A RECIPROCITY FORMULA FOR A COTANGENT SUM

S. BETTIN AND J. B. CONREY

1. Introduction

For a rational number $x = h/k$ with $(h,k) = 1$ and $k > 0$ define

$$c(x) = -\sum_{a=1}^{k-1} \frac{a}{k} \cot \frac{\pi a h}{k}.$$

The value of $c(x)$ is an algebraic number, i.e. $c : \mathbb{Q} \to \overline{\mathbb{Q}}$. Notice that c is odd and is periodic with period 1. Here is a table of c for a few rationals with small denominators:

x	$c(x)$
0	0
1	0
$\frac{1}{2}$	0
$\frac{1}{3}$	$\frac{1}{3\sqrt{3}}$
$\frac{1}{4}$	$\frac{1}{2}$
$\frac{1}{5}$	$\frac{(\sqrt{5}-1)\sqrt{5-\sqrt{5}}+3(\sqrt{5}+1)\sqrt{5+\sqrt{5}}}{10\sqrt{10}}$
$\frac{2}{5}$	$\frac{3(\sqrt{5}-1)\sqrt{5-\sqrt{5}}-(\sqrt{5}+1)\sqrt{5+\sqrt{5}}}{10\sqrt{10}}$
$\frac{1}{6}$	$\frac{7}{3\sqrt{3}}$
$\frac{5}{6}$	$\frac{-7}{3\sqrt{3}}$

Clearly, if $x \in \mathbf{Q}$ then $c(x)$ is contained in the cyclotomic field containing all roots of unity. Also, $ic(h/k)$ is purely imaginary and is in the cyclotomic field $\mathbf{Q}(e^{\pi i/k})$ of $2k$-th roots of unity. It is not hard to see that $c(h/k)$ is contained in the field $\mathbf{Q}(\cot \frac{\pi}{k})$ and that $x = \cot \frac{\pi}{k}$ satisfies the equation

$$\sum_{j=0}^{[(k-1)/2]} (-1)^j \binom{k}{2j+1} x^{k-2j-1} = 0.$$

If k is not a prime number, then this polynomial is reducible; in general the minimal polynomial of $\cot \frac{\pi}{k}$ is of degree $\phi(k)$ if k is not divisible by 4 and is of degree $\phi(k)/2$ when k is divisible by 4.

In this paper we prove the surprising result that $c(x)$ satisfies a reciprocity formula, somewhat analogous to the Dedekind sum, but apparently deeper. Let, as usual, $d(n)$ denote the number of positive divisors of n and let

$$E_1(z) = 1 - 4\sum_{n=1}^{\infty} d(n)e(nz)$$

be the weight 1 holomorphic Eisenstein series. Then $E_1(z)$ is periodic with period 1 but when $z \to -1/z$ it satisfies a period relation as follows. Let

$$\psi(z) = E_1(z) - (1/z)E_1(-1/z).$$

Using the theory of period functions of Maass forms developed by Lewis and Zagier [LZ] it can be shown (see Lemma 1) that $\psi(z)$ extends to an analytic function on the complex plane minus the non-positive real axis.

Theorem 1. *Let* $g(x) = \frac{ix}{2}\psi(x)$. *Then*

$$xc(x) + c(1/x) - \frac{1}{\pi\,\mathrm{Den}(x)} = g(x)$$

for all rational numbers $x > 0$, *where* $\mathrm{Den}(x) > 0$ *is the denominator of* x *when written in lowest terms.*

The function g, and in particular the Taylor coefficients at $x = 1$, have some remarkable properties. For $|x| < 1$, the function $g(x)$ may be expressed as

$$g(1+x) = \frac{1}{\pi}\sum_{n=0}^{\infty}(-1)^n g_n x^n$$

where $g_0 = -1$, $g_1 = -1/2$ and for $n \geq 2$,

$$g_n = \frac{1}{n(n+1)} + 2b_n + 2\sum_{j=0}^{n-2}\binom{n-1}{j} b_{j+2}$$

where

$$b_n = \frac{\zeta(n)B(n)}{n}$$

with B_n denoting the nth Bernoulli number. The coefficients are rational polynomials in π; for example, the coefficient of x^{20} is

$$\frac{1}{420} + \frac{\pi^2}{36} - \frac{19\pi^4}{600} + \frac{646\pi^6}{19845} - \frac{323\pi^8}{13500} + \frac{4199\pi^{10}}{343035} - \frac{154226363\pi^{12}}{36569373750} + \frac{1292\pi^{14}}{1403325}$$
$$-\frac{248571091\pi^{16}}{2170943775000} + \frac{1924313689\pi^{18}}{288905366499750} - \frac{30489001321\pi^{20}}{252669361772953125};$$

numerically, this is

$$0.00238095 + 0.274156 - 3.08462 + 31.2954 - 227.022 + 1146.32 - 3897.98 + 8398.51$$
$$-10308.6 + 5918.59 - 1058.25 = 0.0499998087\ldots.$$

