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Minimal energy on a class of graphs

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The energy of a graph G, denoted by $E(G)$, is defined to be the sum of absolute values of all eigenvalues of G. Let $\mathscr{U}_n$ denote the set of connected $(n, n)-$ graphs, i.e., the connected graphs with n vertices and n edges. For any graph $G \in \mathscr{U}_n$, if $d(v) = r(\geqslant 2)$ for each vertex v in the unique cycle of G, G is said to be $cycle-r-regular$ $(n, n)-$ graph. In this paper, $cycle-3-regular$ $(n, n)-$ graph with minimal energy is uniquely determined.

KEY WORDS: $cycle-3-regular(n, n)-$ graph, energy of graph, spectrum of graph, matching.

AMS subject classifications: 05C35, 05C50, 05C90.

1. Introduction

Let G be a connected graph with n vertices and $A(G)$ its adjacency matrix. The characteristic polynomial $\phi(G; \lambda)$ of $A(G)$ is defined as

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

where I is the unit matrix of order n.

All n roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of the equation $\phi(G; \lambda) = 0$ are called to be eigenvalues of G. It's evident that each λ_i $(i = 1, 2, \ldots n)$ 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

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that $E(G)$ can be expressed as the coulson integral formula

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

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

Since the energy of a graph can be used to approximate the total π-electron energy of the molecule, it has been intensively studied by many scholars. It's both interesting and significant to determine the graph with extremal energies among a given class of graphs. Numerous results on this subject haven been put forwarded. For more details see [1–9]; for some recent research along these lines see [10–22]. The interested reader may also refer to [23, 24] for the mathematical properties.

As usual, we begin with some notations and terminologies.

Let $G =< V(G), E(G) >$ be a graph with $n = |V(G)|$ vertices and $\varepsilon = |E(G)|$ edges. If $n = \varepsilon$, then G is said to be a $(n,n)-$graph.

It's easy to see that any connected $(n,n)-$graph contains exactly one cycle. Let $\mathscr{U}_n$ denote the set of connected $(n,n)-$ graphs.

Let $\mathscr{U}_n^r = \{G \in \mathscr{U}_n | d(x) = r$ for any vertex $x \in V(C_l)\}$, where $r \geqslant 2$ and C_l is the unique cycle in G. Any graph in $\mathscr{U}_n^r$ is said to be a $cycle-r-regular$ graph. Since $\mathscr{U}_n^2$ contains exactly one single element, we will always suppose that $r \geqslant 3$.

Let G be a connected $(n,n)-$ graph and C_l the unique cycle of length $l(3 \leqslant l \leqslant n)$ in it. If $n \geqslant l+1$, then G has at least a vertex with degree one, which is also named pendent vertex. Let $V_1(G)$ denote the set of pendent vertices in G. Let $d_G(x,\ y)$ denote the length of the shortest path connecting vertices x and y in G, namely, the distance between x and y. Let $d_G(x, C_l) = min\{d_G(x,y)|y \in V(C_l)\ and\ x \notin\ V(C_l)\}$. Let $V_2(G)$ denote the subset of $V_1(G)$ such that for any vertex x in $V_2(G)$ there exists $d_G(x, C_l) = max\{d_G(y, C_l)|\ y \in V_1(G)\}$.

Let P_n be path on n vertices and its vertices be ordered successively as $x_1,\ x_2,\dots,x_n$. By P_n^k we denote the graph obtained from P_n by attaching exactly one pendent edge to each of the vertices $x_k,\ x_{k+1},\ \dots,x_n$, respectively. Here, $P_1^1 = P_2$ and $P_2^1 = P_4$.

Let the vertices of C_l be ordered successively as $y_1,\ y_2,\dots,y_l$. Denote by $C_n^l(t_1,\ t_2,\dots,t_l)$, the graph obtained from C_l by attaching exactly t_i pendent edges to the vertex y_i for $i = 1, 2,\dots,l$, where $t_i \geqslant 0$ and $\sum_{i=1}^{l} t_i = n-l$. Here, $C_l^l(0,\ 0,\dots,0) = C_l$. Let $C_{2l}^l(1,\ 1,\dots,1)^{\circ}S_{n-2l+1}$ be the graph obtained by fusing the center of the star S_{n-2l+1} with one pendent vertex of $C_{2l}^l(1,\ 1,\ \dots,1)$.

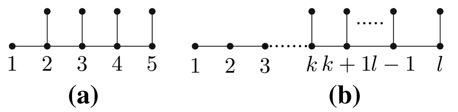

Figure 1. (a). P_5^2; (b). P_l^k.

