J Math Chem (2012) 50:2637–2647
DOI 10.1007/s10910-012-0052-4

ORIGINAL PAPER

The proof of a conjecture on the comparison of the energies of trees

Hai-Ying Shan · Jia-Yu Shao

Received: 15 June 2012 / Accepted: 9 July 2012 / Published online: 24 July 2012

Abstract The energy of a graph is defined as the sum of the absolute values of the eigenvalues of the graph. In this paper, we first present a new method to directly compare the energies of two bipartite graphs, then also present some new techniques to compare the quasi-orders of some bipartite graphs. As the applications of these methods, we prove that a conjecture proposed by Wang and Kang (J Math Chem 47(3):937–958, 2010) is true. At the same time, our results also provide the simplified proofs of the main results of Wang and Kang (J Math Chem 47(3):937–958, 2010) and Li and Li (Electron J Linear Algebra 17:414–425, 2008).

Keywords Bipartite graph · Tree · Energy · k-Claw attaching operation · Quasi-ordering

Mathematics Subject Classification (2000) 05C50

1 Introduction

Let G be a graph with n vertices and A be its adjacency matrix. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A, then the *energy* of G, denoted by $\mathbb{E}(G)$, is defined [2,3] as $\mathbb{E}(G) = \sum_{i=1}^{n} |\lambda_i|$.

Definition 1.1 A tree T is called a caterpillar if the graph obtained by deleting all the pendant vertices of T is a path. A caterpillar of order n obtained from a path

H.-Y. Shan (✉) · J.-Y. Shao
Department of Mathematics, Tongji University, Shanghai 200092, People's Republic of China
e-mail: shan_haiying@tongji.edu.cn

J.-Y. Shao
e-mail: jyshao@tongji.edu.cn

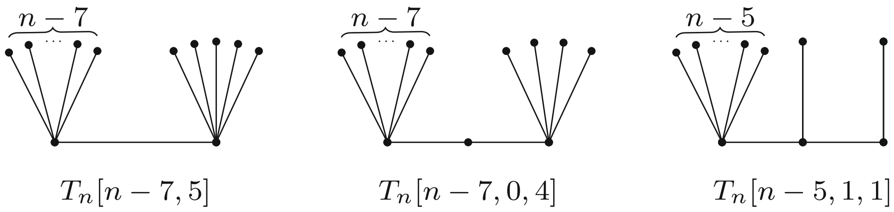

Fig. 1 The trees $T_n[n-7,5]$, $T_n[n-7,0,4]$ and $T_n[n-5,1,1]$

$v_1v_2,\ldots,v_{d-1}$ by adding $n_i (n_i \geq 0)$ pendent edges to v_i $(i = 1,\ldots,d-1)$ is denoted by $T_n[n_1, n_2, \ldots, n_{d-1}]$, where $\sum_{i=1}^{d-1} n_i + d - 1 = n$.

When $n_1 \geq 1$ and $n_{d-1} \geq 1$, then the diameter of $T_n[n_1, n_2, \ldots, n_{d-1}]$ is d.

Graphs with extremal energies are extensively studied in literature. Gutman [1] determined the first four smallest energy trees of order n. Li and Li [5] determined the 5 and 6th smallest energy trees of order n. Wang and Kang [8] determined the 7–9th smallest energy trees of order n. Using our notations given above, these results can be summarized as the following:

Theorem 1.1 [1,5,8] *If $n \geq 46$, then the following nine trees are the first nine smallest energy trees of order n : $T_n[n-1]$, $T_n[n-3,1]$, $T_n[n-4,2]$, $T_n[n-4,0,1]$, $T_n[n-5,3]$, $T_n[n-5,0,2]$, $T_n[n-6,4]$, $T_n[n-6,0,3]$, $T_n[1,n-5,1]$ (Fig. 1).*

In [8], Wang and Kang further proposed the following conjecture:

Conjecture 1.1 (Wang–Kang) *If $n \geq 7117599$, then the 10–12th smallest energy trees of order n are $T_n[n-7,5]$, $T_n[n-7,0,4]$ and $T_n[n-5,1,1]$.*

In view of Theorem 1.1, this conjecture is equivalent to the comparisons of the energies of the following pairs of trees:

$$\mathbb{E}(T_n[n-7,5]) < \mathbb{E}(T_n[n-7,0,4]) < \mathbb{E}(T_n[n-5,1,1]) < \mathbb{E}(T),$$

for all n-vertex trees $T \notin \mathbb{T}_{12}$ where $\mathbb{T}_{12}$ is the set of 12 trees of order n consisting of the 9 trees in Theorem 1.1 and the 3 trees in Conjecture 1.1.

