$

Note that $P^*\backslash e_2u_{n-3}u_{n-2} = P^{**}\backslash e_{n-3}u_{n-3}u_{n-2}\,$, $P^*\backslash u_2u_3e_{n-3} = P^{**}\backslash u_2u_3e_2\,$, and that $P^*\backslash u_2u_3u_{n-3}u_{n-4} = P^{**}\backslash u_2u_3u_{n-3}u_{n-4}\,$. Then

$$b_k(P^{**}) - b_k(P^*) = (w_2^2 - 1)\big[P^*\backslash e_2u_{n-3}u_{n-2} - P^*\backslash u_2u_3e_{n-3}\big] \geq 0$$

and there exists at least one index k such that $b_k(P^{**}) - b_k(P^*) > 0$. Thus $P^* \prec P^{**}$, a contradiction to the hypothesis. Thus we have $i \geq 3$. Similarly we can get $j \leq n-3$.

Now assume otherwise that $i = j-1$. For the case that $i \geq 4$ (or $j \leq n-4$), we can also construct a new path which has larger energy than P^* with the similar technique by exchanging the edges e_3 and e_i (or e_j and e_{n-3}), which contradicts to the hypothesis. Thus we have $3 = i = j-1 = n-4$, which leads $n = 7$. This finishes the proof of Claim 15. □

For $n = 7$, combining Lemma 13, Lemma 6 of [7], and the above Claim, P^* is either $x\,1\,z\,s\,1\,y$ or $x\,1\,s\,z\,1\,y$. Assertion 2 holds immediately. Thus we always assume that $n \geq 8$. Let $\bar{P}_n = u_1e_1u_2 \ldots u_{n-1}e_{n-1}u_n$ be the un-weighted path of order n.

Then P^* is E-equivalent to the graph, denoted by $\tilde{P}$, which is a weighted 2-split graph of P^* on the edges e_1, e_i, e_j, and e_{n-1}, respectively, where the edge e'_h parallels to e_h, and $w(e'_h) = \sqrt{(w(e_h))^2 - 1}$ for each $h = 1, i, j, n-1$.

For convenience, let $M = \{e'_h \,|\, h = 1, i, j, n-1\}$ and $w'_h = w(e'_h)$ for $h = 1, i, j, n-1$. We divide all Sachs graphs of $\tilde{P}$, having k vertices, into five parts: those that contain no edges of M, those that contain exactly one edge of M, those that contain exactly two edges of M, those that contain exactly three edges of M and those that contain all edges of M. Denote by $b_k^t(\tilde{P})$ for $t = 0, 1, 2, 3, 4$ the sum of the weights of all above five types of Sachs graphs, respectively. Obviously, $b_k^0(\tilde{P}) = b_k(\bar{P}_n)$, which is regardless the choice of the indices i and j. Combining Claim 15 with Lemmas 4 and 6, we have

$$\begin{aligned} b_k^1(\tilde{P}) &= [w_1'^2 + w_{n-1}'^2]\, b_{k-2}(\bar{P}_{n-2}) + w_i'^2\, b_{k-2}(\bar{P}_n \backslash u_i u_{i+1}) + w_j'^2\, b_{k-2}(\bar{P}_n \backslash u_j u_{j+1}) \\ &\leq \big[w_1'^2 + w_{n-1}'^2\big] b_{k-2}(\bar{P}_{n-2}) + \big[w_i'^2 + w_j'^2\big] b_{k-2}(\bar{P}_{n-4} \cup \bar{P}_2) \end{aligned}$$

