

Maximum energy bicyclic graphs containing two odd cycles with one common vertex

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Abstract

The energy of a graph is the sum of the absolute values of all eigenvalues of its adjacency matrix. Let $P_n^{6,6}$ be the graph obtained from two copies of C_6 joined by a path P_{n-10} . In 2001, Gutman and Vidović [I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: A computer experiment, J. Chem. Inf. Comput. Sci. 41 (2001) 1002–1005] conjectured that the bicyclic graph with the maximal energy is $P_n^{6,6}$. This conjecture is true for bipartite bicyclic graphs. For non-bipartite bicyclic graphs, Ji and Li [An approach to the problem of the maximal energy of bicyclic graphs, MATCH Commun. Math. Comput. Chem. 68 (2012) 741–762] proved the conjecture for bicyclic graphs which have exactly two edge-disjoint cycles such that one of them is even and the other is odd. This paper is to prove the conjecture for bicyclic graphs containing two odd cycles with one common vertex.

Keywords: Maximal energy; Bicyclic graphs; Eigenvalues; Characteristic polynomial; Odd cycles

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1 Introduction

Graphs considered in this paper are all connected and simple, that is, have no loops and parallel edges. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. An edge $e \in E(G)$ with end vertices v_i and v_j is usually denoted by $v_i v_j$. As usual, let P_n and C_n be the path and cycle of order n . Let P_n^l denote the unicyclic graph obtained by connecting a vertex of C_l with a terminal vertex of P_{n-l} and $P_n^{k,l}$ denote

the graph obtained from two cycles C_k and C_l joined by a path $P_{n-k-l+2}$. Denote by $G(n, l)$ the set of all n order connected unicyclic graphs which contain cycle C_l as its subgraph.

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

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

It is important that $\phi(G, x)$ satisfies the following recursion relation

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

where $\mathcal{C}(uv)$ is the set of cycles containing edge uv . With respect to the coefficients of the characteristic polynomial of a graph, let G be a graph with characteristic polynomial $\sum_{k=0}^n a_k x^{n-k}$. Then for $k \geq 1$,

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

where $L_k(G)$ denotes the set of Sachs subgraphs of G with k vertices, that is, the subgraphs 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, $a_0 = 1$. This is the famous Sachs Theorem [3]. In particular, if G is a tree, the characteristic polynomial of G can be expressed as

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

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

For a graph G , let $\lambda_1, \lambda_2, \dots, \lambda_n$ denote the eigenvalues of $\phi(G, x)$. The energy of G is defined as

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

This definition was put forward by Gutman [5] in 1978. The following formula is also well known

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

where $i^2 = -1$. Furthermore, in the book of Gutman and Polansky [7], the above equation was converted into an explicit formula as follows:

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

which is called the Coulson integral formula.

Let $b_i(G) = |a_i(G)|$ for $0 \leq i \leq n$. If $(-1)^k a_{2k}(G)$ and $(-1)^k a_{2k+1}(G)$ have the uniform sign, respectively, then Equation (1) is reduced to

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

Define the quasi-order \preceq and write $G_1 \preceq G_2$ if $b_i(G_1) \leq b_i(G_2)$ for all $1 \leq i \leq n$. Thus for any two graphs G_1 and G_2 , if $(-1)^k a_{2k}(G_1)$, $(-1)^k a_{2k+1}(G_1)$, $(-1)^k a_{2k}(G_2)$ and $(-1)^k a_{2k+1}(G_2)$ have the uniform sign, respectively, we can obtain $\mathcal{E}(G_1) \leq \mathcal{E}(G_2)$ if $G_1 \preceq G_2$. Since 1980s, the extremal energy $\mathcal{E}(G)$ of a graph G has been studied extensively. Many results have been discovered on acyclic, unicyclic, bicyclic and bipartite graphs by this quasi-order method; see [4, 6, 9, 11, 15].

In [2], Caporossi et al. proposed the following conjecture on the unicyclic graphs with maximal energy.

Conjecture 1.1 *Among all unicyclic graphs on n vertices, the cycle C_n has maximal energy if $n \leq 7$ and $n = 9, 10, 11, 13$ and 15 . For all other values of n , the unicyclic graph with maximal energy is P_n^6 .*

By quasi-order method, Hou et al. [9] obtained $\mathcal{E}(G) < \mathcal{E}(P_n^6)$ for any connected, unicyclic and bipartite graph G on n vertices and $G \notin \{C_n, P_n^6\}$. One of the authors Li [12] and Andriantiana [1] independently proved that $\mathcal{E}(C_n) < \mathcal{E}(P_n^6)$, and then completely determined that P_n^6 is the only graph which attains the maximum value of the energy among all the unicyclic bipartite graphs for $n = 8, 12, 14$ and $n \geq 16$, which partially solved the above conjecture. In [13], by employing the Coulson integral formula and some knowledge of real analysis, especially by using certain combinatorial techniques, Huo et al. completely solved this conjecture. However, they found that for $n = 4$ the conjecture is not true, and P_4^3 should be the unicyclic graph with maximal energy.

In [8], Gutman and Vidović proposed a conjecture on the bicyclic graphs with the maximal energy.

Conjecture 1.2 *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 $P_n^{6,6}$.*

Let G be the bipartite bicyclic graph that is not the graph $R_{a,b}$ obtained from two cycles C_a and C_b ($a, b \geq 10$ and $a \equiv b \equiv 2 \pmod{4}$) joined by an edge. One of the authors Li and

Zhang [16] showed $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6})$ with equality if and only if $G \cong P_n^{6,6}$. Subsequently, Huo et al. [11] solved $\mathcal{E}(R_{a,b}) < \mathcal{E}(P_n^{6,6})$ by using the Coulson integral formula. Thus, the above conjecture for bipartite bicyclic graphs has been completely solved.

For any non-bipartite bicyclic graph G with two edge-disjoint cycles such that one of them is even and the other is odd, Ji and Li [14] proved that $(-1)^k a_{2k}(G)$ and $(-1)^k a_{2k+1}(G)$ have uniform sign, respectively. And they obtained $\mathcal{E}(G) < \mathcal{E}(P_n^{6,6})$.

So far, Conjecture 1.2 is open for bicyclic graphs containing two odd cycles. In this paper, we will consider bicyclic graphs containing exactly two odd cycles with one common vertex. Let $\mathcal{D}_n^{r,s}$ be the class of all bicyclic graphs which have exactly two cycles C_r and C_s satisfying that they have just one common vertex. We will prove the following propositions.

Proposition 1.3 *Conjecture 1.2 is true for bicyclic graphs in $\mathcal{D}_n^{2p+1,2q+1}$ where $p, q \geq 1$ and $p + q \geq 3$, and $n = 12, 14$ and $n \geq 16$.*

Proposition 1.4 *Conjecture 1.2 is true for bicyclic graphs in $\mathcal{D}_n^{3,3}$ where $n \geq 12$.*

From Propositions 1.3 and 1.4 we can directly get our following main result.

Theorem 1.5 *Conjecture 1.2 is true for bicyclic graphs that contain two odd cycles with one common vertex.*

2 Preliminaries

To prove Propositions 1.3 and 1.4, we need some known and new results, so we will divide this section into two parts. We first provide some known results which will be used later and then give some new lemmas.

2.1 Known results

First we list some knowledge on real analysis, we refer the readers to [17] for details.

Theorem 2.1 [17] *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 very useful result which will be frequently used in our proofs.

Theorem 2.2 [7] Let $n \in \{4k, 4k + 1, 4k + 2, 4k + 3\}$. Then for even i ,

$$b_i(P_n) > b_i(P_2 \cup P_{n-2}) > b_i(P_4 \cup P_{n-4}) > \cdots > b_i(P_{2k} \cup P_{n-2k}) > b_i(P_{2k+1} \cup P_{n-2k-1}) \\ > b_i(P_{2k-1} \cup P_{n-2k+1}) > \cdots > b_i(P_3 \cup P_{n-3}) > b_i(P_1 \cup P_{n-1}).$$

Recall that $G(n, l)$ is the set of all n order connected unicyclic graphs which contain cycle C_l as its subgraph. In the study of unicyclic graphs with maximal energy, Hou et al. [9] got the following result.

Theorem 2.3 [9] Let $G \in G(n, l)$ where $l \not\equiv 0 \pmod{4}$. Then $b_i(G) \leq b_i(P_n^l)$.

On the bicyclic graphs, Ji and Li [14] obtained two results which will be used in the sequel.

Theorem 2.4 [14] Let G be a bicyclic graph which has exactly two edge-disjoint cycles C_t and C_l satisfying that t is even and $l = 2p + 1$ is odd. Then for $i \geq 0$, we have

$$(i) \quad (-1)^i a_{2i} \geq 0;$$

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

Theorem 2.5 [14] Let G be a bicyclic graph which has exactly two edge-disjoint cycles satisfying that one is even and the other is odd. Then $\mathcal{E}(G) < \mathcal{E}(P_n^{6,6})$ for $n = 12, 14$ and $n \geq 16$.

The following lemma is a well-known conclusion due to Gutman [6].

Theorem 2.6 [6] If G_1 and G_2 are two graphs with the same number of vertices, then

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

2.2 New lemmas

In the proof of Proposition 1.3, we will use bicyclic graphs which have exactly two vertex-disjoint cycles such that one is even and the other is odd. Ji and Li [14] obtained that Equation (2) holds for these graphs. What is more, they gave a result of b_i when $b_{2i}(G) = (-1)^i a_{2i}(G)$ and $b_{2i+1}(G) = (-1)^i a_{2i+1}(G)$. Based on the definition of $b_i(G)$ in this paper, we provide a similar result.

Lemma 2.7 Let G be a bicyclic graph where has exactly two vertex-disjoint cycles satisfying that one is even and the other is odd. If uv is an edge of a cycle C_r with $r \not\equiv 0 \pmod{4}$, then

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-r}(G - C_r).$$

Proof. Let $L_i(G)$ be the set of the Sachs subgraphs with i vertices of G . Without loss of generality, we assume that the even cycle of G is C_{2p} and the odd cycle is C_{2q+1} .

Case 1. uv is an edge of the cycle C_{2p} and p is odd.

If i is odd, then $i - 2$ and $i - 2p$ are also odd. Since the graphs $G - uv$, $G - u - v$ and $G - C_{2p}$ all contain the odd cycle C_{2q+1} , we have

$$a_i(G - uv) = \begin{cases} 0, & i < 2q + 1; \\ 2 \sum_{S \in L_i(G-uv)} (-1)^{\frac{i-2q+1}{2}}, & i \geq 2q + 1, \end{cases}$$

$$a_{i-2}(G - u - v) = \begin{cases} 0, & i < 2q + 3; \\ 2 \sum_{S \in L_{i-2}(G-u-v)} (-1)^{\frac{i-2q-1}{2}}, & i \geq 2q + 3, \end{cases}$$

and

$$a_{i-2p}(G - C_{2p}) = \begin{cases} 0, & i < 2q + 2p + 1; \\ 2 \sum_{S \in L_{i-2p}(G-C_{2p})} (-1)^{\frac{i-2p-2q+1}{2}}, & i \geq 2q + 2p + 1. \end{cases}$$

According to p being odd, we obtain

$$\begin{aligned} b_i(G) &= |a_i(G)| = |a_i(G - uv) - a_{i-2}(G - u - v) - 2a_{i-2p}(G - C_{2p})| \\ &= |a_i(G - uv)| + |a_{i-2}(G - u - v)| + 2|a_{i-2p}(G - C_{2p})| \\ &= b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-2p}(G - C_{2p}). \end{aligned}$$

Similarly, if i is even, then $i - 2$ is even and $i - 2p$ is also even. Since there are no even cycles in the graphs $G - uv$, $G - u - v$ and $G - C_{2p}$, we get

$$a_i(G - uv) = \sum_{S \in L_i(G-uv)} (-1)^{\frac{i}{2}},$$

$$a_{i-2}(G - u - v) = \sum_{S \in L_{i-2}(G-u-v)} (-1)^{\frac{i-2}{2}},$$

and

$$a_{i-2p}(G - C_{2p}) = \sum_{S \in L_{i-2p}(G-C_{2p})} (-1)^{\frac{i-2p}{2}}$$

for $i \geq 2p$. Thus,

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-2p}(G - C_{2p}).$$

Case 2. uv is an edge of the cycle C_{2q+1} .

