MATCH
Communications in Mathematical
and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. 82 (2019) 443-458

ISSN 0340 - 6253

Ordering of Connected Bipartite Unicyclic Graphs with Large Energies*

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(Received October 11, 2018)

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 $\lfloor \frac{n-5}{2} \rfloor$ 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 π-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 $\phi(G, x) = \sum_{i=0}^{n} a_i(G) x^{n-i}$.

*This research is supported by NSFC (No. 11371372); supported by the Fundamental Research Funds for the Central Universities (No. 22120180254).

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

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

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

Assume that

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

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

$$E(G)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln(\sum_{i=0}^{\lfloor n/2\rfloor} b_{2i}(G)x^{2i})dx. \tag{2}$$

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

Defintion 1.1 Let G_1 and G_2 be two bipartite graphs of order n. If $b_{2i}(G_1)\le b_{2i}(G_2)$ for all i with $0\le i\le\lfloor n/2\rfloor$, 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]:

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

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

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

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

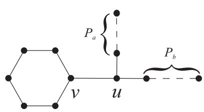

Fig. 1. The graph $C_6(a,b)$

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_7^6, 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 $\lfloor \frac{n-5}{2} \rfloor$ largest energies of connected bipartite unicyclic graphs with $n \geq 78$ vertices.

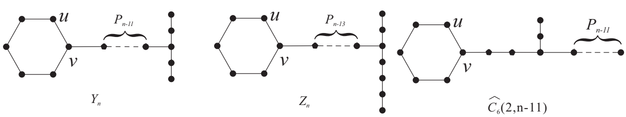

Fig. 2. The graphs Y_n, Z_n and $\widehat{C_6}(2, n-11)$

Denote by $\mathcal{BU}(n)$ 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^6_{n-4} (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^6_{n-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^6_9 (see Fig. 2). Now we give the main result of this paper.

Theorem 1.1 *Let $G \in \mathcal{BU}(n)$, $k = \lfloor \frac{n-7}{2} \rfloor$, $t = \lfloor \frac{k}{2} \rfloor$ 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:*

$$\begin{aligned} &C_6(0, n-7) \leftharpoonup C_6(2, n-9) \leftharpoonup C_6(4, n-11) \leftharpoonup Y_n \leftharpoonup C_6(6, n-13) \leftharpoonup \cdots \\ &\leftharpoonup C_6(2t, n-7-2t) \leftharpoonup C_6(2l+1, n-8-2l) \leftharpoonup \cdots \leftharpoonup C_6(9, n-16) \leftharpoonup \widehat{C_6}(2, n-11) \\ &\leftharpoonup C_6(7, n-14) \leftharpoonup Z_n. \end{aligned}$$

2 The basic strategy of the proof of Theorem 1.1

Let $\mathcal{BU}(n, l)$ 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 $\mathcal{A}(n)$:*

$$\begin{aligned} &C_6(0, n-7) \leftharpoonup C_6(2, n-9) \leftharpoonup C_6(4, n-11) \leftharpoonup \cdots \leftharpoonup C_6(2t, n-7-2t) \\ &\qquad \leftharpoonup C_6(2l+1, n-8-2l) \leftharpoonup \cdots \leftharpoonup C_6(5, n-12) \leftharpoonup C_6(3, n-10) \leftharpoonup C_6(1, n-8). \end{aligned}$$

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

$$\mathcal{BU}_1 = \{G \mid G \in \mathcal{BU}(n, l), l \neq 6\};$$

$$\mathcal{BU}_2 = \{G \mid G \in \mathcal{BU}(n, 6), |N(G)| \neq 1\};$$

$$\mathcal{BU}_3 = \{G \mid G \in \mathcal{BU}(n, 6), |N(G)| = 1\}.$$

It follows that $\mathcal{BU}(n) = \mathcal{BU}_1 \cup \mathcal{BU}_2 \cup \mathcal{BU}_3$ and $\mathcal{A}(n) \subseteq \mathcal{BU}_3$.

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 $G \in \mathcal{BU}_1$, we have $G \rightharpoonup Z_n$.

(R_2): For any $G \in \mathcal{BU}_2$, we have $G \rightharpoonup Z_n$.

(R_3): (1) $C_6(5, n-12) \rightharpoonup Z_n \rightharpoonup C_6(7, n-14)$;
(2) $C_6(6, n-13) \rightharpoonup Y_n \rightharpoonup C_6(4, n-11)$;
(3) $C_6(7, n-14) \rightharpoonup \widehat{C_6}(2, n-11) \rightharpoonup C_6(9, n-16)$;
(4) For any $G \in \mathcal{BU}_3 \backslash \mathcal{A}(n)$, if $G \neq Y_n, Z_n, \widehat{C_6}(2, n-11)$, then we have $G \rightharpoonup Z_n$.

