Complete Solution to a Conjecture on the Maximal Energy of Unicyclic Graphs*

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Abstract

For a given simple graph G, the energy of G, denoted by $E(G)$, is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. Let P_n^ℓ be the unicyclic graph obtained by connecting a vertex of C_ℓ with a leaf of $P_{n-\ell}$. In [G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39**(1999) 984–996], Caporossi et al. conjectured that the unicyclic graph with maximal energy is C_n if $n \le 7$ and $n = 9, 10, 11, 13, 15$, and P_n^6 for all other values of n. In this paper, by employing the Coulson integral formula and some knowledge of real analysis, especially by using certain combinatorial technique, we completely solve this conjecture. However, it turns out that for $n = 4$ the conjecture is not true, and P_4^3 should be the unicyclic graph with maximal energy.

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1 Introduction

For a given simple graph G of order n, denote by $A(G)$ the adjacency matrix of G. The characteristic polynomial of $A(G)$ is usually called the characteristic polynomial of G, denoted by

$$\phi(G, x) = \det(xI - A(G)) = x^n + a_1 x^{n-1} + \cdots + a_n,$$

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If G is a bipartite graph, the characteristic polynomial of G has the form

$$\phi(G,x)=\sum_{k=0}^{\lfloor n/2\rfloor} a_{2k}x^{n-2k}=\sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k b_{2k}x^{n-2k},$$

where $b_{2k}=(-1)^k a_{2k}$ and $b_{2k}\geq 0$ for all $k=1,\ldots,\lfloor n/2\rfloor$, especially $b_0=a_0=1$. In particular, if G is a tree, the characteristic polynomial of G can be expressed as

$$\phi(G,x)=\sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k m(G,k)x^{n-2k},$$

where $m(G,k)$ is the number of k-matchings of G.

For a graph G, let $\lambda_1,\lambda_2,\ldots,\lambda_n$ denote the eigenvalues of $\phi(G,x)$. The *energy* of G is defined as

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

This definition was put forward by Gutman [6] in 1978. The following formula is also well-known

$$E(G)=\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}\log|x^n\phi(G,i/x)|\mathrm{d}x,$$

where $i^2=-1$. Furthermore, in the book of Gutman and Polansky [10], the above equality was converted into an explicit formula as follows:

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

For more results about graph energy, we refer the readers to the survey of Gutman, Li and Zhang [8].

For two given trees, or bipartite graphs G_1 and G_2, according to the corresponding coefficients of the characteristic polynomials, one can introduce a quasi order to compare the values of $E(G_1)$ and $E(G_2)$. Actually, the quasi order method is commonly used to compare the energies of pairs of such graphs. However, for general graphs, it is difficult to define such a quasi order. If, for two trees, or bipartite graphs, the above quantities $m(T,k)$ or $|a_k(G)|$ can not be compared uniformly, then the quasi order method is invalid, and this happened very often. Recently, for these quasi-order incomparable problems, we find an efficient approach to determine which one attains the extremal value of the energy, such as our earlier papers [13]–[18].

Let C_n be the cycle of order n, P_n the path of order n, and P_n^ℓ the unicyclic graph obtained by connecting a vertex of C_ℓ with a leaf of $P_{n-\ell}$. In [2], Caporossi et al. proposed the following conjecture on the unicyclic graph with maximal energy.

Conjecture 1 *Among all unicyclic graphs on n vertices, the cycle C_n has maximal energy if $n\leq 7$ and $n=9,10,11,13$ and 15. For all other values of n, the unicyclic graph with maximal energy is P_n^6.*

In [12], the authors proved the following Theorem 1 that is weaker than the above conjecture, namely that $E(P_n^6)$ is maximal within the class of the unicyclic bipartite n-vertex graphs differing from C_n. And they also claimed that the energy of C_n and P_n^6 is quasi-order incomparable.

Theorem 1 *Let G be any connected, unicyclic and bipartite graph on n vertices and $G \ncong C_n$. Then $E(G) < E(P_n^6)$.*

Very recently, our another paper [17] and Andriantiana [1] independently proved that $E(C_n) < E(P_n^6)$, and then completely determined that P_n^6 is the only graph which attains the maximum value of the energy among all the unicyclic bipartite graphs for $n = 8, 12, 14$ and $n \geq 16$, which partially solves the above conjecture.

Theorem 2 *For $n = 8, 12, 14$ and $n \geq 16$, $E(P_n^6) > E(C_n)$.*

In this paper, by employing the Coulson integral formula (details on the formula can be found in [3] and [10] pp.139-147, as well as in the recent works [9, 20]) and some knowledge of real analysis, especially by using certain combinatorial technique, we completely solve this conjecture by proving the following theorem and corollary. However, we find that for $n = 4$ the conjecture is not true, and P_4^3 should be the unicyclic graph with maximal energy.

Theorem 3 *Among all unicyclic graphs of order $n \geq 16$, the unicyclic graph with maximal energy is P_n^6.*

Corollary 1 *Among all unicyclic graphs on n vertices, the cycle C_n has maximal energy if $n \leq 7$ but $n \neq 4$, and $n = 9, 10, 11, 13$ and 15; P_4^3 has maximal energy if $n = 4$. For all other values of n, the unicyclic graph with maximal energy is P_n^6.*

2 Preliminaries

Let $G(n, \ell)$ be the set of all connected unicyclic graphs on n vertices that contain the cycle C_ℓ as a subgraph. Denote by $C(n, \ell)$ the set of all unicyclic graphs obtained from C_ℓ by adding to it $n - \ell$ pendent vertices. In the following, we list some results given in [12] which will be used in the sequel.

