# Determining the Conjugated Trees with the Third- through the Sixth-Minimal Energies

Bofeng Huo[1,2], Xueliang Li[1], Yongtang Shi[1], Lusheng Wang[3]

[1]Center for Combinatorics and LPMC-TJKLC
Nankai University, Tianjin 300071, China
E-mail: huobofeng@mail.nankai.edu.cn; lxl@nankai.edu.cn; shi@nankai.edu.cn
[2]Department of Mathematics and Information Science
Qinghai Normal University, Xining 810008, China
[3]Department of Computer Science, City University of Hong Kong
Tat Chee Avenue, Kowloon, Hong Kong SAR, China
E-mail: cswangl@cityu.edu.hk

(Received January 27, 2010)

## Abstract

For a simple graph $G$, the energy $E(G)$ is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. A conjugated tree is a tree that has a perfect matching. The conjugated trees $F_n$ and $B_n$ with the minimal and second-minimal energies were determined by Zhang and Li. They also figured out that the conjugated trees with the third- and fourth-minimal energies are $L_n$ or $M_n$. However, they could not determine which is the third, and the other is the fourth. Recently, S. Li and N. Li further investigated the conjugated trees with the third-, through the sixth-minimal energies. As a result, they figured out that these trees must be among the trees $L_n$, $M_n$, $I_n$ and $W^*_{\frac{n}{2}}$. They then showed that the energy of $M_n$ is smaller than that of $I_n$, and the energy of $L_n$ is smaller than that of $W^*_{\frac{n}{2}}$, but they could not give a total ordering of the 4 trees. For comparing of the energies, a common used method is to compare the number of $k$-matchings in each concerned tree, but it is often invalid for further comparing. This paper is aimed at solving the above unsolved problems by giving the energies of the 4 trees a total ordering, that is, completely determining the conjugated trees with the third-, forth-, fifth- and sixth-minimal energies. Our method uses the well-known Coulson integral formula.

## 1 Introduction

For a given simple graph $G$ of order $n$, denote by $A(G)$ the adjacency matrix of $G$. The characteristic polynomial of $A(G)$

$$\phi(G;x) = \det(xI - A(G)) = x^n + a_1 x^{n-1} + \cdots + a_n,$$

is usually called the characteristic polynomial of $G$. It is well-known [4] that the characteristic polynomial of a bipartite graph $G$ takes the form

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

where $b_{2k} = (-1)^k a_{2k}$ and $b_{2k} \geq 0$ for all $k = 1, \ldots, \lfloor \frac{n}{2} \rfloor$, especially $b_0 = a_0 = 1$. Furthermore, the characteristic polynomial of a tree $T$ can be expressed as

$$\phi(T;x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(T,k) x^{n-2k},$$

where $m(T,k)$ denotes the number of $k$-matchings of $T$.

The energy is a graph parameter stemming from the Hückel moleculear orbital (HMO) approximation for the total $\pi$-electron energy, see [7] for details. If $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the eigenvalues of the adjacency matrix $A(G)$, the energy of a graph $G$ is then defined as

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

For calculating the energy, Coulson [3] deduced the following formula

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[ n - \frac{ix\phi'(G,ix)}{\phi(G,ix)} \right] \mathrm{d}x. \tag{1}$$

It was then derived into a handy formula [7, 9]

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log |x^n \phi(G; i/x)| \mathrm{d}x.$$

Moreover, Gutman and Polansky [9] converted Eq.(1) into an explicit formula as follows:

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left[ \left( \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k a_{2k} x^{2k} \right)^2 + \left( \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k a_{2k+1} x^{2k+1} \right)^2 \right] \mathrm{d}x,$$

where $a_1, a_2, \ldots, a_n$ are the coefficients of the characteristic polynomial of $G$. In particular, the energy of a bipartite graph $G$ takes the form

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left[ 1 + \sum_{k=1}^{\lfloor \frac{n}{2} \rfloor} (-1)^k a_{2k} x^{2k} \right] \mathrm{d}x,$$

and the energy of a tree $T$ [9] can be expressed as

$$E(T) = \frac{2}{\pi}\int_0^{+\infty} x^{-2}\log\left[1+\sum_{k=1}^{\lfloor \frac{n}{2}\rfloor} m(T,k)x^{2k}\right]\mathrm{d}x,$$

where $m(G,k)$ is the number of $k$-matchings of $T$.

