

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

Bofeng Huo^{1,2}, Xueliang Li¹, Yongtang Shi¹, Lusheng Wang³

¹Center 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

²Department of Mathematics and Information Science
Qinghai Normal University, Xining 810008, China

³Department 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 $A(G)$

$$\phi(G; x) = \det(xI - A(G)) = x^n + a_1x^{n-1} + \dots + a_n,$$

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 $k = 1, \dots, \lfloor \frac{n}{2} \rfloor$, 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 molecular orbital (HMO) approximation for the total π -electron energy, see [7] for details. If $\lambda_1, \lambda_2, \dots, \lambda_n$ 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

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

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

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

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

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

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

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

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

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

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 $E(T_1) \leq E(T_2)$ if $m(T_1, k) \leq m(T_2, k)$ 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 $m(T_1, k) \leq m(T_2, k)$ holds for all $k \geq 0$, then we define $T_1 \preceq T_2$. Thus $T_1 \preceq T_2$ implies $E(T_1) \leq E(T_2)$ [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 $|a_k(G_1)| \leq |a_k(G_2)|$ for all $k \geq 0$, and $G_1 \preceq G_2$ implies $E(G_1) \leq E(G_2)$. 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 $E(G_1) \leq E(G_2)$. 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*

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

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 Φ_n the class of trees of order n that have perfect matchings. For the minimal energy tree in Φ_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 Φ_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.*

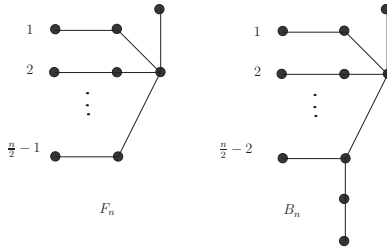


Figure 1: The trees F_n and B_n .

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

Lemma 2.3. [22] *In the class Φ_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 Φ_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 Φ_n , the trees with the third-, fourth-, 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.*

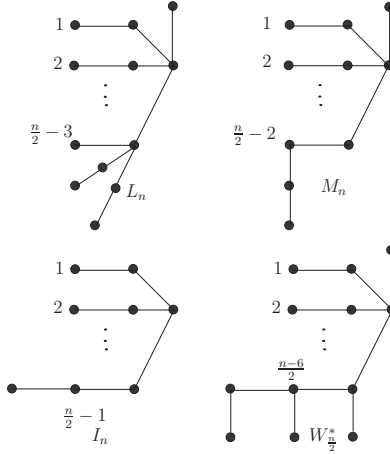


Figure 2: The trees L_n, M_n, I_n and $W_{\frac{n}{2}}^*$.

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

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

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

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

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

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 $n \rightarrow \infty$; and

(3) the integration $g(n) = \int_a^{+\infty} f(x, n)dx$ 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 $\lim_{n \rightarrow \infty} \int_a^{+\infty} f(x, n)dx = \int_a^{+\infty} \varphi(x)dx$.

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 $X = \frac{B}{A+C} - \frac{C}{A+C} \geq -\frac{C}{A+C} > -1$. □

Now we give our main result of this 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

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

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.,

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

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 $n \geq 13$,

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

and

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

It follows that

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

and

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

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

Notice that $f(x, n)$ is a pointwise convergent sequence, i.e., $\lim_{n \rightarrow +\infty} f(x, n)$ 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 δ 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 $\varphi(x)$ 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 $[\delta, +\infty)$,

$$\lim_{n \rightarrow +\infty} \int_{\delta}^{+\infty} f(x, n) dx = \int_{\delta}^{+\infty} \lim_{n \rightarrow +\infty} f(x, n) dx = \int_{\delta}^{+\infty} \varphi(x) dx.$$

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

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

Consequently,

$$\begin{aligned} \int_0^{+\infty} f(x, n) dx &= \int_0^{\delta} f(x, n) dx + \int_{\delta}^{+\infty} f(x, n) dx \\ &< \int_0^{\delta} \varphi(x) dx + \int_{\delta}^{+\infty} \varphi(x) dx + \epsilon = \int_0^{+\infty} \varphi(x) dx + \epsilon. \end{aligned}$$

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

$$\int_0^{+\infty} f(x, n) dx < \int_0^{+\infty} \varphi(x) dx + \epsilon = 0.$$

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

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 $M_n < I_n$ and $L_n < W_{\frac{n}{2}}^*$, 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. \square

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
$n = 84$	-0.6×10^{-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, Acyclic systems with extremal Hückel π -electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.
- [6] I. Gutman, Acyclic 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 Applications*, 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 acyclic 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 acyclic conjugated molecules with minimal energies, *Discr. Appl. Math.* **92** (1999) 71–84.
- [23] B. Zhou, F. Li, On minimal energies of trees of a prescribed diameter, *J. Math. Chem.* **39** (2006) 465–473.
- [24] V. A. Zorich, *Mathematical Analysis I & II*, Moscow Center for Continuous Mathematical Education, Moscow, 2002.