THE POSITIVITY OF NUMBER SEQUENCES AND THE RAMANUJAN GRAPHS

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Abstract. Let $X$ denote a connected $(q+1)$-regular undirected graph of finite order $n$. The graph $X$ is called Ramanujan whenever $|\lambda| \leq 2q^{\frac{1}{2}}$ for all nontrivial eigenvalues $\lambda$ of $X$. We consider the variant $\Xi(u)$ of the Ihara zeta function $Z(u)$ of $X$ defined by

$$
\Xi(u) = \begin{cases} 
(1-u)(1-qu)(1-q^{\frac{1}{2}}u)^{2n-2}(1-u^2)^{\frac{n(q-1)}{2}}Z(u) & \text{if } X \text{ is nonbipartite,} \\
(1-q^2u^2)(1-q^{\frac{1}{2}}u)^{2n-4}(1-u^2)^{\frac{n(q-1)}{2}+1}Z(u) & \text{if } X \text{ is bipartite.}
\end{cases}
$$

The functional equation for $\Xi(u)$ is $\Xi(q^{-1}u^{-1}) = \Xi(u)$. Let $\{h_k\}_{k=1}^{\infty}$ denote the number sequence given by

$$
du \ln \Xi(q^{-\frac{1}{2}}u) = \sum_{k=0}^{\infty} h_{k+1}u^{k}.
$$

In this paper we establish the equivalence of the following statements: (i) $X$ is Ramanujan; (ii) $h_k \geq 0$ for all $k \geq 1$; (iii) $h_k \geq 0$ for infinitely many even $k \geq 2$. Furthermore we derive the Hasse–Weil bound for the Ramanujan graphs.

Keywords: Hasse–Weil bound, Ihara zeta function, Li’s criterion, Ramanujan graphs.

1. Introduction

The motivation of this paper originates from developing a graph theoretical counterpart of the following sufficient and necessary condition for the Riemann hypothesis. Recall that the Riemann zeta function $\zeta(s)$ is the analytic continuation of

$$
\sum_{n=1}^{\infty} \frac{1}{n^s}.
$$

The negative even integers are trivial zeros of $\zeta(s)$ and the Riemann hypothesis asserts that the real part of every nontrivial zero of $\zeta(s)$ is $\frac{1}{2}$. The Riemann xi function $\xi(s)$ is a variation of $\zeta(s)$ defined by

$$
\xi(s) = \frac{1}{2}s(s-1)\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\zeta(s)
$$

where $\Gamma(s)$ is the Gamma function. The functional equation for $\xi(s)$ is

$$
\xi(1-s) = \xi(s).
$$

Let $\{\lambda_k\}_{k=1}^{\infty}$ denote the number sequence given by

$$
\frac{d}{dz} \ln \xi\left(\frac{1}{1-z}\right) = \sum_{k=0}^{\infty} \lambda_{k+1}z^{k}.
$$

Li’s criterion [3] states the Riemann hypothesis holds if and only if $\lambda_k \geq 0$ for all $k \geq 1$.

Fix two integers $q \geq 1$ and $n \geq 3$. Assume that $X$ is a connected $(q+1)$-regular undirected graph of finite order $n$. A walk is a nonempty finite sequence of edges which joins vertices. The

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length of a walk is the number of edges in the walk. A cycle is meant to be a closed walk. A cycle is said to be geodesic if all shifted cycles are backtrackless. For all \( k \geq 1 \) let \( N_k \) denote the number of geodesic cycles on \( X \) of length \( k \). The \textit{Ihara zeta function} \( Z(u) \) of \( X \) is the analytic continuation of

\[
\exp \left( \sum_{k=1}^{\infty} \frac{N_k}{k} u^k \right).
\]

The poles of \( Z(u) \) with values \( \pm 1 \) and \( \pm q^{-1} \) are called trivial poles. Recall that an eigenvalue of \( X \) with absolute value \( q + 1 \) is called a trivial eigenvalue. The graph \( X \) is said to be \textit{Ramanujan} whenever

\[
|\lambda| \leq 2q^{\frac{1}{2}}
\]

for all nontrivial eigenvalues \( \lambda \) of \( X \). The graph \( X \) is Ramanujan if and only if all nontrivial poles of \( Z(u) \) have the same absolute value \( q^{-\frac{1}{2}} \), which is similar to the Riemann hypothesis by writing \( u = q^{-s} \).