with equality holding if and only if $i = 3$ and $j = n-3$. Similarly,

$$\begin{aligned} b_k^2(\tilde{P}) &= w_1'^2\, w_i'^2\, b_{k-4}(\bar{P}_{n-2} \backslash u_{i-2}\, u_{i-1}) + w_1'^2\, w_j'^2\, b_{k-4}(\bar{P}_{n-2} \backslash u_{j-2} u_{j-1}) \\ &+ w_1'^2\, w_{n-1}'^2\, b_{k-4}(\bar{P}_{n-4}) + w_i'^2\, w_j'^2\, b_{k-4}(\bar{P}_n \backslash u_i u_{i+1} u_j u_{j+1}) \\ &+ w_i'^2\, w_{n-1}'^2\, b_{k-4}(\bar{P}_{n-2} \backslash u_i u_{i+1}) + w_j'^2\, w_{n-1}'^2\, b_{k-4}(\bar{P}_{n-2} \backslash u_j u_{j+1}) \\ &\leq \big[w_1'^2\, w_i'^2 + w_j'^2\, w_{n-1}'^2 + w_1'^2\, w_{n-1}'^2\big] b_{k-4}(\bar{P}_{n-4}) \\ &+ \big[w_1'^2\, w_j'^2 + w_i'^2\, w_{n-1}'^2\big] b_{k-4}(\bar{P}_{n-6} \cup \bar{P}_2) + w_i'^2\, w_j'^2\, b_{k-4}(\bar{P}_{n-8} \cup 2\bar{P}_2) \end{aligned}$$

with equality holding if and only if $i = 3$ and $j = n-3$,

$$\begin{aligned} b_k^3(\tilde{P}) &= w_i'^2\, w_j'^2\, w_{n-1}'^2\, b_{k-6}(\bar{P}_{n-2} \backslash u_i u_{i+1} u_j u_{j+1}) + w_1'^2\, w_j'^2\, w_{n-1}'^2\, b_{k-6}(\bar{P}_{n-4} \backslash u_{j-2} u_{j-1}) \\ &+ w_1'^2\, w_i'^2\, w_{n-1}'^2\, b_{k-6}(\bar{P}_{n-4} \backslash u_{i-2} u_{i-1}) + w_1'^2\, w_i'^2\, w_j'^2\, b_{k-6}(\bar{P}_{n-2} \backslash u_{i-2} u_{i-1} u_{j-2} u_{j-1}) \\ &\leq \big[w_1'^2 + w_{n-1}'^2\big] w_i'^2\, w_j'^2\, b_{k-6}(\bar{P}_{n-8} \cup \bar{P}_2) + \big[w_i'^2 + w_j'^2\big] w_1'^2\, w_{n-1}'^2\, b_{k-6}(\bar{P}_{n-6}) \end{aligned}$$

with equality holding if and only if $i = 3$ and $j = n-3$, and

$$\begin{aligned} b_k^4(\tilde{P}) &= w_1'^2\, w_i'^2\, w_j'^2\, w_{n-1}'^2\, b_{k-8}(\bar{P}_{i-3} \cup \bar{P}_{j-i-2} \cup \bar{P}_{n-j-3}) \\ &\leq w_1'^2\, w_i'^2\, w_j'^2\, w_{n-1}'^2\, b_{k-8}(\bar{P}_{n-8}) \end{aligned}$$

with equality holding if and only if either $i = 3$ and $j = n-3$, or $i = 3$ and $j = 5$, or $i = n-5$ and $j = n-3$. Consequently, $b_k(\tilde{P})$ attains the unique maximum value if and only if $i = 3$ and $j = n-3$. The result hence follows.

Assertion 3. $P^* = x\ 1\ z\ \overbrace{1\ \ldots\ 1}^{n-7}\ s\ 1\ y$.

Combining Assertion 2 with Lemma 6 of [7], P^* is either P_1 or P_2 or P_3, where

$$\begin{aligned} P_1 &= x\ 1\ z\ \overbrace{1\ \ldots\ 1}^{n-7}\ s\ 1\ y \\ P_2 &= x\ 1\ s\ \overbrace{1\ \ldots\ 1}^{n-7}\ z\ 1\ y \\ P_3 &= x\ 1\ y\ \overbrace{1\ \ldots\ 1}^{n-7}\ s\ 1\ z\,. \end{aligned}$$

