A generalization of the Riemann-Siegel formula

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Abstract

The celebrated Riemann-Siegel formula compares the Riemann zeta function on the critical line with its partial sums, expressing the difference between them as an expansion in terms of decreasing powers of the imaginary variable t. Siegel anticipated that this formula could be generalized to include the Hardy-Littlewood approximate functional equation, valid in any vertical strip. We give this generalization for the first time. The asymptotics contain Mordell integrals and an interesting new family of polynomials.

1 Introduction

1.1 The approximate functional equation

The functional equation for the Riemann zeta function $\zeta(s)$ may be written as

$$\zeta(s) = \chi(s)\zeta(1-s) \tag{1.1}$$

for

$$\chi(s) := \pi^{s-1/2}\Gamma\left(\frac{1-s}{2}\right)\Gamma\left(\frac{s}{2}\right)^{-1}.$$

Hardy and Littlewood gave the following approximation for $\zeta(s)$ in [HL23]. The notation $s = \sigma + it$ for the real and imaginary parts of s is assumed from here on.

Theorem 1.1 (The Hardy-Littlewood approximate functional equation)**.** *Let $I \subset \mathbb{R}$ be a finite interval. Let s be any complex number in the vertical strip described by $\sigma \in I$ and $t \geqslant 2\pi$. Then for all $\alpha, \beta \in \mathbb{R}_{\geqslant 1}$ with $t = 2\pi\alpha\beta$, we have*

$$\zeta(s) = \sum_{n \leqslant \alpha} \frac{1}{n^s} + \chi(s) \sum_{n \leqslant \beta} \frac{1}{n^{1-s}} + O\Big(\alpha^{-\sigma} + t^{1/2-\sigma}\beta^{\sigma-1}\Big) \tag{1.2}$$

where the implied constant depends only on I.

The sums in (1.2), and similar sums below, are over all positive integers n satisfying the given conditions. Our use of the big O notation is as in [HL23] and [IK04, p. 7], for example. Writing $f(x) = O(g(x))$ (or equivalently $f(x) \ll g(x)$) means that, for an explicitly specified range X, there is an implied constant $C > 0$ so that $|f(x)| \leqslant C \cdot g(x)$ for all $x \in X$. Similarly, the notation extends to functions of more than one variable. With this convention, the implied constant in Theorem 1.1 may depend on I, but gives a bound that is valid for all s, α and β satisfying the given conditions. In this way, for instance, the qualifier "as $t \to \infty$" is not needed for (1.2).

Hardy and Littlewood used Theorem 1.1 to estimate the second and fourth moments of ζ on the critical line with real part $1/2$. See for example [Tit86, Chapter 7], [Ivi85, Chapters 5,8,15] for more on the important general moment problem and [Sou09] for descriptions of more recent results and conjectures.

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If α and β are similar in size then the error in (1.2) is about $O(t^{-\sigma/2})$ and hence small for t large and σ positive. Thus, $\zeta_\alpha(s) := \sum_{n\leqslant\alpha} n^{-s} + \chi(s)\sum_{n\leqslant\alpha} n^{-1+s}$ gives a good approximation to $\zeta(s)$ when t is close to $2\pi\alpha^2$. For positive fixed α, the function $\zeta_\alpha(s)$ is interesting in its own right. It is shown in [GM13, Thm. 1.5] that, in a natural sense, 100% of its zeros are simple and lie on the critical line.

Following Siegel in [Sie32, Eq. (36)], we define

$$\vartheta(s) := (i/2)\log\chi(s)$$

for $s \in \mathbb{C}$ with s outside the intervals $(-\infty, 0] \cup [1, \infty)$. The requirement $\vartheta(1/2) = 0$ specifies the branch uniquely; see Section 4.1 for more details. (We do not use the common notation $\vartheta(t)$ for $(i/2)\log\chi(1/2+it)$ as it is not well suited for working off the critical line.) As a consequence of Corollary 4.3 we have, for example,

$$i\vartheta(s) = \left(\frac{s}{2} - \frac{1}{4}\right)\log\frac{|t|}{2\pi} - \frac{it}{2} - \operatorname{sgn}(t)\frac{i\pi}{8} + O\left(\frac{1}{|t|}\right)$$

for all $t \neq 0$ with the implied constant depending on σ. Also $\vartheta(s)$ satisfies the relations

$$\vartheta(1-s) = -\vartheta(s), \qquad \overline{\vartheta(s)} = -\vartheta(\overline{s}). \tag{1.3}$$

