Unicyclic Bipartite Graphs with Maximum Energy

Eric Ould Dadah Andriantiana
Department of Mathematical Sciences
Mathematics Division
Stellenbosch University
Private Bag X1, Matieland 7602
South Africa
ericoda@sun.ac.za
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Abstract

The sum of the absolute values of the eigenvalues of a graph $G$ is called energy of $G$. Let $P_6^8$ be the graph obtained by merging a vertex of the six vertex cycle $C_6$ and an end vertex of the $n-5$ vertex path. In this paper we prove that for $n = 8, 12, 14$ or $n \geq 16$ we have $E(P_6^8) > E(C_n)$. Combined with a result in [Y. Hou, I. Gutman, C.-W. Woo, Unicyclic graphs with maximal energy, Linear Algebra Appl. 356 (2002) 27-36] this means that $P_6^8$ is the connected unicyclic bipartite graph of order $n$, for the values listed above, with maximal energy.

1 Introduction

For any graph $G$ of order $n$, we denote by $\lambda_1(G), \lambda_2(G), \cdots, \lambda_n(G)$ its eigenvalues. The graph invariant defined by

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

is called energy of $G$. Within the framework of the Hückel molecular orbital [1] approximation, the calculation of the total $\pi$-electron energy in a conjugated hydrocarbon can be reduced to that of the energy of the corresponding graph. An alternative expression
of $E(G)$ is given as a Coulson integral [1] by

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log \left[ \left( \sum_{j=0}^{\lfloor n/2 \rfloor} (-1)^j a_{2j} x^{2j} \right)^2 + \left( \sum_{j=0}^{\lfloor n/2 \rfloor} (-1)^j a_{2j+1} x^{2j+1} \right)^2 \right] dx , \quad (2)$$

where $a_0, a_1, \cdots, a_n$ are the coefficients of the characteristic polynomial of $G$ written in the form

$$\phi(G, x) = \sum_{i=0}^{n} a_i x^{n-i} . \quad (3)$$

Formula (2) has been very helpful for the study of extremal energy in various classes of graphs (see for instance [2–4]).

Among the most popular classes of graphs are unicyclic graphs and bipartite graphs. The former class consists of all graphs which contain exactly one cycle, and a graph belongs to the latter class if its set of vertices can be partitioned into two subsets in such a way that every edge has its ends in different sets. In this paper we aim to show that $P_n^6$, which results from merging an end vertex of a $n - 5$ vertex path and a vertex in a 6 vertex cyclic graph, is the connected unicyclic bipartite graph of order $n$ with maximal energy. A very important step leading to this objective was achieved in [5] where it is proven that

**Theorem 1.** $P_n^6$ has the maximal energy among all connected unicyclic bipartite $n$-vertex graphs, except the circuit $C_n$.

Therefore, what is left is to compare the energy of the two graphs $P_n^6$ and $C_n$ for a fixed positive integer $n$. Our main result is that for $n = 8, 12, 14$ or $n \geq 16$ we have

$$E(C_n) < E(P_n^6) . \quad (4)$$

This partially proves the conjecture:

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

## 2 Lower bound for $E(P_n^6)$

Since $P_n^6$ is bipartite (see Figure 1), its characteristic polynomials is of the form [1]

$$\phi(P_n^6, x) = \det(xI_n - A(P_n^6)) = \sum_{k \geq 0} (-1)^k b_k(P_n^6) x^{n-2k} \quad (5)$$

Since $P_n^6$ is bipartite (see Figure 1), its characteristic polynomials is of the form [1]
where $A(P_n^6)$ is an adjacency matrix of $P_n^6$ and $I_n$ is the identity matrix of order $n$. Hence, using equation (2), the Coulson integral expression of the energy of $P_n^6$ is given by

$$E(P_n^6) = \frac{2}{\pi} \int_0^{\infty} \frac{1}{x^2} \log \left( \sum_{k \geq 0} b_k (P_n^6)^2 x^{2k} \right) \, dx .$$

(6)