From the above one can see that if $T_1$ and $T_2$ are two trees with the same number of vertices, it is clear that $E(T_1) \le E(T_2)$ if $m(T_1,k) \le m(T_2,k)$ for all $k = 1,\dots,\lfloor \frac{n}{2}\rfloor$. So there exists a partial ordering $\preceq$ in the set of trees by comparing the number of $k$-matchings in each concerned tree, that is, for two trees $T_1$ and $T_2$ with $n$ vertices, if $m(T_1,k) \le m(T_2,k)$ holds for all $k \ge 0$, then we define $T_1 \preceq T_2$. Thus $T_1 \preceq T_2$ implies $E(T_1) \le E(T_2)$ [5, 10, 21]. Similarly, a partial ordering can be defined for bipartite graphs [18] and unicyclic graphs [11]. These relations have been established for numerous pairs of graphs [2, 5, 6, 11–16, 18, 19, 21–23]. For two bipartite graphs $G_1$ and $G_2$, we call $G_1 \preceq G_2$ if $|a_k(G_1)| \le |a_k(G_2)|$ for all $k \ge 0$, and $G_1 \preceq G_2$ implies $E(G_1) \le E(G_2)$. The above mentioned method is commonly used to compare the energies of two trees or bipartite graphs. However, for general graphs, it is hard to define such a partial ordering, since in this case, Coulson integral formula can not be used to determine whether $G_1 \preceq G_2$ implies $E(G_1) \le E(G_2)$. If, for two trees or bipartite graphs, the above quantities $m(T,k)$ or $|a_k(G)|$ can not be compared uniformly, then the common comparing method is invalid, and this happened very often. For examples, paper [13] could not determine the unicyclic bipartite graph with maximal energy; papers [15, 20] could not determine the tree with the fourth maximal energy; paper [17] could not determine the bicyclic graph with maximal energy; paper [16] could not determine the tree with two maximum degree vertices that has maximal energy; paper [22] could not determine the conjugated trees with the third- and fourth-minimal energies; paper [14] could not determine the conjugated trees with the third- through the sixth-minimal energies, etc. In this paper, we will employ Coulson integral formula to solve the last two undetermined cases, i.e., to determine the conjugated trees with the third- , forth-, fifth- and sixth-minimal energies. For more results on graph energy, we refer to [7, 8], and for terminology and notation not defined here, we refer to Bondy and Murty [1].

The following lemma is a well-known result due to Gutman [7], which will be used in the sequel.

**Lemma 1.1.** *If $G_1$ and $G_2$ are two graphs with the same number of vertices, then*

$$E(G_1) - E(G_2) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \log\frac{\phi(G_1;ix)}{\phi(G_2;ix)}\mathrm{d}x.$$

## 2 Main results

Denote by $X_n$ the star $K_{1,n-1}$, $Y_n$ the tree obtained by attaching a pendant edge to a pendant vertex of the star $K_{1,n-2}$, $Z_n$ by attaching two pendant edges to a pendant vertex of $K_{1,n-3}$ and $W_n$ by attaching a $P_3$ to a pendant vertex of $K_{1,n-3}$. In [5], Gutman gave the following result.

**Lemma 2.1.** *For any tree $T$ of order $n$, if $T \neq X_n, Y_n, Z_n, W_n$, then $X_n \prec Y_n \prec Z_n \prec W_n \prec T$.*

Denoted by $\Phi_n$ the class of trees of order $n$ that have perfect matchings. For the minimal energy tree in $\Phi_n$, Gutman proposed two conjectures in [6]. Later, Zhang and Li [22] confirmed that both conjectures are true by using the partial ordering relation $\preceq$.