We now show that $P_1 \succ P_2$ and $P_1 \succ P_3$. Applying Lemma 4, we have

$$\begin{aligned} b_k(P_1) &= b_k(P_1 \backslash e_3) + z^2\, b_{k-2}(P_1 \backslash u_3 u_4) \\ &= b_k(P_1 \backslash e_3 e_{n-3}) + s^2\, b_{k-2}(P_1 \backslash e_3 u_{n-3} u_{n-2}) \\ &+ z^2\, b_{k-2}(P_1 \backslash u_3 u_4 e_{n-3}) + z^2 s^2\, b_{k-4}(P_1 \backslash u_3 u_4 u_{n-3} u_{n-2}) \end{aligned}$$

and

$$\begin{aligned} b_k(P_2) &= b_k(P_2 \backslash e_{n-3}) + s^2\, b_{k-2}(P_2 \backslash u_3 u_4) \\ &= b_k(P_2 \backslash e_3 e_{n-3}) + z^2\, b_{k-2}(P_2 \backslash e_{n-3} u_{n-3} u_{n-2}) \\ &+ s^2\, b_{k-2}(P_2 \backslash u_3 u_4 e_3) + z^2 s^2\, b_{k-4}(P_2 \backslash u_3 u_4 u_{n-3} u_{n-2})\,. \end{aligned}$$

This implies

$$b_k(P_1) - b_k(P_2) = (s^2 - z^2)[b_{k-2}(P_1 \backslash e_3 u_{n-3} u_{n-2}) - b_{k-2}(P_1 \backslash u_3 u_4 e_{n-3})] \geq 0\,.$$

Consequently, $P_1 \succ P_2$. By a similar method, we conclude that $P_1 \succ P_3$.

Hence, the result follows. □

4 The path achieving maximal energy in $\mathcal{P}(n, m)$ for $m \leq n+3$

Definition 16. *Let G be an un-weighted graph, $e \in G$ a cut edge, and $G_e(k)$ denote the graph obtained by replacing e with an un-weighted path of length $k+1$* (for simplicity, we abbreviate $G_e(k)$ by $G(k)$). *Then $G(k)$ is referred to as a k-subdivision graph of G on the cut edge e. We also agree that $G(0) = G$.*

In [27], Shan et al. introduced a method for comparing the energies of two k-subdivision bipartite graphs $G(k)$ and $H(k)$ when these are quasi-order incomparable, as follows.

Lemma 17. [27, Theorem 3.1(1)] *Let $G(k)$, $H(k)$ be $k-$subdivision graphs on some cut edges of the un-weighted bipartite graphs G and H of order n, respectively ($k \geq 0$), and $g_k = \tilde{\phi}(G(k), \lambda)$ and $h_k = \tilde{\phi}(H(k), \lambda)$ for each k. If $h_1\, g_0 - h_0\, g_1 > 0$ for all $\lambda > 0$, then*

$$\mathcal{E}(H(k)) - \mathcal{E}(G(k)) > \mathcal{E}(H(0)) - \mathcal{E}(G(0)) \qquad \text{for all } k > 0.$$

One can easily verify that this result is equally well applicable in the case of weighted graphs when the edge e described in Definition 16 and all subdivided edges having weight 1. Hence, we have

Lemma 18. *Let $n \geq 5$, $P_n^* = a\ \overbrace{1\ \ldots\ 1}^{n-3}\ b \in \mathcal{P}(n,m)$ and $P_n^{**} = a+1\ \overbrace{1\ \ldots\ 1}^{n-3}\ b-1 \in \mathcal{P}(n,m)$. If $a \geq b \geq 2$, then $\mathcal{E}(P_n^{**}) > \mathcal{E}(P_n^*)$.*

Proof. P_n^* and P_n^{**} respectively can be considered as $(n-4)$-subdivision graphs of P_4^* and P_4^{**} on their middle edges, where each subdivided edge has weight 1. Let $g_i = \tilde{\phi}(P_{i+4}^*, \lambda)$ and $h_i = \tilde{\phi}(P_{i+4}^{**}, \lambda)$ for $i = 0, 1, \ldots, n-4$. By direct calculation,

$$\begin{aligned} g_0 &= \lambda^4 + (a^2+1+b^2)\lambda^2 + a^2b^2 \\ g_1 &= \lambda^5 + (a^2+2+b^2)\lambda^3 + (a^2+a^2b^2+b^2)\lambda \\ h_0 &= \lambda^4 + ((a+1)^2+(b-1)^2+1)\lambda^2 + (a+1)^2(b-1)^2 \\ h_1 &= \lambda^5 + ((a+1)^2+(b-1)^2+2)\lambda^3 + \big[(a+1)^2+(b-1)^2+(a+1)^2(b-1)^2\big]\lambda\,. \end{aligned}$$