First, we need an explicit expression for $Q_n(x) = \sum_{k \geq 0} b_k (P_n^6)x^{2k}$ in terms of $n$ and $x$. This will help us to evaluate the right-hand side of the equation (6). $Q_n(x)$ and $\phi(P_n^6, x)$ are related as follows for all $n \geq 6$:

$$(x/i)^n \phi_n(P_n^6, i/x) = (x/i)^n \sum_{k \geq 0} (-1)^k b_k (P_n^6)^k (i/x)^{n-2k} = \sum_{k \geq 0} (-1)^k b_k (P_n^6)^k i^{-n} (i/n-2k)x^{n-x-n+2k} = \sum_{k \geq 0} b_k (P_n^6)x^{2k} = Q_n(x) .$$

(7)

If we label the vertices of $P_n^6$ as in Figure 1, then the corresponding adjacency matrix is

$$A(P_n^6) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 \end{bmatrix} .$$

(8)
Therefore the characteristic polynomial of $P_n^6$ is

$$\phi(P_n^6, x) = \begin{vmatrix} x & -1 & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 \\
-1 & x & -1 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & -1 & x & -1 & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & -1 & x & -1 & 0 & \cdots & 0 & 0 \\
-1 & 0 & 0 & 0 & -1 & x & \cdots & \cdots & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & x & \cdots & \cdots & -1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & -1 & x \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 \end{vmatrix}. \quad (9)$$

In particular, after computation of the corresponding determinant, we have

$$\phi(P_6^6, x) = x^6 - 6x^4 + 9x^2 - 4, \quad (10)$$

$$\phi(P_7^6, x) = x^7 - 7x^5 + 13x^3 - 7x \quad (11)$$

and consequently, using equation (7), we obtain

$$Q_6(x) = (x/i)^6((i/x)^6 - 6(i/x)^4 + 9(i/x)^2 - 4)$$

$$= 1 + 6x^2 + 9x^4 + 4x^6 \quad (12)$$

$$Q_7(x) = (x/i)^7((i/x)^7 - 7(i/x)^5 + 13(i/x)^3 - 7(i/x))$$

$$= 1 + 7x^2 + 13x^4 + 7x^6. \quad (13)$$

The importance of equation (9) is that it allows us to derive a recurrence relation for the sequence of polynomials $(\phi(P_n^6, x))_{n \geq 6}$. For $n \geq 8$, expanding the determinant on the right-hand side of equation (9) with respect to its last row we obtain

$$\phi(P_n^6, x) = x\phi(P_{n-1}^6, x) - \phi(P_{n-2}^6, x). \quad (14)$$

Via equation (7) we now can deduce a recurrence relation for the sequence $(Q_n(x))_{n \geq 6}$:

$$Q_n(x) = (x/i)^n\phi_n(i/x)$$

$$= (x/i)^n\frac{i}{x}\phi_{n-1}(i/x) - (x/i)^n\phi_{n-2}(i/x)$$

$$= (x/i)^{n-1}\phi_{n-1}(i/x) + x^2(x/i)^{n-2}\phi_{n-2}(i/x)$$

$$= Q_{n-1}(x) + x^2Q_{n-2}(x). \quad (15)$$
This linear recurrence relation has characteristic equation
\[ X^2 - X - x^2 = 0 \]  
which has two roots
\[ D_1(x) = \frac{1 + \sqrt{1 + 4x^2}}{2} \]
and
\[ D_2(x) = \frac{1 - \sqrt{1 + 4x^2}}{2} . \]

Therefore, the explicit expression for \( Q_n(x) \) must be of the form
\[ Q_n(x) = C_1(x)D_1^n(x) + C_2(x)D_2^n(x) \]

where \( C_1(x) \) and \( C_2(x) \) satisfy the system of equations
\[
\begin{cases}
C_1(x)D_1^6(x) + C_2(x)D_2^6(x) = Q_6(x) = 1 + 6x^2 + 9x^4 + 4x^6 \\
C_1(x)D_1^7(x) + C_2(x)D_2^7(x) = Q_7(x) = 1 + 7x^2 + 13x^4 + 7x^6 .
\end{cases}
\]

