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Bipartite Unicyclic Graphs with Large Energy

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Abstract

Let G be a graph with n vertices and $\lambda_1, \lambda_2, \dots, \lambda_n$ be n eigenvalues of its adjacency matrix A(G). The energy of G, denoted by E(G), is defined to be the summation $\sum_{i=1}^{n} |\lambda_i|$. Denote by \mathcal{BU}_n the set of connected bipartite unicyclic graphs on n vertices. For $n \geq l+1$, let P_n^l be graph obtained by identifying one pendent vertex of the path P_{n-l+1} with any vertex of the cycle C_l . Recently, I. Gutman^[7] and Y. Hou^[10] determined that P_n^6 is the unique graph with the greatest energy among all graphs in $\mathcal{BU}_n \setminus \{C_n\}$. Let $\mathcal{BU}_n^* = \mathcal{BU}_n \setminus \{C_n, P_n^l, l = 4, 5, \dots, n-1\}$. It is proved in this paper that for $n \geq 13$, $M_n^{6,3}$ is the graph with maximal energy among all graphs in \mathcal{BU}_n^* , where $M_n^{6,3}$ is the graph obtained by joining (by a new edge) any vertex of the hexagon with the vertex 3 of the path P_{n-6} .

1 Introduction

Let G be a connected graph with n vertices and A(G) be its adjacency matrix. The characteristic polynomial of A(G) is defined to be

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

which is also said to be the characteristic polynomial of G. All n roots $\lambda_1, \lambda_2, \dots, \lambda_n$ of $\phi(G; x)$ are called to be eigenvalues of G. It's not difficult to see that each λ_i $(i = 1, 2, \dots, n)$ is real since A(G) is symmetric.

The energy of G, denoted by E(G), is defined to be $\sum_{i=1}^{n} |\lambda_i|$. It's well known that E(G) can

be expressed as the coulson integral formula

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

where a_0, a_1, \dots, a_n are coefficients of characteristic polynomial of G.

Since the energy of a graph can be used to estimate approximately the total π -electron energy of the molecule, it has been intensively studied by many scholars. For more details see [3-10]; for some recent research along these lines see [11-22]. The interested reader may also refer to [23,24] for the mathematical properties of E(G).

As usual, we begin with some notations and terminologies. For a graph G, we use V(G)and E(G) to denote its set of vertices and edges, respectively. Let $d_G(v)$ denote the degree of vertex v, namely the number of edges incident with v in G. By $d_G(x, y)$ we mean the length of the shortest path connecting vertices x and y, i.e., the distance between x and y in G. Let $V_p(G)$ denote the set of pendent vertices in G. By S_n , C_n and P_n we denote respectively the star graph, the cycle graph and the path graph with n vertices. Let $P_n^l(n \ge l+1)$ be graph obtained by identifying one pendent vertex of the path P_{n-l+1} with any vertex of the cycle C_l . Denote by K_n^l $(n \ge l+2)$ the graph obtained from P_{n-1}^l by attaching one pendent edge to one neighbor (lying on C_l) of the unique 3-degree vertex of P_{n-1}^l . By R_n^l $(n \ge l+4)$ we denote the graph obtained by attaching a path of length 2 to one neighbor (lying on C_l) of the unique 3-degree vertex of P_{n-2}^l . Let $Q_n^l(n \ge l+5)$ be graph obtained by identifying the middle-point of the path P_5 with the unique pendent vertex of P_{n-4}^l . Fig.1. illustrate P_n^l , K_n^l , R_n^l and Q_n^l , respectively.





Denote by \mathcal{U}_n and \mathcal{BU}_n the set of connected unicyclic graphs and bipartite unicyclic graphs on *n* vertices, respectively. Let *G* be any graph in \mathcal{U}_n and *v* the vertex lying on its unique cycle. If $d_G(v) \ge 3$, then v is said to be a branched vertex. For a given vertex $x \notin V(C_l)$ in G, let $d_G(x, C_l) = min\{d_G(x, y)|y \in V(C_l)\}$, where C_l is the cycle in G.

Let $\mathcal{BU}_n^* = \mathcal{BU}_n \setminus \{C_n, P_n^l, l = 4, 5, \cdots, n-1\}$. For any graph $G \in \mathcal{BU}_n^*$, let C_l be the cycle of length l in G. Then $n \geq l+2$, i.e., $V_p(G) \neq \emptyset$. Let $\mathcal{BU}_{n,1}^* = \{G \in \mathcal{BU}_n^* | \text{there exists } x \in V_p(G) \text{ such that } d_G(x, C_l) = 1\}$. Set $\mathcal{BU}_{n,2}^* = \mathcal{BU}_n^* \setminus \mathcal{BU}_{n,1}^*$. Let $\mathcal{BU}_{n,2}^{*b}$ denote the subset of $\mathcal{BU}_{n,2}^*$ such that for any $G \in \mathcal{BU}_{n,2}^{*b}$, there's exactly one branched vertex in the unique cycle of G. Denote by $\mathcal{BU}_{n,2}^{*a}$ the set $\mathcal{BU}_{n,2}^* \setminus \mathcal{BU}_{n,2}^{*b}$. By $\mathcal{BU}_{n,2}^{*b}(l)$ we mean the subset of $\mathcal{BU}_{n,2}^{*b}$ such that for each graph G in $\mathcal{BU}_{n,2}^{*b}(l)$, G has a unique cycle of length l. Similarly, we can define respectively the sets $\mathcal{BU}_{n,1}(l)$, $\mathcal{BU}_{n,2}^{*a}(l)$, $\mathcal{U}_n(l)$ and $\mathcal{BU}_n(l)$ in this way.

In this paper, we determined the graph with maximal energy among all graphs in \mathcal{BU}^*_n .

2 Lemmas and Results

Sachs theorem [25] states that

$$a_i(G) = \sum_{S \in L_i} (-1)^{k(S)} 2^{c(S)}, \tag{2}$$

where L_i denote the set of Sachs graphs G with *i* vertices, k(S) is number of components of S and c(S) is the number of cycles contained in S.