Lemma 1 *Let $G \in G(n, \ell)$ and $n > \ell$. If G has maximal energy in $G(n, \ell)$, then G is either P_n^ℓ or, when $\ell = 4r$, a graph from $C(n, \ell)$.*

Lemma 2 *Let $G \in C(n, \ell)$ and $n > \ell$. If ℓ is even with $\ell \geq 8$ or $\ell = 4$, then $E(G) < E(P_n^6)$.*

Lemma 3 *Let ℓ be even and $\ell \geq 8$ or $\ell = 4$. Then $E(P_n^\ell) < E(P_n^6)$.*

Form Lemmas 1–3 and Theorem 2, we conclude that for any n-vertex unicyclic graph G, if the length of the unique cycle of G is even and $n = 8, 12, 14$ and $n \geq 16$, then $E(G) < E(P_n^6)$; if the length of the unique cycle of G is odd and $G \in G(n, \ell)$, then $E(G) < E(P_n^\ell)$. For proving Theorem 3, we only need to show that $E(P_n^\ell) < E(P_n^6)$ for every odd ℓ and $n \geq 16$.

In the remainder of this section, we will introduce some lemmas and notations. At first, we recall some knowledge on real analysis, for which we refer the readers to [21].

Lemma 4 *For any real number $X > -1$, we have*

$$\frac{X}{1+X} \leq \log(1+X) \leq X.$$

In particular, $\log(1+X) < 0$ *if and only if* $X < 0$.

The following lemma on the difference of the energies of two graphs is a well-known result due to Gutman [7], which will be used in the sequel.

Lemma 5 *If G_1 and G_2 are two graphs with the same number of vertices, then*

$$E(G_1) - E(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \log \left| \frac{\phi(G_1, ix)}{\phi(G_2, ix)} \right| \mathrm{d}x.$$

Now we present one basic formula of the characteristic polynomial $\phi(G, x)$, which can be found in [4].

Lemma 6 *Let uv be an edge of G . Then*

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

where $\mathcal{C}(uv)$ is the set of cycles containing uv . In particular, if uv is a pendant edge with pendant vertex v , then $\phi(G, x) = x\,\phi(G - v, x) - \phi(G - u - v, x)$.

From Lemma 6, we can easily obtain the following lemma.

Lemma 7 *For any positive integer $t \leq n - 2$, $\phi(P_n^t, x) = x\phi(P_{n-1}^t, x) - \phi(P_{n-2}^t, x)$. In particular, $\phi(P_n^6, x) = x\phi(P_{n-1}^6, x) - \phi(P_{n-2}^6, x)$.*

Now for convenience, we introduce some notations as follows, which will be well used in this sequel.

$$Y_1(x) = \frac{x + \sqrt{x^2 - 4}}{2}, \qquad Y_2(x) = \frac{x - \sqrt{x^2 - 4}}{2}.$$

It is easy to verify that $Y_1(x) + Y_2(x) = x$, $Y_1(x)Y_2(x) = 1$, $Y_1(ix) = \frac{x+\sqrt{x^2+4}}{2}i$ and $Y_2(ix) = \frac{x-\sqrt{x^2+4}}{2}i$. We define

$$Z_1(x) = -iY_1(ix) = \frac{x + \sqrt{x^2 + 4}}{2}, \; Z_2(x) = -iY_2(ix) = \frac{x - \sqrt{x^2 + 4}}{2}.$$

Observe that $Z_1(x) + Z_2(x) = x$ and $Z_1(x)Z_2(x) = -1$. In addition, for $x > 0$, $Z_1(x) > 1$ and $-1 < Z_2(x) < 0$; for $x < 0$, $0 < Z_1(x) < 1$ and $Z_2(x) < -1$. In the rest of this paper, we abbreviate $Z_j(x)$ to Z_j for $j = 1, 2$.

3 Main results

First, we introduce some more notations, which will be used frequently later.

$$A_1(x) = \frac{Y_1(x)\phi(P_8^6, x) - \phi(P_7^6, x)}{(Y_1(x))^9 - (Y_1(x))^7}, \qquad A_2(x) = \frac{Y_2(x)\phi(P_8^6, x) - \phi(P_7^6, x)}{(Y_2(x))^9 - (Y_2(x))^7},$$
$$B_1(x) = \frac{Y_1(x)\phi(P_{t+2}^t, x) - \phi(P_{t+1}^t, x)}{(Y_1(x))^{t+3} - (Y_1(x))^{t+1}}, \quad B_2(x) = \frac{Y_2(x)\phi(P_{t+2}^t, x) - \phi(P_{t+1}^t, x)}{(Y_2(x))^{t+3} - (Y_2(x))^{t+1}},$$
$$C_1(x) = \frac{Y_1(x)(x^2-1) - x}{(Y_1(x))^3 - Y_1(x)}, \qquad C_2(x) = \frac{Y_2(x)(x^2-1) - x}{(Y_2(x))^3 - Y_2(x)}.$$

By some calculations, we can get that $\phi(P_8^6, x) = x^8 - 8x^6 + 19x^4 - 16x^2 + 4$ and $\phi(P_7^6, x) = x^7 - 7x^5 + 13x^3 - 7x$, and then

$$A_1(ix) = -\frac{Z_1 f_8 + f_7}{Z_1^2 + 1} Z_2^7, \quad A_2(ix) = -\frac{Z_2 f_8 + f_7}{Z_2^2 + 1} Z_1^7,$$

where $f_8 = \phi(P_8^6, ix) = x^8 + 8x^6 + 19x^4 + 16x^2 + 4$ and $f_7 = i\phi(P_7^6, ix) = x^7 + 7x^5 + 13x^3 + 7x$.

Lemma 8 *For $n \geq 7$ and odd integer $3 \leq t \leq n$, the characteristic polynomials of P_n^6 and P_n^t have the following forms:*

$$\phi(P_n^6, x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n$$

and

$$\phi(P_n^t, x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n$$

where $x \neq \pm 2$.

