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On unicyclic conjugated molecules with minimal energies

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The energy of a graph is defined as the sum of the absolute values of all the eigenvalues of the graph. Let $U(k)$ be the set of all unicyclic graphs with a perfect matching. Let $C_{g(G)}$ be the unique cycle of G with length $g(G)$, and $M(G)$ be a perfect matching of G. Let $U^0(k)$ be the subset of $U(k)$ such that $g(G) \equiv 0 \pmod 4$, there are just $g/2$ independence edges of $M(G)$ in $C_{g(G)}$ and there are some edges of $E(G)\backslash M(G)$ in $G \backslash C_{g(G)}$ for any $G \in U^0(k)$. In this paper, we discuss the graphs with minimal and second minimal energies in $U^*(k) = U(k)\backslash U^0(k)$, the graph with minimal energy in $U^0(k)$, and propose a conjecture on the graph with minimal energy in $U(k)$.

KEY WORDS: energy, unicyclic graph, characteristic polynomial, eigenvalue, perfect matching

AMS subject classification: 05C50, 05C35

1. Introduction

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

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

The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ 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 then defined as $E(G) = \sum_{i=0}^{n} |\lambda_i|$. It is known that [7] $E(G)$ can be expressed as the Coulson integral formula

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

Since the energy of a graph can be used to approximate the total π-electron energy of the molecule, it has been intensively studied (see [2, 5, 8, 9, 10, 13, 14]). For a survey of the mathematical properties and results on $E(G)$, see the recent review [6].

In [14], Zhang and Li studied the minimal energies of acyclic conjugated molecules. In this paper, we discuss the minimal energies about unicylic graphs with a perfect matching.

Let $U(k)$ be the set of all unicyclic graphs on $2k$ vertices with a perfect matching. Let $C_g(G)$ be the unique cycle of G with length $g(G)$, and $M(G)$ be a perfect matching of G. Let $U^0(k)$ be the subset of $U(k)$ such that $g(G) \equiv 0 \pmod 4$, there are just $g/2$ independence edges of $M(G)$ in $C_{g(G)}$ and there are some edges of $E(G) \backslash M(G)$ in $G \backslash C_{g(G)}$ for any $G \in U^0(k)$. Let $S_3^1(k)$ be the graph on $2k$ vertices obtained from C_3 by attaching one pendant edge and $k-2$ paths of length 2 together to one of the three vertices of C_3. Let $S_4^1(k)$ be the graph obtained from C_4 by attaching one path P of length 2 to one vertex of C_4 and then attaching $k-3$ paths of length 2 to the second vertex of the path P (figure 1).

Let $S_4^2(k)$ be the graph on $2k$ vertices obtained from C_4 by attaching $k-2$ paths of length 2 to one of the four vertices of C_4. Let $S_4^3(n,k)$ be the graph on $2k$ vertices obtained from C_4 by attaching one pendant edge and $k-3$ paths of

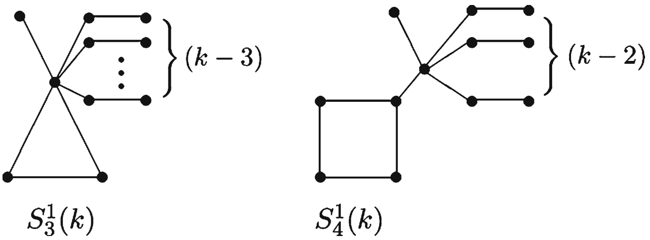

Figure 1. Graphs $S_3^1(k)$ and $S_4^1(k)$.

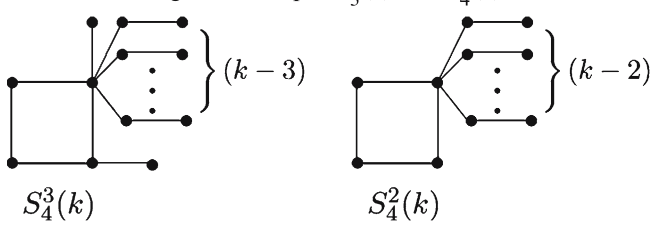

Figure 2. Graphs $S_4^3(k)$ and $S_4^2(k)$.

length 2 together to one of the four vertices of C_4, and one pendant edge to the adjacent vertex of C_4, respectively (see figure 2).