In Sect. 2 of this paper, we present a new method of directly comparing the energies of two k-claw attaching bipartite graphs $G_u(k)$ and $H_v(k)$. As the application of this method, we prove that the Conjecture 1.1 proposed by Wang and Kang is true under the weaker requirement $n \geq 59$. We also give an example to show that Conjecture 1.1 does not hold when $n = 58$.

Also, the results we obtained in the proof of Conjecture 1.1 actually include the main results of [8] and [5] (without using the result of Theorem 1.1). In this sense, we also provide a simplified proof of the main results of [8] which originally need a very long proof.

The characteristic polynomial $\det(xI - A)$ of the adjacency matrix A of a graph G is also called the characteristic polynomial of G, written as $\phi(G,x) = \sum_{i=0}^{n} a_i(G)x^{n-i}$.

In this paper, we write $b_i(G) = |a_i(G)|$, and also write $\widetilde{\phi}(G,x) = \sum_{i=0}^{n} b_i(G)x^{n-i}$.

If G is a bipartite graph, then it is well known that $\phi(G,x)$ has the form

$$\phi(G,x)=\sum_{i=0}^{\lfloor\frac{n}{2}\rfloor}a_{2i}(G)x^{n-2i}=\sum_{i=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^i b_{2i}(G)x^{n-2i} \tag{1}$$

and thus

$$\widetilde{\phi}(G,x)=\sum_{i=0}^{\lfloor\frac{n}{2}\rfloor}b_{2i}(G)x^{n-2i}. \quad (b_{2i}(G)=|a_{2i}(G)|=(-1)^i a_{2i}(G)) \tag{2}$$

In case G is a forest, then $b_{2i}(G)=m(G,i)$, the number of i-matchings of G.

When G is a bipartite graph of order n. Then by (1) and (2) we have

$$\phi(G,ix)=i^n\widetilde{\phi}(G,x) \quad (G \text{ is bipartite, } i=\sqrt{-1}) \tag{3}$$

The starting point of our discussions is the following integral formula (4) for the energy differences of two bipartite graphs G_1 and G_2 of order n given in [7]:

$$\mathbb{E}(G_1)-\mathbb{E}(G_2)=\frac{2}{\pi}\int_0^{+\infty}\ln\frac{\widetilde{\phi}(G_1,x)}{\widetilde{\phi}(G_2,x)}\mathrm{d}x \tag{4}$$

The method of the quasi-order relation "$\preccurlyeq$" is an important tool in the study of graph energy, which was first defined by Gutman and Polansky in [4], and can be equivalently defined as in the following definitions 1.1 and 1.2.

Definition 1.2 Let $f(x)=\sum_{i=0}^{n}a_i x^{n-i}$ and $g(x)=\sum_{i=0}^{n}b_i x^{n-i}$ be two monic polynomials of degree n with nonnegative coefficients.

(1) If $a_i \le b_i$ for all $0\le i\le n$, then we write $f(x)\preccurlyeq g(x)$.
(2) If $f(x)\preccurlyeq g(x)$ and $f(x)\neq g(x)$, then we write $f(x)\prec g(x)$.

Definition 1.3 Let G_1 and G_2 be two bipartite graphs of order n. Then we write $G_1\preccurlyeq G_2$ if $\widetilde{\phi}(G_1,x)\preccurlyeq\widetilde{\phi}(G_2,x)$, write $G_1\prec G_2$ if $\widetilde{\phi}(G_1,x)\prec\widetilde{\phi}(G_2,x)$ and write $G_1\sim G_2$ if $\widetilde{\phi}(G_1,x)=\widetilde{\phi}(G_2,x)$.

According to the integral formula (4), we have for two bipartite graphs G_1 and G_2 of order n that,

$$G_1\preccurlyeq G_2 \Longrightarrow \mathbb{E}(G_1)\le\mathbb{E}(G_2) \quad \textit{and} \quad G_1\prec G_2\Longrightarrow\mathbb{E}(G_1)<\mathbb{E}(G_2).$$

2 A new method of directly comparing the energies of two k-claw attaching bipartite graphs

In the study of many problems of graph energies, the method of quasi-order is an efficient method. But unfortunately, in some cases the two graphs under consideration are quasi-order incomparable (for example, the 8 and 9th smallest energy trees, and the 11 and 12th smallest energy trees in Wang–Kang's Conjecture 1.1). In such cases, we need some new methods to directly compare the energies of two bipartite graphs. In this section, we will give one such method which will be one of the main techniques in the proof of our main result. At the end of this section, we will also give a new technique (in Theorem 2.3) for the comparison of the quasi-orders concerning the different coalescences of bipartite graphs.

Let u be a vertex of a graph G. A k-claw attaching graph of G at u, denoted by $G_u(k)$, is the graph obtained from G by attaching k new pendant edges to G at the vertex u.

