An Approach to the Problem of the Maximal Energy of Bicyclic Graphs

Shengjin Ji, Jing Li

Center for Combinatorics and LPMC-TJKLC

Nankai University, Tianjin 300071, China

E-mail: jsj@cfc.nankai.edu.cn; lj02013@163.com

(Received November 22, 2011)

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. Let C_n be the cycle and $P_n^{6,6}$ be the graph obtained from two copies of C_6 joined by a path of order $n-10$. Let $\mathscr{C}_n$ be the class of bicyclic graphs which have exact two edge-disjoint cycles satisfying that one is even, the other is odd. In [I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: a computer experiment, *J. Chem. Inf. Sci.* **41**(2001),1002–1005.], Gutman and Vidović conjectured that the bicyclic graph with maximal energy is $P_n^{6,6}$, for $n = 14$ and $n \geq 16$. Recently, Huo et al. proved that the assertion is true for bipartite bicyclic graphs. In the paper, we first show that for the graphs in $\mathscr{C}_n$ the coefficients of characteristic polynomials have uniform sign. Besides, we extend the correctness of the assertion from bipartite bicyclic graphs to $\mathscr{C}_n$.

1 Introduction

Let G be a graph of order n and $A(G)$ be its adjacency matrix . The characteristic polynomial $\phi(G,x)$ (or $\phi(G)$ for short) of G is defined as

$$\phi(G,x) = det(xI - A(G)) = \sum_{i=0}^{n} a_i x^{n-i}. \tag{1}$$

The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\phi(G,\lambda) = 0$ are called the eigenvalues of G.

With respect to the coefficients of the characteristic polynomial of a graph, we propose the famous Sachs Theorem [2].

Let G be a graph with characteristic polynomial $\sum_{k=0}^{n} a_k x^{n-k}$. Then for $k \geq 1$,

$$a_k = \sum_{S \in L_k} (-1)^{\omega(S)} 2^{c(S)} \tag{2}$$

where L_k denotes the set of Sachs subgraphs of G with k vertices, that is, the subgraph in which every component is either a K_2 or a cycle; $\omega(S)$ is the number of connected components of S and $c(S)$ is the number of cycles contained in S. In addition, $a_0 = 1$.

Two basic properties of the characteristic polynomial $\phi(G)$[2] will be introduced.

Proposition 1.1. *If $G_1, G_2, \ldots, G_r$ are the connected components of a graph G, then*

$$\phi(G) = \prod_{i=1}^{r} \phi(G_i).$$

Proposition 1.2. *Let uv be an edge of G. Then*

$$\phi(G,x) = \phi(G-uv,x) - \phi(G-u-v,x) - 2\sum_{C \in \mathcal{C}(uv)} \phi(G-C,x),$$

where $\mathcal{C}(uv)$ is the set of cycles containing uv. In particular, if uv is a pendent edge with pendent vertex v, then $\phi(G,x) = x\phi(G-v,x) - \phi(G-u-v,x)$.

The *energy* of G, denoted by $E(G)$, is defined as $E(G) = \sum_{i=0}^{n} |\lambda_i|$. This definition was proposed by Gutman [5]. The *Coulson integral formula* [1] is

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

where $i^2 = -1$. Moreover, it is known from [1] that the above equality can be expressed an explicit formula as follows:

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

where $a_1, a_2, \ldots, a_n$ are the coefficients of the characteristic polynomial $\phi(G, x)$. Formally, We usually note $(-1)^i a_{2i} = b_{2i}$ and $(-1)^i a_{2i+1} = b_{2i+1}$. For more results about graph energy, we refer readers to the recent survey of Gutman, Li and Zhang[10].

Since 1980s, the extremal energy $E(G)$ of a graph G has been studied extensively. Many results have been discovered on acyclic, unicyclic, bicyclic and bipartite graphs. But the quasi-order method people used before is not always valid. Recently, for these quasi-order incomparable problems, we find an efficient way to determine which one attains the extremal value of the energy, refer to [13, 15–19].

In the paper, the graphs under our consideration are finite, connected and simple. The order of G is the number of vertices in G, denoted by $|G|$. Let P_n and C_n denote the path and cycle with n vertices, respectively. Let P_n^ℓ be the unicyclic graph obtained by joining a vertex of C_ℓ with a leaf of $P_{n-\ell}$ and $P_n^{6,\ell}$ be the graph obtained from two cycles C_6 and C_ℓ joined by a path $P_{n-\ell-4}$. If the path have just one vertex(namely, P_1), then $P_n^{6,\ell} \cong P_{\ell+5}^{6,\ell}$. Denote by $R_{a,b}$ the graph obtained from two cycles C_a and C_b ($a, b \geq 10$ and $a \equiv b \equiv 2 \pmod 4$) connected by an edge. Let $\mathscr{B}_n$ be the class of all bipartite bicyclic graphs that are not the graph $R_{a,b}$. Let $\mathscr{C}_n$ be the class of bicyclic graphs which have exact two edge-disjoint cycles satisfying that one is even, the other is odd.

Huo et al. [18], recently, obtained a beautiful result that P_n^6 is the only graph with the maximal energy among all unicyclic graphs. In [9], Gutman and Vidović proposed a conjecture on the bicyclic graph with the maximal energy.

Conjecture 1.3. *For $n = 14$ and $n \geq 16$ the bicyclic molecular graph of order n with maximal energy is the molecular graph of the α, β diphenyl-polyene $C_6H_5(CH)_{n-12}C_6H_5$, or denoted by $P_n^{6,6}$.*

On the bipartite bicyclic graphs, Li and Zhang(2007)[20] discussed assertion on $\mathscr{B}_n$, as follows.

Theorem 1.4. *If $G \in \mathscr{B}_n$ and $n \geq 16$, then $E(G) \leq E(P_n^{6,6})$ with equality if and only if $G \cong P_n^{6,6}$.*

But the authors couldn't compare the energy of $P_n^{6,6}$ with that of $R_{a,b}$. Recently, Huo et al. [16] solve the problem. Thus, the above conjecture for bipartite bicyclic graphs has been completely solved.

Theorem 1.5. *For $n-t, t \geq 10$ and $n-t \equiv t \equiv 2\,(mod\,4)$, $E(R_{n-t,t}) < E(P_n^{6,6})$.*

In the paper, we will confirm that the Conjecture 1.3 is also true on the class $\mathscr{C}_n$.

Theorem 1.6. *Let $G \in \mathscr{C}_n \backslash \{G_1, G_2, G_3, G_4\}$, $n \geq \ell + 5$, then $E(G) \leq E(P_n^{6,\ell})$ with equality if and only if $G \cong P_n^{6,\ell}$.*

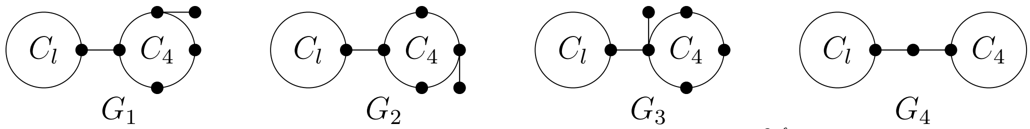

Fig.1 The graphs are incomparable with $P_{\ell+5}^{6,\ell}$.

Theorem 1.7. *If $G \in \mathscr{C}_n$, then $E(G) < E(P_n^{6,6})$ for $n = 12, 14$ and $n \geq 16$.*

For several kind of graphs, we cannot use the quasi-order method to get the extremal energy graph, but we can use it to simplify the class of graphs. As we known, the necessary condition to use the quasi-order method that is the coefficients of the characteristic polynomials of graphs must have uniform sign. So the following lemma will be very important.

Lemma 1.8. *If $G \in \mathscr{C}_n$ contains an odd cycle of length ℓ, $\ell = 2p+1$, for all $i \geq 0$, we have : $(i)\ (-1)^i a_{2i} \geq 0$;*

$(ii)\ (-1)^i a_{2i+1} \geq 0 (resp. \leq 0)$ if p is odd $(resp.\, even)$.

2 Proof of some Lemmas

The proof of Lemma 1.8

Proof. Let $L_{2i}^{(1)}$ and $L_{2i+1}^{(1)}$ denote the *Sachs subgraph* of G containing an even cycle, $L_{2i}^{(2)} = L_{2i} \backslash L_{2i}^{(1)}$ and $L_{2i+1}^{(2)} = L_{2i+1} \backslash L_{2i+1}^{(1)}$, besides, $m(G,k)$ is the number of the k-matching of G. We first show $(-1)^i a_{2i} \geq 0$. From Eq.(2) (Sachs Theorem), we have

$$(-1)^i a_{2i} = (-1)^i \left(\sum_{S \in L_{2i}^{(1)}} (-1)^{\omega(S)} 2^{c(S)} + \sum_{S \in L_{2i}^{(2)}} (-1)^{\omega(S)} 2^{c(S)} \right) \tag{3}$$

According to the property of Sachs subgraph, the following two cases should be considered.

Case 1. The length of the even cycle is $\ell = 4k + 2$.

If $2i < 4k + 2$, then $(-1)^i a_{2i} = m(G, i) > 0$.

