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Unicyclic Bipartite Graphs with Maximum Energy

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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_n^6 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 $\mathrm{E}(P_n^6) > \mathrm{E}(C_n)$. 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_n^6 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

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

is called energy of G. Within the framework of the Hückel molecular orbital [1] approximation, the calculation of the total π-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

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

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

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

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]

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

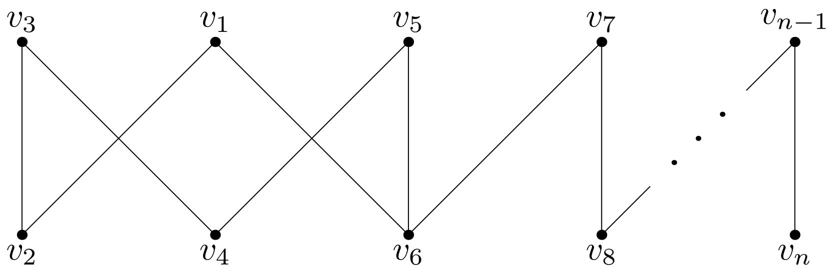

Figure 1: P_n^6, emphasizing that it is bipartite

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

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

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 $n \geq 6$:

$$\begin{aligned}
(x/i)^n \phi_n(P_n^6, i/x) &= (x/i)^n \sum_{k \geq 0} (-1)^k b_k(P_n^6)(i/x)^{n-2k} \\
&= \sum_{k \geq 0} (-1)^k b_k(P_n^6) i^{-n} i^{n-2k} x^n x^{-n+2k} \\
&= \sum_{k \geq 0} b_k(P_n^6) x^{2k} \\
&= Q_n(x) \ .
\end{aligned} \tag{7}$$

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

$$A(P_n^6) = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 1 & 0 & \ldots & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & \ldots & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & \ldots & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & \ldots & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 1 & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & \ddots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0
\end{bmatrix} . \tag{8}$$

Therefore the characteristic polynomial of P_n^6 is

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

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

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

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

and consequently, using equation (7), we obtain

$$\begin{aligned} Q_6(x) &= (x/i)^6((i/x)^6 - 6(i/x)^4 + 9(i/x)^2 - 4) \\ &= 1 + 6x^2 + 9x^4 + 4x^6 \end{aligned} \tag{12}$$

$$\begin{aligned} Q_7(x) &= (x/i)^7((i/x)^7 - 7(i/x)^5 + 13(i/x)^3 - 7(i/x)) \\ &= 1 + 7x^2 + 13x^4 + 7x^6\ . \end{aligned} \tag{13}$$

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

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

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

$$\begin{aligned} Q_n(x) &= (x/i)^n\phi_n(i/x) \\ &= (x/i)^n\frac{i}{x}\phi_{n-1}(i/x) - (x/i)^n\phi_{n-2}(i/x) \\ &= (x/i)^{n-1}\phi_{n-1}(i/x) + x^2(x/i)^{n-2}\phi_{n-2}(i/x) \\ &= Q_{n-1}(x) + x^2Q_{n-2}(x)\ . \end{aligned} \tag{15}$$

This linear recurrence relation has characteristic equation

$$X^2 - X - x^2 = 0 \tag{16}$$

which has two roots

$$D_1(x) = \frac{1+\sqrt{1+4x^2}}{2} \tag{17}$$

and

$$D_2(x) = \frac{1-\sqrt{1+4x^2}}{2}\ . \tag{18}$$

Therefore, the explicit expression for $Q_n(x)$ must be of the form

$$Q_n(x) = C_1(x)D_1^n(x) + C_2(x)D_2^n(x) \tag{19}$$

where $C_1(x)$ and $C_2(x)$ satisfy the system of equations

$$\begin{cases} C_1(x)D_1^6(x) + C_2(x)D_2^6(x) = Q_6(x) = 1 + 6x^2 + 9x^4 + 4x^6 \\ \\ C_1(x)D_1^7(x) + C_2(x)D_2^7(x) = Q_7(x) = 1 + 7x^2 + 13x^4 + 7x^6\ . \end{cases} \tag{20}$$