The coalescence of two graphs G and H with respect to vertex u in G and vertex v in H, denoted by $G_u \cdot H_v$ (sometimes abbreviated as $G \cdot H$), is the graph obtained by identifying the vertices u and v. In particular, if H is the star $K_{1,k}$ and v is its central vertex, then $G \cdot H = G_u(k)$, the k-claw attaching graphs G at u.

For the sake of simplicity, the polynomials $\phi(G, x)$ and $\widetilde{\phi}(G, x)$ will be denoted by $\phi(G)$ and $\widetilde{\phi}(G)$.

Theorem 2.1 [6]

$$\phi(G \cdot H) = \phi(G)\phi(H - v) + \phi(G - u)\left(\phi(H) - x\phi(H - v)\right) \tag{5}$$

If G and H are both bipartite graphs, then from formulae (3) and (5) we have:

$$\widetilde{\phi}(G \cdot H) = \widetilde{\phi}(G)\widetilde{\phi}(H - v) + \widetilde{\phi}(G - u)\left(\widetilde{\phi}(H) - x\widetilde{\phi}(H - v)\right) \tag{6}$$

In case when $G \cdot H = G_u(k)$, we have $\widetilde{\phi}(H - v) = x^k$ and $\widetilde{\phi}(H) - x\widetilde{\phi}(H - v) = kx^{k-1}$. Thus (6) will become the following:

$$\widetilde{\phi}(G_u(k)) = x^{k-1}\left(x\widetilde{\phi}(G) + k\widetilde{\phi}(G - u)\right). \tag{7}$$

Let u, v be vertices of bipartite graphs G and H with the same order, respectively. $G_u(k)$ and $H_v(k)$ are k-claw attaching graph of G, H. In the following, we write:

$$D(G_u, H_v) = \widetilde{\phi}(H)\widetilde{\phi}(G - u) - \widetilde{\phi}(G)\widetilde{\phi}(H - v)$$
$$D_1 = \{x > 0 | D(G_u, H_v) > 0\},\ D_2 = \{x > 0 | D(G_u, H_v) < 0\}$$

and

$$D_3 = \{x > 0 | D(G_u, H_v) = 0\}$$

Then obviously we have: $D_1 \cup D_2 \cup D_3 = (0, +\infty)$.

We also write

$$d_k(x) = \frac{\widetilde{\phi}(H_v(k))}{\widetilde{\phi}(G_u(k))} = \frac{x\widetilde{\phi}(H) + k\widetilde{\phi}(H - v)}{x\widetilde{\phi}(G) + k\widetilde{\phi}(G - u)} \quad \text{and} \quad d(x) = \frac{\widetilde{\phi}(H - v)}{\widetilde{\phi}(G - u)}$$

then it is easy to see that for $x > 0$, we have

$$x \in D_1 \Leftrightarrow \frac{\widetilde{\phi}(H-v,x)}{\widetilde{\phi}(G-u,x)} < \frac{\widetilde{\phi}(H,x)}{\widetilde{\phi}(G,x)},$$
$$x \in D_2 \Leftrightarrow \frac{\widetilde{\phi}(H-v,x)}{\widetilde{\phi}(G-u,x)} > \frac{\widetilde{\phi}(H,x)}{\widetilde{\phi}(G,x)},$$
$$x \in D_3 \Leftrightarrow \frac{\widetilde{\phi}(H-v,x)}{\widetilde{\phi}(G-u,x)} = \frac{\widetilde{\phi}(H,x)}{\widetilde{\phi}(G,x)}.$$

Now let

$$ED(k) = \mathbb{E}(H_v(k)) - \mathbb{E}(G_u(k)) \quad \text{and} \quad ED = \mathbb{E}(H-v) - \mathbb{E}(G-u).$$

According to the integral formula (4) and (7), we have

$$ED = \frac{2}{\pi}\int_0^{+\infty} \ln \frac{\widetilde{\phi}(H-v)}{\widetilde{\phi}(G-u)} \mathrm{d}x = \frac{2}{\pi}\int_0^{+\infty} \ln d(x) dx$$

and

$$ED(k) = \frac{2}{\pi}\int_0^{+\infty} \ln \frac{x\widetilde{\phi}(H) + k\widetilde{\phi}(H-v)}{x\widetilde{\phi}(G) + k\widetilde{\phi}(G-u)} \mathrm{d}x = \frac{2}{\pi}\int_0^{+\infty} \ln d_k(x) dx \tag{8}$$

Under the above notations, we have the following properties for the function $d_k(x)$:

Lemma 2.1 *Let $x > 0$ be fixed. Then for all $0 \le l < k$ we have:*

(1) *If $x \in D_1$, then $d(x) < d_k(x) < d_l(x)$;*
(2) *If $x \in D_2$, then $d(x) > d_k(x) > d_l(x)$;*
(3) *If $x \in D_3$, then $d(x) = d_k(x) = d_l(x)$.*

