Unicyclic graphs with large energy

Eric Ould Dadah Andriantiana [1] and Stephan Wagner [2]

Department of Mathematical Sciences
Mathematics Division
Stellenbosch University
Private Bag X1, Matieland 7602
South Africa

Abstract

We study the energy (i.e., the sum of the absolute values of all eigenvalues) of so-called tadpole graphs, which are obtained by joining a vertex of a cycle to one of the ends of a path. By means of the Coulson integral formula and careful estimation of the resulting integrals, we prove two conjectures on the largest and second-largest energy of a unicyclic graph due to Caporossi, Cvetković, Gutman and Hansen and Gutman, Furtula and Hua respectively. Moreover, we characterise the non-bipartite unicyclic graphs whose energy is largest.

Key words: Maximum Energy, unicyclic graphs, Coulson formula
2010 MSC: 05C35, 05C50, 92E10

1 Introduction

The energy $\mathrm{E}(G)$ of a graph G, defined as the sum of the absolute values of its eigenvalues, certainly belongs to the most popular graph invariants in chemical graph theory. It originates from the pi-electron energy in the Hückel molecular orbital model [6–8], but has also gained purely mathematical interest on its own right. Maximum and minimum values of the energy are known for various classes of graphs, and in some cases also the second-largest/second-smallest

Email address: `ericoda@sun.ac.za,swagner@sun.ac.za` (Stephan Wagner).
[1] Supported by the German Academic Exchange Service (DAAD), in association with the African Institute for Mathematical Sciences (AIMS). Code No.: A/11/07858.
[2] This material is based upon work supported by the National Research Foundation of South Africa under grant number 70560.

and further values as well as the corresponding extremal graphs; see the review [10], the recent papers [2,12,13,16,19–26], and the references cited therein.

One of the graph classes that has been quite thoroughly studied is the class of all unicyclic graphs, i.e., connected graphs with only one unique cycle. The study of these graphs is motivated by the chemical background as well as the fact that unicyclic graphs are very similar to trees, so that many of the techniques that apply to trees can still be used.

Among all unicyclic graphs with a given number $n \geq 6$ of vertices, the minimum energy is attained for the graph that results from connecting two leaves of a star by an edge; the second-smallest, third-smallest, ..., sixth-smallest values and the corresponding graphs are also all known [4,13,20,22]. On the other hand, the converse question for the largest possible energy of a unicyclic graph appears to be somewhat more intricate. In answering this question, the so-called tadpole graphs P_n^k, which are obtained by merging an end of a path of length $n-k$ with a cycle of length k, play an essential role. The following was originally found by means of an extensive computer search:

Conjecture 1 ([3,11]). *Among the set U_n of all unicyclic graphs of order $n \geq 7$, 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 (see Figure 1).*

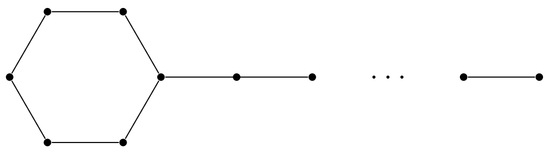

Fig. 1. The graph P_n^6

Substantial progress on this conjecture was already made shortly afterwards in a paper of Hou, Gutman and Woo [14], who proved the following:

Theorem 2 ([14]). *Let $G(n,k)$ be the set of all unicyclic graphs of order n and girth k, and let $C(n,k)$ be the set of all unicyclic graphs obtained from a cycle C_k of length k by adding $n-k$ pendant vertices to it. Suppose that $G \in G(n,k)$, $n \geq k$. If G has maximum energy in $G(n,k)$, then G is either P_n^k or, when $k \equiv 0 \mod 4$, a graph from $C(n,k)$.*

By virtue of this theorem, the authors of [14] were also able to prove the following for the slightly narrower class of unicyclic bipartite graphs:

Theorem 3 ([14]). *P_n^6 has the largest energy among all unicyclic bipartite n-vertex graphs, except possibly the cycle C_n.*

The fact that P_n^6 "wins" over C_n for almost all n was proved only very recently in two independent papers:

Theorem 4 ([1,18]). *For all $n \geq 7$, $n \neq 9, 10, 11, 13, 15$, we have* $\mathrm{E}(C_n) < \mathrm{E}(P_n^6)$.

The more general Conjecture 1 was settled very recently by Huo, Li and Shi in [17]. The aim of the present paper is to provide an alternative approach to this problem; while the proof given in [17] is simpler in some respects, the main benefit of our method is that it gives more precise information on the actual value of the maximum energy of an n-vertex unicyclic graph and the gap between P_n^6 and other graphs of the form P_n^k (it turns out that, for fixed k, the difference of the energies converges to a constant as $n \to \infty$). We are also able to prove additional results by means of our method:

Theorem 5. *Let D_n be the graph obtained by joining a vertex of the cycle C_6 and the third vertex in P_{n-6} by an edge (see Figure 2). For $n \geq 28$, D_n is the unicyclic graph with second-largest energy.*

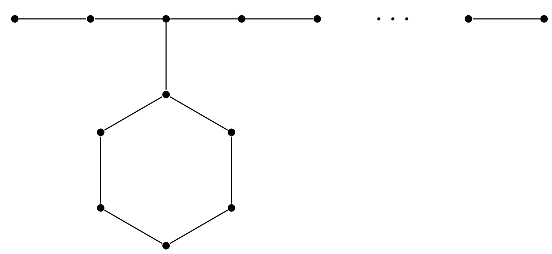

Fig. 2. The graph D_n

This was conjectured in [9] for bipartite unicyclic graphs, but it still holds in the non-bipartite case. In order to prove this theorem, we can make use of the following result:

Theorem 6 ([15]). *Let $G \in U_n \setminus \{P_n^k | k = 3, 4, \ldots, n\}$ be a bipartite unicyclic graph. For $n \geq 13$, if $G \neq D_n$, we have* $\mathrm{E}(G) < \mathrm{E}(D_n)$.

This shows that it is sufficient to compare D_n to all tadpole graphs P_n^k once Conjecture 1 has been verified. In the following section, we gather some auxiliary tools. We then proceed to determine a relatively simple integral representation for $\mathrm{E}(P_n^k)$, which is used to study the behaviour of P_n^k as k varies. This leaves us with only a few cases that are studied in more detail to prove Conjecture 1 as well as Theorem 5. Another result that we obtain as a consequence of our estimates is the following:

Theorem 7. *Among all non-bipartite unicyclic graphs in U_n ($n \geq 3$), P_n^3 has maximum energy if n is even, and C_n has maximum energy if n is odd.*

2 Preliminaries

As most other results on the energy of graphs, our proof is based on the Coulson integral

