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The Conjecture About the Comparison for Resolvent Energies of Cycles and Stars

Zhibin Du[a,b], Kinkar Chandra Das[c,*]

[a] *School of Software, South China Normal University, Foshan, 528225, China*

[b] *School of Mathematics and Statistics, Zhaoqing University, Zhaoqing 526061, China*
zhibindu@126.com

[c] *Department of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea*
E-mail: kinkardas2003@gmail.com

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Abstract

The resolvent energy of a graph G of order n is defined as $ER(G) = \sum_{i=1}^{n} (n - \lambda_i)^{-1}$, where λ_1, $\lambda_2, \ldots, \lambda_n$ are the eigenvalues of G. Gutman *et al.* [Resolvent energy of graphs, MATCH Commun. Math. Comput. Chem. 75 (2016) 279–290] proposed a conjecture that $ER(S_n) < ER(C_n)$ holds for all $n \geq 4$, where S_n and C_n are the star and the cycle of order n, respectively. In this note, we confirm this conjecture.

1 Introduction

Let G be a graph on n vertices. Also let $A(G)$ be the adjacency matrix of G and denote by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ the eigenvalues of $A(G)$. The properties of the adjacency eigenvalues, especially spectral radius, studied recently in [4] and the reference therein. The resolvent matrix of $A(G)$ is

$$R_A(z) = (zI_n - A(G))^{-1},$$

and its eigenvalues are $\frac{1}{z-\lambda_i}$, $i = 1, 2, \ldots, n$.

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*Corresponding author

The energy of graphs is one of the most well-known and meaningful topological indices in theoretical chemistry, which is defined as [8]

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

For its basic properties and applications, including various lower and upper bounds, see the book [13], the surveys [9,12], the recent papers [3,4] and the references cited therein.

Recently, Gutman *et al.* [10] proposed a new type of energy, called resolvent energy, based on the spectrum (eigenvalues) of the resolvent matrix

$$R_G(n) = (n\, I_n - A(G)^{-1}.$$

Notices that the eigenvalues of $R_G(n)$ are $\frac{1}{n-\lambda_i}$, $i = 1, 2, \ldots, n$, thus the resolvent energy of G is naturally defined as [10,11]

$$ER(G) = \sum_{i=1}^{n} \frac{1}{n - \lambda_i}.$$

For its basic properties and applications, including various lower and upper bounds, see the recent papers [2,5,7,16,17] and the references cited therein. The resolvent energy belongs to a general class of cumulative vertex centrality measures based on closed walks, originally put forward by Estrada and Higham in [6].
Let S_n denote the star on n vertices, and C_n the n-vertex cycle, for $n \geq 3$. Gutman *et al.* [10] proposed the following conjecture:

Conjecture 1. [10] *The inequality*

$$ER(S_n) < ER(C_n)$$

holds for all $n \geq 4$. *Consequently, any tree has smaller ER-value than any unicyclic graph of the same order.*

Das [2] solved Conjecture 1 when n is even. Now we completely settle Conjecture 1, by a unified method no matter n is even or odd.

2 Proof for Conjecture 1

In this section we give a proof of Conjecture 1. For this aim, we need the following results.

Lemma 2. *For $n \geq 3$,*

$$\frac{n}{\sqrt{n^2-4}} - \frac{1}{n^4} > \frac{2n}{n^2-n+1} + \frac{n-2}{n}.$$

Proof. We have to prove that

$$\frac{n}{\sqrt{n^2-4}} > \frac{2n}{n^2-n+1} + \frac{n-2}{n} + \frac{1}{n^4} = \frac{n^6-n^5+3n^4-2n^3+n^2-n+1}{n^4(n^2-n+1)},$$

that is,

$$n^{10}\,(n^2-n+1)^2 > (n^2-4)\,(n^6-n^5+3n^4-2n^3+n^2-n+1)^2,$$

that is,

$$14\,n^{10} - 24\,n^9 + 46\,n^8 - 52\,n^7 + 45\,n^6 - 42\,n^5 + 41\,n^4 - 22\,n^3 + 11\,n^2 - 8n + 4 > 0,$$

which is always true as $n \geq 3$. ∎

The spectra of stars and cycles are well-known, e.g., see [1, p. 72].

Lemma 3. *The eigenvalues of S_n are $\pm\sqrt{n-1}$, and 0 of multiplicity $n-2$. The eigenvalues of C_n are $2\cos\frac{2k\pi}{n}$ for $k = 1, 2, \ldots, n$.*

As a consequence, we obtain the expressions of resolvent energies of stars and cycles:

$$ER(S_n) = \frac{2n}{n^2-n+1} + \frac{n-2}{n}$$

and

$$ER(C_n) = \sum_{k=1}^{n} \frac{1}{n - 2\cos\frac{2k\pi}{n}}.$$

So Conjecture 1 is equivalent to verify the following inequality:

$$\sum_{k=1}^{n} \frac{1}{n - 2\cos\frac{2k\pi}{n}} > \frac{2n}{n^2-n+1} + \frac{n-2}{n}.$$

In the following, we will complete this task by establishing two inequalities: For $n \geq 3$,

$$\sum_{k=1}^{n} \frac{1}{n - 2\cos\frac{2k\pi}{n}} > \frac{n}{\sqrt{n^2-4}} - \frac{1}{n^4} > \frac{2n}{n^2-n+1} + \frac{n-2}{n}.$$

By Lemma 2, we have the second part. So we have to prove the first inequality:

$$\sum_{k=1}^{n} \frac{1}{n - 2\cos\frac{2k\pi}{n}} > \frac{n}{\sqrt{n^2-4}} - \frac{1}{n^4}$$

for $n \geq 3$.