If $2i = 4k + 2$, then $(-1)^i a_{2i} = 2 + m(G, 2k + 1) > 0$.

If $2i > 4k+2$, then $(-1)^i a_{2i} = (-1)^i (2 \sum_{S \in L_{2i}^{(1)}} (-1)^{\frac{2i-4k-2}{2}+1} + \sum_{S \in L_{2i}^{(2)}} (-1)^i) = 2 \sum_{S \in L_{2i}^{(1)}} (-1)^{2i} + \sum_{S \in L_{2i}^{(2)}} (-1)^{2i} > 0$.

Case 2. The length of the even cycle is $\ell = 4k$.

If $2i < 4k$, then $(-1)^i a_{2i} = m(G, 2k) > 0$.

If $2i = 4k$, then $(-1)^i a_{2i} = -2 + m(G, 2k) \geq 0$, since C_{4k} has two $2k$-matchings.

If $2i > 4k$, then $(-1)^i a_{2i} = (-1)^i (2 \sum_{S \in L_{2i}^{(1)}} (-1)^{\frac{2i-4k}{2}+1} + \sum_{S \in L_{2i}^{(2)}} (-1)^i) = -2(m(G - C_{4k}, i - 2k)) + m(G, i) \geq -2(m(G - C_{4k}, i - 2k)) + m(G - C_{4k}, i - 2k) m(C_{4k}, 2k) = 0$.

We now consider $(-1)^i a_{2i+1}$, there are two cases to be executed.

Case 1. $2i + 1 \geq (2p + 1) + \ell$, ℓ is the length of the even cycle and $2p + 1$ is that of the odd cycle.

$$\begin{aligned} (-1)^i a_{2i+1} &= (-1)^i \left(4 \sum_{S \in L_{2i+1}^{(1)}} (-1)^{\frac{2i+1-(2p+1)-\ell}{2}+2} + 2 \sum_{S \in L_{2i+1}^{(2)}} (-1)^{\frac{2i+1-(2p+1)}{2}+1} \right) \\ &= 4 \sum_{S \in L_{2i+1}^{(1)}} (-1)^{p+\frac{\ell}{2}} + 2 \sum_{S \in L_{2i+1}^{(2)}} (-1)^{1-p}. \end{aligned}$$

If $\ell = 4k + 2$, then $p + \frac{\ell}{2}$ and $1 - p$ have the same parity.

If $\ell = 4k$ then $p + \frac{\ell}{2}$ and $1 - p$ have different parity. In this case, finding the difference between $|4\sum_{S\in L_{2i+1}^{(1)}}(-1)^{p-\frac{\ell}{2}}|$ and $|2\sum_{S\in L_{2i+1}^{(2)}}(-1)^{1-p}|$ is necessary. By the way,

$$\begin{aligned}|2\sum_{S\in L_{2i+1}^{(2)}}(-1)^{1-p}| &= 2m(G-C_{2p+1}, i-p)\\ &\geq 2m(G-C_{2p+1}-C_\ell, i-p-\ell/2)\times m(C_\ell, \ell/2)\\ &= |4\sum_{S\in L_{2i+1}^{(1)}}(-1)^{p+\frac{\ell}{2}}|,\end{aligned}$$

Thus, if p is even, $(-1)^i a_{2i+1} < 0$; otherwise, $(-1)^i a_{2i+1} > 0$, the result holds.

Case 2. $2p+1 \leq 2i+1 < (2p+1)+l$.

From Eq.3, we have $(-1)^i a_{2i+1} = 2\sum_{S\in L_{2i+1}^{(2)}}(-1)^{1-p}$. So $(-1)^i a_{2i+1} < 0$, for even p; $(-1)^i a_{2i+1} > 0$, otherwise. The proof is thus completed. □

In view of Lemma 1.8, the quasi-order method is applicable to $\mathscr{C}_n$. It will play a key role in the proof of Theorem 1.7

Now, in order to simplified the proof of Theorem 1.6, we define some notations. The distance of two cycles C_1 and C_2 of the graph G is $d_G(C_1, C_2) = min\{d(x,y)|\, x \in C_1 \text{ and } y \in C_2\}$, the corresponding path is marked as xTy. If C_1 and C_2 have a common vertex, we define $d_G(C_1, C_2) = 0$. We refer to $P_m^{s,\ell}$ as the *brace* of the bicyclic graph G, if G contains $P_m^{s,\ell}$ as its induced subgraph. Let C_n^ℓ be the set of all unicyclic graphs with n vertices and with a cycle C_ℓ, and $C(n,\ell)$ denote the collection of all unicyclic graphs obtained from C_ℓ by adding to it $n-\ell$ pendent vertices. We define T_s to be a forest with s vertices. we will write $d_G(C_1, C_2)$ by $d(G)$ for short.

Lemma 2.1. *Let $n = 4k, 4k+1, 4k+2$ or $4k+3$. Then*

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

Lemma 2.2. *If $\ell\,(\geq 3)$ is odd and $n > t \geq \ell+3$, we have $P_n^\ell \cup P_4 \succ P_t^\ell \cup P_{n-t+4}$.*

Proof. By Proposition 1.2, we get

$$\begin{aligned}b_i(P_n^\ell\cup P_4) &= b_i(P_t^\ell\cup P_{n-t}\cup P_4) + b_{i-2}(P_{t-1}^\ell\cup P_{n-t-1}\cup P_4),\\ b_i(P_t^\ell\cup P_{n-t+4}) &= b_i(P_t^\ell\cup P_{n-t}\cup P_4) + b_{i-2}(P_t^\ell\cup P_{n-t-1}\cup P_3).\end{aligned}$$

From the above equalities, we only need to compare $b_{i-2}(P_{t-1}^{\ell}\cup P_{n-t-1}\cup P_4)$ with $b_{i-2}(P_t^{\ell}\cup P_{n-t-1}\cup P_3)$, where

$$\begin{aligned} b_{i-2}(P_{t-1}^{\ell}\cup P_{n-t-1}\cup P_4) &= b_{i-2}(P_{t-1}\cup P_{n-t-1}\cup P_4)+b_{i-4}(P_{\ell-2}\cup P_{n-t-1}\cup P_{t-\ell-1}\cup P_4)\\ &\quad + 2b_{i-\ell-2}(P_{n-t-1}\cup P_{t-\ell-1}\cup P_4),\\ b_{i-2}(P_t^{\ell}\cup P_{n-t-1}\cup P_3) &= b_{i-2}(P_t\cup P_{n-t-1}\cup P_3)+b_{i-4}(P_{\ell-2}\cup P_{t-\ell}\cup P_{n-t-1}\cup P_3)\\ &\quad + 2b_{i-\ell-2}(P_{t-\ell}\cup P_{n-t-1}\cup P_3). \end{aligned}$$

If $t-\ell=3$, then $P_{t-\ell-1}\cup P_4\succ P_{t-\ell}\cup P_3$; if $t-\ell=4$,then $P_{t-\ell-1}\cup P_4\cong P_{t-\ell}\cup P_3$; if $t-\ell\geq 5$, then $P_{t-\ell-1}\cup P_4\succ P_{t-\ell}\cup P_3$. Meanwhile, $P_{t-1}\cup P_4\succ P_t\cup P_3$. Thus $b_{i-2}(P_{t-1}^{\ell}\cup P_{n-t-1}\cup P_4)\succ b_{i-2}(P_t^{\ell}\cup P_{n-t-1}\cup P_3)$, the result holds. □

In terms of Proposition 1.2 and the property of the coefficients of characteristic polynomial, we can easily deduce the following lemma.

Lemma 2.3. *Let G be a graph in $\mathscr{C}_n$.*

(a) If G contains a cycle C_r and uv is an edge on this cycle, then

$$\begin{aligned} b_i(G) &= b_i(G-uv)+b_{i-2}(G-u-v)-2b_{i-r}(G-C_r) \quad \text{if } r\equiv 0(mod\, 4)\\ b_i(G) &= b_i(G-uv)+b_{i-2}(G-u-v)+2b_{i-r}(G-C_r) \quad \text{if } r\not\equiv 0(mod\, 4). \end{aligned}$$

(b) If uv is a cut edge of G, then $b_i(G)=b_i(G-uv)+b_{i-2}(G-u-v)$.

Next, we shall introduce some results given in [12] which will be used in the context.

Lemma 2.4. *Let $G\in C_n^{\ell}$ and $n>\ell$. If G has maximal energy in C_n^{ℓ}, then G is either P_n^{ℓ} or, when $\ell=4r$, a graph from $C(n,\ell)$.*

Lemma 2.5. *Let $G\in C(n,\ell)$ and $n>\ell$. If ℓ is even with $\ell\geq 8$ or $\ell=4$, then $E(G)<E(P_n^6)$.*

Lemma 2.6. *Let ℓ be even and $\ell\geq 8$ or $\ell=4$, then $E(P_n^{\ell})<E(P_n^6)$.*

Proof of Theorem1.6: We will use three lemmas, which lay out as follows, to display the proceeding of the proof Theorem 1.6. In the following proof, we will use the conclusion of Lemma 2.1, 2.2, 2.4, 2.5 and 2.6.