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

where $a_1, a_2, \ldots, a_n$ are the coefficients of the characteristic polynomial

$$\phi(G,x) = \sum_{k=0}^{n} a_k x^{n-k}$$

of G. For unicyclic graphs, it is known that the coefficients $b_{2j} = (-1)^j a_{2j}$ and $b_{2j+1} = (-1)^j a_{2j+1}$ are all positive, and so the integral is an increasing function of each of these coefficients. This property is frequently exploited to compare the energies of different graphs. For our purposes, however, it is more convenient to work directly with the characteristic polynomial: the above integral can also be written in any of the following forms:

$$\begin{aligned}
\mathrm{E}(G) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{dx}{x^2}\log\left(x^{2n}\phi(G,i/x)\phi(G,-i/x)\right)\\
&= \frac{1}{\pi}\int_{0}^{+\infty}\frac{dx}{x^2}\log\left(x^{2n}\phi(G,i/x)\phi(G,-i/x)\right)\\
&= \frac{1}{\pi}\int_{0}^{+\infty}\frac{dx}{x^2}\log\left(x^{2n}\phi(G,i/x)\overline{\phi(G,i/x)}\right)\\
&= \frac{2}{\pi}\int_{0}^{+\infty}\frac{dx}{x^2}\log\left(x^{n}|\phi(G,i/x)|\right).
\end{aligned}$$

Since

$$\frac{d}{du}\frac{1}{\sinh u} = -\frac{\cosh u}{\sinh^2 u},$$

the change of variable

$$x = \frac{1}{2\sinh u}$$

leads us to

$$\begin{aligned}
\mathrm{E}(G) &= \frac{2}{\pi}\int_{0}^{+\infty} du\frac{\cosh u}{2\sinh^2 u}(4\sinh^2 u)\log\left(\frac{1}{2^n\sinh^n u}|\phi(G,2i\sinh u)|\right)\\
&= \frac{4}{\pi}\int_{0}^{+\infty}\log\left(\frac{|\phi(G,2i\sinh u)|}{2^n\sinh^n u}\right)\cosh u\,du, \qquad (1)
\end{aligned}$$

which is the expression for the energy that we will mostly work with. In order to determine the characteristic polynomials of the graphs we are interested in, we also need the following properties:

Lemma 8 ([5]). *Let uv be an edge of a graph 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, then

$$\phi(G,x) = x\phi(G-uv,x) - \phi(G-u-v,x).$$

It is convenient to set $\phi(\varnothing,x)=1$.

3 The energy of the tadpole graph P_n^k

3.1 A formula for $\mathrm{E}(P_n^k)$

In order to determine $\mathrm{E}(P_n^k)$ using (1), we need an explicit expression for $\phi(P_n^k, 2i\sinh u)$. Using Lemma 8 we obtain

$$\begin{aligned}\phi(P_k,x) &= x\phi(P_{k-1},x) - \phi(P_{k-2},x), \\ \phi(C_k,x) &= x\phi(P_k,x) - \phi(P_{k-2},x) - 2, \\ \phi(P_n^{n-1},x) &= x\phi(C_{n-1},x) - \phi(P_{n-2},x)\end{aligned} \tag{2}$$

and

$$\phi(P_n^k,x) = x\phi(P_{n-1}^k,x) - \phi(P_{n-2}^k,x). \tag{3}$$

Note that

$$\phi(P_n^n,x) = \phi(C_n,x).$$

The characteristic equation

$$q^2 - xq + 1 = q^2 - 2iq\sinh u + 1 = 0 \tag{4}$$

of the linear recurrence (2) (taking $x = 2i\sinh u$) has the two roots

$$q_1 = \frac{x+\sqrt{x^2-4}}{2} = ie^u \tag{5}$$

and

$$q_2 = \frac{x-\sqrt{x^2-4}}{2} = (ie^u)^{-1}. \tag{6}$$

Together with the initial values $\phi(P_0, 2i\sinh u) = 1$ and $\phi(P_1, 2i\sinh u) = 2i\sinh u$ we get, after some calculations,

$$\phi(P_k, 2i\sinh u) = \frac{e^{2u}}{1+e^{2u}}(ie^u)^k + \frac{1}{1+e^{2u}}(ie^u)^{-k}.$$

Hence

$$\begin{aligned}\phi(C_k, 2i\sinh u) &= \frac{e^{2u}}{1+e^{2u}}((ie^u)^k - (ie^u)^{k-2}) + \frac{1}{1+e^{2u}}((ie^u)^{-k} - (ie^u)^{-k+2}) - 2\\ &= (ie^u)^k + (ie^u)^{-k} - 2\\ &= (ie^u)^k + (-ie^{-u})^k - 2,\end{aligned}$$

and

$$\begin{aligned}&\phi(P_k^{k-1}, 2i\sinh u)\\ &= i(e^u - e^{-u})((ie^u)^{k-1} + (-ie^{-u})^{k-1} - 2) - \frac{e^{2u}}{1+e^{2u}}(ie^u)^{k-2} - \frac{1}{1+e^{2u}}(ie^u)^{-k+2}\\ &= \frac{e^{2u}+1-e^{-2u}}{1+e^{2u}}(ie^u)^k - \frac{e^{4u}-e^{2u}-1}{1+e^{2u}}(-ie^{-u})^k - 2i(e^u - e^{-u}).\end{aligned}$$

The characteristic polynomial of the linear recurrence relation (3) is the same as (4), and consequently has the two roots given in (5) and (6). Hence, the explicit expression of $\phi(P_n^k, 2i\sinh u)$ is of the form

$$\phi(P_n^k, 2i\sinh u) = A(ie^u)^n + B(ie^u)^{-n},$$

where A and B are such that

$$\begin{cases} A(ie^u)^k + B(ie^u)^{-k} = \phi(P_k^k, 2i\sinh u) = (ie^u)^k + (ie^u)^{-k} - 2,\\ A(ie^u)^{k+1} + B(ie^u)^{-k-1} = \phi(P_{k+1}^k, 2i\sinh u)\\ \qquad = \frac{e^{2u}+1-e^{-2u}}{1+e^{2u}}(ie^u)^{k+1} - \frac{e^{4u}-e^{2u}-1}{1+e^{2u}}(-ie^{-u})^{k+1} - 2i(e^u - e^{-u}).\end{cases}$$

Solving the system of equations we get

$$A = \frac{e^{2u}(e^{2u}+2)}{(1+e^{2u})^2} + \frac{2(ie^u)^{2-k}}{1+e^{2u}} + \frac{(ie^u)^{2(2-k)}}{(1+e^{2u})^2}$$

and

$$B = \frac{(ie^u)^{2k}}{(1+e^{2u})^2} - \frac{2(ie^u)^k}{1+e^{2u}} + \frac{2e^{2u}+1}{(1+e^{2u})^2}.$$

Therefore we obtain

$$\begin{aligned}\phi(P_n^k, 2i\sinh u) &= \left(\frac{e^{2u}(e^{2u}+2)}{(1+e^{2u})^2} + \frac{2(ie^u)^{2-k}}{1+e^{2u}} + \frac{(ie^u)^{2(2-k)}}{(1+e^{2u})^2}\right)(ie^u)^n\\ &\quad + \left(\frac{(ie^u)^{2k}}{(1+e^{2u})^2} - \frac{2(ie^u)^k}{1+e^{2u}} + \frac{2e^{2u}+1}{(1+e^{2u})^2}\right)(ie^u)^{-n}\end{aligned}$$

which implies

$$\begin{aligned}|\phi(P_n^k, 2i\sinh u)| = e^{nu}\Bigg| &\frac{e^{2u}(e^{2u}+2)}{(1+e^{2u})^2} + \frac{2(ie^u)^{2-k}}{1+e^{2u}} + \frac{(ie^u)^{2(2-k)}}{(1+e^{2u})^2} + \frac{(ie^u)^{2k-2n}}{(1+e^{2u})^2}\\ &- \frac{2(ie^u)^{k-2n}}{1+e^{2u}} + \frac{(2e^{2u}+1)(ie^u)^{-2n}}{(1+e^{2u})^2}\Bigg|.\end{aligned}$$