Set $b_i(G) = |a_i(G)|$ $(i = 0, 1 \cdots, n)$. From Eq.(2), we find that $b_2(G)$ is equal to the number of edges of G. Let m(G, k) denote the number of k-matchings of a graph G. If G contains no cycle, then $b_{2k}(G) = m(G, k)$ and $b_{2k+1}(G) = 0$ for each $k \ge 0$. It's both consistent and convenient to define $b_k(G) = 0$ and m(G; k) = 0 for the case when k < 0.

In [8], Y. Hou obtained the following result.

Lemma 1. Let $G \in \mathcal{U}_n(l)$. Then $(-1)^k a_{2k} \ge 0$ for all $k \ge 0$; and $(-1)^k a_{2k+1} \ge 0$ (resp. ≤ 0) for all $k \ge 0$ if l = 2r + 1 and r is odd (resp. even).

From Eq.(1) and lemma 1, we obtain

$$E(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{1}{x^2} ln \left[\left(\sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_{2i} x^{2i} \right)^2 + \left(\sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_{2i+1} x^{2i+1} \right)^2 \right] dx.$$
(3)

It follows from (3) that E(G) is a strictly increasing function of $b_i(G)$ for $i = 0, 1, \dots, n$. That is to say, for any two unicyclic graphs G_1 and G_2 , there exists

$$b_i(G_1) \ge b_i(G_2) \text{ for all } i \ge 0 \Rightarrow E(G_1) \ge E(G_2).$$
 (4)

If $b_i(G_1) \ge b_i(G_2)$ holds for all $i \ge 0$, then we write $G_1 \succeq G_2$ or $G_2 \preceq G_1$. If $G_1 \succeq G_2$ and there exists some i_0 such that $b_{i_0}(G_1) > b_{i_0}(G_2)$, then we write $G_1 \succ G_2$.

According to the above relations, the following lemma follows readily.

Lemma 2. Let G_1 and G_2 be two graphs. Then $G_1 \succeq G_2$ implies that $E(G_1) \ge E(G_2)$ and $G_1 \succ G_2$ implies that $E(G_1) > E(G_2)$.

The following lemma is crucial to the proof of our main result.

Lemma 3. Let G be a unicyclic graph on n vertices with its cycle being C_l . Let uv be an edge in E(G), we have

(a). If $uv \in C_l$, then $b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) - 2b_{i-l}(G - C_l)$ if $l \equiv 0 \pmod{4}$ and $b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-l}(G - C_l)$ if $l \not\equiv 0 \pmod{4}$;

(b). If $uv \notin C_l$, then $b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v)$. In particular, if uv is a pendent edge with pendent vertex v, then $b_i(G) = b_i(G - v) + b_{i-2}(G - u - v)$.

Proof. Recall that

$$\phi(G;x) = \phi(G - uv;x) - \phi(G - u - v;x) - 2\sum_{C \in \mathscr{C}_{uv}} \phi(G - C;x),$$
(5)

where \mathscr{C}_{uv} denotes the set of cycles containing uv.

One can easily obtain the desired result by equating the coefficients of x^{n-i} on both sides of Eq.(5). \Box

F. Li and B. Zhou obtained the following result in [21].

Lemma 4. Let G be a unicyclic graph in \mathscr{U}_n and G' the graph obtained from G by deleting at least one edge outside its unique cycle. Then $G' \prec G$.

I. Gutman [3] show that n-vertex path P_n is the unique graph with the maximal energy among all all acyclic graphs on n vertices. The following lemma could be found in [1] as proposition 9.

Lemma 5. Let T be a tree of order $n \ge 6$ not isomorphic to P_n . Then $E(T) \le E(T_n^2)$ with equality if and only if $T \cong T_n^2$, where T_n^2 is the tree obtained by pasting one endpoint of P_{n-4} to the middle vertex of P_5 . (See Fig.2. for T_n^2).

In addition to the trees with maximal and second-maximal energy, also the trees with thirdmaximal, fourth-maximal, ... energy are determined by F. Zhang and H. Li [6].



 T_n^2 with $n \ge 8$ vertices.

Fig.2.

Lemmas 6—8 given below are due to Y. Hou in [10].

Lemma 6. Let $G \in \mathscr{U}_n(l)$ with $l \not\equiv 0 \pmod{4}$. If $G \ncong P_n^l$, then $G \prec P_n^l$.

Let C(n, l) be the set of unicyclic graphs obtained from C_l by attaching to it n - l pendent vertices.

Lemma 7. Let $G \in \mathscr{U}_n(l)$ with $l \equiv 0 \pmod{4}$. If $G \ncong \mathcal{C}(n,l), P_n^l$, then $G \prec P_n^l$.

Lemma 8. Let G be any connected graph in \mathscr{U}_n and $G \not\cong C_n$. Then $E(G) \leq E(P_n^6)$ with equality only if l = 6.

Lemma 9. Suppose $4 \le l \le n-6$. If $l \ne 4, 6$, then $P_{l-2} \cup T_{n-l}^2 \le P_4 \cup T_{n-6}^2 \le P_2 \cup T_{n-4}^2$.

Proof. From [3], we know that $P_2 \cup P_{n-2} \succeq P_4 \cup P_{n-4} \succeq P_i \cup P_{n-i}$ for any integer $1 \le i \le n-1$ and $i \ne 2, 4$. Note that

$$\begin{split} m(P_{l-2}\cup T^2_{n-l};k) &= m(P_{l-2}\cup P_2\cup P_{n-l-2};k) + m(P_{l-2}\cup P_2\cup P_{n-l-5};k-1), \\ m(P_4\cup T^2_{n-6};k) &= m(P_4\cup P_2\cup P_{n-8};k) + m(P_4\cup P_2\cup P_{n-11};k-1), \\ m(P_2\cup T^2_{n-4};k) &= m(P_2\cup P_2\cup P_{n-6};k) + m(P_2\cup P_2\cup P_{n-9};k-1). \end{split}$$