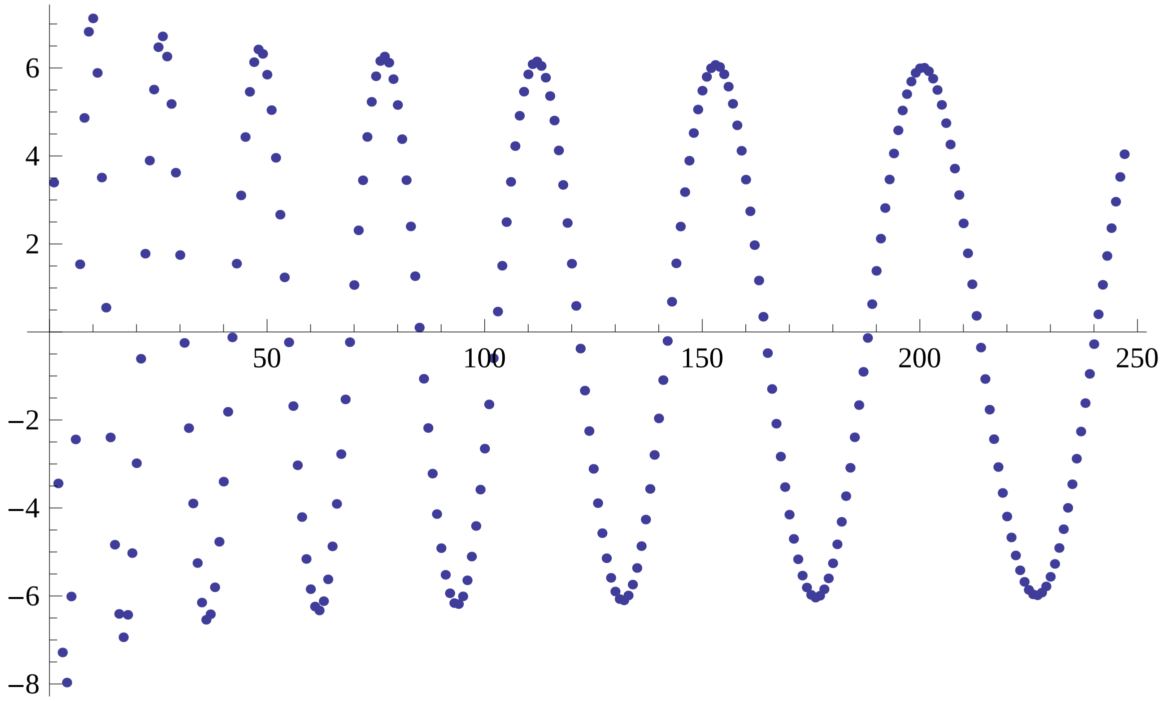

FIGURE 1. The plot of $n^{3/4}e^{2\sqrt{\pi n}}(g_n - 1/n)$ for $4 \leq n \leq 250$.

Notice how close this number is to $1/20$. Here is a table of the g_n for $3 \leq n \leq 10$ which illustrates how close g_n is to $1/n$.

n	3	4	5	6	7	8	9	10
$1/n$	0.333333	0.25	0.2	0.166667	0.142857	0.125	0.111111	0.1
g_n	0.357489	0.252001	0.199257	0.166023	0.142544	0.124888	0.111088	0.100007

Theorem 2. *We have*

$$g_n - \frac{1}{n} \sim 2^{5/4}\pi^{3/4}n^{-3/4}e^{-2\sqrt{\pi n}}\sin(2\sqrt{\pi n} + 3\pi/8)$$

as $n \to \infty$.

The remarkable asymptotics for $g_n - 1/n$ stated here were conjectured by Don Zagier (private communication). We remark that $c(x)$ is (nearly) an example of what Zagier calls a "quantum modular form" (see [Zag1]).

Corollary 1. *The numbers* $c(x)$ *can be computed to within a prescribed accuracy in a time that is polynomial in* $\log \mathrm{Den}(x)$.

The function $c(x)$ arises in a natural way in the Nyman–Beurling, Baez-Duarte reformulation of the Riemann Hypothesis (described below).

The results of this paper can be extended to a family of cotangent sums containing c; see [BC] where the same authors investigate these sums and provide other applications of the analytic continuation of the period function $\psi(x)$.

We would like to thank Ozlem Imamoglu for pointing us in the direction of period functions and we would like to thank Don Zagier for some enlightening conversations and helpful suggestions with this paper.

2. FURTHER BACKGROUND AND SOME PICTURES

The cotangent sum $c(x)$ arises in analytic number theory in the value at 0

$$D(0,x) = \frac{1}{4} + \frac{i}{2}c(x)$$

of $D(s,x)$, the Estermann function, defined for $\Re s > 1$ and $\Im x \geq 0$ by

$$D(s,x) = \sum_{n=1}^{\infty} \frac{d(n)e(nx)}{n^s}$$

where $d(n)$ is the number of positive integer divisors of n. In the case that $x \in \mathbb{Q}$, it is known that Estermann's function has a double pole at $s = 1$, and is analytic in the whole rest of the plane, and satisfies a functional equation which relates $D(1-s,x)$ with $D(s,x^*)$ and $D(s,-x^*)$, where, for $x \in \mathbb{Q}/\mathbb{Z}$ we define the involution $* : \mathbb{Q}/\mathbb{Z} \to \mathbb{Q}/\mathbb{Z}$ by $\mathrm{Den}(x^*) = \mathrm{Den}(x)$ and $\mathrm{Den}(x)^2 xx* \equiv 1 \bmod \mathrm{Den}(x)$. We have

