Ordering of Connected Bipartite Unicyclic Graphs with Large Energies

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Abstract

The energy of a graph is the sum of the absolute value of the eigenvalues of its adjacency matrix. In this paper, the first $\left\lfloor \frac{n-5}{2} \right\rfloor$ largest energies of connected bipartite unicyclic graphs on $n \geq 78$ vertices are determined which generalize some known results.

1 Introduction

Let $G$ be a simple undirected graph with $n$ vertices and $A(G)$ be its adjacency matrix. Let $\lambda_1(G), \cdots, \lambda_n(G)$ be the eigenvalues of $A(G)$. Then the energy of $G$, denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i(G)|$ (see [4]). The study on the graph energy originated from the total $\pi$-electron energy of conjugated hydrocarbons, which has an important implication on thermodynamics and molecular structure. Its details can be found in an appropriate textbook [3].

The characteristic polynomial $\det(xI - A(G))$ of the adjacency matrix $A(G)$ of a graph $G$ is also called the characteristic polynomial of $G$, written as $\phi(G, x) = \sum_{i=0}^{n} a_i(G)x^{n-i}$.

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If $G$ is a bipartite graph, then it is well known that $\phi(G, x)$ has the form

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

(1)

where $b_{2i}(G) = |a_{2i}(G)| = (-1)^ia_{2i}(G)$.

Assume that

$$\tilde{\phi}(G, x) = \sum_{i=0}^{\lfloor n/2 \rfloor} b_{2i}(G)x^{n-2i}.$$ 

The energy of a bipartite graph $G$ on $n$ vertices can be expressed in terms of the Coulson integral formula [5]:

$$E(G) = \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \ln(\sum_{i=0}^{\lfloor n/2 \rfloor} b_{2i}(G)x^{2i})dx.$$  

(2)

Thus, by Eq. (2), $E(G)$ is a strictly monotonically increasing function of those numbers $b_{2i}(G)$ ($i = 0, 1, \ldots, \lfloor n/2 \rfloor$) for bipartite graphs. This observation provides a way of comparing the energies of a pair of bipartite graphs as follows.

**Definition 1.1** Let $G_1$ and $G_2$ be two bipartite graphs of order $n$. If $b_{2i}(G_1) \leq b_{2i}(G_2)$ for all $i$ with $0 \leq i \leq \lfloor n/2 \rfloor$, 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 $b_{2j}(G_1) < b_{2j}(G_2)$, then we write $G_1 \prec G_2$. If $b_{2j}(G_1) = b_{2j}(G_2)$ for all $j$, we write $G_1 \sim G_2$.

According to the Coulson integral formula, we have the quasi-order method of comparing the energies for two bipartite graphs $G_1$ and $G_2$ of order $n$ that [5]:

$$G_1 \preceq G_2 \Rightarrow E(G_1) \leq E(G_2)$$

$$G_1 \prec G_2 \Rightarrow E(G_1) < E(G_2).$$

In this paper, for sake of conciseness, we introduce the symbol "$\Rightarrow G_1 \rightarrow G_2$" as follows:

$$E(G_1) < E(G_2) \Leftrightarrow G_1 \rightarrow G_2.$$
Throughout this paper, we use $P_n$ and $C_n$ to denote the $n$-vertex path and $n$-vertex cycle, respectively. Let $P_n^l$ be the graph obtained by joining some vertex of $C_l$ and one of the end vertices of $P_{n-l}$ ($n > l$). Let $a$ and $b$ be nonnegative integers. We denote by $C_6(a, b)$ the graph obtained by attaching two pendent paths of length $a$ and $b$ to the unique pendent vertex of $P_n^6$, respectively (see Fig. 1). It is easy to see that $C_6(a, b) = C_6(b, a)$ and $P_n^6 = C_6(0, n - 7)$.

Using the above quasi-order method, Hou et al. [8] proved that for $n \geq 7$, $P_n^6$ has the maximal energy among all connected unicyclic bipartite $n$-vertex graphs except for $C_n$. Gutman and Hou [7] shown that $E(P_n^6) > E(C_n)$ by some numerical calculations for $n \geq 12$, but they did not give a rigorous mathematical proof. In [9], Hua further investigated the second-maximal energy of bipartite unicyclic graph. By means of an appropriate computer search and some numerical calculations, Gutman et al. [6] determined the $n$-vertex bipartite unicyclic graphs with maximal, second-maximal and third-maximal energy. But they could not give a rigorous mathematical proof. Thus they posed the following conjecture.

**Conjecture 1** For all $n \geq 11$, the $n$-vertex bipartite unicyclic graph with maximal energy is $C_6(0, n - 7)$. For all $n \geq 23$, the $n$-vertex bipartite unicyclic graph with second-maximal energy is $C_6(2, n - 9)$. For all $n \geq 27$, the $n$-vertex bipartite unicyclic graph with third-maximal energy is $C_6(4, n - 11)$.

Recently, using the Coulson integral formula for the energy of a graph, Huo et al. [11] and Andriantiana [1] independently proved that the bipartite unicyclic graph with maximal energy is $C_6(0, n - 7)$ for $n \geq 11$. In [10], Huo et al. further characterized the unicyclic graph with maximal energy. Furthermore, Andriantiana and Wagner [2] showed that the unicyclic graph with second-maximal energy is $C_6(2, n - 9)$ for $n \geq 28$; Zhu and Yang [18] proved that the $n$-vertex bipartite unicyclic graph with third-maximal energy is $C_6(4, n - 11)$ for $n \geq 27$. Therefore the above conjecture has been completely solved. In this paper, we will give the first $\left\lfloor \frac{n-5}{2} \right\rfloor$ largest energies of connected bipartite unicyclic graphs with $n \geq 78$ vertices.