Since

$$\begin{aligned}
&\int_0^{+\infty} \log\left(\frac{e^{nu}}{(2\sinh u)^n}\right)\cosh u\,du \\
&\qquad\qquad = -n\int_0^{+\infty} \log(1-e^{-2u})d(\sinh u) \\
&\qquad\qquad = -n\left(\Big[\log(1-e^{-2u})\sinh u\Big]_0^{+\infty} - \int_0^{+\infty}(\sinh u)d(\log(1-e^{-2u}))\right) \\
&\qquad\qquad = n\int_0^{+\infty} e^{-u}du = n,
\end{aligned}$$

we end up with

$$\mathrm{E}(P_n^k) = \frac{4n}{\pi} + \frac{4}{\pi}\int_0^{+\infty} \log(Q_n^k(u))\cosh u\ \ du, \tag{7}$$

where

$$\begin{aligned}
Q_n^k(u) &= \Bigg|\frac{e^{2u}(e^{2u}+2)}{(1+e^{2u})^2} + \frac{2(ie^u)^{2-k}}{1+e^{2u}} + \frac{(ie^u)^{2(2-k)}}{(1+e^{2u})^2} + \frac{(ie^u)^{2k-2n}}{(1+e^{2u})^2} \\
&\qquad\qquad\qquad - \frac{2(ie^u)^{k-2n}}{1+e^{2u}} + \frac{(2e^{2u}+1)(ie^u)^{-2n}}{(1+e^{2u})^2}\Bigg| \\
&= \Bigg|\frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - 2e^{2u}\frac{(ie^u)^{-k}-(ie^u)^{k-2(n+1)}}{e^{2u}+1} \\
&\qquad\qquad + \frac{(ie^u)^{-2k+4}+(ie^u)^{2k-2n}}{(e^{2u}+1)^2} + \frac{2e^{2u}+1}{(e^{2u}+1)^2}(ie^u)^{-2n}\Bigg|.
\end{aligned} \tag{8}$$

If we fix k and let $n \to \infty$, we obtain the following result:

Proposition 9. *For any fixed $k \geq 3$, we have*

$$\begin{aligned}
&\lim_{n\to\infty}\left(\mathrm{E}(P_n^k) - \frac{4n}{\pi}\right) = C(k) \\
&\qquad := \frac{4}{\pi}\int_0^{+\infty}\log\left|\frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - 2e^{2u}\frac{(ie^u)^{-k}}{e^{2u}+1} + \frac{(-e^{2u})^{2-k}}{(e^{2u}+1)^2}\right|\cosh u\ \ du.
\end{aligned}$$

An analogous result holds if we fix $\ell = n-k$:

Proposition 10. *For any fixed $\ell \geq 0$, we have*

$$\begin{aligned}
&\lim_{n\to\infty}\left(\mathrm{E}(P_n^{n-\ell}) - \frac{4n}{\pi}\right) = D(\ell) \\
&\qquad\qquad := \frac{4}{\pi}\int_0^{+\infty}\log\left|\frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} + \frac{(-e^{2u})^{-\ell}}{(e^{2u}+1)^2}\right|\cosh u\ \ du.
\end{aligned}$$

Finally, we can let k and $n-k$ tend to ∞ simultaneously:

Proposition 11. *If both k and $n-k$ go to infinity, then*

$$\begin{aligned}\mathrm{E}(P_n^k) - \frac{4n}{\pi} &\to \frac{4}{\pi}\int_0^{+\infty} \cosh u \log \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2}\, du \\ &= \frac{6\sqrt{2}}{\pi}\arctan\sqrt{2} + \frac{4}{\pi} - 4 \approx -0.146499.\end{aligned}$$

For example, $C(3) \approx -0.037$, $C(4) \approx -0.866$, $C(5) \approx -0.084$, $C(6) \approx 0.118$, $D(0) = 0$, $D(1) \approx -0.246$, $D(2) \approx -0.087$, $D(3) \approx -0.200$. Figure 3 shows plots of more values of $C(k)$ and $D(l)$.

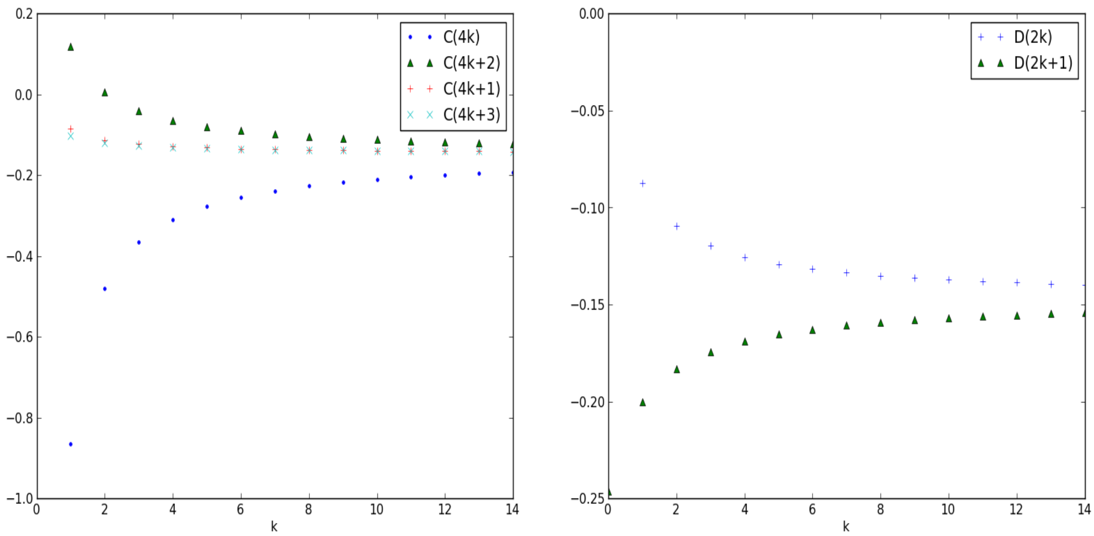

Fig. 3. Plot of the functions $C(k)$ and $D(l)$

In the following, it will be convenient to use the following abbreviation:

$$f_{a,n,r}(j) = a^j + (-1)^r a^{n-j}.$$

Let us note some basic properties of this function:

Lemma 12. *For all non-negative integers n, r and $a \in (0,1)$, the function $f_{a,n,r}(j)$ is positive and decreasing on $[0, n/2)$.*

Proof. For all $j \in [0, n/2)$ we know that $j < n - j$, and since $a \in (0,1)$ it is clear that $a^j > |(-1)^r a^{n-j}|$, therefore $f_{a,n,r}(j) > 0$ for all $j \in [0, n/2)$.