$$D(s,x) \quad = \quad 2G(s)^2\,\mathrm{Den}(x)^{1-2s}\big(\cos\pi s\; D(1-s,-x^*) - D(1-s,x^*)\big) \tag{1}$$

where

$$G(s) = -i(2\pi)^{s-1}\Gamma(1-s).$$

These properties of D are useful in studying the asymptotics of the mean square of the Riemann zeta-function multiplied by a Dirichlet polynomial (see [BCHB]), which are needed, for example, for theorems which give a lower bound for the proportion of zeros of the Riemann zeta-function on the critical-line. See also [C] and [I]. The sum

$$V(h,k) := \sum_{a=1}^{k-1} \left(\left(\frac{ah}{k}\right)\right) \cot\frac{\pi a}{k} = -c(x^*),$$

known as the Vasyunin sum, arises in the study of the Riemann zeta-function by virtue of the formula (valid for $(h,k) = 1$):

$$\begin{aligned} b_{h,k} &:= \frac{1}{2\pi\sqrt{hk}} \int_{-\infty}^{\infty} |\zeta(1/2+it)|^2 (h/k)^{it} \frac{dt}{\frac{1}{4}+t^2} \\ &= \frac{\log 2\pi - \gamma}{2}\left(\frac{1}{h}+\frac{1}{k}\right) + \frac{k-h}{2hk}\log\frac{h}{k} - \frac{\pi}{2hk}\left(V(h,k)+V(k,h)\right); \end{aligned} \tag{2}$$

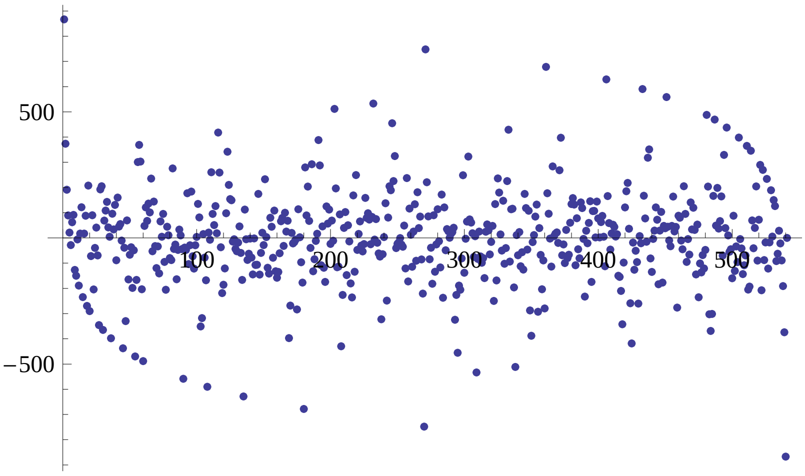

Figure 2. List plot of $c(h/541)$ for $1 \le h \le 541$.

(see [LR], for example), This formula is relevant to the Nyman-Beurling-Baez-Duarte-Vasyunin approach to the Riemann hypothesis which asserts that the Riemann Hypothesis is true if and only if $\lim_{N\to\infty} d_N = 0$ where

$$d_N^2 = \inf_{A_N} \frac{1}{2\pi} \int_{-\infty}^{\infty} |1 - \zeta A_N(1/2+it)|^2 \, \frac{dt}{\frac{1}{4}+t^2}$$

where the inf is over all Dirichlet polynomials $A_N(s) = \sum_{n=1}^{N} a_n n^{-s}$ of length N; see [Bag] for a nice account of the Nyman-Beurling approach to the Riemann Hypothesis with Baez-Duarte's significant contribution, and see [BDBLS] and [LR] for information about the Vasyunin sums, as well as interesting numerical experiments about d_N and the minimizing Dirichlet polynomials A_N. Thus, d_N^2 is a quadratic expression in the unknown quantities a_m with coefficients given in terms of the Vasyunn sums. The reciprocity formula presented in this paper for these sums reveals a previously unknown structure present in this quadratic expression for d_N^2.

Another expression for the $b_{h,k}$ is given by

$$b_{h,k} = \int_0^\infty \left\{ \frac{1}{hx} \right\} \left\{ \frac{1}{kx} \right\} \, dx$$

where $\{x\} = x - [x]$ is the fractional part of x.

Figure 2 shows a plot of the points $(x, c(x))$, for a fixed value of $\mathrm{Den}(x)$. Figure 3 illustrates a plot of $(x, c(x^*))$ with a fixed value of $\mathrm{Den}(x)$. Figure 4 shows the sum of $V(h,k)+V(k,h)$, which was studied in [BBDLS]. Finally, Figure 5 shows a plot of $xc(x) + c(1/x) - \frac{1}{\pi \,\mathrm{Den}(x)} = g(x)$.