![Fig. 2. The graphs $Y_n$, $Z_n$ and $\hat{C}_6(2, n - 11)$](image-url)
Denote by $BU(n)$ the set of all connected bipartite unicyclic graphs with $n$ vertices. Denote by $Y_n$ the graph obtained by attaching two pendent paths of length 2 to the unique pendent vertex of $P_{n-4}^6$ (see Fig. 2). Denote by $Z_n$ the graph obtained by attaching two pendent paths of length 2 and 4 to the unique pendent vertex of $P_{n-6}^6$ (see Fig. 2). Denote by $\widehat{C}_6(2, n-11)$ the graph obtained by attaching two pendent paths of length 2 and $n-11$ to the unique pendent vertex of $P_{9}^6$ (see Fig. 2). Now we give the main result of this paper.

**Theorem 1.1** Let $G \in BU(n)$, $k = \lfloor \frac{n-7}{2} \rfloor$, $t = \lfloor \frac{k}{2} \rfloor$ and $l = \lfloor \frac{k-1}{2} \rfloor$. If $n \geq 78$, then the $n$-vertex connected bipartite unicyclic graphs with the first $\lfloor \frac{n-5}{2} \rfloor$ largest energies are as follows:

\[
C_6(0, n-7) \leftarrow C_6(2, n-9) \leftarrow C_6(4, n-11) \leftarrow Y_n \leftarrow C_6(6, n-13) \leftarrow \cdots
\]

\[
\leftarrow C_6(2t, n-7 - 2t) \leftarrow C_6(2t + 1, n-8 - 2t) \leftarrow \cdots \leftarrow C_6(9, n-16) \leftarrow \widehat{C}_6(2, n-11)
\]

\[
\leftarrow C_6(7, n-14) \leftarrow Z_n.
\]

2 The basic strategy of the proof of Theorem 1.1

Let $BU(n, l)$ be the set of connected bipartite unicyclic graphs of order $n$ with one unique cycle of length $l$. Let $\mathcal{A}(n) = \{C_6(a, b) \mid 0 \leq a \leq b, a + b = n - 7\}$. In [18], Zhu and Yang gave the following result:

**Lemma 2.1** Let $k = \lfloor \frac{n-7}{2} \rfloor$, $t = \lfloor \frac{k}{2} \rfloor$ and $l = \lfloor \frac{k-1}{2} \rfloor$. Then we have the following quasi-order relation in $\mathcal{A}(n)$:

\[
C_6(0, n-7) \leftarrow C_6(2, n-9) \leftarrow C_6(4, n-11) \leftarrow \cdots \leftarrow C_6(2l, n-7 - 2t)
\]

\[
\leftarrow C_6(2l + 1, n-8 - 2t) \leftarrow \cdots \leftarrow C_6(5, n-12) \leftarrow C_6(3, n-10) \leftarrow C_6(1, n-8).
\]

Let $C_6 = v_1v_2v_3v_4v_5v_6v_1$ be the unique cycle of $BU(n, 6)$. For a graph $G \in BU(n, 6)$, let $N(G) = \{v_i \mid d_G(v_i) \geq 3, i = 1, 2, ..., 6\}$. Then we can classify the graphs in $BU(n)$ into the following three classes.

\[
BU_1 = \{G \mid G \in BU(n, l), l \neq 6\};
\]

\[
BU_2 = \{G \mid G \in BU(n, 6), |N(G)| \neq 1\};
\]

\[
BU_3 = \{G \mid G \in BU(n, 6), |N(G)| = 1\}.
\]
It follows that $BU(n) = BU_1 \cup BU_2 \cup BU_3$ and $A(n) \subseteq BU_3$.

For $n \geq 78$, our basic strategy of the proof of Theorem 1.1 is to prove the following results $(R_1)-(R_3)$:

$(R_1)$: For any $G \in BU_1$, we have $G \rightarrow Z_n$.

$(R_2)$: For any $G \in BU_2$, we have $G \rightarrow Z_n$.

$(R_3)$: (1) $C_6(5, n - 12) \rightarrow Z_n \rightarrow C_6(7, n - 14)$;
(2) $C_6(6, n - 13) \rightarrow Y_n \rightarrow C_6(4, n - 11)$;
(3) $C_6(7, n - 14) \rightarrow \hat{C}_6(2, n - 11) \rightarrow C_6(9, n - 16)$;
(4) For any $G \in BU_3 \setminus A(n)$, if $G \neq Y_n, Z_n, \hat{C}_6(2, n - 11)$, then we have $G \rightarrow Z_n$.

It is easy to see that we can prove Theorem 1.1 by combining Lemma 2.1 and the above results $(R_1)-(R_3)$. We will prove the result $(R_1)$ in section 3. Then we will prove the results $(R_2)$ and $(R_3)$ in sections 4 and 5, respectively.

3 The proof of $(R_1)$

The quasi-order method mentioned above can be used to compare the energies of two bipartite graphs. However, it sometimes does not work [18]. In [17], Shan et al. presented a new method of comparing the energies of two subdivision bipartite graphs.

Definition 3.1 [17] Let $e$ be a cut edge of a graph $G$, and let $G_e(k)$ denote the graph obtained by replacing $e$ with a path of length $k+1$ (for simplicity of notations, we usually abbreviate $G_e(k)$ by $G(k)$). We say that $G(k)$ is a $k$-subdivision graph of $G$ on the cut edge $e$. We also set $G(0)=G$.