Then

$$\begin{aligned} h_1\, g_0 - g_1\, h_0 &= (1+a-b)\big[-b^2+b^3+a^3(-1+2b)+a^2(-1+b+2b^2)+\lambda^2 \\ &+ b\lambda^2 + a(-1+2b)(b^2+\lambda^2)\big]\lambda > 0 \end{aligned}$$

for all $\lambda > 0$, since $a \geq b \geq 2$.

From Example 9 in [3], we have

$$\mathcal{E}(P_4^*) = \mathcal{E}(P_4^{**})\,.$$

Consequently, combining this with Lemma 17,

$$\mathcal{E}(P_n^{**}) - \mathcal{E}(P_n^*) > \mathcal{E}(P_4^{**}) - \mathcal{E}(P_4^*) = 0$$

for each n ($n \geq 5$). Hence, the result follows. □

Theorem 19. *Let $n \geq 5$ and $n \leq m \leq n+3$. The path with weight sequence $\{m-n+2, 1, \ldots, 1\}$, where the weight of one of the pendent edges equals $m-n+2$, is the unique tree in $\mathcal{T}(n,m)$ with maximum energy.*

Proof. For $m = n$, since the weight sequence of each tree in $\mathcal{T}(n,n)$ must be $\{2, \overbrace{1, \ldots, 1}^{n-2}\}$, the result follows from Lemma 11.

For $m = n+1$, the weight sequence of each tree in $\mathcal{T}(n, n+1)$ may be either $\{3, \overbrace{1, \ldots, 1}^{n-2}\}$ or $\{2, 2, \overbrace{1, \ldots, 1}^{n-3}\}$. Then combining with Lemmas 11, 12, and 18 the result follows.

For $m = n+2$, the weight sequence of each tree in $\mathcal{T}(n, n+2)$ may be either $\{2, 2, 2, \overbrace{1, \ldots, 1}^{n-4}\}$ or $\{3, 2, \overbrace{1, \ldots, 1}^{n-3}\}$ or $\{4, \overbrace{1, \ldots, 1}^{n-2}\}$. Then combining with Lemma 11, 12, and Theorem 14, the path with energy $\hat{\mathbb{E}}(n, n+2)$ is either $P_n^1 = 4\ \overbrace{1\ \ldots\ 1}^{n-2}$ or $P_n^2 = 3\ \overbrace{1\ \ldots\ 1}^{n-2}\ 2$ or $P_n^3 = 2\ 1\ 2\ \overbrace{1\ \ldots\ 1}^{n-5}\ 2$. Applying Lemma 18, it suffices to show that $\mathcal{E}(P_n^2) > \mathcal{E}(P_n^3)$.

If $n = 5$, then by direct calculation we get $\mathcal{E}(P_5^2) = 10.7704$ and $\mathcal{E}(P_5^3) = 10$. The result follows.

For $n \geq 6$, note that P_n^2 and P_n^3 respectively can be considered as $(n-6)$-subdivision graphs of $P_6^2 = u_1 3 u_2 1 u_3 1 u_4 1 u_5 2 u_6$ and $P_6^3 = u_1 2 u_2 1 u_3 2 u_4 1 u_5 2 u_6$ on the edge $u_4 u_5$, where each subdivided edge has weight 1. Let $h_i = \tilde{\phi}(P_{i+6}^2, \lambda)$ and $g_i = \tilde{\phi}(P_{i+6}^3, \lambda)$ for $i = 0, 1, \ldots, n-6$. By direct calculation we get

$$\begin{aligned} g_0 &= 64 + 57\lambda^2 + 14\lambda^4 + \lambda^6 \\ h_0 &= 36 + 63\lambda^2 + 16\lambda^4 + \lambda^6 \\ g_1 &= 100\lambda + 70\lambda^3 + 15\lambda^5 + \lambda^7 \\ h_1 &= 85\lambda + 78\lambda^3 + 17\lambda^5 + \lambda^7 . \end{aligned}$$

