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ORIGINAL PAPER

Some results on energy of unicyclic graphs with *n* vertices

Ying Liu

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Abstract A unicyclic graph is a connected graph whose number of edges is equal to the number of vertices. Hou (J Math Chem 29:163–168, 2001) first considered the minimal energy for general unicyclic graphs. In this paper, we determine the unicyclic graphs with the minimal energy in $\mathcal{U}_n^l$ and the unicyclic graphs with the first forth smallest energy in $\mathcal{U}_n$ $(n \geq 13)$ vertices.

Keywords Unicyclic graphs · Energy · Characteristic polynomial

1 Introduction

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

$$\phi(G; x) = |xE - A(G)| = \sum_{i=0}^{n} a_i x^{n-i} \tag{1}$$

where E is the unit matrix of order n.

The eigenvalues $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ of $\phi(G; x) = 0$ are called the eigenvalues of G. Since $A(G)$ is symmetric, all eigenvalues of G are real. The energy of a graph G is defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i(G)|.$$

Y. Liu (✉)
College of Mathematics and Information, Shanghai Lixin University of Commerce,
Shanghai 201620, China
e-mail: lymaths@126.com

This concept was introduced by [5] and is intensively studied in Chemistry, since it is closely related to the total π-electron energy of the molecular in conjugated hydrocarbons. For more details on the chemical aspects and mathematical properties of $E(G)$ see [3,4].

The energy problems of some special graphs have been extensively investigated see [10,11], etc. Minimal energy of unicyclic graphs are usually harder than those of acyclic graphs. Hou [6] first considered it for general unicyclic graphs. Recently, the minimal energy of unicyclic graphs with perfect matching has been presented in [8,9].

Let G be a graph with n vertices and the characteristic polynomial of G be (1). Set $b_i(G) = |a_i(G)|$ $(0 \leq i \leq n)$. Notice that $b_0(G) = 1$ and $b_2(G)$ is the number of edges of G. Let $m(G, k)$ $(k \geq 1)$ be the number of k-matchings of G and define $m(G, 0) = 1, m(G, k) = 0$ $(k < 0)$. $E(G)$ can be expressed as the Coulson integral formula in (1)

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

From Eq. 2, we have

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

and it follows that $E(G)$ is a monotonically increasing function of $b_i(G)$ $(0 \leq i \leq n)$, that is, if G_1, G_2 are unicyclic graphs, and

$$b_i(G_1) \geq b_i(G_2) \tag{4}$$

for all $i \geq 0$, then

$$E(G_1) \geq E(G_2) \tag{5}$$

and equality holds if and only if $b_i(G_1) \geq b_i(G_2)$ for all i. If (4) holds for all i, then we write $G_1 \succeq G_2$, and we write $G_1 \succ G_2$ if $E(G_1) > E(G_2)$.

A unicyclic graph is a connected graph whose number of edges is equal to the number of vertices. Let $\mathcal{U}_n$ and $\mathcal{U}_n^l$ denote the set unicyclic graphs with n vertices, the set unicyclic graphs with n vertices and the cycle C_l, respectively. In this paper, we determine the unicyclic graph with the minimal energy in $\mathcal{U}_n^l$ and the unicyclic graphs with the first forth smallest energy in $\mathcal{U}_n$ $(n \geq 13)$ vertices.

2 The minimal energy in $\mathcal{U}_n^l$

The following lemmas are necessary for our main results.

Lemma 1 ([2]) *Let G be a graph and uv be an edge of G. Then*

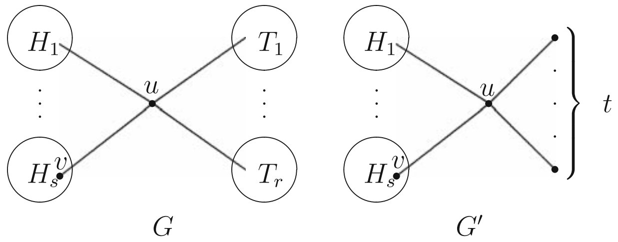


Fig. 1 The graphs of order n

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

Lemma 2 ([2]) *Let T be a tree with n vertices and $T \notin \{K_{1,n-1}, T(1,n-3)\}$. Then*

$$T \succ T(1,n-3) \succ K_{1,n-1},$$

where $T(1,n-3)$ is obtained from P_2 by attaching one pendent vertex and $n-3$ pendent vertices at P_2, respectively.