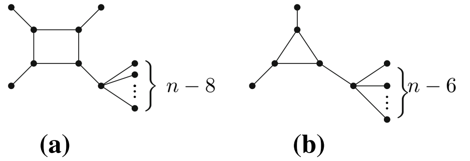

Figure 2. (a). $C_8^4(1, 1, 1, 1)^{\text{o}} S_{n-7}$;$(b)$. $C_6^3(1, 1, 1)^{\text{o}} S_{n-5}$.

As examples, we illustrate P_5^2 and P_l^k in figure 1 and $C_8^4(1, 1, 1, 1)^{\text{o}} S_{n-7}$ and $C_6^3(1, 1, 1)^{\text{o}} S_{n-5}$ in figure 2, respectively.

Denote, as usual, $mK_1 (m \geqslant 1)$ m copies of isolated vertex K_1.

In this work, we investigate the minimal energy for graphs in $\mathscr{U}_n^3$. It's mathematically proved that $C_6^3(1, 1, 1)^{\text{o}} S_{n-5}$ is the unique graph with minimal energy among all graphs in $\mathscr{U}_n^3$.

2. Lemmas and results

We begin with a well-known result due to Sachs [25] which reads as follows

Lemma 1. Let G be a graph on n vertices with characteristic polynomial $\phi(G; x) = \sum_{i=0}^{n} a_i x^{n-i}$. Then

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

where L_i denotes the set of Sachs graphs with i vertices (namely, the graph with its component being either K_2 or a cycle), $k(S)$ is number of components of S and $c(S)$ is the number of cycles contained in S.

Let $b_i(G) = |a_i(G)| (i = 0, 1, \ldots, n)$. It can be easily seen from equation (2) that $b_2(G)$ equals exactly the number of edges of G. In addition, $b_0(G) = 1$.

Let $m(G, k)$ denote the number of $k-$matchings of a graph G, where $k-$matchings is a set of edges of size k in which any two edges share no common vertices. In particular, if G contains no cycle, i.e., G is acyclic, then $b_{2k}(G) = m(G, k)$ and $b_{2k+1}(G) = 0$ for each $k \geqslant 0$. It's both consistent and convenient to define $b_k(G) = 0$ and $m(G, k) = 0$ for the case when $k < 0$.

In Ref [5], Y. Hou obtained the following result:

Lemma 2. Let G be a unicyclic graph with its cycle C_l. Then $(-1)^k a_{2k} \geqslant 0$ for all $k \geqslant 0$; and $(-1)^k a_{2k+1} \geqslant 0$ $(resp. \leqslant 0)$ for all $k \geqslant 0$ if $l = 2r + 1$ and r is odd $(resp.$ $even)$.

By means of lemma 2, equation (1) is now reduced to

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

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

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

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

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

Lemma 3. Let G_1 and G_2 be two unicyclic graphs. Then $G_1 \succeq G_2$ implies that $E(G_1) \geqslant E(G_2)$ and $G_1 \succ G_2$ implies that $E(G_1) > E(G_2)$.

Lemma 4. 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 $l \equiv 0 (mod\ 4)$ and $b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-l}(G - C_l)$ if $l \not\equiv 0 (mod\ 4)$;

(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

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

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 equation (5). □

F. Li obtained the following result in Ref. [22].

Lemma 5. 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 $G' \prec G$.

Denote by $\mathscr{U}_n^3(l)$ the subset of $\mathscr{U}_n^3$ such that for any graph $G \in \mathscr{U}_n^3(l)$, G has a cycle of length l. It's obvious that G has at least $2l$ vertices.

Theorem 6. Let $G \in \mathscr{U}_n^3(l)$. Then $E(G) \geqslant E(C_{2l}^l(1, 1, \ldots, 1)^{\circ} S_{n-2l+1})$. Equality holds if and only if $G \cong C_{2l}^l(1, 1, \ldots, 1)^{\circ} S_{n-2l+1}$.

Proof. By lemma 3, it suffices to prove that if $G \ncong C_{2l}^l(1, 1, \ldots, 1)^{\circ} S_{n-2l+1}$, then $G \succ C_{2l}^l(1, 1, \ldots, 1)^{\circ} S_{n-2l+1}$.

We proceed by induction on $n - 2l$.

When $n - 2l = 0$, we have $G \cong C_{2l}^l(1, 1, \ldots, 1)^{\circ} S_1$ since $G \in \mathscr{U}_n^3(l)$. Therefore, the result follows.

