

Minimal Energy on Unicyclic Graphs

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Abstract For a simple graph G , the energy $E(G)$ is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. Let \mathcal{U}_n denote the set of all connected unicyclic graphs with order n , and $\mathcal{U}_n^r = \{G \in \mathcal{U}_n \mid d(x) = r \text{ for any vertex } x \in V(C_\ell)\}$, where $r \geq 2$ and C_ℓ is the unique cycle in G . Every unicyclic graph in \mathcal{U}_n^r is said to be a cycle- r -regular graph. In this paper, we completely characterize that $C_9^3(2, 2, 2) \circ S_{n-8}$ is the unique graph having minimal energy in \mathcal{U}_n^4 . Moreover, the graph with minimal energy is uniquely determined in \mathcal{U}_n^r for $r = 3, 4$.

Keywords graph energy; unicyclic graph; matching; quasi-order.

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1. Introduction

Let G be a graph of order n and $A(G)$ the adjacency matrix of G . The characteristic polynomial of G is

$$\phi(G, x) = \det(\lambda I - A(G)) = \sum_{i=0}^n a_i \lambda^{n-i}. \quad (1.1)$$

The roots $\lambda_1, \lambda_2, \dots, \lambda_n$ of $\phi(G, \lambda) = 0$ are called the eigenvalues of G . Since $A(G)$ is symmetric, all the eigenvalues of G are real.

The energy of G , denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^n |\lambda_i|$. It is known from [1] that $E(G)$ can be expressed as the Coulson integral formula

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln \left[\left(\sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i a_{2i} x^{2i} \right)^2 + \left(\sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i a_{2i+1} x^{2i+1} \right)^2 \right] dx, \quad (1.2)$$

where a_0, a_1, \dots, a_n are coefficients of characteristic polynomial $\phi(G, x)$ of G .

The graphs under our consideration are finite, connected and simple. Let P_n , C_n and S_n denote the path, cycle and star with n vertices, respectively. Let \mathcal{U}_n denote the set of all connected unicyclic graphs of order n .

Let $\mathcal{U}_n^r = \{G \in \mathcal{U}_n \mid d(x) = r \text{ for any vertex } x \in V(C_\ell)\}$, where $r \geq 2$ and C_ℓ is the unique cycle in G . Every graph in \mathcal{U}_n^r is said to be a cycle- r -regular graph. Since \mathcal{U}_n^2 contains exactly

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one single element, we will suppose $r \geq 3$. Let G be a connected unicyclic graph and C_ℓ the unique cycle of length ℓ ($3 \leq \ell \leq n$) of G . Let the vertices of P_n be ordered successively as x_1, x_2, \dots, x_n . Then, the graph P_n^k is obtained from P_n by attaching exactly two pendent edges to each of the vertices x_k, x_{k+1}, \dots, x_n , respectively; for example, $P_2^2 = S_4$. $P_n^{k,1}$ is the graph obtained from P_n^k by joining just one pendent vertex to the vertex x_1 with $k \geq 2$ (as shown in Figure 1).

Let the vertices of C_ℓ be ordered successively as y_1, y_2, \dots, y_ℓ . Let $C_n^\ell(s_1, s_2, \dots, s_\ell)$ denote the graph obtained from C_ℓ by attaching exactly s_i pendent edges to the vertex y_i for $i = 1, 2, \dots, \ell$, where $s_i \geq 0$ and $\sum_{i=1}^\ell s_i = n - \ell$. Clearly, $C_\ell^\ell(0, 0, \dots, 0) \cong C_\ell$. Let $C_{\ell(s+1)}^\ell(s, s, \dots, s) \circ S_{n-\ell(s+1)+1}$ (For convenience, simply denote it by $C_{\ell(s+1)}^\ell \cdot S_{n-\ell(s+1)+1}$) be the graph obtained by fusing the center of the star $S_{n-\ell(s+1)+1}$ with one pendent vertex of $C_{\ell(s+1)}^\ell(s, s, \dots, s)$, where $s \geq 1$ (as shown in Figure 2).

Since 1980s, the energy $E(G)$ of a graph G has been studied extensively. And many researchers have obtained lots of beautiful results for, such as, acyclic graphs, unicyclic graphs, bicyclic graphs, tricyclic graphs and bipartite graphs. Readers can refer to [3–11, 13–20] and book [12] for more details.