We define the function \( \Xi(u) \) by

\[
\Xi(u)^{-1} = \begin{cases} 
(1 - u)(1 - qu)(1 - q^{\frac{1}{2}} u)^{2n-2}(1 - u^2)^{n(q-1)} Z(u) & \text{if } X \text{ is nonbipartite}, \\
(1 - q^2 u^2)(1 - q^{\frac{1}{2}} u)^{2n-4}(1 - u^2)^{n(q-1)} Z(u) & \text{if } X \text{ is bipartite}.
\end{cases}
\]

The function \( \Xi(u) \) is considered as the \textit{Ihara xi function} which satisfies the functional equation

\[ \Xi(q^{-\frac{1}{2}} u^{-1}) = \Xi(u). \]

If we set \( u = q^{-s} \), then this becomes a functional equation relating \( 1 - s \) and \( s \) similar to the Riemann xi function.

\textbf{Definition 1.1.} Let \( \{h_k\}_{k=1}^{\infty} \) denote the number sequence given by

\[
\frac{d}{du} \ln (q^{\frac{1}{2}} u) = \sum_{k=0}^{\infty} h_{k+1} u^k.
\]

The main results of this paper are as follows:

\textbf{Theorem 1.2.} If there is a positive even integer \( k \) with \( h_k \geq 0 \) then

\[
|\lambda| \leq \begin{cases} 
1 + \frac{\sqrt{4n-7}}{4n-7} q^{\frac{1}{2}} & \text{if } X \text{ is nonbipartite}, \\
1 + \frac{\sqrt{2n-7}}{2n-7} q^{\frac{1}{2}} & \text{if } X \text{ is bipartite}
\end{cases}
\]

for all nontrivial eigenvalues \( \lambda \) of \( X \).

\textbf{Theorem 1.3.} The following are equivalent:

(i) \( X \) is Ramanujan.

(ii) \( h_k \geq 0 \) for all \( k \geq 1 \).

(iii) \( h_k \geq 0 \) for infinitely many even \( k \geq 2 \).

\textbf{Theorem 1.4.} (i) If \( X \) is nonbipartite, then \( X \) is Ramanujan if and only if

\[
|N_k - q^k - 1| \leq 2(n - 1)q^{\frac{k}{2}} \quad \text{for all odd } k;
\]

\[
|N_k - n(q - 1) - q^k - 1| \leq 2(n - 1)q^{\frac{k}{2}} \quad \text{for all even } k.
\]

(ii) If \( X \) is bipartite, then \( X \) is Ramanujan if and only if

\[
|N_k - n(q - 1) - 2q^k - 2| \leq 2(n - 2)q^{\frac{k}{2}} \quad \text{for all even } k.
\]
Theorem 1.2 is an improvement of the implication from Theorem 1.3(iii) to Theorem 1.3(i). The equivalence of Theorem 1.3(i), (ii) is an analogue of Li’s criterion. Theorem 1.4 is an analogue of the Hasse–Weil bound [8].

The paper is organized as follows: In §2 we give some preliminaries on \( \mathbb{Z}(u) \) and \( \Xi(u) \). In §3 we derive three formulae for \( \{h_k\}_{k=1}^\infty \). In §4 we prove Theorems 1.2–1.4. In §5 we discuss the behavior of \( \{h_{2k}\}_{k=1}^\infty \) when \( X \) is not Ramanujan.