**Lemma 2.2.** *[22] In the class $\Phi_n$, $E(T)$ is minimal for the tree $F_n$, and $E(T) = E(F_n)$ if and only if $T = F_n$, where $F_n$ is obtained by attaching a pendant edge to each vertex of the star $K_{1,\frac{n}{2}-1}$, see Figure 1.*

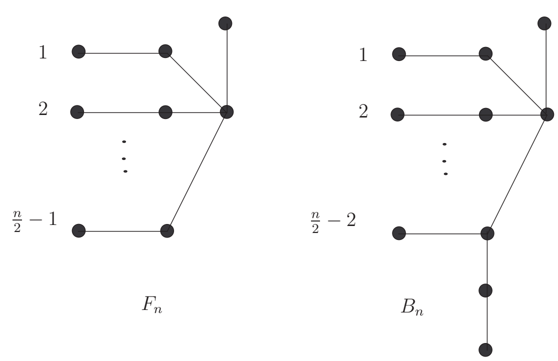


Figure 1: The trees $F_n$ and $B_n$.

For the trees with the second-, third-, and forth-minimal energies in $\Phi_n$, they obtained the following results.

**Lemma 2.3.** *[22] In the class $\Phi_n$, the tree attained the second-minimal energy is $B_n$, where $B_n$ is the tree obtained from $F_{n-2}$ by attaching a $P_3$ to the 2-degree vertex of a pendant edge (see Figure 1), and $E(T) = E(B_n)$ if and only if $T = B_n$.*

**Lemma 2.4.** *[22] In the class $\Phi_n$, the trees attained the third- and forth-minimal energies are among the trees $L_n$ and $M_n$, where $L_n$ is the tree obtained from $F_{n-4}$ by attaching two $P_3$'s to the 2-degree vertex of a pendant edge, and $M_n$ is obtained from $F_{n-2}$ by attaching a $P_3$ to a 1-degree vertex to form a path of length 6, see Figure 2. Furthermore, $L_n$ and $M_n$ are not comparable by the partial ordering relation $\preceq$.*

Denote by $I_n$ the tree obtained by attaching a $P_3$ to a 1-degree vertex of $X_{\frac{n}{2}-1}$ and attaching a pendant edge to each other 1-degree vertex of $X_{\frac{n}{2}-1}$, and $W^*_{\frac{n}{2}}$ the tree obtained by attaching a pendant edge to each vertex of $W_{\frac{n}{2}}$, see Figure 2. Recently, S. Li and N. Li [14] proved the following result.

**Lemma 2.5.** *In the class $\Phi_n$, the trees with the third-, forth-, fifth- and sixth-minimal energies are among the trees $L_n$, $M_n$, $I_n$ and $W^*_{\frac{n}{2}}$. Furthermore, $M_n \prec I_n$ and $L_n \prec W^*_{\frac{n}{2}}$, but $I_n$ and $L_n$ are not comparable.*

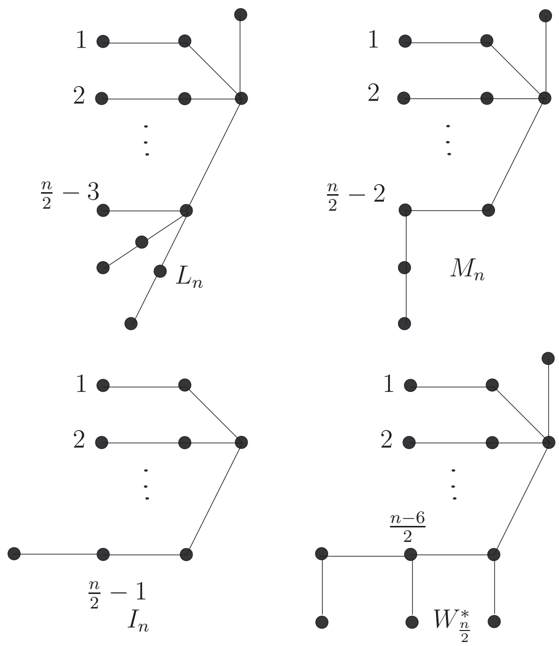


Figure 2: The trees $L_n$, $M_n$, $I_n$ and $W^*_{\frac{n}{2}}$.