If i is odd, then $i - 2$ is odd and $i - (2q + 1)$ is even. Since $G - uv$ and $G - u - v$ have no odd cycles, we get $a_i(G - uv) = 0$ and $a_{i-2}(G - u - v) = 0$. Hence,

$$\begin{aligned} b_i(G) &= |a_i(G - uv)| + |a_{i-2}(G - u - v)| + 2|a_{i-(2q+1)}(G - C_{2q+1})| \\ &= b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-(2q+1)}(G - C_{2q+1}). \end{aligned}$$

If i is even, then $i - 2$ is even and $i - (2q + 1)$ is odd. Because $G - C_{2q+1}$ has no odd cycle, we have $a_{i-(2q+1)}(G - C_{2q+1}) = 0$. Moreover, since C_{2p} is the subgraph of $G - uv$ and $G - u - v$, we obtain the number of components of each Sachs subgraph with i vertices of $G - uv$ is $\frac{i}{2}$ or $\frac{i-2p+2}{2}$ and the number of components of each Sachs subgraph with $i - 2$ vertices of $G - u - v$ is $\frac{i-2}{2}$ or $\frac{i-2p}{2}$. Thus $a_i(G - uv)$ and $a_{i-2}(G - u - v)$ have different signs. We get

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-(2q+1)}(G - C_{2q+1}).$$

Therefore, we complete the proof. \square

Let $G \in \mathcal{D}_n^{2p+1, 2q+1}$ with $p - q \equiv 0 \pmod{2}$. Next we prove $(-1)^k a_{2k}(G)$ and $(-1)^k a_{2k+1}(G)$ have the uniform sign and then give the expression of $b_i(G)$.

Lemma 2.8 *If $G \in \mathcal{D}_n^{2p+1, 2q+1}$ and $p - q \equiv 0 \pmod{2}$, we have*

$$(i) \quad (-1)^i a_{2i} \geq 0;$$

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

Proof. Let $m(G, k)$ be the number of the k -matchings of G . From Sachs Theorem, we have

$$(-1)^i a_{2i} = (-1)^i \cdot (-1)^i m(G, i) \geq 0.$$

Thus, (i) holds.

For $(-1)^i a_{2i+1}$. Without loss of generality, we suppose that $p \leq q$. Let S_{2p+1} and S_{2q+1} be the sets of Sachs subgraphs with $2i + 1$ vertices of G containing cycles C_{2p+1} and C_{2q+1} , respectively.

If $2i + 1 < 2p + 1$, then $(-1)^i a_{2i+1} = 0$.

If $2p + 1 \leq 2i + 1 < 2q + 1$, then

$$(-1)^i a_{2i+1} = 2 \sum_{S \in S_{2p+1}} (-1)^i (-1)^{i-p+1} = 2 \sum_{S \in S_{2p+1}} (-1)^{p-1}.$$

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

If $2i + 1 \geq 2q + 1$, then

$$\begin{aligned} (-1)^i a_{2i+1} &= 2 \sum_{S \in \mathcal{S}_{2p+1}} (-1)^i (-1)^{i-p+1} + 2 \sum_{S \in \mathcal{S}_{2q+1}} (-1)^i (-1)^{i-q+1} \\ &= 2 \sum_{S \in \mathcal{S}_{2p+1}} (-1)^{p-1} + 2 \sum_{S \in \mathcal{S}_{2q+1}} (-1)^{q-1}. \end{aligned}$$

Since $p - q \equiv 0 \pmod{2}$, we get the result. \square

Lemma 2.9 *Let $G \in \mathcal{D}_n^{2p+1, 2q+1}$ and $p - q \equiv 0 \pmod{2}$. If uv is an edge of cycle C_r with $r = 2p + 1$ or $2q + 1$, then*

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-r}(G - C_r).$$

If uv is a cut edge of G , then

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v).$$

Proof. The definition of $L_i(G)$ is the same as that provided in Lemma 2.7. If uv is an edge in the cycle of G , without loss of generality, we suppose that uv is an edge of cycle C_{2p+1} . Then

$$b_i(G) = |a_i(G)| = |a_i(G - uv) - a_{i-2}(G - u - v) - 2a_{i-(2p+1)}(G - C_{2p+1})|.$$

When i is odd, $i - 2$ is odd and $i - (2p + 1)$ is even. We have

$$a_i(G - uv) = \begin{cases} 0, & i < 2q + 1; \\ 2 \sum_{S \in L_i(G-uv)} (-1)^{\frac{i-2q+1}{2}}, & i \geq 2q + 1. \end{cases}$$

For $a_{i-2}(G - u - v)$, if u or v is a common vertex of C_{2p+1} and C_{2q+1} , then $a_{i-2}(G - u - v) = 0$. Otherwise,

$$a_{i-2}(G - u - v) = \begin{cases} 0, & i < 2q + 3; \\ 2 \sum_{S \in L_{i-2}(G-u-v)} (-1)^{\frac{i-2q-1}{2}}, & i \geq 2q + 3. \end{cases}$$

And

$$a_{i-(2p+1)}(G - C_{2p+1}) = \sum_{S \in L_{i-(2p+1)}(G-C_{2p+1})} (-1)^{\frac{i-2p-1}{2}}$$

when $i \geq 2p + 1$.

Since $p - q \equiv 0 \pmod{2}$, we have $a_i(G - uv)$ and $a_{i-2}(G - u - v)$ ($a_{i-(2p+1)}(G - C_{2p+1})$) have different signs for every i . Hence,

$$b_i(G) = |a_i(G - uv)| + |a_{i-2}(G - u - v)| + 2|a_{i-(2p+1)}(G - C_{2p+1})|$$

$$= b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-(2p+1)}(G - C_{2p+1}).$$

When i is even, $i - 2$ is even and $i - (2p + 1)$ is odd. Analogously, we have $a_i(G - uv) = \sum_{S \in L_i(G-uv)} (-1)^{\frac{i}{2}}$ and $a_{i-2}(G - u - v) = \sum_{S \in L_{i-2}(G-u-v)} (-1)^{\frac{i-2}{2}}$. Since there is no odd cycle in $G - C_{2p+1}$, we have $a_{i-(2p+1)}(G - C_{2p+1}) = 0$. Thus,

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-(2p+1)}(G - C_{2p+1}).$$

If uv is a cut edge of G , then we have

$$b_i(G) = |a_i(G)| = |a_i(G - uv) - a_{i-2}(G - u - v)|.$$

When i is odd, $i - 2$ is also odd. The number of components of each Sachs subgraph with i vertices of $G - uv$ is 0 or $\frac{i-2p+1}{2}$ or $\frac{i-2q+1}{2}$. The number of components of each Sachs subgraph with $i - 2$ vertices of $G - u - v$ is 0 or $\frac{i-2p-1}{2}$ or $\frac{i-2q-1}{2}$. According to $p - q \equiv 0 \pmod{2}$, it follows that $a_i(G - uv)$ and $a_{i-2}(G - u - v)$ have different signs. Hence,

$$\begin{aligned} b_i(G) &= |a_i(G - uv)| + |a_{i-2}(G - u - v)| \\ &= b_i(G - uv) + b_{i-2}(G - u - v). \end{aligned}$$

When i is even, $i - 2$ is also even. Since the number of components of each Sachs subgraph with i vertices of $G - uv$ is $\frac{i}{2}$ and the number of components of each Sachs subgraph with $i - 2$ vertices of $G - u - v$ is $\frac{i-2}{2}$, $a_i(G - uv)$ and $a_{i-2}(G - u - v)$ have different signs. Thus,

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v).$$

The proof is now complete. □

Remark 2.10 *As we know, for non-bipartite graphs with uniform signs of $(-1)^k a_{2k}$ and $(-1)^k a_{2k+1}$, respectively, we also can compare their energies by quasi-order method, that is, by directly proving $b_i(G_1) \leq b_i(G_2)$ for all $0 \leq i \leq n$ to obtain $\mathcal{E}(G_1) \leq \mathcal{E}(G_2)$. Thus by Lemma 2.8, we can use this method to compare the energies of graphs belonging to $\mathcal{D}_n^{2p+1, 2q+1}$ with $p - q \equiv 0 \pmod{2}$ and other graph H such that $(-1)^k a_{2k}(H)$ and $(-1)^k a_{2k+1}(H)$ have uniform sign, respectively.*

For the graph $G \in \mathcal{D}_n^{2p+1, 2q+1}$ with $p - q \not\equiv 0 \pmod{2}$, we find the result of Lemma 2.8 may not hold. In this case, if we get $b_i(G) \leq b_i(H)$ for all $0 \leq i \leq n$ and H is the graph such that $(-1)^k a_{2k}(H)$ and $(-1)^k a_{2k+1}(H)$ have uniform sign, respectively, then by

$$\left(\sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k a_{2k}(G) x^{2k} \right)^2 + \left(\sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k a_{2k+1}(G) x^{2k+1} \right)^2$$

$$\leq \left(\sum_{k=0}^{\lfloor n/2 \rfloor} b_{2k}(G)x^{2k} \right)^2 + \left(\sum_{k=0}^{\lfloor n/2 \rfloor} b_{2k+1}(G)x^{2k+1} \right)^2$$

for all $0 \leq k \leq \lfloor n/2 \rfloor$ and Equation (2), we can obtain

$$\begin{aligned} \mathcal{E}(G) &\leq \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left[\left(\sum_{k=0}^{\lfloor n/2 \rfloor} b_{2k}(G)x^{2k} \right)^2 + \left(\sum_{k=0}^{\lfloor n/2 \rfloor} b_{2k+1}(G)x^{2k+1} \right)^2 \right] dx \\ &\leq \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left[\left(\sum_{k=0}^{\lfloor n/2 \rfloor} b_{2k}(H)x^{2k} \right)^2 + \left(\sum_{k=0}^{\lfloor n/2 \rfloor} b_{2k+1}(H)x^{2k+1} \right)^2 \right] dx \\ &= \mathcal{E}(H). \end{aligned} \tag{3}$$

For convenience, we give some notations. Denote by $C(l)$ the induced subgraph of G consisting of the cycle C_l and all the trees with a vertex on C_l . For a graph $G \in \mathcal{D}_n^{2p+1, 2q+1}$, denote the two cycles $C_{2p+1} = v_0v'_1 \cdots v'_{2p}$ and $C_{2q+1} = v_0v_1 \cdots v_{2q}$. Let T_i (resp. T'_i) be the subtree of G such that T_i (resp. T'_i) and C_{2q+1} (resp. C_{2p+1}) have a unique common vertex v_i (resp. v'_i). Denote by F_i and F'_i the forests obtained from $T_i - v_i$ and $T'_i - v'_i$, respectively. Let $|C(2p+1) - F_0| = 2p+1+l$ and $|C(2q+1)| = 2q+1+k$.

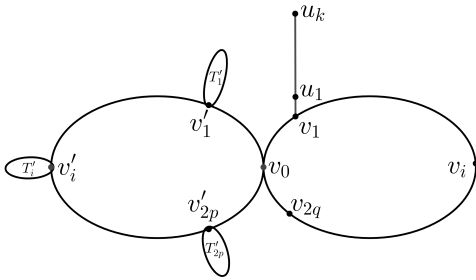


Figure 1: Graph H .

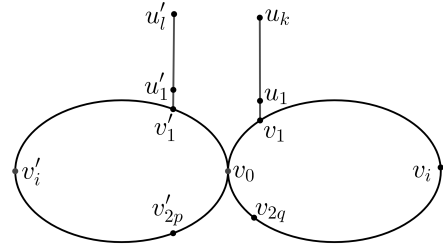


Figure 2: Graph $H_n(2p+1, l; 2q+1, k)$ with $k+l = n - 2p - 2q - 1$.

