MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **70** (2013) 97-118

ISSN 0340 - 6253

On Minimal Energies of Unicyclic Graphs with Perfect Matching[1]

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(Received December 10, 2012)

Abstract

The energy of a graph is the sum of the absolute values of the eigenvalues of its adjacency matrix. We denote by $\mathbb{U}(2n)$ the set of all unicyclic graphs of order $2n$ with a perfect matching. Let $\mathbb{B}(2n) = \{G \in \mathbb{U}(2n) |$ the length of the unique cycle of G is divisible by $4\}$ and $\mathbb{A}(2n) = \mathbb{U}(2n) \setminus \mathbb{B}(2n)$. W. Wang, in the paper "Ordering of unicyclic graphs with perfect matchings by minimal energies", *MATCH Commun. Math. Comput. Chem.* **66** (2011) 927–942, [1], posed a conjecture about ordering of graphs in $\mathbb{A}(2n)$ by minimal energies. We now characterize the graphs in $\mathbb{U}(2n)$ with the first seven minimal energies and offer an answer to the conjecture.

1 Introduction

Let G be a simple graph with n vertices and $A(G)$ its adjacency matrix. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of $A(G)$. Then the energy of G, denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$ (see [2–4]). The theory of graph energy is well developed nowadays. Its details can be found in the recent book [5] and reviews [6], and in the references therein.

One of the fundamental questions that is encountered in the study of graph energy is which graphs (from a given class) have the maximal and minimal energy. A remarkably large number of papers were published on such extremal problems (see [5, Chapter 7]).

[1]Supported by the National Natural Science Foundation of China No. 71173145 and Shanghai Project 085.

One of the graph classes that has been quite thoroughly studied is the class of all unicyclic graphs [7-27], i.e., connected graphs with one unique cycle. A number of results concerning the extremal energies of various families of unicyclic graphs has been obtained as follows: unicyclic graphs with maximal energies [7,11,14]; bipartite unicyclic graphs with maximal energies [8,9,10,12,13]; unicyclic graphs with minimal energies [15-18]; unicyclic graphs with a perfect matching [19-23]; unicyclic graphs with a given diameter [24]; unicyclic graphs with given number of pendent vertices [25,26].

The characteristic polynomial $\det(xI - A(G))$ of the adjacency matrix $A(G)$ of a graph G is also called the characteristic polynomial of G, is written as $\phi(G,x) = \sum_{i=0}^{n} a_i(G)\, x^{n-i}$. Using these coefficients of $\phi(G,x)$, the energy $E(G)$ of a graph G with n vertices can be expressed by the following Coulson integral formula [4]:

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

Throughout this paper, we write $b_i(G) = |a_i(G)|$. It is easy to see that $b_0(G) = 1$, $b_1(G) = 0$, and $b_2(G)$ equals the number of edges of G.

About the signs of the coefficients of the characteristic polynomials of unicyclic graphs, the following results were shown in [15].

Lemma 1.1 [15]. Let G be a unicyclic graph and the length of the unique cycle of G be ℓ. Then we have the following.

(1) $b_{2i}(G) = (-1)^i\, a_{2i}(G)$;

(2) $b_{2i+1}(G) = (-1)^i\, a_{2i+1}(G)$, if G contains a cycle of length ℓ with $\ell \not\equiv 1\ (mod\ 4)$;

(3) $b_{2i+1}(G) = (-1)^{i+1}\, a_{2i+1}(G)$, if G contains a cycle of length ℓ with $\ell \equiv 1\ (mod\ 4)$.

From Lemma 1.1, the Coulson integral formula (1) can be rewritten as the following form (in terms of $b_i(G)$) for unicyclic graphs as follows.

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

It follows that $E(G)$ is a strictly monotonically increasing function of those numbers $b_i(G)$, $i = 0, 1, \ldots, n$, for unicyclic graphs. This in turn provides a way of comparing the energies of a pair of unicyclic graphs. That is to say, the method of the quasi-ordering relation " $\preceq$ ", outlined in the book [4] on the set of forests, can be generalized to the set of unicyclic graphs as follows.

Definition 1.1. Let G_1 and G_2 be two unicyclic graphs of order n. If $b_i(G_1) \leq b_i(G_2)$ for all i with $1 \leq i \leq n$, then we write $G_1 \preceq G_2$.

Furthermore, if $G_1 \preceq G_2$ and there exists at least one index j such that $b_j(G_1) < b_j(G_2)$, then we write that $G_1 \prec G_2$. If $b_i(G_1) = b_i(G_2)$ for all i, we write $G_1 \sim G_2$. According to the Coulson integral formula (2), we have for two unicyclic G_1 and G_2 of order n that

$$G_1 \preceq G_2 \implies E(G_1) \leq E(G_2)$$
$$G_1 \prec G_2 \implies E(G_1) < E(G_2) .$$

In this paper, for the sake of conciseness, we introduce the symbols " $\rightharpoonup$ " as follows.

$$E(G_1) < E(G_2) \Longleftrightarrow G_1 \rightharpoonup G_2 .$$

In the following of this paper, we always assume that the order of a graph G is $2n$. We denote by $\mathbb{U}(2n)$ the set of all unicyclic graphs of order $2n$ with a perfect matching. Let $\mathbb{B}(2n) = \{G \in \mathbb{U}(2n)|$ the length of the unique cycle of G is divisible by 4$\}$ and $\mathbb{A}(2n) = \mathbb{U}(2n) \backslash \mathbb{B}(2n)$. Let $A_i\,(i = 1, 2, 3, 4)$ and $B_i\,(i = 1, 2, 3)$ be the graphs shown in Figure 1. Let $L_i\,(i = 1, 2, 3, 4)$ be the graphs shown in Figure 2.

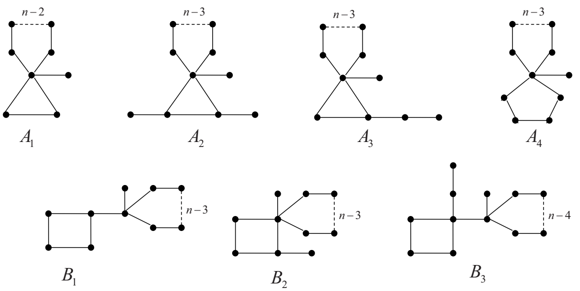

Fig. 1. The graphs in $\mathbb{U}(2n)$ with the first seven minimal energies.

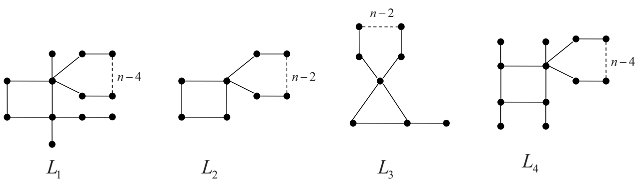

Fig. 2. Some candidate graphs in $\mathbb{U}(2n)$.

