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Asymptotic Expressions for Resolvent Energies of Paths and Cycles

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Abstract

The resolvent energy of an n-vertex graph G is a newly proposed graph-spectrum-based invariant, which is defined as $ER(G) = \sum_{i=1}^{n} \frac{1}{n-\lambda_i}$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G. A lot of properties for the resolvent energy of graphs have been established. In this paper, we will focus on the resolvent energies of paths and cycles, and reveal that the resolvent energies of the path P_n and the cycle C_n are, respectively, asymptotically equal to $\frac{n+1}{\sqrt{n^2-4}}$ and $\frac{n}{\sqrt{n^2-4}}$. Furthermore, we also show that for any tree or unicyclic graph G, when its order is sufficiently large, $ER(G) \approx 1$.

1 Introduction

Let G be a graph on n vertices, and $\mathbf{A}(G)$ be the adjacency matrix of G. Denote by $\lambda_1, \lambda_2, \ldots, \lambda_n$ the eigenvalues of G (i.e., the eigenvalues of $\mathbf{A}(G)$). In particular, the eigenvalues of G form the spectrum of G.

The resolvent matrix of $\mathbf{A}(G)$ is defined as [13]

$$\mathcal{R}_G(z) = (z\mathbf{I}_n - \mathbf{A}(G))^{-1},$$

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where z is a complex variable, and $\mathbf{I}_n$ represents the identity matrix of order n. Clearly, $\mathcal{R}(z)$ is definable when $z \neq \lambda_i$ for $i = 1, 2, \ldots, n$, in that case, the eigenvalues of $\mathcal{R}(z)$ are

$$\frac{1}{z-\lambda_1}, \frac{1}{z-\lambda_2}, \ldots, \frac{1}{z-\lambda_n}.$$

The energy of graphs is one of the most well-known and meaningful topological indices in theoretical chemistry, which is defined as [5]

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

The energy of graphs is investigated extensively and intensively in the past several decades, and result in a large number of results, e.g., see the monograph [12]. In the recent one decade, based on the spectra (eigenvalues) of more matrices induced by graphs, not confined to the adjacency matrix, other types of energies of graphs were emerged, e.g., Laplacian energy [10], skew energy [1], incidence energy [11]. More results on a variety of energies of graphs can also be referred to the monograph [9].

Recently, Gutman *et al.* [6] proposed a new type of energy, called resolvent energy, based on the spectrum (eigenvalues) of the resolvent matrix

$$\mathcal{R}_G(n) = (n\mathbf{I}_n - \mathbf{A}(G))^{-1} .$$

Notices that the eigenvalues of $\mathcal{R}_G(n)$ are

$$\frac{1}{n-\lambda_1}, \frac{1}{n-\lambda_2}, \ldots, \frac{1}{n-\lambda_n},$$

thus the resolvent energy of G is naturally defined as [6, 7]

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

As the pioneering paper for the resolvent energy of graphs, Gutman *et al.* [6] revealed some interesting and remarkable properties for the resolvent energy of graphs, including the relationship between the resolvent energy and spectral moments of graphs, some bounds for the resolvent energy of graphs, the extremal resolvent energy of trees. Later, the extremal resolvent energies of unicyclic graphs, bicyclic graphs, and tricyclic graphs are determined in [2].

In the light of the spectra of paths and cycles are well-known, and motivated by [4, 8], we are aware of that the definition of definite integral is one of the feasible ways to estimate the graph-spectrum-based invariants for paths and cycles. Based on that, in this paper we put our emphasis on the estimation of resolvent energies of paths and cycles, and deduce that the resolvent energies of the path P_n and the cycle C_n are, respectively, asymptotically equal to $\frac{n+1}{\sqrt{n^2-4}}$ and $\frac{n}{\sqrt{n^2-4}}$. Furthermore, we also show that for any tree or unicyclic graph G, when its order is sufficiently large, $ER(G) \approx 1$.

2 Preliminaries

The spectra of paths and cycles are well-known, e.g., see [3, pp. 72–73].

Lemma 2.1 *The eigenvalues of P_n are $2\cos\frac{k\pi}{n+1}$ for $k = 1, 2, \ldots, n$, and the eigenvalues of C_n are $2\cos\frac{2k\pi}{n}$ for $k = 1, 2, \ldots, n$.*

The calculation of the following two integrals is easy, thus we omit the proof here.

Lemma 2.2 *For fixed n, we have*

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

which implies that

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

From the definition of definite integral, we can get the following lemma immediately.