Next, let us show that $f_{a,n,r}$ is decreasing. For all $j \in [0, n/2)$ we have

$$\begin{aligned}f'_{a,n,r}(j) &= \log a (a^j + (-1)^{r+1} a^{n-j}) \\ &< 0 \text{ for } j \in [0, n/2),\end{aligned}$$

which completes the proof. $\square$

Remark 13. It follows from the above observation that $f_{a,n,r}$ is increasing for $j \in [\frac{n}{2}, n]$ if r is even (since $f_{a,n,r}(j) = f_{a,n,r}(n-j)$) while $f_{a,n,r}$ is still decreasing for $j \geq \frac{n}{2}$ if r is odd (since $f_{a,n,r}(j) = -f_{a,n,r}(n-j)$).

3.2 The behaviour of $\mathrm{E}(P_n^k)$ *for different values of* k

In this section, we are interested in the behaviour of the energy of P_n^k as k varies. To this end, we need to distinguish two cases depending on the parity of n as well as three cases for the residue class of k modulo 4.

Case 1: n is an odd integer.

(a) $k \equiv 0 \mod 4$: From (8) we have

$$\begin{aligned} Q_n^k(u) &= \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - \frac{2e^{2u}}{e^{2u}+1}\left(e^{-ku} - e^{-(2n+2-k)u}\right) \\ &\qquad + \frac{e^{-2(k-2)u} - e^{-2(n-k)u}}{(e^{2u}+1)^2} - \frac{2e^{2u}+1}{(e^{2u}+1)^2}e^{-2nu} \\ &< \frac{e^{4u}+2e^{2u}+1}{(e^{2u}+1)^2} + \frac{e^{-2(k-2)u}-1}{(e^{2u}+1)^2} < 1 \end{aligned}$$

and consequently

$$\mathrm{E}(P_n^k) < \frac{4n}{\pi}.$$

As we will see, this implies that no P_n^k, for $k \equiv 0 \mod 4$ and odd n, can be a candidate for the maximum energy in U_n because $\mathrm{E}(P_n^6) > \frac{4n}{\pi}$ (see inequalities (14) and (15)). They cannot be candidates for the second-largest energy in U_n either, because $\mathrm{E}(D_n) > \frac{4n}{\pi}$ for $n \geq 23$ (see inequalities (16) and (17)).

(b) $k \equiv 2 \mod 4$:

$$\begin{aligned} Q_n^k(u) &= \Bigg| \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} + 2e^{2u}\frac{e^{-ku} - e^{-(2n+2-k)u}}{e^{2u}+1} \\ &\qquad + \frac{e^{-2(k-2)u} - e^{-2(n-k)u}}{(e^{2u}+1)^2} - \frac{2e^{2u}+1}{(e^{2u}+1)^2}e^{-2nu} \Bigg| \\ &= \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} + \frac{2e^{2u}}{e^{2u}+1} f_{e^{-u},2(n+1),1}(k) \\ &\qquad + \frac{e^{4u}}{(e^{2u}+1)^2} f_{e^{-2u},n+2,1}(k) - \frac{2e^{2u}+1}{(e^{2u}+1)^2}e^{-2nu}. \end{aligned} \tag{9}$$

Equation (9) shows that $Q_n^k(u)$ is decreasing as a function of k in $[0, n]$ just as $f_{e^{-u},2(n+1),1}(k)$ and $f_{e^{-2u},n+2,1}(k)$ are. Therefore we conclude that for all integers $n \geq k > 10$ (where $k \equiv 2 \mod 4$) and all real $u > 0$ we have $Q_n^6(u) > Q_n^{10}(u) > Q_n^k(u)$, which implies that

$$\mathrm{E}(P_n^6) > \mathrm{E}(P_n^{10}) > \mathrm{E}(P_n^k).$$

(c) k is odd ($k \equiv 1 \mod 4$ or $k \equiv 3 \mod 4$): For this case, what we obtain from (8) is

$$\begin{aligned}
(Q_n^k(u))^2 &= \Bigg| \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} \pm 2i \frac{e^{-(k-2)u} + e^{-(2n-k)u}}{e^{2u}+1} \\
&\qquad - \frac{e^{-2(k-2)u} - e^{-2(n-k)u}}{(e^{2u}+1)^2} - \frac{2e^{2u}+1}{(e^{2u}+1)^2} e^{-2nu} \Bigg|^2 \\
&= \left(\frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - \frac{e^{-2(k-2)u} - e^{-2(n-k)u}}{(e^{2u}+1)^2} - \frac{2e^{2u}+1}{(e^{2u}+1)^2} e^{-2nu} \right)^2 \\
&\qquad + \left(2 \frac{e^{-(k-2)u} + e^{-(2n-k)u}}{e^{2u}+1} \right)^2 .
\end{aligned}$$

Consider the second derivative of $\log((Q_n^k(u))^2)$ with respect to k, which is

$$\begin{aligned}
\frac{\partial^2}{\partial k^2} \log\left((Q_n^k(u))^2\right) &= \frac{(Q_n^k(u))^2 \frac{\partial^2}{\partial k^2}(Q_n^k(u))^2 - \left(\frac{\partial}{\partial k}(Q_n^k(u))^2\right)^2}{(Q_n^k(u))^4} \\
&= \frac{u^2}{(e^{2u}+1)^8 (Q_n^k(u))^4} \cdot \Sigma,
\end{aligned}$$

where Σ is a sum of 79 terms of the form ae^{bu}, which are all positive. It follows that

$$\frac{\partial^2}{\partial k^2} \mathrm{E}(P_n^k) > 0,$$

which implies that $\mathrm{E}(P_n^k)$ is convex as a function of k in this case (by differentiation under the integral sign). This shows that the maximum occurs at one of the ends.

Case 2: n is an even integer.

(a) For $k \equiv 0 \mod 4$, we get

$$\begin{aligned} Q_n^k(u) &= \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - 2e^{2u}\frac{e^{-ku}+e^{-(2(n+1)-k)u}}{e^{2u}+1} \\ &\qquad + e^{4u}\frac{e^{-2ku}+e^{-2(n+2-k)u}}{(e^{2u}+1)^2} + \frac{2e^{2u}+1}{(e^{2u}+1)^2}e^{-2nu} \\ &= \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - 2(e^{4u}+e^{2u})\frac{e^{-ku}+e^{-(2(n+1)-k)u}}{(e^{2u}+1)^2} \\ &\qquad + e^{4u}\frac{e^{-2ku}+e^{-2(n+2-k)u}}{(e^{2u}+1)^2} + \frac{2e^{2u}+1}{(e^{2u}+1)^2}e^{-2nu} \\ &< \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - 2(e^{4u}+e^{2u})\frac{e^{-(2(n+1)-k)u}}{(e^{2u}+1)^2} + \frac{e^{-2(n-k)u}}{(e^{2u}+1)^2} \\ &< \frac{e^{2u}(e^{2u}+2)+1}{(e^{2u}+1)^2} = 1. \end{aligned}$$

Exactly as in the corresponding subcase for odd n, this implies

$$\mathrm{E}(P_n^k) < \frac{4n}{\pi}$$

for all integers $n \geq k > 0$ with $k \equiv 0 \mod 4$. Therefore P_n^k cannot be the unicyclic graph with largest or second-largest energy in this case (see again inequalities (14), (15), (16) and (17)).