Solving the system of equations we obtain
\[
C_2(x) = \frac{(x^2 + 1)((4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} - 1 - 7x^2 - 10x^4)}{2D_2^6(x)\sqrt{1 + 4x^2}} ,
\]
\[
C_1(x) = \frac{(x^2 + 1)((4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} + 1 + 7x^2 + 10x^4)}{2D_1^6(x)\sqrt{1 + 4x^2}}
\]

and therefore
\[
Q_n(x) = \frac{(x^2 + 1)((4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} + 10x^4 + 7x^2 + 1)}{2\sqrt{1 + 4x^2}} \left( \frac{1 + \sqrt{1 + 4x^2}}{2} \right)^{n-6} \\
+ \frac{(x^2 + 1)((4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} - 10x^4 - 7x^2 - 1)}{2\sqrt{1 + 4x^2}} \left( \frac{1 - \sqrt{1 + 4x^2}}{2} \right)^{n-6} \\
= \frac{(x^2 + 1)((4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} + 10x^4 + 7x^2 + 1)}{2\sqrt{1 + 4x^2}} \left( 1 + \frac{(4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} - 10x^4 - 7x^2 - 1}{(4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} + 10x^4 + 7x^2 + 1} \left( \frac{1 - \sqrt{1 + 4x^2}}{2} \right)^{n-6} \right).
\]

With this expression of \( Q_n(x) \), equation (6) leads to
\[
E(P_n^6) = \frac{2}{\pi} ((n - 6)I_1 + I_2 + I_4 - I_3 + I_5(n))
\]
where \( I_1, I_2, I_3, I_4, I_5(n) \) are described as follows:

\[
I_1 = \int_0^{+\infty} \frac{1}{x^2} \log(D_1(x)) \, dx = 2 , \quad (25)
\]

\[
I_2 = \int_0^{+\infty} \frac{\log(x^2 + 1)}{x^2} \, dx = \pi , \quad (26)
\]

\[
I_3 = \int_0^{+\infty} \frac{\log(\sqrt{4x^2 + 1})}{x^2} \, dx = \pi . \quad (27)
\]

Unlike the three first integrations whose exact values can be obtained via easy integration by parts, for the next two we content ourselves with some bounds,

\[
I_4 = \int_0^{+\infty} \frac{\log((4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} + 10x^4 + 7x^2 + 1) - \log(2)}{x^2} \, dx \\
= - \int_0^{+\infty} (\log((4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} + 10x^4 + 7x^2 + 1) - \log(2)) \, d\left(\frac{1}{x}\right) x \\
= - \left[ \frac{\log((4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} + 10x^4 + 7x^2 + 1) - \log(2)}{x} \right]_{x \to +\infty}^{x \to 0} \\
+ \int_0^{+\infty} \frac{80x^5 + 76x^3 + 14x + (40x^3 + 14x)\sqrt{1 + 4x^2}}{16x^7 + 24x^5 + 9x^3 + x + (10x^5 + 7x^3 + x)\sqrt{1 + 4x^2}} \, dx \\
= \int_0^{+\infty} \frac{80x^4 + 76x^2 + 14 + (40x^2 + 14)\sqrt{1 + 4x^2}}{16x^6 + 24x^4 + 9x^2 + 1 + (10x^4 + 7x^2 + 1)\sqrt{1 + 4x^2}} \, dx \\
= \int_0^{+\infty} \frac{2(4x^2 + 1)(10x^2 + 7) + (40x^2 + 14)\sqrt{1 + 4x^2}}{(x^2 + 1)(4x^2 + 1)^2 + (10x^4 + 7x^2 + 1)\sqrt{1 + 4x^2}} \, dx \\
= \int_0^{+\infty} \frac{20x^2 + 14 + 40x^2 + 14}{(x^2 + 1)(4x^2 + 1)\sqrt{1 + 4x^2} + 10x^4 + 7x^2 + 1} \, dx . \quad (28)
\]

Expressing \( x \) in terms of a new variable \( y \) defined by \( x = \frac{1}{4} \left( \frac{1}{y} - y \right) \), \( y \in (0, 1) \), leads to
a rational integral

\[ I_4 = 4 \int_0^1 \frac{(y + 1)^2(y^2 + 1)(5y^4 + 10y^3 + 26y^2 + 10y + 5)}{(y + 1)^4(y^6 + y^5 + 7y^4 - 2y^3 + 7y^2 + y + 1)} \, dy \]

\[ = 8 \int_0^1 \frac{1}{(y + 1)^2} \, dy + 4 \int_0^1 \frac{3y^4 + 2y^3 + 10y^2 + 2y + 3}{y^6 + y^5 + 7y^4 - 2y^3 + 7y^2 + y + 1} \, dy \]

\[ = 4 + 4 \int_0^1 \frac{3y^4 + 2y^3 + 10y^2 + 2y + 3}{y^6 + y^5 + 7y^4 - 2y^3 + 7y^2 + y + 1} \, dy . \quad (29) \]

