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

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Abstract

The energy of a simple graph G, denoted by $E(G)$, is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. Denote by C_n the cycle, and P_n^6 the unicyclic graph obtained by connecting a vertex of C_6 with a leaf of P_{n-6}. Caporossi et al. conjectured that the unicyclic graph with maximal energy is P_n^6 for $n = 8, 12, 14$ and $n \geq 16$. In"Y. Hou, I. Gutman and C. Woo, Unicyclic graphs with maximal energy, *Linear Algebra Appl.* **356**(2002), 27–36", the authors proved 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 energies of C_n and P_n^6 is quasi-order incomparable and left this as an open problem. In this paper, by utilizing the Coulson integral formula and some knowledge of real analysis, especially by employing certain combinatorial techniques, we show that the energy of P_n^6 is greater than that of C_n for $n = 8, 12, 14$ and $n \geq 16$, which completely solves this open problem and partially solves the above conjecture.

Keywords: energy; Coulson integral formula; unicyclic bipartite graph

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1 Introduction

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

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

It is well-known [3] that the characteristic polynomial of a bipartite graph G takes the form

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

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

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

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

For a graph G, let $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the eigenvalues of its characteristic polynomial. The energy of a graph G is defined as

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

This definition was proposed by Gutman [5]. 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 [8], 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 reader to the recent survey of Gutman et al. [7].

For two trees T_1 and T_2 of the same order, one can introduce a quasi order $\preceq$ in the set of trees, namely, if $m(T_1, k) \leq m(T_2, k)$ holds for all $k \geq 0$, then define $T_1 \preceq T_2$, and so $T_1 \preceq T_2$ implies $E(T_1) \leq E(T_2)$ (e.g. [4]). Similarly, one can generalize the quasi order to the cases of bipartite graphs (e.g. [15]) and unicyclic graphs (e.g. [9]). The quasi order method is commonly used to compare the energies of two trees, bipartite graphs and unicyclic 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 common comparing method is invalid, and this happened very often. Recently, for these quasi-order incomparable problems, we find an efficient way to determine which one attains the extremal value of the energy, see [11–14].

Let C_n be the cycle, and P_n^6 be the unicyclic graph obtained by connecting a vertex of C_6 with a leaf of P_{n-6}. In [2], Caporossi et al. proposed a conjecture on the unicyclic graphs with the maximum energy.

Conjecture 1.1. *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.*

Theorem 1.2. *Let G be any connected, unicyclic and bipartite graph on n vertices and $G \ncong C_n$. Then $E(G) < E(P_n^6)$.*

In [10], the authors proved Theorem 1.2 that is weaker than the above conjecture, namely, $E(P_n^6)$ is maximal within the class of the unicyclic bipartite n-vertex graphs differing from C_n. And they also claimed that the energies of C_n and P_n^6 is quasi-order incomparable. In this paper, we will employ the Coulson integral formula and some knowledge of analysis, especially by using certain combinatorial techniques, to show that $E(C_n) < E(P_n^6)$, and then completely determine that P_n^6 is the only graph which attains the maximum value of the energies among all the unicyclic bipartite graphs, which partially solves the above conjecture.

Theorem 1.3. *For $n = 8, 12, 14$ and $n \geq 16$, $E(P_n^6) > E(C_n)$.*

2 Main results

We recall some knowledge on real analysis, for which we refer to [16].

Lemma 2.1. *For any real number $X > -1$, we have*

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

The following lemma is a well-known result due to Gutman [6], which will be used in the sequel.

Lemma 2.2. *If G_1 and G_2 are two graphs with the same number of vertices, then*

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

In the following, we list some basic properties of the characteristic polynomial $\phi(G, x)$, which can be found in [3].

Lemma 2.3. *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 pendent edge with pendent vertex v, then $\phi(G, x) = x\,\phi(G - v, x) - \phi(G - u - v, x)$.

Now we can easily obtain the following lemma from Lemma 2.3.

Lemma 2.4. $\phi(P_n^6, x) = x\phi(P_{n-1}^6, x) - \phi(P_{n-2}^6, x)$ *and* $\phi(C_n, x) = \phi(P_n, x) - \phi(P_{n-2}, x) - 2$.