Lemma 2.7. *If $G \in \mathscr{C}_n$ and contains the brace $P_m^{s,\ell}$, $s(\geq 8)$ is even and ℓ is odd. Then $P_n^{6,\ell} \succ G$.*

Proof. Let C_ℓ be the odd cycle of G. And $C(\ell)$ denote the induced subgraph of G consisting of the cycle C_ℓ and all the trees with a vertex on C_ℓ, let $|C(\ell)| = t(\geq \ell)$. Notice that if $d(P_n^{6,\ell}) \leq 1$, then $|(P_n^{6,\ell})| = \ell + 5$ or $\ell + 6$. But $|G| \geq \ell + 7$. Hence we may assume that $d(P_n^{6,\ell}) \geq 2$.

If $d(P_n^{6,\ell}) = 2$, then $G \cong P_{n+7}^{8,\ell}$. Choosing a right edge $e = uv$ and by Proposition 1.2 and Lemma 2.3, we can find

$$b_i(G) = b_i(P_{\ell+7}^{\ell}) + b_{i-2}(P_6 \cup P_{\ell-1}) - 2b_{i-8}(P_{\ell-1}),$$
$$b_i(P_{\ell+7}^{6,\ell}) = b_i(P_{\ell+7}^{\ell}) + b_{i-2}(P_{\ell+1}^{\ell} \cup P_4) + 2b_{i-6}(_{\ell+1}^{\ell}).$$

and

$$P_6 \cup P_{\ell-1} \cong P_6 \cup P_2 \prec P_4^3 \cup P_4 \cong P_{\ell+1}^{\ell} \cup P_4 \qquad \text{when } \ell = 3,$$
$$P_6 \cup P_{\ell-1} \prec P_4 \cup P_{\ell+1} \prec P_4 \cup P_{\ell+1}^{\ell} \qquad \text{when } \ell \geq 5,$$

therefore, $b_i(G) \leq b_i(P_{\ell+7}^{6,\ell})$.

If $d(P_n^{6,\ell}) \geq 3$, and $d(G) = 0$, by choosing a proper edge uv, we can get

$$\begin{aligned} b_i(G) &= b_i(C_n^s) + b_{i-2}(P_{\ell-2} \cup T_{n-\ell}) + 2b_{i-\ell}(T_{n-\ell}) \\ &\leq b_i(P_n^6) + b_{i-2}(P_{\ell-2} \cup P_{n-\ell}^6) + 2b_{i-\ell}(P_{n-\ell}^6) = b_i(P_n^{6,\ell}) \qquad \text{while } |C(\ell)| = t = \ell, \\ b_i(G) &= b_i(C_n^{\ell}) + b_{i-2}(T_{t-1} \cup T_{n-t-1}) + (-1)^{(1+s/2)} 2b_{i-s}(T_{n-s}) \\ &\leq b_i(P_n^{\ell}) + b_{i-2}(P_4 \cup P_{n-6}^{\ell}) + 2b_{i-6}(P_{n-6}^{\ell}) = b_i(P_n^{6,\ell}) \quad \text{while } |C(\ell)| = t \geq \ell + 1. \end{aligned}$$

If $d(G) = 1$ and $|C(\ell)| = t \geq \ell$, then by choosing an appropriate edge uv, we have

$$\begin{aligned} b_i(G) &= b_i(C_t^{\ell} \cup C_{n-t}^s) + b_{i-2}(T_{t-1} \cup T_{n-t-1}) \\ &\leq b_i(P_t^{\ell} \cup P_{n-t}^6) + b_{i-2}(P_{t-1} \cup P_{n-t-1}) \\ &= b_i(P_t^{\ell} \cup P_{n-t}^6) + b_{i-2}(P_t^{\ell} - u \cup P_{n-t-1}^6) = b_i(P_n^{6,\ell}). \end{aligned}$$

If $d(G) \geq 2$, and $C(\ell) = t \geq \ell$, then by choosing a right edge uv, we get

$$\begin{aligned} b_i(G) &= b_i(C_t^{\ell} \cup C_{n-t}^s) + b_{i-2}(T_{t-1} \cup C_{n-t-1}^s) \\ &\leq b_i(P_t^{\ell} \cup P_{n-t}^6) + b_{i-2}(P_t^{\ell} - u \cup P_{n-t-1}^6) = b_i(P_n^{6,\ell}). \end{aligned}$$

So we complete the proof. $\square$

Analogously, using the same discussion as the above lemma, one can determine the following two assertions, where, the proceeding will be omitted.

Lemma 2.8. *Let $G \in \mathscr{C}_n$ contain the brace $P_m^{6,\ell}$, we have $P_n^{6,\ell} \succ G$.*

Lemma 2.9. *If $G \in \mathscr{C}_n \backslash \{G_1, G_2, G_3, G_4\}$ contains $P_m^{4,\ell}$ as its brace, then $P_n^{6,\ell} \succ G$.*

Combining Lemma 2.7 to 2.9, we finally finish the proof of Theorem 1.6.

3 Proof of Theorem 1.7

Before exhibiting the proceeding of the proof of Theorem 1.7, we shall prepare some knowledge on real analysis [23].

Lemma 3.1. *For any real number $X > -1$, we have*

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

In particular, $\log(1+X) < 0$ if and only if $X < 0$.

The following lemma is a well-known conclusion due to Gutman [7] which will be used later.

Lemma 3.2. *If G_1 and G_2 are two graphs with the same number of vertices, then*

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

We can easily obtain the following recursive equations by means of Proposition 1.1 and Proposition 1.2.

Lemma 3.3. *For any positive number $n \geq 8$, we get*

$$\phi(P_n, x) = x\phi(P_{n-1}, x) - \phi(P_{n-2}, x),$$
$$\phi(P_n^6, x) = x\phi(P_{n-1}^6, x) - \phi(P_{n-2}^6, x);$$

for any positive integer number $n \geq \ell+6$, we have

$$\phi(P_n^{6,\ell},x)=\phi(P_n^6,x)-\phi(P_{\ell-2},x)\phi(P_{n-\ell}^6,x)-2\phi(P_{n-\ell}^6,x),$$
$$\phi(P_{\ell+5}^{6,\ell},x)=\phi(P_{\ell+5}^6,x)-\phi(P_5,x)\phi(P_{\ell-2},x)-2\phi(P_5,x).$$

Next, we define some notions for convenience as follows, which will be well used in the sequel.

$$Y_1(x)=\frac{x+\sqrt{x^2-4}}{2}, \qquad Y_2(x)=\frac{x-\sqrt{x^2-4}}{2}.$$

It is easy to check that $Y_1(x)+Y_2(x)=x$, $Y_1(x)Y_2(x)=1$, $Y_1(ix)=\frac{x+\sqrt{x^2+4}}{2}i$ and $Y_2(ix)=\frac{x-\sqrt{x^2+4}}{2}i$. furthermore, we mark

$$Z_1(x)=-iY_1(ix)=\frac{x+\sqrt{x^2+4}}{2}, \quad Z_2(x)=-iY_2(ix)=\frac{x-\sqrt{x^2+4}}{2}.$$

Note that $Z_1(x)+Z_2(x)=x$, $Z_1(x)Z_2(x)=-1$. Moreover, $Z_1(x)>1$ and $-1<Z_2(x)$ <0, if $x>0$; $0<Z_1(x)<1$ and $Z_2(x)<-1$, otherwise. We abbreviate $Z_j(x)$ to Z_j for $j=1,2$, in the remainder of the section. Now we introduce some notions, which will be used frequently in the sequel.

$$A_1(x)=\frac{Y_1(x)\phi(P_8^6,x)-\phi(P_7^6,x)}{(Y_1(x))^9-(Y_1(x))^7} \qquad A_2(x)=\frac{Y_2(x)\phi(P_8^6,x)-\phi(P_7^6,x)}{(Y_2(x))^9-(Y_2(x))^7},$$
$$B_1(x)=\frac{Y_1(x)(x^2-1)-x}{(Y_1(x))^3-Y_1(x)}, \qquad B_2(x)=\frac{Y_2(x)(x^2-1)-x}{(Y_2(x))^3-Y_2(x)},$$
$$C_1(x)=\frac{Y_1(x)\phi(P_{13}^{6,6},x)-\phi(P_{12}^{6,6},x)}{(Y_1(x))^{14}-(Y_1(x))^{12}}, \quad C_2(x)=\frac{Y_2(x)\phi(P_{13}^{6,6},x)-\phi(P_{12}^{6,6},x)}{(Y_2(x))^{14}-(Y_2(x))^{12}},$$
$$D_1(x)=A_1(x)(1-B_1(x)(Y_2(x))^2)-B_2(x)(Y_2(x))^{2\ell-2}-2(Y_2(x))^{\ell}),$$
$$D_2(x)=A_2(x)(1-B_2(x)(Y_1(x))^2)-B_1(x)(Y_1(x))^{2\ell-2}-2(Y_1(x))^{\ell}),$$
$$D_1'(x)=A_1(x)-(B_1(x))^2(Y_2(x))^2-B_1(x)B_2(x)(Y_2(x))^{12},$$
$$D_2'(x)=A_2(x)-(B_2(x))^2(Y_1(x))^2-B_1(x)B_2(x)(Y_1(x))^{12}.$$