2. The Ihara zeta and \( \Xi \) functions

Let \( \text{Spec}(X) \) denote the spectrum of \( X \); that is the multiset of all eigenvalues of \( X \) with geometric multiplicities. Ihara’s theorem [2] states that \( Z(u) \) is a rational function of the form

\[
Z(u)^{-1} = (1 - u^2)^{\frac{n(q-1)}{2}} \prod_{\lambda \in \text{Spec}(X)} (1 - \lambda u + qu^2).
\]

Substituting (3) into (2) yields that

\[
\Xi^{-1}(u) = \begin{cases} 
\frac{(1 - u)(1 - qu)(1 - q^{\frac{1}{2}}u)^{2n-2}}{\prod_{\lambda \in \text{Spec}(X)} (1 - \lambda u + qu^2)} & \text{if } X \text{ is nonbipartite}, \\
\frac{(1 - u^2)(1 - q^2u^2)(1 - q^{\frac{1}{2}}u)^{2n-4}}{\prod_{\lambda \in \text{Spec}(X)} (1 - \lambda u + qu^2)} & \text{if } X \text{ is bipartite}.
\end{cases}
\]

Let \( \text{Spec}^*(X) \) denote the multiset of all nontrivial eigenvalues of \( X \) with geometric multiplicities. Since \( X \) is a connected \((q + 1)\)-regular undirected graph, it follows that

\[
\text{Spec}^*(X) = \begin{cases} 
\text{Spec}(X) \setminus \{q + 1\} & \text{if } X \text{ is nonbipartite}, \\
\text{Spec}(X) \setminus \{\pm(q + 1)\} & \text{if } X \text{ is bipartite}.
\end{cases}
\]

Combined with (4) we obtain that

\[
\Xi(u) = \prod_{\lambda \in \text{Spec}^*(X)} \frac{1 - \lambda u + qu^2}{(1 - q^{\frac{1}{2}}u)^2}.
\]

**Proposition 2.1.** \( \Xi(u) \) satisfies the functional equation \( \Xi(q^{-1}u^{-1}) = \Xi(u) \).

**Proof.** It is routine to verify the proposition by using (5). \qed

3. Formulae for \( h_k \)

Recall the sequence \( \{h_k\}_{k=1}^\infty \) from Definition 1.1. In this section we give two combinatorial formulae for \( \{h_k\}_{k=1}^\infty \) and a formula for \( \{h_{2k}\}_{k=1}^\infty \) in terms of the Chebyshev polynomials.

**Proposition 3.1.** (i) If \( X \) is nonbipartite then

\[
h_k = \begin{cases} 
2(n - 1) + q^{\frac{k}{2}} + q^{-\frac{k}{2}} - q^{-\frac{k}{2}}N_k & \text{for all odd } k, \\
2(n - 1) + q^{\frac{k}{2}} + q^{-\frac{k}{2}} - q^{-\frac{k}{2}}(N_k - n(q - 1)) & \text{for all even } k.
\end{cases}
\]

(ii) If \( X \) is bipartite then

\[
h_k = \begin{cases} 
2(n - 2) & \text{for all odd } k, \\
2(n - 2 + q^{\frac{k}{2}} + q^{-\frac{k}{2}}) - q^{-\frac{k}{2}}(N_k - n(q - 1)) & \text{for all even } k.
\end{cases}
\]
Proof. Taking logarithm on (1) yields that
\[
\ln Z(u) = \sum_{k=1}^{\infty} \frac{N_k}{k} u^k.
\]
Evaluate \(h_k\) by using (2) and (6) directly. □

Let \(\{T_k(x)\}_{k=0}^{\infty}\) denote the polynomials defined by
\[
xT_k(x) = T_{k+1}(x) + T_{k-1}(x)
\]
for all \(k \geq 1\) with \(T_0(x) = 2\) and \(T_1(x) = x\) [1, §2.3]. Note that \(\frac{1}{2}T_k(2x)\) is the \(k\)th Chebyshev polynomial of the first kind for all \(k \geq 0\) [6].

**Lemma 3.2** ([1, 6]). \(T_k(x + x^{-1}) = x^k + x^{-k}\) for all \(k \geq 0\).

Given a multiset \(S\) of numbers and a constant \(c\), we let \(cS\) denote the multiset consisting of \(cs\) for all \(s \in S\).