Lemma 2.3 *Let $f(x)$ be an integrable function with respect to x over the interval $[a, b]$, and t be a fixed positive integer.*

(i) If $f(x)$ is an increasing function on $x \in [a, b]$, then

$$\frac{b-a}{t} \sum_{k=0}^{t-1} f\left(a + \frac{(b-a)k}{t}\right) \leqslant \int_a^b f(x)dx \leqslant \frac{b-a}{t} \sum_{k=1}^{t} f\left(a + \frac{(b-a)k}{t}\right).$$

(ii) If $f(x)$ is a decreasing function on $x \in [a, b]$, then

$$\frac{b-a}{t} \sum_{k=1}^{t} f\left(a + \frac{(b-a)k}{t}\right) \leqslant \int_a^b f(x)dx \leqslant \frac{b-a}{t} \sum_{k=0}^{t-1} f\left(a + \frac{(b-a)k}{t}\right).$$

Let $\phi(G, \lambda)$ be the characteristic polynomial of G, i.e., the characteristic polynomial of the adjacency matrix $\mathbf{A}(G)$.

In [6], Gutman *et al.* showed that one may calculate the resolvent energy of graphs by using only the characteristic polynomial of that graph without knowing the spectrum.

Lemma 2.4 [6, Theorem 8] *Let G be a graph on n vertices. Then*

$$ER(G) = \frac{\phi'(G,n)}{\phi(G,n)}\,,$$

where $\phi'(G,\lambda)$ is the derivative of $\phi(G,\lambda)$.

3 Asymptotic expression for resolvent energy of paths

In this section, we present the asymptotic expression for the resolvent energy of paths, i.e.,

$$ER(P_n) \approx \frac{n+1}{\sqrt{n^2-4}}$$

when n is sufficiently large.

First we establish the lower and upper bounds for $ER(P_n)$.

Lemma 3.1 *For $n \geqslant 3$, we have*

$$ER(P_n) \geqslant \frac{n+1}{\sqrt{n^2-4}} - \frac{1}{n-2}\,.$$

Proof: First, from Lemma 2.1, we know that the eigenvalues of P_n are $2\cos\frac{k\pi}{n+1}$ for $k = 1, 2, \ldots, n$, thus

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

From Lemma 2.2, we know that $\frac{1}{n-2\cos x}$ is an integrable function with respect to x over the interval $[0, \pi]$. Moreover, note that the function $\frac{1}{n-2\cos x}$ is a decreasing function on $x \in [0, \pi]$, now from Lemma 2.3 (ii), by setting $f(x) = \frac{1}{n-2\cos x}$, $a = 0$, $b = \pi$, and $t = n + 1$, we can get that

$$\begin{aligned}
\int_0^{\pi} \frac{1}{n-2\cos x}dx &\leqslant \frac{\pi}{n+1}\sum_{k=0}^{n} \frac{1}{n-2\cos\frac{k\pi}{n+1}} \\
&= \frac{\pi}{n+1}\left(\sum_{k=1}^{n} \frac{1}{n-2\cos\frac{k\pi}{n+1}} + \frac{1}{n-2\cos 0}\right) \\
&= \frac{\pi}{n+1}\left(ER(P_n) + \frac{1}{n-2}\right)\,.
\end{aligned}$$

Finally, together with $\int_0^{\pi} \frac{1}{n-2\cos x}dx = \frac{\pi}{\sqrt{n^2-4}}$ from Lemma 2.2, we have

$$ER(P_n) \geqslant \frac{n+1}{\sqrt{n^2-4}} - \frac{1}{n-2}\,,$$

as desired. ■

Similar to the proof of Lemma 3.1, we can get a upper bound for $ER(P_n)$.

Lemma 3.2 *For $n \geqslant 3$, we have*

$$ER(P_n) \leqslant \frac{n+1}{\sqrt{n^2-4}} - \frac{1}{n+2}.$$

Combining Lemmas 3.1 and 3.2, we have

$$\frac{n+1}{\sqrt{n^2-4}} - \frac{1}{n-2} \leqslant ER(P_n) \leqslant \frac{n+1}{\sqrt{n^2-4}} - \frac{1}{n+2},$$

which is equivalent to

$$\frac{1}{n+2} \leqslant \frac{n+1}{\sqrt{n^2-4}} - ER(P_n) \leqslant \frac{1}{n-2}.$$

Now we can deduce the asymptotic expression for $ER(P_n)$ easily.

Proposition 3.1 *The resolvent energy of the cycle P_n is asymptotically equal to $\frac{n+1}{\sqrt{n^2-4}}$, i.e.,*

$$ER(P_n) = \frac{n+1}{\sqrt{n^2-4}} + o(1).$$

So when n is sufficiently large,

$$ER(P_n) \approx \frac{n+1}{\sqrt{n^2-4}},$$

and the error is between $\frac{1}{n+2}$ and $\frac{1}{n-2}$.