By some simple calculations, we have that $\phi(P_8^6,x)=x^8-8x^6+19x^4-16x^2+4$, $\phi(P_7^6,x)=x^7-7x^5+13x^3-7x$, $\phi(P_{13}^{6,6},x)=x^{13}-14x^{11}+74x^9-188x^7+245x^5-158x^3+40x$ and $\phi(P_{12}^{6,6},x)=x^{12}-13x^{10}+62x^8-138x^6+153x^4-81x^2+16$, and then

$$A_1(ix)=-\frac{Z_1f_8+f_7}{Z_1^2+1}Z_2^7, \quad A_2(ix)=-\frac{Z_2f_8+f_7}{Z_2^2+1}Z_1^7,$$
$$C_1(ix)=\frac{Z_1g_{13}+g_{12}}{Z_1^2+1}Z_2^{12}, \quad C_2(ix)=\frac{Z_2g_{13}+g_{12}}{Z_2^2+1}Z_1^{12},$$

where $f_8 = x^8 + 8x^6 + 19x^4 + 16$, $f_7 = x^7 + 7x^5 + 13x^3 + 7x$, $g_{13} = x^{13} + 14x^{11} + 74x^9 + 188x^7 + 245x^5 + 158x^3 + 40x$ and $g_{12} = x^{12} + 13x^{10} + 62x^8 + 138x^6 + 153x^4 + 81x^2 + 16$. In [16, 18], $A_j(ix)$ and $C_j(ix)$ possess of the good property that their signs are always positive, i.e., $A_j(ix), C_j(ix) > 0$ for all real number x, $j = 1, 2$. For convenience, we abbreviate $A_j(ix)$, $B_j(ix)$ and $C_j(ix)$ to A_j, B_j and C_j for $j = 1, 2$, respectively.

The following lemma will be used in the showing of the later results, due to Huo et al. [15, 17, 18].

Lemma 3.4. *For $n \geq 7$ and $x \neq \pm 2$, the characteristic polynomials of P_n and P_n^6 possess the following forms,*

$$\phi(P_n, x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n$$

and

$$\phi(P_n^6, x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n.$$

Lemma 3.5. *For $n \geq 12$, $\ell \geq 3$ and $x \neq \pm 2$, the characteristic polynomials of $P_n^{6,6}$ and $P_n^{6,\ell}$ have the following forms,*

$$\phi(P_n^{6,6}, x) = C_1(x)(Y_1(x))^n + C_2(x)(Y_2(x))^n,$$

$$\phi(P_n^{6,\ell}, x) = D_1(x)(Y_1(x))^n + D_2(x)(Y_2(x))^n, \text{ for } n \geq \ell + 6,$$

$$\phi(P_n^{6,\ell}, x) = D_1'(x)(Y_1(x))^n + D_2'(x)(Y_2(x))^n - 2(x^5 - 4x^3 + 3x), \text{ for } n = \ell + 5.$$

Proof. Note that, $\phi(P_n^{6,6})$ satisfies the recursive formula $f(n, x) = xf(n-1, x) - f(n-2, x)$ in terms of the Lemma 3.3. Therefore, the form of the general solution of the linear homogeneous recursive relation is $f(n, x) = F_1(x)(Y_1(x))^n + F_2(x)(Y_2(x))^n$. By some simple calculations, together with the initial values $\phi(P_{12}^{6,6})$ and $\phi(P_{13}^{6,6})$, we can get that $F_i(x) = C_i(x)$, $i = 1, 2$. From Lemma 3.3, Lemma 3.4 and Proposition 1.1, by means of elementary calculations, it is easy to deduce the above formula of $\phi(P_n^{6,\ell}, x)$ and $\phi(P_{\ell+5}^{6,\ell}, x)$. □

In view of Lemma 3.5, we can get the following forms of $D_j(ix)$ and $D_j'(ix)$ $(j = 1, 2)$ by some simplifications,

$$D_1(ix) = D_{11}(x) + D_{12}(x)(i)^\ell, \qquad D_1'(ix) = A_1 + B_1^2 Z_2^2 - B_1 B_2 Z_2^{12},$$

$$D_2(ix) = D_{21}(x) + D_{22}(x)(i)^\ell, \qquad D_2'(ix) = A_2 + B_2^2 Z_1^2 - B_1 B_2 Z_1^{12},$$

where,

$$D_{11}(x) = A_1(1 + B_1 Z_2^2 - B_2 Z_2^{2\ell-2}), \quad D_{12}(x) = 2A_1 Z_2^{\ell},$$
$$D_{21}(x) = A_2(1 + B_2 Z_1^2 - B_1 Z_1^{2\ell-2}), \quad D_{22}(x) = 2A_2 Z_1^{\ell}.$$

By the above simplification and Lemma 3.4, there are no barrier to acquire the simplifying form.

$$|\phi(P_n^{6,6}, ix)|^2 = C_1^2 Z_1^{2n} + C_2^2 Z_2^{2n} + (-1)^n 2C_1C_2, \tag{4}$$

$$|\phi(P_n^{6,\ell}, ix)|^2 = (D_{11}^2 + D_{12}^2)Z_1^{2n} + (D_{21}^2 + D_{22}^2)Z_2^{2n} + (-1)^n 2(D_{11}D_{21} + D_{12}D_{22}), \tag{5}$$

$$|\phi(P_{\ell+5}^{6,\ell}, ix)|^2 = (D_1')^2 Z_1^{2\ell+10} + (D_2')^2 Z_2^{2\ell+10} + 2D_1'D_2' + 4(x^5 + 4x^3 + 3x)^2. \tag{6}$$

Proof of Theorem 1.7: In order to showing our main result, we first verify two assertions which regard as the ingredient parts of the proceeding of the proof.

Theorem 3.6. *If $n \geq \ell + 6$ and ℓ is odd, we have $E(P_n^{6,\ell}) - E(P_n^{6,6}) < 0$.*

Proof. From the above analysis, our work is just to show that $E(P_n^{6,\ell}) < E(P_n^{6,6})$, for any positive number $n \geq \ell + 6$ and $\ell(\geq 3)$ is odd. By Lemma 3.2, we have

$$E(P_n^{6,\ell}) - E(P_n^{6,6}) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \log\left|\frac{\phi(P_n^{6,\ell}; ix)}{\phi(P_n^{6,6}; ix)}\right| \mathrm{d}x.$$

We shall distinguish two cases by means of the parity of n.

Case 1. n is odd and $n \geq 17$. First of all, we shall show that the integrand $\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|$ is monotonically decreasing on n.

$$\begin{aligned}
&\log\left|\frac{\phi(P_{n+2}^{6,\ell}; ix)}{\phi(P_{n+2}^{6,6}; ix)}\right| - \log\left|\frac{\phi(P_n^{6,\ell}; ix)}{\phi(P_n^{6,6}; ix)}\right| \\
&= \frac{1}{2}\log\left|\frac{\phi(P_{n+2}^{6,\ell}; ix)\phi(P_n^{6,6}; ix)}{\phi(P_{n+2}^{6,6}; ix)\phi(P_n^{6,\ell}; ix)}\right|^2 = \frac{1}{2}\log\left(1 + \frac{K(n,\ell,x)}{H(n,\ell,x)}\right),
\end{aligned}$$

where $K(n,\ell,x) = |\phi(P_{n+2}^{6,\ell}; ix)\phi(P_n^{6,6}; ix)|^2 - |\phi(P_{n+2}^{6,6}; ix)\phi(P_n^{6,\ell}; ix)|^2$ and $H(n,\ell,x) = |\phi(P_{n+2}^{6,6}; ix)\phi(P_n^{6,\ell}; ix)|^2 > 0$. From Lemma 3.1, we only need to verify $K(n,\ell,x) < 0$. By means of some directed calculations, we arrive at

$$K(n,t,x) = \gamma(\ell,x)(Z_1^4 - Z_2^4) + \alpha(\ell,x)Z_1^{2n}(Z_1^4 - 1) + \beta(\ell,x)Z_2^{2n}(1 - Z_2^4),$$

where, $\gamma(\ell,x) = C_2^2(D_{11}^2 + D_{12}^2) - C_1^2(D_{21}^2 + D_{22}^2)$, $\alpha(\ell,x) = 2C_1^2(D_{11}D_{21} + D_{12}D_{22}) - 2C_1C_2(D_{11}^2 + D_{12}^2)$ and $\beta(\ell,x) = 2C_1C_2(D_{21}^2 + D_{22}^2) - 2C_1^2(D_{11}D_{21} + D_{12}D_{22})$. we now discuss the sign of $\alpha(\ell,x), \beta(\ell,x)$ and $\gamma(\ell,x)$.