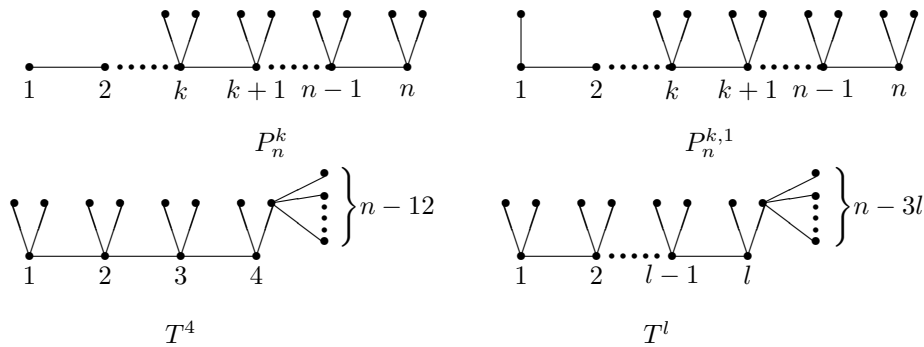


Figure 1 Graphs used in the proof of Theorem 3.4

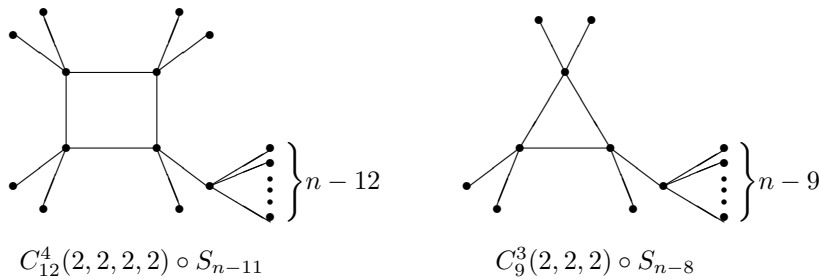


Figure 2 Graphs used in the proof of Lemma 3.5

Recently, Wang et al. [19] characterized that $C_6^3(1, 1, 1) \circ S_{n-5}$ is the unique graph with minimal energy among all graphs in \mathcal{U}_n^3 . In this paper, we will investigate the minimal energy for graphs in \mathcal{U}_n^4 , and obtain that $C_9^3(2, 2, 2) \circ S_{n-8}$ is the unique graph with minimal energy in \mathcal{U}_n^4 . Moreover, the graph with minimal energy is uniquely determined in \mathcal{U}_n^r for $r = 3, 4$.

2. Some lemmas

Let G be a graph with characteristic polynomial $\phi(G, \lambda) = \sum_{i=0}^n a_i \lambda^{n-i}$. Sachs Theorem states [2] that for $i \geq 1$,

$$a_i = \sum_{S \in L_i} (-1)^{p(S)} 2^{c(S)}, \quad (2.1)$$

where L_i denotes the set of Sachs subgraphs of G with i vertices, that is, the subgraphs in which every component is either a K_2 or a cycle, $p(S)$ is the number of components of S and $c(S)$ is the number of cycles contained in S . Let $b_i(G) = |a_i|$ ($i = 0, 1, \dots, n$). Clearly, $b_0(G) = 1$ and $b_2(G)$ equals the number of edges of G .

Let $m(G; k)$ denote the number of matchings of size k in a graph G . For convenience, let $m(G; 0) = 1$ and $m(G; k) = 0$ for all $k < 0$. If G is a bipartite graph, then $b_{2k}(G) = m(G; k)$ and $b_{2k+1}(G) = 0$.

Lemma 2.1 ([2]) *Let $e = uv$ be an edge of a graph G with $n \geq 2$ vertices. Then the $m(G; k)$ for the k -matchings of G is determined by*

$$m(G; k) = m(G - uv; k) + m(G - u - v; k - 1)$$

for $k = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$, where $m(G; 0) = 1$.