In [19], Li et al. proved that the unique graph in $\mathbb{U}(2n)$ with minimal energy is A_1 or B_1. Li and Li [20] have further shown that the unique graph in $\mathbb{U}(2n)$ with the minimal energy is B_1 by directly comparing the energies of A_1 and B_1. Recently, Wang [1] posed a conjecture about ordering of the graphs in $\mathbb{A}(2n)$ by minimal energies as follows.

Conjecture 1. Let $G \in \mathbb{A}(2n)$ and $G \neq A_i\,(i = 1, 2, 3, 4), B_i\,(i = 1, 2)$, L_2, L_3, L_4. If $n \geq 45$, then

$$B_1 \rightharpoonup A_1 \rightharpoonup B_2 \rightharpoonup A_2 \rightharpoonup A_3 \rightharpoonup A_4 \rightharpoonup L_2 \rightharpoonup L_3 \rightharpoonup L_4 \rightharpoonup G\ .$$

Wang [1] pointed out that in order to prove the above conjecture, we only need to prove that $B_1 \rightharpoonup A_1$ and $A_3 \rightharpoonup A_4$. In this paper, by Lemmas 7.5 and 7.8 in Section 7, we show that the above conjecture is true. In fact, when the conjecture is true, we only can determine the graphs in $\mathbb{A}(2n)$ with the first five minimal energies for $n \geq 45$.

Motivated by the above conjecture, in this paper, we characterize the graphs in $\mathbb{U}(2n)$ with the first seven minimal energies in the following theorem which is the main result of this paper.

Theorem 1.1. Let $G \in \mathbb{U}(2n)$ and $G \neq A_i\,(i = 1, 2, 3, 4), B_i\,(i = 1, 2, 3)$. If $n \geq 191$, then

$$B_1 \rightharpoonup A_1 \rightharpoonup B_2 \rightharpoonup A_2 \rightharpoonup A_3 \rightharpoonup A_4 \rightharpoonup B_3 \rightharpoonup G.$$

2 The basic strategy of the proof of Theorem 1.1

In this section, we outline the basic strategy of the proof of Theorem 1.1. Denote by $K(G)$ the number of perfect matchings of a graph G. We first quote the following basic property about the number of perfect matchings of unicyclic graphs.

Lemma 2.1 [21]. Let $G \in \mathbb{U}(2n)$ and C_ℓ be the unique cycle of G . If at least one vertex of C_ℓ is attached by a forest of odd order, then $K(G) = 1$. Otherwise, $K(G) = 2$.

Let $\mathbb{B}(2n) = \{G \in \mathbb{U}(2n)|$ the length of the unique cycle of G is divisible by $4\}$ and $\mathbb{A}(2n) = \mathbb{U}(2n)\backslash\mathbb{B}(2n)$. By Lemma 2.1, we can classify the graphs in $\mathbb{B}(2n)$ into two classes as follows.

$$\begin{aligned} \mathbb{C}(2n) &= \{G \in \mathbb{B}(2n)|K(G) = 1\} \\ \mathbb{D}(2n) &= \{G \in \mathbb{B}(2n)|K(G) = 2\}\ . \end{aligned}$$

Next, in order to further classify the graphs in $\mathbb{D}(2n)$ into two classes, we introduce some notations in what follows.

Throughout this paper, we denote by $M(G)$ a perfect matching of a graph G. Let $\hat{G} = G - M(G) - S_0$, where S_0 is the set of isolated vertices in $G - M(G)$. We call $\hat{G}$ the capped graph of G and G the original graph of $\hat{G}$. For example, the capped graphs of L_1, B_3, L_2 are shown in Figure 3.

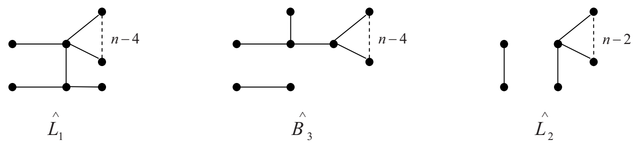

Fig. 3. The capped graphs of L_1, B_3, L_2 .

Denote by $\mathcal{E}(G)$ the edge set of a graph G. Let $G \in \mathbb{D}(2n)$. Then $K(G) = 2$. By Lemma 2.1 and the fact that a tree contains at most one perfect matching, we can see that $\mathcal{E}(G - C_\ell) \cap \mathcal{E}(\hat{G})$ is identical under two different perfect matchings of G. Thus we can classify the graphs in $\mathbb{D}(2n)$ into the following two classes.

$$\begin{aligned}\mathbb{E}(2n) &= \{G \in \mathbb{D}(2n) | \mathcal{E}(G - C_\ell) \cap \mathcal{E}(\hat{G}) \neq \emptyset\} \\ \mathbb{F}(2n) &= \{G \in \mathbb{D}(2n) | \mathcal{E}(G - C_\ell) \cap \mathcal{E}(\hat{G}) = \emptyset\} .\end{aligned}$$

It is easy to see that

$$\mathbb{U}(2n) = \mathbb{A}(2n) \cup \mathbb{C}(2n) \cup \mathbb{E}(2n) \cup \mathbb{F}(2n)$$

and $B_2 \in \mathbb{C}(2n)$, $B_3 \in \mathbb{E}(2n)$ and $L_2 \in \mathbb{F}(2n)$.

For $n \geq 191$, our basic strategy of the proof of Theorem 1.1 is to prove the following results $(R1) - (R5)$:

(R_1) $B_3 \rightharpoonup L_1$

$B_3 \rightharpoonup L_2$

$B_3 \rightharpoonup L_3$

$B_1 \rightharpoonup A_1 \rightharpoonup B_2 \rightharpoonup A_2 \rightharpoonup A_3 \rightharpoonup A_4 \rightharpoonup B_3$.

(R_2) For any $G \in \mathbb{A}(2n) \backslash \{A_1, A_2, A_3, A_4, L_3\}$, we have $L_1 \rightharpoonup G$.

(R_3) For any $G \in \mathbb{C}(2n)\backslash\{B_2, L_1\}$, we have $L_1 \rightharpoonup G$.

(R_4) For any $G \in \mathbb{E}(2n)\backslash\{B_1, B_3, \}$, we have $B_3 \rightharpoonup G$.

(R_5) For any $G \in \mathbb{F}(2n)\backslash\{L_2\}$, we have $L_2 \rightharpoonup G$.

It is easy to see that we can prove Theorem 1.1 by combining the above results (R_1)–(R_5). We first prove (R_2)–(R_5) in Sections 3 to 6, respectively. Finally, we prove (R_1) in Section 7.

3 Proof of ($\mathbf{R_2}$)

An i-matching is a disjoint union of i edges in G. The number of i-matchings is denoted by $m(G, i)$. We agree that $m(G, 0) = 1$ and $m(G, i) = 0 (i < 0)$. In order to compare the energies of two unicyclic graphs by using the method of quasi-ordering, we need to compute the numbers $b_i(G)$. On $b_i(G)$, we can easily obtain the following results.