Then

$$h_1\, g_0 - h_0\, g_1 = \lambda(1840 + 1017\lambda^2 + 174\lambda^4 + 9\lambda^6) > 0$$

for all $\lambda > 0$. Thus, by Lemma 17, $\mathcal{E}(P_n^2) - \mathcal{E}(P_n^3) > \mathcal{E}(P_5^2) - \mathcal{E}(P_5^3) > 0$ for each n ($n \geq 6$).

For $m = n+3$, the weight sequence of each tree in $\mathcal{T}(n, n+3)$ may be either $W_1 = \{5, \overbrace{1, \ldots, 1}^{n-2}\}$ or $W_2 = \{4, 2, \overbrace{1, \ldots, 1}^{n-3}\}$ or $W_3 = \{3, 3, \overbrace{1, \ldots, 1}^{n-3}\}$ or $W_4 = \{3, 2, 2, \overbrace{1, \ldots, 1}^{n-4}\}$ or $W_5 = \{2, 2, 2, 2, \overbrace{1, \ldots, 1}^{n-5}\}$. By Lemma 18,

$$\hat{\mathbb{E}}(n, W_1) > \hat{\mathbb{E}}(n, W_2) > \hat{\mathbb{E}}(n, W_3)\,.$$

Then it suffices to show that $\hat{\mathbb{E}}(n, W_3) > \hat{\mathbb{E}}(n, W_4)$ and $\hat{\mathbb{E}}(n, W_4) > \hat{\mathbb{E}}(n, W_5)$.

We first show that $\hat{\mathbb{E}}(n, W_3) > \hat{\mathbb{E}}(n, W_4)$. From Lemma 14, the paths with energies $\hat{\mathbb{E}}(n, W_3)$ and $\hat{\mathbb{E}}(n, W_4)$ are $P_n^3 = 3\ \overbrace{1\ \ldots\ 1}^{n-4}\ 3$ and $P_n^4 = 3\ 1\ 2\ \overbrace{1\ \ldots\ 1}^{n-5}\ 2$, respectively. By direct calculation, we show that $\mathcal{E}(P_5^3) = 12.6332$ and $\mathcal{E}(P_5^4) = 11.9056$. Thus the result follows if $n = 5$.

For $n \geq 6$, note that P_n^3 and P_n^4 respectively can be considered as $(n-6)$-subdivision graphs of $P_6^3 = u_1 3 u_2 1 u_3 2 u_4 1 u_5 2 u_6$ and $P_6^4 = u_1 3 u_2 1 u_3 1 u_4 1 u_5 3 u_6$ on the edge $u_4 u_5$, where each subdivided edge has weight 1. Let $g_i = \tilde{\phi}(P_{i+6}^4, \lambda)$ and $h_i = \tilde{\phi}(P_{i+6}^3, \lambda)$ for $i = 0, 1, \ldots, n-6$. By direct calculation we obtain

$$\begin{aligned} g_0 &= 144 + 102\lambda^2 + 19\lambda^4 + \lambda^6 \\ h_0 &= 81 + 118\lambda^2 + 21\lambda^4 + \lambda^6 \\ g_1 &= 220\lambda + 120\lambda^3 + 20\lambda^5 + \lambda^7 \\ h_1 &= 180\lambda + 138\lambda^3 + 22\lambda^5 + \lambda^7\,. \end{aligned}$$

Then

$$h_1\, g_0 - h_0\, g_1 = \lambda(8100 + 2552\lambda^2 + 264\lambda^4 + 9\lambda^6) > 0$$

for all $\lambda > 0$. Thus $\hat{\mathbb{E}}(n, W_3) > \hat{\mathbb{E}}(n, W_4)$ for each n (≥ 6).

We next show that $\hat{\mathbb{E}}(n, W_4) > \hat{\mathbb{E}}(n, W_5)$.