Lemma 2.11 *Let $G \in \mathcal{D}_n^{2p+1, 2q+1}$. If $p - q \equiv 0 \pmod{2}$ and $1 \leq p \leq q$, then we have $\mathcal{E}(G) \leq \mathcal{E}(B_n(2p+1; 2q+1, k+l))$ where the graph $B_n(2p+1; 2q+1, k+l)$ is shown in Figure 3.*

Proof. Firstly, we prove $b_i(G) \leq b_i(H)$, where the graph H is shown in Figure 1. By Theorem 2.3 and Lemma 2.9, we have

$$b_i(G) = b_i(G - v_0v'_1) + b_{i-2}(G - v_0 - v'_1) + 2b_{i-(2p+1)}(G - C_{2p+1})$$

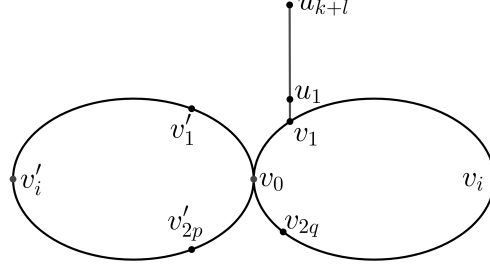


Figure 3: Graph $B_n(2p+1; 2q+1, k+l)$ with $k+l = n - 2p - 2q - 1$.

$$\begin{aligned}
&= b_i(G - v_0v'_1 - v_0v'_{2p}) + b_{i-2}(G - v_0v'_1 - v_0 - v'_{2p}) + b_{i-2}(G - v_0 - v'_1) \\
&+ 2b_{i-(2p+1)}(G - C_{2p+1}) \\
&= b_i((C(2p+1) - T_0) \cup C(2q+1)) \\
&+ b_{i-2}((C(2p+1) - T_0 - T'_{2p}) \cup (C(2q+1) - T_0) \cup F'_{2p} \cup F_0) \\
&+ b_{i-2}((C(2p+1) - T_0 - T'_1) \cup F'_1 \cup F_0 \cup (C(2q+1) - T_0)) \\
&+ 2b_{i-(2p+1)}(F_0 \cup F'_1 \cup \dots \cup F'_{2p} \cup (C(2q+1) - T_0)) \\
&\leq b_i((C(2p+1) - T_0) \cup P_{2q+1+k}^{2q+1}) + b_{i-2}((C(2p+1) - T_0 - T'_{2p}) \cup P_{2q+k} \cup F'_{2p}) \\
&+ b_{i-2}((C(2p+1) - T_0 - T'_1) \cup F'_1 \cup P_{2q+k}) + 2b_{i-(2p+1)}(F'_1 \cup \dots \cup F'_{2p} \cup P_{2q+k}) \\
&= b_i(H - v_0v'_1 - v_0v'_{2p}) + b_{i-2}(H - v_0v'_1 - v_0 - v'_{2p}) + b_{i-2}(H - v_0 - v'_1) \\
&+ 2b_{i-(2p+1)}(H - C_{2p+1}) \\
&= b_i(H - v_0v'_1) + b_{i-2}(H - v_0 - v'_1) + 2b_{i-(2p+1)}(H - C_{2p+1}) \\
&= b_i(H).
\end{aligned}$$

Next, we prove $b_i(H) \leq b_i(H_n(2p+1, l; 2q+1, k))$, where the graph $H_n(2p+1, l; 2q+1, k)$ is shown in Figure 2. Similarly, by Theorem 2.3 and Lemma 2.9, we get

$$\begin{aligned}
b_i(H) &= b_i(H - v_0v_1) + b_{i-2}(H - v_0 - v_1) + 2b_{i-(2q+1)}(H - C_{2q+1}) \\
&= b_i(H - v_0v_1 - v_0v_{2q}) + b_{i-2}(H - v_0v_1 - v_0 - v_{2q}) + b_{i-2}(H - v_0 - v_1) \\
&+ 2b_{i-(2q+1)}(H - C_{2q+1}) \\
&= b_i(P_{2q+k} \cup (C(2p+1) - F_0)) + b_{i-2}((C(2p+1) - T_0) \cup P_{2q+k-1}) \\
&+ b_{i-2}((C(2p+1) - T_0) \cup P_k \cup P_{2q-1}) + 2b_{i-(2q+1)}((C(2p+1) - T_0) \cup P_k) \\
&\leq b_i(P_{2p+l+1}^{2p+1} \cup P_{2q+k}) + b_{i-2}(P_{2p+l} \cup P_{2q+k-1}) \\
&+ b_{i-2}(P_{2p+l} \cup P_k \cup P_{2q-1}) + 2b_{i-(2q+1)}(P_{2p+l} \cup P_k) \\
&= b_i(H_n(2p+1, l; 2q+1, k) - v_0v_1 - v_0v_{2q}) \\
&+ b_{i-2}(H_n(2p+1, l; 2q+1, k) - v_0v_1 - v_0 - v_{2q})
\end{aligned}$$

$$\begin{aligned}
& + b_{i-2}(H_n(2p+1, l; 2q+1, k) - v_0 - v_1) + 2b_{i-(2q+1)}(H_n(2p+1, l; 2q+1, k) - C_{2q+1}) \\
& = b_i(H_n(2p+1, l; 2q+1, k) - v_0v_1) + b_{i-2}(H_n(2p+1, l; 2q+1, k) - v_0 - v_1) \\
& + 2b_{i-(2q+1)}(H_n(2p+1, l; 2q+1, k) - C_{2q+1}) \\
& = b_i(H_n(2p+1, l; 2q+1, k)).
\end{aligned}$$

Finally, by Theorem 2.2 and Lemma 2.9, we obtain

$$\begin{aligned}
& b_i(H_n(2p+1, l; 2q+1, k)) \\
& = b_i(H_n(2p+1, l; 2q+1, k) - v'_1u'_1) + b_{i-2}(H_n(2p+1, l; 2q+1, k) - v'_1 - u'_1) \\
& = b_i(B_{n-l}(2p+1; 2q+1, k) \cup P_l) + b_{i-2}((B_{n-l}(2p+1; 2q+1, k) - v'_1) \cup P_{l-1}) \\
& = b_i(B_{n-l}(2p+1; 2q+1, k) \cup P_l) + b_{i-2}(P_{2p+2q+k} \cup P_{l-1}) \\
& + b_{i-4}(P_{2p-1} \cup P_k \cup P_{2q-1} \cup P_{l-1}) + 2b_{i-(2q+3)}(P_{2p-1} \cup P_k \cup P_{l-1}) \\
& \leq b_i(B_{n-l}(2p+1; 2q+1, k) \cup P_l) + b_{i-2}((B_{n-l-1}(2p+1; 2q+1, k-1) - v_0v'_1) \cup P_{l-1}) \\
& + b_{i-4}(P_{2p-1} \cup P_{2q+k-1} \cup P_{l-1}) + 2b_{i-(2p+3)}(P_{2q+k-1} \cup P_{l-1}) \\
& = b_i(B_n(2p+1; 2q+1, k+l) - u_ku_{k+1}) + b_{i-2}(B_n(2p+1; 2q+1, k+l) - u_k - u_{k+1}) \\
& = b_i(B_n(2p+1; 2q+1, k+l)).
\end{aligned}$$

In the above result, if $k = 0$, we assume that $u_k = v_1$ and $B_{n-l-1}(2p+1; 2q+1, k-1) = P_{n-l-1}^{2p+1}$. Then we have $b_i(G) \leq b_i(B_n(2p+1; 2q+1, k+l))$. By Lemma 2.8, we can get $\mathcal{E}(G) \leq \mathcal{E}(B_n(2p+1; 2q+1, k+l))$, the result holds. \square

3 Proof of Proposition 1.3

In order to prove Proposition 1.3, we divide into four cases based on the difference in length between the two odd cycles. First we prove the result about graphs in $\mathcal{D}_n^{2p+1, 2q+1}$ where $|q-p| \geq 3$.

Lemma 3.1 *Let $G \in \mathcal{D}_n^{2p+1, 2q+1}$ where $|q-p| \geq 3$ and $p, q \geq 1$. Then we have $\mathcal{E}(G) < \mathcal{E}(P_n^{6,6})$ for $n = 12, 14$ and $n \geq 16$.*

Proof. Without loss of generality, we suppose that $q-p \geq 3$. Then $q \geq 4$. Let $|C(2p+1)| = t \geq 2p+1$, we have $n-t \geq 2q \geq 8$.

When i is odd, choose edge v_0v_1 of cycle C_{2q+1} , according to the definition of $b_i(G)$ we get

$$\begin{aligned}
b_i(G) & = |a_i(G - v_0v_1) - a_{i-2}(G - v_0 - v_1) - 2a_{i-(2q+1)}(G - C_{2q+1})| \\
& \leq b_i(G - v_0v_1) + 2b_{i-(2q+1)}(G - C_{2q+1})
\end{aligned}$$

$$\leq b_i(P_n^{2p+1}) + 2b_{i-(2q+1)}(P_{n-(2q+1)}).$$

Since $q - p \geq 3$, $2q - 2p - 6 \geq 0$, it follows that $b_{i-(2q+1)}(P_{n-(2q+1)}) \leq b_{i-(2p+7)}(P_{n-(2q+1)} \cup P_{2q-2p-6}) \leq b_{i-(2p+7)}(P_{n-(2p+7)})$. Thus

$$\begin{aligned} b_i(G) &\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+7)}(P_{n-(2p+7)}) \\ &= b_i(P_n^{2p+1}) + b_{i-6}(P_{n-6}^{2p+1}) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_4 \cup P_{n-6}^{2p+1}) + 2b_{i-6}(P_{n-6}^{2p+1}) \\ &= b_i(P_n^{2p+1,6}). \end{aligned}$$

When i is even, we consider the following two cases.

Case 1. $t \geq 4$.

Pick edge v_0v_1 of cycle C_{2q+1} , we have

$$\begin{aligned} b_i(G) &= |a_i(G - v_0v_1) - a_{i-2}(G - v_0 - v_1) - 2a_{i-(2q+1)}(G - C_{2q+1})| \\ &\leq b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{t-1} \cup P_{n-t-1}) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_4 \cup P_{n-6}) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_4 \cup P_{n-6}^{2p+1}) + 2b_{i-6}(P_{n-6}^{2p+1}) \\ &= b_i(P_n^{2p+1,6}). \end{aligned}$$

By Inequality (3) and Theorems 2.4 and 2.5, we get $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,6}) < \mathcal{E}(P_n^{6,6})$.

Case 2. $t=3$, then we have $p = 1$. Hence, $q \geq 4$.

Choose edge $v_0v'_1$ of cycle C_{2p+1} , we obtain

$$\begin{aligned} b_i(G) &\leq b_i(G - v_0v'_1) + b_{i-2}(G - v_0 - v'_1) \\ &\leq b_i(P_n^{2q+1}) + b_{i-2}(P_1 \cup P_{n-3}) \\ &= b_i(P_n) + b_{i-2}(P_{2q-1} \cup P_{n-(2q+1)}) + b_{i-2}(P_1 \cup P_{n-3}). \end{aligned}$$

Note that $n - (2q + 1) \geq 2$. If $n - (2q + 1) \geq 3$, then by Theorem 2.2, we have $b_{i-2}(P_{2q-1} \cup P_{n-(2q+1)}) \leq b_{i-2}(P_4 \cup P_{n-6})$. Hence,

$$\begin{aligned} b_i(G) &\leq b_i(P_n) + b_{i-2}(P_4 \cup P_{n-6}) + b_{i-2}(P_1 \cup P_{n-3}) \\ &\leq b_i(P_n^6) + b_{i-2}(P_1 \cup P_{n-3}^6) \\ &= b_i(P_n^{3,6}). \end{aligned}$$

When $n - (2q + 1) = 2$, it follows that

$$b_i(G) \leq b_i(P_n) + b_{i-2}(P_2 \cup P_{n-4}) + b_{i-2}(P_1 \cup P_{n-3})$$

$$\begin{aligned}
&= b_i(P_n) + b_{i-2}(P_2 \cup P_{n-6} \cup P_2) + b_{i-4}(P_2 \cup P_{n-7} \cup P_1) + b_{i-2}(P_1 \cup P_{n-3}) \\
&= b_i(P_n) + b_{i-2}(P_2 \cup P_{n-6} \cup P_2) + b_{i-4}(P_1 \cup P_1 \cup P_{n-7} \cup P_1) \\
&\quad + b_{i-6}(P_{n-7} \cup P_1) + b_{i-2}(P_1 \cup P_{n-3}) \\
&\leq b_i(P_n) + b_{i-2}(P_2 \cup P_{n-6} \cup P_2) + b_{i-4}(P_1 \cup P_{n-6} \cup P_1) + b_{i-6}(P_{n-6}) + b_{i-2}(P_1 \cup P_{n-3}) \\
&\leq b_i(P_n) + b_{i-2}(P_4 \cup P_{n-6}) + b_{i-6}(P_{n-6}) + b_{i-2}(P_1 \cup P_{n-3}) \\
&\leq b_i(P_n^6) + b_{i-2}(P_1 \cup P_{n-3}^6) \\
&= b_i(P_n^{3,6}).
\end{aligned}$$

By Inequality (3) and Theorems 2.4 and 2.5, we have $\mathcal{E}(G) \leq \mathcal{E}(P_n^{3,6}) < \mathcal{E}(P_n^{6,6})$ for $n = 12, 14$ and $n \geq 16$. So we complete the proof. \square

In the following, we will discuss graphs in $\mathcal{D}_n^{2p+1, 2q+1}$ where $|q - p| < 3$ one by one. For the graphs in $\mathcal{D}_n^{2p+1, 2p+5}$ and $\mathcal{D}_n^{2p+1, 2p+1}$, they satisfy the condition of Lemma 2.11, so we first consider these graphs.

Lemma 3.2 *Let $G \in \mathcal{D}_n^{2p+1, 2p+5}$ where $p \geq 1$. We have $\mathcal{E}(G) < \mathcal{E}(P_n^{6,6})$ for $n = 12, 14$ and $n \geq 16$.*

Proof. By Lemma 2.11, we just prove that $\mathcal{E}(B_n(2p+1; 2p+5, n - (4p+5))) < \mathcal{E}(P_n^{6,6})$.