Proof. By Lemma 7, we notice that $\phi(P_n^6, x)$ satisfies the recursive formula $f(n, x) = xf(n-1, x) - f(n-2, x)$. Therefore, the general solution of this linear homogeneous recurrence relation is $f(n, x) = D_1(x)(Y_1(x))^n + D_2(x)(Y_2(x))^n$. By some elementary calculations, we can easily obtain that $D_i(x) = A_i(x)$ for $\phi(P_n^6, x)$, $i = 1, 2$, from the initial values $\phi(P_8^6, x)$, $\phi(P_7^6, x)$. Similarly, the required expression of $\phi(P_n^t, x)$ can be obtained by the analogous method. ∎

Employing a method similar to the proof of Lemma 8, we can obtain

Lemma 9 *For positive integer $t \geq 3$, we have*

$$\begin{aligned}\phi(P_{t+2}^t, x) = &\big(C_1(x)(Y_1(x))^{t-2}((Y_1(x))^4 - x^2 + 1)\big)\\ &+ \big(C_2(x)(Y_2(x))^{t-2}((Y_2(x))^4 - x^2 + 1)\big) - 2(x^2 - 1);\end{aligned}$$
$$\phi(P_{t+1}^t, x) = \big(C_1(x)(Y_1(x))^{t-2}((Y_1(x))^3 - x)\big) + \big(C_2(x)(Y_2(x))^{t-2}((Y_2(x))^3 - x)\big) - 2x.$$

Proof. By Lemma 6, we notice that $\phi(P_n, x)$ satisfies the recursive formula $f(n, x) = xf(n-1, x) - f(n-2, x)$. Therefore, the general solution of this linear homogeneous recurrence relation is $f(n, x) = D_1(x)(Y_1(x))^n + D_2(x)(Y_2(x))^n$. By some elementary calculations, we can easily obtain that $D_i(x) = C_i(x)$ for $\phi(P_n, x)$, $i = 1, 2$, from the initial values $\phi(P_2, x)$, $\phi(P_1, x)$. According to Lemma 6, we have

$$\begin{aligned}\phi(P^t_{t+2}, x) =& \phi(P_{t+2}, x) - \phi(P_{t-2}, x)\phi(P_2, x) - 2\phi(P_2, x);\\ \phi(P^t_{t+1}, x) =& \phi(P_{t+1}, x) - \phi(P_{t-2}, x)\phi(P_1, x) - 2\phi(P_1, x).\end{aligned}$$

Therefore, we can obtain the required expression for $\phi(P^t_{t+2}, x)$ and $\phi(P^t_{t+1}, x)$. ∎

Notice that $(x^2 + 1)Z_1 + x = Z_1^3$ and $(x^2 + 1)Z_2 + x = Z_2^3$. By some simplifications, we can get the following corollary from Lemma 9.

Corollary 2 $B_1(ix) = B_{11}(t, x) + B_{12}(t, x) \cdot i^t$ *and* $B_2(ix) = B_{21}(t, x) + B_{22}(t, x) \cdot i^t$, *where*

$$B_{11}(t, x) = \frac{Z_1^2(Z_1^2 + 2)}{(Z_1^2 + 1)^2} - \frac{Z_2^{2t-2}}{x^2 + 4}, \qquad B_{12}(t, x) = \frac{-2Z_2^{t-2}}{Z_1^2 + 1},$$

$$B_{21}(t, x) = \frac{Z_2^2(Z_2^2 + 2)}{(Z_2^2 + 1)^2} - \frac{Z_1^{2t-2}}{x^2 + 4}, \qquad B_{12}(t, x) = \frac{-2Z_1^{t-2}}{Z_2^2 + 1}.$$

For brevity of the exposition, we denote

$$g_1 = \frac{Z_1^2(Z_1^2 + 2)}{(Z_1^2 + 1)^2}, \quad g_2 = \frac{Z_2^2(Z_2^2 + 2)}{(Z_2^2 + 1)^2}, \quad m_1 = \frac{-2}{Z_1^2 + 1}, \quad m_2 = \frac{-2}{Z_2^2 + 1}, \quad h = \frac{1}{x^2 + 4}.$$

Observe that each of g_i, m_i, h is a real function only in x, $i = 1, 2$.

From now on, we use A_j and B_{jk} instead of $A_j(ix)$ and $B_{jk}(t, x)$ for $j, k = 1, 2$, respectively. According to Lemma 8 and Corollary 2, it is no hard to get the following simplifications.

$$\left|\phi(P^6_n, ix)\right|^2 = A_1^2 Z_1^{2n} + A_2^2 Z_2^{2n} + (-1)^n 2A_1A_2, \tag{1}$$

$$\left|\phi(P^t_n, ix)\right|^2 = (B_{11}^2 + B_{12}^2)Z_1^{2n} + (B_{21}^2 + B_{22}^2)Z_2^{2n} + (-1)^n 2(B_{11}B_{21} + B_{12}B_{22}). \tag{2}$$

Proof of Theorem 3.

From the analysis in the above section, we only need to show that $E(P^t_n) < E(P^6_n)$ for every odd $t \le n$ and $n \ge 16$. By Lemma 5,

$$E(P^t_n) - E(P^6_n) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \log\left|\frac{\phi(P^t_n, ix)}{\phi(P^6_n, ix)}\right| \mathrm{d}x.$$

We distinguish two cases in terms of the parity of n.

Case 1. n is odd and $n \ge 17$.