Let G be a graph and $G - u = T_1 \cup \cdots \cup T_r \cup H_1 \cup \cdots \cup H_s$ where u is a cut vertex and T_i $(1 \le i \le r)$ are trees with $\sum_{i=1}^{r} |V(T_i)| = t$. If G' is obtained from G by replacing $T_1 \cup \cdots \cup T_r$ by t pendent vertices, we say that G' is obtained from G by *Grafting I* (see Fig. 1).

Lemma 3 *If G' is obtained from G $(G \ne G')$ by Grafting I (see Fig. 1), then*

$$E(G) > E(G').$$

Proof We prove the result by induction on s, and denote v is adjacent to u in H_s.

If $s = 0$, then $G' = K_{1,t} \ne G'$, then by Lemma 2, we get $G \succ G'$. Suppose that the result holds for $s = p - 1$ $(p \ge 1)$, then we prove the result holds if $s = p$. Since

$$\begin{aligned} G - u - v = \; & (T_1 \cup \cdots \cup T_r) \cup (H_1 \cup \cdots \cup H_{s-1}) \cup (H_s - v) \\ & \succ tP_1 \cup (H_1 \cup \cdots \cup H_{s-1}) \cup (H_s - v) = G' - u - v, \end{aligned}$$

and by induction we have

$$G - uv = (G - H_s) \cup H_s \succ (G' - H_s) \cup H_s = G' - uv.$$

From Lemma 1, the proof is completed. □

Let $G \in \mathcal{U}_n^l$ with v_1 attaching a rooted tree $K_{1,s}$ $(s \ge 1)$ and $i = \min\{j | v_j \in V(C_l), d(v_j) \ge 3 \text{ and } 2 \le j \le l\}$. Suppose that v_i attaching a rooted tree $K_{1,t}$ $(t \ge 1)$, if G'' is obtained from deleting a pendent vertex at v_i and adding a pendent edge at v_1, we say that G'' is obtained from G by *Grafting II*. Obviously, $G'' \in \mathcal{U}_n^l$.

Lemma 4 *If G'' is obtained from G ($G \neq G''$) by Grafting II, then*

$$E(G) > E(G'').$$

Proof Suppose that $s + t = q$. Let u be a pendent vertex at v_1 and v be a pendent vertex at v_i. We prove the results by induction on q.

If $q = 2$, then $s = t = 1$. By Lemma 2.4 in [7], we have

$$G - v_1 v_l \succ G'' - v_1 v_l,$$

and

$$G - v_1 - v_l \supset G'' - v_1 - v_l,$$

so by Lemma 1, we have $G \succ G''$.

If $s + t = q - 1$ ($q \geq 3$), then the result holds. Let u be a pendent vertex at v_1. Now we approve $s + t = q$. By induction, we have

$$G - v_1 u \succ G'' - v_1 u,$$

and

$$G - v_1 - u \supset G'' - v_1 - u,$$

so by Lemma 1, we have $G \succ G''$. So the result is followed. □

Combining Lemma 3 with Lemma 4, we can determine the first minimal energy in $\mathcal{U}_n^l$.

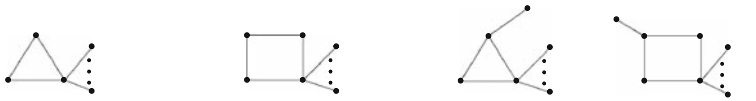
Theorem 5 *If $G \in \mathcal{U}_n^l - S_n^l$, then*

$$E(G) > E(S_n^l),$$

where S_n^l is obtained from C_l by attaching $n - l$ pendent vertices at a vertex v of C_l.

3 The minimal energy in $\mathcal{U}_n$

A unicyclic graph is a connected graph whose number of edges is equal to the number of vertices. It is easy to see that each unicyclic graph can be obtained by attaching rooted trees to the vertices of a cycle C_l of length l. Thus if $R_1, \ldots, R_l$ are l rooted trees (of orders $n_1, \ldots, n_l$, say), then we adopt the notation $U_l(R_1, \ldots, R_l)$ (or simply $U(R_1, \ldots, R_l)$ sometime for convenience) to denote the unicyclic graph G (of order $n = n_1 + \cdots + n_l$) obtained by attaching the rooted tree R_i to the vertex v_i of a cycle $C_l = v_1 v_2 \ldots v_l v_1$ (i.e., by identifying the root of R_i with the vertex v_i) for $i = 1, \ldots, l$.