Case 1. $p \geq 2$.

Subcase 1.1. $n - (4p+5) \geq 3$ or $n = 4p+6$.

When i is odd, by Lemmas 2.7 and 2.9, we get

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + 2b_{i-(2p+5)}(G - C_{2p+5}) \\
&= b_i(P_n^{2p+1}) + 2b_{i-(2p+5)}(P_{2p} \cup P_{n-(4p+5)}) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+5)}(P_{n-2p-9} \cup P_4) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_{n-2p-7} \cup P_4) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{n-6}^{2p+1} \cup P_4) \\
&\leq b_i(P_n^{2p+1,6}).
\end{aligned}$$

For $n - (4p+5) \geq 3$, if $2p = 4$, it follows that $P_{2p} \cup P_{n-(4p+5)} = P_{n-2p-9} \cup P_4$. When $2p \geq 6$, if $2p \leq n - (4p+5)$, then $n - 2p - 9 = n - (4p+5) + 2p - 4 \geq 8$, so $P_{2p} \cup P_{n-(4p+5)} \preceq P_4 \cup P_{n-2p-9}$ by Theorem 2.2. If $2p > n - (4p+5)$, then $n - 2p - 9 = n - (4p+5) + 2p - 4 \geq 3 + 6 - 4 \geq 5$ and $P_{2p} \cup P_{n-(4p+5)} \preceq P_4 \cup P_{n-2p-9}$.

For $n = 4p+6$, $P_{2p} \cup P_{n-(4p+5)} = P_{2p} \cup P_1 \preceq P_{2p-3} \cup P_4 = P_{n-2p-9} \cup P_4$.

Thus, the first inequality above holds.

When i is even, we have

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{2p} \cup P_{2p+3} \cup P_{n-(4p+5)}) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{n-6}^{2p+1} \cup P_4) \\
&\leq b_i(P_n^{2p+1,6}).
\end{aligned}$$

Thus by Equation (2) and Theorems 2.4 and 2.5, $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,6}) < \mathcal{E}(P_n^{6,6})$ for $n = 12, 14$ and $n \geq 16$.

Subcase 1.2. $n = 4p + 7$.

When i is odd, we can find

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + 2b_{i-(2p+5)}(G - C_{2p+5}) \\
&= b_i(P_n^{2p+1}) + 2b_{i-(2p+5)}(P_{2p} \cup P_2) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_{2p} \cup P_2 \cup P_2) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_{2p} \cup P_4) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{4p+1}^{2p+1} \cup P_4) \\
&\leq b_i(P_n^{2p+1,6}).
\end{aligned}$$

When i is even, we have

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{2p} \cup P_{2p+3} \cup P_2) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+2} \cup P_{2p+3}) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{4p+1}^{2p+1} \cup P_4) \\
&\leq b_i(P_n^{2p+1,6}).
\end{aligned}$$

Thus $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,6}) < \mathcal{E}(P_n^{6,6})$.

Subcase 1.3. $n = 4p + 5$.

When i is odd, we have

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + 2b_{i-(2p+5)}(G - C_{2p+5}) \\
&= b_i(P_n^{2p+1}) + 2b_{i-(2p+5)}(P_{2p}) \\
&\leq b_i(P_n^{2p-1}) + 2b_{i-(2p+5)}(P_{2p}) \\
&\leq b_i(P_n^{2p-1}) + 2b_{i-(2p+1)}(P_{2p} \cup P_4) + 4b_{i-(2p+5)}(P_{2p}) \\
&= b_i(P_n^{2p-1}) + b_{i-2}(P_{4p-1}^{2p-1} \cup P_4) + 2b_{i-6}(P_{4p-1}^{2p-1})
\end{aligned}$$

$$= b_i(P_n^{2p-1,6}).$$

When i is even, we obtain

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{2p} \cup P_{2p+3}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-1} \cup P_{2p+4}) + b_{i-2}(P_{2p} \cup P_{2p+3}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+4}) + b_{i-4}(P_{2p-4} \cup P_1 \cup P_{2p+4}) + b_{i-2}(P_{2p} \cup P_{2p+3}) \\
&\leq b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+4}) + b_{i-4}(P_4 \cup P_{4p-3}) + b_{i-2}(P_4 \cup P_{4p-1}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+4}) + b_{i-4}(P_4 \cup P_{2p-3} \cup P_{2p}) \\
&\quad + b_{i-6}(P_4 \cup P_{2p-4} \cup P_{2p-1}) + b_{i-2}(P_4 \cup P_{4p-1}) \\
&\leq b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_{2p+6}) + b_{i-4}(P_4 \cup P_{2p-3} \cup P_{2p}) + b_{i-6}(P_{4p-1}) + b_{i-2}(P_4 \cup P_{4p-1}) \\
&\leq b_i(P_n^{2p-1}) + b_{i-2}(P_{4p-1}^{2p-1} \cup P_4) + 2b_{i-6}(P_{4p-1}^{2p-1}) \\
&= b_i(P_n^{2p-1,6}).
\end{aligned}$$

Thus $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p-1,6}) < \mathcal{E}(P_n^{6,6})$.

Case 2. $p = 1$, that is, $G \cong B_n(3; 7, n - 9)$.

When i is odd, we get

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + 2b_{i-(2p+5)}(G - C_{2p+5}) \\
&= b_i(P_n^3) + 2b_{i-7}(P_2 \cup P_{n-9}) \\
&\leq b_i(P_n^3) + 2b_{i-5}(P_4 \cup P_{n-9}) \\
&= b_i(P_n^3) + b_{i-2}(P_{n-6}^3 \cup P_4) \\
&\leq b_i(P_n^{3,6}).
\end{aligned}$$

When i is even, we have

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v'_1) + b_{i-2}(G - v_0 - v'_1) \\
&\leq b_i(P_n) + b_{i-2}(P_2 \cup P_5 \cup P_{n-9}) + b_{i-2}(P_1 \cup P_{n-3}) \\
&\leq b_i(P_n) + b_{i-2}(P_4 \cup P_{n-6}) + b_{i-2}(P_1 \cup P_{n-3}) \\
&\leq b_i(P_n^6) + b_{i-2}(P_{n-3}^6 \cup P_1) \\
&\leq b_i(P_n^{3,6}).
\end{aligned}$$

Thus $\mathcal{E}(G) \leq \mathcal{E}(P_n^{3,6}) < \mathcal{E}(P_n^{6,6})$. Hence we complete the proof. \square

Lemma 3.3 *Let $G \in \mathcal{D}_n^{2p+1, 2p+1}$ where $p \geq 2$. Then $\mathcal{E}(G) < \mathcal{E}(P_n^{6,6})$ for $n = 12, 14$ and $n \geq 16$.*

Proof. By Lemma 2.11, we have $\mathcal{E}(G) \leq \mathcal{E}(B_n(2p+1; 2p+1, n - (4p+1)))$. Next, we prove that $\mathcal{E}(B_n(2p+1; 2p+1, n - (4p+1))) < \mathcal{E}(P_n^{6,6})$. Let $l = n - (4p+1)$.

When i is odd, we divide into three cases.

Case 1. $l = 1$ or $l \geq 3$.

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + 2b_{i-(2p+1)}(G - C_{2p+1}) \\
&= b_i(P_n^{2p+1}) + 2b_{i-(2p+1)}(P_{2p} \cup P_l) \\
&\leq b_i(P_n^{2p-1}) + 2b_{i-(2p+1)}(P_{2p+l-4} \cup P_4) \\
&= b_i(P_n^{2p-1}) + b_{i-2}(P_{4p+l-5}^{2p-1} \cup P_4) \\
&= b_i(P_n^{2p-1}) + b_{i-2}(P_{n-6}^{2p-1} \cup P_4) \\
&\leq b_i(P_n^{2p-1,6}).
\end{aligned}$$

If $l = 1$, it is obvious that $b_{i-(2p+1)}(P_{2p} \cup P_l) \leq b_{i-(2p+1)}(P_{2p+l-4} \cup P_4)$.

For $l \geq 3$. If $2p + l - 4 < 4$, then $2p + l < 8$. Since $2p \geq 4$ and $l \geq 3$, it follows that $2p + l \geq 7$. So $2p + l = 7$, that is, $p = 2$ and $l = 3$. Thus $b_{i-(2p+1)}(P_{2p} \cup P_l) = b_{i-(2p+1)}(P_4 \cup P_3) = b_{i-(2p+1)}(P_{2p+l-4} \cup P_4)$. If $2p + l - 4 \geq 4$, Since $2p \geq 4$ and $l \geq 3$, it is easy to get that $b_{i-(2p+1)}(P_{2p} \cup P_l) \leq b_{i-(2p+1)}(P_{2p+l-4} \cup P_4)$. Hence, the first inequality above holds.

Case 2. $l = 2$.

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + 2b_{i-(2p+1)}(G - C_{2p+1}) \\
&= b_i(P_n^{2p+1}) + 2b_{i-(2p+1)}(P_{2p} \cup P_2) \\
&= 2b_{i-(2p+1)}(P_{2p+2}) + 2b_{i-(2p+1)}(P_{2p-2} \cup P_2 \cup P_2) + 2b_{i-(2p+3)}(P_{2p-3} \cup P_1 \cup P_2) \\
&\leq 2b_{i-(2p+1)}(P_{2p+2}) + 2b_{i-(2p+1)}(P_{2p-2} \cup P_4) + 2b_{i-(2p-1)}(P_{2p+3} \cup P_1) \\
&= 2b_{i-(2p-1)}(P_{2p+4}) + 2b_{i-(2p+1)}(P_{2p-2} \cup P_4) \\
&= b_i(P_{4p+3}^{2p-1}) + b_{i-2}(P_{4p-3}^{2p-1} \cup P_4) \\
&\leq b_i(P_n^{2p-1,6}).
\end{aligned}$$

Case 3. $l = 0$.

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + 2b_{i-(2p+1)}(G - C_{2p+1}) \\
&= b_i(P_n^{2p+1}) + 2b_{i-(2p+1)}(P_{2p}) \\
&= 2b_{i-(2p+1)}(P_{2p}) + 2b_{i-(2p+1)}(P_{2p-4} \cup P_4) + 2b_{i-(2p+3)}(P_{2p-5} \cup P_3) \\
&= 2b_{i-(2p+1)}(P_{2p}) + 2b_{i-(2p+1)}(P_{2p-4} \cup P_4) + 2b_{i-(2p+3)}(P_{2p-5} \cup P_2 \cup P_1) \\
&\quad + 2b_{i-(2p+5)}(P_{2p-5} \cup P_1) \\
&\leq 2b_{i-(2p+1)}(P_{2p}) + 2b_{i-(2p+1)}(P_{2p-4} \cup P_4) + 2b_{i-(2p-1)}(P_{2p+1} \cup P_1) + 2b_{i-(2p+5)}(P_{2p-4})
\end{aligned}$$

$$\begin{aligned}
&= 2b_{i-(2p-1)}(P_{2p+2}) + 2b_{i-(2p+1)}(P_{2p-4} \cup P_4) + 2b_{i-(2p+5)}(P_{2p-4}) \\
&= b_i(P_{4p+1}^{2p-1}) + b_{i-2}(P_{4p-5}^{2p-1} \cup P_4) + b_{i-6}(P_{4p-5}^{2p-1}) \\
&\leq b_i(P_n^{2p-1,6}).
\end{aligned}$$

When i is even, we get

$$\begin{aligned}
b_i(G) &= b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{2p} \cup P_l \cup P_{2p-1}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-1} \cup P_{2p+l}) + b_{i-2}(P_{2p} \cup P_l \cup P_{2p-1}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+l}) + b_{i-4}(P_{2p-4} \cup P_1 \cup P_{2p+l}) + b_{i-2}(P_{2p} \cup P_l \cup P_{2p-1}) \\
&\leq b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+l}) + b_{i-4}(P_1 \cup P_{4p+l-4}) + b_{i-2}(P_4 \cup P_{4p+l-5}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+l}) + b_{i-4}(P_1 \cup P_{2p-3} \cup P_{2p+l-1}) \\
&\quad + b_{i-6}(P_1 \cup P_{2p-4} \cup P_{2p+l-2}) + b_{i-2}(P_4 \cup P_{4p+l-5}) \\
&\leq b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_{2p+l+2}) + b_{i-6}(P_{4p+l-5}) + b_{i-2}(P_4 \cup P_{4p+l-5}) \\
&\leq b_i(P_n^{2p-1}) + b_{i-2}(P_{4p+l-5}^{2p-1} \cup P_4) + 2b_{i-6}(P_{4p+l-5}^{2p-1}) \\
&= b_i(P_n^{2p-1,6}).
\end{aligned}$$

Thus $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p-1,6}) < \mathcal{E}(P_n^{6,6})$. \square

For graphs in $\mathcal{D}_n^{2p+1,2p+3}$, they do not satisfy Lemma 2.11. Here we use Inequality (3) and prove directly by Theorems 2.2–2.5 and Lemma 2.7.