Lemma 3.1 [15]. Let G be a unicyclic graph and C_ℓ its unique cycle of length ℓ. Let r be a positive integer. Then,

$$b_{2i+1}(G) = \begin{cases} 0 & \ell = 2r\,. \\ 2m(G - C_\ell\,, i - (\ell - 1)/2) & \ell = 2r + 1\,. \end{cases} \tag{3}$$

$$b_{2i}(G) = \begin{cases} m(G, i) & \ell = 2r + 1\,. \\ m(G, i) + 2m(G - C_\ell\,, i - \ell/2) & \ell = 4r + 2\,. \\ m(G, i) - 2m(G - C_\ell\,, i - \ell/2) & \ell = 4r\,. \end{cases} \tag{4}$$

It is easy to see that $\mathcal{E}(G) = \mathcal{E}(\hat{G}) \cup M(G)$. Thus each i-matching Ω of G can be partitioned into two parts: $\Omega = \Phi \cup \Psi$, where $\Phi \subseteq \mathcal{E}(\hat{G})$ and $\Psi \subseteq M(G)$. Let $r_j^{(2i)}(G)$ be the number of ways to choose i independent edges in G such that just j edges are in $\hat{G}$. We agree that $r_0^{(0)}(G) = 1$ and $r_j^{(2i)}(G) = 0\,(i < 0)$. For example, $r_0^{(2i)}(G) = \binom{n}{i}$ and $r_1^{(2i)}(G) = n\binom{n-2}{i-1}$.

Thus we have

$$m(G, i) = \sum_{j=0}^{i} r_j^{(2i)}(G) = p + \sum_{j=2}^{i} r_j^{(2i)}(G)$$

where

$$p = \binom{n}{i} + n\binom{n-2}{i-1}\,.$$

By using formula (4), we get the following two formulas that are frequently used in the rest of this paper.

$$b_{2i}(G) \geq p + \sum_{j=2}^{i} r_j^{(2i)}(G) \qquad \ell \not\equiv 0 \ (mod\ 4) \tag{5}$$

$$b_{2i}(G) = p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-\ell/2} r_j^{(2i-\ell)}(G - C_\ell) \qquad \ell \equiv 0 \ (mod\ 4)\,. \tag{6}$$

In order to prove (R_2), we quote the following lemma.

Lemma 3.2 [1]. Let $G \in \mathbb{U}(2n)$ with $n \geq 5$. If $G \neq A_i\,(i = 1, 2, 3, 4), B_2,\ L_2,\ L_3$, then $m(\hat{G}, 2) \geq 2n - 7$.

Proof of $(\mathbf{R_2})$. Let $G \in \mathbb{A}(2n)\backslash\{A_1, A_2, A_3, A_4, L_3\}$ and C_ℓ be the unique cycle of G. Then $\ell \not\equiv 0$ $(mod\ 4)$, which implies that $G \neq B_2,\ L_2$. By Lemma 3.2, we have $m(\hat{G}, 2) \geq 2n - 7$.

By using formula (5) and the fact that two independent edges in $\hat{G}$ are at most incident with four different edges in $M(G)$, we have

$$\begin{aligned} b_{2i}(G) &\geq p + \sum_{j=2}^{i} r_j^{(2i)}(G) \geq p + r_2^{(2i)}(G) \\ &\geq p + m(\hat{G}, 2)\begin{pmatrix} n-4 \\ i-2 \end{pmatrix} \geq p + (2n-7)\begin{pmatrix} n-4 \\ i-2 \end{pmatrix}. \end{aligned}$$

By using formula (6) and some calculation, we have

$$\begin{aligned} b_{2i}(L_1) &= p + \sum_{j=2}^{i} r_j^{(2i)}(L_1) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(L_1 - C_4) \\ &= p + (2n-7)\begin{pmatrix} n-4 \\ i-2 \end{pmatrix} - \begin{pmatrix} n-3 \\ i-2 \end{pmatrix}. \end{aligned} \tag{7}$$

Therefore, $b_{2i}(G) \geq b_{2i}(L_1)$ and $b_4(G) > b_4(L_1)$. Further, $b_{2i+1}(G) \geq 0 = b_{2i+1}(L_1)$. This implies that $G \succ L_1$. Then $L_1 \rightharpoonup G$. □

4 Proof of $(\mathbf{R_3})$

Let $G \in \mathbb{C}(2n)$ and C_ℓ be the unique cycle of G. Then we have $\ell \equiv 0$ $(mod\ 4)$ and G contains only one perfect matching. In order to prove the result (R_3), we will take two steps to consider the problem: $\ell = 4$ and $\ell \geq 8$. First, we consider the case when $\ell = 4$.

Lemma 4.1. Let $G \in \mathbb{C}(2n)$ with $n \geq 5$ and C_ℓ be the unique cycle of G. Assume that $G \neq B_2,\ L_1$. If $\ell = 4$, then $L_1 \rightharpoonup G$.

Proof. By formula (7) we have

$$b_{2i}(L_1) = p + (2n-7)\binom{n-4}{i-2} - \binom{n-3}{i-2}.$$

Let β_1 be the number of ways to choose two independent edges in $\hat{G}$ such that at least one edge is not in $\mathcal{E}(C_4)$ and β_2 the number of ways to choose two independent edges in $\hat{G}$ such that two edges are both in $\mathcal{E}(C_4)$. We consider the following two cases.

Case 1: $\mathcal{E}(C_4) \cap M(G) = \emptyset$.

Then $\mathcal{E}(C_4) \subseteq \mathcal{E}(\hat{G})$ from which follows $\beta_1 \geq 2(n-4)$ and $\beta_2 = 2$, implying $r_2^{2i}(G) \geq (2n-6)\binom{n-4}{i-2}$. Since $\beta_2 = 2$, we have $r_{j+2}^{2i}(G) \geq 2 \cdot r_j^{2i-4}(G-C_4)$ for all $1 \leq j \leq i-2$. By using formula (6) we have

$$\begin{aligned}
b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(G-C_4) \\
&= p + r_2^{2i}(G) - 2r_0^{2i-4}(G-C_4) + \sum_{j=3}^{i} r_j^{(2i)}(G) - 2\sum_{j=1}^{i-2} r_j^{(2i-4)}(G-C_4) \\
&= p + r_2^{2i}(G) - 2\binom{n-4}{i-2} + \sum_{j=1}^{i-2}\left(r_{j+2}^{(2i)}(G) - 2r_j^{(2i-4)}(G-C_4)\right) \\
&\geq p + (2n-8)\binom{n-4}{i-2} \\
&\geq p + (2n-7)\binom{n-4}{i-2} - \binom{n-3}{i-2} = b_{2i}(L_1)\ .
\end{aligned}$$

Further $b_4(L_1) < b_4(G)$, which implies that $L_1 \prec G$. Then $L_1 \rightharpoonup G$.