Lemma 3.1 [17] Let $G$ be a bipartite graph of order $n$ and let $G(k)$ be a $k$-subdivision graph (of order $n+k$) of $G$ on some cut edge $e$. Then we have:

$$\tilde{\phi}(G(k+2), x) = x\tilde{\phi}(G(k+1), x) + \tilde{\phi}(G(k), x) \quad (k \geq 0).$$

From the proof of Lemma 1.1 in [15], we have the following result.

Lemma 3.2 Let $G(k), H(k)$ be $k$-subdivision graphs on some cut edges of the bipartite graphs $G$ and $H$ of order $n$, respectively ($k \geq 0$). Write $g_k = \tilde{\phi}(G(k), x)$, $h_k = \tilde{\phi}(H(k), x)$, $f_k = h_{k+1}g_k - h_kg_{k+1}$ and $DE(k) = E(H(k)) - E(G(k))$. If $f_0$ is a polynomial with nonnegative coefficients, then

$$DE(2l) < DE(2k) < DE(2k + 1) < DE(2l + 1)$$

holds for all $k > l \geq 0$. 

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Lemma 3.3  [18] Let $G \in \mathcal{BU}_1$, if $G \neq C_n, P_n^{n-2}, P_n^{10}$, we have $G \rightarrow P_n^{10}$.

Now, we will use Lemma 3.2 to prove $P_n^{10} \rightarrow Z_n$ for $n \geq 15$.

Lemma 3.4 If $n \geq 14$, then $P_n^{10} \rightarrow Z_n$.

Proof. Let $G = P_{14}^{10}$, $H = Z_{14}$. Then $P_n^{10}$ and $Z_n$ are $k$-subdivision of $G$ and $H$ on some cut edges ($k = n - 14$), respectively.

By some calculations we get:

$$f_0 = x(1 + x^2)(1 + 3x^2 + x^4)(24 + 160x^2 + 371x^4 + 398x^6 + 235x^8 + 79x^{10} + 14x^{12} + x^{14})$$

and $DE(0) = 0.00077$, $DE(1) = 0.0766$.

By Lemma 3.2, we have for $n \geq 14$, $E(P_n^{10}) < E(Z_n)$.

Next we prove $P_n^{n-2} \rightarrow Z_n$ when $n \geq 16$ and $n$ is even. We need the following results.

Lemma 3.5  [18] Let $h_n$ and $g_n$ be monic polynomials of degree $n$ about $x$ with nonnegative coefficients satisfying that $h_n = xh_{n-1} + h_{n-2}$ and $g_n = xg_{n-1} + g_{n-2}$. Let $p(x)$ be a nonzero polynomial with nonnegative coefficients. Write $a_n = \frac{h_n + p(x)}{g_n}$ and $b_n = \frac{h_n - p(x)}{g_n}$. For each fixed $x > 0$ and $n \geq 9$, we have:

1. If $a_{n-8} > a_{n-4}$, then $a_{n-4} > a_n$.

2. If $b_{n-8} < b_{n-4}$, then $b_{n-4} < b_n$.

Lemma 3.6  [18] Let $h_n, g_n, a_n, b_n, p(x)$ be defined as above. Then $\lim_{n \to \infty} a_n$ and $\lim_{n \to \infty} b_n$ exist.

Lemma 3.7  [18] (1) If $n = 4k$, then we have:

(i) $\tilde{\phi}(C_n, x) = \tilde{\phi}(P_n, x) + \tilde{\phi}(P_{n-2}, x) - 2$;

(ii) $\tilde{\phi}(P_n^{n-2}, x) = \tilde{\phi}(P_n, x) + (x^2 + 1)\tilde{\phi}(P_{n-4}, x) + 2(x^2 + 1)$.

(2) If $n = 4k + 2$, then we have:

(i) $\tilde{\phi}(C_n, x) = \tilde{\phi}(P_n, x) + \tilde{\phi}(P_{n-2}, x) + 2$;

(ii) $\tilde{\phi}(P_n^{n-2}, x) = \tilde{\phi}(P_n, x) + (x^2 + 1)\tilde{\phi}(P_{n-4}, x) - 2(x^2 + 1)$.

Lemma 3.8  [18] (1) Let $h_n = \tilde{\phi}(P_n, x) + \tilde{\phi}(P_{n-2}, x)$. Then $h_n = xh_{n-1} + h_{n-2}$.

(2) Let $h' = \phi(P_n, x) + (x^2 + 1)\tilde{\phi}(P_{n-4}, x)$. Then $h' = xh'_{n-1} + h'_{n-2}$.

Lemma 3.9 If $n \geq 16$ and $n$ is even, then $P_n^{n-2} \rightarrow Z_n$. 
Proof. Let \( h_n = \tilde{\phi}(P_n, x) + (x^2 + 1)\tilde{\phi}(P_{n-4}, x) \). From Lemmas 3.7 and 3.8, we have

\[
\tilde{\phi}(P_n^{n-2}, x) = \begin{cases} 
  h_n + 2(x^2 + 1) & n = 4k \\
  h_n - 2(x^2 + 1) & n = 4k + 2 
\end{cases}
\]

and \( h_n = xh_{n-1} + h_{n-2} \). Let \( g_n = \tilde{\phi}(Z_n, x) \). By Lemma 3.1, we can see that \( g_n = xg_{n-1} + g_{n-2} \). Write \( d_n = \frac{\tilde{\phi}(P_n^{n-2}, x)}{\tilde{\phi}(Z_n, x)} \). We assume that \( x > 0 \) in the following. We consider the following two cases.