Hence, with $\chi(s) = e^{-2i\vartheta(s)}$, we may write the functional equation (1.1) in the symmetric form

$$e^{i\vartheta(s)}\zeta(s) = e^{i\vartheta(1-s)}\zeta(1-s). \tag{1.4}$$

It follows that Theorem 1.1 has the equivalent restatement:

Theorem 1.2 (The Hardy-Littlewood approximate functional equation, symmetric version)**.** *Let $I \subset \mathbb{R}$ be a finite interval. Let s be any complex number in the vertical strip described by $\sigma \in I$ and $t \geqslant 2\pi$. Then for all $\alpha, \beta \in \mathbb{R}_{\geqslant 1}$ with $t = 2\pi\alpha\beta$, we have*

$$e^{i\vartheta(s)}\zeta(s) = e^{i\vartheta(s)}\sum_{n\leqslant\alpha}\frac{1}{n^s} + e^{i\vartheta(1-s)}\sum_{n\leqslant\beta}\frac{1}{n^{1-s}} + O\left(\frac{\lambda^{1/2-\sigma}\left(\lambda^{1/2}+\lambda^{-1/2}\right)}{t^{1/4}}\right) \tag{1.5}$$

where $\lambda := \sqrt{\alpha/\beta}$ and the implied constant depends only on I.

We used that

$$t = 2\pi\alpha\beta \quad \text{and} \quad \lambda = \sqrt{\frac{\alpha}{\beta}} \quad \implies \quad \alpha = \lambda\sqrt{\frac{t}{2\pi}} \quad \text{and} \quad \beta = \frac{1}{\lambda}\sqrt{\frac{t}{2\pi}}. \tag{1.6}$$

1.2 The Riemann-Siegel formula

The Riemann-Siegel formula is one of the key results in the theory of the zeta function. It gives a detailed description of what is happening inside the error terms in Theorems 1.1 and 1.2, at least in the case where the lengths of the partial sums are the same: $\alpha = \beta$ and $\lambda = 1$. Of course Riemann's researches predate those of Hardy and Littlewood by many years. The formula was discovered by Siegel in Riemann's unpublished notes and appeared in [Sie32]. Siegel's classic paper has been recently translated in [BS18] and we use their page numbering, corresponding to the version of the paper appearing in his collected works.

Most major computations verifying the Riemann hypothesis are based on the Riemann-Siegel formula; see for example [Bre79], [OS88], [Gou04], [BH18] and the contained references. It also appears in theoretical work where precise knowledge of $\zeta(s)$ on the critical line is required, such as [Fen05, PT15, Pol19].

Let

$$\Psi(u) := \frac{\cos(\pi(u^2/2 - u - 1/8))}{\cos(\pi u)}, \tag{1.7}$$

which may be seen to be an entire function. The following result in a slightly different notation is given in [Sie32, Eqns. (32), (33)].

Theorem 1.3 (The Riemann-Siegel formula for $\sigma \in I$)**.** *Let $I \subset \mathbb{R}$ be a finite interval and let s be any complex number in the vertical strip described by $\sigma \in I$ and $t \geqslant 2\pi$. Suppose $\alpha := \sqrt{t/(2\pi)}$ has fractional part $a \in [0,1)$. Then we have*

$$\zeta(s) = \sum_{n \leqslant \alpha} \frac{1}{n^s} + \chi(s) \sum_{n \leqslant \alpha} \frac{1}{n^{1-s}} + \frac{(-1)^{\lfloor \alpha \rfloor}(2\pi)^s e^{\pi i s/2}}{\Gamma(s)(e^{2\pi i s}-1)} \exp\left(\left(\frac{s}{2}-\frac{1}{4}\right)\log\frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8}\right)$$
$$\times \left(\frac{2\pi}{t}\right)^{1/4} \sum_{k=0}^{N-1} a_k(s) \sum_{r=0}^{\lfloor k/2 \rfloor} \frac{i^{r-k} \cdot k!}{r!(k-2r)!} \frac{\Psi^{(k-2r)}(2a)}{4^r (2\pi)^{k/2-r}} + O\left(\frac{1}{t^{N/6+\sigma/2}}\right). \quad (1.8)$$

The implied constant depends only on I and $N \in \mathbb{Z}_{\geqslant 0}$.