Case 2: $\mathcal{E}(C_4) \cap M(G) \neq \emptyset$.

If $|\mathcal{E}(C_4) \cap M(G)| = 2$, then G contains two different perfect matchings which contradicts with the condition that $G \in \mathbb{C}(2n)$. Then $|\mathcal{E}(C_4) \cap M(G)| = 1$, which implies that $\beta_2 = 1$. We consider the following two subcases.

Subcase 2.1: $\mathcal{E}(G - C_4) \cap \mathcal{E}(\hat{G}) = \emptyset$.

Since $G \neq B_2, L_1$ and by using formula (6),

$$\begin{aligned}
b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(G-C_4) \\
&= p + r_2^{2i}(G) + \sum_{j=3}^{i} r_j^{(2i)}(G) - 2r_0^{2i-4}(G-C_4)
\end{aligned}$$

$$\geq \ p + r_2^{2i}(G) - 2r_0^{2i-4}(G - C_4)$$

$$\geq \ p + (n-3)\binom{n-4}{i-2} + (n-3)\binom{n-4}{i-2} - \binom{n-3}{i-2}$$

$$\geq \ p + (2n-7)\binom{n-4}{i-2} - \binom{n-3}{i-2} = b_{2i}(L_1)\ .$$

It is further $b_4(L_1) < b_4(G)$, which implies $L_1 \prec G$. It follows that $L_1 \rightharpoonup G$.

Subcase 2.2: $\mathcal{E}(G - C_4) \cap \mathcal{E}(\hat{G}) \neq \emptyset$.

By using formula (6), we have

$$\begin{aligned} b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(G - C_4) \\ &\geq p + \beta_1 \binom{n-4}{i-2} - r_0^{2i-4}(G - C_4) - r_1^{2i-4}(G - C_4) \\ &\geq p + (2n-6)\binom{n-4}{i-2} - \binom{n-3}{i-2} - \binom{n-5}{i-2} \\ &\geq p + (2n-7)\binom{n-4}{i-2} - \binom{n-3}{i-2} = b_{2i}(L_1)\ . \end{aligned}$$

Further, $b_4(L_1) < b_4(G)$, implying $L_1 \prec G$. It follows that $L_1 \rightharpoonup G$.

This completed the proof. □

Next, we consider the case when $\ell \geq 8$.

Lemma 4.2. Let $G \in \mathbb{C}(2n)$ with $n \geq 8$ and C_ℓ be the unique cycle of G. If $\ell \geq 8$, then $L_1 \rightharpoonup G$.

Proof. Since $G \in \mathbb{C}(2n)$, we have that G contains only one perfect matching, which implies that $|\mathcal{E}(C_\ell) \cap M(G)| \leq \ell/2 - 1$. We consider the following two cases.

Case 1: $|\mathcal{E}(C_\ell) \cap M(G)| = \ell/2 - 1$.

Then $|\mathcal{E}(C_\ell) \cap E(\hat{G})| = \ell/2 + 1$. Let M_1 and M_2 be two different perfect matchings of C_ℓ. We further consider the following two subcases.

Case 1.1: $M_1 \not\subseteq \mathcal{E}(\hat{G})$ and $M_2 \not\subseteq \mathcal{E}(\hat{G})$.

Then Both M_1 and M_2 contain at least two edges of $\hat{G}$. Moreover one of them contains at least threes edges of $\hat{G}$. Let M_0 be a matching in $G - C_\ell$ with cardinality $i - \ell/2$. Then there are two matchings $M_1 \cup M_0$ and $M_2 \cup M_0$ with cardinality i corresponding to M_0.

By using formula (6) we have

$$\begin{aligned} b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-\ell/2} r_j^{(2i-\ell)}(G-C_\ell) \\ &\geq p + \beta_0 \binom{n-4}{i-2} - r_0^{2i-\ell}(G-C_\ell) \\ &= p + \beta_0 \binom{n-4}{i-2} - \binom{n-(\ell/2-1)-2}{i-\ell/2} \end{aligned}$$

where β_0 denote the number of ways to choose two independent edges in $\hat{G}$ such that at least one edge is in $\mathcal{E}(C_\ell)$.

Let $C_\ell = v_1v_2\cdots v_\ell v_1$ and T_i be the trees planted at v_i for $1 \leq i \leq \ell$. Let m_i be the number of edges of $\hat{G}$ in T_i. Then we have

$$\begin{aligned} \beta_0 &\geq \left[\binom{\ell/2-1}{2} + (m_1+m_2+\cdots+m_l)(\ell/2+1-2)\right] \\ &= \left[\binom{\ell/2-1}{2} + (n-\ell/2-1)(\ell/2+1-2)\right] \\ &= n(\ell/2-1) - (\ell/2-1)(\ell/4+2)\ . \end{aligned}$$

Let $f(x) = n(\frac{x}{2}-1) - (\frac{x}{2}-1)(\frac{x}{4}+2)$. Then $f'(x) = \frac{1}{4}(2n-x-3) \geq 0$ when $x \leq 2n-3$. Since $8 \leq \ell \leq 2n$, we have $\beta_0 = f(\ell) \geq min\{f(8), f(2n)\} = f(8) = 3n-12$. It follows that

$$\begin{aligned} b_{2i}(G) &\geq p + (3n-12)\binom{n-4}{i-2} - \binom{n-(\ell/2-1)-2}{i-\ell/2} \\ &\geq p + (3n-12)\binom{n-4}{i-2} - \binom{n-5}{i-4} \\ &\geq p + (2n-7)\binom{n-4}{i-2} - \binom{n-3}{i-2} = b_{2i}(L_1)\ . \end{aligned}$$

Further, $b_4(L_1) < b_4(G)$, which implies $L_1 \prec G$. Then $L_1 \rightharpoonup G$.

Case 1.2: $M_1 \subseteq \mathcal{E}(\hat{G})$ or $M_2 \subseteq \mathcal{E}(\hat{G})$.

Without loss of generality, we assume that $M_1 \subseteq \mathcal{E}(\hat{G})$. Then $|M_1 \cap \mathcal{E}(\hat{G})| = \ell/2 \geq 4$ and $|M_2 \cap \mathcal{E}(\hat{G})| = 1$. By using formula (6) we have

$$\begin{aligned} b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-\ell/2} r_j^{(2i-\ell)}(G-C_\ell) \\ &\geq p + \beta_3 \binom{n-4}{i-2} - r_0^{2i-\ell}(G-C_\ell) \\ &= p + \beta_3 \binom{n-4}{i-2} - \binom{n-(\ell/2-1)-2}{i-\ell/2} \end{aligned}$$

where β_3 denote the number of ways to choose two independent edges in $\hat{G}$ such that at least one edge is in M_1 and no edge is in M_2.