Hence the result follows. \Box

Lemma 10. Suppose (i, j, k) is a 3-element ordered pair with $1 \le i \le j \le k$ and i+j+k = n. If $(i, j, k) \ne (2, 2, n - 4), (2, 4, n - 6)$, then $P_i \cup P_j \cup P_k \preceq P_2 \cup P_4 \cup P_{n-6} \preceq P_2 \cup P_2 \cup P_{n-4}$. **Proof.** If $j \neq 2$, then

$$\begin{array}{rcl} P_i \cup (P_j \cup P_k) & \preceq & P_i \cup (P_4 \cup P_{j+k-4}) \\ \\ & = & P_4 \cup (P_i \cup P_{j+k-4}) \\ \\ & \preceq & P_4 \cup (P_2 \cup P_{i+j+k-6}) = P_2 \cup (P_4 \cup P_{n-6}) \end{array}$$

Similarly, if $i \neq 2$, we can show that $P_i \cup P_j \cup P_k \leq P_2 \cup P_4 \cup P_{n-6}$. Since $P_2 \cup P_4 \cup P_{n-6} \leq P_2 \cup P_2 \cup P_{n-4}$, then the result follows. \Box

Theorem 11. Let $G \in \mathcal{BU}^*_{n,1}$ with $n \ge 8$ vertices. If $G \ncong K_n^6$, then $G \prec K_n^6$.

Proof. Let G be any graph in $\mathcal{BU}^*_{n,1}$ and C_l be the unique cycle in G. Since $G \ncong P_n^l$, G has at least two pendent vertices. Let v be the pendent vertex in G such that $d_G(v, C_l) = 1$ and u its unique neighbor. Note that G - v - u is a acyclic graph on n - 2 vertices. So $G - v - u \preceq P_{n-2}$. Since $G - v \ncong C_{n-1}$, then $G - v \preceq P_{n-1}^6$ by lemma 8. According to lemma 3(b), we get

$$b_{2k}(G) = b_{2k}(G-v) + b_{2k-2}(G-v-u)$$

$$\leq b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2})$$

$$= b_{2k}(K_n^6).$$

If $G \ncong K_n^6$, we can always find a positive integer k_0 such that $b_{2k_0}(G) < b_{2k_0}(K_n^6)$. This completes the proof. \Box

Lemma 12. Let $G \in \mathcal{BU}_{n}^{*b}{}_{2}(l)$ with n = l + 3, then $G \preceq K_{n}^{l}$.

Proof. Obviously G_1 is the single element in $\mathcal{BU}_{n,2}^{*b}(l)$ (see Fig.3. for G_1). In view of lemma 3(b), we obtain

$$\begin{split} b_{2k}(K_{l+3}^l) - b_{2k}(G_1) &= b_{2k-2}(P_{l+1}) - b_{2k-2}(C_l) \\ &= m(P_{l+1};k-1) - m(P_l;k-1) - m(P_{l-2};k-2) \pm 2, \end{split}$$

where the last term " ± 2 " should be erased if $2k - 2 \neq l$.

When $2k - 2 \neq l$, $b_{2k}(K_{l+3}^l) - b_{2k}(G_1) = m(P_{l-3}; k-3) \geq 0$. When 2k - 2 = l and $l \equiv 0 \pmod{4}$, we have $b_{2k}(K_{l+3}^l) - b_{2k}(G_1) = m(P_{l-3}; k-3) + 2 > 0$. When 2k - 2 = l and $l \neq 0 \pmod{4}$, we have $b_{2k}(K_{l+3}^l) - b_{2k}(G_1) = m(P_{l-3}; k-3) - 2 = m(P_{l-3}; \frac{l}{2} - 2) - 2 \geq 0$.

Consequently, the result follows. \Box



Fig.3.

Lemma 13. Let $G \in \mathcal{BU}_{n,2}^{*b}(l)$ with n = l + 4, then $G \leq R_n^l$.

Proof. It's evident that G must be one of graphs G_2-G_5 as shown in Fig.3.

According to lemmas 3(b) and 4, one can easily obtain that $G_2 \succ G_4$. In the following, we will show that $R_n^l \succ G_2, G_3, G_5$. Apply lemma 3(b) once again, we obtain

$$\begin{split} b_{2k}(R_{l+4}^l) - b_{2k}(G_2) &= b_{2k}(P_{l+2}^l) + b_{2k-2}(P_{l+2}^l) + b_{2k-2}(P_{l+1}) - b_{2k}(P_{l+3}^l) \\ &\quad -b_{2k-2}(P_2 \cup C_l) \\ &= b_{2k-2}(P_{l+2}^l) + b_{2k-2}(P_{l+1}) - b_{2k-2}(P_{l+1}^l) - b_{2k-2}(C_l) \\ &\quad -b_{2k-4}(C_l) \\ &= \cdots \\ &= b_{2k-2}(P_{l+1}) - b_{2k-2}(C_l). \end{split}$$

Similar to the proof of lemma 12, we can show that $G_2 \preceq R_{l+4}^l$. Similarly,

$$b_{2k}(R_{l+4}^{l}) - b_{2k}(G_{3}) = b_{2k}(P_{l+2}^{l}) + b_{2k-2}(P_{l+2}^{l}) + b_{2k-2}(P_{l+1}) - b_{2k}(P_{l+3}^{l}) - b_{2k-2}(P_{l+1}^{l}) = \cdots = b_{2k-4}(C_{l}) + b_{2k-2}(P_{l+1}) - b_{2k-4}(P_{l-1}) - b_{2k-2}(C_{l}).$$

If $2k - 4 \neq l$ and $2k - 2 \neq l$, then $b_{2k}(R_{l+4}^l) - b_{2k}(G_3) = m(P_{l-3}; k-3) + 2m(P_{l-2}; k-3) \ge 0$. If 2k - 4 = l or 2k - 2 = l, then

$$\begin{array}{rcl} b_{2k}(R_{l+4}^l) - b_{2k}(G_3) & \geq & m(P_{l-3};k-3) + 2m(P_{l-2};k-3) - 2 \\ \\ & \geq & \left\{ \begin{array}{c} 2m(P_{l-2};\frac{l}{2}-1) - 2 = 0, & 2k-4 = l \\ 2m(P_{l-2};\frac{l}{2}-2) - 2 \geq 0, & 2k-2 = l \end{array} \right. \end{array}$$

Thus $G_3 \leq R_{l+4}^l$.

Lemma 14. Let $n \ge 10$ and $4 \le l \le n-4$. If $l \ne 6$, then $R_n^l \prec R_n^6$.