On the other hand, we also take into account the expression for $ER(S_n)$, where S_n represents the star on n vertices. It is easily verified that the characteristic polynomial of S_n is

$$\phi(S_n, \lambda) = \lambda^{n-2}(\lambda^2 - n + 1).$$

From Lemma 2.4, we get

$$ER(S_n) = \frac{n^3 - n^2 + 3n - 2}{n^3 - n^2 + n}.$$

Now combining the resolvent energies of P_n and S_n, we can get the approximate values for the resolvent energies of all trees.

Corollary 3.1 *Let G be a tree on n vertices. If n is sufficiently large, then $ER(G) \approx 1$.*

Proof: Recall that Gutman *et al.* [6] showed that the maximum and minimum resolvent energies of trees are, respectively, attained by S_n and P_n, i.e.,

$$ER(P_n) \leqslant ER(G) \leqslant ER(S_n).$$

Notice that

$$\lim_{n\to\infty} ER(P_n) = \lim_{n\to\infty} ER(S_n) = 1\,,$$

which implies that $ER(P_n) \approx 1$ and $ER(S_n) \approx 1$ when n is sufficiently large, thus $ER(G) \approx 1$ follows. ■

Gutman *et al.* [6] have showed that for any graph G, $ER(G) \geqslant 1$ with equality if and only if G is an edgeless graph. Now Corollary 3.1 reflects that the resolvent energy of every tree is infinitely close to 1 if the order of that tree is sufficiently large.

4 Asymptotic expression for resolvent energy of cycles

In this section, we turn to research the resolvent energy of cycles, and show that

$$ER(C_n) \approx \frac{n}{\sqrt{n^2-4}}$$

when n is sufficiently large.

First, we present the lower and upper bounds for $ER(C_n)$.

Lemma 4.1 *For $n \geqslant 3$,*

(i) if n is even, then

$$ER(C_n) \geqslant \frac{n}{\sqrt{n^2-4}} - \frac{4}{n^2-4}\,;$$

(ii) if n is odd, then

$$ER(C_n) \geqslant \frac{n}{\sqrt{n^2-4}} - \frac{8}{n^2-4}\,.$$

Proof: We only prove (i), i.e., the case when n is even. The proof of (ii) (i.e., the case when n is odd) is similar.

Suppose that n is even.

First, from Lemma 2.1, we know that the eigenvalues of C_n are $2\cos\frac{2k\pi}{n}$ for $k = 1, 2, \ldots, n$, thus

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

Next we consider the relationship between $\int_0^{2\pi} \frac{1}{n-2\cos x}dx$ and $\sum_{k=1}^{n} \frac{1}{n-2\cos\frac{2k\pi}{n}}$ (i.e., $ER(C_n)$). From Lemma 2.2, we know that $\frac{1}{n-2\cos x}$ is an integrable function with respect to x over the intervals $[0,\pi]$ and $[\pi, 2\pi]$.

On one hand, note that the function $\frac{1}{n-2\cos x}$ is a decreasing function on $x \in [0,\pi]$, from Lemma 2.3 (ii), by setting $f(x) = \frac{1}{n-2\cos x}$, $a = 0$, $b = \pi$, and $t = \frac{n}{2}$, we can get that

$$\int_0^{\pi} \frac{1}{n-2\cos x}dx \leqslant \frac{2\pi}{n}\sum_{k=0}^{\frac{n}{2}-1} \frac{1}{n-2\cos\frac{2k\pi}{n}}. \tag{1}$$

On the other hand, note that the function $\frac{1}{n-2\cos x}$ is an increasing function on $x \in [\pi, 2\pi]$, from Lemma 2.3 (i), by setting $f(x) = \frac{1}{n-2\cos x}$, $a = \pi$, $b = 2\pi$, and $t = \frac{n}{2}$, we can get that

$$\begin{aligned}
\int_{\pi}^{2\pi} \frac{1}{n-2\cos x}dx &\leqslant \frac{2\pi}{n}\sum_{k=1}^{\frac{n}{2}} \frac{1}{n-2\cos\left(\pi+\frac{2k\pi}{n}\right)} \\
&= \frac{2\pi}{n}\sum_{k=1}^{\frac{n}{2}} \frac{1}{n-2\cos\frac{2\pi}{n}\left(k+\frac{n}{2}\right)} \\
&= \frac{2\pi}{n}\sum_{k=\frac{n}{2}+1}^{n} \frac{1}{n-2\cos\frac{2k\pi}{n}}.
\end{aligned} \tag{2}$$