Notice that the four trees have small diameters. Their characteristic polynomials can be easily obtained by using the recursion formula in [4] on trees:

$$\phi(M_n; x) = (x^2-1)^{\frac{n}{2}-4}(x^8 - (\tfrac{n}{2}+3)x^6 + (\tfrac{3}{2}n+2)x^4 - (\tfrac{n}{2}+4)x^2 + 1);$$

$$\phi(I_n; x) = (x^2-1)^{\frac{n}{2}-4}(x^8 - (\tfrac{n}{2}+3)x^6 + (\tfrac{3}{2}n+2)x^4 - (n+1)x^2 + 1);$$

$$\phi(L_n; x) = (x^2-1)^{\frac{n}{2}-4}(x^8 - (\tfrac{n}{2}+3)x^6 + (2n-4)x^4 - (\tfrac{n}{2}+3)x^2 + 1);$$

$$\phi(W^*_{\frac{n}{2}}; x) = (x^2-1)^{\frac{n}{2}-4}(x^8 - (\tfrac{n}{2}+3)x^6 + (2n-3)x^4 - (\tfrac{n}{2}+3)x^2 + 1).$$

Before giving our main result, we recall some knowledge on real analysis, for which we refer to [24].

**Lemma 2.6.** *For any real number $X > -1$, we have*

$$\frac{X}{1+X} \leq \log(1+X) \leq X. \tag{2}$$

**Lemma 2.7.** *Let $f(x,n)$ be a real function sequence on real variable $x$ and parameter $n \in \mathbb{N}$. If*

*(1) for any real number $A > a$, $f(x,n)$ is integrable in interval $a \leq x \leq A$, where $a$ is fixed;*

*(2) for any interval $[a, A]$ as above, $f(x,n)$ is uniformly convergent to $\varphi(x)$ as $n \to \infty$; and*

*(3) the integration $g(n) = \int_a^{+\infty} f(x,n)\mathrm{d}x$ is uniformly convergent for $n \in \mathbb{N}$, then the limit function $\varphi(x)$ of the sequence $g(n)$ is integrable in $[a, +\infty]$, and $\lim_{n\to\infty} \int_a^{+\infty} f(x,n)\mathrm{d}x = \int_a^{+\infty} \varphi(x)\mathrm{d}x$.*

The following lemma is useful in the sequel.

**Lemma 2.8.** *Let $A$ be a positive real number, $B$ and $C$ are non-negative. Then $X = \frac{B-C}{A+C} > -1$.*

*Proof.* From the conditions, we get $X = \frac{B}{A+C} - \frac{C}{A+C} \geq -\frac{C}{A+C} > -1$. $\square$

Now we give the main result of our paper.

**Theorem 2.9.** *There exists a fixed positive integer $N_0$, such that for all $n > N_0$, the energy of $I_n$ is smaller than that of $L_n$.*

*Proof.* Clearly, the common comparing method is invalid for $I_n$ and $L_n$, that is, neither $I_n \preceq L_n$ nor $L_n \preceq I_n$. We have to use Coulson integral formula to compare the energies of $I_n$ and $L_n$. By Lemma 1.1 and the characteristic polynomials $\phi(I_n; x)$ and $\phi(L_n; x)$ given above, it is easy to get

$$E(I_n) - E(L_n) = \frac{2}{\pi} \int_0^{+\infty} \log \frac{x^8 + (\frac{n}{2}+3)x^6 + (\frac{3}{2}n+2)x^4 + (n+1)x^2 + 1}{x^8 + (\frac{n}{2}+3)x^6 + (2n-4)x^4 + (\frac{n}{2}+3)x^2 + 1} \mathrm{d}x. \qquad (3)$$

We want to use Lemma 2.7 to finish the proof. The following two steps are distinguished:

**Step 1.** Prove the uniform convergence of the sequence $g(n) = E(I_n) - E(L_n)$.

Denote by $f(x,n)$ the integrand in Eq.(3). By letting $A = x^8 + (\frac{n}{2}+3)x^6 + (\frac{3}{2}n + 2)x^4 + (\frac{n}{2}+3)x^2 + 1$, $B = (\frac{n}{2}-2)x^2$ and $C = (\frac{n}{2}-6)x^4$, we can express $f(x,n)$ as

$$f(x,n) = \log \frac{A+B}{A+C} = \log \left(1 + \frac{B-C}{A+C}\right),$$

i.e.,

$$f(x,n)=\log\left(1+\frac{(-\frac{n}{2}+6)x^4+(\frac{n}{2}-2)x^2}{x^8+(\frac{n}{2}+3)x^6+(2n-4)x^4+(\frac{n}{2}+3)x^2+1}\right).$$