By some easy calculations, we get $\phi(P_8^6, x) = x^8 - 8x^6 + 19x^4 - 16x^2 + 4$ and $\phi(P_7^6, x) = x^7 - 7x^5 + 13x^3 - 7x$. Now for convenience, we introduce some notions as follows

$$\begin{aligned}
Y_1(x) &= \frac{x + \sqrt{x^2 - 4}}{2}, & Y_2(x) &= \frac{x - \sqrt{x^2 - 4}}{2}, \\
C_1(x) &= \frac{Y_1(x)(x^2 - 1) - x}{(Y_1(x))^3 - Y_1(x)}, & C_2(x) &= \frac{Y_2(x)(x^2 - 1) - x}{(Y_2(x))^3 - Y_2(x)}, \\
A_1(x) &= \frac{Y_1(x)\phi(P_8^6, x) - \phi(P_7^6, x)}{(Y_1(x))^9 - (Y_1(x))^7}, & A_2(x) &= \frac{Y_2(x)\phi(P_8^6, x) - \phi(P_7^6, x)}{(Y_2(x))^9 - (Y_2(x))^7}.
\end{aligned}$$

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

$$f_8=x^8+8x^6+19x^4+16x^2+4,\quad f_7=x^7+7x^5+13x^3+7x$$

and

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

Lemma 2.5. *For $n\geq 10$ and $x\neq\pm2$, the characteristic polynomials of P_n^6 and C_n have the following forms*

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

and

$$\phi(C_n,x)=(Y_1(x))^n+(Y_2(x))^n-2.$$

Proof. By Lemma 2.4, 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 $\phi(P_8^6,x)$, $\phi(P_7^6,x)$.

By Lemma 2.4, $\phi(C_n,x)=\phi(P_n,x)-\phi(P_{n-2},x)-2$ and $\phi(P_n,x)$ satisfy the recursive formula $f(n,x)=xf(n-1,x)-f(n-2,x)$. Similarly, we can obtain the general solution of this linear nonhomogeneous recurrence relation from the initial values $\phi(P_1,x)=x$, $\phi(P_2,x)=x^2-1$. $\square$

Proof of Theorem 1.3 For $n=8,12,14$, it is easy to verify $E(P_n^6)>E(C_n)$. In the following, we always suppose $n\geq16$. Using Lemma 2.2, we can deduce

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

From Lemma 2.5, we have

$$\begin{aligned}\phi(C_n,ix)&=(Y_1(ix))^n+(Y_2(ix))^n-2=((Z_2(x))^2(x^2+1)-(Z_2(x))^3x)(Z_1(x))^n\cdot i^n\\&\quad+((Z_1(x))^2(x^2+1)-(Z_1(x))^3x)(Z_2(x))^n\cdot i^n-2,\\ \phi(P_n^6,ix)&=A_1(ix)(Y_1(ix))^n+A_2(ix)(Y_2(ix))^n\\&=\frac{Z_1(x)f_8+f_7}{(Z_1(x))^9+Z_1^7}(Z_1(x))^n\cdot i^n+\frac{Z_2(x)f_8+f_7}{(Z_2(x))^9+(Z_2(x))^7}(Z_2(x))^n\cdot i^n.\end{aligned}$$

Firstly, we will prove that $E(C_n)-E(P_n^6)$ is decreasing in n for $n=4k+j$, $j=1,2,3$, namely,

$$\begin{aligned}&\log\left|\frac{(Y_1(ix))^{n+4}+(Y_2(ix))^{n+4}-2}{A_1(ix)(Y_1(ix))^{n+4}+A_2(ix)(Y_2(ix))^{n+4}}\right|-\log\left|\frac{(Y_1(ix))^n+(Y_2(ix))^n-2}{A_1(ix)(Y_1(ix))^n+A_2(ix)(Y_2(ix))^n}\right|\\&=\log\left(1+\frac{K_0(n,x)}{H_0(n,x)}\right)<0.\end{aligned}$$

Case 1 $n = 4k+2$.

In this case, $H_0(n,x) = \left|\phi(C_n, ix)\cdot\phi(P^6_{n+4}, ix)\right| > 0$ and

$$\begin{aligned}K_0(n,x) =& (A_1(ix) - A_2(ix))\left((Y_2(ix))^4 - (Y_1(ix))^4\right) - 2A_1(ix)(Y_1(ix))^n(1-(Y_1(ix))^4)\\ &- 2A_2(ix)(Y_2(ix))^n(1-(Y_2(ix))^4).\end{aligned}$$

Then, by some elementary calculations, we have

$$\begin{aligned}K_0(n,x) = x(x^2+1)(&x^9 + 9x^7 + 30x^5 + 46x^3 + 28x\\ &+ (Z_2(x))^n(x^5 + 5x^3 + 6x + \sqrt{x^2+4}\,(x^4+3x^2+4))\\ &+ (Z_1(x))^n(x^5 + 5x^3 + 6x - \sqrt{x^2+4}\,(x^4+3x^2+4))).\end{aligned}$$

If $x > 0$, then $Z_1(x) > 1$, $-1 < Z_2(x) < 0$, and we obtain

$$K_0(n,x) = x(x^2+1)(Z_1(x))^n q(n,x) < x(x^2+1)(Z_1(x))^n q(10,x),$$

where

$$\begin{aligned}q(n,x) =&(Z_2(x))^n(x^9 + 9x^7 + 30x^5 + 46x^3 + 28x)\\ &+ (Z_2(x))^{2n}(x^5 + 5x^3 + 6x + \sqrt{x^2+4}\,(x^4+3x^2+4))\\ &+ x^5 + 5x^3 + 6x - \sqrt{x^2+4}\,(x^4+3x^2+4).\end{aligned}$$