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.

Defintion 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:*

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

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 $g_k = \widetilde{\phi}(G(k), x)$, $h_k = \widetilde{\phi}(H(k), x)$, $f_k = h_{k+1}g_k - h_k g_{k+1}$ 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 $k > l \geq 0$.

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

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

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

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 $DE(0) \doteq 0.00077$, $DE(1) \doteq 0.0766$.

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

Next we prove $P_n^{n-2} \rightharpoonup Z_n$ 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) $\widetilde{\phi}(C_n, x) = \widetilde{\phi}(P_n, x) + \widetilde{\phi}(P_{n-2}, x) - 2$;
(ii) $\widetilde{\phi}(P_n^{n-2}, x) = \widetilde{\phi}(P_n, x) + (x^2+1)\widetilde{\phi}(P_{n-4}, x) + 2(x^2+1)$.
(2) If $n = 4k+2$, then we have:
(i) $\widetilde{\phi}(C_n, x) = \widetilde{\phi}(P_n, x) + \widetilde{\phi}(P_{n-2}, x) + 2$;
(ii) $\widetilde{\phi}(P_n^{n-2}, x) = \widetilde{\phi}(P_n, x) + (x^2+1)\widetilde{\phi}(P_{n-4}, x) - 2(x^2+1)$.

Lemma 3.8 *[18] (1) Let $h_n = \widetilde{\phi}(P_n, x) + \widetilde{\phi}(P_{n-2}, x)$. Then $h_n = xh_{n-1} + h_{n-2}$.*
(2) Let $h_n' = \widetilde{\phi}(P_n, x) + (x^2+1)\widetilde{\phi}(P_{n-4}, x)$. Then $h_n' = xh_{n-1}' + h_{n-2}'$.

Lemma 3.9 *If $n \geq 16$ and n is even, then $P_n^{n-2} \rightharpoonup Z_n$.*

Proof. Let $h_n = \widetilde{\phi}(P_n, x) + (x^2+1)\widetilde{\phi}(P_{n-4}, x)$. From Lemmas 3.7 and 3.8, we have

$$\widetilde{\phi}(P_n^{n-2}, x) = \begin{cases} h_n + 2(x^2+1) & n = 4k \\ h_n - 2(x^2+1) & n = 4k+2 \end{cases} \tag{3}$$

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

Case 1. $n = 4k$. Then $d_n = \frac{h_n+2(x^2+1)}{g_n}$. 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

$$\begin{aligned} E(P_n^{n-2}) - E(Z_n) &= \frac{2}{\pi}\int_0^{+\infty} \ln d_n dx \\ &\leq \frac{2}{\pi}\int_0^{+\infty} \ln d_{16} dx \\ &= E(P_{16}^{14}) - E(Z_{16}) \\ &\doteq -0.02341 < 0. \end{aligned}$$

Thus the result holds. ■

Finally, we prove that $C_n \rightharpoonup Z_n$ for $n \geq 36$.

Lemma 3.10 *If $n \geq 36$ and n is even, then $C_n \rightharpoonup Z_n$.*

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

$$\widetilde{\phi}(C_n, x) = \begin{cases} h_n - 2 & n = 4k \\ h_n + 2 & n = 4k+2 \end{cases} \tag{4}$$

and $h_n = xh_{n-1} + h_{n-2}$. Let $g_n = \widetilde{\phi}(Z_n, x)$. By Lemma 3.1, we can see that $g_n = xg_{n-1} + g_{n-2}$. Write $d_n = \frac{\widetilde{\phi}(C_n,x)}{\widetilde{\phi}(Z_n,x)}$. 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 $F(x) = x^2(1+x^2)(2+x^2)(4+x^2)(22+219x^2+797x^4+1379x^6+1249x^8+614x^{10}+162x^{12}+21x^{14}+x^{16})$. 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 $H(x) = -x^2(1+x^2)(4+x^2)(26+386x^2+1517x^4+2731x^6+2691x^8+1581x^{10}+576x^{12}+130x^{14}+17x^{16}+x^{18})$. 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

$$\begin{aligned} E(C_n) - E(Z_n) &= \frac{2}{\pi}\int_0^{+\infty} \ln d_n dx \\ &\leq \frac{2}{\pi}\int_0^{+\infty} \ln d_{38} dx \\ &= E(C_{38}) - E(Z_{38}) \\ &\doteq -0.00013 < 0. \end{aligned}$$