Lemma 2.2 ([7]) *Let G be a unicyclic graph with unique cycle C_ℓ . Then $(-1)^k a_{2k} \geq 0$ for all $k \geq 0$; and $(-1)^k a_{2k+1} \geq 0$ (resp., ≤ 0) for all $k \geq 0$ if $\ell = 2r + 1$ and r is odd (resp., even).*

By Lemma 2.2, Eq. (1.1) can be reduced to

$$E(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[\left(\sum_{i=0}^{\lfloor n/2 \rfloor} b_{2i} x^{2i} \right)^2 + \left(\sum_{i=0}^{\lfloor n/2 \rfloor} b_{2i+1} x^{2i+1} \right)^2 \right] dx. \quad (2.2)$$

It follows from Eq. (2.1) that $E(G)$ is a monotonically increasing function in $b_i(G)$ for $i = 0, 1, \dots, n$. That is, for any two unicyclic graphs G_1 and G_2 , we have

$$b_i(G_1) \geq b_i(G_2) \text{ for all } i \geq 0 \implies E(G_1) \geq E(G_2). \quad (2.3)$$

If $b_i(G_1) \geq b_i(G_2)$ holds for all $i \geq 0$, then we denote $G_1 \succeq G_2$ or $G_2 \preceq G_1$. If $G_1 \succeq G_2$ (or $G_2 \preceq G_1$) and there is some i_0 satisfying $b_{i_0}(G_1) > b_{i_0}(G_2)$, then we denote $G_1 \succ G_2$ (or $G_2 \prec G_1$). Therefore, we have the following relations:

$$\begin{aligned} G_1 \succeq G_2 &\implies E(G_1) \geq E(G_2), \\ G_1 \succ G_2 &\implies E(G_1) > E(G_2), \end{aligned} \quad (2.4)$$

where G_1 and G_2 are two unicyclic graphs.

Lemma 2.3 ([19]) *Let G be a unicyclic graph of order n with unique cycle C_ℓ . Let uv be an edge in $E(G)$. Then we have*

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

(b) If $uv \notin C_\ell$, 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 $b_i(G) = b_i(G - v) + b_{i-2}(G - u - v)$.

Lemma 2.4 ([2, 11]) Let G be an acyclic (or unicyclic) graph of order n , and G' a proper subgraph of G . Then, $G \succ G'$.

By simple calculation, it is not difficult to obtain the next result.

Lemma 2.5 Let P_n be a path with n vertices. Then $m(P_n; k) = \binom{n-k}{k}$ for $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

From Lemmas 2.1 and 2.5, we can easily obtain the following lemma.

Lemma 2.6 Let C_n be a cycle with order n . Then $m(C_n; k) = \frac{n}{k} \binom{n-k-1}{k-1}$.

3. Main results

Denote by $\mathcal{U}_n^4(\ell)$ the subset of \mathcal{U}_n^4 such that the unique cycle of any graph $G \in \mathcal{U}_n^4(\ell)$ has a length ℓ . Let $V_1(G)$ denote the set of pendent vertices of G , and let $d_G(x, y)$ denote the distance between x and y , and $d_G(x, C_\ell) = \min\{d_G(x, y) \mid y \in V(C_\ell) \text{ and } x \notin V(C_\ell)\}$. Let $V_2(G)$ denote the subset of $V_1(G)$ such that for any vertex x in $V_2(G)$ we have $d_G(x, C_\ell) = \max\{d_G(y, C_\ell) \mid y \in V_1(G)\}$.

Theorem 3.1 Let $G \in \mathcal{U}_n^4(\ell)$. Then $E(G) \geq E(C_{3\ell}^\ell \cdot S_{n-3\ell+1})$. Equality holds if and only if $G \cong C_{3\ell}^\ell \cdot S_{n-3\ell+1}$.

Proof By Eq. (2.4), it suffices to prove that if $G \not\cong C_{3\ell}^\ell \cdot S_{n-3\ell+1}$, then $G \succ C_{3\ell}^\ell \cdot S_{n-3\ell+1}$.

We proceed by induction on $n - 3\ell$.

When $n - 3\ell = 0$, we get $G \cong C_{3\ell}^\ell \cdot S_1$ since $G \in \mathcal{U}_n^4(\ell)$. So the statement is true.