$S_n^3 = U(n-3,0,0)$ $S_n^4 = U(n-4,0,0,0)$ $U(n-4,1,0)$ $U(n-5,0,1,0)$

Fig. 2 The unicyclic graphs of order n

In the special case when R_i is a rooted star K_{1,a_i} with the center of the star as its root, we will simplify the notation by replacing R_i by the number a_i.

Let $S(a,b)$ be the tree of order $a+b+2$ obtained from $K_{1,a}$ and $K_{1,b}$ by adding a edge $e = uv$, where u, v are the star centers of $K_{1,a}$ and $K_{1,b}$, respectively.

Let $R(a,b)$ be the rooted tree with $S(a,b)$ as its underlying tree and with the vertex of degree $a+1$ as its root.

Using the above defined notations, we can write the graphs as in Fig. 2.

The following lemmas are needed for the proofs our main results in this section.

Lemma 6 ([6,9]) *Let* $G \in \mathcal{U}_n^l$, *then*

(1) *if* $l = 2r$, *then*

$$b_{2k}(G) = m(G,k) + 2(-1)^{r+1} m(G - C_l, k-r)$$

and $b_{2k+1}(G) = 0$;

(2) *if* $l = 2r+1$, *then* $b_{2k}(G) = m(G,k)$ *and*

$$b_{2k+1}(G) = \begin{cases} 2m(G - C_l, k-r), & 2k+1 \geq l \\ 0, & 2k+1 < l \end{cases}.$$

Lemma 7 ([1]) *Let* G *be a graph and* uv *be an edge of* G, *then*

$$\phi(G;x) = \phi(G - uv; x) - \phi(G - u - v; x) - 2\sum_Z \phi(G - V(Z); x)$$

where Z *is a cycle containing* uv.

Lemma 8 ([6]) *Let* $G \in \mathcal{U}_n^l$ *an* uv *be a pendent edge of* G *with pendent vertex* v, *then*

$$b_i(G) = b_i(G - v) + b_{i-2}(G - v - u).$$

Lemma 9 *Let* S_n^l, $U(n-5,0,1,0) \in \mathcal{U}_n$ $(n \geq 7, l \geq 5)$, *then*

$$S_n^l \succ U(n-5,0,1,0).$$

Proof By Lemma 7, it is not difficult to calculate

$$\phi(U(n-5,0,1,0);x) = x^{n-4}[x^4 - nx^2 + (3n-13)], \tag{6}$$

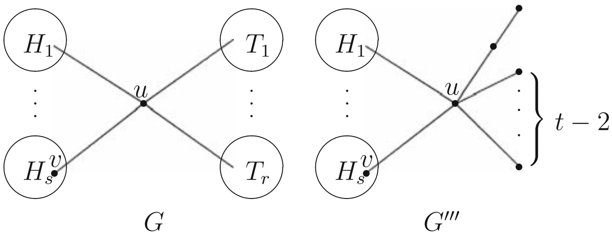


Fig. 3 The graphs of order n

where $b_0(U(n-5, 0, 1, 0)) = 1$, $b_2(U(n-5, 0, 1, 0)) = n$, $b_4(U(n-5, 0, 1, 0)) = 3n - 13$.

Let $n - l = p$, we prove the result by induction on p.

If $p = 0$, then $S_n^l = C_n$. Using Lemma 6, we know that

$$\begin{aligned} b_4(C_n) &\geq m(C_n, 2) - 2 \\ &= m(P_n, 2) + m(P_{n-2}, 1) - 2 \\ &= \frac{(n-3)(n-2)}{2} + (n-3) - 2 \\ &> 3n - 13 = b_4(U(n-5, 0, 1, 0)), \end{aligned}$$

so we can obtain $C_n \succ U(n-5, 0, 1, 0)$ for $n \geq 7, l \geq 5$.

Suppose that the result holds for $p - 1$ ($p \geq 1$), then we prove the result holds if p. Let v be a pendent vertex, then by Lemma 8, we have

$$b_i(S_n^l) = b_i(S_{n-1}^l) + b_{i-2}(P_{l-1}),$$

so by induction, we know for $n \geq 7, l \geq 5$

$$\begin{aligned} b_4(S_n^l) &\geq b_4(S_{n-1}^l) + b_2(P_{l-1}) \\ &\geq 3(n-1) - 13 + l - 2 \geq 3n - 13 = b_4(U(n-5, 0, 1, 0)), \end{aligned}$$

and

$$b_{2k+1}(G) = \begin{cases} 0, & l \neq 2k+1 \\ 2, & l = 2k+1 \end{cases}.$$

Then we complete the proof. □

If G''' is obtained from G by replacing $T_1 \cup \cdots \cup T_r$ by $t - 2$ pendent vertices and a pendent path of length 1, we say that G''' is obtained from G by *Grafting III* (see Fig. 3).