$$\begin{aligned}
\alpha(\ell,x) &= \alpha_0 + \alpha_1 Z_1^{2\ell-4} + \alpha_2 Z_2^{2\ell-4} + \alpha_3 Z_1^{2\ell-2} + \alpha_4 Z_2^{2\ell-2} + \alpha_6 Z_2^{2\ell} + \alpha_8 Z_2^{4\ell-4},\\
\beta(\ell,x) &= \beta_0 + \beta_1 Z_1^{2\ell-4} + \beta_2 Z_2^{2\ell-4} + \beta_3 Z_1^{2\ell-2} + \beta_4 Z_2^{2\ell-2} + \beta_5 Z_1^{2\ell} + \beta_7 Z_1^{4\ell-4},\\
\gamma(\ell,x) &= \gamma_0 + \gamma_3 Z_1^{2\ell-2} + \gamma_4 Z_2^{2\ell-2} + \gamma_5 Z_1^{2\ell} + \gamma_6 Z_2^{2\ell} + \gamma_7 Z_1^{4\ell-4} + \gamma_8 Z_2^{4\ell-4},
\end{aligned}$$

where,

$$\begin{aligned}
&\alpha_0 = 2C_1^2A_1A_2(1 + B_1Z_2^2 + B_2Z_1^2 + 2B_1B_2 - 4) - 2C_1C_2A_1^2(1 + B_1^2Z_2^4 + 2B_1Z_2^2),\\
&\alpha_1 = -2C_1^2A_1A_2B_1^2, \qquad \alpha_2 = -2C_1^2A_1A_2B_2^2,\\
&\alpha_3 = -2C_1^2A_1A_2B_1, \qquad \alpha_4 = -2C_1^2A_1A_2B_2,\\
&\alpha_6 = -4C_1C_2A_1^2(2 - B_1B_2 - Z_1^2B_2), \qquad \alpha_8 = -2C_1C_2A_1^2B_2^2,\\
&\beta_0 = -2C_2^2A_1A_2(1 + B_1Z_2^2 + B_2Z_1^2 + 2B_1B_2 - 4) + 2C_1C_2A_2^2(1 + B_2^2Z_1^4 + 2B_2Z_1^2),\\
&\beta_1 = 2C_2^2A_1A_2B_1^2, \qquad \beta_2 = 2C_2^2A_1A_2B_2^2,\\
&\beta_3 = 2C_2^2A_1A_2B_1, \qquad \beta_4 = 2C_2^2A_1A_2B_2,\\
&\beta_5 = 4C_1C_2A_2^2(2 - B_1B_2 - Z_2^2B_1), \qquad \beta_7 = 2C_1C_2A_2^2B_1^2,\\
&\gamma_0 = C_2^2A_1^2(1 + B_1^2Z_2^4 + 2B_1Z_2^2) - C_1^2A_2^2(1 + B_2^2Z_1^4 + 2B_2Z_1^2),\\
&\gamma_3 = 2C_1^2A_2^2B_1, \qquad \gamma_4 = -2C_2^2A_1^2B_2,\\
&\gamma_5 = 2C_1^2A_2^2(B_1B_2 - 2), \qquad \gamma_6 = 2C_2^2A_1^2(2 - B_1B_2),\\
&\gamma_7 = -C_1^2A_2^2B_1^2, \qquad \gamma_8 = C_2^2A_1^2B_2^2.
\end{aligned}$$

Claim 1. For any real x and positive integer ℓ, $\alpha(\ell,x) < 0$. From the above analysis, we know that A_i, B_i and $C_i > 0$, while $Z_1^2 > 0$ and $Z_2^2 > 0$. Consequently, it not hard to get $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ and $\alpha_8 < 0$. Besides,

$$\alpha_0 = -4C_1^2A_1A_2\frac{(x^2+3)}{x^2+4} - 2C_1C_2A_1^2(1 + B_1^2Z_2^4 + 2B_1Z_2^2) < 0,$$

and

$$\alpha_6 = -2C_1C_2A_1^2\frac{3x^2 + 10 - x\sqrt{x^2+4}}{(x^2+4)} < 0.$$

Therefore, the claim holds.

Claim 2. For any real x and positive integer ℓ, $\beta(\ell,x) > 0$.

Similarly, we can deduce $\beta_1, \beta_2, \beta_3, \beta_4$, and $\beta_7 > 0$. Besides,

$$\beta_0 = 4C_2^2 A_1 A_2 \frac{(x^2+3)}{x^2+4} + 2C_1 C_2 A_2^2 (1 + B_2^2 Z_1^4 + 2B_2 Z_1^2) > 0,$$

and

$$\beta_5 = 2C_1 C_2 A_2^2 \frac{3x^2 + 10 + x\sqrt{x^2+4}}{(x^2+4)} > 0.$$

Hence, the conclusion follows.

Observe that, $Z_1 > 1$ and $0 > Z_2 > -1$ for $x > 0$, we have $Z_1^{2n} \geq Z_1^{2(\ell+6)} > 0$ and $0 < Z_2^{2n} \leq Z_2^{2(\ell+6)}$. Meanwhile, $0 < Z_1 < 1$ and $Z_2 < -1$ for $x < 0$, then $0 < Z_1^{2n} \leq Z_1^{2(\ell+6)}$ and $Z_2^{2n} \geq Z_2^{2(\ell+6)} > 0$. By Claim 1 and 2, $\alpha(\ell, x) < 0$ and $\beta(\ell, x) > 0$. Therefore,

$$K(n, \ell, x) \leq \gamma(\ell, x)(Z_1^4 - Z_2^4) + \alpha(\ell, x) Z_1^{2(\ell+6)}(Z_1^4 - 1) + \beta(\ell, x) Z_2^{2(\ell+6)}(1 - Z_2^4).$$

Claim 3. $f(\ell, x) = \gamma(\ell, x)(Z_1^4 - Z_2^4) + \alpha(\ell, x) Z_1^{2(\ell+6)}(Z_1^4 - 1) + \beta(\ell, x) Z_2^{2(\ell+6)}(1 - Z_2^4)$ is monotonically decreasing on ℓ.

By some simplifications, it is easy to get $f(\ell, x) = d_0 + d_1 Z_1^{2\ell} + d_2 Z_2^{2\ell} + d_3 Z_1^{4\ell} + d_4 Z_2^{4\ell} = d_0 + d_1 (Z_1^2)^{\ell} + d_2 (Z_1^2)^{-\ell} + d_3 (Z_1^2)^{2\ell} + d_4 (Z_1^2)^{-2\ell}$, where,

$$\begin{aligned}
d_0 &= \gamma_0 (Z_1^4 - Z_2^4) + (\alpha_2 Z_1^{16} + \alpha_4 Z_1^{14} + \alpha_6 Z_1^{12})(Z_1^4 - 1) \\
&\quad + (\beta_1 Z_1^{16} + \beta_3 Z_1^{14} + \beta_5 Z_1^{12})(1 - Z_2^4), \\
d_1 &= (\gamma_3 Z_2^2 + \gamma_5)(Z_1^4 - Z_2^4) + \alpha_0 (Z_1^{16} - Z_1^{12}) + \beta_7 (Z_2^{16} - Z_2^{20}), \\
d_2 &= (\gamma_4 Z_1^2 + \gamma_6)(Z_1^4 - Z_2^4) + \alpha_8 (Z_1^{20} - Z_1^{16}) + \beta_0 (Z_2^{12} - Z_2^{16}), \\
d_3 &= \gamma_7 (1 - Z_2^8) + (\alpha_1 Z_1^8 + \alpha_3 Z_1^{10})(Z_1^4 - 1), \\
d_4 &= \gamma_8 (Z_1^8 - 1) + (\beta_2 Z_2^8 + \beta_4 Z_2^{10})(1 - Z_2^4).
\end{aligned}$$

We now mark $n_1(x) = \sqrt{x^2+4}(x^2+2)(x^{16} + 18x^{14} + 138x^{12} + 587x^{10} + 1506x^8 + 2356x^6 + 2145x^4 + 997x^2 + 144)$ and $m_1(x) = x(x^2+4)(x^{16} + 18x^{14} + 140x^{12} + 615x^{10} + 1668x^8 + 2854x^6 + 3005x^4 + 1791x^2 + 472)$. Observe that $(1 - Z_1^4) < 0$ for $x > 0$, $(1 - Z_1^4) > 0$ for $x < 0$; $(1 - Z_2^4) > 0$ for $x > 0$, $(1 - Z_2^4) < 0$ for $x < 0$; $(Z_1^4 - Z_2^4) > 0$ for $x > 0$, $(Z_1^4 - Z_2^4) < 0$ for $x < 0$. Thus, $\alpha_0 (Z_1^{16} - Z_1^{12}) < 0$ for $x > 0$, and then, $\alpha_0 (Z_1^{16} - Z_1^{12}) > 0$ for $x < 0$; $\beta_0 (Z_2^{12} - Z_2^{16}) > 0$ for $x > 0$, and then, $\beta_0 (Z_2^{12} - Z_2^{16}) < 0$ for $x < 0$. Meanwhile, with some operation, we deduce

$$(\gamma_3 Z_2^2+\gamma_5)(Z_1^4-Z_2^4)+\beta_7(Z_2^{16}-Z_2^{20})=-\frac{2C_1A_2^2x(x^2+1)^2(n_1(x)-m_1(x))}{(x^2+x\sqrt{x^2+4}+4)(x^2+4)}, \tag{7}$$

$$(\gamma_4 Z_1^2+\gamma_6)(Z_1^4-Z_2^4)+\alpha_8(Z_1^{20}-Z_1^{16})=-\frac{2C_2A_1^2x(x^2+1)^2(n_1(x)+m_1(x))}{(-x^2+x\sqrt{x^2+4}-4)(x^2+4)}. \tag{8}$$

By means of Claim 1 and 2 and the above discussion, it is not difficult to check that $d_1<0$ and $d_3<0$ for $x>0$, while, $d_2>0$ and $d_4>0$ for $x>0$; $d_1>0$ and $d_3>0$ for $x<0$, while, $d_2<0$ and $d_4<0$ for $x<0$. Therefore, whether $x>0$ or $x<0$, we always conclude that

$$\frac{\partial f(\ell,x)}{\partial t}=(d_1(Z_1^2)^{\ell}-d_2(Z_1^2)^{-\ell}+2d_3(Z_1^2)^{2\ell}-2d_4(Z_1^2)^{-2\ell})\log Z_1^2<0.$$

Thus the proof of Claim 3 is complete.