Now we will prove that the integrand $\log\left|\frac{\phi(P^t_n, ix)}{\phi(P^6_n, ix)}\right|$ is monotonically decreasing in n.

$$\begin{aligned}&\log\left|\frac{\phi(P^t_{n+2}, ix)}{\phi(P^6_{n+2}, ix)}\right| - \log\left|\frac{\phi(P^t_n, ix)}{\phi(P^6_n, ix)}\right|\\ =&\frac{1}{2}\log\frac{\left|\phi(P^t_{n+2}, ix)\cdot\phi(P^6_n, ix)\right|^2}{\left|\phi(P^6_{n+2}, ix)\cdot\phi(P^t_n, ix)\right|^2} = \frac{1}{2}\log\left(1 + \frac{K(n, t, x)}{H(n, t, x)}\right),\end{aligned}$$

where $H(n,t,x) = \left|\phi(P^6_{n+2}, ix)\cdot\phi(P^t_n, ix)\right|^2 > 0$ and

$$K(n,t,x) = \left|\phi(P^t_{n+2}, ix)\cdot\phi(P^6_n, ix)\right|^2 - \left|\phi(P^6_n, ix)\cdot\phi(P^t_n, ix)\right|^2.$$

From Lemma 4, we only need to prove $K(n,t,x) < 0$. By some elementary calculations and simplifications, we can obtain

$$K(n,t,x) = \alpha(t,x)(Z_1^4 - Z_2^4) + \beta(t,x)Z_1^{2n}(Z_1^4 - 1) + \gamma(t,x)Z_2^{2n}(1 - Z_2^4),$$

where $\alpha(t,x) = A_2^2(B_{11}^2 + B_{12}^2) - A_1^2(B_{21}^2 + B_{22}^2)$, $\beta(t,x) = 2A_1^2(B_{11}B_{21} + B_{12}B_{22}) - 2A_1A_2(B_{11}^2 + B_{12}^2)$, $\gamma(t,x) = 2A_1A_2(B_{21}^2 + B_{22}^2) - 2A_2^2(B_{11}B_{21} + B_{12}B_{22})$. In the following, we will discuss the signs of $\alpha(t,x)$, $\beta(t,x)$, $\gamma(t,x)$.

$$\begin{aligned}
\alpha(t,x) &= \alpha_0 + \alpha_1 Z_1^{2t-4} + \alpha_2 Z_2^{2t-4} + \alpha_3 Z_1^{4t-4} + \alpha_4 Z_2^{4t-4},\\
\beta(t,x) &= \beta_0 + \beta_1 Z_1^{2t-2} + \beta_2 Z_2^{2t-2} + \beta_4 Z_2^{4t-4},\\
\gamma(t,x) &= \gamma_0 + \gamma_1 Z_1^{2t-2} + \gamma_2 Z_2^{2t-2} + \gamma_3 Z_1^{4t-4},
\end{aligned}$$

where

$$\alpha_0 = A_2^2 g_1^2 - A_1^2 g_2^2, \qquad \alpha_1 = 2A_1^2 g_2 h Z_1^2 - A_1^2 m_2^2,$$

$$\alpha_2 = A_2^2 m_1^2 - 2A_2^2 g_1 h Z_2^2, \qquad \alpha_3 = -A_1^2 h^2, \qquad \alpha_4 = A_2^2 h^2,$$

$$\beta_0 = -2A_1\left(\frac{2(x^2+3)}{(x^2+4)^2}A_1 + A_2 g_1^2\right), \qquad \beta_1 = -2A_1^2 g_1 h,$$

$$\beta_2 = 2A_1(2A_2 g_1 h - A_1 g_2 h - A_2 m_1^2 Z_1^2), \quad \beta_4 = -2A_1A_2h^2,$$

$$\gamma_0 = 2A_2\left(A_1 g_2^2 + \frac{2(x^2+3)}{(x^2+4)^2}A_2\right), \qquad \gamma_1 = 2A_2(A_1 m_2^2 Z_2^2 + A_2 g_1 h - 2A_1 g_2 h),$$

$$\gamma_2 = 2A_2^2 g_2 h, \qquad \gamma_3 = 2A_1A_2h^2.$$

Claim 1. For any real number x and positive integer t, $\beta(t,x) < 0$.

Notice that $Z_1 f_8 + f_7 = (\frac{x}{2}f_8 + f_7) + \frac{\sqrt{x^2+4}}{2}f_8$, $Z_2 f_8 + f_7 = (\frac{x}{2}f_8 + f_7) - \frac{\sqrt{x^2+4}}{2}f_8$ and

$$\left(\frac{x}{2}f_8 + f_7\right)^2 - \left(\frac{\sqrt{x^2+4}}{2}f_8\right)^2 = -(x^{10} + 10x^8 + 36x^6 + 62x^4 + 51x^2 + 16) < 0.$$

Then $A_1 = -\frac{Z_1 f_8 + f_7}{Z_1^2+1}Z_2^7 > 0$, $A_2 = -\frac{Z_2 f_8 + f_7}{Z_2^2+1}Z_1^7 > 0$ since $Z_1 > 0$ and $Z_2 < 0$. Therefore, $\beta_0 < 0$.

$$\begin{aligned}
\beta_2 = -\frac{A_1(x^2+1)}{(x^2+4)^{\frac{5}{2}}}&(x^9 + 11x^7 + 47x^5 + 93x^3 + 74x\\
&+ \sqrt{x^2+4}(3x^8 + 27x^6 + 85x^4 + 111x^2 + 52)) < 0,
\end{aligned}$$

since

$$(x^9 + 11x^7 + 47x^5 + 93x^3 + 74x)^2 - (x^2 + 4)(3x^8 + 27x^6 + 85x^4 + 111x^2 + 52)^2 < 0. \quad (3)$$

It is easy to check that $\beta_1 < 0$ and $\beta_4 < 0$. Hence, the claim holds.

Claim 2. For any real number x and positive integer t, $\gamma(t, x) > 0$.

Analogously, we can get $\gamma_0 > 0$, $\gamma_2 > 0$ and $\gamma_3 > 0$. From Eq. (3), we have

$$\gamma_1 = \frac{A_2(x^2 + 1)}{(x^2 + 4)^{\frac{5}{2}}}(-(x^9 + 11x^7 + 47x^5 + 93x^3 + 74x) + \sqrt{x^2 + 4}(3x^8 + 27x^6 + 85x^4 + 111x^2 + 52)) > 0.$$

Therefore, $\gamma(t, x) > 0$.