By some simplifications,

$$\begin{aligned}q(10,x) =& -\frac{1}{2}x(x^2+4)(2x^8 + 17x^6 + 47x^4 + 46x^2 + 10)\cdot\\ &(x^{10} + 10x^8 + 35x^6 + 50x^4 + 25x^2 + 2 - \sqrt{x^2+4}(x^9 + 8x^7 + 21x^5 + 20x^3 + 5x)).\end{aligned}$$

Since

$$\left(x^{10} + 10x^8 + 35x^6 + 50x^4 + 25x^2 + 2\right)^2 - \left(\sqrt{x^2+4}\,(x^9 + 8x^7 + 21x^5 + 20x^3 + 5x)\right)^2 = 4,$$

we have $q(10,x) < 0$, and hence $\frac{K_0(n,x)}{H_0(n,x)} < 0$. Similarly, we can prove $\frac{K_0(n,x)}{H_0(n,x)} < 0$ for $x < 0$.

Therefore, we have shown that $E(C_n) - E(P^6_n)$ is decreasing in n for $n = 4k+2$.

Case 2 $n = 4k+j$, $j = 1, 3$.

In this case, $H_0(n,x) = \left|\phi(C_n, ix)\cdot\phi(P^6_{n+4}, ix)\right| > 0$ and

$$\begin{aligned}K_0(n,x) =& \left|((Y_1(ix))^{n+4} + (Y_2(ix))^{n+4} - 2)(A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n)\right|\\ &- \left|(A_1(ix)(Y_1(ix))^{n+4} + A_2(ix)(Y_2(ix))^{n+4})((Y_1(ix))^n + (Y_2(ix))^n - 2)\right|\\ =&\sqrt{p(n,x)} - \sqrt{w(n,x)},\end{aligned}$$

where

$$\begin{aligned}p(n,x) =& \left(A_2(ix)(Z_1(x))^4 + A_1(ix)(Z_2(x))^4 - A_1(ix)(Z_1(x))^{2n+4} - A_2(ix)(Z_2(x))^{2n+4}\right)^2\\ &+ \left(-2A_1(ix)(Z_1(x))^n - 2A_2(ix)(Z_2(x))^n\right)^2,\\ w(n,x) =& \left(A_1(ix)(Z_1(x))^4 + A_2(ix)(Z_2(x))^4 - A_1(ix)(Z_1(x))^{2n+4} - A_2(ix)(Z_2(x))^{2n+4}\right)^2\\ &+ \left(-2A_1(ix)(Z_1(x))^{n+4} - 2A_2(ix)(Z_2(x))^{n+4}\right)^2.\end{aligned}$$

Now we only need to check $p(n,x) - w(n,x) < 0$ for all x and n. First, we suppose $n = 4k+1$. If $x > 0$, then $(Z_1(x))^{2n} > (Z_1(x))^{10}$, $(Z_2(x))^{2n} < (Z_2(x))^{10}$, and we have

$$\begin{aligned}
p(n,x) - w(n,x) = {} & x(x^2+2)^3(x^2+1)^3(x^{11} + 11x^9 + 46x^7 + 92x^5 + 88x^3 + 28x \\
& - 2(Z_1(x))^{2n}(\sqrt{x^2+4}\,(x^2+2) + x) \\
& + 2(Z_2(x))^{2n}(\sqrt{x^2+4}\,(x^2+2) - x)) \\
< {} & p(5,x) - w(5,x) \\
= {} & -x^2(x^2+4)(x^2+1)^4(x^2+2)^3(2x^8 + 19x^6 + 60x^4 + 68x^2 + 14) < 0.
\end{aligned}$$

If $x < 0$, then $(Z_1(x))^{2n} < (Z_1(x))^{10}$, $(Z_2(x))^{2n} > (Z_2(x))^{10}$. Similarly, $p(n,x) - w(n,x) < p(5,x) - w(5,x) < 0$. By the same discussion as the case of $n = 4k+1$, for $n = 4k+3$ and $x > 0$ or $x < 0$, we can deduce that

$$\begin{aligned}
& p(n,x) - w(n,x) < p(7,x) - w(7,x) \\
= & -x^2(x^2+4)(x^2+2)^3(x^2+1)^3 \cdot \\
& (2x^{14} + 30x^{12} + 178x^{10} + 533x^8 + 849x^6 + 690x^4 + 242x^2 + 22) < 0.
\end{aligned}$$

Thus, we have done for $n = 4k+j$, $j = 1,3$.