Using the same method as in Subcase 1.1, we have

$$\beta_3 \geq \left[\binom{\ell/2}{2} + \left(n - \frac{\ell}{2} - 1\right)\left(\frac{\ell}{2} + 1 - 2\right)\right] > \beta_0 \geq 3n - 12 \ .$$

Thus $b_{2i}(L_1) \geq b_{2i}(G)$ and $b_4(L_1) < b_4(G)$. It implies that $L_1 \rightharpoonup G$.

Case 2: $|\mathcal{E}(C_\ell) \cap M(G)| \leq \ell/2 - 2$.

Then $|\mathcal{E}(C_\ell) \cap \mathcal{E}(\hat{G})| \geq \ell/2 + 2 \geq 6$. Let M_1 and M_2 be two different perfect matchings of C_ell. Thus Both M_1 and M_2 contain at least two edges of $\hat{G}$. Since $\ell \geq 8$, we know that M_1 or M_2 contains at least four edges of $\hat{G}$. Take $|\mathcal{E}(C_\ell) \cap \mathcal{E}(\hat{G})| = x$. Then $|\mathcal{E}(C_\ell) \cap M(G)| = \ell - x$. By using formula (6) we have

$$\begin{aligned}
b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-\ell/2} r_j^{(2i-l)}(G - C_\ell) \\
&\geq p + \beta_4 \binom{n-4}{i-2} - r_0^{2i-\ell}(G - C_\ell) \\
&= p + \beta_4 \binom{n-4}{i-2} - \binom{n - (\ell - x) - (2x - \ell)}{i - \ell/2} \\
&= p + \beta_4 \binom{n-4}{i-2} - \binom{n-x}{i-\ell/2} \\
&\geq p + \beta_4 \binom{n-4}{i-2} - \binom{n - \ell/2 - 2}{i - \ell/2}
\end{aligned}$$

where β_4 denote the number of ways to choose two independent edges in $\hat{G}$ such that at least one edge is in $\mathcal{E}(C_\ell)$. Using the same method as in Subcase 1.1, we have

$$\begin{aligned}
\beta_4 &\geq \left[\tfrac{x(x-2)}{2} + (n-x)(x-2)\right] \\
&\geq \left[\tfrac{6(6-2)}{2} + (n-6)(6-2)\right] \geq 4n - 12 \ .
\end{aligned}$$

This implies

$$\begin{aligned}
b_{2i}(G) &\geq p + (4n-12)\binom{n-4}{i-2} - \binom{n-\ell/2-2}{i-\ell/2} \\
&\geq p + (4n-12)\binom{n-4}{i-2} - \binom{n-6}{i-4} \\
&\geq p + (2n-7)\binom{n-4}{i-2} - \binom{n-3}{i-2} = b_{2i}(L_1) \ .
\end{aligned}$$

Thus $b_{2i}(L_1) \leq b_{2i}(G)$ and $b_4(L_1) < b_4(G)$. It implies that $L_1 \rightharpoonup G$. □

Proof of (R_3). The result can be directly derived from Lemmas 4.1 and 4.2. □

5 Proof of $(\mathbf{R}_4)$

Let $G \in \mathbb{E}(2n)$ and C_ℓ be the unique cycle of G. Then we have $\ell \equiv 0$ $(mod\ 4)$ and G contains two different perfect matchings. Moreover, for each perfect matching $M(G)$, we have $\mathcal{E}(G - C_\ell) \cap \mathcal{E}(\hat{G}) \neq \emptyset$. In order to prove the result (R_4), we will take two steps to consider the problem: $\ell = 4$ and $\ell \geq 8$. First, we consider the case when $\ell = 4$.

Lemma 5.1. Let $G \in \mathbb{E}(2n)$ with $n \geq 5$ and C_ℓ be the unique cycle of G. Let $G \neq B_1$, B_3. If $\ell = 4$, then $B_3 \rightharpoonup G$.

Proof. By using formula (6) and some calculation, we have

$$\begin{aligned} b_{2i}(B_3) &= p + \sum_{j=2}^{i} r_j^{(2i)}(B_3) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(B_3 - C_4) \\ &= p + r_2^{(2i)}(B_3) + r_3^{(2i)}(B_3) - 2r_0^{(2i-4)}(B_3 - C_4) - 2r_1^{(2i-4)}(B_3 - C_4) \\ &= p + 2\binom{n-3}{i-2} + 3(n-4)\binom{n-4}{i-2} + (n-4)\binom{n-5}{i-3} \\ &- \binom{n-2}{i-2} - (n-4)\binom{n-4}{i-3}. \end{aligned}$$

Let $C_4 = v_1v_2v_3v_4v_1$. Let m_i be the number of edges in $\mathcal{E}(\hat{G})$ that are adjacent to v_i except two edges of C_4. Take $m_1 + m_2 + m_3 + m_4 = x$. Then we have $1 \leq x \leq n-3$. We consider the following there cases.

Case 1: $x = 1$.

Without loss of generality, we assume that $m_1 = 1$ and $m_2 = m_3 = m_4 = 0$. By using formula (6), and the fact that $G \neq B_1$ and $\mathcal{E}(G - C_4) \cap \mathcal{E}(\hat{G}) \neq \emptyset$, we have

$$\begin{aligned} b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(G - C_4) \\ &\geq p + r_2^{(2i)}(G) + r_3^{(2i)}(G) - 2r_0^{(2i-4)}(G - C_4) - 2r_1^{(2i-4)}(G - C_4) \\ &\geq p + 2\binom{n-3}{i-2} + 3(n-3)\binom{n-4}{i-2} + (n-4)\binom{n-5}{i-3} \\ &- \binom{n-2}{i-2} - (n-4)\binom{n-4}{i-3} \\ &\geq p + 2\binom{n-3}{i-2} + 3(n-4)\binom{n-4}{i-2} + (n-4)\binom{n-5}{i-3} \\ &- \binom{n-2}{i-2} - (n-4)\binom{n-4}{i-3} = b_{2i}(B_3)\,. \end{aligned}$$

Further we have $b_4(B_3) < b_4(G)$, which implies that $B_3 \rightharpoonup G$.

Case 2: $x = 2$.

By using formula (6) and $G \neq B_3$, we have

$$\begin{aligned} b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(G - C_4) \\ &\geq p + r_2^{(2i)}(G) + r_3^{(2i)}(G) - 2r_0^{(2i-4)}(G - C_4) - 2r_1^{(2i-4)}(G - C_4) \\ &\geq p + 2\binom{n-3}{i-2} + 3(n-4)\binom{n-4}{i-2} + (n-5)\binom{n-4}{i-2} \\ &+(n-4)\binom{n-5}{i-3} - \binom{n-2}{i-2} - (n-4)\binom{n-4}{i-3} \geq b_{2i}(B_3)\ . \end{aligned}$$

Further, $b_4(B_3) < b_4(G)$, which implies $B_3 \rightharpoonup G$.

Case 3: $3 \leq x \leq n-3$.