Suppose $t \geqslant 1$ and the above statement is true for the case when $n - 2l < t$.

Now, let $n - 2l = t$. Obviously, $V_2(G) \neq \emptyset$. Let x be any vertex in $V_2(G)$. As $n \geqslant 2l + 1$ and $G \in \mathscr{U}_n^3(l)$, then $d_G(x, C_l) \geqslant 2$. Take x as v and its unique neighbor as u. Using lemma 4(b), we obtain

$$b_i(G) = b_i(G - v) + b_{i-2}(G - v - u) \tag{6}$$

and

$$\begin{aligned} b_i(C_{2l}^l(1, 1, \ldots, 1)^{\circ} S_{n-2l+1}) = {} & b_i(C_{2l}^l(1, 1, \ldots, 1)^{\circ} S_{n-2l}) \\ & + b_{i-2}(C_{2l-1}^l(0, 1, \ldots, 1)). \end{aligned} \tag{7}$$

Noting that $G - v \in \mathscr{U}_{n-1}^3(l)$ and $C_{2l}^l(1, 1, \dots, 1)^{\mathrm{o}} S_{n-2l} \in \mathscr{U}_{n-1}^3(l)$. Then

$$G - v \succeq C_{2l}^l(1, 1, \dots, 1)^{\mathrm{o}} S_{n-2l} \tag{8}$$

with equality if and only if $G - v \cong C_{2l}^l(1, 1, \dots, 1)^{\mathrm{o}} S_{n-2l}$ by induction assumption.

Moreover, $C_{2l-1}^l(0, 1, \dots, 1)$ is a proper subgraph of $G - v - u$, and then

$$G - v - u \succ C_{2l-1}^l(0, 1, \dots, 1). \tag{9}$$

by lemma 5.

From equations.(8) and (9), we get resp.

$$b_i(G - v) \geqslant b_i(C_{2l}^l(1, 1, \dots, 1)^{\mathrm{o}} S_{n-2l}) \tag{10}$$

and

$$b_i(G - v - u) \geqslant b_i(C_{2l-1}^l(0, 1, \dots, 1)). \tag{11}$$

for all $i \geqslant 0$.

Combining equations.(6)–(7) and (10)–(11), we obtain

$$b_i(G) \geqslant b_i(C_{2l}^l(1, 1, \dots, 1)^{\mathrm{o}} S_{n-2l+1}) \tag{12}$$

for all $i \geqslant 0$.

Since $G \ncong C_{2l}^l(1, 1, \dots, 1)^{\mathrm{o}} S_{n-2l+1}$, there must exist some i_0 such that

$$b_{i_0}(G) > b_{i_0}(C_{2l}^l(1, 1, \dots, 1)^{\mathrm{o}} S_{n-2l+1}). \tag{13}$$

(In fact, by equation (9), there must exist some i_0 such that $b_{i_0}(G - v - u) > b_{i_0}(C_{2l-1}^l(0, 1, \dots, 1))$.) Hence, the theorem follows. □

Lemma 7. [25]. Let $e = uv$ be an edge of a graph G on $n \geqslant 2$ vertices. Then the $k-$matchings $m(G; k)$ of G is determined by

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

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

Lemma 8. For $l \geqslant 5$, $E(C_{2l}^l(1, 1, \dots, 1)^{\mathrm{o}} S_1) > E(C_8^4(1, 1, \dots, 1)^{\mathrm{o}} S_{2l-7})$, where $C_8^4(1, 1, \dots, 1)^{\mathrm{o}} S_{n-7}$ is graph as shown in figure 2(a).

Proof. By lemma 3, it's sufficient to prove that $C^{l}_{2l}(1, 1, \ldots, 1)^{\mathrm{o}}S_1) \succ C^4_8$ $(1, 1, \ldots, 1)^{\mathrm{o}}S_{2l-7}$.

We shall prove this by induction on l.
When $l = 5$, by Lemma 4(a), we have

$$b_i(C^5_{10}(1, 1, \ldots, 1)^{\mathrm{o}}S_1) = b_i(P^1_5) + b_{i-2}(P^1_3) + 2b_{i-5}(5K_1), \tag{14}$$

$$b_i(C^4_8(1, 1, \ldots, 1)^{\mathrm{o}}S_3) = b_i(T^{(4)}) + b_{i-2}(P_4 \cup S_3) - 2b_{i-4}(P_3), \tag{15}$$

where $T^{(4)}$ is the tree as indicated in figure 3(a) by setting $l = 4$ and $n = 10$.