(b) For $k \equiv 2 \mod 4$, equation (8) gives

$$\begin{aligned} Q_n^k(u) &= \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} + 2e^{2u}\frac{e^{-ku}+e^{-(2(n+1)-k)u}}{e^{2u}+1} \\ &\qquad + \frac{e^{-2(k-2)u}+e^{-2(n-k)u}}{(e^{2u}+1)^2} + \frac{2e^{2u}+1}{(e^{2u}+1)^2}e^{-2nu}. \end{aligned}$$

Similar to the case of odd n and k, we obtain

$$\frac{\partial^2}{\partial k^2}\log\left(Q_n^k(u)\right) = \frac{Q_n^k(u)\frac{\partial^2}{\partial k^2}Q_n^k(u) - \left(\frac{\partial}{\partial k}Q_n^k(u)\right)^2}{(Q_n^k(u))^2} = \frac{u^2}{(e^{2u}+1)^4(Q_n^k(u))^4}\cdot\Sigma,$$

where Σ is a sum of 27 terms of the form ae^{bu}, which are all positive. It follows that

$$\frac{\partial^2}{\partial k^2}\,\mathrm{E}(P_n^k) > 0,$$

which means that $\mathrm{E}(P_n^k)$ is convex as a function of k. Hence for all integers $k \equiv 2 \mod 4$ such that $n-2 > k > 10$ we have

$$\begin{cases} \max\{\mathrm{E}(P_n^{10}), \mathrm{E}(C_n)\} > \mathrm{E}(P_n^k) & \text{for } n \equiv 2 \mod 4, \\ \max\{\mathrm{E}(P_n^{10}), \mathrm{E}(P_n^{n-2})\} > \mathrm{E}(P_n^k) & \text{for } n \equiv 0 \mod 4. \end{cases}$$

(c) For $k \equiv 3 \mod 4$ or $k \equiv 1 \mod 4$ we get (from (8))

$$\begin{aligned}(Q_n^k(u))^2 &= \left| \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} \pm 2ie^{2u}\frac{e^{-ku}-e^{-(2n+2-k)u}}{e^{2u}+1} \right. \\ &\qquad \left. - \frac{e^{-2(k-2)u}+e^{-2(n-k)u}}{(e^{2u}+1)^2} + \frac{2e^{2u}+1}{(e^{2u}+1)^2}e^{-2nu} \right|^2 \\ &= \left(\frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - e^{4u}\frac{f_{e^{-2u},n+2,2}(k)}{(e^{2u}+1)^2} + \frac{2e^{2u}+1}{(e^{2u}+1)^2}e^{-2nu} \right)^2 \\ &\qquad + \left(2e^{2u}\frac{f_{e^{-u},2n+2,1}(k)}{e^{2u}+1} \right)^2. \end{aligned} \tag{10}$$

We can see from (10) that $Q_n^k(u)$ decreases as a function of k on $[\frac{n+2}{2}, n]$: this is because the two functions $-f_{e^{-2u},n+2,2}$ and $f_{e^{-u},2n+2,1}$ both decrease on this interval. Furthermore, let

$$\begin{aligned}B(u,n) &= e^{2u}(e^{2u}+2) + (2e^{2u}+1)e^{-2nu} \\ &= (e^{2u}+1)^2 + (e^{2u}+1)^2e^{-2nu} - 1 - e^{-2(n-2)u} \\ &= (e^{2u}+1)^2(1+e^{-2nu}) - 1 - e^{-2(n-2)u}\end{aligned}$$

so that we have

$$\begin{aligned}(Q_n^k(u))^2 &= \left(\frac{B(u,n)}{(e^{2u}+1)^2} - e^{4u}\frac{f_{e^{-2u},n+2,2}(k)}{(e^{2u}+1)^2} \right)^2 + \left(2e^{2u}\frac{f_{e^{-u},2n+2,1}(k)}{e^{2u}+1} \right)^2 \\ &= \frac{B^2(u,n)}{(e^{2u}+1)^4} - 2B(u,n)e^{4u}\frac{f_{e^{-2u},n+2,2}(k)}{(e^{2u}+1)^4} \\ &\qquad + e^{8u}\frac{f^2_{e^{-2u},n+2,2}(k)}{(e^{2u}+1)^4} + 4e^{4u}\frac{f^2_{e^{-u},2n+2,1}(k)}{(e^{2u}+1)^2},\end{aligned}$$

and

$$
\begin{aligned}
&\frac{\partial}{\partial k}(Q_n^k(u))^2 \\
&= 4uB(u,n)e^{4u}\frac{f_{e^{-2u},n+2,1}(k)}{(e^{2u}+1)^4} - 4ue^{8u}\frac{f_{e^{-2u},n+2,2}(k)f_{e^{-2u},n+2,1}(k)}{(e^{2u}+1)^4} \\
&\qquad\qquad\qquad\qquad\qquad\qquad - 8ue^{4u}\frac{f_{e^{-u},2n+2,1}(k)f_{e^{-u},2n+2,2}(k)}{(e^{2u}+1)^2} \\
&= 4uB(u,n)e^{4u}\frac{f_{e^{-2u},n+2,1}(k)}{(e^{2u}+1)^4} - 4ue^{8u}\frac{f_{e^{-4u},n+2,1}(k)}{(e^{2u}+1)^4} - 8ue^{4u}\frac{f_{e^{-2u},2n+2,1}(k)}{(e^{2u}+1)^2} \\
&\le \frac{4ue^{4u}}{(e^{2u}+1)^2}\Bigg((1+e^{-2nu})f_{e^{-2u},n+2,1}(k) - \frac{f_{e^{-2u},n+2,1}(k)}{(e^{2u}+1)^2} - e^{4u}\frac{f_{e^{-4u},n+2,1}(k)}{(e^{2u}+1)^2} \\
&\qquad\qquad\qquad\qquad\qquad\qquad - f_{e^{-2u},2n+2,1}(k)\Bigg) \text{ for } k \le \frac{n+2}{2} \\
&= \frac{4ue^{4u}}{(e^{2u}+1)^2}\left(-e^{-2(n+2-k)u} + e^{-2(n+k)u} - \frac{f_{e^{-2u},n+2,1}(k)}{(e^{2u}+1)^2} - e^{4u}\frac{f_{e^{-4u},n+2,1}(k)}{(e^{2u}+1)^2}\right) \\
&< 0.
\end{aligned}
$$

This means that $Q_n^k(u)$ is also decreasing on the interval $[1, \frac{n+2}{2}]$ and thus on the entire interval $[1, n]$. Therefore for all odd k such that $3 < k \le n$ and all $u > 0$ we have

$$Q_n^3(u) > Q_n^k(u)$$

which implies

$$\mathrm{E}(P_n^3) > \mathrm{E}(P_n^k). \tag{11}$$

We can conclude now that the tadpole with largest energy is an element of

$$\begin{cases} \{P_n^3, P_n^6, P_n^{n-2}\} \text{ if } n \equiv 0 \mod 4, \\ \{P_n^3, P_n^6, C_n\} \quad \text{otherwise.} \end{cases} \tag{12}$$