Claim 3. For any real number x and odd $n \geq t$, $K(n, t, x) \leq \alpha(t, x)(Z_1^4 - Z_2^4) + \beta(t, x)Z_1^{2t}(Z_1^4 - 1) + \gamma(t, x)Z_2^{2t}(1 - Z_2^4)$.

Since $Z_1(x) > 1$ and $-1 < Z_2(x) < 0$ for $x > 0$, we have $Z_1^{2n} \geq Z_1^{2t}$ and $Z_2^{2n} \leq Z_2^{2t}$ when $n \geq t$. Since $0 < Z_1(x) < 1$ and $Z_2(x) < -1$ for $x < 0$, we have $Z_1^{2n} \leq Z_1^{2t}$ and $Z_2^{2n} \geq Z_2^{2t}$ when $n \geq t$. From Claims 1 and 2, we have $\beta(t, x) < 0$ and $\gamma(t, x) > 0$ for any real number x. Thus, Claim 3 holds.

Claim 4. $f(t, x) = \alpha(t, x)(Z_1^4 - Z_2^4) + \beta(t, x)Z_1^{2t}(Z_1^4 - 1) + \gamma(t, x)Z_2^{2t}(1 - Z_2^4)$ is monotonically decreasing in t.

It is no difficult to get that $f(t, x) = d_0 + d_1Z_1^{2t} + d_2Z_2^{2t} + d_3Z_1^{4t} + d_4Z_2^{4t} = d_0 + d_1(Z_1^2)^t + d_2(Z_1^2)^{-t} + d_3(Z_1^2)^{2t} + d_4(Z_1^2)^{-2t}$, where

$$d_0 = \alpha_0(Z_1^4 - Z_2^4) + \beta_2(Z_1^4 - 1)Z_1^2 + \gamma_1(1 - Z_2^4)Z_2^2,$$

$$d_1 = \alpha_1(1 - Z_2^8) + \beta_0(Z_1^4 - 1) + \gamma_3(Z_2^4 - Z_2^8),$$

$$d_2 = \alpha_2(Z_1^8 - 1) + \gamma_0(1 - Z_2^4) + \beta_4(Z_1^8 - Z_1^4),$$

$$d_3 = \alpha_3(1 - Z_2^8) + \beta_1(Z_1^2 - Z_2^2),$$

$$d_4 = \alpha_4(Z_1^8 - 1) + \gamma_2(Z_1^2 - Z_2^2).$$

We define $p_1(x) = x^3 + 6x$, $q_1(x) = (3x^2 + 4)\sqrt{x^2 + 4}$, $p_2(x) = x^7 + 9x^5 + 24x^3 + 18x$, $q_2(x) = (x^6 + 7x^4 + 12x^2 + 4)\sqrt{x^2 + 4}$, $p_3(x) = x^{13} + 15x^{11} + 89x^9 + 264x^7 + 405x^5 + 288x^3 + 56x$, $q_3(x) = (x^{12} + 15x^{10} + 85x^8 + 234x^6 + 331x^4 + 220x^2 + 48)\sqrt{x^2 + 4}$. By some calculations, we have

$$d_1 = \frac{x(x^2+4)(x^2+1)^2(x-\sqrt{x^2+4})^7(p_2(x)+q_2(x))(p_3(x)+q_3(x))}{4(x^2+4-x\sqrt{x^2+4})^2(x^2+4+x\sqrt{x^2+4})^4},$$

$$d_2 = \frac{x(x^2+4)(x^2+1)^2(x+\sqrt{x^2+4})^7(p_2(x)-q_2(x))(p_3(x)-q_3(x))}{4(x^2+4+x\sqrt{x^2+4})^2(x^2+4-x\sqrt{x^2+4})^4},$$

$$d_3 = -\frac{x(x^2+1)^2(x-\sqrt{x^2+4})^{14}(p_1(x)+q_1(x))(p_2(x)+q_2(x))^2}{8192(x^2+4+x\sqrt{x^2+4})^4},$$

$$d_4 = -\frac{x(x^2+1)^2(x+\sqrt{x^2+4})^{14}(p_1(x)-q_1(x))(p_2(x)-q_2(x))^2}{8192(x^2+4-x\sqrt{x^2+4})^4}.$$

Since $(p_1(x))^2 - (q_1(x))^2 < 0$, $(p_2(x))^2 - (q_2(x))^2 < 0$ and $(p_3(x))^2 - (q_3(x))^2 < 0$, we deduce that, d_1, $d_3 < 0$ and d_2, $d_4 > 0$ for $x > 0$; d_1, $d_3 > 0$ and d_2, $d_4 < 0$ for $x < 0$. Therefore, no matter what of $x > 0$ or $x < 0$ happens, we always have

$$\frac{\partial f(t,x)}{\partial t} = \left(d_1(Z_1^2)^t - d_2(Z_1^2)^{-t} + 2d_3(Z_1^2)^{2t} - 2d_4(Z_1^2)^{-2t}\right)\log Z_1^2 < 0.$$

The proof of Claim 4 is complete.