In this paper, we show that $S_3^1(k), S_4^3(k)\,(k \geqslant 43)$ are the graphs with minimal and second minimal energies in $U^*(k) = U(k)\backslash U^0(k)$, respectively, $S_4^1(k)$ be the graph with minimal energy in $U^0(k)$. Finally, we give a conjecture on the graph with minimal energy in $U(k)$.

2. Main results

Lemma 1 ([1, 4, 7]). Let G be a graph with characteristic polynomial $\phi(G, \lambda) = \sum_{i=0}^{n} a_i \lambda^{n-i}$. Then for $i \geqslant 1$

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

where L_i denotes the set of Sachs graphs of G with i vertices, that is, the graphs 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. In addition, $a_0 = 1$.

Let $b_{2i}(G) = (-1)^i a_{2i}$ for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$. Clearly, $b_0(G) = 1$ and $b_2(G)$ equals the number of edges of G.

Lemma 2 ([9]). Let $G \in U(k)$, then $b_{2i}(G) \geqslant 0$ for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$.

In view of lemma 2, a quasi-order relation is introduced (see [5]). Let $G, G_0 \in U(k)$ and G_0 be a bipartite graph. If $b_{2i}(G) \geqslant b_{2i}(G_0)$ holds for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$, we say that G is not less than G_0, written as $G \succeq G_0$. Furthermore, if these inequalities sometime are strict, that is, $b_{2i}(G) > b_{2i}(G_0)$ for some i, we say G is more than G_0, written as $G \succ G_0$. Obviously, from (1) and lemma 2 we have the following increasing property on E:

$$G \succ G_0 \Rightarrow E(G) > E(G_0). \tag{2}$$

We denote by $M(G)$ a perfect matching of G, and denote by $\hat{G} = G[E(G)\backslash M(G)]$, where $G[E]$ is the subgraph induced by E, $E(G)\backslash M(G)$ is a set of edges that are not in $M(G)$, but in $E(G)$. For example, $\hat{S}_4^2(k)$, $\hat{S}_4^3(k)$ (see figure 3).

Let $r_j^{(2i)}(G)$ be the number of ways to choose i independence edges in G such that just j edges are of $\hat{G}$. Obviously, $r_0^{(2i)}(G) = \binom{k}{i}$, $r_1^{(2i)}(G) = k\binom{k-2}{i-1}$.

Lemma 3. Let $G \in U^*(k)$, $g(G) \equiv 1 \pmod 2$, $g(G) \geqslant 5$. Then $E(G) > E(S_4^3(k))$.

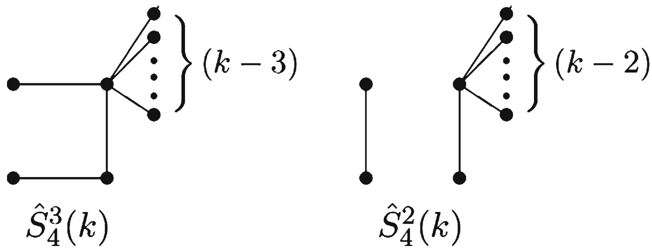

Figure 3. Graphs $\hat{S}_4^3(k)$ and $\hat{S}_4^2(k)$.

Proof. Combining lemmas 1, 2 and the case $g(G) \equiv 1 \pmod 2$, we can obtain

$$\begin{aligned} b_{2i}(S_4^3(k)) &= r_0^{(2i)}(S_4^3(k)) + r_1^{(2i)}(S_4^3(k)) + r_2^{(2i)}(S_4^3(k)) - 2r_0^{(2i-4)}(S_4^3(k)\backslash C_4) \\ &= r_0^{(2i)}(S_4^3(k)) + r_1^{(2i)}(S_4^3(k)) + \binom{k-3}{i-2} + (k-3)\binom{k-4}{i-2} - 2\binom{k-3}{i-2}, \\ b_{2i}(G) &= r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) + \cdots + r_{k-1}^{(2i)}(G). \end{aligned}$$

It suffices to prove that $r_2^{(2i)}(G) \geqslant (k-3)\binom{k-4}{i-2} - \binom{k-3}{i-2}$. Let v_i $(i = 1, 2, \ldots, g)$ be all the vertices of C_g, T_i $(i = 1, 2, \ldots, g)$ be a tree planting at v_i $(v_i \in V(T_i))$, n_i $(i = 1, 2, \ldots, g)$ be the number of edges of $\hat{G}$ in T_i. Obviously, $k - \frac{g+1}{2} \geqslant n_1 + n_2 + \cdots + n_g \geqslant k - g$. Let β_2 be the number of ways to choose two independence edges of $\hat{G}$.