Since P_n^{n-2} (for $n \equiv 0 \mod 4$) is bipartite, we can use Theorem 3 and Theorem 4 to obtain that for all integers $3 < k \le n$ such that $k \neq 6$ the following inequality holds:

$$\mathrm{E}(P_n^k) < \max\{\mathrm{E}(P_n^3), \mathrm{E}(P_n^6)\}$$

if $n \ge 16$. Once we have shown that $\mathrm{E}(P_n^3) < \mathrm{E}(P_n^6)$ for all such n, we also know that the tadpole with second-largest energy must be an element of

$$\begin{cases} \{P_n^3, P_n^{10}, P_n^{n-2}\} \text{ if } n \equiv 0 \mod 4, \\ \{P_n^3, P_n^{10}, C_n\} \quad \text{otherwise.} \end{cases} \tag{13}$$

3.3 Estimating the energy in special cases

We now collect estimates for the energy of the remaining graphs to be considered: first, we consider the graphs P_n^6 and D_n whose energy is estimated from below. On the other hand, we determine upper estimates for $\mathrm{E}(C_n)$, $\mathrm{E}(P_n^3)$, $\mathrm{E}(P_n^{10})$ and $\mathrm{E}(P_n^{n-2})$. Our main theorems are then obtained by combining these estimates. Most of our estimates are obtained from the integral formula (7). For simplicity of notation we use the substitution $z = e^{-u}$.

- From [1] we have the following inequalities:
  - For even $n \geq 6$,

$$\begin{aligned}
\mathrm{E}(P_n^6) &> \frac{4n}{\pi} + \frac{0.370}{\pi} + 2\csc\frac{\pi}{2(n-3)} - \frac{2}{\pi}2(n-3) \\
&> \frac{4n}{\pi} + \frac{0.370}{\pi}.
\end{aligned} \tag{14}$$

  - for odd $n \geq 17$,

$$\begin{aligned}
\mathrm{E}(P_n^6) &> \frac{4n}{\pi} + \frac{0.370}{\pi} + 2\cot\frac{\pi}{2(n-4)} - \frac{2}{\pi}2(n-4) \\
&> \frac{4n}{\pi} + \frac{0.370}{\pi} + 2\cot\frac{\pi}{2(17-4)} - \frac{2}{\pi}2(17-4) \\
&= \frac{4n}{\pi} + \frac{0.370}{\pi} + 2\cot\frac{\pi}{26} - \frac{52}{\pi} \\
&> \frac{4n}{\pi} + \frac{0.116}{\pi}.
\end{aligned} \tag{15}$$

- $\mathrm{E}(D_n)$ is given by

$$\mathrm{E}(D_n) = \frac{4n}{\pi} + \frac{4}{\pi}\int_0^{+\infty} \log\left|\frac{\phi(D_n, 2i\sinh u)}{(ie^u)^n}\right| \cosh u \; du.$$

  Using Lemma 8 we have

$$\phi(D_n, x) = (x^2 - 1)\phi(P_{n-2}^6, x) - x\phi(C_6, x)\phi(P_{n-9}, x),$$

  and hence

$$\begin{aligned}
\phi(D_n, 2i\sinh u) = (-e^{2u} - e^{-2u} + 1)&\phi(P_{n-2}^6, 2i\sinh u) \\
&- i(e^u - e^{-u})\phi(C_6, 2i\sinh u)\phi(P_{n-9}, 2i\sinh u).
\end{aligned}$$

Since

$$
\begin{aligned}
&(-e^{2u}-e^{-2u}+1)\frac{\phi(P^6_{n-2},2i\sinh u)}{(ie^u)^n}\\
&=\frac{(-e^{2u}-e^{-2u}+1)}{(ie^u)^2}\Bigg(\frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2}-2e^{2u}\frac{(ie^u)^{-6}-(ie^u)^{6-2(n-2+1)}}{e^{2u}+1}\\
&\qquad\qquad+\frac{(ie^u)^{-2\cdot 6+4}+(ie^u)^{2\cdot 6-2(n-2)}}{(e^{2u}+1)^2}+\frac{2e^{2u}+1}{(e^{2u}+1)^2}(ie^u)^{-2(n-2)}\Bigg)\\
&=(1+z^4-z^2)\Bigg(\frac{z^{-4}+2z^{-2}+(-1)^n(2z^{2n-6}+z^{2n-4})}{(1+z^{-2})^2}\\
&\qquad\qquad+2\frac{z^4+(-1)^nz^{2n-10}}{1+z^{-2}}+\frac{z^8+(-1)^nz^{2n-16}}{(1+z^{-2})^2}\Bigg)\\
&=\frac{(z^4-z^2+1)^2}{1+z^2}\left(1+2z^2+z^6+(-1)^n(z^{2n-6}+2z^{2n-8}+z^{2n-12})\right)
\end{aligned}
$$

and

$$
\begin{aligned}
&i(e^u-e^{-u})\phi(C_6,2i\sinh u)\frac{\phi(P_{n-9},2i\sinh u)}{(ie^u)^n}\\
&\quad=i(z^{-1}-z)\Big((iz^{-1})^6+(-iz)^6-2\Big)\frac{\frac{1}{1+z^2}(iz^{-1})^{n-9}+\frac{z^2}{1+z^2}(iz^{-1})^{-(n-9)}}{(iz^{-1})^n}\\
&\quad=(z^4-1)(z^4-z^2+1)^2\left(z^2-(-1)^nz^{2n-14}\right),
\end{aligned}
$$

we obtain

$$
\begin{aligned}
\left|\frac{\phi(D_n,2i\sinh u)}{(ie^u)^n}\right|=\frac{(1-z^2+z^4)^2}{1+z^2}\Big(&1+3z^2+z^4-z^8\\
&+(-1)^n(z^{2n-6}+3z^{2n-8}+z^{2n-10}-z^{2n-14})\Big).
\end{aligned}
$$

· For even n, we now have

$$
\begin{aligned}
\left|\frac{\phi(D_n,2i\sinh u)}{(ie^u)^n}\right|&\geq t_1(z,n)\\
&:=\frac{(1-z^2+z^4)^2}{1+z^2}\left(1+3z^2+z^4-z^8-z^{2n-14}\right)
\end{aligned}
$$

and thus

$$
\begin{aligned}
\mathrm{E}(D_n)&>\frac{4n}{\pi}+\frac{2}{\pi}\int_0^1(z^{-2}+1)\log t_1(z,28)dz\text{ for all even }n\geq 28\\
&>\frac{4n}{\pi}+\frac{0.168}{\pi}.
\end{aligned}
\tag{16}
$$

· For odd n we have

$$\left|\frac{\phi(D_n, 2i\sinh u)}{(ie^u)^n}\right| \geq t_2(z,n)$$
$$:= \frac{(1-z^2+z^4)^2}{1+z^2}\left(1+3z^2+z^4-z^8-z^{2n-6}-3z^{2n-8}\right)$$

and thus

$$\begin{aligned}\mathrm{E}(D_n) &\geq \frac{4n}{\pi}+\frac{2}{\pi}\int_0^1 (z^{-2}+1)\log t_2(z,29)dz \text{ for all odd } n\geq 29\\ &> \frac{4n}{\pi}+\frac{0.062}{\pi}.\end{aligned} \tag{17}$$