Proof. By lemma 3(b), we have

$$b_{2k}(R_n^l) = b_{2k}(K_{n-1}^l) + b_{2k-2}(P_{n-2}^l)$$

= $b_{2k}(P_{n-2}^l) + b_{2k-2}(P_{n-2}^l) + b_{2k-2}(P_{n-3}),$
 $b_{2k}(R_n^6) = b_{2k}(P_{n-2}^6) + b_{2k-2}(P_{n-2}^6) + b_{2k-2}(P_{n-3}).$

Since $n-2 \ge l+2$, the lemma follows as expected by lemma 8. \Box

By the same reasoning as employed in lemma 14, we can prove:

Lemma 15. Suppose $n \ge 8$ and $4 \le l \le n-2$. If $l \ne 6$, then $K_n^l \prec K_n^6$.

Lemma 16. For $n \ge 10$, we have $K_n^6 \prec R_n^6$.



Fig.4.

For $2 \leq i \leq n-l-1$ and $n-l \geq 5$, we use $M_n^{l,i}$ to denote the graph obtained by joining a vertex of C_l by a new edge with the i^{th} vertex of path P_{n-l} , where the vertices of P_{n-l} are labelled according to their natural orderings.

Theorem 17. Let $G \in \mathcal{BU}_{n,2}^{*b}$ with $n \ge 13$. If $G \ncong M_n^{n-5,2}$, $M_n^{n-5,3}$, $M_n^{6,3}$ and Q_n^6 , then $G \prec M_n^{6,3}$ or Q_n^6 .

Proof. Let G be any graph in $\mathcal{BU}_{n,2}^{*b}$ and C_l be the unique cycle in it. Since $G \in \mathcal{BU}_{n,2}^{*b}$, then $n \ge l+3$.

If n = l + 3 or l + 4, the result is evidently true from the combination of lemmas 12–16. So we may suppose that $n \ge l + 5$ herein. We shall prove the theorem by distinguishing between two cases.

Case 1. l = 4.

By means of lemmas 3(a) and 5, we have

$$b_{2k}(G) = m(G;k) - 2b_{2k-4}(G - C_4)$$

$$\leq m(G;k)$$

$$\leq m(T_n^2;k) + m(P_2 \cup T_{n-4}^2;k-1)$$

$$= m(Q_n^4;k).$$

In the following, we shall prove that $b_{2k}(Q_n^6) \ge m(Q_n^4;k)$ for all $k \ge 0$. In view of lemma 3(a),

$$b_{2k}(Q_n^6) = m(T_n^2; k) + m(P_4 \cup T_{n-6}^2; k-1) + 2m(T_{n-6}^2; k-3).$$

Thus

$$\begin{array}{lcl} b_{2k}(Q_n^6) - m(Q_n^4;k) &=& m(P_4 \cup T_{n-6}^2;k-1) + 2m(T_{n-6}^2;k-3) - m(P_2 \cup T_{n-4}^2;k-1) \\ &=& m(P_2 \cup P_2 \cup T_{n-6}^2;k-1) + m(T_{n-6}^2;k-2) + 2m(T_{n-6}^2;k-3) \\ && -m(P_2 \cup P_2 \cup T_{n-6}^2;k-1) - m(P_2 \cup T_{n-7}^2;k-2) \\ &=& m(T_{n-6}^2;k-2) - m(T_{n-7}^2;k-2) + 2m(T_{n-6}^2;k-3) - m(T_{n-7}^2;k-3) \\ &\geq& 0. \end{array}$$

So $b_{2k}(Q_n^6) \ge b_{2k}(G)$ and $b_{2k}(Q_n^6) \ge b_{2k}(Q_n^4)$ for all $k \ge 0$ in this case. In particular, $b_6(Q_n^6) > b_6(G)$ and $b_6(Q_n^6) > b_6(Q_n^4)$. Hence $G \prec Q_n^6$ and $Q_n^4 \prec Q_n^6$.

Case 2. $l \ge 6$.

Case 2.1. $G \cong M_n^{l, i}$ for some $2 \le i \le n - l - 1$. (See Fig.4. for $M_n^{l, i}$) In this case, we claim that $G \prec M_n^{6, 3}$. Since $G \not\cong M_n^{n-5, 2} (\cong M_n^{n-5, 4})$, $M_n^{n-5, 3}$, then $n-l \ge 6$.

Firstly, we prove that if $i \neq 3, n-l-2$, then $M_n^{l, i} \prec M_n^{l, 3} (\cong M_n^{l, n-l-2})$. Note that

$$\begin{split} b_{2k}(M_n^{l,i}) &= b_{2k}(C_l \cup P_{n-l}) + b_{2k-2}(P_{l-1} \cup P_{i-1} \cup P_{n-l-i}), \\ b_{2k}(M_n^{l,3}) &= b_{2k}(C_l \cup P_{n-l}) + b_{2k-2}(P_{l-1} \cup P_2 \cup P_{n-l-3}). \end{split}$$

By means of lemma 10, it's not difficult to show that $P_{l-1} \cup P_{i-1} \cup P_{n-l-i} \prec P_{l-1} \cup P_2 \cup P_{n-l-3}$. So there exists some k_0 such that $b_{2k_0}(M_n^{l,3}) > b_{2k_0}(M_n^{l,i})$ and then $M_n^{l,i} \prec M_n^{l,3}$.

Secondly, we will demonstrate that if $l \neq 6$, i.e., $l \geq 8$, then $M_n^{l, 3} \prec M_n^{6, 3}$.

By lemma 3(a), we deduce that

$$b_{2k}(M_n^{l,3}) = b_{2k}(T_1) + b_{2k-2}(P_{l-2} \cup P_{n-l}) \pm 2b_{2k-l}(P_{n-l}),$$

$$b_{2k}(M_n^{6,3}) = b_{2k}(T_2) + b_{2k-2}(P_4 \cup P_{n-6}) + 2b_{2k-6}(P_{n-6}).$$

where T_1 (resp. T_2) is the acyclic graph of order *n* obtained from $M_n^{l,3}$ (resp. $M_n^{6,3}$) by deleting one edge on C_l (resp. C_6) incident with the unique 3-degree vertex of C_l (resp. C_6).