Proof By the definitions we have:

$$d_k(x) - d(x) = \frac{xD(G_u, H_v)}{\widetilde{\phi}(G_u(k))\widetilde{\phi}(G-u)} \tag{9}$$
$$d_k(x) - d_l(x) = \frac{x(l-k)D(G_u, H_v)}{\widetilde{\phi}(G_u(k))\widetilde{\phi}(G_u(l))} \tag{10}$$

So the results (1)–(3) follows easily from (9) and (10). □

From Lemma 2.1 we can obtain the following theorem, which give the upper and lower bound (independent of k) for the energy difference $DE(k) = \mathbb{E}(H_v(k)) - \mathbb{E}(G_u(k))$.

Theorem 2.2 *Let D_1, D_2, D_3, $d_k(x)$ and $d(x)$ be defined as above. Then for $0 \leq l < k$, we have*

(1) $\int_{D_1} \ln d(x)\mathrm{d}x + \int_{D_2} \ln d_l(x)\mathrm{d}x + \int_{D_3} \ln d_l(x)\mathrm{d}x \leq \int_0^{+\infty} \ln d_k(x)\mathrm{d}x$
$\leq \int_{D_1} \ln d_l(x)\mathrm{d}x + \int_{D_2} \ln d(x)\mathrm{d}x + \int_{D_3} \ln d(x)\mathrm{d}x.$
Where (each) equality holds if and only if both D_1 and D_2 are empty.
(2) *If $D_1 = \emptyset$ but $D_2 \neq \emptyset$, then $ED(l) < ED(k) < ED$*
(3) *If $D_2 = \emptyset$ but $D_1 \neq \emptyset$, then $ED < ED(k) < ED(l)$*
(4) *If $D_1 = D_2 = \emptyset$, then $ED(l) = ED(k) = ED$*

Proof (1) We have

$$\int_0^{+\infty} \ln d_k(x)\mathrm{d}x = \int_{D_1} \ln d_k(x)\mathrm{d}x + \int_{D_2} \ln d_k(x)\mathrm{d}x + \int_{D_3} \ln d_k(x)\mathrm{d}x$$

and by Lemma 2.1 we have:

$$\int_{D_1} \ln d(x)\mathrm{d}x < \int_{D_1} \ln d_k(x)\mathrm{d}x < \int_{D_1} \ln d_l(x)\mathrm{d}x \quad (\text{if } D_1 \neq \emptyset, 0 \leq l < k)$$
$$\int_{D_2} \ln d_l(x)\mathrm{d}x < \int_{D_2} \ln d_k(x)\mathrm{d}x < \int_{D_2} \ln d(x)\mathrm{d}x \quad (\text{if } D_2 \neq \emptyset, 0 \leq l < k)$$
$$\int_{D_3} \ln d_l(x)\mathrm{d}x = \int_{D_3} \ln d_k(x)\mathrm{d}x = \int_{D_3} \ln d(x)\mathrm{d}x$$

From these relations (1) follows.

(2) When $D_1 = \emptyset$, the left hand side of the inequality in (1) equals

$$\int_{D_1} \ln d(x)\mathrm{d}x + \int_{D_2} \ln d_l(x)\mathrm{d}x + \int_{D_3} \ln d_l(x)\mathrm{d}x = \int_0^{+\infty} \ln d_l(x)\mathrm{d}x = \frac{\pi}{2}ED(l)$$

and the right hand side of the inequality in (1) equals

$$\int_{D_1} \ln d_l(x)\mathrm{d}x + \int_{D_2} \ln d(x)\mathrm{d}x + \int_{D_3} \ln d(x)\mathrm{d}x = \int_0^{+\infty} \ln d(x)\mathrm{d}x = \frac{\pi}{2}ED$$

So by (8) and result (1) of this theorem (together with $D_2 \neq \emptyset$) we have

$$ED(l) < ED(k) < ED$$

The proof of (3) is similar to (2), and (4) follows directly from (3) of Lemma 2.1. □

The following is a new technique for the comparison of the quasi-orders concerning the different coalescences of bipartite graphs.