Case 1. \( n = 4k \). Then

\[
d_n = h_n + 2\left(x^2 + 1\right) g_n.
\]

By some calculations we have

\[
d_{20} - d_{16} = \frac{F(x)}{g_{16}g_{20}} < 0,
\]

where \( F(x) = -x^2(1 + x^2)(2 + x^2)(48 + 586x^2 + 2167x^4 + 3787x^6 + 3649x^8 + 2087x^{10} + 733x^{12} + 157x^{14} + 19x^{16} + x^{18}) \). By Lemma 3.5(1), we have \( d_{4k} < d_{4k-4} \) when \( k \geq 5 \).

Case 2. \( n = 4k + 2 \). The \( d_n = \frac{h_n - 2(x^2 + 1)}{g_n} \). By some calculations we have:

\[
d_{22} - d_{18} = \frac{H(x)}{g_{18}g_{22}} > 0,
\]

where \( H(x) = x^2(1 + x^2)(152 + 1434x^2 + 5472x^4 + 11143x^6 + 13471x^8 + 10131x^{10} + 4817x^{12} + 1435x^{14} + 257x^{16} + 25x^{18} + x^{20}) \). Thus \( d_{4k+2} < d_{4k+2} \) when \( k \geq 5 \) by Lemma 3.5(2).

From the proof of Lemma 3.6, we can show that \( \lim_{k \to +\infty} d_{4k} = \lim_{k \to +\infty} d_{4k+2} \) exists which implies that \( d_n \leq d_{16} \) for even number \( n \geq 16 \). Thus, if \( n \geq 16 \) and \( n \) is even, then

\[
E(P_{n-2}^n) - E(Z_n) = \frac{2}{\pi} \int_0^{+\infty} \ln d_n \, dx
\]

\[
\leq \frac{2}{\pi} \int_0^{+\infty} \ln d_{16} \, dx
\]

\[
= E(P_{16}^{14}) - E(Z_{16})
\]

\[
= -0.02341 < 0.
\]

Thus the result holds.

Finally, we prove that \( C_n \to Z_n \) for \( n \geq 36 \).

Lemma 3.10 If \( n \geq 36 \) and \( n \) is even, then \( C_n \to Z_n \).

Proof. Let \( h_n = \tilde{\phi}(P_n, x) + \tilde{\phi}(P_{n-2}, x) \). From Lemmas 3.7 and 3.8, we have

\[
\tilde{\phi}(C_n, x) = \begin{cases} 
  h_n - 2 & n = 4k \\
  h_n + 2 & n = 4k + 2 
\end{cases}
\]
and \( h_n = x h_{n-1} + h_{n-2} \). Let \( g_n = \bar{\phi}(Z_n, x) \). By Lemma 3.1, we can see that \( g_n = x g_{n-1} + g_{n-2} \). Write \( d_n = \frac{\bar{\phi}(C_n, x)}{\phi(Z_n, x)} \). We assume that \( x > 0 \) in the following. We consider the following two cases.

Case 1. \( n = 4k \). Then \( d_n = \frac{h_{n-2}}{g_n} \). By some calculations we have

\[
d_{24} - d_{20} = \frac{F(x)}{g_{20} g_{24}} > 0,
\]

where \( F(x) = x^2 (1 + x^2) (4 + x^2) (22 + 219 x^2 + 797 x^4 + 1379 x^6 + 1249 x^8 + 614 x^{10} + 162 x^{12} + 21 x^{14} + x^{16}) \). By Lemma 3.5(2), we have \( d_{4k} > d_{4k-4} \) when \( k \geq 6 \).

Case 2. \( n = 4k + 2 \). Then \( d_n = \frac{h_{n+2}}{g_n} \). By some calculations we have

\[
d_{22} - d_{18} = \frac{H(x)}{g_{18} g_{22}} < 0,
\]

where \( H(x) = -x^2 (1 + x^2) (4 + x^2) (26 + 386 x^2 + 1517 x^4 + 2731 x^6 + 2691 x^8 + 1581 x^{10} + 576 x^{12} + 130 x^{14} + 17 x^{16} + x^{18}) \). Thus \( d_{4k+2} > d_{4k+2} \) when \( k \geq 5 \) by Lemma 3.5(1).

From the proof of Lemma 3.6, we can show that \( \lim_{k \to +\infty} d_{4k} = \lim_{k \to +\infty} d_{4k+2} \) exists which implies that \( d_n \leq d_{38} \) for even number \( n \geq 36 \). Thus, if \( n \geq 36 \) and \( n \) is even, then

\[
E(C_n) - E(Z_n) = \frac{2}{\pi} \int_{0}^{+\infty} \ln d_n \, dx \\
\leq \frac{2}{\pi} \int_{0}^{+\infty} \ln d_{38} \, dx \\
= E(C_{38}) - E(Z_{38}) \\
= -0.00013 < 0.
\]

Thus the result holds.

From Lemmas 3.3, 3.4, 3.9 and 3.10, we have the following.

**Theorem 3.11** If \( G \in BU_1 \), then we have \( G \to Z_n \) (\( n \geq 36 \)).

### 4 The proof of \((R_2)\)

In this section, we will prove the result \((R_2)\). We need to give a notation and introduce some lemmas.