It follows from Claim 3 that for $\ell\geq 11$,

$$\begin{aligned}
K(n,\ell,x)&\leq f(11,x)\\
&=-x^2(x^6+8x^4+19x^2+16)(x^{10}+9x^8+28x^6+35x^4+15x^2+1)\\
&\quad(2x^{34}+84x^{32}+1614x^{30}+18799x^{28}+148264x^{26}+837671x^{24}\\
&\quad+3498049x^{22}+10980708x^{20}+26096742x^{18}+46927728x^{16}\\
&\quad+63358644x^{14}+63262495x^{12}+45628135x^{10}+22990036x^8\\
&\quad+7734802x^6+1635003x^4+196160x^2+10240)(x^2+1)^7<0.
\end{aligned}$$

For $\ell=3,5,7$ and 9, then $n\geq\ell+8$. Thus,

$$\begin{aligned}
K(n,\ell,x)&\leq\gamma(\ell,x)(Z_1^4-Z_2^4)+\alpha(\ell,x)Z_1^{2(\ell+8)}(Z_1^4-1)+\beta(\ell,x)Z_2^{2(\ell+8)}(1-Z_2^4)\\
&<\gamma(\ell,x)(Z_1^4-Z_2^4)+\alpha(\ell,x)Z_1^{2(\ell+6)}(Z_1^4-1)+\beta(\ell,x)Z_2^{2(\ell+6)}(1-Z_2^4)\\
&<\gamma(3,x)(Z_1^4-Z_2^4)+\alpha(3,x)Z_1^{2(3+6)}(Z_1^4-1)+\beta(3,x)Z_2^{2(3+6)}(1-Z_2^4)\\
&=-x^2(x^6+8x^4+19x^2+16)(x^2+1)^7(x^{18}+29x^{16}+341x^{14}+2157x^{12}\\
&\quad+8151x^{10}+19203x^8+28291x^6+24995x^4+11712x^2+2048)<0.
\end{aligned}$$

Therefore, we have verified that the integrand $\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|$ is monotonically decreasing on n. By Claim 3, for $n\geq 17$ and $\ell\geq 11$, $E(P_n^{6,\ell})-E(P_n^{6,6})\leq E(P_{\ell+6}^{6,\ell})-E(P_{\ell+6}^{6,6})\leq E(P_{17}^{6,11})-E(P_{17}^{6,6})<0$; for $n\geq 17$ and $\ell\leq 9$, $E(P_n^{6,\ell})-E(P_n^{6,6})\leq E(P_{17}^{6,\ell})-E(P_{17}^{6,6})<0$.

Table1. The difference between $E(P_{17}^{6,\ell})$ and $E(P_{17}^{6,6})$.

ℓ	3	5	7	9	11
$E(P_{17}^{6,\ell}) - E(P_{17}^{6,6})$	-0.00455	-0.04708	-0.02855	-0.05572	-0.02955

Case 2. n is even and $n \geq 12$.

In terms of Eqs. 4 and 5, we deduce

$$\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|^2 = \log\frac{(D_{11}^2+D_{12}^2)Z_1^{2n}+(D_{21}^2+D_{22}^2)Z_2^{2n}+2(D_{11}D_{21}+D_{12}D_{22})}{C_1^2Z_1^{2n}+C_2^2Z_2^{2n}+2C_1C_2}.$$

When $n\to\infty$,

$$\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|^2 \to \begin{cases} \frac{D_{11}^2+D_{12}^2}{C_1^2} & \text{if } x>0, \\ \frac{D_{21}^2+D_{22}^2}{C_2^2} & \text{if } x<0. \end{cases}$$

Our aim now is to explain

$$\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|^2 < \log\frac{D_{11}^2+D_{12}^2}{C_1^2} \qquad \text{for } x>0 \text{ and}$$

$$\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|^2 < \log\frac{D_{21}^2+D_{22}^2}{C_2^2} \qquad \text{for } x<0.$$

Subcase 2.1 $x>0$.

By means of some simple calculations, we get

$$\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|^2 - \log\frac{D_{11}^2+D_{12}^2}{C_1^2} = \log\left(1+\frac{K_1(n,\ell,x)}{H_1(n,\ell,x)}\right),$$

where $H_1(n,\ell,x)=|\phi(P_n^{6,6};ix)|^2(D_{11}^2+D_{12}^2)>0$ and $K_1(n,\ell,x)=-\gamma(\ell,x)Z_2^{2n}+\alpha(\ell,x)$. We may suppose $\gamma(\ell,x)<0$. Otherwise, $K_1(n,\ell,x)<0$, since $\alpha(\ell,x)<0$ from Claim 1, then we are done.

$$K_1(n,\ell,x)\leq -\gamma(\ell,x)Z_2^{2(\ell+7)}+\alpha(\ell,x)=\bar{d_0}+\bar{d_1}Z_1^{2\ell}+\bar{d_2}Z_2^{2\ell}+\bar{d_3}Z_2^{4\ell}+\bar{d_4}Z_2^{6\ell+10},$$

where, $\bar{d_0}=\alpha_0-\gamma_3Z_2^{16}-\gamma_5Z_2^{14}$, $\bar{d_1}=\alpha_1Z_2^4+\alpha_3Z_2^2-\gamma_7Z_2^{18}$, $\bar{d_2}=-\gamma_0Z_2^{14}+\alpha_2Z_1^4+\alpha_4Z_1^2+\alpha_6$, $\bar{d_3}=-\gamma_4Z_2^{12}-\gamma_6Z_2^{14}+\alpha_8Z_1^4$, and $\bar{d_4}=-\gamma_8$. Because of $\alpha_i<0$ for $i=0,1,2,3,4,5,$ 7, $\gamma_3,\gamma_6,\gamma_8>0$ and $\gamma_4,\gamma_5,\gamma_7<0$, these yield $\bar{d_i}<0$ for $i=3,4$. Besides,

$$\begin{aligned}\bar{d_0} &= \alpha_0-\gamma_3Z_2^{16}-\gamma_5Z_2^{14}\\ &< 2C_1^2A_1A_2(1+B_1Z_2^2+B_2Z_1^2+2B_1B_2-4)-(\gamma_3Z_2^{16}+\gamma_5Z_2^{14})\\ &= C_1^2A_2\frac{x^2+1}{(x^2+4)^2}(n_2(x)-m_2(x))<0,\end{aligned}$$

where, $n_2(x) = \sqrt{x^2+4}(x^{15} + 19x^{13} + 148x^{11} + 604x^9 + 1365x^7 + 1645x^5 + 898x^3 + 118x)$ and $m_2 = x^{16} + 21x^{14} + 184x^{12} + 866x^{10} + 2343x^8 + 3597x^6 + 2842x^2 + 16$. Moreover,

$$\begin{aligned}\bar{d}_1 = &\frac{2C_1^2A_2B_1Z_2^9(x^2+1)}{(Z_1^2+1)(x^2+4)}(x(x^2+4)(2x^6+21x^4+66x^2+57)\\ &+(2x^8+23x^6+88x^4+121x^2+40)\sqrt{x^2+4}) < 0,\end{aligned}$$

$$\begin{aligned}\bar{d}_2 < \gamma_0 Z_2^{14} = -&\frac{Z_2^{14}x}{(x^2+4)^{5/2}}(x^2+1)^6(x^8+11x^6+43x^4+73x^2+50)\\ &(x^6+8x^4+19x^2+16)^2(x^8+9x^6+27x^4+33x^2+12) < 0.\end{aligned}$$

Subcase 2.2 $x < 0$.