Theorem 2.3 *Let u be a non-isolated vertex of a bipartite graph G, v_i be a vertex of a bipartite graph H_i $(i = 1, 2)$. Let $G \cdot H_i$ be the coalescence graph of G and H_i at u and v_i $(i = 1, 2)$. Then we have*

(1) *If $H_1 \succcurlyeq H_2$ and $H_1 - v_1 \succcurlyeq H_2 - v_2$, then $G \cdot H_1 \succcurlyeq G \cdot H_2$. Furthermore, if one of the two conditions is strict, then we have $G \cdot H_1 \succ G \cdot H_2$.*
(2) *For any rooted tree H of order $k+1$ with $G \cdot H \neq G_u(k)$, we have $G \cdot H \succ G_u(k)$.*

Proof (1) By formula (7), we have

$$\widetilde{\phi}(G \cdot H_1) - \widetilde{\phi}(G \cdot H_2) = (\widetilde{\phi}(G) - x\widetilde{\phi}(G-u))(\widetilde{\phi}(H_1 - v_1) - \widetilde{\phi}(H_2 - v_2)) + \widetilde{\phi}(G-u)(\widetilde{\phi}(H_1) - \widetilde{\phi}(H_2)).$$

So the results follow from the hypothesis and the facts $\widetilde{\phi}(G-u) \succ 0$ and $\widetilde{\phi}(G) - x\widetilde{\phi}(G-u) \succ 0$.
(2) Take $H_1 = H$, v_1 be the root of H and $H_2 = K_{1,k}$, v_2 be the center of $K_{1,k}$ in (1). Then obviously we have $H_1 \succcurlyeq K_{1,k} = H_2$. Also $G \cdot H \neq G_u(k)$ implies that $H_1 - v_1 \succ kP_1 = H_2 - v_2$. So we have $G \cdot H \succ G_u(k)$ by result (1). □

3 The inner order of the trees $T_n(i) (1 \le i \le 13)$ in Table 1

In this section, we first define the trees $T_n(i)$ for $n \ge 14$ and $i = 1, 2, \ldots, 13$ in the following Table 1. Then we will prove that $\mathbb{E}(T_n(i)) < \mathbb{E}(T_n(i+1))$ for $i = 1, \ldots, 12$. Here $T_n(13)$ is only an auxiliary graph which will be used in Sect. 4 to help us to prove that $\mathbb{E}(T_n(12)) < \mathbb{E}(T)$ for all n-vertex tree $T \notin \{T_n(i) \mid i = 1, \ldots, 12\}$.

The following lemma can be obtained by directly computing the numbers of 2, 3 and 4-matchings of the corresponding caterpillars.

Lemma 3.1 (1) $\widetilde{\phi}(T_n[a, b]) = x^n + (n-1)x^{n-2} + ab\,x^{n-4}$
(2) $\widetilde{\phi}(T_n[a, b, c]) = x^n + (n-1)x^{n-2} + (a + c + ab + bc + ac)x^{n-4} + abcx^{n-6}$
(3) $\widetilde{\phi}(T_n[a, b, c, d]) = x^n + (n-1)x^{n-2} + (1 + 2a + b + c + 2d + ab + ac + ad + bc + bd + cd)x^{n-4} + (ab + ad + cd + abc + bcd + acd + abd)x^{n-6} + abcdx^{n-8}$

Table 1 The trees $T_n(i)$ with $1 \le i \le 13$ $(n \ge 14)$

i	$T_n(i)$	i	$T_n(i)$	i	$T_n(i)$
1	$T_n[n-1]$	2	$T_n[n-3, 1]$	3	$T_n[n-4, 2]$
4	$T_n[n-4, 0, 1]$	5	$T_n[n-5, 3]$	6	$T_n[n-5, 0, 2]$
7	$T_n[n-6, 4]$	8	$T_n[n-6, 0, 3]$	9	$T_n[1, n-5, 1]$
10	$T_n[n-7, 5]$	11	$T_n[n-7, 0, 4]$	12	$T_n[n-5, 1, 1]$
13	$T_n[n-8, 6]$				

Table 2 The polynomials $\widetilde{\phi}(T_n(i))$ for $i = 1, \ldots, 13$

i	$T_n(i)$	$\widetilde{\phi}(T_n(i))$
1	$T_n[n-1]$	$x^n + (n-1)x^{n-2}$
2	$T_n[n-3, 1]$	$x^n + (n-1)x^{n-2} + (n-3)x^{n-4}$
3	$T_n[n-4, 2]$	$x^n + (n-1)x^{n-2} + (2n-8)x^{n-4}$
4	$T_n[n-4, 0, 1]$	$x^n + (n-1)x^{n-2} + (2n-7)x^{n-4}$
5	$T_n[n-5, 3]$	$x^n + (n-1)x^{n-2} + (3n-15)x^{n-4}$
6	$T_n[n-5, 0, 2]$	$x^n + (n-1)x^{n-2} + (3n-13)x^{n-4}$
7	$T_n[n-6, 4]$	$x^n + (n-1)x^{n-2} + (4n-24)x^{n-4}$
8	$T_n[n-6, 0, 3]$	$x^n + (n-1)x^{n-2} + (4n-21)x^{n-4}$
9	$T_n[1, n-5, 1]$	$x^n + (n-1)x^{n-2} + (2n-7)x^{n-4} + (n-5)x^{n-6}$
10	$T_n[n-7, 5]$	$x^n + (n-1)x^{n-2} + (5n-35)x^{n-4}$
11	$T_n[n-7, 0, 4]$	$x^n + (n-1)x^{n-2} + (5n-31)x^{n-4}$
12	$T_n[n-5, 1, 1]$	$x^n + (n-1)x^{n-2} + (3n-13)x^{n-4} + (n-5)x^{n-6}$
13	$T_n[n-8, 6]$	$x^n + (n-1)x^{n-2} + (6n-48)x^{n-4}$