Now assume $t \geq 1$ and the above result is true when $n - 3\ell < t$. Now let $n - 3\ell = t$. Obviously, $V_2(G) \neq \emptyset$. Let x be any vertex in $V_2(G)$. Since $n \geq 3\ell + 1$ and $G \in \mathcal{U}_n^4(\ell)$, we have $d_G(x, C_\ell) \geq 2$. Take x as v and its unique neighbor as u . From Lemma 2.3, we have

$$b_i(G) = b_i(G - v) + b_{i-2}(G - v - u) \quad (3.1)$$

and

$$b_i(C_{3\ell}^\ell \cdot S_{n-3\ell+1}) = b_i(C_{3\ell}^\ell \cdot S_{n-3\ell}) + b_{i-2}(C_{3\ell}^\ell(1, 2, \dots, 2)). \quad (3.2)$$

Note that $G - v \in \mathcal{U}_{n-1}^4(\ell)$ and $C_{3\ell}^\ell \cdot S_{n-3\ell} \in \mathcal{U}_{n-1}^4(\ell)$. Then

$$G - v \succ C_{3\ell}^\ell \cdot S_{n-3\ell} \quad (3.3)$$

with equality if and only if $G - v \cong C_{3\ell}^\ell \cdot S_{n-3\ell}$ by the induction assumption.

Moreover, since $C_{3\ell}^\ell(1, 2, \dots, 2)$ is a proper subgraph of $G - v - u$, by Lemma 2.4 we have

$$G - v - u \succ C_{3\ell}^\ell(1, 2, \dots, 2). \quad (3.4)$$

From Ineqs. (3.3) and (3.4), for all $i \geq 0$, it is obvious that

$$b_i(G - v) \geq b_i(C_{3\ell}^\ell \cdot S_{n-3\ell}), \quad (3.5)$$

$$b_i(G - v - u) \geq b_i(C_{3\ell}^\ell(1, 2, \dots, 2)). \quad (3.6)$$

Ineqs. (3.1) and (3.2) result in

$$b_i(G) \geq b_i(C_{3\ell}^\ell \cdot S_{n-3\ell+1}).$$

From Ineq. (3.4), there exists some i_0 such that

$$b_{i_0}(G) > b_{i_0}(C_{3\ell}^\ell \cdot S_{n-3\ell+1}).$$

The proof is thus completed. \square

Lemma 3.2 *Let G be a unicyclic graph of $\mathcal{U}_n^4(\ell)$. If $\ell \geq 11$, then $b_{2k} = m(G; k)$ and $b_{2k-1} = 0$ for $1 \leq k \leq 5$.*

Proof If $\ell \geq 11$, it means that the length of the cycle of G is not less than 11. Thus, a Sachs subgraph of G with i vertices does not contain any cycle, for $i \leq 10$. So from Eq. (2.1), the result holds.

From Lemmas 2.5 and 2.6, and by simple computing, we obtain the following two tables, where the graph G in Table 1 is isomorphic to $G \cong C_{3l}^l \cdot S_1$.

G	$b_2(G)$	$b_3(G)$	$b_4(G)$	$b_5(G)$	$b_6(G)$	$b_7(G)$	$b_8(G)$	$b_9(G)$	$b_{10}(G)$
$l = 5$	15	0	75	2	150	0	120	0	32
$l = 6$	18	0	157	0	344	0	468	0	288
$l = 7$	21	0	172	0	651	2	1320	0	1342
$l = 8$	24	0	228	0	1112	0	2944	0	4416
$l = 9$	27	0	297	0	1728	0	5805	2	11610
$l = 10$	30	0	375	0	2550	0	10365	0	18356

Table 1 $G \cong C_{3l}^l \cdot S_1$.

$b_{2k}(G) \setminus G$	$G_1 \cong C_{12}^4 \cdot S_{n-11}$	$G_2 \cong C_{3l}^l \cdot S_1 (3l = n)$
$b_4(G)$	$11n - 90$	$\frac{9}{2}l^2 - \frac{15}{2}l$
$b_6(G)$	$34n - 360$	$\frac{9}{2}l^3 - \frac{45}{2}l^2 + 30l$
$b_8(G)$	$32n - 368$	$\frac{27}{8}l^4 - \frac{135}{4}l^3 + \frac{945}{8}l^2 - \frac{579}{4}l$
$b_{10}(G)$	$8n - 96$	$\frac{81}{40}l^5 - \frac{135}{4}l^4 + \frac{1755}{4}l^3 - \frac{2637}{4}l^2 + \frac{3858}{5}l$

Table 2 The coefficients of characteristic polynomial of two graphs

We next consider the minimal energy on graphs $C_{\ell(s+1)}^\ell \cdot S_{n-\ell(s+1)+1}$. Before exhibiting the first main result, we introduce the following Claim.