Lemma 3.4 *Let $G \in \mathcal{D}_n^{2p+1,2p+3}$ where $p \geq 1$. Then $\mathcal{E}(G) < \mathcal{E}(P_n^{6,6})$ for $n = 12, 14$ and $n \geq 16$.*

Proof. Suppose that $|C(2p+1) - F_0| = 2p+1+l$ and $|C(2p+3)| = 2p+3+k$, then $n = 4p+3+k+l$.

Case 1. $2p+l \geq 3$ and $k = 1$ or $k \geq 3$.

When i is odd, we get

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-(2p+3)}(G - C_{2p+3}) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_k \cup P_{2p+l}) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_4 \cup P_{2p+k+l-4}) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{n-6}^{2p+1} \cup P_4) \\
&\leq b_i(P_n^{2p+1,6}).
\end{aligned}$$

If $3 \leq 2p+l < k$, then $2p+k+l-4 \geq 2p+l \geq 3$. It is obvious that $P_k \cup P_{2p+l} \preceq P_4 \cup P_{2p+k+l-4}$.

For $2p + l \geq k$. Note that $2p + l \geq 3$. If $k = 1$, then $P_k \cup P_{2p+l} = P_1 \cup P_{2p+l} \preceq P_4 \cup P_{2p+l-3} = P_4 \cup P_{2p+k+l-4}$. If $k = 3$, it follows that $2p + k + l - 4 = 2p + l - 1 \geq 2$. Then $P_k \cup P_{2p+l} \preceq P_4 \cup P_{2p+k+l-4}$. If $k \geq 4$, then $2p + k + l - 4 \geq 2p + l \geq k \geq 4$. So $P_k \cup P_{2p+l} \preceq P_4 \cup P_{2p+k+l-4}$.

Therefore, the third inequality above holds.

When i is even, we have

$$\begin{aligned} b_i(G) &\leq b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+l} \cup P_{2p+k+1}) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{n-6}^{2p+1} \cup P_4) \\ &\leq b_i(P_n^{2p+1,6}). \end{aligned}$$

By Inequality (3) and Theorems 2.4 and 2.5, we get $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,6}) < \mathcal{E}(P_n^{6,6})$.

Case 2. $2p + l \geq 3$ and $k = 2$.

Since $n = 4p + 3 + k + l \geq 12$, we have $2p + l \geq 4$. Otherwise $p = 1$ and $l = 1$, thus $n = 10$.

Subcase 2.1. $l \geq 1$.

When i is odd, we have

$$\begin{aligned} b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-(2p+3)}(G - C_{2p+3}) \\ &\leq 2b_{i-(2p+1)}(P_l \cup P_{2p+4}) + 2b_{i-(2p+3)}(P_{2p+l} \cup P_2) \\ &= 2b_{i-(2p+1)}(P_l \cup P_{2p+4}) + 2b_{i-(2p+3)}(P_{2p+l-1} \cup P_1 \cup P_2) + 2b_{i-(2p+5)}(P_{2p+l-2} \cup P_2) \\ &\leq 2b_{i-(2p+1)}(P_l \cup P_{2p+4}) + 2b_{i-(2p+3)}(P_{l-1} \cup P_{2p+3}) + 2b_{i-(2p+5)}(P_{2p+l-2} \cup P_2) \\ &\leq 2b_{i-(2p+1)}(P_l \cup P_{2p+4}) + 2b_{i-(2p+3)}(P_{l-1} \cup P_{2p+3}) \\ &\quad + 2b_{i-(2p+3)}(P_{2p+l-2} \cup P_1 \cup P_3) + 2b_{i-(2p+5)}(P_{2p+l-2} \cup P_2) \\ &= 2b_{i-(2p+1)}(P_{2p+l+4}) + 2b_{i-(2p+3)}(P_{2p+l-2} \cup P_4) \\ &= b_i(P_n^{2p+1}) + b_{i-2}(P_{n-6}^{2p+1} \cup P_4) \\ &\leq b_i(P_n^{2p+1,6}). \end{aligned}$$

When i is even, we get

$$\begin{aligned} b_i(G) &\leq b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+l} \cup P_{2p+3}) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{n-6}^{2p+1} \cup P_4) \\ &\leq b_i(P_n^{2p+1,6}). \end{aligned}$$

Thus $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,6}) < \mathcal{E}(P_n^{6,6})$.

Subcase 2.2. $l = 0$, that is, $n = 4p + 5$.

If p is odd, we prove that $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,2p+4}) < \mathcal{E}(P_n^{6,6})$.

When i is odd, we get

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-(2p+3)}(G - C_{2p+3}) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_2 \cup P_{2p}) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_{2p+2}) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(C_{2p+1} \cup P_{2p+2}) \\
&\leq b_i(P_n^{2p+1,2p+4}).
\end{aligned}$$

When i is even, we have

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v'_1) + b_{i-2}(G - v_0 - v'_1) \\
&= b_i(G - v_0v'_1 - v_0v'_{2p}) + b_{i-2}(G - v_0v'_1 - v_0 - v'_{2p}) + b_{i-2}(G - v_0 - v'_1) \\
&\leq b_i(P_{2p} \cup P_{2p+5}^{2p+3}) + b_{i-2}(P_{2p-1} \cup P_{2p+4}) + b_{i-2}(P_{2p-1} \cup P_{2p+4}) \\
&= b_i(P_{2p} \cup P_{2p+5}) + b_{i-2}(P_{2p} \cup P_{2p+1} \cup P_2) + b_{i-2}(P_{2p-1} \cup P_{2p+4}) + b_{i-2}(P_{2p-1} \cup P_{2p+4}) \\
&= b_i(P_{4p+5}) + b_{i-2}(P_{2p} \cup P_{2p+1} \cup P_2) + b_{i-2}(P_{2p-1} \cup P_{2p+4}) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(C_{2p+1} \cup P_{2p+2}) \\
&\leq b_i(P_n^{2p+1,2p+4}),
\end{aligned}$$

as desired.

If p is even, we prove that $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,2p+2}) < \mathcal{E}(P_n^{6,6})$.

When i is odd, we get

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-(2p+3)}(G - C_{2p+3}) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_2 \cup P_{2p}) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+3}^{2p+1} \cup P_{2p}) \\
&\leq b_i(P_n^{2p+1,2p+2}).
\end{aligned}$$

When i is even, it is analogous to that p is odd,

$$\begin{aligned}
b_i(G) &\leq b_i(P_{4p+5}) + b_{i-2}(P_{2p} \cup P_{2p+1} \cup P_2) + b_{i-2}(P_{2p-1} \cup P_{2p+4}) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+3}^{2p+1} \cup P_{2p}) \\
&\leq b_i(P_n^{2p+1,2p+2}),
\end{aligned}$$

as claimed.

Case 3. $2p + l \geq 3$ and $k = 0$.

Since $n = 4p + 3 + k + l \geq 12$, it follows that $2p + l \geq 5$.

Subcase 3.1. $l = 1$ or $l \geq 3$.

When i is odd, we have

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-(2p+3)}(G - C_{2p+3}) \\
&\leq 2b_{i-(2p+1)}(P_l \cup P_{2p+2}) + 2b_{i-(2p+3)}(P_{2p+l}) \\
&= 2b_{i-(2p+1)}(P_l \cup P_{2p+2}) + 2b_{i-(2p+3)}(P_{2p+l-3} \cup P_3) + 2b_{i-(2p+5)}(P_{2p+l-4} \cup P_2) \\
&\leq 2b_{i-(2p+1)}(P_l \cup P_{2p+2}) + 2b_{i-(2p+3)}(P_{l-1} \cup P_{2p+1}) \\
&\quad + 2b_{i-(2p+5)}(P_{2p+l-4} \cup P_2) + 2b_{i-(2p+3)}(P_{2p+l-4} \cup P_3 \cup P_1) \\
&= 2b_{i-(2p+1)}(P_{2p+l+2}) + 2b_{i-(2p+3)}(P_{2p+l-4} \cup P_4) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(P_{n-6}^{2p+1} \cup P_4) \\
&\leq b_i(P_n^{2p+1,6}).
\end{aligned}$$

When i is even, we get

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+l} \cup P_{2p+1}) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{4p+l-3} \cup P_4) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{n-6}^{2p+1} \cup P_4) \\
&\leq b_i(P_n^{2p+1,6}).
\end{aligned}$$

Thus $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,6}) < \mathcal{E}(P_n^{6,6})$.

Subcase 3.2. $l = 2$, that is, $n = 4p + 5$.

If p is odd, we prove that $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,2p+4}) < \mathcal{E}(P_n^{6,6})$.

When i is odd, we get

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-(2p+3)}(G - C_{2p+3}) \\
&\leq b_i(P_n^{2p+1}) + 2b_{i-(2p+3)}(P_{2p+2}) \\
&= b_i(P_n^{2p+1}) + b_{i-2}(C_{2p+1} \cup P_{2p+2}) \\
&\leq b_i(P_n^{2p+1,2p+4}).
\end{aligned}$$

When i is even, we have

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\
&\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+1} \cup P_{2p+2})
\end{aligned}$$

$$\leq b_i(P_n^{2p+1,2p+4}),$$

as desired.

If p is even, we prove that $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p+1,2p+2}) < \mathcal{E}(P_n^{6,6})$.

When i is odd, we get

$$\begin{aligned} b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-(2p+3)}(G - C_{2p+3}) \\ &\leq 2b_{i-(2p+1)}(P_2 \cup P_{2p+2}) + 2b_{i-(2p+3)}(P_{2p+2}) \\ &= 2b_{i-(2p+1)}(P_2 \cup P_{2p+2}) + 2b_{i-(2p+3)}(P_{2p} \cup P_2) + 2b_{i-(2p+5)}(P_{2p-1} \cup P_1) \\ &\leq 2b_{i-(2p+1)}(P_2 \cup P_{2p+2}) + 2b_{i-(2p+3)}(P_{2p} \cup P_2) + 2b_{i-(2p+3)}(P_{2p+1} \cup P_1) \\ &= 2b_{i-(2p+1)}(P_{2p+4}) + 2b_{i-(2p+3)}(P_{2p} \cup P_2) \\ &= b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+3}^{2p+1} \cup P_{2p}) \\ &\leq b_i(P_n^{2p+1,2p+2}). \end{aligned}$$

When i is even, we have

$$\begin{aligned} b_i(G) &\leq b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+1} \cup P_{2p+2}) \\ &\leq b_i(P_n^{2p+1}) + b_{i-2}(P_{2p+3}^{2p+1} \cup P_{2p}) \\ &\leq b_i(P_n^{2p+1,2p+2}), \end{aligned}$$

as required.

Subcase 3.3. $l = 0$, that is, $n = 4p + 3$. Thus $p \geq 3$.

When i is odd, we have

$$\begin{aligned} b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-(2p+3)}(G - C_{2p+3}) \\ &= 2b_{i-(2p+1)}(P_{2p+2}) + 2b_{i-(2p+3)}(P_{2p}) \\ &= 2b_{i-(2p+1)}(P_{2p+2}) + 2b_{i-(2p+3)}(P_{2p-1} \cup P_1) + 2b_{i-(2p+5)}(P_{2p-2}) \\ &\leq 2b_{i-(2p-1)}(P_{2p+4}) + 2b_{i-(2p+3)}(P_2 \cup P_{2p-2}) + 2b_{i-(2p+5)}(P_{2p-2}) \\ &\leq 2b_{i-(2p-1)}(P_{2p+4}) + 2b_{i-(2p+1)}(P_{2p-2} \cup P_4) + 2b_{i-(2p+5)}(P_{2p-2}) \\ &= b_i(P_{4p+3}^{2p-1}) + b_{i-2}(P_{4p-3}^{2p-1} \cup P_4) + b_{i-6}(P_{4p-3}^{2p-1}) \\ &\leq b_i(P_n^{2p-1,6}). \end{aligned}$$

When i is even, we get

$$\begin{aligned} b_i(G) &\leq b_i(G - v_0v_1) + b_{i-2}(G - v_0 - v_1) \\ &= b_i(P_n^{2p+1}) + b_{i-2}(P_{2p} \cup P_{2p+1}) \end{aligned}$$

$$\begin{aligned}
&= b_i(P_n) + b_{i-2}(P_{2p-1} \cup P_{2p+2}) + b_{i-2}(P_{2p} \cup P_{2p+1}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+2}) + b_{i-4}(P_{2p-4} \cup P_1 \cup P_{2p+2}) \\
&\quad + b_{i-2}(P_{2p} \cup P_{2p-3} \cup P_4) + b_{i-4}(P_{2p} \cup P_{2p-4} \cup P_3) \\
&\leq b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+2}) + b_{i-4}(P_{2p-4} \cup P_4 \cup P_{2p-1}) \\
&\quad + b_{i-2}(P_{2p} \cup P_{2p-3} \cup P_4) + b_{i-4}(P_{2p-3} \cup P_{2p+2}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_2 \cup P_{2p+2}) + b_{i-4}(P_{2p-4} \cup P_4 \cup P_{2p-1}) \\
&\quad + b_{i-2}(P_{2p} \cup P_{2p-3} \cup P_4) + b_{i-4}(P_{2p-3} \cup P_{2p+1} \cup P_1) + b_{i-6}(P_{2p-3} \cup P_{2p}) \\
&= b_i(P_n) + b_{i-2}(P_{2p-3} \cup P_{2p+4}) + b_{i-2}(P_{4p-3} \cup P_4) + b_{i-6}(P_{2p-3} \cup P_{2p}) \\
&\leq b_i(P_n^{2p-1}) + b_{i-2}(P_{4p-3}^{2p-1} \cup P_4) + 2b_{i-6}(P_{4p-3}^{2p-1}) \\
&= b_i(P_n^{2p-1,6}).
\end{aligned}$$

Thus $\mathcal{E}(G) \leq \mathcal{E}(P_n^{2p-1,6}) < \mathcal{E}(P_n^{6,6})$.