It can be seen from equations. (14) and (15) that $b_{2k+1}(C^4_8(1, 1, \ldots, 1)^{\mathrm{o}}S_3) = 0 \leqslant 2b_{(2k+1)-5}(5K_1) = b_{2k+1}(C^5_{10}(1, 1, \ldots, 1)^{\mathrm{o}}S_1)$ for all $k \geqslant 0$.

In what follows, we shall verify that $b_{2k}(C^4_8(1, 1, \ldots, 1)^{\mathrm{o}}S_3) \leqslant b_{2k}(C^5_{10}$ $(1, 1, \ldots, 1)^{\mathrm{o}}S_1)$ for all $k \geqslant 0$. It's easy to see that the statement is true for $k = 0, 1$. So we may assume that $k \geqslant 2$.

Once again, by lemma 4(a), we obtain

$$\begin{aligned} b_{2k}(C^5_{10}(1, 1, \ldots, 1)^{\mathrm{o}}S_1) &= b_{2k}(P^1_5) + b_{2k-2}(P^1_3) \\ &= m(P^1_5; k) + m(P^1_3; k-1), \end{aligned}$$

$$\begin{aligned} b_{2k}(C^4_8(1, 1, \ldots, 1)^{\mathrm{o}}S_3) &= b_{2k}(T^{(4)}) + b_{2k-2}(P_4 \cup P_3) - 2b_{2k-4}(P_3) \\ &= m(T^{(4)}; k) + m(P_4 \cup P_3; k-1) - 2b_{2k-4}(P_3) \\ &\leqslant m(T^{(4)}; k) + m(P_4 \cup P_3; k-1) \end{aligned}$$

Let $f(k) = [m(P^1_5; k) + m(P^1_3; k-1)] - [m(T^{(4)}; k) + m(P_4 \cup P_3; k-1)]$. Then

$$\begin{aligned} f(k) = {} & m(P_2 \cup P^1_4; k) + 2m(P^1_3; k-1) - m(P_3 \cup P^2_4; k) - \\ & m(P^1_3; k-1) - m(P_2 \cup P_4; k-1) - m(P_4; k-2) \\ = {} & \ldots \\ = {} & m(P_4; k-3) - m(P_4; k-2) + m(P_2; k-2) + m(P_2; k-3) \\ = {} & \begin{cases} 0, & 2 \leqslant k \leqslant 3\, and\, k \geqslant 6; \\ 3, & k = 4; \\ 1, & k = 5; \end{cases} \end{aligned}$$

Therefore, $f(k) \geqslant 0$ and then $b_{2k}(C^5_{10}(1, 1, \ldots, 1)^{\mathrm{o}}S_1) \geqslant b_{2k}(C^4_8(1, 1, \ldots, 1)$ ${}^{\mathrm{o}}S_3)$ for all $k \geqslant 0$. In particular, $b_8(C^5_{10}(1, 1, \ldots, 1)^{\mathrm{o}}S_1) > b_8(C^4_8(1, 1, \ldots, 1)^{\mathrm{o}}S_3)$. So the statement is true for the case when $l = 5$.

Let $t \geqslant 6$ and suppose the result is true for $l < t$. Consider the case when $l = t$.

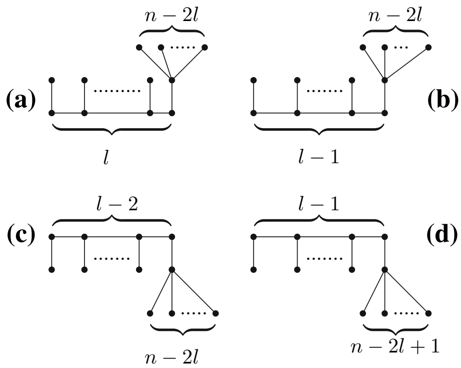

Figure 3. $(a).\, T^{(l)}$; $(b).\, T_1$; $(c).\, T_2$; $(d).\, T_3$.

Obviously, $b_{2k+1}(C_8^4(1,\ 1, \ldots, 1)^{\circ}S_{2t-7}) = -2b_{(2k+1)-4}(S_{2t-7}) = 0$.

If $t \equiv 0(mod\,4)$, $b_{2k+1}(C_{2t}^t(1,\ 1, \ldots, 1)^{\circ}S_1) = -2b_{(2k+1)-t}(tK_1) = 0$, and if $t \not\equiv 0(mod\,4)$, $b_{2k+1}(C_{2t}^t(1,\ 1, \ldots, 1)^{\circ}S_1) = 2b_{(2k+1)-t}(tK_1) \geqslant 0$.