**Proposition 3.3.** For all \(k \geq 1\) the following equation holds:
\[
h_k = 2|\text{Spec}^*(X)| - \sum_{s \in q^{-1/2}\text{Spec}^*(X)} T_k(s).
\]

Proof. Let \(S = q^{-\frac{1}{2}}\text{Spec}^*(X)\). Applying (5) yields that
\[
\ln \Xi(q^{-\frac{1}{2}}u) = \sum_{s \in S} \ln(1 - su + u^2) - 2|S| \ln(1 - u)
\]
\[
= \sum_{s \in S} \ln(1 - su + u^2) + 2|S| \sum_{k=1}^{\infty} \frac{u^k}{k}.
\]
Let \(s \in S\) be given. Write \(s = \alpha + \alpha^{-1}\) for some nonzero complex number \(\alpha\). Then
\[
\ln(1 - su + u^2) = \ln(1 - \alpha u) + \ln(1 - \alpha^{-1} u) = -\sum_{k=1}^{\infty} \frac{\alpha^k + \alpha^{-k}}{k} u^k.
\]
It follows from Lemma 3.2 that \(T_k(s) = \alpha^k + \alpha^{-k}\). By the above comments we have
\[
\ln \Xi(q^{-\frac{1}{2}}u) = \sum_{k=1}^{\infty} \frac{2|S| - \sum_{s \in S} T_k(s)}{k} u^k.
\]
Now the proposition follows by taking differential on both sides of the above equation. □

For convenience we define \((-1) = 1\) and \((-1) = 0\) for all \(k \geq 0\).

**Lemma 3.4** ([1, 6]). \(T_k(x) = \sum_{i=0}^{|\frac{k}{2}|} (-1)^i \left( \binom{k-i}{i} + \binom{k-i-1}{i-1} \right) x^{k-2i}\) for all \(k \geq 0\).

For all \(k \geq 1\) let \(C_k\) denote the number of the cycles on \(X\) of length \(k\) and define \(C_0 = n\).

**Proposition 3.5.** (i) If \(X\) is nonbipartite then
\[
h_k = 2(n - 1) + q^{-\frac{k}{2}} + q^{-\frac{k}{2}} - \sum_{i=0}^{|\frac{k}{2}|} (-1)^i q^{-\frac{k-2i}{2}} \left( \binom{k-i}{i} + \binom{k-i-1}{i-1} \right) C_{k-2i}
\]
for all \(k \geq 1\).
(ii) If $X$ is bipartite then

$$h_k = \begin{cases} 
2(n-2) & \text{for all odd } k, \\
2(n-2 + \frac{k}{2} + q^{-\frac{k}{2}}) - \sum_{i=0}^{\frac{k}{2}} (-1)^i q^{-\frac{k-2i}{2}} \left( \binom{k-i}{i} + \binom{k-i-1}{i-1} \right) C_{k-2i} & \text{for all even } k.
\end{cases}$$

Proof. Evaluate $h_k$ by using Lemmas 3.2, 3.4 and Proposition 3.3 along with the fact

$$\sum_{\lambda \in \text{Spec}^*(X)} \lambda^i = \begin{cases} 
C_i - (q+1)^i & \text{if } X \text{ is nonbipartite,} \\
C_i - (1 + (-1)^i)(q+1)^i & \text{if } X \text{ is bipartite}
\end{cases}$$

for all $i \geq 0$. □

Combining Propositions 3.1 and 3.5 we have the following corollary:

**Corollary 3.6.** The following equation holds:

$$N_k = \begin{cases} 
\frac{k}{2} - 1 \sum_{i=0}^{\frac{k}{2}} (-q)^i \left( \binom{k-i}{i} + \binom{k-i-1}{i-1} \right) C_{k-2i} & \text{for all odd } k, \\
n(q-1) + \frac{k}{2} \sum_{i=0}^{\frac{k}{2}} (-q)^i \left( \binom{k-i}{i} + \binom{k-i-1}{i-1} \right) C_{k-2i} & \text{for all even } k.
\end{cases}$$

4. **Proof of the main results**

In this section we show Theorems 1.2–1.4.