Table 3 n_i, $D_1(i)$, $D_2(i)$, l_i, $ED(l_i)$ and ED for $i \in \{8, 9, 11, 12\}$

i	n_i	$D_1(i)$	$D_2(i)$	l_i	$ED(l_i)$	ED
8	6	$(0, +\infty)$	$\emptyset$	0	1.08+	0
9	7	$\emptyset$	$(0, +\infty)$	39	0.00565+	0.47+
11	7	$(0, +\infty)$	$\emptyset$	0	1.3+	0
12	8	$\emptyset$	$(0, +\infty)$	51	0.0017+	0.4268+

Now we can list all the polynomials $\widetilde{\phi}(T_n(i))$ for $i = 1, \ldots, 13$ in the following Table 2.

Theorem 3.1 *If $n \geq 59$, then $\mathbb{E}(T_n(i)) < \mathbb{E}(T_n(i+1))$ for $1 \leq i \leq 12$.*

Proof—Case 1: $i \in \{8, 9, 11, 12\}$. For this fixed i, take $G = G_i = T_{n_i}(i)$ for some n_i (see Table 3). Let $H = H_i = T_{n_i}(i+1)$ and write $k = n - n_i$.

Let u be the vertex with maximal degree in G, and v be the vertex with maximal degree in H. Then for $n \geq 59$, we can write $T_n(i) = G_u(n - n_i) = G_u(k)$ and $T_n(i+1) = H_v(n - n_i) = H_v(k)$.

Now for such choices of G, H and u, v, we can compute $D(G_u, H_v)$ and the corresponding regions $D_1 = D_1(i)$ and $D_2 = D_2(i)$. We find that exactly one of the two regions $D_1(i)$ and $D_2(i)$ is empty (see Table 3). Thus we see that our G, H and u, v chosen in this way satisfy the hypothesis of (2) or (3) of Theorem 2.2, and so we can conclude by Theorem 2.2 that $ED(k)$ is between ED and $ED(l)$ for all $0 \leq l < k$.

Next, for this fixed i, we take $l = l_i$ as in Table 3. Then $n \geq 59$ implies that $k = n - n_i \geq l_i = l \geq 0$. Thus by Theorem 2.2 we have either $ED(l) < ED(k) < ED$ or $ED < ED(k) < ED(l)$ when $k > l_i$, and obviously $ED(k) = ED(l_i)$ when $k = l_i$.

Finally, we use computer to calculate ED and $ED(l_i)$ (they are all independent of k and n, and thus are fixed when i is fixed). We find that $ED \geq 0$ and $ED(l_i) > 0$

for all $i \in \{8, 9, 11, 12\}$. So from Theorem 2.2 we obtain $ED(k) > 0$, namely $\mathbb{E}(H_v(k)) > \mathbb{E}(G_u(k))$, or equivalently $\mathbb{E}(T_n(i)) < \mathbb{E}(T_n(i+1))$ for all $n \geq 59$, and each fixed $i \in \{8, 9, 11, 12\}$.
Case 2: $i \in \{1, 2, 3, 4, 5, 6, 7, 10\}$. By Table 2 we have $\widetilde{\phi}(T_n(i)) \prec \widetilde{\phi}(T_n(i+1))$. Thus by the integral formula (4) we have $\mathbb{E}(T_n(i)) < \mathbb{E}(T_n(i+1))$. □

Remark 3.1 (1) Among those numbers $ED(l_i)$ and ED in the last two columns of Table 3, the notation $a+$ means a number greater than a.
(2) The two zeros in the last column of Table 3 are accurate values which can be checked by direct computations as follows:
$i = 8$: $\mathbb{E}(H - v) = \mathbb{E}(G - u) = 4$; $i = 11$: $\mathbb{E}(H - v) = \mathbb{E}(G - u) = 2\sqrt{5}$.

4 The proof of Conjecture 1

In this section, we will prove that the Wang–Kang's Conjecture 1 is true for $n \geq 59$. By the results of Sect. 3, we are only left to show that $\mathbb{E}(T_n(12)) < \mathbb{E}(T)$ for all n-vertex tree $T \notin \{T_n(i) \mid i = 1, \ldots, 12\}$.