Claim 1 *For $0 \leq k \leq 5$, $b_{2k}(C_{3\ell}^\ell \cdot S_1) \geq b_{2k}(C_{12}^4 \cdot S_{3\ell-11})$.*

Proof It is trivial to show that $b_{2k}(C_{3\ell}^\ell \cdot S_1) \geq b_{2k}(C_{12}^4 \cdot S_{3\ell-11})$, for $0 \leq k \leq 1$. In view of Eq. (2.1), we only need to consider the following four cases.

Case 1 $k = 2$.

From Table 2, we have that $b_4(C_{3\ell}^\ell \cdot S_1) = \frac{9}{2}\ell^2 - \frac{15}{2}\ell$ and $b_4(C_{12}^4 \cdot S_{3\ell-11}) = 33\ell - 90$.

Now let $f_1(x) = \frac{9}{2}x^2 - \frac{15}{2}x - (33x - 90) = \frac{9}{2}x^2 - \frac{81}{2}x + 90$. From the property of a quadratic function, $f_1(x)$ is a monotonically increasing function on interval $[10, +\infty)$. Moreover, $f_1(10) = 25 > 0$. Therefore, $b_4(C_{3\ell}^\ell \cdot S_1) > b_4(C_{12}^4 \cdot S_{3\ell-11})$.

Case 2 $k = 3$.

From Table 2, it is not difficult to get that $b_6(C_{3\ell}^\ell \cdot S_1) = \frac{9}{2}\ell^3 - \frac{45}{2}\ell^2 + 30\ell$ and $b_6(C_{12}^4 \cdot S_{3\ell-11}) = 102\ell - 360$. By examining the function $f_2(x) = \frac{9}{2}x^3 - \frac{45}{2}x^2 + 30x - (102x - 360) = \frac{9}{2}x^3 - \frac{45}{2}x^2 - 72x + 360$, $f_2 : [10, +\infty) \rightarrow \mathbb{R}$, and its first derivative $f_2'(x) = \frac{27}{2}x^2 - 45x - 72$, we see that $f_2'(x) > 0$ for any x with $10 \leq x \leq +\infty$, hence $f_2(x)$ is a monotonically increasing function, and $f_2(10) = 1790$. So $b_6(C_{3\ell}^\ell \cdot S_1) > b_6(C_{12}^4 \cdot S_{3\ell-11})$.

Case 3 $k = 4$.

From Table 2, we obtain that $b_8(C_{3\ell}^\ell \cdot S_1) = \frac{27}{8}\ell^4 - \frac{135}{4}\ell^3 + \frac{945}{8}\ell^2 - \frac{579}{4}\ell$ and $b_8(C_{12}^4 \cdot S_{3\ell-11}) = 96\ell - 368$. Now we consider the function $f_3(x) = \frac{27}{8}x^4 - \frac{135}{4}x^3 + \frac{945}{8}x^2 - \frac{579}{4}x - (96x - 368) = \frac{27}{8}x^4 - \frac{135}{4}x^3 + \frac{945}{8}x^2 - \frac{963}{4}x + 368$. Moreover, its first derivative $f_3'(x) = \frac{27}{2}x^3 - \frac{405}{4}x^2 + \frac{945}{4}x - \frac{963}{4}$, implies that $f_3'(x) > 0$ for any x with $10 \leq x \leq +\infty$. Hence $b_8(C_{3\ell}^\ell \cdot S_1) > b_8(C_{12}^4 \cdot S_{3\ell-11})$.

Case 4 $k = 5$.