Remark 1. *The nth Taylor coefficient of $\pi g(z)$ at $z = 1$ is the value at π of a rational polynomial of degree n.*

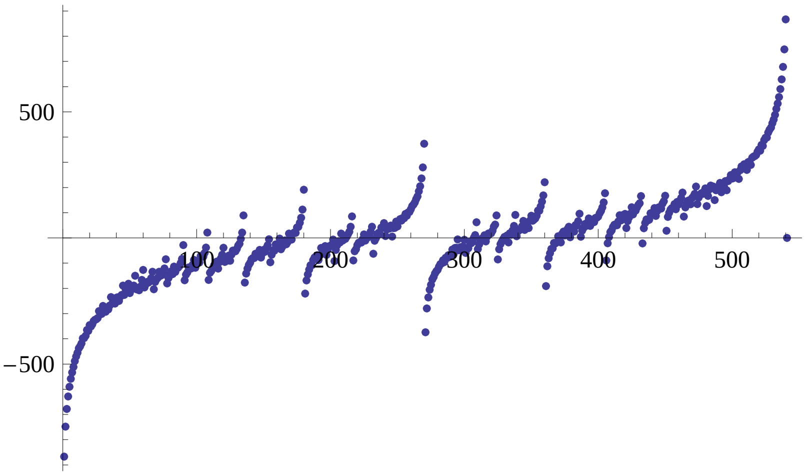

FIGURE 3. List plot of $V(h, 541)$ with $1 \leq h \leq 541$

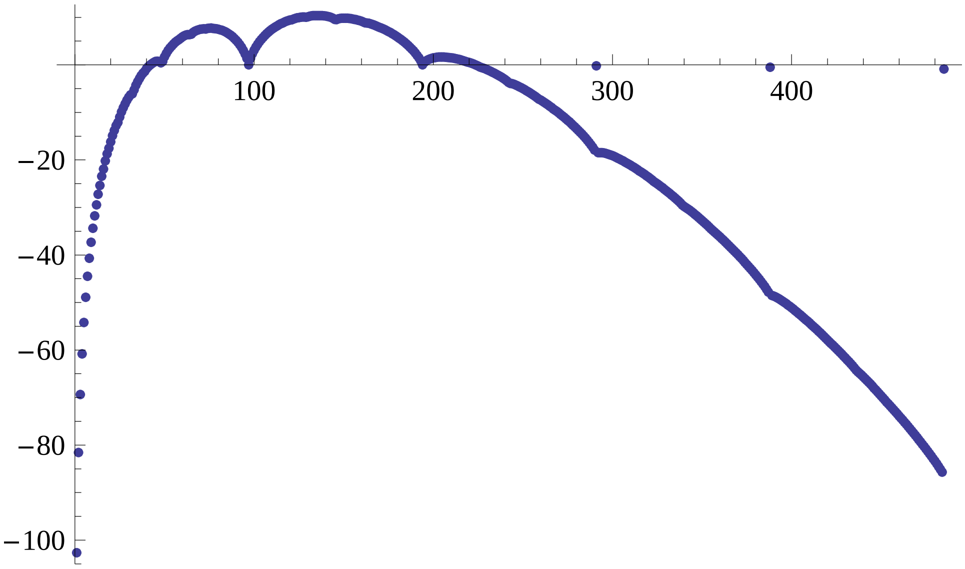

FIGURE 4. The plot of $V(h, 97) + V(97, h)$ for $1 \leq h \leq 5 \times 97$.

We begin with a little background material to set up the proof of Theorem 1. In the course of our proof we will see that g is essentially a period function of a Maass form, not a Maass cusp form but rather of the Eisenstein series $E(z, s)$ at $s = 1/2$.

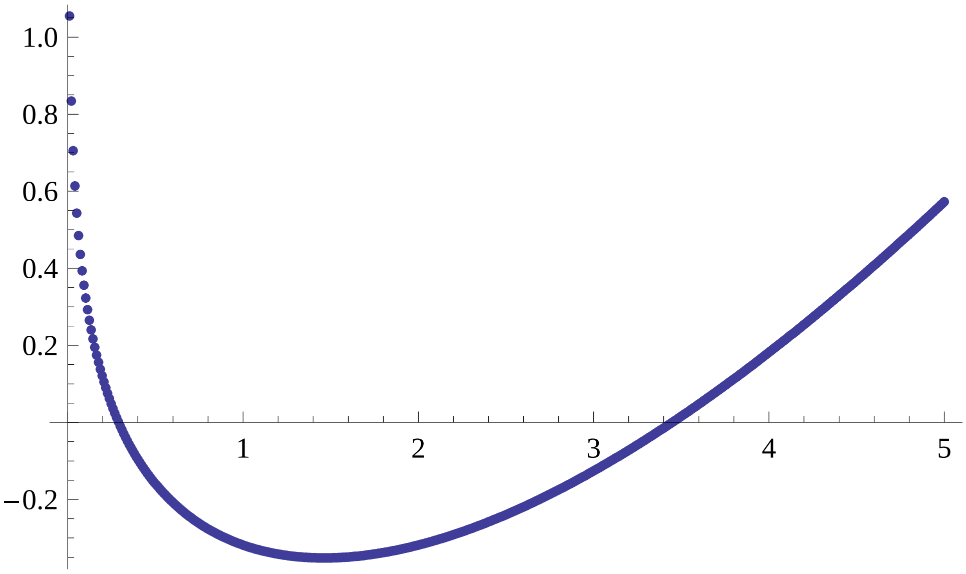

FIGURE 5. The plot of $(h/97, g(h/97))$ for $1 \leq h \leq 5 \times 97$.