Case 4. $2p + l = 2$, that is, $p = 1$ and $l = 0$.

When i is odd, we get

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v_1) + 2b_{i-5}(G - C_5) \\
&\leq b_i(P_n^3) + 2b_{i-5}(P_2 \cup P_{n-7}) \\
&= b_i(P_n^3) + 2b_{i-5}(P_2 \cup P_{n-9} \cup P_2) + 2b_{i-7}(P_2 \cup P_{n-10} \cup P_1) \\
&= b_i(P_n^3) + 2b_{i-5}(P_2 \cup P_{n-9} \cup P_2) + 2b_{i-7}(3P_1 \cup P_{n-10}) + 2b_{i-9}(P_1 \cup P_{n-10}) \\
&\leq b_i(P_n^3) + 2b_{i-5}(P_2 \cup P_{n-9} \cup P_2) + 2b_{i-7}(3P_1 \cup P_{n-10}) + 2b_{i-9}(P_{n-9}) \\
&\leq b_i(P_n^3) + 2b_{i-5}(P_2 \cup P_{n-9} \cup P_2) + 2b_{i-7}(2P_1 \cup P_{n-9}) + 4b_{i-9}(P_{n-9}) \\
&= b_i(P_n^3) + 2b_{i-5}(P_4 \cup P_{n-9}) + 4b_{i-9}(P_{n-9}) \\
&= b_i(P_n^3) + b_{i-2}(P_{n-6}^3 \cup P_4) + 2b_{i-6}(P_{n-6}^3) \\
&= b_i(P_n^{3,6}).
\end{aligned}$$

When i is even, we have

$$\begin{aligned}
b_i(G) &\leq b_i(G - v_0v'_1) + b_{i-2}(G - v_0 - v'_1) \\
&\leq b_i(P_n^5) + b_{i-2}(P_1 \cup P_{n-3}) \\
&= b_i(P_n) + b_{i-2}(P_3 \cup P_{n-5}) + b_{i-2}(P_1 \cup P_{n-3}) \\
&\leq b_i(P_n) + b_{i-2}(P_4 \cup P_{n-6}) + b_{i-2}(P_1 \cup P_{n-3}) \\
&\leq b_i(P_n^6) + b_{i-2}(P_1 \cup P_{n-3}^6) \\
&= b_i(P_n^{3,6}).
\end{aligned}$$

Thus $\mathcal{E}(G) \leq \mathcal{E}(P_n^{3,6}) < \mathcal{E}(P_n^{6,6})$. □

Combining Lemmas 3.1–3.4, we can obtain Proposition 1.3.

4 Proof of Proposition 1.4

In this section, we will prove Proposition 1.4. For convenience, we introduce some notations as follows, which will be used in the sequel. Let

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

And

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

It is easy to verify that

$$Y_1(x) + Y_2(x) = x, \quad Y_1(x)Y_2(x) = 1$$

and

$$Z_1(x) + Z_2(x) = x, \quad Z_1(x)Z_2(x) = -1.$$

What is more, $Z_1(x) > 1$ and $-1 < Z_2(x) < 0$ for $x > 0$; $0 < Z_1(x) < 1$ and $Z_2(x) < -1$ for $x < 0$. In the following, we abbreviate $Z_k(x)$ to Z_k for $k = 1, 2$.

We define

$$A_1(x) = \frac{Y_1(x)\phi(B_7(3; 3, 2), x) - \phi(B_6(3; 3, 1), x)}{(Y_1(x))^8 - (Y_1(x))^6}, \quad A_2(x) = \frac{Y_2(x)\phi(B_7(3; 3, 2), x) - \phi(B_6(3; 3, 1), x)}{(Y_2(x))^8 - (Y_2(x))^6},$$

$$B_1(x) = \frac{Y_1(x)\phi(P_{13}^{6,6}, x) - \phi(P_{12}^{6,6}, x)}{(Y_1(x))^{14} - (Y_1(x))^{12}}, \quad B_2(x) = \frac{Y_2(x)\phi(P_{13}^{6,6}, x) - \phi(P_{12}^{6,6}, x)}{(Y_2(x))^{14} - (Y_2(x))^{12}},$$

$$C_1(x) = \frac{Y_1(x)(x^2 - 1) - x}{(Y_1(x))^3 - Y_1(x)}, \quad C_2(x) = \frac{Y_2(x)(x^2 - 1) - x}{(Y_2(x))^3 - Y_2(x)}.$$

By calculations, we have that

$$\phi(P_{13}^{6,6}, x) = x^{13} - 14x^{11} + 74x^9 - 188x^7 + 245x^5 - 158x^3 + 40x$$

and

$$\phi(P_{12}^{6,6}, x) = x^{12} - 13x^{10} + 62x^8 - 138x^6 + 153x^4 - 81x^2 + 16.$$

Then

$$B_1(ix) = \frac{Z_1g_{13} + g_{12}}{Z_1^2 + 1}Z_2^{12}, \quad B_2(ix) = \frac{Z_2g_{13} + g_{12}}{Z_2^2 + 1}Z_1^{12},$$

where

$$g_{13} = x^{13} + 14x^{11} + 74x^9 + 188x^7 + 245x^5 + 158x^3 + 40x$$

and

$$g_{12} = x^{12} + 13x^{10} + 62x^8 + 138x^6 + 153x^4 + 81x^2 + 16.$$

Huo et al. got that $B_1(ix), B_2(ix) > 0$ in [11].

About the characteristic polynomials of P_n and $P_n^{6,6}$, Huo et al. [10, 11, 12] proposed the following Lemma.

Lemma 4.1 For $n \geq 12$ and $x \neq \pm 2$, the characteristic polynomials of P_n and $P_n^{6,6}$ have the following forms:

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

and

$$\phi(P_n^{6,6}, x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n.$$

Similarly, we can get a characteristic polynomial of $B_n(3; 3, n - 5)$.

Lemma 4.2 For $n \geq 6$ and $x \neq \pm 2$, the characteristic polynomial of $B_n(3; 3, n - 5)$ has the following form:

$$\phi(B_n(3; 3, n - 5), x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n.$$

Proof. Note that $\phi(B_n(3; 3, n - 5), x)$ satisfies the recursive formula $f(n, x) = xf(n - 1, x) - f(n - 2, x)$. Therefore, the form of the general solution of the linear homogeneous recursive relation is $f(n, x) = D_1(x)(Y_1(x))^n + D_2(x)(Y_2(x))^n$. By simple calculations, we can obtain that $D_i(x) = A_i(x)$, $i = 1, 2$, from the initial values $\phi(B_7(3; 3, n - 5), x)$ and $\phi(B_6(3; 3, n - 5), x)$. \square

Lemma 4.3 $A_1(ix) = A_{11}(x) + A_{12}(x) \cdot i$ and $A_2(ix) = A_{21}(x) + A_{22}(x) \cdot i$, where

$$A_{11}(x) = \frac{Z_1^5 + xZ_1^2 + x^3 + x}{Z_1^5 + Z_1^3}, \quad A_{12}(x) = -\frac{2Z_1^2 + 2(x^2 + 1)}{Z_1^5 + Z_1^3},$$

$$A_{21}(x) = \frac{Z_2^5 + xZ_2^2 + x^3 + x}{Z_2^5 + Z_2^3}, \quad A_{22}(x) = -\frac{2Z_2^2 + 2(x^2 + 1)}{Z_2^5 + Z_2^3}.$$

Proof. By $\phi(G, x) = \phi(G - uv, x) - \phi(G - u - v, x) - 2 \sum_{C \in \mathcal{E}(uv)} \phi(G - C, x)$, we have

$$\begin{aligned} \phi(B_7(3; 3, 2), x) &= \phi(P_7^3, x) - \phi(2P_2 \cup P_1, x) - 2\phi(2P_2, x) \\ &= \phi(P_7, x) - \phi(P_1 \cup P_4, x) - 2\phi(P_4, x) - \phi(2P_2 \cup P_1, x) - 2\phi(2P_2, x) \\ &= C_1(x)(Y_1(x))^7 + C_2(x)(Y_2(x))^7 - xC_1(x)(Y_1(x))^4 - xC_2(x)(Y_2(x))^4 \\ &\quad - 2C_1(x)(Y_1(x))^4 - 2C_2(x)(Y_2(x))^4 - x(x^2 - 1)^2 - 2(x^2 - 1)^2 \\ &= C_1(x)(Y_1(x))^4((Y_1(x))^3 - x - 2) + C_2(x)(Y_2(x))^4((Y_2(x))^3 - x - 2) \\ &\quad - (x + 2)(x^2 - 1)^2. \end{aligned}$$

Similarly,

$$\phi(B_6(3; 3, 1), x) = C_1(x)(Y_1(x))^3((Y_1(x))^3 - x - 2) + C_2(x)(Y_2(x))^3((Y_2(x))^3 - x - 2)$$

$$-x(x+2)(x^2-1).$$

Then

$$\begin{aligned} A_1(x) &= \frac{C_1(x)((Y_1(x))^3((Y_1(x))^2-1)(Y_1(x))^3-x-2)-(x+2)(x^2-1)((x^2-1)Y_1(x)-x)}{(Y_1(x))^8-(Y_1(x))^6} \\ &= \frac{(Y_1(x)(x^2-1)-x)(Y_1(x))^2((Y_1(x))^3-x-2)-(x+2)(x^2-1)((x^2-1)Y_1(x)-x)}{(Y_1(x))^8-(Y_1(x))^6} \\ &= \frac{(Y_1(x))^2((Y_1(x))^3-x-2)-(x+2)(x^2-1)}{(Y_1(x))^5-(Y_1(x))^3} \\ &= \frac{(Y_1(x))^5-(x+2)(Y_1(x))^2-(x+2)(x^2-1)}{(Y_1(x))^5-(Y_1(x))^3}. \end{aligned}$$

Therefore,

$$\begin{aligned} A_1(ix) &= \frac{iZ_1^5+(ix+2)Z_1^2-(ix+2)(-x^2-1)}{iZ_1^5+iZ_1^3} \\ &= \frac{Z_1^5+(x-2i)Z_1^2+(x-2i)(x^2+1)}{Z_1^5+Z_1^3} \\ &= \frac{Z_1^5+xZ_1^2+x^3+x}{Z_1^5+Z_1^3}-\frac{2Z_1^2+2(x^2+1)}{Z_1^5+Z_1^3}i. \end{aligned}$$

Similarly, the required expression of $A_2(ix)$ can be obtained by the analogous method. \square

For convenience, we abbreviate $A_{jk}(x)$ and $B_j(ix)$ to A_{jk} and B_j for $j, k = 1, 2$. According to Lemmas 4.1–4.3, it is easy to get the following simplifications.

$$\begin{aligned} |\phi(B_n(3; 3, n-5), ix)|^2 &= (A_{11}^2 + A_{12}^2)Z_1^{2n} + (A_{21}^2 + A_{22}^2)Z_2^{2n} + (-1)^n 2(A_{11}A_{21} + A_{12}A_{22}), \\ |\phi(P_n^{6,6}, ix)|^2 &= B_1^2 Z_1^{2n} + B_2^2 Z_2^{2n} + (-1)^n 2B_1 B_2. \end{aligned}$$

Proof of Proposition 1.4. According to Lemma 2.11, we can obtain that $\mathcal{E}(G) \leq \mathcal{E}(B_n(3; 3, n-5))$ for $G \in \mathcal{D}_n^{3,3}$. Next we just prove $\mathcal{E}(B_n(3; 3, n-5)) < \mathcal{E}(P_n^{6,6})$ for any positive number $n \geq 12$. By Theorem 2.6,

$$\mathcal{E}(B_n(3; 3, n-5)) - \mathcal{E}(P_n^{6,6}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right| dx.$$

We distinguish two cases in terms of the parity of n .