Siegel was also able to bound the error's dependence on N in (1.8) for t large enough. The functions $a_k(s)$ may be defined recursively by $a_{-2}(s) = a_{-1}(s) = 0$, $a_0(s) = 1$ and

$$(k+1)\sqrt{t} \cdot a_{k+1}(s) = -(k+1-\sigma)a_k(s) + i \cdot a_{k-2}(s) \qquad (k \in \mathbb{Z}_{\geqslant 0}). \quad (1.9)$$

Theorem 1.3 is in fact an intermediate result. In what we may call the completed form, the terms on the right of (1.8) are expanded in decreasing powers of t. It is also useful to make things symmetric by multiplying by $e^{i\vartheta(s)}$. This was Riemann's goal, as shown in [Sie32, Eqns. (44), (45)], and the following theorem is stated in [Sie43, p. 143].

Theorem 1.4 (The Riemann-Siegel formula: completed, symmetric version for $\sigma = 1/2$)**.** *Let $a \in [0,1)$ be the fractional part of $\alpha := \sqrt{t/(2\pi)}$. For any $N \in \mathbb{Z}_{\geqslant 0}$, there exist explicit functions of a alone, $C_0(a)$, $C_1(a)$, $C_2(a), \dots$, such that*

$$e^{i\vartheta(s)}\zeta(s) = e^{i\vartheta(s)} \sum_{n \leqslant \alpha} \frac{1}{n^s} + e^{i\vartheta(1-s)} \sum_{n \leqslant \alpha} \frac{1}{n^{1-s}} + (-1)^{\lfloor \alpha \rfloor + 1} \left(\frac{2\pi}{t}\right)^{1/4} \sum_{m=0}^{N-1} \frac{C_m(a)}{t^{m/2}} + O\left(\frac{1}{t^{N/2+1/4}}\right) \quad (1.10)$$

for all $s = 1/2 + it$ with $t \geqslant 2\pi$. The implied constant in (1.10) *depends only on N.*

Riemann computed the initial terms in (1.10) exactly and the first four are

$$C_0(a) = \Psi(2a), \quad (1.11a)$$
$$C_1(a) = -\frac{1}{3}(2\pi)^{-3/2}\Psi^{(3)}(2a), \quad (1.11b)$$
$$C_2(a) = \frac{1}{18}(2\pi)^{-3}\Psi^{(6)}(2a) + \frac{1}{4}(2\pi)^{-1}\Psi^{(2)}(2a), \quad (1.11c)$$
$$C_3(a) = -\frac{1}{162}(2\pi)^{-9/2}\Psi^{(9)}(2a) - \frac{2}{15}(2\pi)^{-5/2}\Psi^{(5)}(2a) - \frac{1}{8}(2\pi)^{-1/2}\Psi^{(1)}(2a). \quad (1.11d)$$

Siegel proved in [Sie32, p. 293] that only derivatives $\Psi^{(r)}(2a)$ for $r \equiv 3m \bmod 4$ appear in $C_m(a)$.

The left side of (1.10) for $s = 1/2 + it$ defines $Z(t)$, Hardy's Z function, and the sums over n may be combined so that (1.10) becomes

$$Z(t) = 2\sum_{n \leqslant \alpha} \frac{\cos(\vartheta(1/2+it) - t\log n)}{n^{1/2}} + (-1)^{\lfloor \alpha \rfloor + 1}\left(\frac{2\pi}{t}\right)^{1/4} \sum_{m=0}^{N-1} \frac{C_m(a)}{t^{m/2}} + O\left(\frac{1}{t^{N/2+1/4}}\right). \quad (1.12)$$

For $t \in \mathbb{R}$ we have that $\vartheta(1/2+it)$ and $Z(t)$ are real. Therefore zeros of $\zeta(s)$ on the critical line correspond to zeros of $Z(t)$. Riemann was able to find the first zeros in the critical strip, as Edwards recounts in [Edw74, Sect. 7.6], although it is not clear if he was using this formula in his calculations. Subsequent work using (1.12) has verified the Riemann hypothesis up to a large height. In these applications it is important to give exact bounds on the error in (1.10), (1.12). This has been achieved, for example, by Titchmarsh for $N = 1$ [Tit86, p. 390] and Gabcke for all $N \leqslant 10$ [Gab79, Eq. (8)]. In this paper we will not give explicit error bounds.