3. LEMMAS

Let

$$\Lambda(s) = \pi^{-\frac{s}{2}}\Gamma(\frac{s}{2})\zeta(s)$$

and

$$Q(s) = \frac{\zeta(s)\zeta(1-s)}{\sin \pi s} = (2\pi)^{-s}\Gamma(s)\zeta(s)^2 \csc\frac{\pi s}{2} = \Lambda(s)^2\Gamma(\frac{s+1}{2})\Gamma(1-\frac{s}{2})/(2\pi^{3/2}).$$

Further, let

$$r(z) = \operatorname*{Res}_{s=1} Q(s)\sin\frac{\pi s}{2}e^{\frac{\pi i s}{2}}z^{-s} = \frac{\log 2\pi z - \gamma - \frac{\pi i}{2}}{2\pi i z}.$$

Lemma 1. *For $\Im z > 0$ let*

$$E_1(z) = 1 - 4\sum_{n=1}^{\infty} d(n)e(nz).$$

Then $\psi(z) := E_1(z) - \frac{1}{z}E_1(\frac{-1}{z})$ extends to an analytic function on $\mathbb{C}'$, the complex plane minus the non-positive real-axis, and is given in that region by

$$\psi(z) = -\frac{1}{z} - 4r(z) - \frac{2}{\pi}\int_{(\frac{-1}{2})} Q(s)z^{-s}\, ds;$$

the integral converges absolutely. In the neighborhood of $z = 1$ *we have*

$$\psi(z) = \frac{2i}{\pi} \sum_{m=0}^{\infty} \psi_m (z-1)^m$$

where

$$\psi_m = \frac{(-1)^m}{m+1} + 2\sum_{n=1}^{m-1} (-1)^{m-n} \binom{m}{n} b_{n+1}.$$

with

$$b_n = \frac{\zeta(n) B_n}{n}$$

for $n \geq 2$.

Proof. The proof is based on the ideas and formulas from the paper of [LZ]. Curiously, they consider the period functions of $E(z,s)$ with $s = 1/2 + it$ for all t *except* $t = 0$, which is exactly the case we need here!

For $\Im z > 0$ we have

$$E_1(z) = 1 - \frac{4}{2\pi i} \int_{(2)} \Gamma(s)\zeta(s)^2 (-2\pi i z)^{-s} \, ds$$

where $|\arg(-2\pi i z)| < \frac{\pi}{2}$. By Cauchy's theorem,

$$\begin{aligned} E_1(z) &= 1 - \frac{4}{2\pi i} \int_{(2)} Q(s) \sin\frac{\pi s}{2} e^{\frac{\pi i s}{2}} z^{-s} \, ds \\ &= 1 - 4r(z) - \frac{4}{2\pi i} \int_{(\frac{1}{2})} Q(s) \sin\frac{\pi s}{2} e^{\frac{\pi i s}{2}} z^{-s} \, ds. \end{aligned}$$

It follows that

$$\psi(z) = 1 - \frac{1}{z} - 4r(z) + \frac{4}{z} r(\frac{-1}{z}) - \frac{4}{2\pi i} \int_{(\frac{1}{2})} Q(s) \sin\frac{\pi s}{2} e^{\frac{\pi i s}{2}} \left(z^{-s} + (\frac{-1}{z})^{1-s} \right) \, ds.$$

Note that by a change of variable $s \to 1-s$, and using the functional equation $Q(1-s) = Q(s)$, we have

$$\frac{1}{2\pi i} \int_{(\frac{1}{2})} Q(s) \sin\frac{\pi s}{2} e^{\frac{\pi i s}{2}} (\frac{-1}{z})^{1-s} \, ds = \frac{1}{2\pi i} \int_{(\frac{1}{2})} Q(s) \cos\frac{\pi s}{2} e^{\frac{\pi i (1-s)}{2}} e^{\pi i s} z^{-s} \, ds$$

since in this context $0 < \arg z < \pi$ and $0 < \arg \frac{-1}{z} < \pi$ so that if we use $\arg(-1) = \pi$ then the identity $\arg \frac{-1}{z} = \arg(-1) - \arg z$ holds. Thus, the integral on the right is

$$\frac{1}{2\pi i} \int_{(\frac{1}{2})} i Q(s) \cos\frac{\pi s}{2} e^{\frac{\pi i s}{2}} z^{-s} \, ds.$$

Part one of the lemma now follows from the fact that

$$\sin\frac{\pi s}{2} e^{\frac{\pi i s}{2}} + i \cos\frac{\pi s}{2} e^{\frac{\pi i s}{2}} = i.$$

Next, we have have an asymptotic expansion for $\psi(x)$ as $x \to 0^+$ which we can obtain by moving the path of integration to $\Re s = -N - 1/2$. We have

$$\psi(x) \;=\; 1 - \frac{1}{x} - 4\frac{\log 2\pi x - \gamma - \frac{\pi i}{2}}{2\pi i x} - 4\frac{\log \frac{2\pi}{x} - \gamma + \frac{\pi i}{2}}{2\pi i} - 4ir_0(x) - \frac{4i}{\pi}\sum_{n=2}^{N}\frac{\zeta(n)B_n}{n}x^{n-1} + O(x^N)$$

where

$$r_0(x) = \operatorname*{Res}_{s=0} Q(s)x^{-s} = \frac{1}{2\pi}(\log 2\pi/x - \gamma);$$

this uses the fact that

$$\begin{aligned}\operatorname*{Res}_{s=-n} Q(s) &= \begin{cases} -\frac{i^n(2\pi)^{n-1}\zeta(-n+1)^2}{(n-1)!} & \text{if } n \text{ is even} \\ 0 & \text{if } n > 1 \text{ is odd} \end{cases} \\ &= \begin{cases} \frac{\zeta(n)B_n}{n\pi} & \text{if } n \text{ is even} \\ 0 & \text{if } n > 1 \text{ is odd} \end{cases}.\end{aligned}$$