To get a lower bound for \( I_4 \), note that for all \( y \in (0, 1) \) we have

\[ \frac{3y^4 + 2y^3 + 10y^2 + 2y + 3}{y^6 + y^5 + 7y^4 - 2y^3 + 7y^2 + y + 1} - \frac{15y^2 - 50y + 60}{20} = \frac{(y - y^2)f(y)}{4y^6 + 4y^5 + 28y^4 - 8y^3 + 28y^2 + 4y + 4} \quad (30) \]

where

\[ f(y) = 3y^6 - 4y^5 + 19y^4 - 45y^3 + 68y^2 - 31y + 6 \]

\[ = 6(-y^2 + 3y - 1)^2 + 2(y^2 - y)^2 + 3y^6 - 4y^5 + 11y^4 - 5y^3 + 5y > 0 . \quad (31) \]

This means that the difference in (30) is positive for all \( y \in (0, 1) \), therefore we deduce that

\[ I_4 > 4 + 4 \int_0^1 \frac{15y^2 - 50y + 60}{20} \, dy = 12 . \quad (32) \]

By numerical integration we get a better estimate for \( I_4 \):

\[ I_4 > 12.1855 . \quad (33) \]

And finally the last term is given by

\[ I_5(n) = \int_0^\infty \frac{1}{x^2} \log \left(1 + \frac{(4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} - 10x^4 - 7x^2 - 1}{(4x^4 + 5x^2 + 1)\sqrt{1 + 4x^2} + 10x^4 + 7x^2 + 1} \left(1 - \sqrt{1 + 4x^2}\right)^{n-6} \right) \, dx. \quad (34) \]

Let us proceed by a change of variable from \( x \) to \( z \) where \( x = \frac{1}{e^z - e^{-z}} \). This gives

\[ dx = -\frac{e^z + e^{-z}}{(e^z - e^{-z})^2} \, dz , \quad \sqrt{1 + 4x^2} = \frac{e^z + e^{-z}}{e^z - e^{-z}} , \quad (35) \]
and

\[ I_5(n) = \int_0^\infty \log \left( 1 + \frac{2e^z + 4e^{-3z} + 2e^{-5z}}{2e^{5z} + 4e^{3z} + 2e^{-z}} \left( e^z - e^{-z} - (e^z + e^{-z}) \right)^{n-6} \right) (e^z + e^{-z}) \, dz \]

\[ = \int_0^\infty \log \left( 1 + \frac{2e^{-5z}(e^{6z} + 2e^{2z} + 1)}{2e^{-z}(e^{6z} + 2e^{4z} + 1)} \right) (-e^{-2z})^{n-6} (e^z + e^{-z}) \, dz \]

\[ = \int_0^\infty \log \left( 1 + \frac{e^{6z} + 2e^{2z} + 1}{e^{6z} + 2e^{4z} + 1} (-1)^{n-4} e^{-2(n-4)z} \right) (e^z + e^{-z}) \, dz . \]

(36)

Let us treat separately two cases depending on the parity of \( n \).

- If \( n \) is even, then \( n-4 \) is even and equation (36) leads to the following inequality which will be needed for the comparison of \( \text{E}(P_6^n) \) and \( \text{E}(C_n) \):

\[ I_5(n) > J_+(n) = \int_0^\infty \log \left( 1 + 1 + \frac{e^{6z}}{e^{2z} + e^{8z} + 2e^{4z}e^{-2(n-4)z}} \right) (e^z + e^{-z}) \, dz \]

\[ = \int_0^\infty \log \left( 1 + e^{-2(n-3)z} \right) (e^z + e^{-z}) \, dz > 0 . \]

(37)