Solving the system of equations we obtain

$$C_2(x) = \frac{(x^2+1)((4x^4+5x^2+1)\sqrt{1+4x^2} - 1 - 7x^2 - 10x^4)}{2D_2^6(x)\sqrt{1+4x^2}}\ , \tag{21}$$

$$C_1(x) = \frac{(x^2+1)((4x^4+5x^2+1)\sqrt{1+4x^2} + 1 + 7x^2 + 10x^4)}{2D_1^6(x)\sqrt{1+4x^2}} \tag{22}$$

and therefore

$$\begin{aligned} Q_n(x) = {} & \frac{(x^2+1)((4x^4+5x^2+1)\sqrt{1+4x^2} + 10x^4 + 7x^2 + 1)}{2\sqrt{1+4x^2}} \left(\frac{1+\sqrt{1+4x^2}}{2}\right)^{n-6} \\ & + \frac{(x^2+1)((4x^4+5x^2+1)\sqrt{1+4x^2} - 10x^4 - 7x^2 - 1)}{2\sqrt{1+4x^2}} \left(\frac{1-\sqrt{1+4x^2}}{2}\right)^{n-6} \\ = {} & \frac{(x^2+1)((4x^4+5x^2+1)\sqrt{1+4x^2} + 10x^4 + 7x^2 + 1)}{2\sqrt{1+4x^2}} \left(\frac{1+\sqrt{1+4x^2}}{2}\right)^{n-6} \\ & \left(1 + \frac{(4x^4+5x^2+1)\sqrt{1+4x^2} - 10x^4 - 7x^2 - 1}{(4x^4+5x^2+1)\sqrt{1+4x^2} + 10x^4 + 7x^2 + 1} \left(\frac{1-\sqrt{1+4x^2}}{1+\sqrt{1+4x^2}}\right)^{n-6}\right)\ . \end{aligned} \tag{23}$$

With this expression of $Q_n(x)$, equation (6) leads to

$$\mathrm{E}(P_n^6) = \frac{2}{\pi}((n-6)I_1 + I_2 + I_4 - I_3 + I_5(n)) \tag{24}$$

where $I_1, I_2, I_3, I_4, I_5(n)$ are described as follows:

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

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

$$I_3 = \int_0^{+\infty} \frac{\log(\sqrt{4x^2+1})}{x^2} dx = \pi\ . \tag{27}$$

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,

$$I_4 = \int_0^{+\infty} \frac{\log((4x^4+5x^2+1)\sqrt{1+4x^2}+10x^4+7x^2+1)-\log(2)}{x^2} dx$$

$$= -\int_0^{+\infty} (\log((4x^4+5x^2+1)\sqrt{1+4x^2}+10x^4+7x^2+1)-\log(2))\, d\left(\frac{1}{x}\right) x$$

$$= -\left[\frac{\log((4x^4+5x^2+1)\sqrt{1+4x^2}+10x^4+7x^2+1)-\log(2)}{x}\right]_{x\to 0}^{x\to+\infty}$$

$$+ \int_0^{+\infty} \frac{80x^5+76x^3+14x+(40x^3+14x)\sqrt{1+4x^2}}{16x^7+24x^5+9x^3+x+(10x^5+7x^3+x)\sqrt{1+4x^2}} dx$$

$$= \int_0^{+\infty} \frac{80x^4+76x^2+14+(40x^2+14)\sqrt{1+4x^2}}{16x^6+24x^4+9x^2+1+(10x^4+7x^2+1)\sqrt{1+4x^2}} dx$$

$$= \int_0^{+\infty} \frac{2(4x^2+1)(10x^2+7)+(40x^2+14)\sqrt{1+4x^2}}{(x^2+1)(4x^2+1)^2+(10x^4+7x^2+1)\sqrt{1+4x^2}} dx$$

$$= \int_0^{+\infty} \frac{(20x^2+14)\sqrt{1+4x^2}+40x^2+14}{(x^2+1)(4x^2+1)\sqrt{1+4x^2}+10x^4+7x^2+1} dx\ . \tag{28}$$

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

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

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

$$= 4 + 4\int_0^1 \frac{3y^4+2y^3+10y^2+2y+3}{y^6+y^5+7y^4-2y^3+7y^2+y+1}\,dy\ . \tag{29}$$

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

$$\frac{3y^4+2y^3+10y^2+2y+3}{y^6+y^5+7y^4-2y^3+7y^2+y+1} - \frac{15y^2-50y+60}{20}$$

$$= \frac{(y-y^2)f(y)}{4y^6+4y^5+28y^4-8y^3+28y^2+4y+4} \tag{30}$$

where

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

$$= 6(-y^2+3y-1)^2 + 2(y^2-y)^2 + 3y^6 - 4y^5 + 11y^4 - 5y^3 + 5y > 0\ . \tag{31}$$