Thus,

$$\psi(x) = -4\frac{\log 2\pi x - \gamma}{2\pi i x} - \frac{4i}{\pi}\sum_{n=2}^{N}\frac{\zeta(n)B_n}{n}x^{n-1} + O(x^N)$$

as $x \to 0^+$. But it follows from the fact that $f(z)$ is periodic with period 1 and the definition of ψ that ψ satisfies the three term relation

$$\psi(x) = \psi(x+1) + (x+1)^{-2s}\psi(\frac{x}{x+1})$$

with $s = 1/2$. Incidentally, this equation is a possible starting point for the theory of Lewis and Zagier: the ψ which are analytic on $\mathbb{C}'$ and satisfy such a 3-term relation together with a growth condition at 0^+ and ∞ are precisely the period functions of Maass cusp forms for $\mathrm{SL}_2(\mathbb{Z})$ and exist only for the values $s = 1/4 + r^2$ where $\lambda = 1/2 + ir$ is an eigenvalue of the hyperbolic Laplacian.

Letting $x \to 0^+$ and substituting the asymptotic expression above in the first and third terms, we find an asymptotic expansion for ψ near 1. To simplify this calculation, let $b_0 = \frac{2\gamma}{\pi i x}$; $b_1 = 0$; and $b_n = \zeta(n)B_n/n$ for $n \geq 2$. Then $\psi(x) = \frac{-2\log 2\pi x}{\pi i x} - \frac{4i}{\pi}\sum_{m=0}^{M} b_m x^{m-1} + O(x^M)$.

We obtain

$$\begin{aligned}\psi(1+x) &= \psi(x)-\frac{1}{x+1}\psi(\frac{x}{x+1})\\ &= \frac{-2\log 2\pi x}{\pi i x}-\frac{-2\log 2\pi\frac{x}{1+x}}{(1+x)\pi i\frac{x}{1+x}}-\frac{4i}{\pi}\sum_{m=0}^{M-1}b_m x^{m-1}(1-(1+x)^{-m})+O(x^M)\\ &= \frac{-2\log(1+x)}{\pi i x}+\frac{4i}{\pi}\sum_{m=2}^{M-1}b_m x^{m-1}\sum_{j=1}^{M-m}\binom{-m}{j}x^j+O(x^M)\\ &= \frac{2i}{\pi}\sum_{m=0}^{M-1}\psi_m x^m+O(x^M),\end{aligned}$$

where

$$\psi_m=\frac{(-1)^m}{m+1}+2\sum_{n=1}^{m-1}(-1)^{n-m}\binom{m}{n}b_{n+1}.$$

Since ψ is analytic in $\mathbb{C}'$ the series $\sum_{m=1}^{\infty}\psi_m z^m$ converges for complex z with $|z|<1$. ☐

Lemma 2. *For a positive rational number x we have*

$$\psi(x)=-2i(c(x)+\frac{1}{x}c(1/x)-\frac{1}{\pi x\,\mathrm{Den}(x)}).$$

Proof. We have

$$\psi(h/k)=\lim_{\delta\to 0^+}\psi((1+i\delta)\frac{h}{k})=\lim_{\delta\to 0^+}\left(E_1((1+i\delta)\frac{h}{k})-\frac{k}{h(1+i\delta)}E_1(\frac{-k}{h(1+i\delta)})\right)$$

where

$$E_1(z)=1-4\sum_{n=1}^{\infty}d(n)e(nz)$$

for $\Im z>0$. Then

$$\begin{aligned}E_1((1+i\delta)\frac{h}{k}) &= 1-4\sum_{n=1}^{\infty}d(n)e(nh/k)e^{-2\pi n\delta h/k}\\ &= 1-\frac{2}{\pi i}\int_{(2)}D(s,h/k)(2\pi\delta h/k)^{-s}\Gamma(s)\;ds\end{aligned}$$

where

$$D(s,h/k)=\sum_{n=1}^{\infty}\frac{d(n)e(nh/k)}{n^s}$$

is Estermann's function. Recall that

$$D(s,h/k)-k^{1-2s}\zeta(s)^2$$

is entire and

$$D(0, h/k) = \frac{1}{4} + \frac{i}{2} c(h/k).$$

Thus, moving the path of integration to the path $(-1/2)$ we find that

$$\begin{aligned} E_1((1+i\delta)\frac{h}{k}) &= 1 - 4 \operatorname*{Res}_{s=1} k^{1-2s} \zeta(s)^2 (2\pi\delta h/k)^{-s} \Gamma(s) - 4D(0, h/k) + O(\delta^{1/2}) \\ &= -4 \frac{\gamma - \log(2\pi\delta hk)}{2\pi\delta h} - 2ic(h/k) + O(\delta^{1/2}). \end{aligned}$$