So $b_{2k+1}(C_{2t}^t(1,\ 1, \ldots, 1)^{\circ}S_1) \geqslant b_{2k+1}(C_8^4(1,\ 1, \ldots, 1)^{\circ}S_{2t-7})$ for all $k \geqslant 0$. Now, we need only to show that $b_{2k}(C_{2t}^t(1,\ 1, \ldots, 1)^{\circ}S_1) \geqslant b_{2k}(C_8^4(1,\ 1, \ldots, 1)^{\circ}S_{2t-7})$ for all $k \geqslant 0$.

From lemma 4(a), we obtain

$$\begin{aligned}
b_{2k}(C_{2t}^t(1,\ 1, \ldots, 1)^{\circ}S_1) &= b_{2k}(P_t^1) + b_{2k-2}(P_{t-2}^1) \pm 2b_{2k-t}(tK_1)\\
&\geqslant m(P_t^1; k) + m(P_{t-2}^1; k-1) - 2\\
&= m(P_2 \cup P_{t-1}^1; k) + 2m(P_{t-2}^1; k-1) - 2\\
&= m(P_{t-1}^1; k) + m(P_{t-1}^1; k-1) + 2m(P_{t-2}^1; k-1) - 2\\
&= [m(P_{t-1}^1; k) + m(P_{t-3}^1; k-1) + 2] + m(P_{t-1}^1; k-1) +\\
&\quad\ m(P_{t-3}^1; k-1) + 2m(P_{t-3}^1; k-2) + 2m(P_{t-4}^1; k-2) - 4\\
&\geqslant b_{2k}(C_{2(t-1)}^{t-1}(1,\ 1, \ldots, 1)^{\circ}S_1) + m(P_{t-1}^1; k-1)\\
&\quad\ + m(P_{t-3}^1; k-1).
\end{aligned}$$

By induction assumption, $b_{2k}(C_{2(t-1)}^{t-1}(1,\ 1, \ldots, 1)^{\circ}S_1) \geqslant b_{2k}(C_8^4(1,\ 1, \ldots, 1)^{\circ}S_{2t-9})$. This gives $b_{2k}(C_{2t}^t(1,\ 1, \ldots, 1)^{\circ}S_1) \geqslant b_{2k}(C_8^4(1,\ 1, \ldots, 1)^{\circ}S_{2t-9}) + m(P_{t-1}^1; k-1) + m(P_{t-3}^1; k-1)$.

By lemma 4 (b) and (a), we have

$$b_{2k}(C_8^4(1,\ 1, \ldots, 1)^{\circ}S_{2t-7}) = b_{2k}(C_8^4(1,\ 1, \ldots, 1)^{\circ}S_{2t-9}) + 2b_{2k-2}(C_7^4(0,\ 1, \ldots, 1))$$

and

$$\begin{aligned} b_{2k-2}(C_7^4(0,\ 1,\ldots,1)) &= b_{2k-2}(P_4^2)+b_{2k-4}(P_4)-2b_{2k-6}(3K_1)\\ &= m(P_4^2;k-1)+m(P_4;k-2)-2b_{2k-6}(3K_1), \end{aligned}$$

respectively.

What remains is to prove that $m(P_{t-1}^1;k-1)+m(P_{t-3}^1;k-1)\geqslant 2[m(P_4^2;k-1)+m(P_4;k-2)]$.

Note that

$$m(P_{t-1}^1;k-1)\geqslant m(P_5^1;k-1)=m(P_4^1;k-1)+m(P_4^1;k-2)+m(P_3^1;k-2),$$

$$m(P_{t-3}^1;k-1)\geqslant m(P_3^1;k-1)=m(P_4;k-1)+m(P_4;k-2)+m(P_2;k-2).$$

Hence,

$$\begin{aligned} m(P_{t-1}^1;k-1)+m(P_{t-3}^1;k-1) &\geqslant m(P_4^1;k-1)+m(P_4^1;k-2)+m(P_3;k-2)\\ &\quad +m(P_4;k-1)+m(P_4;k-2)+m(P_2;k-2)\\ &= m(P_3^1;k-1)+m(P_4;k-1)+2m(P_4;k-2)\\ &\quad +m(P_4^1;k-2)+2m(P_3^1;k-2)+m(P_2;k-2)\\ &= 2m(P_4;k-1)+3m(P_4;k-2)+m(P_4^1;k-2)\\ &\quad +2m(P_3^1;k-2)+2m(P_2;k-2)\\ &\geqslant 2m(P_4;k-1)+6m(P_4;k-2)+2m(P_2;k-2)\\ &= 2[m(P_3^1;k-1)+2m(P_4;k-2)]\\ &= 2[m(P_4^2;k-1)+m(P_4;k-2)]. \end{aligned}$$