Riemann and Siegel gave recursive procedures for calculating the coefficients $C_m(a)$. Gabcke in [Gab79] provided a different method of proof of Theorem 1.4 and a new recursion for the coefficients $C_m(a)$. The starting point in [Gab79] is another unpublished formula of Riemann appearing in [Sie32], namely

$$\zeta(s) = \int_{0\swarrow 1} \frac{z^{-s}e^{\pi i z^2}}{e^{\pi i z} - e^{-\pi i z}}\,dz + \chi(s)\int_{0\searrow 1} \frac{z^{-s}e^{-\pi i z^2}}{e^{\pi i z} - e^{-\pi i z}}\,dz. \tag{1.13}$$

The paths of integration are lines that pass through the interval $(0,1)$ in the indicated direction. We also mention an interesting formal derivation of the $C_m(a)$ by Berry in [Ber95].

As Theorem 1.3 is valid in any vertical strip, it is natural to seek an extension of Theorem 1.4 that is also valid off the critical line. Arias de Reyna in [AdR11] gave a Riemann-Siegel formula for the left integral on the right side of (1.13) that holds in any vertical strip. With the same assumptions as Theorem 1.3, his result may be stated for $\zeta(s)$ as

$$\begin{aligned}\zeta(s) = \sum_{n\leqslant\alpha}\frac{1}{n^s} + \chi(s)\sum_{n\leqslant\alpha}\frac{1}{n^{1-s}} + (-1)^{\lfloor\alpha\rfloor+1}\sum_{k=0}^{N-1}\frac{1}{t^{k/2}}\\ \times\left[t^{-\sigma/2}U(t)\cdot D_k(a,\sigma) + \chi(s)t^{(\sigma-1)/2}\overline{U(t)\cdot D_k(a,1-\sigma)}\right] + O\left(\frac{t^{-\sigma/2}+t^{(\sigma-1)/2}}{t^{N/2}}\right)\end{aligned} \tag{1.14}$$

for $U(t) := \exp\left(-\frac{it}{2}\log\frac{t}{2\pi} + \frac{it}{2} + \frac{i\pi}{8}\right)$ and certain recursively defined functions $D_k(a,\sigma)$ as described in [AdR11, Sect. 2]. The implied constant depends on I and N and is bounded explicitly in [AdR11, Thm. 4.2].

1.3 Main results

In this paper we generalize the Riemann-Siegel formula to the case where the lengths of the partial sums, α and β, may be different, as in the results of Hardy and Littlewood. Siegel himself, in [Sie32, Sect. 4], suggested this should be possible without much difficulty and even gave the function that would be needed in place of Ψ. For $u,\tau\in\mathbb{C}$ with $\mathrm{Re}(\tau)>0$, it is

$$\Upsilon(u;\tau) := \int_{0\nwarrow 1}\frac{e^{-\pi i\tau z^2+2\pi i u z}}{e^{2\pi i z}-1}\,dz \tag{1.15}$$

where the path of integration is again a line crossing the interval $(0,1)$ in the indicated direction. It is straightforward to see that the integral converges rapidly for $\mathrm{Re}(\tau)>0$ and is independent of the choice of line. Siegel used $\Phi(-\tau,u)$ for $\Upsilon(u;\tau)$, so the new notation should avoid confusion.

We need a suitably normalized version of Siegel's function:

$$G(u;\tau) := \tau^{1/4}\exp\left(-\frac{\pi i u^2}{2}+\frac{\pi i}{8}\right)\Upsilon\left(\sqrt{\tau}\cdot u;\tau\right). \tag{1.16}$$

Proposition 3.2 will show that G has the symmetry

$$G(u;1/\tau) = \overline{G(\overline{u};\overline{\tau})}. \tag{1.17}$$

For each τ, $G(u;\tau)$ is holomorphic in u. The notation $G^{(k)}(u;\tau)$ indicates the kth derivative with respect to this variable u. If τ is rational then $G(u;\tau)$ has a more explicit description as seen in (3.13).