- For the cycle C_n, we have explicit formulas that were also used in [1]:

$$\mathrm{E}(C_n) = \begin{cases} 4\cot\frac{\pi}{n} & n\equiv 0 \mod 4,\\ 4\csc\frac{\pi}{n} & n\equiv 2 \mod 4,\\ 2\csc\frac{\pi}{2n} & n \text{ odd.}\end{cases}$$

This gives us a trivial lower bound for odd n:

$$\mathrm{E}(C_n) > \frac{4n}{\pi} \text{ if } n \text{ is odd.}$$

For an upper bound, we notice that $\cot x < \csc x$, and that the function $\csc x - 1/x$ is increasing for $x<\pi$. Hence we have

$$\mathrm{E}(C_n) \leq 4\csc\frac{\pi}{n} \leq \frac{4n}{\pi}+4\csc\frac{\pi}{40}-\frac{160}{\pi} < \frac{4n}{\pi}+\frac{0.165}{\pi} < \mathrm{E}(D_n) \tag{18}$$

for even $n\geq 40$, and the inequality $\mathrm{E}(C_n)<\mathrm{E}(D_n)$ can also be verified directly for even $n\in[28,38]$. Likewise,

$$\mathrm{E}(C_n) = 2\csc\frac{\pi}{2n} \leq \frac{4n}{\pi}+2\csc\frac{\pi}{58}-\frac{116}{\pi} < \frac{4n}{\pi}+\frac{0.057}{\pi} < \mathrm{E}(D_n) \tag{19}$$

for odd $n\geq 29$.

- From (8) we get

$$\begin{aligned}(Q_n^3(u))^2 &= \left|\frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - 2ie^{2u}\frac{e^{-3u}-(-1)^n e^{(1-2n)u}}{e^{2u}+1}\right.\\ &\qquad \left. -\frac{e^{-2u}+(-1)^n e^{(6-2n)u}}{(e^{2u}+1)^2}+\frac{2e^{2u}+1}{(e^{2u}+1)^2}(ie^u)^{-2n}\right|^2\\ &= \left(\frac{z^{-4}+2z^{-2}-z^2-(-1)^n z^{2n-6}+(-1)^n(2z^{2n-2}+z^{2n})}{(z^{-2}+1)^2}\right)^2\\ &\qquad +\left(\frac{2z-2(-1)^n z^{2n-3}}{z^{-2}+1}\right)^2.\end{aligned} \tag{20}$$

· If n is even, then we have

$$\begin{aligned}
&(Q_n^3(u))^2 \\
&= \left(\frac{z^{-4}+2z^{-2}-z^2-z^{2n-6}+2z^{2n-2}+z^{2n}}{(z^{-2}+1)^2}\right)^2 + \left(\frac{2z-2z^{2n-3}}{z^{-2}+1}\right)^2 \\
&\le u_1(z,n) := \left(\frac{1+2z^2-z^6+z^{2n+2}+z^{2n+4}}{(z^2+1)^2}\right)^2 + \left(\frac{2z^3}{z^2+1}\right)^2.
\end{aligned}$$

Therefore

$$\begin{aligned}
\mathrm{E}(P_n^3) &= \frac{4n}{\pi} + \frac{2}{\pi}\int_0^{+\infty} \log((Q_6^3(u))^2)\cosh u\, du \\
&< \frac{4n}{\pi} + \frac{1}{\pi}\int_0^1 (z^{-2}+1)\log u_1(z,28) dz \text{ for all even } n \ge 28 \\
&\le \frac{4n}{\pi} - \frac{0.100}{\pi} < \mathrm{E}(D_n) \qquad (21)
\end{aligned}$$

and

$$\begin{aligned}
\mathrm{E}(P_n^3) &< \frac{4n}{\pi} + \frac{1}{\pi}\int_0^1 (z^{-2}+1)\log u_1(z,6) dz \text{ for all even } n \ge 6 \\
&\le \frac{4n}{\pi} - \frac{0.028}{\pi} < \mathrm{E}(P_n^6). \qquad (22)
\end{aligned}$$

· For odd n we obtain from (20) that

$$\begin{aligned}
(Q_n^3(u))^2 &= \left(\frac{z^{-4}+2z^{-2}-z^2+z^{2n-6}-2z^{2n-2}-z^{2n}}{(z^{-2}+1)^2}\right)^2 + \left(\frac{2z+2z^{2n-3}}{z^{-2}+1}\right)^2 \\
&\le u_2(z,n) := \left(\frac{1+2z^2-z^6+z^{2n-2}}{(z^2+1)^2}\right)^2 + \left(\frac{2z^3+2z^{2n-1}}{z^2+1}\right)^2.
\end{aligned}$$

Hence

$$\begin{aligned}
\mathrm{E}(P_n^3) &\le \frac{4n}{\pi} + \frac{1}{\pi}\int_0^1 (z^{-2}+1)\log u_2(z,15) dz \text{ for } n \ge 15 \\
&\le \frac{4n}{\pi} < \min\{\mathrm{E}(C_n), \mathrm{E}(P_n^6)\}. \qquad (23)
\end{aligned}$$

Furthermore, we also have

$$\mathrm{E}(P_n^3) \le \frac{4n}{\pi} < \mathrm{E}(D_n) \qquad (24)$$

for $n \ge 23$.

- From (8) we get

$$
\begin{aligned}
Q_n^{10}(u) &= \left| \frac{e^{2u}(e^{2u}+2)}{(e^{2u}+1)^2} - 2e^{2u}\frac{(ie^u)^{-10}-(ie^u)^{10-2(n+1)}}{e^{2u}+1} \right. \\
&\qquad \left. + \frac{(ie^u)^{-2\cdot 10+4}+(ie^u)^{2\cdot 10-2n}}{(e^{2u}+1)^2} + \frac{2e^{2u}+1}{(e^{2u}+1)^2}(ie^u)^{-2n} \right| \\
&= \frac{z^{-4}+2z^{-2}+(-1)^n(2z^{2n-2}+z^{2n})+z^{16}+(-1)^n z^{2n-20}}{(z^{-2}+1)^2} \\
&\qquad + 2\frac{z^8+(-1)^n z^{2n-10}}{z^{-2}+1}.
\end{aligned}
$$

  · For even n we have

$$
\begin{aligned}
Q_n^{10}(u) = v_1(z,n) := &\frac{1+2z^2+2z^{2n+2}+z^{2n+4}+z^{20}+z^{2n-16}}{(z^2+1)^2} \\
&+ 2\frac{z^{10}+z^{2n-8}}{z^2+1}.
\end{aligned}
$$

  It follows that

$$
\begin{aligned}
\mathrm{E}(P_n^{10}) &\leq \frac{4n}{\pi} + \frac{2}{\pi}\int_0^1 (z^{-2}+1)\log v_1(z,28)dz \text{ for } n \geq 28 \\
&\leq \frac{4n}{\pi} + \frac{0.092}{\pi} < \mathrm{E}(D_n).
\end{aligned} \tag{25}
$$

  · For odd n we have

$$
\begin{aligned}
Q_n^{10}(u) &= \frac{1+2z^2-2z^{2n+2}-z^{2n+4}+z^{20}-z^{2n-16}}{(z^2+1)^2} + 2\frac{z^{10}-z^{2n-8}}{z^2+1} \\
&\leq v_2(z) := \frac{1+2z^2+z^{20}}{(z^2+1)^2} + \frac{2z^{10}}{z^2+1}.
\end{aligned}
$$