Therefore, $b_{2k}(C_{2t}^t(1,\ 1,\ldots,1)^{o}S_1)\geqslant b_{2k}(C_8^4(1,\ 1,\ldots,1)^{o}S_{2t-7})$ for all $k\geqslant 0$. In particular, $b_6(C_{2t}^t(1,\ 1,\ldots,1)^{o}S_1)>b_6(C_8^4(1,\ 1,\ldots,1)^{o}S_{2t-7})$. This completes the proof. □

Theorem 9. For $l\geqslant 5$ and $n\geqslant 2l$, $E(C_{2l}^l(1,\ 1,\ldots,1)^{o}S_{n-2l+1})>E(C_8^4(1,\ 1,\ldots,1)^{o}S_{n-7})$.

Proof. By lemma 3, it suffices to demonstrate that $C_{2l}^l(1,\ 1,\ldots,1)^{o}S_{n-2l+1}\succ C_8^4(1,\ 1,\ldots,1)^{o}S_{n-7}$. If $n=2l$, the result follows readily by lemma 8. So we may assume that $n\geqslant 2l+1$ in what follows. Using lemma 4(a), we obtain

$$b_i(C_8^4(1,\ 1,\ldots,1)^{o}S_{n-7})=b_i(T^{(4)})+b_{i-2}(P_4\cup S_{n-7})-2b_{i-4}(S_{n-7}),\quad (16)$$

$$b_i(C_{2l}^l(1,\ 1,\ldots,1)^{o}S_{n-2l+1})=b_i(T^{(l)})+b_{i-2}(P_{l-2}^1\cup S_{n-2l+1})-2b_{i-l}(S_{n-2l+1})\quad (17)$$

for $l\equiv 0(mod\,4)$ and

$$b_i(C_{2l}^l(1, 1, \ldots, 1)^{\circ}S_{n-2l+1}) = b_i(T^{(l)}) + b_{i-2}(P_{l-2}^1 \cup S_{n-2l+1}) + 2b_{i-l}(S_{n-2l+1}) \tag{18}$$

for $l \not\equiv 0(mod\,4)$, where $T^{(l)}$ is the tree as indicated in figure 3(a) and $T^{(4)}$ is the tree by setting $l = 4$ in figure 3(a).

Note from Sachs theorem that $b_{2k+1}(C_8^4(1, 1, \ldots, 1)^{\circ}S_{n-7}) = 0$ for any integer $k \geqslant 0$.

If $l \equiv 0(mod\,4)$, then $b_{2k+1}(C_{2l}^l(1, 1, \ldots, 1)^{\circ}S_{n-2l+1}) = -2b_{(2k+1)-l}(S_{n-2l+1}) = 0$ for any integer $k \geqslant 0$, and if $l \not\equiv 0(mod\,4)$, then $b_{2k+1}(C_{2l}^l(1, 1, \ldots, 1)^{\circ}S_{n-2l+1}) = 2b_{(2k+1)-l}(S_{n-2l+1}) \geqslant 0$ for any integer $k \geqslant 0$.

Thus $b_{2k+1}(C_{2l}^l(1, 1, \ldots, 1)^{\circ}S_{n-2l+1}) \geqslant b_{2k+1}(C_8^4(1, 1, \ldots, 1)^{\circ}S_{n-7})$ for all integer $k \geqslant 0$.

Now, what remains is to verify that $b_{2k}(C_{2l}^l(1, 1, \ldots, 1)^{\circ}S_{n-2l+1}) \geqslant b_{2k}(C_8^4(1, 1, \ldots, 1)^{\circ}S_{n-7})$ for all integer $k \geqslant 0$.

It's evident that the above inequality is true for $k = 0, 1$. So we need only consider the case when $k \geqslant 2$.