Applying Theorem 10 in [7], the paths with energies $\hat{\mathbb{E}}(5, W_4)$ and $\hat{\mathbb{E}}(5, W_5)$ are $P_5^4 = 3\ 1\ 2\ 2$ and $P_5^5 = 2\ 2\ 2\ 2$, and the paths with energies $\hat{\mathbb{E}}(6, W_4)$ and $\hat{\mathbb{E}}(6, W_5)$ are $P_6^4 = 3\ 1\ 2\ 1\ 2$ and $P_6^5 = 2\ 1\ 2\ 2\ 2$, respectively. By direct calculation, we have $\mathcal{E}(P_5^4) = 11.9056$, $\mathcal{E}(P_5^4) = 10.9282$, $\mathcal{E}(P_6^4) = 14.4484$, and $\mathcal{E}(P_6^4) = 13.2156$. Thus the result follows for $n = 5, 6$.

For $n \geq 7$, let $P_n^* = 2\ 1\ 3\ \overbrace{1\ \ldots\ 1}^{n-5}\ 2$. Applying Theorem 14, the path with energy $\hat{\mathbb{E}}(n, W_5)$ is $P_n^5 = 2\ 1\ 2\ \overbrace{1\ \ldots\ 1}^{n-7}\ 2\ 1\ 2$. From Theorem 14, it follows that

$\mathcal{E}(P_n^4) > \mathcal{E}(P_n^*)$. Then it suffices to show that $\mathcal{E}(P_n^*) > \mathcal{E}(P_n^5)$. By direct calculation, we get $\mathcal{E}(P_7^*) = 14.9886$ and $\mathcal{E}(P_7^5) = 13.3340$. Then $\mathcal{E}(P_7^*) > \mathcal{E}(P_7^5)$. For $n \geq 8$, note that P_n^* and P_n^5 respectively can be considered as $(n-8)$-subdivision graphs of $P_8^* = u_1 2 u_2 1 u_3 3 u_4 1 u_5 1 u_6 1 u_7 2 u_8$ and $P_8^5 = u_1 2 u_2 1 u_3 2 u_4 1 u_5 2 u_6 1 u_7 2 u_8$ on the edge $u_4 u_5$, where each subdivided edge has weight 1. Let $g_i = \tilde{\phi}(P_{i+8}^5, \lambda)$ and $h_i = \tilde{\phi}(P_{i+8}^*, \lambda)$ for $i = 0, 1, \ldots, n-8$. By direct calculation,

$$\begin{aligned}
g_0 &= \lambda^8 + 19\lambda^6 + 123\lambda^4 + 313\lambda^2 + 256 \\
h_0 &= \lambda^8 + 21\lambda^6 + 134\lambda^4 + 297\lambda^2 + 144 \\
g_1 &= \lambda^9 + 20\lambda^7 + 141\lambda^5 + 410\lambda^3 + 416\lambda \\
h_1 &= \lambda^9 + 22\lambda^7 + 154\lambda^5 + 412\lambda^3 + 344\lambda \\
h_1\, g_0 - h_0\, g_1 &= \lambda(4+\lambda^2)(5+\lambda^2)(1408 + 894\lambda^2 + 171\lambda^4 + 9\lambda^6) > 0
\end{aligned}$$

for all $\lambda > 0$. Thus $\mathcal{E}(P_n^*) > \mathcal{E}(P_n^5)$ for each n (≥ 8).

Consequently, the result follows. □

References

[1] J. Aihara, General rules for constructing Hückel molecular orbital characteristic polynomials, *J. Am. Chem. Soc.* **98** (1976) 6840–6844.

[2] S. Akbari, E. Ghorbani, M. R. Oboudi, Edge addition, singular values and energy of graphs and matrices, *Lin. Algebra Appl.* **430** (2009) 2192–2199.

[3] R. A. Brualdi, J. Y. Shao, S. C. Gong, C. Q. Xu, G. H. Xu, On the extremal energy of integral weighted trees, *Lin. Multilin. Algebra* **60** (2012) 1255–1264.