From Claim 4, it follows that for $t \geq 5$, we have

$$\begin{aligned} K(n,t,x) \leq f(5,x) = & -x^2(x^2+1)^2(x^4+3x^2+1) \\ & \cdot (2x^{12}+31x^{10}+189x^8+574x^6+899x^4+661x^2+160) < 0. \end{aligned}$$

For $t = 3$, one must have $n > t+2$. So

$$\begin{aligned} & K(n,3,x) < \alpha(3,x)(Z_1^4 - Z_2^4) + \beta(3,x)Z_1^{2\times3+4}(Z_1^4-1) + \gamma(3,x)Z_2^{2\times3+4}(1-Z_2^4) \\ = & -x^2(x^2+1)^3(x^2+5)(2x^{12}+23x^{10}+104x^8+238x^6+290x^4+171x^2+32) < 0. \end{aligned}$$

We conclude that the integrand $\log\left|\frac{\phi(P_n^t;ix)}{\phi(P_n^6;ix)}\right|$ is monotonically decreasing in n. Therefore,

t	$E(P_{17}^t) - E(P_{17}^6)$	t	$E(P_{17}^t) - E(P_{17}^6)$
3	-0.05339	11	-0.12030
5	-0.09835	13	-0.11425
7	-0.11405	15	-0.09493
9	-0.12006		

Table 1: The values of $E(P_{17}^t) - E(P_{17}^6)$ for $t \leq 15$.

by Theorem 2, for $n \geq 17$ and $t \geq 17$, $E(P_n^t) - E(P_n^6) < E(P_t^t) - E(P_t^6) < 0$. For $n \geq 17$ and $t \leq 15$, $E(P_n^t) - E(P_n^6) < E(P_{17}^t) - E(P_{17}^6) < 0$ from Table 1.

Case 2. n is even and $n \geq 8$.

From Eqs. (2) and (1), we have

$$\log\left|\frac{\phi(P_n^t,ix)}{\phi(P_n^6,ix)}\right|^2 = \log\frac{(B_{11}^2+B_{12}^2)Z_1^{2n}+(B_{21}^2+B_{22}^2)Z_2^{2n}+2(B_{11}B_{21}+B_{12}B_{22})}{A_1^2Z_1^{2n}+A_2^2Z_2^{2n}+2A_1A_2}.$$

Therefore, when $n\to\infty$, we have

$$\left|\frac{\phi(P_n^t,ix)}{\phi(P_n^6,ix)}\right|^2 \to \begin{cases} \frac{B_{11}^2+B_{12}^2}{A_1^2} & \text{if } x>0 \\ \frac{B_{21}^2+B_{22}^2}{A_2^2} & \text{if } x<0. \end{cases}$$

In this case, we will show

$$\log\left|\frac{\phi(P_n^t,ix)}{\phi(P_n^6,ix)}\right|^2 < \log\frac{B_{11}^2+B_{12}^2}{A_1^2}$$

for $x>0$, and

$$\log\left|\frac{\phi(P_n^t,ix)}{\phi(P_n^6,ix)}\right|^2 < \log\frac{B_{21}^2+B_{22}^2}{A_2^2}$$

for $x<0$. Now we can simplify the expressions of α_i for $i=0,1,2$ as follows:

$$\alpha_0 = \frac{x(x^2+1)^2(x^8+11x^6+43x^4+73x^2+50)(x^8+9x^6+27x^4+33x^2+12)}{(x^2+4)^{5/2}},$$

$$\alpha_1 = -\frac{(p_2(x)+q_2(x))^2(3x^2+10+x\sqrt{x^2+4})(x-\sqrt{x^2+4})^{14}(x^2+1)^2}{4096(x^2-x\sqrt{x^2+4}+4)^2(x^2+x\sqrt{x^2+4}+4)^2(x^2+4)},$$

$$\alpha_2 = \frac{(p_2(x)-q_2(x))^2(3x^2+10-x\sqrt{x^2+4})(x+\sqrt{x^2+4})^{14}(x^2+1)^2}{4096(x^2-x\sqrt{x^2+4}+4)^2(x^2+x\sqrt{x^2+4}+4)^2(x^2+4)}.$$

Subcase 2.1. $x>0$.

By some calculations, we have

$$\log\left|\frac{\phi(P_n^t,ix)}{\phi(P_n^6,ix)}\right|^2 - \log\frac{B_{11}^2+B_{12}^2}{A_1^2} = \log\left(1+\frac{K_1(n,t,x)}{H_1(n,t,x)}\right),$$

where $H_1(n,t,x)=|\phi(P_n^6,ix)|^2(B_{11}^2+B_{12}^2)>0$ and $K_1(n,t,x)=-\alpha(t,x)Z_2^{2n}+\beta(t,x)$. Now we suppose $\alpha(t,x)<0$. Otherwise, $K_1(n,t,x)<0$ since $\beta(t,x)<0$ by Claim 1, and then we are done. Since $-1<Z_2<0$,

$$K_1(n,t,x)\le -\alpha(t,x)Z_2^{2t}+\beta(t,x)=\overline{d}_0+\overline{d}_1Z_1^{2t-2}+\overline{d}_2Z_2^{2t-2}+\overline{d}_3Z_2^{4t-4}+\overline{d}_4Z_2^{6t-4},$$

where $\overline{d}_0=\beta_0-\alpha_1Z_2^4$, $\overline{d}_1=\beta_1-\alpha_3Z_2^2$, $\overline{d}_2=\beta_2-\alpha_0Z_2^2$, $\overline{d}_3=\beta_4-\alpha_2$, $\overline{d}_4=-\alpha_4$. Since $\beta_i<0$ for $i=0,1,2,4$, α_0, α_2, $\alpha_4>0$ and α_1, $\alpha_3<0$, we have $\overline{d}_i<0$ for $i=2,3,4$ and

$$\overline{d}_1=-2A_1^2g_1h+A_1^2h^2Z_2^2=A_1^2h(hZ_2^2-2g_1)=-\frac{A_1^2h(2Z_1^2-Z_2^2+4)}{x^2+4}<0.$$

Denote by $p_0(x) = x^{14} + 19x^{12} + 146x^{10} + 584x^8 + 1300x^6 + 1582x^4 + 928x^2 + 160$ and $q_0(x) = (x^{13} + 17x^{11} + 116x^9 + 404x^7 + 756x^5 + 722x^3 + 272x)\sqrt{x^2+4}$. Then,

$$\overline{d}_0 = -\frac{A_1(x^2+1)}{(Z_1^2+1)^4(Z_2^2+1)^2}\left(p_0(x) + q_0(x)\right) < 0.$$

Thus, for $x > 0$, $K_1(n,t,x) < 0$, and then

$$\log\left|\frac{\phi(P_n^t, ix)}{\phi(P_n^6, ix)}\right|^2 < \log\frac{B_{11}^2 + B_{12}^2}{A_1^2}.$$

Subcase 2.2. $x < 0$.