Moreover,

$$b_{2k}(T_1) = b_{2k}(P_2 \cup P_{n-2}) + b_{2k-2}(P_1 \cup P_l \cup P_{n-l-3})$$

$$b_{2k}(T_2) = b_{2k}(P_2 \cup P_{n-2}) + b_{2k-2}(P_1 \cup P_6 \cup P_{n-9}).$$

Furthermore,

$$\begin{array}{lll} b_{2k-6}(P_{n-6})=m(P_{n-6};k-3)&=&m(P_{n-7};k-3)+m(P_{n-8};k-4)\\ &\geq&m(P_{n-8};k-4)\\ &\geq&\cdots\\ &\geq&m(P_{n-6-(l-6)};k-3-\frac{l-6}{2})\\ &=&m(P_{n-l};k-\frac{l}{2})=b_{2k-l}(P_{n-l}). \end{array}$$

When $n-l \neq 7$, we clearly have $P_1 \cup P_l \cup P_{n-l-3} \leq P_1 \cup P_6 \cup P_{n-9}$ since $l \geq 8$. Thus $T_1 \leq T_2$ and then $M_n^{l,3} \leq M_n^{6,3}$.

When n-l=7,

$$\begin{split} b_{2k}(M_n^{6,3}) - b_{2k}(M_n^{l,3}) &\geq b_{2k-2}(P_4 \cup P_{n-6}) - b_{2k-2}(P_7 \cup P_{n-9}) + b_{2k-2}(P_6 \cup P_{n-9}) \\ &- b_{2k-2}(P_4 \cup P_{n-7}) \\ &= m(P_4 \cup P_{n-8}; k-2) - m(P_5 \cup P_{n-9}; k-2) \geq 0. \end{split}$$

So $M_n^{l, 3} \preceq M_n^{6, 3}$.

Since $b_0(P_{n-6}) = 1 > 0 = b_{6-l}(P_{n-l})$, then $b_6(M_n^{6,3}) > b_6(M_n^{l,3})$. This gives $M_n^{l,3} \prec M_n^{6,3}$. Case 2.2. $G \ncong M_n^{l,i}$ for any $2 \le i \le n-l-1$.

Since $G \in \mathcal{BU}_{n,2}^{*b}$, C_l has exactly one branched vertex. Let u be such a branched vertex and w be one of its neighbors lying on C_l . By lemma 3(a),

$$\begin{aligned} b_{2k}(G) &= b_{2k}(G-uw) + b_{2k-2}(G-u-w) \pm 2b_{2k-l}(G-C_l) \\ &\leq b_{2k}(T_n^2) + b_{2k-2}(P_{l-2} \cup T_{n-l}) \pm 2b_{2k-l}(T_{n-l}), \end{aligned}$$

where T_{n-l} denotes the forest obtained by deleting the cycle C_l from G. As $T_{n-l} \not\cong P_{n-l}$ (otherwise $G \cong P_n^l$ or $M_n^{l, i}$, a contradiction), we have $T_{n-l} \preceq T_{n-l}^2$ by lemma 5. Because $l \ge 6$, we have $P_{l-2} \cup T_{n-l}^2 \preceq P_4 \cup T_{n-6}^2$ by lemma 9.

When $l \equiv 0 \pmod{4}$, we have

$$b_{2k}(G) \le b_{2k}(T_n^2) + b_{2k-2}(P_4 \cup T_{n-6}^2) + 2b_{2k-6}(T_{n-6}^2) = b_{2k}(Q_n^6).$$

Moreover, there exists some k_0 such that $b_{2k_0}(Q_n^6) > b_{2k_0}(G)$ since $G \not\cong Q_n^6$. When $l \not\equiv 0 \pmod{4}$, we have

$$\begin{split} m(T_{n-6}^2;k-3) &= m(T_{n-7}^2;k-3) + m(T_{n-8}^2;k-4) \\ &\geq m(T_{n-8}^2;k-4) \\ &\geq \cdots \\ &\geq m(T_{n-6-(l-6)}^2;k-3-\frac{l-6}{2}) \\ &= m(T_{n-l}^2;k-\frac{l}{2}). \end{split}$$

$$\begin{split} &\text{Hence } b_{2k}(G) \leq b_{2k}(T_n^2) + b_{2k-2}(P_{l-2} \cup T_{n-l}^2) + 2b_{2k-l}(T_{n-l}^2) \leq b_{2k}(T_n^2) + b_{2k-2}(P_4 \cup T_{n-6}^2) + 2b_{2k-6}(T_{n-6}^2) = b_{2k}(Q_n^6). \text{ If } l \neq 6, \text{ there must exist some } k_0' \text{ such that } b_{2k_0'}(Q_n^6) > b_{2k_0'}(G). \end{split}$$

From the combination of cases 1 and 2 it follows the present theorem as expected. \Box

Lemma 18. Let $G \in \mathcal{BU}_{n,2}^{*a}(l)$ with n = l + 4 or l + 5. If $G \ncong R_n^l$, then $G \prec R_n^l$.

Proof. We consider only the case that n = l + 4. Since $G \in \mathcal{BU}_{n,2}^{*a}$, G must have a pendent vertex v such that $d_G(v, C_l) = 2$ and $d_G(u) = 2$, where u is the unique neighbor of v. Note that $G - v \in \mathcal{BU}_{n-1,1}^{*}$, one can easily verify that $G - v \preceq K_{n-1}^{l}$ by lemma 3(b). Similarly, we can demonstrate that $G - u - v \preceq P_{n-2}^{l}$ since $G - u - v \notin \mathcal{C}(n-2,l)$ and $G - u - v \notin C_{n-2}$. By lemma 3(b),

$$b_{2k}(G) = b_{2k}(G-v) + b_{2k-2}(G-u-v) \le b_{2k}(K_{n-1}^l) + b_{2k-2}(P_{n-2}^l) = b_{2k}(R_n^l).$$

If $G \not\cong R_n^l$, we can always find a positive integer k_0 such that $b_{2k_0}(R_n^l) > b_{2k_0}(G)$.