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

$$I_4 > 4 + 4\int_0^1 \frac{15y^2-50y+60}{20}\,dy = 12\ . \tag{32}$$

By numerical integration we get a better estimate for I_4:

$$I_4 > 12.1855\ . \tag{33}$$

And finally the last term is given by

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

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

$$dx = -\frac{e^z+e^{-z}}{(e^z-e^{-z})^2}dz, \qquad \sqrt{1+4x^2} = \frac{e^z+e^{-z}}{e^z-e^{-z}}\,, \tag{35}$$

and

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

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

$$= \int_0^\infty \log\left(1 + \frac{e^{6z} + 2e^{2z} + 1}{e^{6z} + 2e^{4z} + 1}(-1)^{n-4}e^{-2(n-4)z}\right)(e^z + e^{-z})\,dz\ . \tag{36}$$

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 $\mathrm{E}(P_n^6)$ and $\mathrm{E}(C_n)$:

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

$$= \int_0^\infty \log\left(1 + e^{-2(n-3)z}\right)(e^z + e^{-z})\,dz > 0\ . \tag{37}$$

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

$$\log(1+x) = \sum_{k=1}^\infty \frac{(-1)^{k-1}x^k}{k} \tag{38}$$

we get

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

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

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

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

$$= 4(n-3)\sum_{k=1}^\infty \frac{(-1)^{k-1}}{4(n-3)^2k^2 - 1} = \sum_{k=1}^\infty \frac{(-1)^{k-1}2\dfrac{1}{2(n-3)}}{k^2 - \dfrac{1}{(2(n-3))^2}}\ . \tag{39}$$

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

$$\pi\csc\frac{\pi}{2(n-3)}=\frac{1}{\frac{1}{2(n-3)}}+\sum_{k=1}^{\infty}\frac{(-1)^{k-1}2\frac{1}{2(n-3)}}{k^2-\frac{1}{(2(n-3))^2}} \tag{40}$$

to find

$$I_5(n)>J_+(n)=\pi\csc\frac{\pi}{2(n-3)}-2(n-3)\ . \tag{41}$$

Hence for all even integers $n\geq 6$

$$\begin{aligned}\mathrm{E}(P_n^6)&>\frac{4n}{\pi}+\frac{2}{\pi}(I_4-12)+2\csc\frac{\pi}{2(n-3)}-\frac{2}{\pi}2(n-3)\\&=2\csc\frac{\pi}{2(n-3)}+\frac{2}{\pi}(I_4-6)\ .\end{aligned} \tag{42}$$

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.*

$$\begin{aligned}0<I_5(n)&<\int_0^\infty\log\left(1+\frac{1+e^{6z}+2e^{4z}}{1+e^{6z}+2e^{4z}}e^{-2(n-4)z}\right)(e^z+e^{-z})\,dz\\&=\int_0^\infty\log\left(1+e^{-2(n-4)z}\right)(e^z+e^{-z})\,dz\\&=\pi\csc\left(\frac{\pi}{2(n-4)}\right)-2(n-4)\ .\end{aligned} \tag{43}$$

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

$$\begin{aligned}0>I_5(n)>J_-(n)&=\int_0^\infty\log\left(1-\frac{1+e^{6z}+2e^{4z}}{1+e^{6z}+2e^{4z}}e^{-2(n-4)z}\right)(e^z+e^{-z})\,dz\\&=\int_0^\infty\log\left(1-e^{-2(n-4)z}\right)(e^z+e^{-z})\,dz\ .\end{aligned} \tag{44}$$

We still can use the power series

$$\log(1-x)=-\sum_{k=1}^{\infty}\frac{x^k}{k} \tag{45}$$

to obtain

$$J_-(n)=-\int_0^\infty\sum_{k=1}^{\infty}\frac{e^{-2(n-4)kz}}{k}(e^z+e^{-z})\,dz\ . \tag{46}$$

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

$$J_-(n) = \pi \cot \frac{\pi}{2(n-4)} - 2(n-4) \ . \tag{47}$$

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

$$\begin{aligned} \mathrm{E}(P_n^6) &> \frac{4n}{\pi} + \frac{2}{\pi}(I_4 - 12) + 2\cot\frac{\pi}{2(n-4)} - \frac{2}{\pi}2(n-4) \\ &> 2\cot\frac{\pi}{2(n-4)} + \frac{2}{\pi}(I_4 - 4) \ . \end{aligned} \tag{48}$$

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

$$\begin{aligned} \lambda_k &= 2\cos\frac{2i\pi k}{n} \\ &= e^{\frac{2i\pi k}{n}} + e^{-\frac{2i\pi k}{n}}, \ k = 0, 1, \cdots, n-1 \ . \end{aligned} \tag{49}$$