Table 2 implies that $b_{10}(C_{3\ell}^\ell \cdot S_1) = \frac{81}{40}\ell^5 - \frac{135}{4}\ell^4 + \frac{1755}{4}\ell^3 - \frac{2637}{4}\ell^2 + \frac{3858}{5}\ell$ and $b_{10}(C_{12}^4 \cdot S_{3\ell-11}) = 24\ell - 96$. Seeing function $f_4(x) = \frac{81}{40}x^5 - \frac{135}{4}x^4 + \frac{1755}{4}x^3 - \frac{2637}{4}x^2 + \frac{3738}{5}x + 96$ and its first derivative $f_4'(x) = \frac{81}{8}x^4 - 135x^3 + \frac{5265}{4}x^2 - \frac{2637}{2}x + \frac{3738}{5}$, we get that $f_4'(x) > 0$ for any x with $10 \leq x \leq +\infty$. Therefore, $b_{10}(C_{3\ell}^\ell \cdot S_1) > b_{10}(C_{12}^4 \cdot S_{3\ell-11})$.

Theorem 3.3 For $\ell \geq 5$, $E(C_{3\ell}^\ell \cdot S_1) > E(C_{12}^4 \cdot S_{3\ell-11})$.

Proof From Eq. (2.4), it suffices to prove that $C_{3\ell}^\ell \cdot S_1 \succ C_{12}^4 \cdot S_{3\ell-11}$. When $5 \leq \ell \leq 10$, we know, from Table 1, that the conclusion is true by simple comparison. Hence, we now only need to consider the remainder part $\ell \geq 11$.

Since $C_{12}^4 \cdot S_{3\ell-11}$ is bipartite, $b_{2k+1}(G) = 0$ for all $k \geq 0$. Note that the number of i -matchings of $C_{12}^4 \cdot S_{3\ell-11}$ equals 0 for $i \geq 6$. Thus, it suffices to prove $b_{2k}(C_{3\ell}^\ell \cdot S_1) \geq b_{2k}(C_{12}^4 \cdot S_{3\ell-11})$, for $0 \leq k \leq 5$.

By Claim 1, we complete the proof. \square

We now describe an important conclusion which will be used in the proof of the next main result.

Claim 2 If $\ell \geq 5$, then $m(T^\ell; k) + m(P_{\ell-2}^1 \cup S_{n-3\ell+1}; k-1) - m(T^{\ell-1}; k) + m(P_{\ell-3}^1 \cup S_{n-3\ell+4}; k-1) > m(P_{\ell-4}^1 \cup S_{n-3\ell+1}; k-2)$.

Proof Let $f_1(\ell) = m(T^\ell; k) + m(P_{\ell-2}^1 \cup S_{n-3\ell+1}; k-1)$. Then

$$f_1(\ell) = m(T^\ell; k) + m(P_{\ell-2}^1 \cup S_{n-3\ell+1}; k-1)$$

$$\begin{aligned}
&= m(P_{\ell}^{2,1} \cup S_{n-3\ell+1}; k) + m(P_{\ell-1}^1; k-1) + m(P_{\ell-2}^1 \cup S_{n-3\ell+1}; k-1) \\
&= m(P_{\ell-1}^{2,1} \cup P_3 \cup S_{n-3\ell+1}; k) + m(P_{\ell-2}^{2,1} \cup S_{n-3\ell+1}; k-1) + m(P_{\ell-1}^1; k-1) + \\
&\quad m(P_{\ell-3}^1 \cup P_3 \cup S_{n-3\ell+1}; k-1) + m(P_{\ell-4}^1 \cup S_{n-3\ell+1}; k-2) \\
&= m(P_{\ell-1}^{2,1} \cup S_{n-3\ell+1}; k) + 2m(P_{\ell-1}^{2,1} \cup S_{n-3\ell+1}; k-1) + m(P_{\ell-2}^{2,1} \cup S_{n-3\ell+1}; k-1) + \\
&\quad m(P_{\ell-1}^1; k-1) + m(P_{\ell-3}^1 \cup S_{n-3\ell+1}; k-1) + 2m(P_{\ell-3}^1 \cup S_{n-3\ell+1}; k-2) + \\
&\quad m(P_{\ell-4}^1 \cup S_{n-3\ell+1}; k-2), \tag{3.7}
\end{aligned}$$

and

$$\begin{aligned}
f_1(\ell-1) &= m(T^{\ell-1}; k) + m(P_{\ell-3}^1 \cup S_{n-3\ell+4}; k-1) \\
&= m(P_{\ell-1}^{2,1} \cup S_{n-3\ell+4}; k) + m(P_{\ell-2}^1; k-1) + m(P_{\ell-3}^1 \cup S_{n-3\ell+4}; k-1) \\
&= m(P_{\ell-1}^{2,1} \cup S_{n-3\ell+1}; k) + 3m(P_{\ell-1}^{2,1}; k-1) + m(P_{\ell-2}^1; k-1) + \\
&\quad m(P_{\ell-3}^1 \cup S_{n-3\ell+1}; k-1) + 3m(P_{\ell-3}^1; k-2). \tag{3.8}
\end{aligned}$$