When n = l + 5, the lemma can be proved by the same reasoning as used above. So the result follows. \Box

Lemma 19. Let $G \in \mathcal{BU}^{*a}_{n,2}(l)$ with $l \not\equiv 0 \pmod{4}$. If $G \ncong R_n^l$, then $G \prec R_n^l$.

Proof. Let G be any graph in $\mathcal{BU}_{n,2}^{*a}$ and C_l be the unique cycle in G. Since $G \in \mathcal{BU}_{n,2}^{*a}$, then $n \ge l + 4$. We shall prove this lemma by induction on n - l. When n - l = 4 or 5, the lemma is immediate from lemma 18. Suppose that $n - l \ge 6$ and the lemma is true for graphs in $\mathcal{BU}_{n-1,2}^{*a}$ or $\mathcal{BU}_{n-2,2}^{*a}$. Now, let G be graph in $\mathcal{BU}_{n,2}^{*a}$ with $n - l \ge 6$. There're two cases we should distinguish between.

Case 1. $d_G(v, C_l) = 2$ for any $v \in V_p(G)$.

Let S be the set of vertices adjacent to pendent vertices in G. If $d_G(u) = 2$ for some vertex $u \in S$, then by the same method as used in proving lemma 18, we can show that $G \prec R_n^l$ (Here $G \ncong R_n^l$). Suppose that $d_G(u) \ge 3$ for all vertices u in S. Let u be any vertex in S and v be one pendent vertex adjacent to it. Then $G - v \in \mathcal{BU}_{n-1,2}^{*a}$ and thus $G - v \prec R_{n-1}^l$ by induction assumption. Since $d_G(u) \ge 3$, all connected components not containing C_l of G - v - u must be isolated vertices. So by lemma 4, $G - v - u \prec G'$, where G' is the graph by attaching all isolated vertices of G - v - u to any vertex of C_l . Evidently, $G' \in \mathcal{BU}_{n-2,1}^*$ and it's not difficult to obtain that $G' \prec K_{n-2}^l$. By lemmas 3(b) and (6), $K_{n-2}^l \prec R_{n-2}^l$ since $n-2 \ge l+4$ and $l \ne 0 \pmod{4}$.

Therefore $G \prec R_n^l$.

Case 2 There exists some pendent vertex v in $V_p(G)$ such that $d_G(v, C_l) \ge 3$.

Let $w \in V_p(G)$ be the pendent vertex in G such that $d_G(w, C_l) = max\{d_G(x, C_l) | x \in V_p(G)\}$. Obviously $G - w \in \mathcal{BU}^{*a}_{n-1,2}$ and thus $G - w \preceq R^l_{n-1}$ by induction assumption.

Let u be the unique neighbor of w. If G - w - u is connected, then $G - w - u \in \mathcal{BU}^{*a}_{n-2,2}(d_G(w, C_l) \ge 4)$ or $\mathcal{BU}^{*a}_{n-2,1}(d_G(w, C_l) = 3)$.

If $G - w - u \in \mathcal{BU}^*_{n-2,1}$, then $G - w - u \preceq K_{n-2}^l \prec R_{n-2}^l$ (as $n-2 \ge l+4$ and $l \ne 0 \pmod{4}$). If $G - w - u \in \mathcal{BU}^*_{n-2,2}$, then $G - w - u \preceq R_{n-2}^l$ by induction hypothesis.

If G - w - u is disconnected, then $G - w - u \prec G'' \prec K_{n-2}^l \prec R_{n-2}^l$, where G'' is the graph by attaching all isolated vertices of G - w - u to any vertex of C_l .

Combining cases 1 and 2, the proof is completed. \Box

Let G be any graph in \mathcal{U}_n and C_l the unique cycle in G. Given that all vertices of the cycle C_l are ordered successively as v_1, v_2, \dots, v_l . For any $v_i \in V(C_l)$, let $T_{[v_i]}$ denote the connected component containing v_i of $G - v_{i-1}v_i - v_iv_{i+1}$.

Lemma 20. Let $G \in \mathcal{BU}_{n,2}^{*a}(l)$ with $l \equiv 0 \pmod{4}$, $4 \leq l \leq n-4$ and $n \geq 12$. Then $G \prec Q_n^6$ or R_n^6 .

Proof. Since $G \in \mathcal{BU}_{n,2}^{*a}$, then $n \ge l+4$. We consider the following two cases.

Case 1. For some branched vertex $v_i \in V(C_l)$, $n(T_{[v_i]}) = 3$, where $n(T_{[v_i]})$ is the order of $T_{[v_i]}$.

Since $G \in \mathcal{BU}_{n,2}^{*a}(l)$, then $T[v_i] \cong P_3$ and v_i is one end-point of P_3 . Let the vertices of $T[v_i](or P_3)$ be ordered successively as v_i, v'_i, v''_i such that $d(v'_i) = 2$ and $d(v''_i) = 1$. Then $G - v''_i \in \mathcal{BU}_{n-1,1}^{*a}$ and thus $G - v''_i \preceq K_{n-1}^l \prec K_{n-1}^6$ by theorem 11. Moreover, $G - v''_i \prec P_{n-2}^6$ by lemma 8 since $G - v''_i = C_{n-2}$. So $G \prec R_n^6$ in this case.

Case 2. For each branched vertex $v_i \in V(C_l), n(T_{[v_i]}) \ge 4$.

Let v_t be any branched vertex on C_l . We can always find one neighbor, say v'_t , of $v_t(v'_t)$ lies

on C_l) such that

$$b_{2k}(G - v_t v'_t) + b_{2k-2}(G - v_t - v'_t) \le b_{2k}(T_n^2) + b_{2k-2}(P_4 \cup T_{n-6}^2) (by \ lemmas \ 5 \ and \ 9)$$

or

$$b_{2k}(G - v_t v'_t) + b_{2k-2}(G - v_t - v'_t) \le b_{2k}(P_n) + b_{2k-2}(P_2 \cup P_4 \cup P_{n-8})(by \ lemma \ 10).$$