If there exist at least two trees T_i, T_j such that $n_i, n_j > 0 (n_i \geqslant n_j)$. Then $k - \frac{g+1}{2} \geqslant 2n_j$.

$$\beta_2 - (k-3) \geqslant n_j(k - n_j - 2) - k + 3 = n_j k - n_j^2 - 2n_j - k + 3 \geqslant 0.$$

If there is just a tree T_i such that $n_i > 0$, then there exists an edge e of C_g such that e belongs to $E(\hat{G})$ and is not adjacent to v_i. Thus $\beta_2 \geqslant k-1-2$. Then

$$r_2^{(2i)}(G) \geqslant (k-3)\binom{k-4}{i-2}.$$

□

Lemma 4. Let $G \in U^*(k)$. If $g(G) = 3$, and $G \not\cong S_3^1(k)$, then $E(G) > E(S_4^3(k))$.

Proof. Similarly, it suffices to prove that $\beta_2 \geqslant k-3$, where v_i, n_i, β_2 are defined as the same as those in the proof of lemma 3.

Case 1. There is just one edge $e \in M(G)$ in C_3, without loss of generally, let $e = v_1v_2$. Then $n_1 + n_2 + n_3 = k - 2$.

Subcase 1.1: There are at least two trees T_i, T_j such that $n_i, n_j > 0$. Then, similar to the proof of lemma 3, we can obtain $\beta_2 \geqslant k - 3$.

Subcase 1.2: There is just a tree T_i such that $n_i > 0$. If $i = 1$ or 2, then $\beta_2 \geqslant k-3$. If $i = 3$, let $P = v_3u_1 \dots u_{t-2}u_{t-1}u_t$ be the longest path of T_3 from v_3. Then u_t is a pendant edge and $u_{t-2}u_{t-1} \in E(\hat{G})$. Since $G \not\cong S_3^1(k)$, we have $t \geqslant 3$ and so $t-2 \geqslant 1$. Let x be the number of edges of $E(\hat{G})$ that adjacent to u_{t-2}. Then $\beta_2 \geqslant k-2$ when $x = 1$, and $\beta_2 \geqslant (x-1)(k-x) \geqslant k-3$ when $x \geqslant 2$, since $k \geqslant x+2$.

Case 2. There is no edge of $M(G)$ in C_3. Then $\beta_2 \geqslant n_1+n_2+n_3 = k-3$. □

Lemma 5. Let $G \in U^*(k)$. If $g(G) \equiv 2 \pmod 4$, then $E(G) > E(S_4^3(k))$.

Proof. By lemmas 1 and 2, we have

$$b_{2i}(G) = r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) + \cdots + r_k^{(2i)}(G)$$
$$+2[r_0^{(2i-g)}(G\backslash C_g) + r_1^{(2i-g)}(G\backslash C_g) + \cdots + r_{k-g}^{(2i-g)}(G\backslash C_g)].$$

It suffices to prove that $r_2^{(2i)}(G) \geqslant r_2^{(2i)}(S_4^3(k))$. Similar to the proof of lemma 3, we can obtain the inequality. □

Lemma 6. Let $G \in U^*(k)$, $g(G) \equiv 0 \pmod 4$, and $g(G) \geqslant 8$.

(i) If there are less than $\frac{g}{2}-1$ edges of $M(G)$ in $C_g(G)$, then $E(G) > E(S_4^3(k))$.

(ii) If there are just $\frac{g}{2}$ edges of $M(G)$ in $C_g(G)$, then $E(G) > E(S_4^2(k))$.

Proof. (i) By lemmas 1 and 2, we can obtain

$$b_{2i}(G) = r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) + \cdots + r_k^{(2i)}(G)$$
$$-2[r_0^{(2i-g)}(G\backslash C_g) + r_1^{(2i-g)}(G\backslash C_g) + \cdots + r_{k-g}^{(2i-g)}(G\backslash C_g)].$$

Case 1: There are just $\frac{g}{2}-1$ edges of $M(G)$ in $C_g(G)$. Then there are $\frac{g}{2}+1$ edges of $E(\hat{G})$ in $C_g(G)$. Let M_1, M_2 be two matchings in $C_g(G)$ with cardinality $\frac{g}{2}$.