In order to do that, first let us see why the term $\frac{n}{\sqrt{n^2-4}}$ would occur. In fact, it comes from an integral.

Lemma 4. *For a fixed integer $n \geq 3$, we have*

$$\int_0^1 \frac{1}{n - 2\cos 2\pi x} dx = \frac{1}{\sqrt{n^2 - 4}}.$$

In [5], Du has shown that

$$ER(C_n) = \sum_{k=1}^{n} \frac{1}{n - 2\cos\frac{2k\pi}{n}} = \frac{n}{\sqrt{n^2-4}} + o(1),$$

and the error is at most $\frac{8}{n^2-4}$. For our need here, we would like to improve the error term (less than $\frac{1}{n^4}$). We resort to the well-known Euler-Maclaurin summation formula, see [14, p. 181].

Lemma 5 (Euler-Maclaurin summation formula)**.** *If $h(x)$ is an infinitely differentiable function, m is a fixed constant, then*

$$\sum_{0 \leq k \leq n} h\left(\frac{k}{n}\right) = n \int_0^1 h(x)dx + \frac{h(0) + h(1)}{2} + \sum_{1 \leq i \leq m} \frac{B_{2i}}{(2i)!} \frac{1}{n^{2i-1}} h^{(2i-1)}(x)\Big|_0^1 + R_m,$$

where B_{2i}'s are the Bernoulli numbers and R_m is a remainder term satisfying

$$|R_m| \leq \frac{|B_{2m}|}{(2m)!} \frac{1}{n^{2m}} \int_0^1 |h^{(2m)}(x)|dx < \frac{4}{(2\pi n)^{2m}} \int_0^1 |h^{(2m)}(x)|dx.$$

Set $h(x) = \dfrac{1}{n - 2\cos 2\pi x}$. Applying Euler-Maclaurin summation formula (Lemma 5), it leads to

$$\sum_{k=0}^{n} \frac{1}{n - 2\cos\frac{2\pi k}{n}} = n \int_0^1 \frac{1}{n - 2\cos 2\pi x} dx + \frac{1}{n-2} + \sum_{1 \leq i \leq m} \frac{B_{2i}}{(2i)!} \frac{1}{n^{2i-1}} h^{(2i-1)}(x)\Big|_0^1 + R_m,$$

for some positive integer m. Together with Lemma 4, the above equation is equivalent to

$$\sum_{k=1}^{n} \frac{1}{n - 2\cos\frac{2\pi k}{n}} = \frac{n}{\sqrt{n^2-4}} + \sum_{1 \leq i \leq m} \frac{B_{2i}}{(2i)!} \frac{1}{n^{2i-1}} h^{(2i-1)}(x)\Big|_0^1 + R_m.$$

We still need to calculate the higher derivatives of $h(x)$, aiming to estimate the error term. Let us take the first three orders of derivatives of $h(x)$ to explore their patterns:

$$h'(x) = -\frac{4\pi \sin 2\pi x}{(n - 2\cos 2\pi x)^2},$$

$$h''(x) = -\frac{8\pi^2 \cos 2\pi x}{(n - 2\cos 2\pi x)^2} + \frac{32\pi^2 (\sin 2\pi x)^2}{(n - 2\cos 2\pi x)^3}$$

and

$$h'''(x) = \frac{16\pi^3 \sin 2\pi x}{(n - 2\cos 2\pi x)^2} + \frac{192\pi^3 \cos 2\pi x \sin 2\pi x}{(n - 2\cos 2\pi x)^3} - \frac{384\pi^3 (\sin 2\pi x)^3}{(n - 2\cos 2\pi x)^4}.$$

From these derivative expressions, we have two claims:

- The denominator of every term of $h^{(2i-1)}(x)$, for $i \geq 1$, is of the form $(n-2\cos 2\pi x)^s$, for $2 \leq s \leq 2i$.
- Ignore the constant coefficients, the numerator of every term of $h^{(2i-1)}(x)$ is of the form $(\sin 2\pi x)^r(\cos 2\pi x)^t$, for odd $r \geq 1$, and $t \geq 0$ (for our need, the key point here is the exponent r (of $\sin 2\pi x$) is an odd positive integer).