 \mathbf{So}

$$\begin{array}{lll} b_{2k}(G) & = & b_{2k}(G-v_tv_t^{'}) + b_{2k-2}(G-v_t-v_t^{'}) - 2b_{2k-l}(G-C_l) \\ & \leq & b_{2k}(T_n^2) + b_{2k-2}(P_4 \cup T_{n-6}^2) + 2b_{2k-6}(T_{n-6}^2) = b_{2k}(Q_n^6). \end{array}$$

or

$$\begin{array}{lll} b_{2k}(G) & = & b_{2k}(G-v_tv_t^{'})+b_{2k-2}(G-v_t-v_t^{'})-2b_{2k-l}(G-C_l) \\ & \leq & b_{2k}(P_n)+b_{2k-2}(P_2\cup P_4\cup P_{n-8})+2b_{2k-6}(P_2\cup P_{n-8})=b_{2k}(R_n^6). \end{array}$$

In either cases, there exists some k_0 such that $b_{2k_0}(G) < b_{2k_0}(R_n^6)$ or $b_{2k_0}(G) < b_{2k_0}(Q_n^6)$. This proves the lemma. \Box

Theorem 21. Let $G \in \mathcal{BU}_{n,2}^{*a}$ with $n \ge 12$. Then $G \prec Q_n^6$ or R_n^6 .

Proof. Let G be any graph in $\mathcal{BU}_{n,2}^{*a}$ and C_l be the unique cycle in G. If $l \equiv 0 \pmod{4}$, the theorem is true by lemma 20. If $l \not\equiv 0 \pmod{4}$, then $G \preceq R_n^l$ by lemma 19. Since $n \ge 12$, we can easily verify that $R_n^l \preceq R_n^6$ and the theorem follows as desired. \Box

Lemma 22. For $n \geq 13$, we have $M_n^{n-5,2} \prec M_n^{n-5,3} \prec R_n^6$.

Proof. In full analogy with the proof of subcase 2.1 of theorem 17, we can obtain that $M_n^{n-5,2} \prec M_n^{n-5,3}$. In what follows we shall verify that $M_n^{n-5,3} \prec R_n^6$.

By means of lemma 3(a), we have

$$\begin{split} b_{2k}(R_n^6) &= b_{2k}(P_n) + b_{2k-2}(P_2 \cup P_4 \cup P_{n-8}) + 2b_{2k-6}(P_2 \cup P_{n-8}) \\ &= b_{2k}(P_2 \cup P_{n-2}) + b_{2k-2}(P_1 \cup P_{n-3}) + b_{2k-2}(P_2 \cup P_4 \cup P_{n-8}) \\ &+ 2b_{2k-6}(P_{n-8}) + 2b_{2k-8}(P_{n-8}), \end{split}$$

$$\begin{aligned} b_{2k}(M_n^{n-5,3}) &= b_{2k}(T_n^2) + b_{2k-2}(P_5 \cup P_{n-7}) \pm 2b_{2k-(n-5)}(P_5) \\ &= b_{2k}(P_2 \cup P_{n-2}) + b_{2k-2}(P_1 \cup P_2 \cup P_{n-5}) + b_{2k-2}(P_5 \cup P_{n-7}) \\ &\pm 2b_{2k-(n-5)}(P_5). \end{aligned}$$

 So

$$\begin{array}{lll} b_{2k}(R_n^6) - b_{2k}(M_n^{n-5,3}) & = & b_{2k-4}(P_1 \cup P_1 \cup P_{n-6}) + b_{2k-2}(P_2 \cup P_4 \cup P_{n-8}) \\ & & -b_{2k-2}(P_2 \cup P_3 \cup P_{n-7}) - b_{2k-4}(P_1 \cup P_2 \cup P_{n-7}) + \\ & & 2b_{2k-6}(P_{n-8}) + 2b_{2k-8}(P_{n-8}) \mp 2b_{2k-(n-5)}(P_5) \\ & \geq^{(\star)} & b_{2k-4}(P_{n-6}) - b_{2k-4}(P_{n-7}) - b_{2k-6}(P_{n-7}) + 2b_{2k-6}(P_{n-8}) \\ & & + 2b_{2k-8}(P_{n-8}) \mp 2b_{2k-(n-5)}(P_5) \\ & = & -b_{2k-8}(P_{n-9}) + 2b_{2k-6}(P_{n-8}) + 2b_{2k-8}(P_{n-8}) \mp 2b_{2k-(n-5)}(P_5) \\ & \geq & 2b_{2k-6}(P_{n-8}) + b_{2k-8}(P_{n-8}) \mp 2b_{2k-(n-5)}(P_5) \\ & \geq & 0. \end{array}$$

where the inequality (*) holds due to the fact that $P_2 \cup P_4 \cup P_{n-8} \succeq P_2 \cup P_3 \cup P_{n-7}$.

If n is even, $b_{2k-(n-5)}(P_5)=0$ and the inequality (•) is evidently true. Suppose that n is odd. If $n-5 \equiv 0 \pmod{4}$, the inequality (•) holds clearly. If $n-5 \neq 0 \pmod{4}$ and $2k - (n-5) \geq 6$, the result is obvious. If $n-5 \neq 0 \pmod{4}$ and $2k - (n-5) \geq 6$, the result is obvious. If $n-5 \neq 0 \pmod{4}$ and $2k - (n-5) \geq 6$, the result is obvious. If $n-5 \neq 0 \pmod{4}$ and 2k - (n-5) = 4, $b_{2k-6}(P_{n-8}) = 0$ and $b_{2k-8}(P_{n-8}) = b_{n-9}(P_{n-8}) = m(P_{n-8}; \frac{n-9}{2}) = m(P_{n-9}; \frac{n-9}{2}) + m(P_{n-10}; \frac{n-9}{2} - 1) = 1 + m(P_{n-10}; \frac{n-11}{2}) \geq 1 + 2 = b_{2k-(n-5)}(P_5)$. If $n-5 \neq 0 \pmod{4}$ and 2k - (n-5) = 2, then $b_{2k-6}(P_{n-8}) = b_{n-9}(P_{n-8}) = m(P_{n-8}; \frac{n-9}{2}) = \cdots = 1 + m(P_{n-10}; \frac{n-11}{2}) \geq 1 + 2 = 3$ and $b_{2k-8}(P_{n-8}) = b_{n-11}(P_{n-8}) = m(P_{n-8}; \frac{n-11}{2}) = m(P_{n-9}; \frac{n-11}{2}) + m(P_{n-10}; \frac{n-13}{2}) > 2$. Hence $2b_{2k-6}(P_{n-8}) + b_{2k-8}(P_{n-8}) \mp 2b_{2k-(n-5)}(P_5) > 2 \times 3 + 2 - 2 \times 4 = 0$. If $n-5 \neq 0 \pmod{4}$ and 2k - (n-5) = 0, the inequality (•) is immediate by the same method as used above.