A \textit{k-matching} is a disjoint union of \( k \) edges in \( G \). The number of \textit{k-matching} is denoted by \( m(G, k) \). We agree that \( m(G, 0) = 1 \) and \( m(G, k) = 0 \) \((k < 0)\). In order to compare the energies of two bipartite unicyclic graphs by Definition 1.1, we need to compute the numbers \( b_{2k}(G) \).
Lemma 4.1  [8] Let $G \in \mathcal{BU}(n,l)$. Let $r$ be a positive integer. Then we have the following.

$$b_{2i}(G) = \begin{cases} 
  m(G,i) + 2m(G - C_l, i - \frac{l}{2}), & l = 4r + 2 \\
  m(G,i) - 2m(G - C_l, i - \frac{l}{2}), & l = 4r 
\end{cases}$$

Let $C_6 = v_1v_2v_3v_4v_5v_6v_1$. We denote by $C_6(a_1, a_2, a_3, a_4, a_5, a_6)$ the graph obtained by attaching a pendent path of $P_{a_i+1}$ to vertex $v_i$ of $C_6$ for $i = 1, 2, ..., 6$, respectively (see Fig. 3).

Lemma 4.2  If $n \geq 15$, then $C_6(2, n-8, 0, 0, 0, 0) \to Z_n$.

**Proof.** Let $G = C_6(2, 8, 0, 0, 0, 0)$, $H = Z_{16}$. Then $C_6(2, n-8, 0, 0, 0, 0)$ and $Z_n$ are $k$-subdivision of $G$ and $H$ on some cut edges ($k = n - 16$), respectively. By some calculations we get:

$$f_0 = x(1 + x^2)(2 + x^2)(6 + 73x^2 + 284x^4 + 519x^6 + 507x^8 + 283x^{10} + 90x^{12} + 15x^{14} + x^{16})$$

and $DE(0) = 0.0081$, $DE(1) = 0.0315$.

By Lemma 3.2, we have for $n \geq 16$, $E(C_6(2, n-8, 0, 0, 0, 0)) < E(Z_n)$.

Let $u$ be a vertex of a graph $G$, and $T$ be a rooted tree. Let $G_u(T)$ be the graph obtained by attaching $T$ to $G$ such that the root of $T$ is at $u$. When $T$ is a path $P_{k+1}$ with one of its end vertices as the root, then we simply write $G_u(T)$ as $G_u(k)$. The following three lemmas will be used in the proof of Theorem 4.8.

Lemma 4.3  [16] Let $u$ be a vertex of a bipartite graph $G$ and $T$ be a tree of order $k + 1$. If $G_u(T) \neq G_u(k)$, then $G_u(T) \prec G_u(k)$.
Lemma 4.4 [5] Let $G$ be a graph and $uv$ be an edge of $G$. Then
\[ m(G, k) = m(G - uv, k) + m(G - u - v, k - 1) \quad (0 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor). \]

Lemma 4.5 [5] For any $T$ with order $n$, if $T \neq S_n, T \neq P_n$, then
\[ S_n \prec T \prec P_n. \]

Lemma 4.6 [8] Let $G \in G(n, l)$ where $l \not\equiv 0 \mod 4$. If $G \neq P_n^4$, then $G \prec P_n^4$.

Lemma 4.7 [14] Let $u$ be a non-isolated vertex of a bipartite graph $G$, $w_i$ be a vertex of a bipartite graph $H_i$ $(i = 1, 2)$. Let $G \cdot H_i$ be the coalescence graph of $G$ and $H_i$ at $u$ and $w_i$ $(i = 1, 2)$. Then we have:

If $H_1 \succeq H_2$ and $H_1 - w_1 \succeq H_2 - w_2$, then $G \cdot H_1 \succeq G \cdot H_2$. Furthermore, if one of the two conditions is strict, then we have $G \cdot H_1 \succ G \cdot H_2$.

Theorem 4.8 Let $\Gamma \in BU_2$, then we have $\Gamma < Z_n$ $(n \geq 15)$.

Proof. Let $C_6 = v_1v_2v_3v_4v_5v_6v_1$ be the unique cycle of $\Gamma$. Then $|N(\Gamma)| \geq 2$ for $n \geq 15$.

From Lemma 4.3, we have $\Gamma \succeq C_6(a_1, a_2, a_3, a_4, a_5, a_6)$ where $a_1 + a_2 + a_3 + a_4 + a_5 + a_6 = n - 6$. Let $G_1 = C_6(a_1, n - 8 - a_1, 0, 0, 0, 0)$ and $G_2 = C_6(a_1, a_2, a_3, a_4, a_5, a_6)$. Without loss of generality, assume $a_1 = \max\{a_1, a_2, a_3, a_4, a_5, a_6\} > 2$. We will prove $G_2 \succeq G_1$.

Take $G = P_{a_1}$, $H_1 = C_6(0, n - 8 - a_1, 0, 0, 0, 0) = P_6^{n-a_1}$ and $H_2 = C_6(0, a_2, a_3, a_4, a_5, a_6)$.

Let $u$ be an end vertex of $G$ and $w_1, w_2$ be the vertex of $C_6$ in $H_1$ and $H_2$ corresponding to $v_1$, respectively.

It is easy to see that $G_1 = G \cdot H_1$ and $G_2 = G \cdot H_2$. By Lemmas 4.5, 4.6 we have $H_2 \succeq H_1$ and $H_2 - w_2 \succeq H_1 - w_1 = P_{n-a_1-1}$.

Then, $G_2 \prec G_1$ follows from Lemma 4.7.