Analogously, we have

$$\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|^2 - \log\frac{D_{21}^2+D_{22}^2}{C_2^2} = \log\left(1+\frac{K_2(n,\ell,x)}{H_2(n,\ell,x)}\right),$$

where $H_2(n,\ell,x) = |\phi(P_n^{6,6};ix)|^2(D_{21}^2+D_{22}^2) > 0$ and $K_2(n,\ell,x) = \gamma(\ell,x)Z_1^{2n} - \beta(\ell,x)$. We may suppose $\gamma(\ell,x) > 0$. Otherwise, $K_1(n,\ell,x) < 0$, Since $\beta(\ell,x) > 0$ from Claim 2, then we are done.

$$K_2(n,\ell,x) \le \gamma(\ell,x)Z_1^{2(\ell+7)} - \beta(\ell,x) = \tilde{d}_0 + \tilde{d}_1 Z_1^{2\ell} + \tilde{d}_2 Z_2^{2\ell} + \tilde{d}_3 Z_1^{4\ell} + \tilde{d}_4 Z_1^{6\ell+10},$$

where, $\tilde{d}_0 = -\beta_0 + \gamma_4 Z_1^{16} + \gamma_6 Z_1^{14}$, $\tilde{d}_1 = \gamma_0 Z_1^{14} - (\beta_1 Z_2^4 + \beta_3 Z_2^2 + \beta_5)$, $\tilde{d}_2 = \gamma_8 Z_1^{18} - \beta_2 Z_1^4 - \beta_4 Z_1^2$, $\tilde{d}_3 = \gamma_3 Z_1^{12} + \gamma_5 Z_1^{14} - \beta_7 Z_2^4$, and $\tilde{d}_4 = \gamma_7$. Because of $\beta_i > 0$ for $i = 0,1,2,3,4,6,8$, $\gamma_3, \gamma_6, \gamma_8 > 0$ and $\gamma_4, \gamma_5, \gamma_7 < 0$, we acquire $\tilde{d}_i < 0$ for $i = 3,4$. Meanwhile,

$$\begin{aligned}\tilde{d}_0 &= -\beta_0 + \gamma_4 Z_1^{16} + \gamma_6 Z_1^{14}\\ &< 2C_2^2A_1A_2(1 + B_1Z_2^2 + B_2Z_1^2 + 2B_1B_2 - 4) - (\gamma_4 Z_1^{16} + \gamma_6 Z_1^{14})\\ &= C_2^2A_1\frac{x^2+1}{(x^2+4)^2}(n_2(x)+m_2(x)) < 0,\end{aligned}$$

$$\begin{aligned}\tilde{d}_1 < \gamma_0 Z_1^{14} = &\frac{Z_1^{14}x}{(x^2+4)^{5/2}}(x^2+1)^6(x^8+11x^6+43x^4+73x^2+50)\\ &(x^6+8x^4+19x^2+16)^2(x^8+9x^6+27x^4+33x^2+12) < 0,\end{aligned}$$

$$\begin{aligned}\tilde{d}_2 = &\frac{2C_2^2A_1B_2Z_1^9(x^2+1)}{-(Z_2^2+1)(x^2+4)}((2x^8+23x^6+88x^4+121x^2+40)\sqrt{x^2+4}\\ &-x(x^2+4)(2x^6+21x^4+66x^2+57)) < 0.\end{aligned}$$

In terms of the above two subcases, we arrive at

$$E(P_n^{6,\ell})-E(P_n^{6,6})=\frac{1}{\pi}\int_{-\infty}^{+\infty}\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|\mathrm{d}x=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\log\left|\frac{\phi(P_n^{6,\ell};ix)}{\phi(P_n^{6,6};ix)}\right|^2\mathrm{d}x$$
$$<\frac{1}{2\pi}\int_{-\infty}^{0}\log\frac{D_{21}^2+D_{22}^2}{C_2^2}\log\mathrm{d}x+\frac{1}{2\pi}\int_{0}^{+\infty}\frac{D_{11}^2+D_{12}^2}{C_1^2}\mathrm{d}x.$$

Let $n_3=x\sqrt{x^2+4}(x^{28}+27x^{26}+334x^{24}+2512x^{22}+12843x^{20}+47233x^{18}+128815x^{16}+264327x^{14}+409110x^{12}+473270x^{10}+399900x^8+236284x^6+90085x^4+18851x^2+1432)$, $m_3=x^{30}+29x^{28}+386x^{26}+3130x^{24}+17297x^{22}+68989x^{20}+204975x^{18}+461091x^{16}+789186x^{14}+1022232x^{12}+985182x^{10}+683502x^8+321663x^6+91811x^4+12430x^2+352.$ Notice that $(n_3(x))^2-(m_3(x))^2=-4(2x^{10}+24x^8+106x^6+225x^4+248x^2+121)(x^6+8x^4+19x^2+16)^2<0$ for all real x.

When $x>0, Z_2^2<1$, we obtain

$$\begin{aligned}D_{11}^2+D_{12}^2-C_1^2&=A_1^2\frac{Z_2^{4\ell-2}+Z_1^2+4Z_2^2+4}{x^2+4}+2A_1^2Z_2^{2\ell}\frac{Z_1^2+2Z_2^2+2}{(Z_1^2+1)(Z_2^2+1)}-C_1^2\\&\le A_1^2\frac{Z_2^{10}+Z_1^2+4Z_2^2+4}{x^2+4}+2A_1^2Z_2^{6}\frac{Z_1^2+2Z_2^2+2}{(Z_1^2+1)(Z_2^2+1)}-C_1^2\\&=\frac{2(x^2+1)^3}{(x\sqrt{x^2+4}-x^2-4)^2}(n_3(x)-m_3(x))<0.\end{aligned}$$

When $x<0, Z_1^2<1$, we get

$$\begin{aligned}D_{21}^2+D_{22}^2-C_2^2&=A_2^2\frac{Z_1^{4\ell-2}+Z_2^2+4Z_1^2+4}{x^2+4}+2A_2^2Z_1^{2\ell}\frac{Z_2^2+2Z_1^2+2}{(Z_1^2+1)(Z_2^2+1)}-C_2^2\\&\le A_2^2\frac{Z_1^{10}+Z_2^2+4Z_1^2+4}{x^2+4}+2A_2^2Z_1^{6}\frac{Z_2^2+2Z_1^2+2}{(Z_1^2+1)(Z_2^2+1)}-C_2^2\\&=-\frac{2(x^2+1)^3}{(x\sqrt{x^2+4}-x^2-4)^2}(n_3(x)+m_3(x))<0.\end{aligned}$$

Therefore,

$$\frac{1}{2\pi}\int_{-\infty}^{0}\log\frac{D_{21}^2+D_{22}^2}{C_2^2}\mathrm{d}x<0\quad\text{and}\quad\frac{1}{2\pi}\int_{0}^{+\infty}\log\frac{D_{11}^2+D_{12}^2}{C_1^2}\mathrm{d}x<0$$

Thus, $E(P_n^{6,\ell})-E(P_n^{6,6})<0$ for all even n. □

Theorem 3.7. *If $n=\ell+5$ and ℓ is odd, we have $E(P_n^{6,\ell})-E(P_n^{6,6})<0$.*

Proof. Denote $n_4(x)=x^{14}+15x^{12}+95x^{10}+323x^8+628x^6+694x^4+404x^2+128$, $m_4(x)=x\sqrt{x^2+4}(x^8+11x^6+48x^4+96x^2+80)(x^2+1)^2$, $n_5(x)=x\sqrt{x^2+4}(x^{14}+13x^{12}+$

$71x^{10}+213x^8+381x^6+407x^4+238x^2+54)$, $m_5(x)=x^{16}+15x^{14}+95x^{12}+333x^{10}+707x^8+925x^6+712x^4+270x^2+24$, $n_6(x)=x\sqrt{x^2+4}(x^{14}+13x^{12}+71x^{10}+213x^8+379x^6+397x^4+226x^2+58)$ and $m_6(x)=x^{16}+15x^{14}+95x^{12}+333x^{10}+705x^8+917x^6+684x^4+2262x^2+40$. Similarly, when $\ell\to\infty$,

$$\left|\frac{\phi(P^{6,\ell}_{\ell+5};ix)}{\phi(P^{6,6}_{\ell+5};ix)}\right|^2\to\begin{cases}\frac{(D_1')^2}{C_1^2} & \text{if } x>0,\\ \frac{(D_2')^2}{C_2^2} & \text{if } x<0.\end{cases}$$

The next work is to explain

$$\log\left|\frac{\phi(P^{6,\ell}_{\ell+5};ix)}{\phi(P^{6,6}_{\ell+5};ix)}\right|^2<\log\frac{(D_1')^2}{C_1^2}\qquad\text{for } x>0 \text{ and}$$

$$\log\left|\frac{\phi(P^{6,\ell}_{n};ix)}{\phi(P^{6,6}_{n};ix)}\right|^2<\log\frac{(D_2')^2}{C_2^2}\qquad\text{for } x<0\ .$$

Case 1. $x>0$.

By means of some simple calculations, we get

$$\log\left|\frac{\phi(P^{6,\ell}_{\ell+5};ix)}{\phi(P^{6,6}_{\ell+5};ix)}\right|^2-\log\frac{(D_1')^2}{C_1^2}=\log\left(1+\frac{K_3(n,\ell,x)}{H_3(n,\ell,x)}\right),$$

where, $H_3(n,\ell,x)=|\phi(P^{6,6}_{\ell+5};ix)|^2(D_1')^2>0$ and $K_3(n,\ell,x)=(C_1^2(D_2')^2-C_2^2(D_1')^2)Z_2^{2\ell+10}+C_1^2(2D_1'D_2'+4(x^5+4x^3+3x)^2)-2(D_1')^2C_1C_2$. In fact, we may acquire

$$C_1^2(D_2')^2-C_2^2(D_1')^2=-\frac{x(x^2+3)}{(x^2+4)^{3/2}}(x^{10}+12x^8+53x^6+116x^4+130x^2+64)$$
$$(x^2+2)^2(x^2+1)^6(x^{10}+13x^8+61x^6+131x^4+130x^2+32)<0,$$

$$C_1^2(2D_1'D_2'+4(x^5+4x^3+3x)^2)-2(D_1')^2C_1C_2=-C_1\frac{2x(x^2+3)(x^2+2)(x^2+1)^4}{\sqrt{x^2+4}(x^2+x\sqrt{x^2+4}+4)}$$
$$(n_4(x)-m_4(x))<0.$$

Therefore, for $x>0$, $K_3(\ell,x)<0$, we achieve it.