Similarly, we can obtain

$$\log\left|\frac{\phi(P_n^t, ix)}{\phi(P_n^6, ix)}\right|^2 - \log\frac{B_{21}^2 + B_{22}^2}{A_2^2} = \log\left(1 + \frac{K_2(n,t,x)}{H_2(n,t,x)}\right),$$

where $H_2(n,t,x) = \left|\phi(P_n^6, ix)\right|^2 (B_{21}^2 + B_{22}^2) > 0$ and $K_2(n,t,x) = \alpha(t,x)Z_1^{2n} - \gamma(t,x)$. Now we suppose $\alpha(t,x) > 0$. Otherwise, $K_2(n,t,x) < 0$ since $\gamma(t,x) > 0$ by Claim 2, and then we are done. Since $0 < Z_1 < 1$,

$$K_2(n,t,x) \le \alpha(t,x)Z_1^{2t} - \gamma(t,x) = \widetilde{d}_0 + \widetilde{d}_1 Z_1^{2t-2} + \widetilde{d}_2 Z_2^{2t-2} + \widetilde{d}_3 Z_1^{4t-4} + \widetilde{d}_4 Z_1^{6t-4},$$

where $\widetilde{d}_0 = \alpha_2 Z_1^4 - \gamma_0$, $\widetilde{d}_1 = \alpha_0 Z_1^2 - \gamma_1$, $\widetilde{d}_2 = \alpha_4 Z_1^2 - \gamma_2$, $\widetilde{d}_3 = \alpha_1 - \gamma_3$, $\widetilde{d}_4 = \alpha_3$. Since $\gamma_i > 0$ for $i = 0,1,2,3$, α_0, α_1, $\alpha_3 < 0$ and α_2, $\alpha_4 > 0$, we have $\widetilde{d}_i < 0$ for $i = 1,3,4$ and

$$\widetilde{d}_0 = -\frac{A_2(x^2+1)}{(Z_2^2+1)^4(Z_1^2+1)^2}\left(p_0(x) - q_0(x)\right) < 0,$$

$$\widetilde{d}_2 = A_2^2 h^2 Z_1^2 - 2A_2^2 g_2 h = A_2^2 h(hZ_1^2 - 2g_2) = -\frac{A_2^2 h(2Z_2^2 - Z_1^2 + 4)}{x^2+4} < 0.$$

Thus, for $x < 0$, $K_2(n,t,x) < 0$, and then

$$\log\left|\frac{\phi(P_n^t, ix)}{\phi(P_n^6, ix)}\right|^2 < \log\frac{B_{21}^2 + B_{22}^2}{A_2^2}.$$

From the two subcases, we conclude that

$$\begin{aligned} E(P_n^t) - E(P_n^6) &= \frac{1}{\pi}\int_{-\infty}^{+\infty} \log\left|\frac{\phi(P_n^t, ix)}{\phi(P_n^6, ix)}\right| \mathrm{d}x \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \log\left|\frac{\phi(P_n^t, ix)}{\phi(P_n^6, ix)}\right|^2 \mathrm{d}x \\ &< \frac{1}{2\pi}\int_{0}^{+\infty} \log\frac{B_{11}^2 + B_{12}^2}{A_1^2}\mathrm{d}x + \frac{1}{2\pi}\int_{-\infty}^{0} \log\frac{B_{21}^2 + B_{22}^2}{A_2^2}\mathrm{d}x. \end{aligned}$$

Denote $p_4(x) = x^{16} + 14x^{14} + 83x^{12} + 274x^{10} + 551x^8 + 686x^6 + 507x^4 + 190x^2 + 22$, $q_4(x) = (x^{15} + 12x^{13} + 61x^{11} + 172x^9 + 291x^7 + 296x^5 + 167x^3 + 40x)\sqrt{x^2+4}$. Notice that $\frac{Z_1^2}{(Z_1^2+1)^2} = \frac{Z_2^2}{(Z_2^2+1)^2} = \frac{1}{x^2+4}$ and $(p_4(x))^2 - (q_4(x))^2 = 4(x^2+1)^2(2x^{10} + 24x^8 + 104x^6 + 225x^4 + 248x^2 + 121) > 0$ whenever $x > 0$ or $x < 0$. When $x > 0$, $Z_2^2 < 1$, we have

$$\begin{aligned} B_{11}^2 + B_{12}^2 - A_1^2 &= \left(\frac{Z_1^2+2}{x^2+4} - \frac{Z_2^{2t-2}}{x^2+4}\right)^2 + \left(-\frac{2(Z_1^2+1)Z_2^t}{x^2+4}\right)^2 - A_1^2 \\ &= \frac{1}{(x^2+4)^2}\left((Z_1^2+2)^2 + (2Z_1^2+4Z_2^2+4)Z_2^{2t-2} + Z_2^{4t-4}\right) - A_1^2 \\ &< \frac{1}{(x^2+4)^2}\left((Z_1^2+2)^2 + (2Z_1^2+4Z_2^2+4)Z_2^4 + Z_2^8\right) - A_1^2 \\ &= -\frac{p_4(x) - q_4(x)}{(x^2+4)(x^2+2+x\sqrt{x^2+4})} < 0. \end{aligned}$$