Since $G_1 = C_6(a_1, n - 8 - a_1, 0, 0, 0, 0) \prec C_6(2, n - 8, 0, 0, 0, 0)$, We have $\Gamma \prec C_6(2, n - 8, 0, 0, 0, 0)$. By Lemma 4.2, we get $\Gamma < Z_n$. \hfill \blacksquare

5 The proof of $(R_3)$

In this section, we first prove that (1) – (3) of $R_3$ hold.

Lemma 5.1 If $n \geq 41$, then $Z_n \rightarrow C_6(7, n - 14)$.
Proof. Let $G = Z_{41}$, $H = C_6(7, 27)$. Then $Z_n$ and $C_6(7, n - 14)$ are $k$-subdivision of $G$ and $H$ on some cut edges ($k = n - 41$), respectively.

By some calculations we get:

$$f_0 = x(1 + x^2)^3(12 + 339x^2 + 1605x^4 + 3219x^6 + 3406x^8 + 2090x^{10} + 770x^{12} + 168x^{14} + 20x^{16} + x^{18})$$

and $DE(0) \approx 0.00012$, $DE(1) \approx 0.00201$.

By Lemma 3.2, we have for $n \geq 41$, $E(Z_n) < E(C_6(7, n - 14))$.  

Lemma 5.2 If $n \geq 38$, then $C_6(5, n - 12) \rightarrow Z_n$.

Proof. Let $G = C_6(5, 26)$, $H = Z_{38}$. Then $C_6(5, n - 12)$ and $Z_n$ are $k$-subdivision of $G$ and $H$ on some cut edges ($k = n - 38$), respectively.

By some calculations we get:

$$f_0 = x(1 + x^2)^3(2 + x^2)(6 + 120x^2 + 334x^4 + 317x^6 + 136x^8 + 27x^{10} + 2x^{12})$$

and $DE(0) \approx 0.000059$, $DE(1) \approx 0.002223$.

By Lemma 3.2, we have for $n \geq 38$, $E(C_6(5, n - 12)) < E(Z_n)$.  

Lemma 5.3 [18] If $n \geq 27$, then $Y_n \rightarrow C_6(4, n - 11)$.

Lemma 5.4 If $n \geq 19$, then $C_6(6, n - 13) \rightarrow Y_n$.

Proof. Let $G = C_6(6, 6)$, $H = Y_{19}$. Then $C_6(6, n - 13)$ and $Y_n$ are $k$-subdivision of $G$ and $H$ on some cut edges ($k = n - 38$), respectively.

By some calculations we get:

$$f_0 = x^3(1 + x^2)^3(3 + x^2)(41 + 216x^2 + 343x^4 + 245x^6 + 87x^8 + 15x^{10} + x^{12})$$

and $DE(0) \approx 0.0012$, $DE(1) \approx 0.004577$.

By Lemma 3.2, we have for $n \geq 19$, $E(C_6(6, n - 13)) < E(Y_n)$.  

Lemma 5.5 If $n \geq 38$, then $C_6(7, n - 14) \rightarrow 2C_6(2, n - 11)$.

Proof. Let $G = C_6(6, 24)$, $H = 2C_6(2, 27)$. Then $C_6(7, n - 14)$ and $2C_6(2, n - 11)$ are $k$-subdivision of $G$ and $H$ on some cut edges ($k = n - 38$), respectively.

By some calculations we get:

$$f_0 = x(1 + x^2)^3(3 + x^2)(4 + 105x^2 + 461x^4 + 845x^6 + 792x^8 + 408x^{10} + 116x^{12} + 17x^{14} + x^{16})$$
and $DE(0) \doteq 0.000011$, $DE(1) \doteq 0.002229$.

By Lemma 3.2, we have for $n \geq 38$, $E(C_6(n, n-14)) < E(C_6(2, n-11))$. $\blacksquare$

**Lemma 5.6** If $n \geq 78$, then $\tilde{C}_6(2, n-11) \rightarrow C_6(n, n-16)$.

**Proof.** Let $G = \tilde{C}_6(2, 68)$, $H = C_6(9, 63)$. Then $\tilde{C}_6(2, n-11)$ and $C_6(n, n-16)$ are $k$-subdivision of $G$ and $H$ on some cut edges ($k = n-79$), respectively.

By some calculations we get:

$$f_0 = x(x^2 + 3)(x^2 + 1)^2(4 + 148x^2 + 1158x^4 + 4148x^6 + 8223x^8 + 9806x^{10} + 7358x^{12} + 3544x^{14} + 1091x^{16} + 207x^{18} + 22x^{20} + x^{22}).$$

and $DE(0) \doteq 0.000001589$, $DE(1) \doteq 0.000432$.

By Lemma 3.2, we have for $n \geq 79$, $E(\tilde{C}_6(2, n-11)) < E(C_6(9, n-16))$.

For $n = 78$, by directly calculation we have $E(C_6(9, 62)) - E(\tilde{C}_6(2, 67)) \doteq 0.00044$. So the result holds. $\blacksquare$

![Graphs](image_url)

Fig. 4. The graphs $\tilde{C}_6(2, n-8)$ and $C_6 \ast (P_{n-6}(2, 2, n-11), i)$

In the following, we will prove that (4) of $R_3$ holds.