Obviously, for $n\geq 12$ we have $A>0$, $B\geq 0$ and $C\geq 0$. Now let $X=\frac{B-C}{A+C}$. Then from Lemmas 2.8 and 2.6, we get that for all $x\in\mathbb{R}$ and any integer $n\geq 13$,

$$f(x,n)\leq\frac{(-\frac{n}{2}+6)x^4+(\frac{n}{2}-2)x^2}{x^8+(\frac{n}{2}+3)x^6+(2n-4)x^4+(\frac{n}{2}+3)x^2+1}$$

and

$$f(x,n)\geq\frac{(-\frac{n}{2}+6)x^4+(\frac{n}{2}-2)x^2}{(x^8+(\frac{n}{2}+3)x^6+(\frac{3}{2}n+2)x^4+(n+1)x^2+1}.$$

It follows that

$$|f(n,x)|\leq\frac{(-\frac{n}{2}+6)x^4+(\frac{n}{2}-2)x^2}{x^8+(\frac{n}{2}+3)x^6+(2n-4)x^4+(\frac{n}{2}+3)x^2+1},\text{if }\ |x|\leq\sqrt{\frac{n-4}{n-12}}$$

and

$$|f(n,x)|\leq\frac{(\frac{n}{2}-6)x^4-(\frac{n}{2}-2)x^2}{x^8+(\frac{n}{2}+3)x^6+(\frac{3}{2}n+2)x^4+(n+1)x^2+1},\text{if }\ |x|\geq\sqrt{\frac{n-4}{n-12}}.$$

Since for $n\geq 3$ and all $x$, there always have

$$\left(\left(-\frac{n}{2}+6\right)x^4+\left(\frac{n}{2}-2\right)x^2\right)(x^2+1)\leq 2\left(x^8+\left(\frac{n}{2}+3\right)x^6+(2n-4)x^4+\left(\frac{n}{2}+3\right)x^2+1\right)$$

and

$$\left(\left(\frac{n}{2}-6\right)x^4-\left(\frac{n}{2}-2\right)x^2\right)(x^2+1)\leq 2\left(x^8+\left(\frac{n}{2}+3\right)x^6+\left(\frac{3}{2}n+2\right)x^4+(n+1)x^2+1\right),$$

So it is easy to see that for $n\geq 13$ and all $x$,

$$|f(x,n)|\leq\frac{2}{x^2+1},$$

while $\int_0^{+\infty}\frac{2}{x^2+1}\mathrm{d}x=\pi$ is convergent. From the well-known Weierstrass's criterion (for example, see [24]), we can get that $g(n)=E(I_n)-E(L_n)=\frac{2}{\pi}\int_0^{\infty}f(x,n)\mathrm{d}x$ is uniformly convergent.

Notice that $f(x,n)$ is a pointwise convergent sequence, i.e., $\lim_{n\to+\infty}f(x,n)$ exists, and it is a piecewise continuous function:

$$\varphi(x)=\begin{cases}\log\frac{x^4+3x^2+2}{x^4+4x^2+1} & x\neq 0\\ 0 & x=0.\end{cases}$$

**Step 2:** Prove that $f(n,x)$ uniformly converges to $\varphi(x)$ in an interval $I \subset (0,+\infty)$.

For $x \neq 0$, we have

$$\begin{aligned} & f(n,x)-\varphi(x) \\ =& \log\left[\frac{x^8+(\frac{n}{2}+3)x^6+(\frac{3}{2}n+2)x^4+(n+1)x^2+1}{x^8+(\frac{n}{2}+3)x^6+(2n-4)x^4+(\frac{n}{2}+3)x^2+1}\cdot\frac{x^4+4x^2+1}{x^4+3x^2+2}\right] \\ =& \log\left[\frac{x^{12}+(\frac{n}{2}+7)x^{10}+(\frac{7}{2}n+15)x^8+(\frac{15}{2}n+12)x^6+(\frac{11}{2}n+7)x^4+(n+5)x^2+1}{x^{12}+(\frac{n}{2}+6)x^{10}+(\frac{7}{2}n+7)x^8+(\frac{15}{2}n-3)x^6+(\frac{11}{2}n+2)x^4+(n+9)x^2+2}\right]. \end{aligned}$$