A basic elementary inequality which we will use several times in the comparison of the quasi-order relation is the following:

$$xy \geq c(x + y - c), \quad \text{if } x \geq c \quad \text{and} \quad y \geq c \tag{11}$$

Lemma 4.1 *Let $n \geq 15$ and $T = T_n[a, b, c]$ be a caterpillar tree of order n with the diameter $d(T) = 4$, and $T \neq T_n(i)$ for $i = 4, 6, 8, 9, 11, 12$ in Table 1 Then either $T \succ T_n(12)$ or $T \succ T_n(13)$.*

Proof—Case 1: $b = 0$. Since $T \neq T_n(i)$ for $i = 4, 6, 8, 11$, we have $\min\{a, c\} \geq 5$. Thus by Lemma 3.1 and the inequality (4.1) we have $m(T_n[a, 0, c], 2) = ac + a + c \geq 5(a + c - 5) + a + c = 6n - 43$. Then $T = T_n[a, 0, c] \succ T_n(13)$ by Table 2.
Case 2: $b \geq 1$. Since $T \neq T_n(9)$, $T_n(12)$, we have $a \geq 2, c \geq 2$ when $b = 1$, and $a + c \geq 3$ when $b \geq 2$. Thus

$$m(T_n[a, b, c], 3) = abc \geq 2(a + b + c - 3) = 2(n - 6) = 2n - 12.$$

For $m(T, 2)$, we still use Lemma 3.1 and the inequality (4.1) to consider the following two cases:

(1) If $b = 1$, then $m(T, 2) = 2(a + c) + ac \geq 2(a + c) + 2(a + c - 2) = 4n - 20 > 3n - 13$.
(2) If $b \geq 2$, then $m(T, 2) = (b + 1)(a + c) + ac \geq 3(a + b + c - 2) + ac \geq 3(n - 5) + 2 = 3n - 13$

So by Table 2 we always have $T = T_n[a, b, c] \succ T_n(12)$ in this case. □

Lemma 4.2 *Let $n \geq 15$ and T be a non-caterpillar tree of order n with the diameter $d(T) = 4$. Then $T \succ T_n(12)$.*

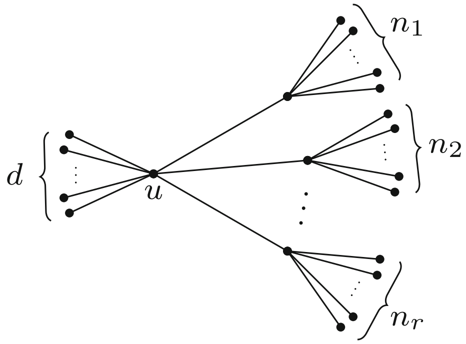

Fig. 2 The non-caterpillar tree $M_n(n_1, \ldots, n_r; d)$

Proof Since T be a non-caterpillar tree of order n with the diameter $d(T) = 4$, the tree obtained from T by deleting all pendant vertices of T is not a path and has diameter 2. So it must be a star $K_{1,r}$ with $r \geq 3$. It follows that T is a tree of the form $M_n(n_1, \ldots, n_r; d)$ as shown in Fig. 2, where $n_1 \geq n_2 \geq \cdots \geq n_r \geq 1$ and $d \geq 0$.
Case 1: $n_1 \geq 2$. By using (2) of Theorem 2.3, we have $T \succ T_n[n_1, a, n_2]$, where $a \geq n_3 + 1 \geq 2$.
By the proof of Case 2 of Lemma 4.1, we also have $T_n[n_1, a, n_2] \succ T_n(12)$. So we get $T \succ T_n(12)$.
Case 2: $n_1 = n_2 = \cdots = n_r = 1$.

If $r = 3$, then $T = M_n(1, 1, 1; n - 7)$. By direct calculation, it is easy to see that $m(T, 2) = 3n - 11$, $m(T, 3) = 3n - 17$. Then by Table 2 we have $T = M_n(1, 1, 1; n - 7) \succ T_n(12)$.

If $r \geq 4$., then by using (2) of Theorem 2.3 again we have $T \succ M_n(1, 1, 1; n - 7) \succ T_n(12)$. □

Lemma 4.3 *Let $n \geq 14$ and T be a caterpillar tree of order n with the diameter $d(T) = 5$. Then $T \succ T_n(12)$.*

Proof By hypothesis, T is a tree of the form $T_n[a, b, c, d]$ (where $a \geq 1, d \geq 1$ and $a + b + c + d = n - 4$).
Case 1: Both b and c are not zero. Then a, b, c, d are all not zero.
By Lemma 3.1 and using the inequalities (11), we have:

$m(T, 2) = 1 + (a + b + c + d) + (a + d)(b + c + 1) + ad + bc$
$\geq 1 + (a + b + c + d) + 2(a + b + c + d - 1) + (a + d - 1) + (b + c - 1) = 4n - 19$,
and also