[4] C. A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, *Proc. Cambridge Phil. Soc.* **36** (1940) 201–203.

[5] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.

[6] D. Cvetković, P. Rowlinson, S. Simić, *An Introduction to the Theory of Graph Spectra*, Cambridge Univ. Press, Cambridge, 2010.

[7] S. C. Gong, X. L. Li, I. Gutman, G. H. Xu, Y. X. Tang, Z. M. Qin, K. Yang, On the maximal energy of trees with fixed weight sequence, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 267–278.

[8] S. C. Gong, G. H. Xu, The characteristic polynomial and the matchings polynomial of a weighted oriented graph, *Lin. Algebra Appl.* **436** (2012) 3597–3607.

[9] A. Graovac, I. Gutman, N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer, Berlin, 1977.

[10] A. Graovac, I. Gutman, N. Trinajstić, T. Živković, Graph theory and molecular orbitals. Application of Sachs theorem, *Theor. Chim. Acta* **26** (1972) 67–78.

[11] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

[12] I. Gutman, Generalizations of a recurrence relation for the characteristic polynomials of trees, *Publ. Inst. Math. (Beograd)* **21** (1977) 75–80.

[13] I. Gutman, The energy of a graph, *Ber. Math.-Statist. Sekt. Forschungsz. Graz.* **103** (1978) 1–22.

[14] I. Gutman, Partial ordering of forests according to their characteristic polynomials, in: A. Hajnal, V. T. Sós (Eds.), *Combinatorics*, North–Holland, Amsterdam, 1978, pp. 429–436.

[15] I. Gutman, Rectifying a misbelief: Frank Harary's role in the discovery of the coefficient–theorem in chemical graph theory, *J. Math. Chem.* **16** (1994) 73–78.

[16] I. Gutman, The energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Lau, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer, Berlin, 2001, pp. 196–211.

[17] I. Gutman, Impact of the Sachs theorem on theoretical chemistry: A participant's testimony, *MATCH Commun. Math. Comput. Chem.* **48** (2003) 17–34.

[18] I. Gutman, X. Li (Eds.), *Graph Energies – Theory and Applications*, Univ. Kragujevac, Kragujevac, 2016.

[19] I. Gutman, X. Li, J. Zhang, Graph energy, in: M. Dehmer, F. Emmert–Streib (Eds.), *Analysis of Complex Networks. From Biology to Linguistics*, Wiley–VCH, Weinheim, 2009, pp. 145–174.

[20] I. Gutman, M. Mateljević, Note on the Coulson integral formula, *J. Math. Chem.* **39** (2006) 259–266.

[21] I. Gutman, J. Y. Shao, The energy change of weighted graphs, *Lin. Algebra Appl.* **435** (2011) 2425–2431.

[22] I. Gutman, F. Zhang, On a quasiordering of bipartite graphs, *Publ. Inst. Math. (Beograd)* **40** (1986) 11–15.

[23] I. Gutman, F. Zhang, On the ordering of graphs with respect to their matching numbers, *Discr. Appl. Math.* **15** (1986) 25–33.

[24] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, new York, 2012.

[25] R. B. Mallion, A. J. Schwenk, N. Trinajstić, A graphical study of heteroconjugated molecules, *Croat. Chem. Acta* **46** (1974) 171–182.

[26] R. B. Mallion, N. Trinajstić, A. J. Schwenk, Graph theory in chemistry – Generalization of Sachs' formula, *Z. Naturforsch.* **29a** (1974) 1481–1484.

[27] H. Y. Shan, J. Y. Shao, L. Zhang, C. X. He, A New method of comparing the energies of subdivision bipartite graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 721–740.

[28] J. Y. Shao, F. Gong, Z. B. Du, The extremal energies of weighted trees and forests with fixed total weight sum, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 879–890.

[29] F. Zhang, Two theorems of comparison of bipartite graphs by their energy, *Kexue Tongbao* **28** (1983) 726–730.

[30] F. Zhang, Z. Lai, Three theorems of comparison of trees by their energy, *Sci. Explor.* **3** (1983) 12–19.