Case 1. n is odd and $n \geq 13$.

We first prove that the integrand $\log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|$ is monotonically decreasing in n when $n \geq 13$.

$$\log \left| \frac{\phi(B_{n+2}(3; 3, n-3), ix)}{\phi(P_{n+2}^{6,6}, ix)} \right| - \log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|$$

$$\begin{aligned}
&= \frac{1}{2} \log \frac{|\phi(B_{n+2}(3; 3, n-3), ix) \cdot \phi(P_n^{6,6}, ix)|^2}{|\phi(B_n(3; 3, n-5), ix) \cdot \phi(P_{n+2}^{6,6}, ix)|^2} \\
&= \frac{1}{2} \log \left(1 + \frac{K(n, x)}{H(n, x)} \right),
\end{aligned}$$

where

$$H(n, x) = |\phi(B_n(3; 3, n-5), ix) \cdot \phi(P_{n+2}^{6,6}, ix)|^2 > 0$$

and

$$K(n, x) = |\phi(B_{n+2}(3; 3, n-3), ix) \cdot \phi(P_n^{6,6}, ix)|^2 - |\phi(B_n(3; 3, n-5), ix) \cdot \phi(P_{n+2}^{6,6}, ix)|^2.$$

From Theorem 2.1, we just need to show $K(n, x) < 0$. By elementary calculations and simplifications, we have

$$\begin{aligned}
K(n, x) &= [(A_{11}^2 + A_{12}^2)B_2^2 - (A_{21}^2 + A_{22}^2)B_1^2](Z_1^4 - Z_2^4) \\
&\quad - 2[(A_{11}^2 + A_{12}^2)B_1B_2 - (A_{11}A_{21} + A_{12}A_{22})B_1^2](Z_1^4 - 1)Z_1^{2n} \\
&\quad - 2[(A_{11}A_{21} + A_{12}A_{22})B_2^2 - (A_{21}^2 + A_{22}^2)B_1B_2](1 - Z_2^4)Z_2^{2n}.
\end{aligned}$$

Claim 1. For any real number x , $A_{11}A_{21} + A_{12}A_{22} < 0$.

Proof. By Lemma 4.3, we have

$$\begin{aligned}
&A_{11}A_{21} + A_{12}A_{22} \\
&= \frac{Z_1^5 + xZ_1^2 + x^3 + x}{Z_1^5 + Z_1^3} \cdot \frac{Z_2^5 + xZ_2^2 + x^3 + x}{Z_2^5 + Z_2^3} + \frac{2Z_1^2 + 2(x^2 + 1)}{Z_1^5 + Z_1^3} \cdot \frac{2Z_2^2 + 2(x^2 + 1)}{Z_2^5 + Z_2^3} \\
&= -\frac{-1 + x(Z_1^3 + Z_2^3) + x(x^2 + 1)(Z_1^5 + Z_2^5) + x^2 + x^2(x^2 + 1)(Z_1^2 + Z_2^2) + x^2(x^2 + 1)^2}{(Z_1^2 + 1)(Z_2^2 + 1)} \\
&\quad - \frac{4 + 4(x^2 + 1)(Z_1^2 + Z_2^2) + 4(x^2 + 1)^2}{(Z_1^2 + 1)(Z_2^2 + 1)} \\
&= -\frac{3 + x(Z_1^3 + Z_2^3) + x(x^2 + 1)(Z_1^5 + Z_2^5) + x^2 + (x^2 + 4)(x^2 + 1)(Z_1^2 + Z_2^2) + (x^2 + 4)(x^2 + 1)^2}{(Z_1^2 + 1)(Z_2^2 + 1)}.
\end{aligned}$$

Since

$$Z_1^3 + Z_2^3 = x^3 + 3x$$

and

$$Z_1^5 + Z_2^5 = x^5 + 5x^3 + 5x,$$

we can obtain $A_{11}A_{21} + A_{12}A_{22} < 0$ for any real number x . Hence, the claim holds. \square

Since $Z_1(x) > 1$ and $-1 < Z_2(x) < 0$ for $x > 0$, we have $Z_1^{2n} \geq Z_1^{26}$ and $Z_2^{2n} \leq Z_2^{26}$ when $n \geq 13$. Since $0 < Z_1(x) < 1$ and $Z_2(x) < -1$ for $x < 0$, we get $Z_1^{2n} \leq Z_1^{26}$ and $Z_2^{2n} \geq Z_2^{26}$ when $n \geq 13$. By Claim 1, we obtain

$$K(n, x) \leq [(A_{11}^2 + A_{12}^2)B_2^2 - (A_{21}^2 + A_{22}^2)B_1^2](Z_1^4 - Z_2^4)$$

$$\begin{aligned}
& -2[(A_{11}^2 + A_{12}^2)B_1B_2 - (A_{11}A_{21} + A_{12}A_{22})B_1^2](Z_1^4 - 1)Z_1^{26} \\
& -2[(A_{11}A_{21} + A_{12}A_{22})B_2^2 - (A_{21}^2 + A_{22}^2)B_1B_2](1 - Z_2^4)Z_2^{26} \\
& = |\phi(B_{15}(3; 3, 10), ix) \cdot \phi(P_{13}^{6,6}, ix)|^2 - |\phi(B_{13}(3; 3, 8), ix) \cdot \phi(P_{15}^{6,6}, ix)|^2.
\end{aligned}$$

It is no difficult to get that

$$\begin{aligned}
\phi(B_{15}(3; 3, 10), ix) &= -(4x^{12} + 42x^{10} + 164x^8 + 294x^6 + 240x^4 + 74x^2 + 4) \\
&\quad - (x^{15} + 16x^{13} + 99x^{11} + 302x^9 + 477x^7 + 372x^5 + 121x^3 + 10x)i, \\
\phi(B_{13}(3; 3, 8), ix) &= (4x^{10} + 34x^8 + 100x^6 + 120x^4 + 52x^2 + 4) \\
&\quad + (x^{13} + 14x^{11} + 72x^9 + 170x^7 + 186x^5 + 82x^3 + 9x)i
\end{aligned}$$

and

$$\begin{aligned}
\phi(P_{15}^{6,6}, ix) &= -(x^{15} + 16x^{13} + 101x^{11} + 324x^9 + 571x^7 + 556x^5 + 279x^3 + 56x)i, \\
\phi(P_{13}^{6,6}, ix) &= (x^{13} + 14x^{11} + 74x^9 + 188x^7 + 245x^5 + 158x^3 + 40x)i.
\end{aligned}$$

By direct calculations, we have

$$\begin{aligned}
K(n, x) &\leq |\phi(B_{15}(3; 3, 10), ix) \cdot \phi(P_{13}^{6,6}, ix)|^2 - |\phi(B_{13}(3; 3, 8), ix) \cdot \phi(P_{15}^{6,6}, ix)|^2 \\
&= -x^2(x^2 + 3)(x^2 + 1)^5(2x^{34} + 80x^{32} + 1456x^{30} + 16024x^{28} + 119483x^{26} + 640628x^{24} \\
&\quad + 2556655x^{22} + 7750232x^{20} + 18036236x^{18} + 32317620x^{16} + 44398154x^{14} + 46211348x^{12} \\
&\quad + 35669955x^{10} + 19725556x^8 + 7395899x^6 + 1714208x^4 + 206016x^2 + 8192) < 0.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\mathcal{E}(B_n(3; 3, n-5)) - \mathcal{E}(P_n^{6,6}) &\leq \frac{1}{\pi} \int_{-\infty}^{+\infty} \log \left| \frac{\phi(B_{13}(3; 3, n-5), ix)}{\phi(P_{13}^{6,6}, ix)} \right| dx \\
&= \mathcal{E}(B_{13}(3; 3, 8)) - \mathcal{E}(P_{13}^{6,6}) \\
&= -0.1676 < 0.
\end{aligned}$$

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

Since

$$\log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 = \log \frac{(A_{11}^2 + A_{12}^2)Z_1^{2n} + (A_{21}^2 + A_{22}^2)Z_2^{2n} + (-1)^n 2(A_{11}A_{21} + A_{12}A_{22})}{B_1^2 Z_1^{2n} + B_2^2 Z_2^{2n} + (-1)^n 2B_1B_2},$$

we have

$$\left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 \rightarrow \begin{cases} \frac{A_{11}^2 + A_{12}^2}{B_1^2}, & x > 0; \\ \frac{A_{21}^2 + A_{22}^2}{B_2^2}, & x < 0 \end{cases}$$

when $n \rightarrow \infty$. Next we will show

$$\log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 < \log \frac{A_{11}^2 + A_{12}^2}{B_1^2}$$

for $x > 0$, and

$$\log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 < \log \frac{A_{21}^2 + A_{22}^2}{B_2^2}$$

for $x < 0$.

Subcase 2.1 $x > 0$.

$$\begin{aligned} & \log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 - \log \frac{A_{11}^2 + A_{12}^2}{B_1^2} \\ &= \log \frac{|\phi(B_n(3; 3, n-5), ix)|^2 \cdot B_1^2}{|\phi(P_n^{6,6}, ix)|^2 \cdot (A_{11}^2 + A_{12}^2)} \\ &= \log \left(1 + \frac{((A_{21}^2 + A_{22}^2)B_1^2 - (A_{11}^2 + A_{12}^2)B_2^2)Z_2^{2n} + 2(A_{11}A_{21} + A_{12}A_{22})B_1^2 - 2(A_{11}^2 + A_{12}^2)B_1B_2}{|\phi(P_n^{6,6}, ix)|^2 \cdot (A_{11}^2 + A_{12}^2)} \right). \end{aligned}$$

Let

$$K_1(n, x) = ((A_{21}^2 + A_{22}^2)B_1^2 - (A_{11}^2 + A_{12}^2)B_2^2)Z_2^{2n} + 2(A_{11}A_{21} + A_{12}A_{22})B_1^2 - 2(A_{11}^2 + A_{12}^2)B_1B_2.$$

By Claim 1, we have

$$2(A_{11}A_{21} + A_{12}A_{22})B_1^2 - 2(A_{11}^2 + A_{12}^2)B_1B_2 < 0.$$

If $(A_{21}^2 + A_{22}^2)B_1^2 - (A_{11}^2 + A_{12}^2)B_2^2 \leq 0$, then $K_1(n, x) < 0$. Hence,

$$\log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 < \log \frac{A_{11}^2 + A_{12}^2}{B_1^2}.$$

Now suppose $(A_{21}^2 + A_{22}^2)B_1^2 - (A_{11}^2 + A_{12}^2)B_2^2 > 0$. Since $-1 < Z_2(x) < 0$ and $n \geq 12$, we get $Z_2^{2n} \leq Z_2^{24}$. Hence,

$$\begin{aligned} K_1(n, x) &\leq ((A_{21}^2 + A_{22}^2)B_1^2 - (A_{11}^2 + A_{12}^2)B_2^2)Z_2^{24} + 2(A_{11}A_{21} + A_{12}A_{22})B_1^2 - 2(A_{11}^2 + A_{12}^2)B_1B_2 \\ &= |\phi(B_{12}(3; 3, 7), ix)|^2 \cdot B_1^2 - |\phi(P_{12}^{6,6}, ix)|^2 \cdot (A_{11}^2 + A_{12}^2) \\ &= |\phi(B_{12}(3; 3, 7), ix)|^2 \cdot \frac{(Z_1g_{13} + g_{12})^2}{(Z_1^2 + 1)^2} Z_2^{24} \\ &\quad - |\phi(P_{12}^{6,6}, ix)|^2 \cdot \frac{(Z_1^5 + xZ_1^2 + x^3 + x)^2 + (2Z_1^2 + 2x^2 + 2)^2}{(Z_1^2 + 1)^2} Z_2^6 \\ &= \frac{Z_2^{22}}{(Z_1^2 + 1)^2} \cdot (|\phi(B_{12}(3; 3, 7), ix)|^2 \cdot (g_{13} - Z_2g_{12})^2 \\ &\quad - |\phi(P_{12}^{6,6}, ix)|^2 \cdot ((Z_1^5 + xZ_1^2 + x^3 + x)^2 + (2Z_1^2 + 2x^2 + 2)^2) \cdot Z_1^{16}). \end{aligned}$$

Since

$$\phi(B_{12}(3; 3, 7), ix) = (x^{12} + 13x^{10} + 60x^8 + 121x^6 + 104x^4 + 30x^2 + 1) - (4x^9 + 30x^7 + 74x^5 + 68x^3 + 18x)i$$

and

$$\phi(P_{12}^{6,6}, ix) = x^{12} + 13x^{10} + 62x^8 + 138x^6 + 153x^4 + 81x^2 + 16,$$

by calculations, we get

$$\begin{aligned} K_1(n, x) \leq & \frac{Z_2^{22}}{(Z_1^2 + 1)^2} \cdot ((-x^2 - 2)(x^2 + 1)^6(x^{30} + 38x^{28} + 650x^{26} + 6638x^{24} + 45235x^{22} \\ & + 217640x^{20} + 762306x^{18} + 1973232x^{16} + 3787141x^{14} + 5347554x^{12} + 5442680x^{10} \\ & + 3844902x^8 + 1767427x^6 + 473164x^4 + 60192x^2 + 2048) - x(x^2 + 1)^5(x^8 + 11x^6 \\ & + 39x^4 + 49x^2 + 16)(x^{24} + 28x^{22} + 343x^{20} + 2445x^{18} + 11336x^{16} + 36074x^{14} \\ & + 80758x^{12} + 127760x^{10} + 140831x^8 + 104274x^6 + 48307x^4 + 12235x^2 + 1256)\sqrt{x^2 + 4}). \end{aligned}$$

Because $x > 0$, we can obtain $K_1(n, x) < 0$ and $\log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 < \log \frac{A_{11}^2 + A_{12}^2}{B_1^2}$.