It can be easily seen that

$$-2b_{2k-4}(S_{n-7}) = \begin{cases} -2, & k = 2; \\ -2(n-8), & k = 3; \\ 0, & k \geqslant 4; \end{cases} \tag{19}$$

Moreover, we have the following:

(1). If $l \equiv 1\, or\, 3(mod\,4)$, then $2b_{2k-l}(S_{n-2l+1}) = 0$ for all $k \geqslant 0$;

(2). If $l \equiv 2(mod\,4)$, then $2b_{2k-l}(S_{n-2l+1}) = \begin{cases} 2, & k = \frac{l}{2}; \\ 2(n-2l), & k = \frac{l}{2}+1; \\ 0, & 2 \leqslant k \leqslant \frac{l}{2}-1 \\ & or\ k \geqslant \frac{l}{2}+2. \end{cases}$

(3). If $l \equiv 0(mod\,4)$, then $-2b_{2k-l}(S_{n-2l+1}) = \begin{cases} -2, & k = \frac{l}{2}; \\ -2(n-2l), & k = \frac{l}{2}+1; \\ 0, & 2 \leqslant k \leqslant \frac{l}{2}-1 \\ & or\ k \geqslant \frac{l}{2}+2. \end{cases}$

Let $g(l) = b_{2k}(T^{(l)}) + b_{2k-2}(P_{l-2}^1 \cup S_{n-2l+1})$. Since $T^{(l)}$ and $P_{l-2}^1 \cup S_{n-2l+1}$ are all acyclic graphs, then $g(l) = m(T^{(l)}; k) + m(P_{l-2}^1 \cup S_{n-2l+1}; k-1)$ by Sachs theorem.

So, by lemma 7, we obtain

$$\begin{aligned}
g(l) - g(l-1) &= [m(T^{(l)}; k) + m(P^1_{l-2} \cup S_{n-2l+1}; k-1)] - [m(T^{(l-1)}; k) \\
&\quad + m(P^1_{l-3} \cup S_{n-2l+3}; k-1)] \\
&= [m(T_1 \cup P_2; k) + m(T_2; k-1) + m(P_2 \cup P^1_{l-3} \cup S_{n-2l+1}; k-1) \\
&\quad + m(P^1_{l-4} \cup S_{n-2l+1}; k-2)] - [m(T_3; k) + m(P^2_{l-1}; k-1) \\
&\quad + m(P^1_{l-3} \cup S_{n-2l+2}; k-1) + m(P^1_{l-3}; k-2)] \\
&= m(T_1; k) + m(T_1; k-1) + m(T_2; k-1) + m(P^1_{l-3} \cup S_{n-2l+1}; k-1) \\
&\quad + m(P^1_{l-3} \cup S_{n-2l+1}; k-2) + m(P^1_{l-4} \cup S_{n-2l+1}; k-2) - m(T_1; k) \\
&\quad - 2m(P^2_{l-1}; k-1) - m(P^1_{l-3} \cup S_{n-2l+1}; k-1) - 2m(P^1_{l-3}; k-2) \\
&= m(T_1; k-1) + m(T_2; k-1) + m(P^1_{l-3} \cup S_{n-2l+1}; k-2) \\
&\quad + m(P^1_{l-4} \cup S_{n-2l+1}; k-2) - 2m(P^2_{l-1}; k-1) - 2m(P^1_{l-3}; k-2),
\end{aligned} \tag{20}$$

where T_1, T_2 and T_3 are graphs as illustrated in figure 2(b),(c) and (d). Bearing in mind that

$$m(T_1; k-1) = m(P^2_{l-1} \cup S_{n-2l+1}; k-1) + m(P^1_{l-2}; k-2), \tag{21}$$

$$m(T_2; k-1) = m(P^2_{l-2} \cup S_{n-2l+1}; k-1) + m(P^1_{l-3}; k-2), \tag{22}$$

$$m(P^1_{l-3} \cup S_{n-2l+1}; k-2) > m(P^1_{l-3}; k-2), \tag{23}$$

$$m(P^2_{l-1} \cup S_{n-2l+1}; k-1) > m(P^2_{l-1}; k-1). \tag{24}$$

In view of equations. (21)–(24), equation. (20) is reduced to

$$\begin{aligned}
g(l) - g(l-1) > m(P^2_{l-2} \cup S_{n-2l+1}; k-1) + m(P^1_{l-2}; k-2) \\
+ m(P^1_{l-4} \cup S_{n-2l+1}; k-2) - m(P^2_{l-1}; k-1).
\end{aligned}$$

Since $n \geqslant 2l+1$, then

$$m(P^2_{l-2} \cup S_{n-2l+1}; k-1) \geqslant m(P^2_{l-2} \cup P_2; k-1) = m(P^2_{l-2}; k-1) + m(P^2_{l-2}; k-2). \tag{25}$$

Note that

$$m(P^2_{l-1}; k-1) = m(P^1_{l-2}; k-1) + m(P^1_{l-3}; k-2) = m(P^2_{l-2}; k-1) + 2m(P^1_{l-3}; k-2). \tag{26}$$

Consequently,

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

The above inequality holds due to the fact that both P_{l-2}^{1} and P_{l-2}^{2} contain P_{l-3}^{1} as proper subgraph.