Thus the result holds. ■

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

Theorem 3.11 *If $G \in \mathcal{BU}_1$, then we have $G \rightharpoonup Z_n$ $(n \geq 36)$.*

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 *k-matching* is a disjoint union of k edges in G. The number of *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.*

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

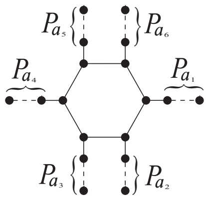

Fig. 3. The graph $C_6(a_1, a_2, a_3, a_4, a_5, a_6)$

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 $C_6(2, n-8, 0, 0, 0, 0) \rightharpoonup Z_n$.*

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 $DE(0) \doteq 0.0081$, $DE(1) \doteq 0.0315$.

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

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*

$$m(G,k) = m(G-uv,k) + m(G-u-v,k-1) \quad (0 \le k \le \lfloor \frac{n}{2} \rfloor).$$

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 $G \neq P_n^l$ then $G \prec P_n^l$.*

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 $H_1 \succcurlyeq H_2$ and $H_1 - w_1 \succcurlyeq H_2 - w_2$, then $G \cdot H_1 \succcurlyeq G \cdot H_2$. 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 $\Gamma \in \mathcal{BU}_2$, then we have $\Gamma \prec Z_n$ $(n \ge 15)$.*

Proof. Let $C_6 = v_1v_2v_3v_4v_5v_6v_1$ be the unique cycle of Γ. Then $|N(\Gamma)| \ge 2$ for $n \ge 15$. From Lemma 4.3, we have $\Gamma \preceq C_6(a_1,a_2,a_3,a_4,a_5,a_6)$ 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 $G_2 \preceq G_1$. 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 $H_2 \preceq H_1$ and $H_2 - w_2 \preceq H_1 - w_1 = P_{n-a_1-1}$.

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 $\Gamma \prec Z_n$. ∎

5 The proof of (R_3)

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

Lemma 5.1 *If $n \ge 41$, then $Z_n \rightharpoonup C_6(7, n-14)$.*

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 $DE(0) \doteq 0.00012$, $DE(1) \doteq 0.00201$.

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

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

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 $DE(0) \doteq 0.000059$, $DE(1) \doteq 0.002223$.

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

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

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

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 $DE(0) \doteq 0.0012$, $DE(1) \doteq 0.004577$.

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

Lemma 5.5 *If $n \geq 38$, then $C_6(7, n-14) \rightharpoonup \widehat{C_6}(2, n-11)$.*

Proof. Let $G = C_6(6, 24)$, $H = \widehat{C_6}(2, 27)$. Then $C_6(7, n-14)$ and $\widehat{C_6}(2, n-11)$ 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 $n \geqslant 38$, $E(C_6(7, n-14)) < E(\widehat{C_6}(2, n-11))$. ■

Lemma 5.6 *If $n \geq 78$, then $\widehat{C_6}(2, n-11) \rightharpoonup C_6(9, n-16)$.*

Proof. Let $G = \widehat{C_6}(2, 68)$, $H = C_6(9, 63)$. Then $\widehat{C_6}(2, n-11)$ and $C_6(9, n-16)$ 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 $n \geqslant 79$, $E(\widehat{C_6}(2, n-11)) < E(C_6(9, n-16))$

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

$\widetilde{C_6}(2,n-8)$ $C_6 * (P_{n-6}(2,2,n-11),i)$

Fig. 4. The graphs $\widetilde{C_6}(2, n-8)$ and $C_6 * (P_{n-6}(2, 2, n-11), i)$

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 pendant 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 $\widetilde{C_6}(2, n-8)$ 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 $C_6 * (P_{n-6}(2, 2, n-11), i)$ be the graph obtained by joining the vertex w_i of $P_{n-6}(2, 2, n-11)$ with some vertex, say v_1, of the cycle C_6 (see Fig. 4). Let $P_6 * (P_{n-6}(2, 2, n-11), i) = C_6 * (P_{n-6}(2, 2, n-11), i) - v_1v_2$, where v_2 is the vertex of the cycle of $C_6 * (P_{n-6}(2, 2, n-11), i)$ 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 $G(0) \preccurlyeq H(0)$ and $G(1) \preccurlyeq H(1)$, then we have $G(k) \preccurlyeq H(k)$ 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:

$\widetilde{\phi}(G(0)) = 19x + 129x^3 + 322x^5 + 391x^7 + 252x^9 + 87x^{11} + 15x^{13} + x^{15}$;

$\widetilde{\phi}(H(0)) = 23x + 145x^3 + 347x^5 + 410x^7 + 259x^9 + 88x^{11} + 15x^{13} + x^{15}$;

$\widetilde{\phi}(G(1)) = 4 + 68x^2 + 297x^4 + 574x^6 + 581x^8 + 326x^{10} + 101x^{12} + 16x^{14} + x^{16}$;

$\widetilde{\phi}(H(1)) = 4 + 76x^2 + 325x^4 + 612x^6 + 606x^8 + 334x^{10} + 102x^{12} + 16x^{14} + x^{16}$.

Then $G(0) \prec H(0), G(1) \prec H(1)$. By Lemma 5.8, we have $\widetilde{C_6}(2, n-8) \prec Z_n$. ■

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

Proof. Let $G = C_6 * (P_{10}(2, 2, 5), 3)$, $H = Z_{16}$. Then $C_6 * (P_{n-6}(2, 2, n-11), 3)$ 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 $DE(0) \doteq 0.04092$, $DE(1) \doteq 0.04633$.

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

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 $C_6 * (P_{n-6}(2, 2, n-11), i) \preceq C_6 * (P_{n-6}(2, 2, n-11), 3)$ for $i = 2, \ldots, n-9$.*

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

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

By some calculations we have $P_1 \cup P_5 \prec P_2 \cup P(2,2,1)$ and $P_1 \cup P_6 \prec P_2 \cup P(2,2,2)$. Then by Lemma 5.8, we have $H_2 - v_2 \prec H_1 - v_1$ for $i = n-9$.

Since $P_2 \cup P_2 \cup P_{n-11}$ is subgraph of $P_2 \cup P(2,2,n-14)$, $H_2 - v_2 \prec H_1 - v_1$ for $i = n-10$.

Since $\widetilde{\phi}(P_2 \cup P(2,2,n-14),x) = \widetilde{\phi}(2P_2 \cup P_{n-11},x) + \widetilde{\phi}(2P_2 \cup P_1 \cup P_{n-14},x)$

$\widetilde{\phi}(P_{i-1} \cup P(2,2,n-11-i),x) = \widetilde{\phi}(P_2 \cup P_{i-1} \cup P_{n-8-i},x) + \widetilde{\phi}(P_{i-1} \cup P_2 \cup P_1 \cup P_{n-11-i},x)$.

By Lemma 5.11, we have

$P_{i-1} \cup P_{n-8-i} \preceq P_2 \cup P_{n-11}$ and $P_{i-1} \cup P_{n-i-11} \preceq P_2 \cup P_{n-14}$ for $2 \le i \le n-11$.

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

Then $H_2 - v_2 \prec H_1 - v_1$ for $2 \le i \le n-9$. Let $G = P_7^6$ and u be the vertex of degree 1 of G. By Lemma 4.7, we have $C_6 * (P_{n-6}(2,2,n-11),i) \preceq C_6 * (P_{n-6}(2,2,n-11),3)$. ■

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 $a \le b$, $c \le d$, $a+b = c+d$, 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 $G_u(a,b) \prec G_u(c,d)$.

Theorem 5.14 *Let $G \in \mathcal{BU}_3 \backslash \mathcal{A}_n$. If $G \ne Y_n, Z_n, \widehat{C_6}(2,n-11)$, 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 $d_G(v_1) \ge 3$. We consider the following two cases.

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

Case 2. $d_G(v_1) = 3$. Since $G \in \mathcal{BU}_3 \backslash \mathcal{A}_n$, we have $G - C_6 \ne P_{n-6}$. We distinguish the following two subcases.

Subcase 2.1. $G - C_6 \ne P_{n-6}(2,2,n-11)$. 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 $G \notin \mathcal{A}_n$, $G \neq Y_n$, 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 $G = C_6 * (P_{n-6}(2,2,n-11), i)$. Note that $G = Y_n$ when $i = 1$; $G = \widehat{C_6}(2, n-11)$ when $i = n-8$. By Lemmas 4.1 we have $C_6 * (P_{n-6}(2,2,n-11), i) \preceq C_6 * (P_{n-6}(2,2,n-11), 3)$ for for $2 \leq i \leq n-9$. Then by Lemma 5.10, we can get $C_6 * (P_{n-6}(2,2,n-11), i) \prec Z_n$ when $2 \leqslant i \leqslant n-9$. So we have $G \prec Z_n$. We complete the proof. ■

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