The first claim is clear, while the second one can be deduced by induction. From the two claims, we know that ignore the constant coefficients, each term of $h^{(2i-1)}(x)$ is of the form $\dfrac{(\sin 2\pi x)^r(\cos 2\pi x)^t}{(n-2\cos 2\pi x)^s}$, for $s \geq 2$, odd $r \geq 1$, and $t \geq 0$. When we go ahead from $h^{(2i-1)}(x)$ to $h^{(2i+1)}(x)$, we would take the second derivative of $\dfrac{(\sin 2\pi x)^r(\cos 2\pi x)^t}{(n-2\cos 2\pi x)^s}$, it is not hard to see that the factor related to $\sin 2\pi x$ would become $(\sin 2\pi x)^r$, $(\sin 2\pi x)^{r+2}$, or $(\sin 2\pi x)^{r-2}$ (with $r \geq 3$), as desired.

As a consequence, $\left.\dfrac{(\sin 2\pi x)^r(\cos 2\pi x)^t}{(n-2\cos 2\pi x)^s}\right|_0^1 = 0$ since the existence of $\sin 2\pi x$. Furthermore, it means that

$$\frac{B_{2i}}{(2i)!}\frac{1}{n^{2i-1}}\,h^{(2i-1)}(x)\Big|_0^1 = 0$$

for any $i \geq 1$, thus

$$\sum_{1\leq i\leq m}\frac{B_{2i}}{(2i)!}\frac{1}{n^{2i-1}}\,h^{(2i-1)}(x)\Big|_0^1 = 0$$

for any m.

At this stage, we have

$$\sum_{k=1}^{n}\frac{1}{n-2\cos\frac{2\pi k}{n}} = \frac{n}{\sqrt{n^2-4}} + R_m.$$

Clearly, our desired inequality

$$\sum_{k=1}^{n}\frac{1}{n-2\cos\frac{2k\pi}{n}} > \frac{n}{\sqrt{n^2-4}} - \frac{1}{n^4}$$

comes from $R_m > -\frac{1}{n^4}$, or equivalently, $|R_m| < \frac{1}{n^4}$, for some positive integer m. Recall that

$$|R_m| < \frac{4}{(2\pi n)^{2m}}\int_0^1 |h^{(2m)}(x)|dx.$$

Set $m = 2$. It is easy to verify that

$$h^{(4)}(x) \quad = \quad \frac{32\pi^4\cos 2\pi x}{(n-2\cos 2\pi x)^2} + \frac{384\pi^4(\cos 2\pi x)^2}{(n-2\cos 2\pi x)^3} - \frac{512\pi^4(\sin 2\pi x)^2}{(n-2\cos 2\pi x)^3}$$

$$-\frac{4608\pi^4\cos 2\pi x(\sin 2\pi x)^2}{(n-2\cos 2\pi x)^4}+\frac{6144\pi^4(\sin 2\pi x)^4}{(n-2\cos 2\pi x)^5}.$$

Further,

$$\begin{aligned}
|h^{(4)}(x)| &\le \left|\frac{32\pi^4\cos 2\pi x}{(n-2\cos 2\pi x)^2}\right|+\left|\frac{384\pi^4(\cos 2\pi x)^2}{(n-2\cos 2\pi x)^3}\right|+\left|\frac{512\pi^4(\sin 2\pi x)^2}{(n-2\cos 2\pi x)^3}\right| \\
&\quad+\left|\frac{4608\pi^4\cos 2\pi x(\sin 2\pi x)^2}{(n-2\cos 2\pi x)^4}\right|+\left|\frac{6144\pi^4(\sin 2\pi x)^4}{(n-2\cos 2\pi x)^5}\right| \\
&\le \frac{32\pi^4}{(n-2\cos 2\pi x)^2}+\frac{384\pi^4}{(n-2\cos 2\pi x)^3}+\frac{512\pi^4}{(n-2\cos 2\pi x)^3} \\
&\quad+\frac{4608\pi^4}{(n-2\cos 2\pi x)^4}+\frac{6144\pi^4}{(n-2\cos 2\pi x)^5} \\
&< \frac{32\pi^4}{(n-2\cos 2\pi x)^2}+\frac{384\pi^4}{(n-2\cos 2\pi x)^2}+\frac{512\pi^4}{(n-2\cos 2\pi x)^2} \\
&\quad+\frac{4608\pi^4}{(n-2\cos 2\pi x)^2}+\frac{6144\pi^4}{(n-2\cos 2\pi x)^2} \\
&= \frac{11680\pi^4}{(n-2\cos 2\pi x)^2}.
\end{aligned}$$

So

$$|R_2|<\frac{4}{(2\pi n)^4}\int_0^1\frac{11680\pi^4}{(n-2\cos 2\pi x)^2}dx=\frac{2920}{n^3(n^2-4)^{\frac{3}{2}}}<\frac{1}{n^4}$$

for $n\ge 55$, here we need to use the integral

$$\int_0^1\frac{1}{(n-2\cos 2\pi x)^2}dx=\frac{n}{(n^2-4)^{\frac{3}{2}}}.$$

It means that

$$\sum_{k=1}^{n}\frac{1}{n-2\cos\frac{2k\pi}{n}}>\frac{n}{\sqrt{n^2-4}}-\frac{1}{n^4}$$

holds for $n\ge 55$. By Sage [15], one can easily check that the above result holds also for $3\le n\le 54$. This completes the proof.

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