Similarly,

$$\begin{aligned} E_1(\frac{-k}{h(1+i\delta)}) &= 1 - 4 \sum_{n=1}^{\infty} d(n) e(-nk/h) e^{-2\pi n\delta k/(h(1+i\delta))} \\ &= 1 - \frac{2}{\pi i} \int_{(2)} D(s, -k/h) (2\pi\delta k/(h(1+i\delta)))^{-s} \Gamma(s)\, ds \\ &= -4 \frac{\gamma - \log(2\pi\delta hk/(1+i\delta))}{2\pi k\delta/(1+i\delta)} - 2ic(-k, h) + O(\delta^{1/2}). \end{aligned}$$

Now

$$\begin{aligned} &E_1((1+i\delta)\frac{h}{k}) - \frac{k}{h(1+i\delta)} E_1(\frac{-k}{h(1+i\delta)}) \\ &= -4 \frac{-\log(1+i\delta)}{2\delta\pi h} - 2i(c(h/k) - \frac{k}{h(1+i\delta)} c(-k/h)) \\ &\to -2i(c(h/k) + \frac{k}{h} c(k/h) - \frac{1}{\pi h}). \end{aligned}$$

□

4. Proof of Theorem 1

It follows from Lemmas 1 and 2 that, with $x = h/k$,

$$g(x) = g(h/k) = \frac{h}{k} c(h/k) + c(k/h) - \frac{1}{\pi k} = \frac{1}{2} i x \psi(x)$$

so that

$$\begin{aligned} \pi g(1+x) &= -1 - \frac{x}{2} + \left(\frac{1}{6} + \frac{\pi^2}{18}\right) x^2 + \left(-\frac{1}{12} - \frac{\pi^2}{36}\right) x^3 + \dots \\ &= -1 - \frac{x}{2} + \sum_{n=2}^{\infty} \left(\frac{1}{n(n+1)} + 2b_n + 2 \sum_{j=0}^{n-2} \binom{n-1}{j} b_{j+2} \right) (-1)^n x^n \\ &\approx -1 - 0.5x + 0.715x^2 - 0.357x^3 + 0.252x^4 - 0.199x^5 + 0.166x^6 + \dots \end{aligned}$$

where

$$b_n = \frac{\zeta(n)B_n}{n}.$$

5. ESTIMATE FOR THE COEFFICIENTS OF g

Theorem 2 asserts that the coefficients g_n satisfy

$$g_n - \frac{1}{n} \sim 2^{5/4}\pi^{3/4}n^{-3/4}e^{-2\sqrt{\pi n}}\sin(2\sqrt{\pi n} + 3\pi/8)$$

Proof. We have that

$$\pi g(x) = \frac{\pi i x}{2}\psi(x)$$

where

$$\psi(x) = -\frac{1}{x} - 4r(x) - \frac{2}{\pi}\int_{(\frac{-1}{2})} \frac{\zeta(s)\zeta(1-s)}{\sin \pi s} x^{-s}\, ds$$

with

$$r(x) = \frac{\log 2\pi x - \gamma - \frac{\pi i}{2}}{2\pi i x}.$$

Thus,

$$\begin{aligned} \pi g(x) &= -\log 2\pi x + \gamma - i\int_{(\frac{-1}{2})} \frac{\zeta(s)\zeta(1-s)}{\sin \pi s} x^{1-s}\, ds \\ &= -\log 2\pi x + \gamma - i\int_{(\frac{3}{2})} \frac{\zeta(s)\zeta(1-s)}{\sin \pi s} x^{s}\, ds. \end{aligned}$$

By definition

$$\begin{aligned} g_n &= \frac{(-1)^n\pi g^{(n)}(1)}{n!} = \frac{1}{n} - \frac{i(-1)^n}{n!}\int_{(\frac{3}{2})} \frac{\zeta(s)\zeta(1-s)}{\sin \pi s} s(s-1)\dots(s-n+1)\, ds \\ &= \frac{1}{n} - I_n, \end{aligned}$$

say. By the functional equation for $\zeta(s)$ and basic properties of $\Gamma(s)$,

$$\begin{aligned} I_n &= -\frac{i}{n!}\int_{(\frac{3}{2})} \frac{\zeta(s)\zeta(1-s)}{\sin \pi s}\frac{\Gamma(n-s)}{\Gamma(-s)}\, ds \\ &= -\frac{2i}{\pi n!}\int_{(\frac{3}{2})} \zeta(s)^2\Gamma(s)\Gamma(1-s)(2\pi)^{-s}\Gamma(s)\cos\frac{\pi s}{2}\frac{\Gamma(n-s)}{\Gamma(-s)}\, ds \\ &= \frac{2i}{\pi n!}\int_{(\frac{3}{2})} \zeta(s)^2\Gamma(s)\Gamma(s+1)\Gamma(n-s)(2\pi)^{-s}\cos\frac{\pi s}{2}\, ds. \end{aligned}$$