Subcase 1.1: If $M_1 \not\subset E(\hat{G})$ and $M_2 \not\subset E(\hat{G})$, then M_1, M_2 contain at least two edges of $E(\hat{G})$, and one of those contains at least three edges of $E(\hat{G})$. Let M_0 be a matching in $G\backslash C_g(G)$ with cardinality $i-\frac{g}{2}$ such that it contains at least one edge of $E(\hat{G})$, then there are two matchings $M_1 \cup M_0, M_2 \cup M_0$ with cardinality i corresponding to M_0. Thus

$$b_{2i}(G) \geqslant r_0^{(2i)}(G) + r_1^{(2i)}(G) + \beta_2^0 \begin{pmatrix} k-4 \\ i-2 \end{pmatrix} - \begin{pmatrix} k-\frac{g}{2} \\ i-\frac{g}{2} \end{pmatrix},$$

where β_2^0 be the number of ways to choose two independence edges of $E(\hat{G})$ such that at least one edge in $C_g(G)$. Let $n_1, n_2, \dots, n_g$ be defined as the same as those in the proof of lemma 3.

$$\begin{aligned}\beta_2^0 &\geqslant \left(\tfrac{g}{2}+1-2\right)\left(n_1+n_2+\cdots+n_g\right)+\binom{\frac{g}{2}-1}{2}\\ &=\left(\tfrac{g}{2}-1\right)\left(k-\tfrac{g}{2}-1\right)+\binom{\frac{g}{2}-1}{2}\\ &=k\left(\tfrac{g}{2}-1\right)-\binom{\frac{g}{2}-1}{2}\\ &\geqslant k-3.\end{aligned}$$

Subcase 1.2: Without loss of generally, let $M_1 \subset E(\hat{G})$, then M_2 contains just one edge of $E(\hat{G})$. Similarly, we have

$$b_{2i}(G) \geqslant r_0^{(2i)}(G)+r_1^{(2i)}(G)+\beta_2^*\binom{k-4}{i-2}-\binom{k-\frac{g}{2}}{i-\frac{g}{2}},$$

where β_2^* be the number of ways to choose two independence edges of $E(\hat{G})$ such that at least one edge in M_1 and no edge in M_2. Then

$$\begin{aligned}\beta_2^* &\geqslant \left(\tfrac{g}{2}-1\right)\left(n_1+n_2+\cdots+n_g\right)+\binom{\frac{g}{2}}{2}\\ &=\left(\tfrac{g}{2}-1\right)\left(k-\tfrac{g}{2}-1\right)+\binom{\frac{g}{2}}{2}\\ &\geqslant k-3.\end{aligned}$$

Since $\binom{k-3}{i-2} \geqslant \binom{k-\frac{g}{2}-1}{i-\frac{g}{2}}$, we can obtain $b_{2i}(G) \geqslant b_{2i}(S_4^3(k))$ for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$, and these equalities do not always hold.

Case 2: There are at most $\frac{g}{2}-2$ edges of $M(G)$ in $C_g(G)$. Then M_1, M_2 contain at least two edges of $E(\hat{G})$. Similar to case 1, we can have $b_{2i}(G) \geqslant b_{2i}(S_4^3(k))$ for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$, and these equalities do not always hold. Thus $G \succ S_4^2(k)$, $E(G) > E(S_4^2(k))$.

(ii) There are just $\frac{g}{2}$ edges of $M(G)$ in $C_g(G)$. By lemmas 1 and 2 and $G \in U^*(k)$, we have

$$
\begin{aligned}
b_{2i}(S_4^2(k)) &= r_0^{(2i)}(S_4^3(k)) + r_1^{(2i)}(S_4^3(k)) + r_2^{(2i)}(S_4^3(k)) - 2r_0^{(2i-4)}(S_4^3(k)\backslash C_4)\\
&= r_0^{(2i)}(S_4^3(k)) + r_1^{(2i)}(S_4^3(k)) + \tbinom{k-2}{i-2} + (k-2)\tbinom{k-3}{i-2} - 2\tbinom{k-2}{i-2},\\
b_{2i}(G) &= r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) + \cdots + r_k^{(2i)}(G) - 2r_0^{(2i-g)}(G\backslash C_g)\\
&\geqslant r_0^{(2i)}(G) + r_1^{(2i)}(G) + \beta_2'\tbinom{k-3}{i-2} - \binom{k-\frac{g}{2}}{i-\frac{g}{2}},
\end{aligned}
$$