By using formula (6) we have

$$\begin{aligned} b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(G - C_4) \\ &\geq p + r_2^{(2i)}(G) + r_3^{(2i)}(G) - 2r_0^{(2i-4)}(G - C_4) - 2r_1^{(2i-4)}(G - C_4) \\ &\geq p + x\binom{n-3}{i-2} + 2(n-x-2)\binom{n-4}{i-2} + (x-1)(n-x-2)\binom{n-4}{i-2} \\ &+(x-1)(n-x-2)\binom{n-5}{i-3} - \binom{n-2}{i-2} - (n-4)\binom{n-4}{i-3} \\ &\geq p + 3\binom{n-3}{i-2} + 4(n-5)\binom{n-4}{i-2} + 2(n-5)\binom{n-5}{i-3} \\ &- \binom{n-2}{i-2} - (n-4)\binom{n-4}{i-3} \geq b_{2i}(B_3)\ . \end{aligned}$$

Further, $b_4(B_3) < b_4(G)$, which implies that $B_3 \rightharpoonup G$.

This completes the proof. □

Next, we consider the case when $\ell \geq 8$.

Lemma 5.2. Let $G \in \mathbb{E}(2n)$ with $n \geq 5$ and C_ℓ be the unique cycle of G. If $\ell \geq 8$, then $B_3 \rightharpoonup G$.

Proof. By using formula (6) we have

$$b_{2i}(G) \;=\; p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-\ell/2} r_j^{(2i-l)}(G - C_\ell)$$

$$\begin{aligned}
&\geq\; p+2\binom{n-3}{i-2}+(\beta_5-1)\binom{n-4}{i-2}+\frac{\ell}{2}\binom{n-4}{i-3}\\
&+\;\left(n-\frac{\ell}{2}-1\right)\binom{n-5}{i-3}-r_0^{2i-\ell}(G-C_\ell)-r_1^{2i-\ell}(G-C_\ell)\\
&\geq\; p+2\binom{n-3}{i-2}+(\beta_5-1)\binom{n-4}{i-2}+(n-1)\binom{n-5}{i-3}\\
&-\;\binom{n-\ell/2}{i-\ell/2}-(n-\ell/2-1)\binom{n-\ell/2-2}{i-\ell/2-1}\\
&\geq\; p+2\binom{n-3}{i-2}+(\beta_5-1)\binom{n-4}{i-2}+(n-1)\binom{n-5}{i-3}\\
&-\;\binom{n-4}{i-2}-(n-5)\binom{n-6}{i-5}
\end{aligned}$$

where β_5 denotes the number of ways to choose two independent edges in $\hat{G}$ such that at least one edge is in $\mathcal{E}(C_\ell)$.

Using the same method as in Subcase 1.1 of Lemma 4.2, we have

$$\beta_5 \geq \binom{\ell/2}{2}+\left(n-\frac{\ell}{2}\right)\left(\frac{\ell}{2}-1\right)\geq 3n-6\ .$$

Then,

$$\begin{aligned}
b_{2i}(G)\;&\geq p+2\binom{n-3}{i-2}+3(n-4)\binom{n-4}{i-2}+(n-4)\binom{n-5}{i-3}\\
&-\binom{n-2}{i-2}-(n-4)\binom{n-4}{i-3}=b_{2i}(B_3)\ .
\end{aligned}$$

Further, $b_4(B_3)<b_4(G)$, implying $B_3 \rightharpoondown G$.

This completes the proof. □

Proof of ($\mathbf{R_4}$). The result can be directly derived from Lemmas 5.1 and 5.2. □.

6 Proof of ($\mathbf{R_5}$)

Let $G\in\mathbb{F}(2n)$ and C_ℓ be the unique cycle of G. Then we have $\ell\equiv 0\ (mod\ 4)$ and G contains two different perfect matchings. Moreover, $\mathcal{E}(G-C_\ell)\cap\mathcal{E}(\hat{G})=\emptyset$ for each perfect matching $M(G)$ of G. In order to prove the result (R_5), we will take two steps to consider the problem: $\ell=4$ and $\ell\geq 8$. First, we consider the case when $\ell=4$.

Lemma 6.1. Let $G \in \mathbb{F}(2n)$ with $n \geq 5$ and C_ℓ be the unique cycle of G. Let $G \neq L_2$. If $\ell = 4$, then $L_2 \rightharpoonup G$.

Proof. By using formula (6), we have

$$\begin{aligned} b_{2i}(L_2) &= p + \sum_{j=2}^{i} r_j^{(2i)}(L_2) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(L_2 - C_4) \\ &= p + r_2^{(2i)}(L_2) - 2r_0^{(2i-4)}(L_2 - C_4) \\ &= p + \binom{n-2}{i-2} + (n-2)\binom{n-3}{i-2} - 2\binom{n-2}{i-2} \\ &= p + (n-2)\binom{n-3}{i-2} - \binom{n-2}{i-2}. \end{aligned}$$

By using formula (6), and the fact that $G \neq L_2$ and $\mathcal{E}(G - C_4) \cap \mathcal{E}(\hat{G}) = \emptyset$, we have

$$\begin{aligned} b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-2} r_j^{(2i-4)}(G - C_4) \\ &\geq p + r_2^{(2i)}(G) - 2r_0^{(2i-4)}(G - C_4) \\ &\geq p + \binom{n-2}{i-2} + (n-2)\binom{n-3}{i-2} + \binom{n-4}{i-2} - 2\binom{n-2}{i-2} \\ &= p + (n-2)\binom{n-3}{i-2} + \binom{n-4}{i-2} - \binom{n-2}{i-2} \geq b_{2i}(L_2)\ . \end{aligned}$$

Further, $b_4(L_2) < b_4(G)$, which implies $L_2 \rightharpoonup G$.

By this the proof is completed. □

Next, we consider the case when $\ell \geq 8$.

Lemma 6.2. Let $G \in \mathbb{F}(2n)$ with $n \geq 5$ and C_ℓ be the unique cycle of G. If $\ell \geq 8$, then $L_2 \rightharpoonup G$.