Lemma 10 *If G''' is obtained from G and $G''' \notin \{G, G'\}$ by Grafting III (see Fig. 3), then*

$$E(G) > E(G''').$$

Proof We prove the result by induction on s, and denote v is adjacent to u in H_s. If $s = 0$, then $G''' = T(1, n-3) \neq K_{1,t}$, then by Lemma 2, we get $G \succ G'''$. Suppose that the result holds for $s = p-1$ $(p \geq 1)$, then we prove the result holds if $s = p$. Since

$$\begin{aligned} G - u - v &= (T_1 \cup \cdots \cup T_r) \cup (H_1 \cup \cdots \cup H_{s-1}) \cup (H_s - v) \\ &\succ (t-2)P_1 \cup P_2 \cup (H_1 \cup \cdots \cup H_{s-1}) \cup (H_s - v) = G''' - u - v, \end{aligned}$$

and by induction we have

$$G - uv = (G - H_s) \cup H_s \succ (G''' - H_s) \cup H_s = G''' - uv.$$

From Lemma 1, the proof is completed. □

Lemma 11 *Let $U(n-5, 0, 1, 0), U(R(n-5, 1), 0, 0) \in \mathcal{U}_n$ with $n \geq 13$, then*

$$E(U(R(n-5, 1), 0, 0)) > E(U(n-5, 0, 1, 0)).$$

Proof By Lemma (7) we have

$$\begin{aligned} \phi(U(R(n-5,1),0,0); x) &= x^{n-6}(x-1)(x+1)[x^4 - (n-1)x^2 - 2x + n - 5] \\ &= x^{n-6}(x-1)(x+1)g(x), \\ \phi(U(n-5,0,1,0); x) &= x^{n-4}[x^4 - nx^2 + (3n-13)] = x^{n-4}f(x), \end{aligned}$$

where $g(x) = f(x) + (x^2 - 2x - 2n + 8) = f(x) + h(x)$. Let x_i, y_i $(1 \leq i \leq 2)$ be the roots of $f(x) = 0$ and $g(x) = 0$, respectively.

It is not difficult to calculate that

$$\begin{aligned} f\left(\frac{7}{4}\right) &= -\frac{1}{256}(16n + 927), \quad f\left(\frac{3}{2}\right) = \frac{1}{12}(12n - 127), \\ f\left(\frac{\sqrt{n}}{2}\right) &= -\frac{1}{16}\left(3n^2 - 48n + 208\right), \quad f(\sqrt{n-1}) = 2(n-6), \end{aligned}$$

and

$$\begin{aligned} g\left(\frac{3}{4}\right) &= \frac{1}{256}(112n - 1439), \quad g(1) = -5, \\ g\left(\frac{\sqrt{n}}{2}\right) &= -\frac{1}{16}(3n^2 - 20n + 16\sqrt{n} + 80), \ g(\sqrt{n-1}) = n - 2\sqrt{n-1} - 5. \end{aligned}$$

If $n \geq 13$, then we have

$$\frac{3}{2} < x_1 < \frac{7}{4}, \quad \frac{\sqrt{n}}{2} < x_2 < \sqrt{n-1},$$

and

$$\frac{3}{4} < y_1 < 1, \quad \frac{\sqrt{n}}{2} < y_2 < \sqrt{n-1}.$$

It is easy to check $g(x_2) < 0$, so we can obtain $x_2 < y_2$ and $x_1 < 7/4 < 1 + y_1$, then

$$E(U(R(n-5,1),0,0)) = 2(1+y_1+y_2) > 2(x_1+x_2) = E(U(n-5,0,1,0)).\square$$

Theorem 12 *If* $G \in \mathcal{U}_n - \{S_n^3, S_n^4, \ U(n-4,1,0), \ U(n-5,0,1,0)\}$ *with* $n \geq 13$*, then*

$$G \succ U(n-5,0,1,0).$$

Proof We will discuss according to l.