So

$$
\begin{aligned}
g(l) &> g(l-1)+m(P_{l-4}^{1}\cup S_{n-2l+1}; k-2)\\
&> g(l-2)+m(P_{l-4}^{1}\cup S_{n-2l+1}; k-2)\\
&> \dots\\
&> g(4)+m(P_{l-4}^{1}\cup S_{n-2l+1}; k-2). \qquad (27)
\end{aligned}
$$

When $l \not\equiv 0(mod\ 4)$, by equations. (16), (18)–(19),(27) and (i)-(ii), we have $b_{2k}(C_{2l}^{l}(1,\ 1,\dots,1)^{o}S_{n-2l+1}) \geqslant b_{2k}(C_{8}^{4}(1,\ 1,\dots,1)^{o}S_{n-7})$ for all integer $k \geqslant 0$.

When $l \equiv 0(mod\ 4)$, we have

$$
m(P_{l-4}^{1}\cup S_{n-2l+1}; k-2)-2b_{2k-l}(S_{n-2l+1}) >
$$

$$
\begin{cases}
\binom{l-4}{\frac{l}{2}-3}(n-2l)-2>0, & k=\frac{l}{2};\\
\binom{l-4}{\frac{l}{2}-2}(n-2l)-2(n-2l)>0, & k=\frac{l}{2}+1;\\
0, & k\neq \frac{l}{2}, \frac{l}{2}+1;
\end{cases}
$$

Hence,

$$
\begin{aligned}
b_{2k}(C_{2l}^{l}(1,\ 1,\dots,1)^{o}S_{n-2l+1}) &= g(l)-2b_{2k-l}(S_{n-2l+1})\\
&> g(4)+m(P_{l-4}^{1}\cup S_{n-2l+1}; k-2)-2b_{2k-l}(S_{n-2l+1})\\
&> g(4)\\
&\geqslant g(4)-2b_{2k-4}(S_{n-7})\\
&= b_{2k}(C_{8}^{4}(1,\ 1,\dots,1)^{o}S_{n-7}).
\end{aligned}
$$

From the above discussion, we know that there must exist some k_0 such that $b_{2k_0}(C_{2l}^{l}(1,\ 1,\dots,1)^{o}S_{n-2l+1}) > b_{2k_0}(C_{8}^{4}(1,\ 1,\dots,1)^{o}S_{n-7})$. This completes the proof. □

Lemma 10. For $n \geqslant 8$, $E(C_8^4(1, 1, 1, 1)^{\circ} S_{n-7}) > E(C_6^3(1, 1, 1)^{\circ} S_{n-5})$.

Proof. One can easily get that

$$\phi(C_6^3(1, 1, 1)^{\circ} S_{n-5}) = x^{n-6}[x^6 - nx^4 - 2x^3 + (5n-24)x^2 + 2(n-6)x - (3n-17)], \quad (28)$$

$$\phi(C_8^4(1, 1, 1, 1)^{\circ} S_{n-7}) = x^{n-8}[x^8 - nx^6 + (7n-38)x^4 - (13n-96)x^2 + (3n-23)]. \quad (29)$$

Hence, by equations. (3), (28) and (29), we have $E(C_n^4(1, 1, 1, n-7)) - E(C_n^3(1, 1, n-5)) = \frac{1}{\pi}\int_0^{+\infty} \frac{1}{x^2} ln \frac{f_1(x)}{f_2(x)} dx$, where $f_1(x) = [1 + nx^2 + (7n-38)x^4 + (13n-96)x^6 + (3n-23)x^8]^2$ and $f_2(x) = [1 + nx^2 + (5n-24)x^4 + (3n-17)x^6]^2 + [(2x^3) + 2(n-5)x^5]^2$. The the result follows by a simple calculation. □

Summarizing theorems 6, 9 and lemma 10, we arrive at

Theorem 11. For $n \geqslant 6$, $C_6^3(1, 1, 1)^{\circ} S_{n-5}$ has the minimal energy among all graphs in $\mathscr{U}_n^3$, where $C_6^3(1, 1, 1)^{\circ} S_{n-5}$ is graph as shown in figure 2(b).

Remark. It seems that graph with minimal energy in $\mathscr{U}_n^r (r \geqslant 4)$ should have a similar structure as the one with minimal energy in $\mathscr{U}_n^3$. So the same reasoning should work well for discussing the minimal energy for graphs in $\mathscr{U}_n^r (r \geqslant 4)$.

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