**Lemma 4.1.** For all $k \geq 1$ the coefficient $h_k \geq 0$ if and only if

$$\frac{1}{2|\text{Spec}^*(X)|} \sum_{s \in q^{-1/2}\text{Spec}^*(X)} T_k(s) \leq 1.$$

Proof. Immediate from Proposition 3.3 □

**Lemma 4.2** ([6]). $T_k(2 \cos \theta) = 2 \cos k \theta$ for all $k \geq 0$ and all real numbers $\theta$.

**Lemma 4.3.** If $s$ is a real number with $|s| \leq 2$ then $|T_k(s)| \leq 2$ for all $k \geq 0$.

Proof. Immediate from Lemma 4.2 □

**Lemma 4.4.** If $X$ is Ramanujan then $|T_k(s)| \leq 2$ for all $k \geq 0$ and all $s \in q^{-1/2}\text{Spec}^*(X)$.

Proof. Since $X$ is Ramanujan if and only if $|s| \leq 2$ for all $s \in q^{-1/2}\text{Spec}^*(X)$, the lemma is immediate from Lemma 4.3 □

**Lemma 4.5** ([6]). $T_k(x) = 2 \left( \frac{x}{2} \right)^k \sum_{i=0}^{\lfloor \frac{k}{2} \rfloor} \left( \frac{x}{2} \right)^i \left( 1 - \left( \frac{x}{2} \right)^{-2} \right)^i$ for all $k \geq 0$.

**Lemma 4.6.** If $s$ is a real number with $|s| > 2$ then $T_k(s) > 0$ for all even $k \geq 0$.

Proof. Immediate from Lemma 4.5 □
Proposition 4.7. Let $S$ denote a nonempty finite multiset consisting of real numbers. If there is a positive even integer $k$ with

$$
\frac{1}{2|S|} \sum_{s \in S} T_k(s) \leq 1
$$

then $|s| \leq 1 + \frac{\sqrt{4|S|} - 3}{\sqrt{4|S|} - 3 + 1}$ for all $s \in S$.

Proof. For convenience let

$$
\varepsilon = \frac{\sqrt{4|S|} - 3 - 1}{\sqrt{4|S|} - 3 + 1}.
$$

Suppose on the contrary that there is a real number $t \in S$ with

$$
|t| > 1 + \frac{\sqrt{4|S|} - 3}{\sqrt{4|S|} - 3 + 1}.
$$

Using (8) yields that $1 - \left(\frac{t}{2}\right)^2 > 1 - (1 - \varepsilon)^2 = 2\varepsilon - \varepsilon^2$. Since $0 < \varepsilon < 1$ we have $\varepsilon^2 < 2\varepsilon - \varepsilon^2$. Combined with Lemma 4.5 this implies

$$
\frac{1}{2} T_k(t) > \left(\frac{t}{2}\right)^k \sum_{i=0}^{\frac{k}{2}} \binom{k}{2i} \varepsilon^{2i} = \left(\frac{t}{2}\right)^k \frac{(1 + \varepsilon)^k + (1 - \varepsilon)^k}{2}.
$$

By Lemmas 4.3 and 4.6 we have $T_k(s) \geq -2$ for all $s \in S \setminus \{t\}$.

Combining (7) with the above comments yields that

$$
|S| \geq \frac{1}{2} \sum_{s \in S} T_k(s) = \frac{1}{2} T_k(t) + \frac{1}{2} \sum_{s \in S \setminus \{t\}} T_k(s) > \left(\frac{1}{2}\right)^k \frac{(1 + \varepsilon)^k + (1 - \varepsilon)^k}{2} - (|S| - 1).
$$

It leads to

$$
\left(\frac{t}{2}\right)^k < \frac{4|S| - 2}{(1 + \varepsilon)^k + (1 - \varepsilon)^k}.
$$