Case 2. $x<0$.

By means of some simply calculations, we get

$$\log\left|\frac{\phi(P^{6,\ell}_{\ell+5};ix)}{\phi(P^{6,6}_{\ell+5};ix)}\right|^2-\log\frac{(D_2')^2}{C_2^2}=\log\left(1+\frac{K_4(n,\ell,x)}{H_4(n,\ell,x)}\right),$$

where, $H_4(n,\ell,x) = |\phi(P^{6,6}_{\ell+5};ix)|^2(D'_2)^2 > 0$ and $K_4(n,\ell,x) = (C_2^2(D'_1)^2 - C_1^2(D'_2)^2)$ $Z_1^{2\ell+10} + C_2^2(2D'_1D'_2 + 4(x^5+4x^3+3x)^2) - 2(D'_2)^2C_1C_2$. Actually, we can determine

$$C_2^2(D'_1)^2 - C_1^2(D'_2)^2 = \frac{x(x^2+3)}{(x^2+4)^{3/2}}(x^{10}+12x^8+53x^6+116x^4+130x^2+64)$$
$$(x^2+2)^2(x^2+1)^6(x^{10}+13x^8+61x^6+131x^4+130x^2+32) < 0,$$

$$C_2^2(2D'_1D'_2+4(x^5+4x^3+3x)^2) - 2(D'_2)^2C_1C_2 = -C_2\frac{2x(x^2+3)(x^2+2)(x^2+1)^4}{\sqrt{x^2+4}(x\sqrt{x^2+4}-x^2-4)}$$
$$(n_4(x)+m_4(x)) < 0.$$

Therefore, for $x<0$, $K_4(\ell,x)<0$, and then we finish the case.

From the above analysis, we can arrive at

$$E(P^{6,\ell}_{\ell}) - E(P^6_{\ell+5}) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\log\left|\frac{\phi(P^{6,\ell}_{\ell+5};ix)}{\phi(P^{6,6}_{\ell+5};ix)}\right|\mathrm{d}x = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\log\left|\frac{\phi(P^{6,\ell}_{\ell+5};ix)}{\phi(P^{6,6}_{\ell+5};ix)}\right|^2\mathrm{d}x$$
$$< \frac{1}{2\pi}\int_{-\infty}^{0}\log\frac{(D'_2)^2}{C_2^2}\mathrm{d}x + \frac{1}{2\pi}\int_{0}^{+\infty}\log\frac{(D'_1)^2}{C_1^2}\mathrm{d}x.$$

Observe that, when $x>0$, we have

$$D'_1 - C_1 = \frac{x^2+1}{x^2+x\sqrt{x^2+4}+4}(n_5(x)-m_5(x)) < 0$$
$$D'_1 + C_1 = -\frac{x^2+1}{x^2+x\sqrt{x^2+4}+4}(n_6(x)-m_6(x)) > 0.$$

So we deduce $(D'_1)^2 - C_1^2 < 0$.

Besides, when $x<0$, we have

$$D'_2 - C_2 = \frac{x^2+1}{x\sqrt{x^2+4}-x^2-4}(n_5(x)+m_5(x)) < 0$$
$$D'_2 + C_2 = -\frac{x^2+1}{x\sqrt{x^2+4}-x^2-4}(n_6(x)+m_6(x)) > 0.$$

So we conclude $(D'_2)^2 - C_2^2 < 0$. □

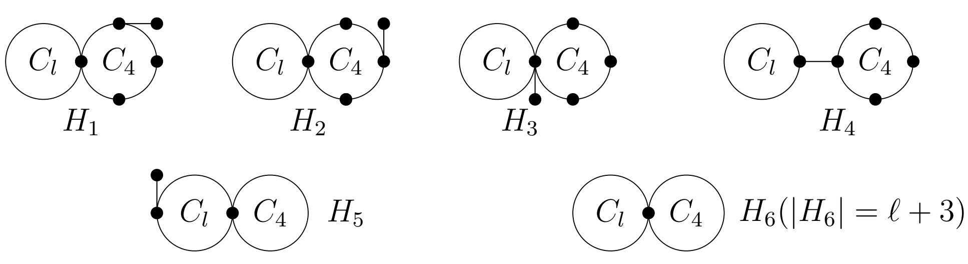

Fig.2 All the graphs with $P^{4,\ell}_m$ as its *brace* and $n \le \ell+4$.

According to the above two theorems, we already verified Theorem 1.7 for $n \geq \ell + 5$ except the four graphs as in Figure 1. In the rest of the section, we just consider them and the graphs with fewer vertices, which is shown in Figure 2. By Proposition 1.2, Lemma 2.1 and Lemma 2.3 , we now have the following assertion.

Observation 3.8. (i) *For* $n = \ell + 5$, $G_1 \succ G_2 \succ G_3$ *but* G_1 *are incomparable with* G_4*;* (ii) *For* $n = \ell + 4$, $H_1 \succ H_i$, $i = 2, 3, 5$, *while* H_1 *is incomparable with* H_4.

Now, there are five graphs, i.e. G_1, G_4, H_1, H_4 and H_6(see Figure 1 and 2), that we want to show their energies also smaller than that of $P_n^{6,6}$ for $n \leq \ell+5$, by the Observation 3.8, Theorem 3.6 and Thoerem 3.7. Fortunately, we proved them, but here, we omit the proof. Since the proceeding is similar to that of Theorem 3.7. Therefore, we complete the whole proof of Theorem 1.7. □

Acknowledgement: The authors S. Ji and J. Li are supported by NSFC and "the Fundamental Research Funds for the Central Universities".

References

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

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

[3] G. Caporossi, D. Cvetković, I. Gutman and P. Hansen, Variable neighborhood search for extremal graphs.2. Finding graphs with extremal energy, *J. Chem. Inform. Comput. Sci.* **39**(1999),984–996.

[4] B. Furtula, S. Radenković, I. Gutman, Bicyclic molecular graphs with the greatest energy, *J. Serb. chem. Soc.* **73**(4)(2008),431–433.

[5] I. Gutman, Acylclic systems with extremal Hückel π-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 Applications, Springer-Verlag, Berlin.* 2001, pp.196–211.

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

[9] I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: a computer experiment, *J. Chem. Inf. Sci.* **41**(2001),1002-1005.

[10] I. Gutman, X. Li, J. Zhang, Graph Eenergy, in: M. Dehmer, F.Emmert-Streb(Eds.), Analysis of Complex Networks: *From Biology to Linguistics, Wiley-VCH Verlag, Weinheim.* (2009),145-174.

[11] Y. Hou, Bicyclic graphs with minimal energy, *Linear and Multilinear Algebra.* **49**(2001),347–354.

[12] Y. Hou, I. Gutman and C. Woo, Unicyclic graphs with maximal energy, *Linear Algebra Appl.* **365**(2002),27–36.

[13] B. Huo, S. Ji, X. Li, Note on unicyclic graphs with given number of pendent vertices and minimal energy, *Linear Algebra Appl.* **433** (2010),1381–1387.

[14] B. Huo, S. Ji, X. Li, Solutions to unsolved problems on the minimal eneries of two classes of graphs, *MATCH Commun. Math. Comput. Chem.* **66(3)**(2011),943–958.

[15] B. Huo, S. Ji, X. Li, Y. Shi, Complete solution to a conjecture on the fourth maximal energy tree, *MATCH Commun. Math. Comput. Chem.* **66(3)**(2011),903–912.

[16] B. Huo, S. Ji, X. Li, Y. Shi, Complete Solution to a Problem on the Maximal Energy of Bicyclic Bipartite Graphs, *Linear Algebra Appl.* **435** (2011) 804–810.

[17] B. Huo, X. Li, Y. Shi, Complete solution to a problem on the maximal energy of unicyclic bipartite graphs, *Linear Algebra Appl.* **434**(2011),1370–1377.

[18] B. Huo, X. Li, Y. Shi, Complete solution to a conjecture on the maximal energy of uncicyclic graphs, *European J. Combin.* **32**(2011),662–673.

[19] B. Huo, X. Li, Y. Shi, L. Wang, Determining the conjugated trees with the third through the sixth minimal energies, *MATCH Commun. Math. Comput. Chem.* **65**(2011),521–532.

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

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

[22] X. Li, J. Zhang, B. Zhou, On unicyclic conjugated molecules with minimal energies, *J. Math. Chem.* **42**(2007), 729–740.

[23] V.A. Zorich, Mathematical Analysis, *MCCME.* 2002.