Let $P_n(a, b, c)$ be a tree of order $n$ obtained by attaching three pendent paths of length $a$, $b$ and $c$ to an isolated vertex with one of their end vertices, respectively, where $a+b+c = n-1$. We denote by $\tilde{C}_6(2, n-8)$ the graph obtained by attaching two pendent paths of length 2 and $n-8$ to some vertex of $C_6$ (see Fig. 4). Labeling the vertices of $P_{n-6}(2, 2, n-1)$ with $w_1, w_2, \cdots, w_{n-6}$, let $C_6 \ast (P_{n-6}(2, 2, n-11), i)$ be the graph obtained by joining the vertex $v_i$ of $P_{n-6}(2, 2, n-11)$ with some vertex, say $v_1$, of the cycle $C_6$ (see Fig. 4). Let $P_6 \ast (P_{n-6}(2, 2, n-11), i) = C_6 \ast (P_{n-6}(2, 2, n-11), i) - v_1v_2$, where $v_2$ is the vertex of the cycle of $C_6 \ast (P_{n-6}(2, 2, n-11), i)$ which is adjacent to $v_1$. The following lemma is an alternative form of Theorem 3.6 in [12].

**Lemma 5.7** [12] Let $T$ be a tree of order $n$. If $T \neq P_n, P_n(2, 2, n-5)$, then $m(T, i) \leq m(P_n(2, 4, n-7), i)$, the equality holds if and only if $T = P_n(2, 4, n-7)$. 


Lemma 5.8 [17] Let $e, e'$ be cut edges of bipartite graphs $G$ and $H$ of order $n$, respectively. If $G(0) \preceq H(0)$ and $G(1) \preceq H(1)$, then we have $G(k) \preceq H(k)$ for all $k \geq 2$, with $G(k) \sim H(k)$ if and only if both the two relations $H(0) \sim G(0)$ and $H(1) \sim G(1)$ hold.

Lemma 5.9 If $n \geq 15$, then $\widetilde{C}_6(2, n - 8) \prec Z_n$.

Proof. Let $G = \widetilde{C}_6(2, 7), H = Z_{15}$. Then for $n \geq 15$, $\widetilde{C}_6(2, n - 8)$ and $Z_n$ are $(n - 15)$-subdivision graph of $G$ and $H$, respectively.

By some calculations we get:

$$\begin{align*}
\tilde{\phi}(G(0)) &= 19x + 129x^3 + 322x^5 + 391x^7 + 252x^9 + 87x^{11} + 15x^{13} + x^{15}; \\
\tilde{\phi}(H(0)) &= 23x + 145x^3 + 347x^5 + 410x^7 + 259x^9 + 88x^{11} + 15x^{13} + x^{15}; \\
\tilde{\phi}(G(1)) &= 4 + 68x^2 + 297x^4 + 574x^6 + 581x^8 + 326x^{10} + 101x^{12} + 16x^{14} + x^{16}; \\
\tilde{\phi}(H(1)) &= 4 + 76x^2 + 325x^4 + 612x^6 + 606x^8 + 334x^{10} + 102x^{12} + 16x^{14} + x^{16}.
\end{align*}$$

Then $G(0) \prec H(0), G(1) \prec H(1)$. By Lemma 5.8, we have $\widetilde{C}_6(2, n - 8) \prec Z_n$. $\blacksquare$

Lemma 5.10 If $n \geq 16$, then $C_6 \ast (P_{n-6}(2, 2, n-11), 3) \rightarrow Z_n$.

Proof. Let $G = C_6 \ast (P_{10}(2, 2, 5), 3), H = Z_{16}$. Then $C_6 \ast (P_{n-6}(2, 2, n-11), 3)$ and $Z_n$ are $k$-subdivision of $G$ and $H$ on some cut edges ($k = n - 16$), respectively.

By some calculations we get:

$$f_0 = x^3(1 + x^2)^5(47 + 216x^2 + 211x^4 + 84x^6 + 15x^8 + x^{10})$$

and $DE(0) = 0.04092, DE(1) = 0.04633$.

By Lemma 3.2, we have for $n \geq 16$, $E(C_6 \ast (P_{n-6}(2, 2, n-11), 3)) < E(Z_n)$. $\blacksquare$

The following lemma is an alternative form of Theorem 2.2 in [13] which will be used to compare the matching numbers of two trees.

Lemma 5.11 [13] Let $a + b = c + d$ with $0 \leq a \leq b$ and $0 \leq c \leq d$. Let $a < c$. Then we have:

1. If $a$ is even, then $m(P_a \cup P_b, i) \geq m(P_c \cup P_d, i)$. Furthermore, there exists at least one index $i$ such that the above inequality is strict.
2. If $a$ is odd, then $m(P_a \cup P_b, i) \leq m(P_c \cup P_d, i)$. Furthermore, there exists at least one index $i$ such that the above inequality is strict.

Lemma 5.12 If $n \geq 14$, then $C_6 \ast (P_{n-6}(2, 2, n-11), i) \leq C_6 \ast (P_{n-6}(2, 2, n-11), 3)$ for $i = 2, \ldots, n - 9$. 

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Proof. Take $H_1 = H_2 = P_{n-6}(2,2,n-11)$, $v_1 = w_3$ and $v_2 = w_i$. Then $H_1 - v_1 = P_2 \cup P(2,2,n-14)$ and

$$H_2 - v_2 = \begin{cases} P_{i-1} \cup P(2,2,n-11-i) & \text{if } 2 \leq i \leq n-11; \\ P_2 \cup P_2 \cup P_{n-11} & \text{if } i = n-10; \\ P_1 \cup P_{n-8} & \text{if } i = n-9. \end{cases}$$

By some calculations we have $P_1 \cup P_5 < P_2 \cup P(2,2,1)$ and $P_1 \cup P_6 < P_2 \cup P(2,2,2)$. Then by Lemma 5.8, we have $P_{i-1} \cup P(2,2,n-11)$ is subgraph of $P_2 \cup P(2,2,n-14)$, $H_2 - v_2 < H_1 - v_1$ for $i = n-10$.