$m(T, 3) > ab + cd + ad \geq (a + b - 1) + (c + d - 1) + ad \geq n - 5$.
So by Table 2 we have $T = T_n[a, b, c, d] \succ T_n(12)$.
Case 2: One of b and c is zero, say $b = 0$. By Lemma 3.1 and using the inequality (11), we have:

$m(T, 2) \geq 1 + 2(a + c + d) + (a + c)d \geq 1 + 2(a + c + d) + a + c + d - 1 = 3(n - 4) = 3n - 12$,
and $m(T, 3) \geq (a + c)d \geq a + c + d - 1 = n - 5$. So by Table 2 we have $T = T_n[a, b, c, d] \succ T_n(12)$. □

Theorem 4.1 *Let $n \geq 15$. $T \notin \{T_n(1), \ldots, T_n(12)\}$. Then either $T \succ T_n(12)$ or $T \succcurlyeq T_n(13)$.*

Proof—Case 1: $d(T) = 3$. Then $T = T_n[a, b]$ with $a \geq 6$ and $b \geq 6$ by hypothesis. By Lemma 3.1 and the inequality (4.1) we have $m(T, 2) = ab \geq 6(a + b - 6) = 6n - 48$. So $T \succcurlyeq T_n(13)$.
Case 2: $d(T) = 4$.
If T is a caterpillar tree, then by Lemma 4.1 we have either $T \succ T_n(12)$ or $T \succ T_n(13)$.
If T is a non-caterpillar tree, then by Lemma 4.2 we have $T \succ T_n(12)$.
Case 3: $d(T) \geq 5$. By using (2) of Theorem 2.3 several times, we can obtain some tree $T' = T_n[a, b, c, d]$ with $a \geq 1$, $d \geq 1$ such that $T \succcurlyeq T'$. By Lemma 4.3, we have $T' \succ T_n(12)$. So in this case we have $T \succ T_n(12)$. □

Theorem 4.2 *Let $n \geq 59$. Then the tree $T_n(i)$ is the ith smallest energy tree of order n for $i = 1, 2, \ldots, 12$. Consequently, the Wang–Kang's Conjecture 1.1 is true.*

Proof By Theorem 3.1, we already know that $\mathbb{E}(T_n(i)) < \mathbb{E}(T_n(i+1))$ for $1 \leq i \leq 12$.
Now suppose that $T \notin \{T_n(1), \ldots, T_n(12)\}$. By Theorem 4.1 we have either $T \succ T_n(12)$ or $T \succcurlyeq T_n(13)$.
In the first case, we have $\mathbb{E}(T) > \mathbb{E}(T_n(12))$. In the second case, we have $\mathbb{E}(T) \geq \mathbb{E}(T_n(13)) > \mathbb{E}(T_n(12))$ by Theorem 3.1. Thus we always have $\mathbb{E}(T) > \mathbb{E}(T_n(12))$ when $T \notin \{T_n(1), \ldots, T_n(12)\}$. This proves that the tree $T_n(i)$ is the ith smallest energy tree of order n for $i = 1, 2, \ldots, 12$. Consequently, Conjecture 1 is true. □

Remark 4.1 By using a computer we can obtain that $\mathbb{E}(T_{58}(12)) - \mathbb{E}(T_{58}(13)) \doteq 0.0024212 > 0$. This example shows that Conjecture 1 does not hold when $n = 58$.

Remark 4.2 Since the results of Theorem 4.2 already include the main results of [8] and [5], our results actually also provide the simplified proofs of the main results of [8] and [5].

Acknowledgments This study was supported by NSF of China No.10731040 and the Fundamental Research Funds for the Central Universities.

References

1. I. Gutman, Acyclic systems with extremal Hückel π-electron energy. Theor. Chem. Acta **45**(2), 79–87 (1977)
2. I. Gutman, The energy of a graph. Ber. Math. Stat. Sekt. Forsch. Graz **103**, 1–22 (1978)
3. I. Gutman, The energy of a graph: old and new results, in *Algebraic Combinatorics and Applications*, ed. by A. Betten, A. Kohnert, R. Laue, A. Wassermann (Springer–Verlag, Berlin, 2001), pp. 196–211
4. I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry* (Springer, Berlin, 1986)
5. S. Li, N. Li, On minimal energies of trees with given diameter. Electron. J. Linear Algebra **17**, 414–425 (2008)
6. A. Schwenk, Computing the characteristic polynomial of a graph, in *Graphs and Combinatorics*, ed. by R. Bari, F. Harary (Springer, Berlin, 1974), pp. 153–172
7. 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**(3), 721–740 (2012)
8. W.H. Wang, L.Y. Kang, Ordering of the trees by minimal energies. J. Math. Chem. **47**(3), 937–958 (2010)