Using the expression of \( \log(1+x) \) as a power series

\[ \log(1+x) = \sum_{k=1}^\infty \frac{(-1)^{k-1}x^k}{k} \]

we get

\[ J_+(n) = \int_0^\infty \sum_{k=1}^\infty \frac{(-1)^{k-1}e^{-2(n-3)kz}}{k} (e^z + e^{-z}) \, dz \]

\[ = \sum_{k=1}^\infty \frac{(-1)^{k-1}}{k} \int_0^\infty \left( e^{-(2(n-3)k-1)z} + e^{-(2(n-3)k+1)z} \right) \, dz \]

\[ = \sum_{k=1}^\infty \frac{(-1)^{k-1}}{k} \left( \left[ \frac{e^{-(2(n-3)k-1)z}}{-(2(n-3)k-1)} \right]_{z=0}^{z=\infty} + \left[ \frac{e^{-(2(n-3)k+1)z}}{-(2(n-3)k+1)} \right]_{z=0}^{z=\infty} \right) \]

\[ = \sum_{k=1}^\infty \frac{(-1)^{k-1}}{k} \left( \frac{1}{2(n-3)k - 1} + \frac{1}{2(n-3)k + 1} \right) \]

\[ = 4(n-3) \sum_{k=1}^\infty \frac{(-1)^{k-1}}{4(n-3)^2k^2 - 1} = \sum_{k=1}^\infty \frac{(-1)^{k-1}2(n-3)}{k^2 - \frac{1}{(2(n-3))^2}} . \]

(39)
Now, we use Euler’s partial fraction expansion of $\pi \csc(\pi z)$ for $z = \frac{1}{2(n-3)}$

$$\pi \csc \frac{\pi}{2(n-3)} = \frac{1}{2(n-3)} + \sum_{k=1}^{\infty} \frac{(-1)^{k-1}2}{k^2 - \frac{1}{(2(n-3))^2}}$$

(40)

to find

$$I_5(n) > J_+(n) = \pi \csc \frac{\pi}{2(n-3)} - 2(n-3) .$$

(41)

Hence for all even integers $n \geq 6$

$$E(P_n^6) > \frac{4n}{\pi} + \frac{2}{\pi}(I_4 - 12) + 2 \csc \frac{\pi}{2(n-3)} - \frac{2}{\pi}2(n-3)$$

$$= 2 \csc \frac{\pi}{2(n-3)} + \frac{2}{\pi}(I_4 - 6) .$$

(42)

**Remark 1.** Similarly, we can also obtain an upper bound for $I_5(n)$ which helps to see that $I_5(n)$ tends to zero when $n$ tends to infinity.

$$0 < I_5(n) < \int_0^{\infty} \log \left( 1 + \frac{1 + e^{6z} + 2e^{4z}e^{-2(n-4)z}}{1 + e^{6z} + 2e^{4z}} \right) (e^z + e^{-z}) \, dz$$

$$\quad = \int_0^{\infty} \log \left( 1 + e^{-2(n-4)z} \right) (e^z + e^{-z}) \, dz$$

$$\quad = \pi \csc \left( \frac{\pi}{2(n-4)} \right) - 2(n-4) .$$

(43)

- If $n$ is odd, then $n - 4$ is also odd and equation (36) leads to

$$0 > I_5(n) > J_-(n) = \int_0^{\infty} \log \left( 1 - \frac{1 + e^{6z} + 2e^{4z}e^{-2(n-4)z}}{1 + e^{6z} + 2e^{4z}} \right) (e^z + e^{-z}) \, dz$$

$$\quad = \int_0^{\infty} \log \left( 1 - e^{-2(n-4)z} \right) (e^z + e^{-z}) \, dz .$$

(44)

We still can use the power series

$$\log(1 - x) = -\sum_{k=1}^{\infty} \frac{x^k}{k}$$

(45)

to obtain

$$J_-(n) = -\int_0^{\infty} \sum_{k=1}^{\infty} \frac{e^{-2(n-4)kz}}{k} (e^z + e^{-z}) \, dz .$$

(46)
Similar way as in the previous case, using the Euler’s partial fraction expansion of \( \pi z \cot(\pi z) \) instead of that of \( \pi \csc(\pi z) \) leads to

\[
J_-(n) = \pi \cot \left( \frac{\pi}{2(n-4)} \right) - 2(n-4) .
\]  
(47)