Combining (1) and (2), we have

$$\begin{aligned}
\int_0^{2\pi} \frac{1}{n-2\cos x}dx &= \int_0^{\pi} \frac{1}{n-2\cos x}dx + \int_{\pi}^{2\pi} \frac{1}{n-2\cos x}dx \\
&\leqslant \frac{2\pi}{n}\left(\sum_{k=0}^{\frac{n}{2}-1} \frac{1}{n-2\cos\frac{2k\pi}{n}} + \sum_{k=\frac{n}{2}+1}^{n} \frac{1}{n-2\cos\frac{2k\pi}{n}}\right) \\
&\leqslant \frac{2\pi}{n}\left(\sum_{k=0}^{n} \frac{1}{n-2\cos\frac{2k\pi}{n}} - \frac{1}{n-2\cos\pi}\right) \\
&= \frac{2\pi}{n}\left(\sum_{k=1}^{n} \frac{1}{n-2\cos\frac{2k\pi}{n}} + \frac{1}{n-2\cos 0} - \frac{1}{n-2\cos\pi}\right) \\
&= \frac{2\pi}{n}\left(ER(C_n) + \frac{1}{n-2} - \frac{1}{n+2}\right) \\
&= \frac{2\pi}{n}\left(ER(C_n) + \frac{4}{n^2-4}\right).
\end{aligned}$$

Finally, together with $\int_0^{2\pi} \frac{1}{n-2\cos x}dx = \frac{2\pi}{\sqrt{n^2-4}}$ from Lemma 2.2, we have

$$ER(C_n) \geqslant \frac{n}{\sqrt{n^2-4}} - \frac{4}{n^2-4}.$$

So (i) follows.

For the case when n is odd, similar to the arguments for the case when n is even as above, we can deduce that

$$ER(C_n) \geqslant \frac{n}{\sqrt{n^2-4}} + 2\left(\frac{1}{n+2\cos\frac{\pi}{n}} - \frac{1}{n-2}\right)$$

$$\geqslant \frac{n}{\sqrt{n^2-4}} + 2\left(\frac{1}{n+2} - \frac{1}{n-2}\right)$$
$$= \frac{n}{\sqrt{n^2-4}} - \frac{8}{n^2-4}\,.$$

So (ii) follows. ■

Similar to the proof of Lemma 4.1, we can get a upper bound for $ER(C_n)$.

Lemma 4.2 *For $n \geqslant 3$,*

(i) if n is even, then

$$ER(C_n) \leqslant \frac{n}{\sqrt{n^2-4}} + \frac{4}{n^2-4}\,;$$

(ii) if n is odd, then

$$ER(C_n) \leqslant \frac{n}{\sqrt{n^2-4}} + \frac{8}{n^2-4}\,.$$

Combining Lemmas 4.1 and 4.2, we have

$$\frac{n}{\sqrt{n^2-4}} - \frac{8}{n^2-4} \leqslant ER(C_n) \leqslant \frac{n}{\sqrt{n^2-4}} + \frac{8}{n^2-4}\,,$$

which is equivalent to

$$\left|ER(C_n) - \frac{n}{\sqrt{n^2-4}}\right| \leqslant \frac{8}{n^2-4}\,.$$

Now the asymptotic expression for $ER(C_n)$ follows easily.

Proposition 4.1 *The resolvent energy of the cycle C_n is asymptotically equal to $\frac{n}{\sqrt{n^2-4}}$, i.e.,*

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

So when n is sufficiently large,

$$ER(C_n) \approx \frac{n}{\sqrt{n^2-4}}\,,$$

and the error is at most $\frac{8}{n^2-4}$.

On the other hand, let us consider the resolvent energy of S_n^+, where S_n^+ is the unicyclic graph obtained from S_n by adding an edge between two terminal vertices. It is easily verified that the characteristic polynomial of S_n^+ is

$$\phi(S_n^+, \lambda) = \lambda^{n-4}(\lambda^4 - n\lambda^2 - 2\lambda + n - 3)\,.$$

From Lemma 2.4, we get

$$ER(S_n^+) = \frac{n^5 - n^4 + 2n^3 - n^2 - n + 12}{n^5 - n^4 - n^2 - 3n}\,.$$

Finally combining the resolvent energies of C_n and S_n^+, we get the approximate values for the resolvent energies of all unicyclic graphs.

Corollary 4.1 *Let G be a unicyclic graph on n vertices. If n is sufficiently large, then $ER(G) \approx 1$.*

Proof: Recall that Allem *et al.* [2] showed that the maximum and minimum resolvent energies of unicyclic graphs are, respectively, attained by S_n^+ and C_n, i.e.,

$$ER(C_n) \leqslant ER(G) \leqslant ER(S_n^+)\,.$$

Notice that

$$\lim_{n\to\infty} ER(C_n) = \lim_{n\to\infty} ER(S_n^+) = 1\,,$$

which implies that $ER(C_n) \approx 1$ and $ER(S_n^+) \approx 1$ when n is sufficiently large, thus $ER(G) \approx 1$ follows. ■

As a consequence of Corollary 4.1, it follows that the resolvent energy of every unicyclic graph is infinitely close to 1 if the order of that unicyclic graph is sufficiently large.

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