Similar to the above, by letting $A = x^{12}+(\frac{n}{2}+6)x^{10}+(\frac{7}{2}n+7)x^8+(\frac{15}{2}n-3)x^6+(\frac{11}{2}n+2)x^4+(n+5)x^2+1$, $B = x^{10}+8x^8+15x^6+5x^4$ and $C = 4x^2+1$, we can express the above $f(n,x)-\varphi(x)$ as

$$f(n,x)-\varphi(x) = \log\frac{A+B}{A+C} = \log\left(1+\frac{B-C}{A+C}\right),$$

i.e.,

$$\begin{aligned} & f(n,x)-\varphi(x) \\ =& \log\left[1+\frac{x^{10}+8x^8+15x^6+5x^4-4x^2-1}{x^{12}+(\frac{n}{2}+6)x^{10}+(\frac{7}{2}n+7)x^8+(\frac{15}{2}n-3)x^6+(\frac{11}{2}n+2)x^4+(n+9)x^2+2}\right]. \end{aligned}$$

It is easy to see that $A>0$, $B\geq 0$ and $C\geq 0$. From Lemmas 2.8 and 2.6, we get that for any $x\neq 0$, $x\in\mathbb{R}$ and any positive integer $n$, we have

$$f(n,x)-\varphi(x) \leq \frac{x^{10}+8x^8+15x^6+5x^4-4x^2-1}{x^{12}+(\frac{n}{2}+6)x^{10}+(\frac{7}{2}n+7)x^8+(\frac{15}{2}n-3)x^6+(\frac{11}{2}n+2)x^4+(n+9)x^2+2}$$

and

$$f(n,x)-\varphi(x) \geq \frac{x^{10}+8x^8+15x^6+5x^4-4x^2-1}{x^{12}+(\frac{n}{2}+7)x^{10}+(\frac{7}{2}n+15)x^8+(\frac{15}{2}n+12)x^6+(\frac{11}{2}n+7)x^4+(n+5)x^2+1}.$$

If $x^{10}+8x^8+15x^6+5x^4-4x^2-1\geq 0$,

$$|f(n,x)-\varphi(x)| \leq \frac{x^{10}+8x^8+15x^6+5x^4-4x^2-1}{x^{12}+(\frac{n}{2}+6)x^{10}+(\frac{7}{2}n+7)x^8+(\frac{15}{2}n-3)x^6+(\frac{11}{2}n+2)x^4+(n+9)x^2+2};$$

and if $x^{10}+8x^8+15x^6+5x^4-4x^2-1\leq 0$,

$$|f(n,x)-\varphi(x)| \leq \frac{-(x^{10}+8x^8+15x^6+5x^4-4x^2-1)}{x^{12}+(\frac{n}{2}+7)x^{10}+(\frac{7}{2}n+15)x^8+(\frac{15}{2}n+12)x^6+(\frac{11}{2}n+7)x^4+(n+5)x^2+1}.$$

It is not hard to verify that for $n\geq 3$ and any $x\in[\delta,+\infty)$, $x^{10}+8x^8+15x^6+5x^4-4x^2-1\geq 0$, and

$$|f(n,x)-\varphi(x)| \leq \frac{4}{\sqrt{n}},$$

where $\delta$ is the only positive root of the polynomial $x^{10}+8x^8+15x^6+5x^4-4x^2-1$ and $\delta \in (0.6750, 0.6751)$, which proves that $f(x,n)$ uniformly converges to $\phi(x)$ in the interval $I=[\delta,+\infty)$.

Finally, we turn to showing the conclusion of the theorem.