Proof. By using formula (6) and the fact that $\mathcal{E}(G - C_\ell) \cap \mathcal{E}(\hat{G}) = \emptyset$, we have

$$\begin{aligned} b_{2i}(G) &= p + \sum_{j=2}^{i} r_j^{(2i)}(G) - 2\sum_{j=0}^{i-\ell/2} r_j^{(2i-l)}(G - C_\ell) \\ &\geq p + r_2^{(2i)}(G) - 2r_0^{(2i-\ell)}(G - C_\ell) \\ &\geq p + \beta_6\binom{n-3}{i-2} - r_0^{(2i-\ell)}(G - C_\ell) \\ &\geq p + \beta_6\binom{n-3}{i-2} - \binom{n-\ell/2}{i-\ell/2} \\ &\geq p + \beta_6\binom{n-3}{i-2} - \binom{n-2}{i-2} \end{aligned}$$

where β_6 is the number of ways of choosing two independent edges of $\mathcal{E}(\hat{G})$, such that these are adjacent to a same edge in $M(G)$. Then $\beta_6 \geq (n-\ell/2)+\ell/2 = n$, which implies

$$b_{2i}(G) \geq p + n \begin{pmatrix} n-3 \\ i-2 \end{pmatrix} - \begin{pmatrix} n-2 \\ i-2 \end{pmatrix} \geq b_{2i}(L_2) \ .$$

Further, $b_4(L_2) < b_4(G)$, implying $L_2 \rightharpoonup G$. □

Proof of (R_5). The result can be directly derived from Lemmas 6.1 and 6.2. □

7 Proof of $(\mathbf{R}_1)$

From Section 2 to Section 6, the quasi-ordering method is always used to compare the energies of two unicyclic graphs. However, if the quantities $b_i(G)$ cannot be compared uniformly, then the common comparing method is invalid, and this happens quite often. Recently much effort has been made to tackle these quasi-ordering incomparable problems. Efficient approaches to solve these problems can be found in [1,11-14,17,18,20,27-36]. In particular, by means of the Coulson integral formula for the energy difference of two graphs, Huo et al. determined the fourth energy tree [28] and the maximal energy unicyclic graph [14]. Recently, Shan et al. [35] presented a new method of comparing the energies of subdivision bipartite graphs which can also be used to tackle these quasi-ordering incomparable problems. By using this method, they determined the first $3n-84$ (when n is odd) and $3n-87$ (when n is even) largest energy trees in [36].

In this section, we use the the Coulson integral formula for the energy difference of two graphs to compare the energies of two unicyclic graphs which are quasi-ordering incomparable. The following lemma is a well known result due to Gutman [6], which will be used in the sequel.

Lemma 7.1 [6]. Let $\phi_1(x)$ and $\phi_2(x)$ be two characteristic polynomials of two graphs G_1 and G_2 with the same order, respectively. Then

$$E(G_1) - E(G_2) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \log\left|\frac{\phi_1(ix)}{\phi_2(ix)}\right| dx = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \log\frac{p_1^2(x)+q_1^2(x)}{p_2^2(x)+q_2^2(x)}\, dx \qquad (8)$$

where $\phi_1(ix) = p_1(x) + i\, q_1(x)$ and $\phi_2(ix) = p_2(x) + i\, q_2(x)$.

By using formula (8), we can prove the following results.

Lemma 7.2. If $n \geq 5$, then $B_3 \rightharpoonup L_1$.

Proof. By some calculation we have

$$\begin{aligned}\phi(B_3,x) &= x^2(x^2-1)^{n-5}(x^8-(n+5)x^6+(6n-1)x^4-(6n-1)x^2+8)\\ \phi(L_1,x) &= (x^2-1)^{n-5}(x^{10}-(n+5)x^8+(5n+2)x^6-(5n+1)x^4+(n+4)x^2-1)\ .\end{aligned}$$

By using formula (8) we have

$$E(B_3)-E(L_1)=\frac{1}{\pi}\int_{-\infty}^{+\infty}\log F(x)\,dx=\frac{2}{\pi}\int_{0}^{+\infty}\log F(x)\,dx$$

where

$$F(x)=\frac{x^2(x^8+(n+5)x^6+(6n-1)x^4+(6n-1)x^2+8)}{x^{10}+(n+5)x^8+(5n+2)x^6+(5n+1)x^4+(n+4)x^2+1}\ .$$

Write

$$f(t,x)=\frac{\tilde{\phi}_1}{\tilde{\phi}_2}=\frac{x^2(x^8+(t+5)x^6+(6t-1)x^4+(6t-1)x^2+8)}{x^{10}+(t+5)x^8+(5t+2)x^6+(5t+1)x^4+(t+4)x^2+1}\ .$$

Then

$$f'_t(t,x)=\frac{x^4(x^2+1)(x^4+x^2-1)(x^6+7x^4+9x^2+2)}{(\tilde{\phi}_2)^2}$$

which has only one positive real root, equal to $\sqrt{(\sqrt{5}-1)/2}$. Therefore $f(n,x)$ strictly decreases when $x\in\left(0,\sqrt{(\sqrt{5}-1)/2}\right)$ and strictly increases when $x\in\left[\sqrt{(\sqrt{5}-1)/2},+\infty\right)$. Take

$$f(+\infty,x)=\lim_{n\to+\infty}f(n,x)=\frac{x^2(x^6+6x^4+6x^2)}{x^8+5x^6+5x^4+x^2}=\frac{x^6+6x^4+6x^2}{x^6+5x^4+5x^2+1}\ .$$

It follows that

$$\begin{aligned}E(B_3)-E(L_1) &= \frac{2}{\pi}\int_0^{+\infty}\log f(n,x)\,dx\\ &\le \frac{2}{\pi}\int_0^{\sqrt{\frac{\sqrt{5}-1}{2}}}\log f(5,x)\,dx+\frac{2}{\pi}\int_{\sqrt{\frac{\sqrt{5}-1}{2}}}^{+\infty}\log f(+\infty,x)\,dx\\ &\doteq \frac{2}{\pi}(-0.851236+0.502351)<0\ .\end{aligned}$$

Thus, $B_3 \rightharpoonup L_1$ for $n\ge 5$. □

Lemma 7.3. If $n\ge 5$, then $B_3\rightharpoonup L_2$.

Proof. By some calculation we obtain

$$\phi(B_3,x) = x^2(x^2-1)^{n-5}(x^8-(n+5)x^6+(6n-1)x^4-(6n-1)x^2+8)$$

$$\phi(L_2,x) \;=\; x^2(x^2-1)^{n-3}(x^4-(n+3)x^2+2n)\ .$$

Using formula (8) we have

$$E(B_3)-E(L_2)=\frac{2}{\pi}\int_0^{+\infty}\log\frac{x^8+(n+5)x^6+(6n-1)x^4+(6n-1)x^2+8}{(x^2+1)^2(x^4+(n+3)x^2+2n)}\,dx\ .$$

Write

$$f(t,x)=\frac{\tilde{\phi}_1}{\tilde{\phi}_2}=\frac{x^8+(t+5)x^6+(6t-1)x^4+(6t-1)x^2+8}{(x^2+1)^2(x^4+(t+3)x^2+2t)}\ .$$

Then

$$f'_t(t,x)=\frac{(x^2+1)^2(2x^4+x^2-2)(x^4+7x^2+8)}{(\tilde{\phi}_2)^2}$$

which has only one positive real root, equal to $\sqrt{(\sqrt{17}-1)/4}$. Therefore $f(n,x)$ strictly decreases when $x\in\left(0,\sqrt{(\sqrt{17}-1)/4}\right)$ and strictly increases when $x\in\left[\sqrt{(\sqrt{17}-1)/4},+\infty\right)$. Take

$$f(+\infty,x)=\lim_{n\to+\infty}f(n,x)=\frac{x^6+6x^4+6x^2}{(x^2+1)^2(x^2+2)}\ .$$

If $n\geq 90$, then

$$\begin{aligned}E(B_3)-E(L_2) &= \frac{2}{\pi}\int_0^{+\infty}\log f(n,x)\,dx\\ &\leq \frac{2}{\pi}\int_0^{\sqrt{\frac{\sqrt{17}-1}{4}}}\log f(90,x)dx+\frac{2}{\pi}\int_{\sqrt{\frac{\sqrt{17}-1}{4}}}^{+\infty}\log f(+\infty,x)\,dx\\ &\doteq \frac{2}{\pi}(-0.944366+0.942722)<0\ .\end{aligned}$$

Further, $B_3 \rightharpoonup L_2$ for $5\leq n\leq 89$. Thus, $B_3 \rightharpoonup L_2$ for $n\geq 5$. □

Lemma 7.4. If $n\geq 5$, then $B_3 \rightharpoonup L_3$.