When $x < 0$, $Z_1^2 < 1$, we have

$$\begin{aligned} B_{21}^2 + B_{22}^2 - A_2^2 &= \left(\frac{Z_2^2+2}{x^2+4} - \frac{Z_1^{2t-2}}{x^2+4}\right)^2 + \left(-\frac{2(Z_2^2+1)Z_1^t}{x^2+4}\right)^2 - A_2^2 \\ &= \frac{1}{(x^2+4)^2}\left((Z_2^2+2)^2 + (2Z_2^2+4Z_1^2+4)Z_1^{2t-2} + Z_1^{4t-4}\right) - A_2^2 \\ &< \frac{1}{(x^2+4)^2}\left((Z_2^2+2)^2 + (2Z_2^2+4Z_1^2+4)Z_1^4 + Z_1^8\right) - A_2^2 \\ &= -\frac{p_4(x) + q_4(x)}{(x^2+4)(x^2+2-x\sqrt{x^2+4})} < 0. \end{aligned}$$

So

$$\int_0^{+\infty} \log\frac{B_{11}^2 + B_{12}^2}{A_1^2}\mathrm{d}x < 0 \quad \text{and} \quad \int_{-\infty}^0 \log\frac{B_{21}^2 + B_{22}^2}{A_2^2}\mathrm{d}x < 0.$$

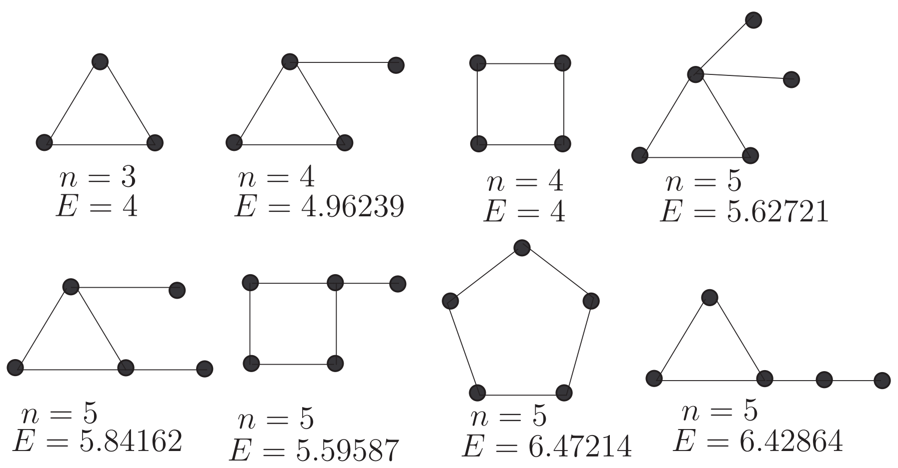

Figure 1: All unicyclic graphs and its energies for $n \leq 5$.

Therefore, $E(P_n^t) - E(P_n^6) < 0$ when n is even. ∎

n	t	$E(P_n^t) - E(P_n^6)$	n	t	$E(P_n^t) - E(P_n^6)$
6	3	−0.45075	6	5	−0.53412
7	3	0.22026	7	5	0.19680
8	3	−0.31283	8	5	−0.37252
8	7	−0.42994	9	3	0.08604
9	5	0.04987	9	7	0.05443
10	3	−0.26573	10	5	−0.31918
10	7	−0.35115	10	9	−0.40167
11	3	0.02396	11	5	−0.01682
11	7	−0.02469	11	9	−0.01186
12	3	−0.24081	12	5	−0.29174
12	7	−0.31698	12	9	−0.34102
12	11	−0.38894	13	3	−0.01237
13	5	−0.05536	13	7	−0.06773
13	9	−0.06719	13	11	−0.05081
14	3	−0.22520	14	5	−0.27486
14	7	−0.29740	14	9	−0.31438
14	11	−0.33517	14	13	−0.38193
15	3	−0.03635	15	5	−0.08055
15	7	−0.09506	15	9	−0.09897
15	11	−0.09481	15	13	−0.07658
16	3	−0.21447	16	5	−0.26340
16	7	−0.28459	16	9	−0.29873
16	11	−0.31223	16	13	−0.33141
16	15	−0.37761			

Table 2: Values of $E(P_n^t) - E(P_n^6)$ for $n \leq 16$ and odd t.

Proof of Corollary 1.

There are only two unicyclic graphs of order 4, which are shown in Figure 1. Observe that P_4^3 has maximal energy for $n = 4$. From Lemmas 1–3, and Theorems 2 and 3, we only need to show that for $n \leq 16$ $(n \neq 4)$ and any odd t with $3 \leq t \leq n$, $E(P_n^t) < E(P_n^6)$ or $E(P_n^t) < E(C_n)$. From Table 2, we can see that $E(P_n^t) < E(P_n^6)$ for $6 \leq n \leq 16$ except for $n = 7, 9, 11$ and some t. In such cases, we can check that $E(P_n^t) < E(C_n)$ from Table 3. For $n = 3, 5$, we consider all the unicyclic graphs. All such graphs and their energies are shown in Figure 1, in which our results are verified. Finally, we calculate the energies of C_n and P_n^6 for $n = 7, 9, 10, 11, 13, 15$, and verify that $E(C_n) > E(P_n^6)$ in these cases. ∎

n	t	$E(P_n^t)$	$E(C_n)$	n	t	$E(P_n^t)$	$E(C_n)$
7	3	8.94083	8.98792	7	5	8.91737	8.98792
9	3	11.47069	11.51754	9	5	11.43452	11.51754
9	7	11.43908	11.51754	11	3	14.00732	14.05335
n	t	$E(P_n^t)$	$E(C_n)$	n	t	$E(P_n^t)$	$E(C_n)$
7	6	8.72057	8.98792	9	6	11.38465	11.51754
10	6	12.93214	12.94427	11	6	13.98336	14.05335
13	6	16.55965	16.59246	15	6	19.12546	19.13354

Table 3: Values of $E(P_n^t)$ and $E(C_n)$ for $n = 7, 9, 11, 13, 15$ and some t.

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