Note that, since $n \geq 3\ell+1$, we have

$$m(P_{\ell-1}^{2,1} \cup S_{n-3\ell+1}; k-1) \geq m(P_{\ell-1}^{2,1} \cup P_2; k-1) = m(P_{\ell-1}^{2,1}; k-1) + m(P_{\ell-1}^{2,1}; k-2). \tag{3.9}$$

Meanwhile,

$$\begin{aligned}
m(P_{\ell-1}^1; k-1) &= m(P_{\ell-2}^1 \cup P_3; k-1) + m(P_{\ell-3}^1; k-2) \\
&= m(P_{\ell-2}^1; k-1) + 2m(P_{\ell-2}^1; k-2) + m(P_{\ell-3}^1; k-2), \tag{3.10}
\end{aligned}$$

$$\begin{aligned}
m(P_{\ell-1}^{2,1}; k-1) &= m(P_{\ell-2}^{2,1} \cup P_3; k-1) + m(P_{\ell-3}^{2,1}; k-2) \\
&= m(P_{\ell-2}^{2,1}; k-1) + 2m(P_{\ell-2}^{2,1}; k-2) + m(P_{\ell-3}^{2,1}; k-2), \tag{3.11}
\end{aligned}$$

and

$$\begin{aligned}
m(P_{\ell-2}^{2,1} \cup S_{n-3\ell+1}; k-1) &> m(P_{\ell-2}^{2,1}; k-1), \\
m(P_{\ell-3}^1 \cup S_{n-3\ell+1}; k-2) &> m(P_{\ell-3}^1; k-2). \tag{3.12}
\end{aligned}$$

Combining the above Eqs. (3.7) through (3.12) with Lemma 2.4, we obtain

$$\begin{aligned}
f_1(\ell) - f_1(\ell-1) &\geq m(P_{\ell-2}^1; k-2) + m(P_{\ell-4}^1 \cup S_{n-3\ell+1}; k-2) \\
&> m(P_{\ell-4}^1 \cup S_{n-3\ell+1}; k-2).
\end{aligned}$$

Therefore, the result holds. \square

Theorem 3.4 For $\ell \geq 5$, $E(C_{3\ell}^\ell \cdot S_{n-3\ell+1}) > E(C_{12}^4 \cdot S_{n-11})$.

Proof By Lemma 2.3, we conclude that

$$b_i(C_{12}^4 \cdot S_{n-11}) = b_i(T^4) + b_{i-2}(P_2^1 \cup S_{n-11}) - 2b_{i-4}(S_{n-11}),$$

while for $\ell \equiv 0 \pmod{4}$,

$$b_i(C_{3\ell}^\ell \cdot S_{n-3\ell+1}) = b_i(T^\ell) + b_{i-2}(P_{\ell-2}^1 \cup S_{n-3\ell+1}) - 2b_{i-\ell}(S_{n-3\ell+1}),$$

and for $\ell \not\equiv 0 \pmod{4}$,

$$b_i(C_{3\ell}^\ell \cdot S_{n-3\ell+1}) = b_i(T^\ell) + b_{i-2}(P_{\ell-2}^1 \cup S_{n-3\ell+1}) + 2b_{i-\ell}(S_{n-3\ell+1}).$$

Let $f_1(\ell) = b_{2k}(T^\ell) + b_{2k-2}(P_{\ell-2}^1 \cup S_{n-3\ell+1})$. From (2.1) (Sachs Theorem), we also have $f_1(\ell) = m(T^\ell; k) + m(P_{\ell-2}^1 \cup S_{n-3\ell+1}; k-1)$.