(1) $l \geq 5$.
Using Theorem 5 and Lemma 9, we have

$$G \succeq S_n^l \succeq S_n^5 \succ U(n-4,1,0).$$

(2) $l = 4$.
(a) The number of rooted vertex is 1.
Then by Lemma 10, we have

$$G \succeq U(R(n-6,1),0,0,0).$$

And

$$\phi(U(R(n-6,1),0,0,0)) = x^{n-6}[x^6 - nx^4 + (3n-12)x^2 - (2n-12)],$$

if $n \geq 6$, then $U(R(n-6,1),0,0,0) \succ U(n-5,1,0,0)$.
(b) The number of rooted vertex is 2.
Then using Lemmas 3 and 4, we have

$$G \succeq U(s,0,n-4-s,0) \succeq U(n-6,0,2,0) \succ U(n-5,0,1,0),$$

or

$$G \succeq U(s,n-4-s,0,0) \succeq U(n-5,1,0,0).$$

By Lemma 7, we have

$$\phi(U(n-5,1,0,0)) = x^{n-6}[x^6 - nx^4 + (3n-13)x^2 - (n-5)],$$

then if $n \geq 6$, we have $U(n-5,1,0,0) \succ U(n-5,0,1,0)$.

(c) The number of rooted vertex is greater than 2.
Then combining Lemmas 3 and 4 with Subcase 2.2, we have

$$G \succeq U(n_1, n_2, n_3, n_4) \succ \min\{U(s, n-4-s, 0, 0), (s, 0, n-4-s, 0)\} \succ U(n-5, 0, 1, 0).$$

(3) $l = 3$.
(a) The number of rooted vertex is 1.
Then by Lemmas 10 and 11, we have

$$G \succeq U(R(n-5, 1), 1, 0) \succ U(n-5, 0, 1, 0).$$

(b) The number of rooted vertex is 2.
Then by Lemmas 3 and 4, we have

$$G \succeq U(n-5, 2, 0).$$

And

$$\phi(n-5, 2, 0) = x^{n-4}[x^4 - nx^2 - 2x + 3n - 13],$$

so comparing b_i with (6), we have $G \succeq U(n-5, 2, 0) \succ U(n-5, 0, 1, 0)$.
(c) The number of rooted vertex is 3.
Then by using Lemmas 3 and 4, we have

$$G \succeq U(n_1, n_2, n_3) \succeq U(n-5, 1, 1).$$

By Lemma 7, we have

$$\phi(n-5, 1, 1) = x^{n-6}[x^6 - nx^4 - 2x^3 + (3n-12)x^2 - (n-5)],$$

by comparing b_i with (6), we know $G \succ U(n-5, 0, 1, 0)$.

□

Lemma 13 *Let* $U(n-5, 0, 1, 0)$, $U(n-4, 1, 0)$, $S_n^4 \in \mathcal{U}_n$ *with* $n \geq 7$, *then*

$$U(n-5, 0, 1, 0) \succ U(n-4, 1, 0) \succ S_n^4.$$

Proof It is not difficult to calculate

$$\phi(U(n-4, 1, 0)) = x^{n-4}[x^4 - nx^2 - 2x + (2n-7)],$$
$$\phi(S_n^4) = x^{n-4}[x^4 - nx^2 + (2n-8)],$$

by comparing b_i, we have $U(n-4, 1, 0) \succ S_n^4$.

Next we prove the first inequality. Since

$$E(U(n-5,0,1,0)) - E(U(n-4,1,0)) = \frac{1}{\pi}\int_0^{+\infty} \frac{1}{x^2} \ln \frac{[1+nx^2+(3n-13)x^4]^2}{[1+nx^2+(2n-7)x^4]^2+(2x^3)^2} dx,$$

we set

$$r(x) = [1+nx^2+(3n-13)x^4]^2 - [1+nx^2+(2n-7)x^4]^2 - (2x^3)^2 = x^4[(5n^2-50n+120)x^4 + (2n^2-12n-4)x^2 + (2n-12)],$$

if $n \geq 7$, then $r(x) \geq 0$, so $E(U(n-5,0,1,0)) > E(U(n-4,1,0))$. The proof is completed. □

Combining Theorem 12 and Lemma 13, we obtain the main result in this section.

Theorem 14 *Let* $G \in \mathcal{U}_n - \{S_n^3, S_n^4, U(n-4,1,0),\ U(n-5,0,1,0)\}$ *with* $n \geq 13$*, then*

(1) $E(G) > E(U(n-5,0,1,0))$;
(2) $E(U(n-5,0,1,0)) > E(U(n-4,1,0)) > E(S_n^4) > E(S_n^3)$.

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