where β_2' is the number of ways to choose two independence edges of $E(\hat{G})$ such that both are adjacent to one edge of $M(G)$. Without loss of generality, let $v_1v_2, v_3v_4, \ldots, v_{g-1}v_g \in E(\hat{G})$. Then

$$
\begin{aligned}
\beta_2' &\geqslant n_3 + n_g + n_2 + n_4 + \cdots + n_{g-2} + n_1 + g\\
&= k - \tfrac{g}{2} + \tfrac{g}{2} > k-2.
\end{aligned}
$$

Combining $\binom{k-2}{i-2} \geqslant \binom{k-\frac{g}{2}}{i-\frac{g}{2}}$, we can obtain $G \succ S_4^2(k)$, $E(G) > E(S_4^2(k))$. □

Similarly, we have

Lemma 7. Let $G \in U^*(k)$, $g(G) = 4$. (i) If there is just one edge of $M(G)$ in C_4, then $E(G) > E(S_4^3(k))$. (ii) If there are just two edges of $M(G)$ in C_4, then $E(G) > E(S_4^2(k))$.

Lemma 8 [4]. Let uv be an edge of G, then

$$\phi(G,\lambda) = \phi(G-uv,\lambda) - \phi(G-u-v,\lambda) - 2\sum_{C\in\mathcal{C}(uv)}\phi(G-C,\lambda),$$

where $\mathcal{C}(uv)$ is the set of cycles containing uv; In particular, if uv is a pendant edge with pendant vertex v, then

$$\phi(G,\lambda) = \lambda\phi(G-v,\lambda) - \phi(G-u-v,\lambda).$$

Lemma 9 [12]. $\phi(S_4^3(k),\lambda) < \phi(S_4^2(k),\lambda)$ *for all* $\lambda \geqslant \lambda(S_4^1(k))$. In particular, $\lambda_1(S_4^3(k)) > \lambda_1(S_4^2(k))$.

Lemma 10 [3]. $S_3^1(k)$ is the graph with maximal spectral radius in $U(k)$.

From [9,11,12] and lemma 8, we can get

Lemma 11. Let G be a graph with characteristic polynomial $\phi(G,\lambda)$. Then

$$\phi(S_4^3(k),\lambda) = (\lambda^2-1)^{k-4}(\lambda^8-(k+4)\lambda^6+(3k+2)\lambda^4-(k+3)\lambda^2+1),$$
$$\phi(S_4^2(k),\lambda) = \lambda^2(\lambda^2-1)^{k-3}(\lambda^4-(k+3)\lambda^2+2k),$$
$$\phi(S_3^1(k),\lambda) = (\lambda^2-1)^{k-2}(\lambda^4-(k+4)\lambda^2-2\lambda+1),$$
$$\phi(S_4^1(k),\lambda) = \lambda^2(\lambda^2-1)^{k-4}(\lambda^6-(k+4)\lambda^4+4k\lambda^2-6).$$

Lemma 12. $E(S_4^2(k)) > E(S_4^3(k))$ for $k \geqslant 29$.

Proof. Let x_1, x_2, x_3, x_4 $(x_1 > x_2 \geqslant x_3 \geqslant x_4)$ be the positive roots of $f(x) = x^8 - (k+4)x^6 + (3k+2)x^4 - (k+3)x^2 + 1 = 0$. Let y_1, y_2 $(y_1 > y_2)$ be the two positive roots of $g(y) = y^4 - (k+3)y^2 + 2k = 0$. For convenience, we give the Appendix table. It suffices to prove that $x_1 + x_2 + x_3 + x_4 < y_1 + y_2 + 1$ for $k \geqslant 50$.