When $\ell \equiv 0 \pmod{4}$, we arrive at

$$m(P_{\ell-4}^1 \cup S_{n-3\ell+1}; k-2) - 2b_{2k-\ell}(S_{n-3\ell+1}) > \begin{cases} \left(\frac{\ell-4}{2}-3\right)(n-3\ell) - 2 > 0 & k = \frac{\ell}{2}; \\ \left(\frac{\ell-4}{2}-2\right)(n-3\ell) - 2(n-3\ell) > 0 & k = \frac{\ell}{2} + 1; \\ 0 & k \neq \frac{\ell}{2}, \frac{\ell}{2} + 1. \end{cases}$$

By Claim 2, we have

$$\begin{aligned} b_{2k}(C_{3\ell}^\ell \cdot S_{n-3\ell+1}) &= f_1(\ell) - 2b_{2k-\ell}(S_{n-3\ell+1}) \\ &> f_1(\ell-1) + m(P_{\ell-4}^1 \cup S_{n-3\ell+1}; k-2) - 2b_{2k-\ell}(S_{n-3\ell+1}) \\ &> f_1(\ell-1) \geq f_1(4) \geq f_1(4) - 2b_{2k-4}(S_{n-11}) \\ &= b_{2k}(C_{12}^4 \cdot S_{n-11}). \end{aligned}$$

When $\ell \not\equiv 0 \pmod{4}$, from Claim 2, we get

$$\begin{aligned} b_{2k}(C_{3\ell}^\ell \cdot S_{n-3\ell+1}) &= f_1(\ell) + 2b_{2k-\ell}(S_{n-3\ell+1}) \\ &> f_1(\ell-1) + m(P_{\ell-4}^1 \cup S_{n-3\ell+1}; k-2) + 2b_{2k-\ell}(S_{n-3\ell+1}) \\ &> f_1(\ell-1) \geq f_1(4) \geq f_1(4) - 2b_{2k-4}(S_{n-11}) \\ &= b_{2k}(C_{12}^4 \cdot S_{n-11}). \end{aligned}$$

So we conclude that $b_{10}(C_{3\ell}^\ell \cdot S_{n-3\ell+1}) > b_{10}(C_{12}^4 \cdot S_{n-11})$.

Thus the proof is completed. \square

Lemma 3.5 For $n \geq 12$, $E(C_{12}^4 \cdot S_{n-11}) > E(C_9^3 \cdot S_{n-8})$.

Proof Note that

$$\begin{aligned} \phi(C_9^3 \cdot S_{n-8}) &= x^{n-8}(x^8 - nx^6 - 2x^5 + (8n-54)x^4 + 2(n-9)x^3 - (14n-118)x^2 + 4(n-9)), \\ \phi(C_{12}^4 \cdot S_{n-11}) &= x^{n-10}(x^{10} - nx^8 + (11n-90)x^6 - (3n-336)x^4 + (32n-368)x^2 + (8n-96)), \end{aligned}$$

where the graphs $C_{12}^4 \cdot S_{n-11}$ and $C_9^3 \cdot S_{n-8}$ refer to Figure 2. Therefore, from Eq. (2.2), we have

$$E(C_{12}^4 \cdot S_{n-11}) - E(C_9^3 \cdot S_{n-8}) = \frac{1}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \frac{h_1(x)}{h_2(x)} dx,$$

where $h_1(x) = (1 + nx^2 + (11n-90)x^4 + (3n-336)x^6 + (32n-368)x^8 + (8n-96)x^{10})^2$ and $h_2(x) = (1 + nx^2 + (8n-54)x^4 + (14n-118)x^6 + 4(n-9)x^8)^2 + (2x^3 + 2(n-9)x^5)^2$. Then, by a simple calculation, we can obtain the result.

Combining Lemma 3.5 and Theorem 3.1 with Theorem 3.4, we get the main result of the paper.

Theorem 3.6 For $n \geq 9$, $C_9^3 \cdot S_{n-8}$ has the minimal energy among all graphs in \mathcal{U}_n^4 .

Therefore, from [19, Theorem 11] and Theorem 3.6, we have an additional result as the next corollary.

Corollary 3.7 For $n \geq 9$, $C_9^3(1, 1, 1) \cdot S_{n-5}$ has the minimal energy among all graphs in \mathcal{U}_n^r for $r = 3, 4$.

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