Subcase 2.2. $x < 0$.

$$\begin{aligned} & \log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 - \log \frac{A_{21}^2 + A_{22}^2}{B_2^2} \\ &= \log \frac{|\phi(B_n(3; 3, n-5), ix)|^2 \cdot B_2^2}{|\phi(P_n^{6,6}, ix)|^2 \cdot (A_{21}^2 + A_{22}^2)} \\ &= \log \left(1 + \frac{((A_{11}^2 + A_{12}^2)B_2^2 - (A_{21}^2 + A_{22}^2)B_1^2)Z_1^{2n} + 2(A_{11}A_{21} + A_{12}A_{22})B_2^2 - 2(A_{21}^2 + A_{22}^2)B_1B_2}{|\phi(P_n^{6,6}, ix)|^2 \cdot (A_{21}^2 + A_{22}^2)} \right). \end{aligned}$$

Let

$$K_2(n, x) = ((A_{11}^2 + A_{12}^2)B_2^2 - (A_{21}^2 + A_{22}^2)B_1^2)Z_1^{2n} + 2(A_{11}A_{21} + A_{12}A_{22})B_2^2 - 2(A_{21}^2 + A_{22}^2)B_1B_2.$$

By Claim 1, we have

$$2(A_{11}A_{21} + A_{12}A_{22})B_2^2 - 2(A_{21}^2 + A_{22}^2)B_1B_2 < 0.$$

If $(A_{11}^2 + A_{12}^2)B_2^2 - (A_{21}^2 + A_{22}^2)B_1^2 \leq 0$, then $K_2(n, x) < 0$. Hence,

$$\log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 < \log \frac{A_{21}^2 + A_{22}^2}{B_2^2}.$$

Now suppose $(A_{11}^2 + A_{12}^2)B_2^2 - (A_{21}^2 + A_{22}^2)B_1^2 > 0$. Since $0 < Z_1(x) < 1$ and $n \geq 12$, we have $Z_1^{2n} \leq Z_1^{24}$. Therefore,

$$K_2(n, x) \leq ((A_{11}^2 + A_{12}^2)B_2^2 - (A_{21}^2 + A_{22}^2)B_1^2)Z_1^{24} + 2(A_{11}A_{21} + A_{12}A_{22})B_2^2 - 2(A_{21}^2 + A_{22}^2)B_1B_2$$

$$\begin{aligned}
&= |\phi(B_{12}(3; 3, 7), ix)|^2 \cdot B_2^2 - |\phi(P_{12}^{6,6}, ix)|^2 \cdot (A_{21}^2 + A_{22}^2) \\
&= |\phi(B_{12}(3; 3, 7), ix)|^2 \cdot \frac{(Z_2 g_{13} + g_{12})^2}{(Z_2^2 + 1)^2} Z_1^{24} \\
&\quad - |\phi(P_{12}^{6,6}, ix)|^2 \cdot \frac{(Z_2^5 + xZ_2^2 + x^3 + x)^2 + (2Z_2^2 + 2x^2 + 2)^2}{(Z_2^2 + 1)^2} Z_1^6 \\
&= \frac{Z_1^{22}}{(Z_2^2 + 1)^2} \cdot (|\phi(B_{12}(3; 3, 7), ix)|^2 \cdot (g_{13} - Z_1 g_{12})^2 \\
&\quad - |\phi(P_{12}^{6,6}, ix)|^2 ((Z_2^5 + xZ_2^2 + x^3 + x)^2 + (2Z_2^2 + 2x^2 + 2)^2) \cdot Z_2^{16}) \\
&= \frac{Z_1^{22}}{(Z_2^2 + 1)^2} \cdot ((-x^2 - 2)(x^2 + 1)^6 (x^{30} + 38x^{28} + 650x^{26} + 6638x^{24} + 45235x^{22} \\
&\quad + 217640x^{20} + 762306x^{18} + 1973232x^{16} + 3787141x^{14} + 5347554x^{12} + 5442680x^{10} \\
&\quad + 3844902x^8 + 1767427x^6 + 473164x^4 + 60192x^2 + 2048) + x(x^2 + 1)^5 (x^8 + 11x^6 \\
&\quad + 39x^4 + 49x^2 + 16)(x^{24} + 28x^{22} + 343x^{20} + 2445x^{18} + 11336x^{16} + 36074x^{14} \\
&\quad + 80758x^{12} + 127760x^{10} + 140831x^8 + 104274x^6 + 48307x^4 + 12235x^2 + 1256)\sqrt{x^2 + 4}).
\end{aligned}$$

Because $x < 0$, we can obtain $K_2(n, x) < 0$ and $\log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 < \log \frac{A_{21}^2 + A_{22}^2}{B_2^2}$.

From the two subcases, we have

$$\begin{aligned}
\mathcal{E}(B_n(3; 3, n-5)) - \mathcal{E}(P_n^{6,6}) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \log \left| \frac{\phi(B_n(3; 3, n-5), ix)}{\phi(P_n^{6,6}, ix)} \right|^2 dx \\
&< \frac{1}{2\pi} \int_0^{+\infty} \log \frac{A_{11}^2 + A_{12}^2}{B_1^2} dx + \frac{1}{2\pi} \int_{-\infty}^0 \log \frac{A_{21}^2 + A_{22}^2}{B_2^2} dx.
\end{aligned}$$

When $x > 0$, we can obtain

$$\begin{aligned}
A_{11}^2 + A_{12}^2 - B_1^2 &= \frac{(Z_1^5 + xZ_1^2 + x^3 + x)^2 + (2Z_1^2 + 2x^2 + 2)^2}{(Z_1^5 + Z_1^3)^2} - \frac{(Z_1 g_{13} + g_{12})^2}{(Z_1^2 + 1)^2} \cdot Z_1^{24} \\
&= \frac{Z_2^{22}}{(Z_1^2 + 1)^2} (((Z_1^5 + xZ_1^2 + x^3 + x)^2 + (2Z_1^2 + 2x^2 + 2)^2) Z_1^{16} - (g_{13} - Z_2 g_{12})^2) \\
&= \frac{Z_2^{22}}{2(Z_1^2 + 1)^2} ((-x^2 - 1)(x^2 + 2)(4x^{18} + 72x^{16} + 560x^{14} + 2484x^{12} + 6911x^{10} \\
&\quad + 12285x^8 + 13476x^6 + 8396x^4 + 2521x^2 + 239) + x(-x^2 - 1)(4x^{18} + 72x^{16} \\
&\quad + 568x^{14} + 2596x^{12} + 7573x^{10} + 14471x^8 + 17790x^6 + 13282x^4 + 5345x^2 \\
&\quad + 863)\sqrt{x^2 + 4}) \\
&< 0.
\end{aligned}$$

When $x < 0$, we have

$$A_{21}^2 + A_{22}^2 - B_2^2 = \frac{(Z_2^5 + xZ_2^2 + x^3 + x)^2 + (2Z_2^2 + 2x^2 + 2)^2}{(Z_2^5 + Z_2^3)^2} - \frac{(Z_2 g_{13} + g_{12})^2}{(Z_2^2 + 1)^2} \cdot Z_1^{24}$$

$$\begin{aligned}
&= \frac{Z_1^{22}}{(Z_2^2 + 1)^2} (((Z_2^5 + xZ_2^2 + x^3 + x)^2 + (2Z_2^2 + 2x^2 + 2)^2)Z_2^{16} - (g_{13} - Z_1g_{12})^2) \\
&= \frac{Z_2^{22}}{2(Z_1^2 + 1)^2} ((-x^2 - 1)(x^2 + 2)(4x^{18} + 72x^{16} + 560x^{14} + 2484x^{12} + 6911x^{10} \\
&\quad + 12285x^8 + 13476x^6 + 8396x^4 + 2521x^2 + 239) + x(x^2 + 1)(4x^{18} + 72x^{16} \\
&\quad + 568x^{14} + 2596x^{12} + 7573x^{10} + 14471x^8 + 17790x^6 + 13282x^4 + 5345x^2 \\
&\quad + 863)\sqrt{x^2 + 4}) \\
&< 0.
\end{aligned}$$

Therefore,

$$\frac{1}{2\pi} \int_0^{+\infty} \log \frac{A_{11}^2 + A_{12}^2}{B_1^2} dx < 0$$

and

$$\frac{1}{2\pi} \int_{-\infty}^0 \log \frac{A_{21}^2 + A_{22}^2}{B_2^2} dx < 0.$$

Hence, $\mathcal{E}(B_n(3; 3, n - 5)) < \mathcal{E}(P_n^{6,6})$ when n is even. The entire proof of Proposition 1.4 is now complete. \square

5 Concluding remarks

In this paper we prove that Conjecture 1.2 holds for the bicyclic graphs containing exactly two odd cycles with one common vertex. So far, Conjecture 1.2 is true for the following cases:

Case 1: G is bipartite bicyclic graph ([16] and [11]).

Case 2: G is bicyclic graph which has exactly two edge-disjoint cycles such that one of them is even and the other is odd ([14]).

Case 3: G is bicyclic graph which contains exactly two odd cycles with one common vertex (Theorem 1.5 of this paper).

In order to completely solve Conjecture 1.2, one just needs to consider the remaining two cases, one of bicyclic graphs that contain two odd cycles with no common vertex and the other of bicyclic graphs that contain two odd cycles with at least one common edge. We think the latter case is much more difficult.

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References

- [1] E. Andriantiana, Unicyclic bipartite graphs with maximum energy, *MATCH Commun. Math. Comput. Chem.* 66 (2011) 913–926.
- [2] G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* 39 (1999) 984–996.
- [3] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs-Theory and Application*, Academic Press, New York, 1980.
- [4] I. Gutman, Acyclic systems with extremal Hückel π -electron energy, *Theoret. Chim. Acta (Berlin)* 45 (1977) 79–87.
- [5] I. Gutman, The energy of a graph, *Ber. Math. Statist. Sect. Forschungsz. Graz.* 103 (1978) 1–22.
- [6] 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.
- [7] I. Gutman, O. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.
- [8] I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: A computer experiment, *J. Chem. Inf. Comput. Sci.* 41 (2001) 1002–1005.
- [9] Y. Hou, I. Gutman, C. Woo, Unicyclic graphs with maximal energy, *Linear Algebra Appl.* 356 (2002) 27–36.
- [10] 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 (2011) 903–912.
- [11] B. Huo, S. Ji, X. Li, Y. Shi, Solution to a conjecture on the maximal energy of bipartite bicyclic graphs, *Linear Algebra Appl.* 435 (2011) 804–810.
- [12] 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.

- [13] B. Huo, X. Li, Y. Shi, Complete solution to a conjecture on the maximal energy of unicyclic graphs, *European J. Combin.* 32 (2011) 662–673.
- [14] S. Ji, J. Li, An approach to the problem of the maximal energy of bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* 68 (2012) 741–762.
- [15] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.
- [16] X. Li, J. Zhang, On bicyclic graphs with maximal energy, *Linear Algebra Appl.* 427 (2007) 87–98.
- [17] V. A. Zorich, *Mathematical Analysis*, MCCME, 2002.