When $k \geqslant 50$, $f(0) > 0$, $f(0.145) < 0$, $f(0.62)$, $f(\frac{\sqrt{5}+1}{2}) < 0$, $f(\sqrt{k+\frac{6}{5}}) > 0$; $g(1.4) < 0$, $g(\sqrt{k+1}) > 0$, $g(\sqrt{k+2}) < 0$. Then we can obtain that $x_4 < 0.145$, $x_3 < 0.62$, $x_2 < 1.618$, $x_1 < \sqrt{k+\frac{6}{5}}$, $y_2 > 1.4$, $y_1 > \sqrt{k+1}$. Furthermore, by lemma 9 we have $\sqrt{k+\frac{6}{5}} > x_1 > y_1 > \sqrt{k+1}$, $y_1 > x_1 - (\sqrt{k+\frac{6}{5}} - \sqrt{k+1}) > x_1 - 0.0143$. Thus, we have

$$\begin{aligned} x_1 + x_2 + x_3 + x_4 &< 0.145 + 0.62 + 1.618 + x_1 \\ &= 2.383 + x_1 \\ &< 1 + 1.4 + x_1 - 0.0143 < 1 + y_1 + y_2. \end{aligned}$$

□

Lemma 13. $E(S_4^3(k)) > E(S_3^1(k))$ for $k \geqslant 43$.

Proof. Let t_1, t_2 $(t_1 > t_2)$ be the two positive roots of $h(t) = t^4 - (k+3)t^2 - 2t + 1 = 0$. By lemma 11, we have

$$E(S_4^3(k)) = 2k - 8 + 2(x_1 + x_2 + x_3 + x_4),$$
$$E(S_3^1(k)) = 2k - 4 + 2(t_1 + t_2).$$

It suffices to prove $x_1 + x_2 + x_3 + x_4 > t_1 + t_2 + 2$ for $k \geqslant 51$. When $k \geqslant 51$, $f(0) > 0$, $f(\frac{\sqrt{5}-1}{2}) < 0$, $f(1.597) > 0$, $f(\frac{\sqrt{5}+1}{2}) < 0$ and $h(0) > 0, h(0.12) < 0$. Then $x_2 + x_3 + x_4 - y_2 - 2 \geqslant 0.618 + 1.597 - 0.12 - 2 = 0.095 = \varepsilon$. Thus $x_2 + x_3 + x_4 > 2 + t_2 + \varepsilon$.

We will prove $t_1 < x_1 + \varepsilon$. It suffices to prove $h(x_1 + \varepsilon) > 0$. When $k \geqslant 51$, $x_1 > \sqrt{k+1} > 7.1$. Then

$$\begin{aligned}
\frac{h(t)}{t^2} &= t^2-(k+2)-\tfrac{2}{t}+\tfrac{1}{t^2}\\
&= t^2-(k+2)+(\tfrac{1}{t}-1)^2-1,\\
\frac{h(x_1+\varepsilon)}{(x_1+\varepsilon)^2} &\geqslant (x_1+\varepsilon)^2-(k+2)+0.7381-1\\
&= x_1^2-(k+1)+2\varepsilon x_1+\varepsilon^2-1.2619\\
&\geqslant 2\varepsilon x_1-1.2619>0.
\end{aligned}$$

We have $h(x_1+\varepsilon)>0$, and $x_1+x_2+x_3+x_4>t_1+t_2+2$. □

Combining the Appendix table and lemmas 3–8, 12 and 13, we can obtain

Theorem 1. (i) When $5 \leqslant k \leqslant 28$, $S_4^2(k)$ is the graph with minimal energy in $U^*(k)$. (ii) When $29 \leqslant k \leqslant 42$, $S_4^3(k)$ is the graph with minimal energy in $U^*(k)$. (iii) When $k \geqslant 43$, $S_3^1(k)$, $S_4^3(k)$ are the graphs with minimal and second minimal energies in $U^*(k)$, respectively,

Lemma 14. Let $G \in U^0(k)$, $g(G)=4$, $G \ncong S_4^1(k)$. Then $E(G)>E(S_4^1(k))$.

Proof. Let x be the number of edges in $E(\hat{G})$ that are adjacent to vertices of C_4 except for two edges in C_4. Since there are just two edges of $M(G)$, $G\backslash C_4$ contains some edges of $E(\hat{G})$. Then $1 \leqslant x \leqslant k-3$. By lemmas 1 and 2, we can obtain