Therefore, for this case we have the following lower bound for \( E(P_n^6) \):

\[
E(P_n^6) > \frac{4n}{\pi} + \frac{2}{\pi} (I_4 - 12) + 2 \cot \left( \frac{\pi}{2(n-4)} \right) - \frac{2}{\pi} 2(n-4)
\]
\[
> 2 \cot \left( \frac{\pi}{2(n-4)} \right) + \frac{2}{\pi} (I_4 - 4) .
\]  
(48)

3 Energy of the cyclic graph with vertices \( n \)

Let us denote by \( C_n \) the cyclic graph with \( n \) vertices. The eigenvalues of \( C_n \) can be computed explicitly [8], they are

\[
\lambda_k = 2 \cos \frac{2i\pi k}{n} = e^{\frac{2i\pi k}{n}} + e^{-\frac{2i\pi k}{n}} , \quad k = 0, 1, \cdots, n - 1 .
\]  
(49)

Summing the geometric series one obtains

\[
E(C_n) = \begin{cases} 
4 \cot \left( \frac{\pi}{n} \right) & \text{if } n = 4l , \\
2 \csc \left( \frac{\pi}{2n} \right) & \text{if } n = 4l + 1 \text{ or } n = 4l + 3 , \\
4 \csc \frac{\pi}{n} & \text{if } n = 4l + 2 .
\end{cases}
\]  
(50)

4 Comparison between \( E(P_n^6) \) and \( E(C_n) \)

We are only concerned with \( n \geq 6 \) corresponding to \( \frac{\pi}{n} \in (0, \frac{\pi}{6}] \).

- For \( n = 4l, 2 \leq l \in \mathbb{N} \), the Taylor expansion of \( \cot \) shows that for \( \frac{\pi}{2} > x > 0 \)

\[
\cot(x) < \frac{1}{x} .
\]  
(51)

from equations (32) and (37) we know that \( I_4 > 12 \) and \( I_5(4l) > 0 \), respectively. Hence, it follows that

\[
E(C_{4l}) = 4 \cot \left( \frac{\pi}{4l} \right) < \frac{16l}{\pi} + \frac{2}{\pi} (I_4 - 12 + I_5(4l)) = E(P_n^6) .
\]  
(52)
• For $n = 4l + 2, 1 \leq l \in \mathbb{N}$ inequality (42) and equation (50) lead to

$$E(P_n^6) - E(C_n) > D(n) = 2 \csc \frac{\pi}{2(n-3)} - 4 \csc \frac{\pi}{n} + \frac{2}{\pi}(I_4 - 6).$$  \hspace{1cm} (53)

Computing the particular value of $D(n)$ at $n = 4 \cdot 3 + 2$ using the lower bound for $I_4$ in equation (33) we have

$$D(14) \geq 0.01532.$$  \hspace{1cm} (54)

Let us define a function $f_D : [6, \infty) \to \mathbb{R}$ by

$$f_D(x) = 2 \csc \frac{\pi}{2(x-3)} - 4 \csc \frac{\pi}{x} + \frac{2}{\pi}(I_4 - 6).$$  \hspace{1cm} (55)

Note that for all integers $n \in [6, \infty)$ we have $f_D(n) = D(n)$. Clearly $f_D$ is differentiable in $[6, \infty)$. Aiming to prove that the sequence $(D(n))_{n \in \mathbb{N}}$ is increasing we are going to prove that $f_D$ is an increasing function in $[6, \infty)$. The derivative of $f_D$ at any point $x \in [6, \infty)$ is given by

$$f'_D(x) = \frac{2\pi}{2(x-3)^2} \cos \frac{\pi}{2(x-3)} \csc^2 \frac{\pi}{2(x-3)} - \frac{4\pi}{x^2} \cos \frac{\pi}{x} \csc^2 \frac{\pi}{x} \cos \frac{\pi}{x} \csc^2 \frac{\pi}{x}$$

$$= \frac{4}{\pi} \left( \frac{\pi}{2(x-3)} \right)^2 \cos \frac{\pi}{2(x-3)} \csc^2 \frac{\pi}{2(x-3)} - \frac{4\pi}{x^2} \cos \frac{\pi}{x} \csc^2 \frac{\pi}{x} \cos \frac{\pi}{x} \csc^2 \frac{\pi}{x}$$

$$= \frac{4}{\pi} \left( f \left( \frac{\pi}{2(x-3)} \right) - f \left( \frac{\pi}{x} \right) \right)$$  \hspace{1cm} (56)