Notice that from the above we know that for $x \in [0,\delta]$, we have

$$f(n,x)-\varphi(x) \leq 0.$$

On the other hand, from Lemma 2.7 and the above two steps, we get that in the interval $[\delta,+\infty)$,

$$\lim_{n\to+\infty}\int_{\delta}^{+\infty} f(x,n)\mathrm{d}x = \int_{\delta}^{+\infty}\lim_{n\to+\infty} f(x,n)\mathrm{d}x = \int_{\delta}^{+\infty}\varphi(x)\mathrm{d}x.$$

That is, for an arbitrarily small $\epsilon>0$, there exists a positive integer $N$, such that for any $n>N$,

$$\int_{\delta}^{+\infty}\varphi(x)\mathrm{d}x-\epsilon < \int_{\delta}^{+\infty} f(x,n)\mathrm{d}x < \int_{\delta}^{+\infty}\varphi(x)\mathrm{d}x+\epsilon.$$

Consequently,

$$\begin{aligned}\int_{0}^{+\infty} f(x,n)\mathrm{d}x &= \int_{0}^{\delta} f(x,n)\mathrm{d}x + \int_{\delta}^{+\infty} f(x,n)\mathrm{d}x\\ &< \int_{0}^{\delta}\varphi(x)\mathrm{d}x + \int_{\delta}^{+\infty}\varphi(x)\mathrm{d}x+\epsilon = \int_{0}^{+\infty}\varphi(x)\mathrm{d}x+\epsilon.\end{aligned}$$

It is not difficult to get that $\int_0^{+\infty}\varphi(x)\mathrm{d}x=\alpha\approx -0.110823$. If we take $\epsilon=|\alpha|$, there exists a positive integer $N_0$, such that for any $n>N_0$

$$\int_{0}^{+\infty} f(x,n)\mathrm{d}x < \int_{0}^{+\infty}\varphi(x)\mathrm{d}x+\epsilon=0.$$

Thus $E(I_n)<E(L_n)$ for any $n>N_0$, which completes the proof. □

The following is an easy consequence, which determines the conjugated trees with the third- through the sixth-minimal energies.

**Theorem 2.10.** *There exists a fixed positive integer $N_0$, such that for all $n>N_0$, $E(M_n)<E(I_n)<E(L_n)<E(W^*_{\frac{n}{2}})$.*

*Proof.* It is known from [14] that $M_n \prec I_n$ and $L_n \prec W^*_{\frac{n}{2}}$, implying that $E(M_n)<E(I_n)$ and $E(L_n)<E(W^*_{\frac{n}{2}})$. The conclusion then follows immediately from Theorem 2.9. □

By running a computer with Maple programm, we get the following table:

Table. The difference between $E(I_n)$ and $E(L_n)$.

| $n$ | $\varepsilon(I_n) - \varepsilon(L_n)$ | $n$ | $\varepsilon(I_n) - \varepsilon(L_n)$ |
|---|---|---|---|
| $n = 8$ | 0.154368 | $n = 10$ | 0.133281 |
| $n = 12$ | 0.117005 | $n = 14$ | 0.103962 |
| $n = 16$ | 0.093213 | $n = 18$ | 0.084161 |
| $n = 20$ | 0.076404 | $n = 22$ | 0.069664 |
| $n = 24$ | 0.063737 | $n = 26$ | 0.058475 |
| $n = 28$ | 0.053762 | $n = 30$ | 0.049510 |
| $n = 32$ | 0.045649 | $n = 34$ | 0.042123 |
| $n = 36$ | 0.038887 | $n = 38$ | 0.035904 |
| $n = 40$ | 0.033143 | $n = 42$ | 0.030577 |
| $n = 44$ | 0.028185 | $n = 46$ | 0.025949 |
| $n = 48$ | 0.023852 | $n = 50$ | 0.021881 |
| $n = 52$ | 0.020023 | $n = 54$ | 0.018269 |
| $n = 56$ | 0.016609 | $n = 58$ | 0.015035 |
| $n = 60$ | 0.013541 | $n = 62$ | 0.012118 |
| $n = 64$ | 0.010763 | $n = 66$ | 0.009470 |
| $n = 68$ | 0.008235 | $n = 70$ | 0.007052 |
| $n = 72$ | 0.005920 | $n = 74$ | 0.004834 |
| $n = 76$ | 0.003791 | $n = 78$ | 0.002788 |
| $n = 80$ | 0.001824 | $n = 82$ | 0.000895 |
| $n = 84$ | $-0.6 \times 10^{-8}$ | $n = 86$ | $-0.000864$ |
| $n = 88$ | $-0.001697$ | $n = 90$ | $-0.002503$ |
| $n = 92$ | $-0.003282$ | $n = 94$ | $-0.004036$ |
| $n = 96$ | $-0.004765$ | $n = 98$ | $-0.005473$ |
| $n = 100$ | $-0.006158$ | $n = 102$ | $-0.006824$ |