Employing the methods of Riemann and Siegel, we first extend Theorem 1.3 to the case of general α and β. This gives the intermediate result, Theorem 2.1, proved in Section 2. Interesting work in a similar direction to Theorem 2.1 is found in Chapter 4 of [FL22], also based on the techniques in [Sie32]. Our main theorem, given after the next definitions, is a completed, symmetric Riemann-Siegel formula that is valid in any vertical strip and that allows the partial sums to have different lengths. Write the quantity we are interested in estimating as

$$R(s;\alpha,\beta) := e^{i\vartheta(s)}\zeta(s) - e^{i\vartheta(s)}\sum_{n\leqslant\alpha}\frac{1}{n^s} - e^{i\vartheta(1-s)}\sum_{n\leqslant\beta}\frac{1}{n^{1-s}}. \tag{1.18}$$

With (1.3) and (1.4) it satisfies the symmetry

$$R(s;\alpha,\beta)=\overline{R(1-\overline{s};\beta,\alpha)}. \tag{1.19}$$

Throughout this work we will use the notation

$$a:=\alpha-\lfloor\alpha\rfloor, \qquad b:=\beta-\lfloor\beta\rfloor, \qquad \lambda:=\sqrt{\frac{\alpha}{\beta}}. \tag{1.20}$$

Theorem 1.5. *Let $I\subset\mathbb{R}$ be a finite interval. Let s be any complex number in the vertical strip described by $\sigma\in I$ and $t\geqslant 2\pi$. Then for all $\alpha,\beta\in\mathbb{R}_{\geqslant 1}$ with $t=2\pi\alpha\beta$, we have*

$$\begin{aligned}R(s;\alpha,\beta)&=(-1)^{\lfloor\alpha\rfloor\lfloor\beta\rfloor+1}\exp\bigl(\pi i(2a\beta-2b\alpha+a^2\lambda^{-2}-b^2\lambda^2)/2\bigr)\\&\quad\times\left(\frac{2\pi}{t}\right)^{1/4}\sum_{n=0}^{N-1}\frac{\lambda^{1/2-s}}{t^{n/2}}\left[\sum_{r=0}^{3n}\frac{G^{(r)}(a\lambda^{-1}+b\lambda;\lambda^2)}{(2\pi)^{r/2}}\cdot P_{n,3n-r}\left(\left(\frac{\pi}{2}\right)^{1/2}(a\lambda^{-1}-b\lambda),\sigma\right)\right]\\&\quad+O\left(\frac{\lambda^{1/2-\sigma}(\lambda+\lambda^{-1})^{3N+1/2}}{t^{N/2+1/4}}\right)\end{aligned} \tag{1.21}$$

using the notation from (1.18) *and* (1.20). *The implied constant depends only on $N\in\mathbb{Z}_{\geqslant 0}$ and I. The function $G(u;\tau)$ in* (1.21) *is the normalized Mordell integral defined in* (1.16) *and $P_{n,k}(x,\sigma)$ is a polynomial in x and σ, of degree k in x, that is given explicitly in* (6.1).

The simplest case of Theorem 1.5 has $N=0$. Then the sum is empty, equaling zero, and we find

$$R(s;\alpha,\beta)=O\left(\frac{\lambda^{1/2-\sigma}(\lambda+\lambda^{-1})^{1/2}}{t^{1/4}}\right)$$

recovering Hardy and Littlewood's Theorem 1.2. When $N=1$ we obtain the next term in the asymptotic expansion:

$$\begin{aligned}R(s;\alpha,\beta)&=(-1)^{\lfloor\alpha\rfloor\lfloor\beta\rfloor+1}\exp\bigl(\pi i(2a\beta-2b\alpha+a^2\lambda^{-2}-b^2\lambda^2)/2\bigr)\\&\quad\times\left(\frac{2\pi}{t}\right)^{1/4}\lambda^{1/2-s}G(a\lambda^{-1}+b\lambda;\lambda^2)+O\left(\frac{\lambda^{1/2-\sigma}(\lambda+\lambda^{-1})^{3+1/2}}{t^{1/2+1/4}}\right)\end{aligned} \tag{1.22}$$

since, as we will see, $P_{0,0}(x,\sigma)=1$. For $N=2$, the next term contains derivatives of G times the polynomials $P_{1,0}(x,\sigma)=-1/3$,

$$P_{1,1}(x,\sigma)=-ix, \quad P_{1,2}(x,\sigma)=x^2-i\bigl(\sigma-\tfrac{1}{2}\bigr), \quad P_{1,3}(x,\sigma)=\tfrac{i}{3}x^3+\bigl(\sigma-\tfrac{1}{2}\bigr)x. \tag{1.23}$$