$$\begin{aligned}
b_{2i}(G) &= r_0^{(2i)}(G)+r_1^{(2i)}(G)+r_2^{(2i)}(G)+\cdots+r_k^{(2i)}(G)\\
&\quad -2\left[r_0^{(2i-4)}(G\backslash C_4)+r_1^{(2i-4)}(G\backslash C_4)+\cdots+r_{k-4}^{(2i-4)}(G\backslash C_4)\right]\\
&\geqslant r_0^{(2i)}(G)+r_1^{(2i)}(G)+x\tbinom{k-3}{i-2}+2(k-2-x)\tbinom{k-4}{i-2}\\
&\quad +(x-1)\tbinom{k-4}{i-2}-\tbinom{k-2}{i-2}-(k-2-x)\tbinom{k-4}{i-3}\\
&= r_0^{(2i)}(G)+r_1^{(2i)}(G)+x\left[\tbinom{k-3}{i-2}-\tbinom{k-4}{i-2}+\tbinom{k-4}{i-3}\right]\\
&\quad +2(k-2)\tbinom{k-4}{i-2}-\tbinom{k-4}{i-2}-(k-2)\tbinom{k-4}{i-3}\\
&\geqslant r_0^{(2i)}(G)+r_1^{(2i)}(G)+1\cdot\left[\tbinom{k-3}{i-2}-\tbinom{k-4}{i-2}+\tbinom{k-4}{i-3}\right]\\
&\quad +2(k-2)\tbinom{k-4}{i-2}-\tbinom{k-4}{i-2}-(k-2)\tbinom{k-4}{i-3}\\
&= b_{2i}(S_4^1(k)),
\end{aligned}$$

where the equality holds if and only if $G \cong S_4^1(k)$. So, we have $G \succ S_4^1(k)$, $E(G)>E(S_4^1(k)$. □

Lemma 15. Let $G \in U^0(k)$, $g(G) \geqslant 8$. Then $E(G)>E(S_4^1(k))$.

Proof. By lemmas 1 and 2, we can obtain

$$
\begin{aligned}
b_{2i}(S_4^1(k)) &= r_0^{(2i)}(S_4^1(k)) + r_1^{(2i)}(S_4^1(k)) + r_2^{(2i)}(S_4^1(k)) r_3^{(2i)}(S_4^1(k)) \\
&\quad -2[r_0^{(2i-4)}(S_4^1(k)\backslash C_4) + r_1^{(2i-4)}(S_4^1(k)\backslash C_4)] \\
&= r_0^{(2i)}(S_4^1(k)) + r_1^{(2i)}(S_4^1(k)) + \binom{k-3}{i-2} + 2(k-3)\binom{k-4}{i-2} \\
&\quad -\binom{k-2}{i-2} - (k-3)\binom{k-4}{i-3}
\end{aligned}
$$

$$
\begin{aligned}
b_{2i}(G) &= r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) + \cdots + r_k^{(2i)}(G) \\
&\quad -2[r_0^{(2i-g)}(G\backslash C_g) + r_1^{(2i-g)}(G\backslash C_g) + \cdots + r_{k-g}^{(2i-g)}(G\backslash C_g)] \\
&\geqslant r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) - r_0^{(2i-g)}(G\backslash C_g) - r_1^{(2i-g)}(G\backslash C_g) \\
&\geqslant r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) - \begin{pmatrix} k-\frac{g}{2} \\ i-\frac{g}{2} \end{pmatrix} - (k-\tfrac{g}{2}-1)\begin{pmatrix} k-\frac{g}{2}-2 \\ i-\frac{g}{2}-1 \end{pmatrix}.
\end{aligned}
$$

Let v_i $(i = 1, 2, \ldots, g)$ be all the vertices of C_g, T_i $(i = 1, 2, \ldots, g)$ be a tree planting at v_i $(v_i \in V(T_i))$, v_i $(i = 1, 2, \ldots, g)$ be the number of edges in $\hat{G}$. Obviously, $n_1 + n_2 + \cdots + n_g = k - \frac{g}{2}$. Let β_2 be the number of ways to choose two independence edges of $\hat{G}$ such that at least one edge in $C_{g(G)}$. Then

$$
\begin{aligned}
\beta_2 &\geqslant (\tfrac{g}{2}-1)(n_1 + n_2 + \cdots + n_g) + \binom{\frac{g}{2}}{2} \\
&= (\tfrac{g}{2}-1)(k - \tfrac{g}{2}) + \binom{\frac{g}{2}}{2} \\
&\geqslant 2k + 5.
\end{aligned}
$$

We have $r_2^{(2i)}(G) > \binom{k-3}{i-2} + 2(k-3)\binom{k-4}{i-2}$. Since $\binom{k-2}{i-2} > \binom{k-\frac{g}{2}}{i-\frac{g}{2}}$, $(k-3)\binom{k-4}{i-3} > (k-\frac{g}{2}-1)\begin{pmatrix} k-\frac{g}{2}-2 \\ i-\frac{g}{2}-1 \end{pmatrix}$. We have $G \succ S_4^1(k)$, $E(G) \geqslant E(S_4^1(k))$. □

Using lemmas 14 and 15, it is not difficult to obtain the following theorem.