Since $k$ is even the inequality (9) implies that

$$
\left(\frac{t}{2}\right)^k \leq \frac{1}{(1 - \varepsilon)^k}.
$$

Combining (10) and (11) we see that

$$
\frac{1}{(1 - \varepsilon)^k} < \frac{4|S| - 2}{(1 + \varepsilon)^k + (1 - \varepsilon)^k}.
$$

Using the setting (8) it is routine to verify that both sides of (12) are equal, a contradiction. The proposition follows. \qed

Proof of Theorem 1.2. By Lemma 4.1 when $X$ is nonbipartite the result follows by applying Proposition 4.7 with $S$ replaced by $q^{-1/2}\text{Spec}^*(X)$.

Since $k$ is even and by Lemma 3.4 the polynomial $T_k(x)$ is an even function. Combined with Lemma 4.1 when $X$ is bipartite the result follows by applying Proposition 4.7 with $S$ chosen as the multiset of all positive numbers and a half number of zeros in $q^{-1/2}\text{Spec}^*(X)$. \qed

Proof of Theorem 1.3. (i) $\Rightarrow$ (ii): Combine Lemmas 4.1 and 4.4

(ii) $\Rightarrow$ (iii): It is obvious.

(iii) $\Rightarrow$ (i): Immediate from Theorem 1.2.
Lemma 4.8. If $X$ is Ramanujan then
\[ h_k \leq \begin{cases} 
4(n-1) & \text{if } X \text{ is nonbipartite,} \\
4(n-2) & \text{if } X \text{ is bipartite}
\end{cases} \]
for all $k \geq 1$.

Proof. By Proposition 3.3 and Lemma 4.4 the coefficient $h_k \leq 4|\text{Spec}^*(X)|$ for all $k \geq 1$. □

Proof of Theorem 1.4. Combine Theorem 1.3(i), (ii) and Proposition 3.1 along with Lemma 4.8. □

5. Behavior of $h_{2k}$

We end this paper with a remark on \{h_{2k}\}_{k=1}^{\infty} under the assumption that $X$ is not Ramanujan. Let $S$ denote the set of all nonzero complex numbers $\alpha$ with $\alpha + \alpha^{-1} \in q^{-1/2}\text{Spec}^*(X)$. For those $s \in q^{-1/2}\text{Spec}^*(X)$ with $|s| \leq 2$ the corresponding numbers $\alpha \in S$ have the same absolute value 1. By the assumption that $X$ is not Ramanujan there exists an $s \in q^{-1/2}\text{Spec}^*(X)$ with $|s| > 2$ and the corresponding numbers $\alpha \in S$ are real and $\alpha \neq \pm 1$. Let
\[ \mu = \max_{\alpha \in S} |\alpha| > 1. \]

Since the function $f(x) = x + x^{-1}$ is increasing on $(1, \infty)$, it follows that
\[ \mu + \mu^{-1} = \max_{\alpha \in S} |\alpha| + |\alpha|^{-1} = \max_{s \in q^{-1/2}\text{Spec}^*(X)} |s|. \]

Using Lemma 3.2 yields that
\[ \lim_{k \to \infty} \frac{T_{2k}(\alpha + \alpha^{-1})}{\mu^{2k}} = \begin{cases} 
0 & \text{if } \mu > |\alpha| \text{ and } \mu > |\alpha|^{-1}, \\
1 & \text{else}
\end{cases} \]
for all $\alpha \in S$. It follows from Proposition 3.3 that $h_{2k}$ is asymptotic to $-m\mu^{2k}$ as $k$ approaches to $\infty$, where $m$ is the number of $s \in q^{-1/2}\text{Spec}^*(X)$ with $|s| = \mu + \mu^{-1}$. Therefore the following corollary holds:

Corollary 5.1. If $X$ is not Ramanujan then
\[ q^{-\frac{1}{2}} \max |\lambda| = \lim_{k \to \infty} \sqrt{\frac{h_{2k+2}}{h_{2k}}} + \sqrt{\frac{h_{2k}}{h_{2k+2}}} \]
where max is over all nontrivial eigenvalues $\lambda$ of $X$.

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