Proof. By some calculation we have

$$\begin{aligned}\phi(L_3,x) &= (x^2-1)^{n-3}(x^6-(n+3)x^4-2x^3+(2n+1)x^2+2x-1)\\ \phi(L_2,x) &= x^2(x^2-1)^{n-3}(x^4-(n+3)x^2+2n)\ .\end{aligned}$$

Thus, $L_2 \prec L_3$, which implies that $L_2 \rightharpoonup L_3$. By Lemma 7.3, $B_3 \rightharpoonup L_3$. □

In [5], Li and Li have shown the following result by directly comparing the energies of B_1 and A_1.

Lemma 7.5 [20]. I f $n\geq 5$, then $B_1 \rightharpoonup A_1$.

Wang [1] has shown the following results by means of the theorem of zero points.

Lemma 7.6. If $n \geq 7$, then $A_1 \rightharpoonup B_2$.

Lemma 7.7. If $n \geq 4$, then $B_2 \rightharpoonup A_2 \rightharpoonup A_3$.

In order to prove the result (R_1), we only need to prove that $A_3 \rightharpoonup A_4$ and $A_4 \rightharpoonup B_3$.

Lemma 7.8. If $n \geq 4$, then $A_3 \rightharpoonup A_4$.

Proof. By some calculation we have

$$\begin{aligned}\phi(A_3, x) &= (x^2-1)^{n-4}(x^8-(n+4)x^6-2x^5+(3n+4)x^4+4x^3-(n+5)x^2-2x+1)\\ \phi(A_4, x) &= (x^2-1)^{n-4}(x^8-(n+4)x^6+(3n+5)x^4-2x^3-(n+6)x^2+2x+1)\ .\end{aligned}$$

Write

$$\begin{aligned}p_1 &= x^8+(n+4)x^6+(3n+4)x^4+(n+5)x^2+1\\ q_1 &= 2x^5+4x^3+2x\\ p_2 &= x^8+(n+4)x^6+(3n+5)x^4+(n+6)x^2+1\\ q_2 &= 2x^3+2x\ .\end{aligned}$$

By using formula (8),

$$E(A_3)-E(A_4) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\log\frac{p_1^2+q_1^2}{p_2^2+q_2^2}\,dx$$

and it can be shown that

$$(p_1^2+q_1^2)-(p_2^2+q_2^2) = -x^2(x^2+1)(2x^8+(2n+4)x^6+(6n-3)x^4+(2n+3)x^2+2) \leq 0\ .$$

It follows that $E(A_3) < E(A_4)$, that is, $A_3 \rightharpoonup A_4$. □

Lemma 7.9. If $n \geq 191$, then $A_4 \rightharpoonup B_3$.

Proof. By some calculation we have

$$\begin{aligned}\phi(A_4, x) &= (x^2-1)^{n-4}(x^8-(n+4)x^6+(3n+5)x^4-2x^3-(n+6)x^2+2x+1)\\ \phi(B_3, x) &= x^2(x^2-1)^{n-5}(x^8-(n+5)x^6+(6n-1)x^4-(6n-1)x^2+8)\ .\end{aligned}$$

By using formula (8), we get

$$E(A_4)-E(B_3) = \frac{1}{\pi}\int_0^{+\infty}\log F_1(x)\,dx < \frac{1}{\pi}\int_0^{+\infty}\log F_2(x)\,dx$$

where

$$F_1(x) = \frac{(x^2+1)^2\,[(x^8+(n+4)x^6+(3n+5)x^4+(n+6)x^2+1)^2+(2x^3+2x)^2]}{x^4(x^8+(n+5)x^6+(6n-1)x^4+(6n-1)x^2+8)^2}$$

$$F_2(x) = \frac{(x^2+1)^2\,[(x^8+(n+4)x^6+(3n+5)x^4+(n+6)x^2+1)^2+(2x^3+2x)^2]}{x^4(x^8+(n+5)x^6+(6n-1)x^4+(6n-1)x^2+6)^2}\,.$$

Write

$$\begin{aligned} p_1 &= x^8+(t+4)x^6+(3t+5)x^4+(t+6)x^2+1 \\ q_1 &= 2x^3+2x \\ p_2 &= x^8+(t+5)x^6+(6t-1)x^4+(6t-1)x^2+6 \\ f(t,x) &= \frac{(x^2+1)^2\,[p_1^2+q_1^2]}{x^4p_2^2}\,. \end{aligned}$$

Then

$$\begin{aligned} f'_t(t,x) &= \frac{(x^2+1)^2}{x^4}\cdot\frac{2p_1p_2^2(x^6+3x^4+x^2)-2p_2(p_1^2+q_1^2)(x^6+6x^4+6x^2)}{p_2^4} \\ &\leq \frac{(x^2+1)^2}{x^4}\cdot\frac{2p_1p_2\left((x^6+3x^4+x^2)p_2-(x^6+6x^4+6x^2)p_1\right)}{p_2^4} \\ &= \frac{(x^2+1)^2}{x^4}\cdot\frac{2p_1p_2\left(-x^4(2x^8+20x^6+59x^4+65x^2+25)\right)}{p_2^4} < 0\,. \end{aligned}$$

Thus $f(n,x)$ about n strictly decreases when $x \in (0,+\infty)$. When $n \geq 300$, it implies that

$$\begin{aligned} E(A_4)-E(B_3) &< \frac{1}{\pi}\int_0^{+\infty}\log f(n,x)\,dx < \frac{1}{\pi}\int_0^{+\infty}\log f(300,x)\,dx \\ &\doteq -0.0335098 < 0\,. \end{aligned}$$

Further, by some calculation we obtain $A_4 \rightharpoonup B_3$ for $191 \leq n \leq 299$. Therefore, $B_3 \rightharpoonup L_2$ for $n \geq 191$. □

Proof of ($\mathbf{R_1}$). The result can be directly derived from Lemmas 7.2 to 7.9. □

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