Theorem 2. $S_4^1(k)$ is the graph with minimal energy in $U^0(k)$.

By theorems 1 and 2, lemmas 14 and 15, and the Appendix table, we can obtain

Theorem 3. Either $S_3^1(k)$ or $S_4^1(k)$ is the graph with minimal energies in $U(k)$.

Remark. We can obtain the energies of $S_3^1(k)$ or $S_4^1(k)$ by computation for some positive integer k. When $k = 100, 1000, 10000$, the result of the computation is $E(S_3^1(k)) > E(S_4^1(k))$. But we have not found a proper way to prove it. So, we propose

Conjecture 1. $S_4^1(k)$ is the graph with minimal energies in $U(k)$.

Table 1
Appendix table.

$n = 2k$	$E(S_4^1(k))$	$E(S_3^1(k))$	$E(S_4^2(k))$	$E(S_4^3(k))$
$k = 5$	12.6598	11.4066	11.5696	11.9997
$k = 6$	14.9516	13.7663	13.9820	14.3547
$k = 7$	17.2319	16.1047	16.3626	16.6890
$k = 8$	19.5020	18.4251	18.7178	19.0058
$k = 9$	21.7628	20.7601	21.0521	21.3076
$k = 10$	24.0153	23.0219	23.3689	23.5965
$k = 11$	26.2602	25.3019	25.6707	25.8739
$k = 12$	28.4982	27.5715	27.9595	28.1411
$k = 13$	30.7297	29.8318	30.2368	30.3992
$k = 14$	32.9553	32.0870	32.5039	32.6839
$k = 15$	35.1754	34.0064	34.7619	34.8913
$k = 16$	37.3904	36.5652	37.0116	37.1268
$k = 17$	39.6006	38.7960	39.2538	39.3559
$k = 18$	41.8064	41.0209	41.4991	41.5793
$k = 19$	44.0079	43.2403	43.7182	43.7972
$k = 20$	46.2055	45.4545	45.9414	46.0101
$k = 21$	48.3994	47.6641	48.1592	48.2183
$k = 22$	50.5897	49.8691	50.3720	50.4221
$k = 23$	52.7767	52.0700	52.5801	52.6218
$k = 24$	54.9605	54.2669	54.7838	54.8176
$k = 25$	57.1413	56.4602	56.9834	57.0098
$k = 26$	56.4602	58.6499	59.1791	59.1985
$k = 27$	61.4944	60.8362	61.3712	61.3839
$k = 28$	63.6669	63.0194	63.5597	63.5661
$k = 29$	65.8370	65.1996	65.7450	65.7454
$k = 30$	68.0046	67.3770	67.9272	67.3922
$k = 31$	70.1699	69.5516	70.1065	70.0957
$k = 32$	72.3331	71.7236	72.2829	72.2669
$k = 33$	74.4941	73.8931	74.4566	74.4357
$k = 34$	76.6530	76.0623	76.6277	76.6020
$k = 35$	78.8100	78.2251	78.7964	78.7662
$k = 36$	80.9651	80.3878	80.9627	80.9281
$k = 37$	83.1184	82.5483	83.1268	83.0880
$k = 38$	85.2669	84.7068	85.2886	85.2458
$k = 39$	87.4197	86.8634	87.4484	87.4017
$k = 40$	89.5678	89.0180	89.6062	89.5558
$k = 41$	91.7144	91.1709	91.7621	91.7080
$k = 42$	93.8594	93.3219	93.9161	93.8585
$k = 43$	96.0029	95.4713	96.0683	96.0074
$k = 44$	98.1449	97.6090	98.2187	98.1546
$k = 45$	100.2856	99.7652	100.3675	100.3002
$k = 46$	102.4249	101.9099	102.5146	102.4443
$k = 47$	104.5628	104.0530	104.6602	104.5869
$k = 48$	106.6994	106.1947	106.8043	106.7281
$k = 49$	108.3350	108.8348	108.9469	108.8679
$k = 50$	110.4739	110.9690	111.0880	111.0064

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