We can see immediately that $I_n \ll_A n^{-A}$ for any fixed $A > 0$, just by moving the path of integration to the line with real part A and using trivial estimates for Γ. To get a formula which is asymptotic as $n \to \infty$ we expand $\zeta(s)^2$ into a Dirichlet series and integrate term-by-term. We re-express the resulting integrals as convolution integrals. Thus, we have

$$I_n \;=\; \frac{-4}{n!}\sum_{m=1}^{\infty} d(m) I_n(m)$$

where

$$I_n(x) = \frac{1}{2\pi i}\int_{(\frac{3}{2})} \Gamma(s)\Gamma(s+1)\Gamma(n-s)(2\pi x)^{-s}\cos\frac{\pi s}{2}\,ds;$$

the main term arises from the $m = 1$ term of this sum. Recall that

$$\frac{1}{2\pi i}\int_{(3/2)} \Gamma(s)\Gamma(s+1)u^{-s}\,ds = 2u^{1/2}K_1(2\sqrt{u})$$

where K_1 denotes the K-Bessel function of index 1. Also

$$\frac{1}{2\pi i}\int_{(3/2)} \Gamma(n-s)u^{-s}\,ds = u^{-n}e^{-1/u}.$$

Thus,

$$I_n(x) = \Re\int_0^{\infty} \sqrt{2\pi i u}\,K_1(2\sqrt{2\pi i u})x^{-n}u^n e^{-\frac{u}{x}}\frac{du}{u}.$$

Replacing u by ux here we have

$$I_n(x) = \Re\sqrt{2\pi i x}\int_0^{\infty} \sqrt{u}\,K_1(2(1+i)\sqrt{\pi u x})u^n e^{-u}\frac{du}{u}.$$

Now

$$K_1(z) = \sqrt{\frac{\pi}{2z}}e^{-z}\left(1 + \frac{3}{8z} + O(1/|z|^2)\right).$$

Thus

$$I_n(x) = \Re\pi^{3/4}x^{1/4}e^{\frac{\pi i}{8}}2^{\frac{-3}{4}}\int_0^{\infty} u^{\frac{1}{4}}e^{-2(1+i)\sqrt{\pi u x}}\left(1 + \frac{3}{16(1+i)\sqrt{\pi u x}} + O(\frac{1}{ux})\right)u^n e^{-u}\frac{du}{u}.$$

The proof of Theorem 1 is now completed by an appeal to Stirling's formula for $n!$ and

Lemma 3. *For fixed complex numbers A and α we have, as $n \to \infty$,*

$$J_n := \int_0^{\infty} u^{\alpha}e^{-A\sqrt{u}}u^n e^{-u}\frac{du}{u} = \sqrt{2\pi}e^{\frac{A^2}{8}}e^{-A\sqrt{n}}e^{-n}n^{n+\alpha-\frac{1}{2}}(1 + \frac{C}{\sqrt{n}} + O(\frac{1}{n}))$$

where

$$C = -\frac{4\alpha-1}{8}A - \frac{A^3}{96}.$$

□

We remark that Zagier conjectured an asymptotic series for g_n of the shape

$$g_n - \frac{1}{n} = e^{-2\sqrt{\pi n}} \left(\sum_{\substack{k=3\\ k\equiv 1 \bmod 2}}^{M} \frac{C_k \sin(2\sqrt{\pi n} + D_k)}{n^{k/4}} + O(n^{-M/4}) \right),$$

for certain constants C_k and D_k, an assertion that may be proven by the techniques used here.

5.1. **Proof of Lemma 3.**

Proof. We let $u = vn$ to see that

$$J_n = n^{n+\alpha} \int_0^\infty e^{-A\sqrt{vn}} e^{n(\log v - v)} v^\alpha \frac{dv}{v}.$$

Next, letting $v = w + 1$ we find that for any small fixed $\delta > 0$,

$$\begin{aligned} J_n &= n^{n+\alpha} \int_{-1}^\infty e^{-A\sqrt{n+nw}} e^{n(\log(w+1)-(w+1))} \frac{dw}{(1+w)^{1-\alpha}} \\ &= e^{-n} n^{n+\alpha} \int_{-\delta}^{\delta} e^{-A\sqrt{n+nw}} e^{-nw^2/2} (1 + nw^3/3 + O(nw^4)) \frac{dw}{(1+w)^{1-\alpha}} (1 + O(e^{-n\delta^2/2}). \end{aligned}$$

Now let $w = t/\sqrt{n}$. Then

$$J_n = e^{-A\sqrt{n}} e^{-n} n^{n+\alpha-1/2} \int_{-\delta\sqrt{n}}^{\delta\sqrt{n}} e^{A\sqrt{n} - A\sqrt{n+\sqrt{n}t}} e^{-t^2/2} (1 + \frac{t^3}{3\sqrt{n}} + \frac{(\alpha-1)t}{\sqrt{n}} + O(1/n))\, dt.$$

Now

$$\sqrt{n} - \sqrt{n + \sqrt{n}t} = \frac{-\sqrt{n}t}{\sqrt{n} + \sqrt{n+\sqrt{n}t}} = \frac{-t}{2} + \frac{t^2}{8\sqrt{n}} + O(t^3/n).$$

Thus,

$$J_n = e^{-A\sqrt{n}} e^{-n} n^{n+\alpha-1/2} \int_{-\infty}^{\infty} e^{-t^2/2 - At/2} (1 + \frac{At^2}{8\sqrt{n}} + \frac{t^3}{3\sqrt{n}} + \frac{(\alpha-1)t}{\sqrt{n}} + O(1/n))\, dt.$$

We evaluate the integrals after which the lemma follows. □

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University of Bristol

American Institute of Mathematics