Since $\overline{\phi}(P_2 \cup P(2,2,n-14), x) = \overline{\phi}(2P_2 \cup P_{n-11}, x) + \overline{\phi}(2P_2 \cup P_{i-1} \cup P_{n-11-i}, x)$

By Lemma 5.11, we have $P_{i-1} \cup P_{n-8-i} \leq P_2 \cup P_{i-1} \cup P_{n-11-i}$ and $P_{i-1} \cup P_{n-8-i} \leq P_2 \cup P_{n-14}$ for $2 \leq i \leq n-11$.

Hence $P_{i-1} \cup P(2,2,n-11-i) \leq P_2 \cup P(2,2,n-14)$ for $2 \leq i \leq n-11$.

Then $H_2 - v_2 < H_1 - v_1$ for $2 \leq i \leq n-9$. Let $G = P_i^v$ and $u$ be the vertex of degree 1 of $G$. By Lemma 4.7, we have $C_6 \ast (P_{n-6}(2,2,n-11), i) \leq C_6 \ast (P_{n-6}(2,2,n-11), 3)$. 

**Lemma 5.13** [16] Let $u$ be a vertex of a bipartite graph $G$. Denote by $G_u(a,b)$ the graph obtained by attaching to $G$ two pendent paths of length $a$ and $b$ at $u$ (as shown in Fig.4).

Let $a,b,c,d$ be nonnegative integers with $a \leq b$, $c \leq d$, $a + b = c + d$, and $a < c$. If $u$ is a non-isolated vertex of a bipartite graph $G$, then the following statements are true:

1. If $a$ is even, then $G_u(a,b) \succ G_u(c,d)$;
2. If $a$ is odd, then $G_u(a,b) < G_u(c,d)$.

**Theorem 5.14** Let $G \in BU_3 \setminus A_n$. If $G \neq Y_n, Z_n, \overline{C_6}(2,n-11)$, then $G \prec Z_n$.

**Proof.** Let $C_6 = v_1v_2v_3v_4v_5v_6v_1$ be the unique cycle of $G$. Since $|N(G)| = 1$, without loss of generality, we assume that $d_G(v_1) \geq 3$. We consider the following two cases.

Case 1. $d_G(v_1) \geq 4$. From Lemmas 4.3 and 5.13, we can get that the graph with maximal energy in this case is $\overline{C_6}(2,n-8)$. Furthermore, by Lemma 5.9, we get $G \prec Z_n$.

Case 2. $d_G(v_1) = 3$. Since $G \in BU_3 \setminus A_n$, we have $G - C_6 \neq P_{n-6}$. We distinguish the following two subcases.

Subcase 2.1. $G - C_6 \neq P_{n-6}(2,2,n-11)$. From Lemma 4.1, we can get the following
two equations:

\[ b_{2k}(G) = m(G, k) + 2m(G - C_6, k - 3); \]
\[ b_{2k}(Z_n) = m(Z_n, k) + 2m(P_{n-6}(2, 4, n - 13), k - 3). \]

Since \( G - C_6 \neq P_{n-6}, P_{n-6}(2, 2, n - 11) \), by Lemma 5.7, we have \( m(G - C_6, k - 3) \leq m(P_{n-6}(2, 4, n - 13), k - 3) \). Then \( m(P_4 \cup (G - C_6), k - 1) \leq m(P_4 \cup P_{n-6}(2, 4, n - 13), k - 1) \). Moreover, from Lemma 4.4,

\[ m(G, k) = m(G - v_1v_2, k) + m(P_4 \cup (G - C_6), k - 1); \]
\[ m(Z_n, k) = m(P_n(2, 4, n - 7), k) + m(P_4 \cup P_{n-6}(2, 4, n - 13), k - 1). \]

Since \( G \not\in \mathcal{A}_n, G \neq Y_n \), we get \( G - v_1v_2 \neq P_n, P_n(2, 2, n - 5) \). From Lemma 5.7, we have \( m(G - v_1v_2, k) \leq m(P_n(2, 4, n - 7), k) \), the equality holds if and only if \( G - v_1v_2 = P_n(2, 4, n - 7) \). Hence \( b_{2k}(G) \leq b_{2k}(Z_n) \). Since \( G \neq Z_n \), we have \( G - v_1v_2 \neq P_n(2, 4, n - 7). \) Then \( G \prec Z_n. \)

Subcase 2.2. \( G - C_6 = P_{n-6}(2, 2, n - 11) \). Then \( G = C_6 \ast (P_{n-6}(2, 2, n - 11), i) \). Note that \( G = Y_n \) when \( i = 1 \); \( G = C_6(2, n - 11) \) when \( i = n - 8 \). By Lemmas 4.1 we have \( C_6 \ast (P_{n-6}(2, 2, n - 11), i) \preceq C_6 \ast (P_{n-6}(2, 2, n - 11), 3) \) for \( 2 \leq i \leq n - 9 \). Then by Lemma 5.10, we can get \( C_6 \ast (P_{n-6}(2, 2, n - 11), i) \prec Z_n \) when \( 2 \leq i \leq n - 9 \). So we have \( G \prec Z_n. \) We complete the proof.

References