From the table one can see that for $n$ even, $E(I_n) > E(L_n)$ for $n = 8$ up to 82, while $E(I_n) < E(L_n)$ for $n = 84$ up to 102. The table can be continued with $E(I_n) < E(L_n)$. Thus, we guess that $E(I_n) < E(L_n)$ holds for $n \geq 84$, i.e., the moment $N_0$ could be taken as 82. Yet, we have not found a proper way to show this.

**Remark.** The method employed in this paper might be extended to comparing the energies of the two graphs $P_n^6$ and $C_n$ ($n$ even) candidated as the unicyclic bipartite graph with maximal energy in [13], of the two trees candidated as the tree with the fourth-maximal energy in [20], and of those candidated graphs mentioned in the end of the introduction.

**Acknowledgement.** The authors B. Huo, X. Li and Y. Shi are supported by NSFC No.10831001, PCSIRT and the "973" program. The author Lusheng Wang is fully supported by a grant from the Research Grants Council of the Hong Kong SAR [Project No. CityU 121207]. The authors are very grateful to Prof. Ivan Gutman for helpful comments and suggestions.

## References


[1] J.A. Bondy, U.S.R. Murty, *Graph Theory*, Springer-Verlag, Berlin, 2008.

[2] A. Chen, A. Chang, W.C. Shiu, Energy ordering of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **55**(2006) 95–102.

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

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

[5] I. Gutman, Acylclic systems with extremal Hückel $\pi$-electron energy, *Theor. Chim. Acta* **45**(1977) 79–87.

[6] I. Gutman, Acylclic conjugated molecules, trees and their energies, *J. Math. Chem.* **1**(1987) 123–143.

[7] I. Gutman, *The Energy of a Graph: Old and New Results*, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Allications*, Springer-Verlag, Berlin, 2001, pp. 196–211.

[8] 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.

[9] I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.

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

[11] Y. Hou, Unicyclic graphs with minimal energy, *J. Math. Chem.* **29**(2001) 163–168.

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

[13] Y. Hou, I. Gutman, C. Woo, Unicyclic graphs with maximal energy, *Lin. Algebra Appl.* **356**(2002) 27–36.

[14] S. Li, N. Li, On minimal energies of acylclic conjugated molecules, *MATCH Commun. Math. Comput. Chem.* **61**(2009) 341–349.

[15] S. Li, X. Li, The fourth maximal energy of acyclic graphs, *MATCH Commun. Math. Comput. Chem.* **61**(2009) 383–394.

[16] X. Li, X. Yao, J. Zhang, I. Gutman, Maximum energy trees with two maximum degree vertices, *J. Math. Chem.* **45**(2009) 962–973.

[17] X. Li, J. Zhang, On bicyclic graphs with maximal energy, *Lin. Algebra Appl.* **427**(2007) 87–98.

[18] X. Li, J. Zhang, L. Wang, On bipartite graphs with minimal energy, *Discr. Appl. Math.* **157**(2009) 869–873.

[19] W. Lin, X. Guo, H. Li, On the extremal energies of trees with a given maximum degree, *MATCH Commun. Math. Comput. Chem.* **54**(2005) 363–378.

[20] H. Shan, J. Shao, S. Li, X. Li, On a conjecture on the tree with fourth greatest energy, *MATCH Commun. Math. Comput. Chem.* **64**(2009) 181–188.

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

[22] F. Zhang, H. Li, On acylclic conjugated molecules with minimal energies, *Discr. Appl. Math.* **92**(1999) 71–84.

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

[24] V.A. Zorich, *Mathematical Analysis I & II*, Original Russian edition published by MCCME, Moscow, Russia, 2002. Springer 2004, XV, Hardcover.