From above arguments we conclude that $b_{2k}(R_n^6) \ge b_{2k}(M_n^{n-5,3})$ and $b_6(R_n^6) > b_6(M_n^{n-5,3})$, which proved the lemma. \Box

Theorem 23. Let $G \in \mathcal{BU}^*_n$ with $n \ge 13$. Then $M_n^{6,3}$ has the maximal energy among all graphs in \mathcal{BU}^*_n .

Proof. According to theorems 11, 17 and 21 and lemmas 16 and 22, we need only to prove that $M_n^{6,3} > R_n^6, Q_n^6$.

Using lemma 3, we obtain

$$b_{2k}(M_n^{6,3}) = b_{2k}(P_2 \cup P_{n-2}^6) + b_{2k-2}(P_1 \cup C_6 \cup P_{n-9}),$$
(6)

$$b_{2k}(R_n^6) = b_{2k}(P_2 \cup P_{n-2}^6) + b_{2k-2}(P_1 \cup P_{n-3}),$$
(7)

$$b_{2k}(Q_n^6) = b_{2k}(P_2 \cup P_{n-2}^6) + b_{2k-2}(P_1 \cup P_2 \cup P_{n-5}^6).$$
(8)

To prove that $M_n^{6,3} \succ R_n^6$, it's sufficient to prove that $C_6 \cup P_{n-9} \succ P_{n-3}$ by Eqs.(6) and (7). In view of lemma 3, we obtain

$$b_{2k}(C_6 \cup P_{n-9}) = b_{2k}(P_6 \cup P_{n-9}) + b_{2k-2}(P_4 \cup P_{n-9}) + 2b_{2k-6}(P_{n-9}),$$

$$b_{2k}(P_{n-3}) = b_{2k}(P_6 \cup P_{n-9}) + b_{2k-2}(P_5 \cup P_{n-10}).$$

It's easy to see that $b_6(C_6 \cup P_{n-9}) > b_6(P_{n-3})$. Therefore $C_6 \cup P_{n-9} \succ P_{n-3}$ and then $M_n^{6,3} \succ R_n^6$.

Next, we shall prove that $M_n^{6,3} \succ Q_n^6$. Combining Eqs.(6) and (8), we need only to prove that $C_6 \cup P_{n-9} \succ P_2 \cup P_{n-5}^6$. In view of lemma 3(b), we obtain

$$\begin{split} b_{2k}(C_6 \cup P_{n-9}) &= b_{2k}(C_6 \cup P_2 \cup P_{n-11}) + b_{2k-2}(C_6 \cup P_1 \cup P_{n-12}), \\ b_{2k}(P_2 \cup P_{n-5}^6) &= b_{2k}(C_6 \cup P_2 \cup P_{n-11}) + b_{2k-2}(P_2 \cup P_5 \cup P_{n-12}). \end{split}$$

In what follows, we shall prove that $C_6 \cup P_1 \cup P_{n-12} \succ P_2 \cup P_5 \cup P_{n-12}$. Once again by lemma 3, we have

$$\begin{split} b_{2k}(C_6 \cup P_1 \cup P_{n-12}) &= b_{2k}(P_6 \cup P_1 \cup P_{n-12}) + b_{2k-2}(P_4 \cup P_1 \cup P_{n-12}) + 2b_{2k-6}(P_1 \cup P_{n-12}) \\ &= b_{2k}(P_1 \cup P_2 \cup P_4 \cup P_{n-12}) + b_{2k-2}(P_1 \cup P_1 \cup P_3 \cup P_{n-12}) + b_{2k-2}(P_1 \cup P_2 \cup P_2 \cup P_{n-12}) + b_{2k-4}(P_{n-12}) + 2b_{2k-6}(P_{n-12}), \end{split}$$

$$\begin{aligned} b_{2k}(P_2 \cup P_5 \cup P_{n-12}) &= b_{2k}(P_2 \cup P_2 \cup P_3 \cup P_{n-12}) + b_{2k-2}(P_2 \cup P_1 \cup P_2 \cup P_{n-12}) \\ &= b_{2k}(P_1 \cup P_1 \cup P_2 \cup P_3 \cup P_{n-12}) + b_{2k-2}(P_2 \cup P_3 \cup P_{n-12}) + b_{2k-2}(P_1 \cup P_2 \cup P_2 \cup P_2 \cup P_{n-12}). \end{aligned}$$

Obviously, $P_1 \cup P_2 \cup P_4 \cup P_{n-12} \succ P_1 \cup P_1 \cup P_2 \cup P_3 \cup P_{n-12}$. So $b_{2k}(C_6 \cup P_1 \cup P_{n-12}) - b_{2k}(P_2 \cup P_3 \cup P_{n-12})$

$$\geq b_{2k-2}(P_1 \cup P_1 \cup P_3 \cup P_{n-12}) - b_{2k-2}(P_2 \cup P_3 \cup P_{n-12}) \\ + b_{2k-4}(P_{n-12}) + 2b_{2k-6}(P_{n-12}) \\ = b_{2k-2}(P_3 \cup P_{n-12}) - b_{2k-2}(P_3 \cup P_{n-12}) - b_{2k-4}(P_3 \cup P_{n-12}) \\ + b_{2k-4}(P_{n-12}) + 2b_{2k-6}(P_{n-12}) \\ = \cdots = 0.$$

It's evident that there exists some k_0 such that $b_{2k_0}(C_6 \cup P_1 \cup P_{n-12}) > b_{2k_0}(P_2 \cup P_5 \cup P_{n-12})$. So $C_6 \cup P_1 \cup P_{n-12} \succ P_2 \cup P_5 \cup P_{n-12}$ and then $C_6 \cup P_{n-9} \succ P_2 \cup P_{n-5}^6$. This completes the proof. \Box

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