Therefore, we have shown that $E(C_n) - E(P_n^6)$ is decreasing in n for $n = 4k+j$, $j = 1,2,3$. So, when $n = 4k+2$, $E(C_n) - E(P_n^6) < E(C_{18}) - E(P_{18}^6) \doteq -0.03752 < 0$; when $n = 4k+1$, $E(C_n) - E(P_n^6) < E(C_{17}) - E(P_{17}^6) \doteq -0.00961 < 0$; when $n = 4k+3$, $E(C_n) - E(P_n^6) < E(C_{19}) - E(P_{19}^6) \doteq -0.02290 < 0$.

Finally, we will deal with the case of $n = 4k$. Notice that in this case both $\phi(C_n, ix)$ and $\phi(P_n^6, ix)$ are polynomials of x with all real coefficients. When $n \to \infty$,

$$\frac{(Y_1(ix))^n + (Y_2(ix))^n - 2}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n} \to \begin{cases} \frac{1}{A_1(ix)} & \text{if } x > 0 \\ \frac{1}{A_2(ix)} & \text{if } x < 0. \end{cases}$$

In this case, we will show

$$\log \frac{(Y_1(ix))^n + (Y_2(ix))^n - 2}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n} < \log \frac{1}{A_1(ix)}$$

for $x > 0$ and

$$\log \frac{(Y_1(ix))^n + (Y_2(ix))^n - 2}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n} < \log \frac{1}{A_2(ix)}$$

for $x < 0$. In the following we only check the case of $x > 0$ as the case of $x < 0$ is similar. Assume

$$\log \frac{(Y_1(ix))^n + (Y_2(ix))^n - 2}{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n} - \log \frac{1}{A_1(ix)} = \log \left(1 + \frac{K_1(n,x)}{H_1(n,x)}\right),$$

by some elementary calculations, we obtain $H_1(n,x) > 0$ and

$$\begin{aligned}
& K_1(n,x) = -\frac{x^2+1}{x^2+4} \cdot \\
& \left(x^8 + 9x^6 + 28x^4 + 36x^2 + 16 + ((Z_2(x))^n - 1)\sqrt{x^2+4}\,(x^7 + 7x^5 + 16x^3 + 14x)\right) \\
& < -\frac{x^2+1}{x^2+4} \cdot \left(x^8 + 9x^6 + 28x^4 + 36x^2 + 16 - \sqrt{x^2+4}\,(x^7 + 7x^5 + 16x^3 + 14x)\right) < 0,
\end{aligned}$$

since

$$\left(x^8+9x^6+28x^4+36x^2+16\right)^2-\left(\sqrt{x^2+4}\,(x^7+7x^5+16x^3+14x)\right)^2$$
$$=4x^8+48x^6+204x^4+368x^2+256>0.$$

Notice that if $x>0$, then $A_1(ix)=\frac{Z_1(x)f_8+f_7}{(Z_1(x))^9+Z_1^7}>0$, and if $x<0$, then $A_2(ix)=\frac{Z_2(x)f_8+f_7}{(Z_2(x))^9+Z_2^7}=\frac{Z_1(x)\cdot(Z_2(x)f_8+f_7)}{Z_1(x)\cdot\left((Z_2(x))^9+Z_2^7\right)}=\frac{f_8-Z_1(x)f_7}{(Z_2(x))^8+Z_2^6}>0$. Thus, by Lemma 2.1, we have

$$\frac{1}{\pi}\int_0^{+\infty}\log\frac{1}{A_1(ix)}\mathrm{d}x<\frac{1}{\pi}\int_0^{+\infty}\left(\frac{1}{A_1(ix)}-1\right)\mathrm{d}x\doteq-0.047643;$$
$$\frac{1}{\pi}\int_{-\infty}^{0}\log\frac{1}{A_2(ix)}\mathrm{d}x<\frac{1}{\pi}\int_0^{+\infty}\left(\frac{1}{A_2(ix)}-1\right)\mathrm{d}x\doteq-0.047643.$$

Therefore,

$$E(C_n)-E(P_n^6)<\frac{1}{\pi}\int_0^{+\infty}\log\frac{1}{A_1(ix)}\mathrm{d}x+\int_{-\infty}^{0}\log\frac{1}{A_2(ix)}\mathrm{d}x<-0.047643-0.047643<0.$$

The proof is now completed. □

Remark. One of the referees points out that at about the same time Andriantiana in [1] independently obtained the same result. We have carefully read paper [1], and found that the main idea of our paper is different from his. In our paper we get result by showing the monotonicity and considering the limit function of the integrand of $E(C_n)-E(P_n^6)$. While, in [1] he compares the energy of two graphs by using the estimation of $E(P_n^6)$ and the exact (known) eigenvalues of C_n. Our method is more general than his, since it can be used to compare energies of some other pairs of graphs. Our similar idea was used in earlier papers [11–14].

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