Summing the geometric series one obtains

$$\mathrm{E}(C_n) = \begin{cases} 4\cot\frac{\pi}{n} \text{ if } n = 4l\,, \\ 2\csc\frac{\pi}{2n} \text{ if } n = 4l+1 \text{ or } n = 4l+3\,, \\ 4\csc\frac{\pi}{n} \text{ if } n = 4l+2\ . \end{cases} \tag{50}$$

4 Comparison between $\mathrm{E}(P_n^6)$ and $\mathrm{E}(C_n)$

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 $\frac{\pi}{2} > x > 0$

  $$\cot(x) < \frac{1}{x}\,, \tag{51}$$

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

  $$\mathrm{E}(C_{4l}) = 4\cot\frac{\pi}{4l} < \frac{16l}{\pi} + \frac{2}{\pi}(I_4 - 12 + I_5(4l)) = \mathrm{E}(P_{4l}^6) \ . \tag{52}$$

- For $n = 4l + 2, 1 \leq l \in \mathbb{N}$ inequality (42) and equation (50) lead to

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

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

$$D(14) \geq 0.01532\ . \tag{54}$$

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

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

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 $(D(n))_{6 \leq n}$ 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

$$\begin{aligned} f_D'(x) &= \frac{2\pi}{2(x-3)^2}\cos\frac{\pi}{2(x-3)}\csc^2\frac{\pi}{2(x-3)} - \frac{4\pi}{x^2}\cos\frac{\pi}{x}\csc^2\frac{\pi}{x} \\ &= \frac{4}{\pi}\left(\frac{\pi}{2(x-3)}\right)^2\cos\frac{\pi}{2(x-3)}\csc^2\frac{\pi}{2(x-3)} - \frac{4}{\pi}\left(\frac{\pi}{x}\right)^2\cos\frac{\pi}{x}\csc^2\frac{\pi}{x} \\ &= \frac{4}{\pi}\left(f\left(\frac{\pi}{2(x-3)}\right) - f\left(\frac{\pi}{x}\right)\right) \end{aligned} \tag{56}$$

where the function f is defined by

$$f(x) = x^2 \cos x \csc^2 x \tag{57}$$

and for all x the expression of its derivative is

$$\begin{aligned} f'(x) &= \frac{(2x\cos x - x^2\sin x)\sin^2 x - 2x^2\cos x\sin x\cos x}{\sin^4 x} \\ &= \frac{2x\cos x\sin x - x^2\sin^2 x - 2x^2\cos^2 x}{\sin^3 x} \\ &= \frac{x(2\cos x\sin x - x - x\cos^2 x)}{\sin^3 x} \\ &\leq \frac{x(2x\cos x - x - x\cos^2 x)}{\sin^3 x} \\ &= -\frac{x^2(1-\cos x)^2}{\sin^3 x} < 0 \end{aligned} \tag{58}$$

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

$$D(4l+2) \geq D(14) > 0 \ . \tag{59}$$

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

$$\mathrm{E}(P^6_{4l+2}) > \mathrm{E}(C_{4l+2}) \tag{60}$$

holds.

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

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

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

$$\begin{aligned} f_D : [6, \infty) &\longrightarrow \mathbb{R} \\ x &\longmapsto 2\cot\frac{\pi}{2(x-4)} - 2\csc\frac{\pi}{2x} + \frac{2}{\pi}(I_4 - 4) \end{aligned}$$

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

$$\begin{aligned} f'_D(x) &= 2\frac{\dfrac{\pi}{2(x-4)^2}}{\sin^2\dfrac{\pi}{2(x-4)}} - 2\frac{\dfrac{\pi}{2x^2}\cos\dfrac{\pi}{2x}}{\sin^2\dfrac{\pi}{2x}} \\ &> \frac{4}{\pi}\left(\frac{\dfrac{\pi}{2(x-4)}}{\sin\dfrac{\pi}{2(x-4)}}\right)^2 - \frac{4}{\pi}\left(\frac{\dfrac{\pi}{2x}}{\sin\dfrac{\pi}{2x}}\right)^2 \ . \end{aligned} \tag{62}$$

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

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

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

$$\mathrm{E}(P^6_{4l+1}) > \mathrm{E}(C_{4l+1}) \tag{64}$$

and

$$\mathrm{E}(P^6_{4l+3}) > \mathrm{E}(C_{4l+3}) \ . \tag{65}$$

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*

$$\lim_{n\to+\infty} \mathrm{E}(P_n^6) - \mathrm{E}(C_n) = \frac{2}{\pi}(I_4 - 12) > 0\ . \tag{67}$$

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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