  This implies

$$
\begin{aligned}
\mathrm{E}(P_n^{10}) &\leq \frac{4n}{\pi} + \frac{2}{\pi}\int_0^1 (z^{-2}+1)\log v_2(z)dz \\
&\leq \frac{4n}{\pi} + \frac{0.016}{\pi} < \mathrm{E}(D_n).
\end{aligned} \tag{26}
$$

- For even $n \equiv 0 \mod 4$, using (8) we have

$$
\begin{aligned}
&Q_n^{n-2}(u) \\
&= \frac{e^{4u}+2e^{2u}+2e^{-2(n-1)u}+e^{-2nu}}{(e^{2u}+1)^2} + 2\frac{e^{-(n-4)u}+e^{-(n+2)u}}{e^{2u}+1} + \frac{e^{-2(n-4)u}+e^{-4u}}{(e^{2u}+1)^2} \\
&= w(z,n) := \frac{1+2z^2+2z^{2n+2}+z^{2n+4}+z^{2n-4}+z^8}{(z^2+1)^2} + 2\frac{z^{n-2}+z^{n+4}}{z^2+1}.
\end{aligned}
$$

This implies that

$$\begin{aligned}\mathrm{E}(P_n^{n-2}) &\leq \frac{4n}{\pi} + \frac{2}{\pi}\int_0^1 (z^{-2}+1)\log w(z,28)dz \text{ for } n \geq 28 \\ &\leq \frac{4n}{\pi} - \frac{0.02}{\pi} < \mathrm{E}(D_n). \end{aligned} \tag{27}$$

3.4 Main theorems, conclusion

We are now ready to collect all estimates and prove our three main results: Conjecture 1, Theorem 5 and Theorem 7, which all follow now by appropriately combining the inequalities obtained in the preceding sections: the results of Section 3.2 have already reduced the number of possibilities considerably (see observations (12) and (13)), and the remaining cases are all covered by the estimates in Section 3.3.

In particular, we obtain Conjecture 1 by combining our observation (12) with Theorem 4, Theorem 3 and the inequalities (22) and (23).

Theorem 5 is a combination of observation (13), Theorem 6 and inequalities (18), (19), (21), (24), (25), (26) and (27).

Finally, Theorem 7 follows immediately from inequality (11) for even n and for odd n from inequality (23) (for $n \geq 15$; the remaining cases can be checked directly) together with the observation that $\mathrm{E}(P_n^k)$ is a convex function in k for odd k.

It is very likely that the same approach can also be used to characterise the unicyclic graph with third-largest, fourth-largest, ... energy, although the number of cases to be considered will become considerable. Propositions 9, 10 and 11 also show that there are lots of unicyclic graphs whose energy comes close (within a constant) to the maximum value.

References

[1] E. O. D. Andriantiana, Unicyclic bipartite graphs with maximum energy, MATCH Commun. Math. Comput. Chem., in press, 2011.

[2] Y. Cao, A. Lin, R. Luo, X. Zha, On the minimal energy of unicyclic Hückel molecular graphs possessing Kekulé structures, Discrete Appl. Math. 157 (5) (2009) 913–919.

[3] 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 (3) (1999) 984–996.

[4] A. Chen, A. Chang, W. C. Shiu, Energy ordering of unicycle graphs, MATCH Commun. Math. Comput. Chem. 55 (1) (2006) 95–102.

[5] D. M. Cvetković, M. Doob, H. Sachs, Spectra of Graphs – Theory and Application, Academic Press, New York, 1980.

[6] I. Gutman, Acyclic systems with extremal Hückel pi-electron energy, Theor. Chim. Acta 45 (1977) 79–87.

[7] I. Gutman, The energy of a graph, Ber. Math.-Statist. Sekt. Forsch. Graz (100–105) (1978) Ber. No. 103, 22.

[8] I. Gutman, The energy of a graph: old and new results, in: Algebraic combinatorics and applications (Gößweinstein, 1999), Springer, Berlin, 2001, pp. 196–211.

[9] I. Gutman, B. Furtula, H. Hua, Bipartite unicyclic graphs with maximal, second-maximal, and third-maximal energy, MATCH Commun. Math. Comput. Chem. 58 (2007) 75–82.

[10] I. Gutman, X. Li, J. Zhang, Graph energy, in: M. Dehmer, F. Emmert-Streib (eds.), Analysis of Complex Networks. From Biology to Linguistics, Wiley-VCH Verlag, Weinheim, 2009, pp. 145–174.

[11] I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: A computer experiment, J. Chem. Inf. Comput. Sci. 41 (3) (2001) 1002–1005.

[12] C. Heuberger, S. G. Wagner, Chemical trees minimizing energy and Hosoya index, J. Math. Chem. 46 (1) (2009) 214–230.

[13] Y. Hou, Unicyclic graphs with minimal energy, J. Math. Chem. 29 (3) (2001) 163–168.

[14] Y. Hou, I. Gutman, C.-W. Woo, Unicyclic graphs with maximal energy, Linear Algebra Appl. 356 (2002) 27–36, special issue on algebraic graph theory (Edinburgh, 2001).

[15] H. Hua, Bipartite unicyclic graphs with large energy, MATCH Commun. Math. Comput. Chem. 58 (1) (2007) 57–73.

[16] B. Huo, S. Ji, X. Li, Note on unicyclic graphs with given number of pendent vertices and minimal energy, Linear Algebra and its Applications 433 (7) (2010) 1381–1387.

[17] B. Huo, X. Li, Y. Shi, Complete solution to a problem on the maximal energy of unicyclic graphs, preprint, `http://arxiv.org/abs/1011.4658`.

[18] B. Huo, X. Li, Y. Shi, Complete solution to a problem on the maximal energy of unicyclic bipartite graphs, Linear Algebra and its Applications 434 (5) (2011) 1370–1377.

[19] J. Li, X. Li, Note on bipartite unicyclic graphs of given bipartition with minimal energy, MATCH Commun. Math. Comput. Chem. 64 (1) (2010) 61–64.

[20] S. Li, X. Li, Z. Zhu, On minimal energy and Hosoya index of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 61 (2) (2009) 325–339.

[21] X. Li, Y. Li, Note on conjugated unicyclic graphs with minimal energy, MATCH Commun. Math. Comput. Chem. 64 (1) (2010) 141–144.

[22] Y. Liu, Some results on energy of unicyclic graphs with n vertices, J. Math. Chem. 47 (1) (2010) 1–10.

[23] H.-Y. Shan, J.-Y. Shao, S. Li, X. Li, On a conjecture on the tree with fourth greatest energy, MATCH Commun. Math. Comput. Chem. 64 (1) (2010) 181–188.

[24] W.-H. Wang, L.-Y. Kang, Ordering of the trees by minimal energies, J. Math. Chem. 47 (3) (2010) 937–958.

[25] X. Yao, Maximum energy trees with one maximum and one second maximum degree vertex, MATCH Commun. Math. Comput. Chem. 64 (1) (2010) 217–230.

[26] B. Zhang, Remarks on minimal energies of unicyclic bipartite graphs, MATCH Commun. Math. Comput. Chem. 61 (2) (2009) 487–494.