where the function $f$ is defined by

$$f(x) = x^2 \cos x \csc^2 x$$  \hspace{1cm} (57)

and for all $x$ the expression of its derivative is

$$f'(x) = \frac{(2x \cos x - x^2 \sin x) \sin^2 x - 2x^2 \cos x \sin x \cos x}{\sin^4 x}$$

$$= \frac{2x \cos x \sin x - x^2 \sin^2 x - 2x^2 \cos^2 x}{\sin^3 x}$$

$$= \frac{x(2 \cos x \sin x - x - x \cos^2 x)}{\sin^3 x}$$

$$\leq \frac{x(2 \cos x - x - x \cos^2 x)}{\sin^3 x}$$

$$= \frac{x^2(1 - \cos x)^2}{\sin^3 x} < 0$$  \hspace{1cm} (58)
meaning that $f$ is a decreasing function on $(0, \frac{\pi}{6}]$. Equation (56) implies that for all $x \in [6, \infty)$ we have $f'(D(x)) > 0$. Therefore, for all $l \geq 3$ we have

$$D(4l + 2) \geq D(14) > 0.$$  \hfill (59)

Finally, this implies that whenever $l \geq 3$ the inequality

$$E(P_{4l+2}^6) > E(C_{4l+2})$$  \hfill (60)

holds.

- For the two cases $6 \leq n = 4l + 1$ or $6 \leq n = 4l + 3$, using the corresponding expression of $E(C_n)$ in (50) and the inequality (48) we obtain

$$E(P_n^6) - E(C_n) > D(n) = 2 \cot \frac{\pi}{2(n - 4)} - 2 \csc \frac{\pi}{2n} + \frac{2}{\pi} (I_4 - 4).$$  \hfill (61)

Exactly as in the previous case, we can associate a continuous function $f_D$ to the sequence $(D(n))_{6 \leq n}$ defined by

$$f_D : [6, \infty) \longrightarrow \mathbb{R}$$

$$x \mapsto 2 \cot \frac{\pi}{2(x - 4)} - 2 \csc \frac{\pi}{2x} + \frac{2}{\pi} (I_4 - 4)$$

which has a derivative at any point $x \in [6, \infty)$ given by

$$f'_D(x) = 2 - \frac{2(x - 4)^2}{\sin^2 \frac{\pi}{2(x - 4)}} - 2 \frac{2x^2 \cos \frac{\pi}{2x}}{\sin^2 \frac{\pi}{2x}}$$

$$> 4 \left( \frac{2(x - 4)}{\sin \frac{\pi}{2(x - 4)}} \right)^2 - 4 \left( \frac{\pi}{\sin \frac{\pi}{2x}} \right)^2. \hfill (62)$$

Since the function $g(x) = x / \sin x$ is positive and increasing and $2(x - 4) < 2x$ inequality (62) gives $f'_D(x) > 0$. Therefore $f_D$, and consequently the sequence $(D(n))_{6 \leq n}$, is increasing. This implies that for all integers $l \geq 4$ we have

$$D(4l + 3) \geq D(4l + 1) \geq D(17) \approx 0.0066 > 0.$$  \hfill (63)

It follows that for all integers $l \geq 4$ we have

$$E(P_{4l+1}^6) > E(C_{4l+1})$$  \hfill (64)

and

$$E(P_{4l+3}^6) > E(C_{4l+3}).$$  \hfill (65)
Remark 2. From equation (43) for even \( n \) and equation (47) for odd \( n \), it follows that
\[
\lim_{n \to +\infty} I_5(n) = 0, \tag{66}
\]
and therefore in view of equations (24) and (50) we deduce that
\[
\lim_{n \to +\infty} E(P_n^6) - E(C_n) = \frac{2}{\pi}(I_4 - 12) > 0. \tag{67}
\]

In summary, the results (52), (60), (64), (65) and Theorem 1 lead clearly to the following theorem

**Theorem 2.** Among all connected unicyclic bipartite graphs on \( n \geq 6 \) vertices the graph \( P_n^6 \) has maximal energy except for \( n = 10 \).

We believe that a similar method can be used to improve the result in [9] aiming to prove claims in [10] on the \( n \)-vertex unicyclic bipartite graph with second or third maximal energy.

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**References**