We may take λ as fixed in these results but this is not necessary; Theorem 1.5 produces asymptotics whenever λ and $1/\lambda$ have order of magnitude less than $t^{1/6}$.

For $\sigma=1/2$ and $\alpha=\beta$ in Theorem 1.5 (so that $\lambda=1$ and $\alpha=\sqrt{t/2\pi}$), we recover the Riemann-Siegel formula, Theorem 1.4, as the expression

$$R(s;\alpha,\alpha)=(-1)^{\lfloor\alpha\rfloor+1}\left(\frac{2\pi}{t}\right)^{1/4}\sum_{n=0}^{N-1}\frac{1}{t^{n/2}}\left[\sum_{r=0}^{3n}\frac{G^{(r)}(2a;1)}{(2\pi)^{r/2}}\cdot P_{n,3n-r}(0,1/2)\right]+O\left(\frac{1}{t^{N/2+1/4}}\right). \tag{1.24}$$

This agrees with the forms of (1.10) and (1.11) since $G(u;1)=\Psi(u)$ by (3.14) and, as shown after Lemma 6.3, the numbers $P_{n,3n-r}(0,1/2)$ are zero unless $r\equiv 3n \bmod 4$. The more general case of s with $\sigma\in I$ and $\alpha=\beta$ has only the difference that $P_{n,3n-r}(0,1/2)$ in (1.24) is replaced by $P_{n,3n-r}(0,\sigma)$ and we obtain a simpler form of (1.14).

Our normalizations in Theorem 1.5 are guided by the symmetry (1.19). If we define a transformation $\mathcal{T}$ on functions of s, α and β as

$$\mathcal{T}f(s;\alpha,\beta):=\overline{f(1-\overline{s};\beta,\alpha)} \tag{1.25}$$

then $R(s;\alpha,\beta)$ is invariant under $\mathcal{T}$. All the components on the right side of (1.21) are also invariant under $\mathcal{T}$. For example $\exp\bigl(\pi i(2a\beta - 2b\alpha + a^2\lambda^{-2} - b^2\lambda^2)/2\bigr)$ gets mapped to itself since $\mathcal{T}$ switches a and b and sends λ to $1/\lambda$. That $\mathcal{T}$ sends $G^{(r)}(a\lambda^{-1}+b\lambda;\lambda^2)$ to itself follows from (1.17); see Proposition 3.2. We prove that $P_{n,k}(\sqrt{\pi/2}(a\lambda^{-1}-b\lambda),\sigma)$ is invariant under $\mathcal{T}$ in Theorem 6.1. The invariance of the right side of (1.21) under $\mathcal{T}$ is required for the final step in the proof of Theorem 1.5 to obtain the correct error term.

The functions $G(u;\tau)$ appearing in (1.21) are Mordell integrals and have many fascinating properties and connections, some of which have only been discovered recently [Zwe02, CR15, DRZ17]. In Section 3 we establish the various results about them we will need, including bounds, functional equations and the linear independence of their derivatives.

A preliminary form of Theorem 1.5 is proved in Section 5 after some explicit series expansions related to $\vartheta(s)$ are found in Section 4. The proof is completed in Section 6. The polynomials $P_{n,k}(x,\sigma)$ in (1.21) seem to be new and we also make an initial study of some of their properties in Section 6. Their description in (6.1) is given in terms of Bernoulli, Hermite and De Moivre polynomials.

N	Theorem 1.5	
1	$-0.08810545388 + 0.10864755195i$	
3	$-0.08764536572 + 0.10936255272i$	
5	$-0.08764522833 + 0.10936268294i$	
	$-0.08764522824 + 0.10936268305i$	R

Table 1: The approximations of Theorem 1.5 to $R = R(1/2 + 600i; 30/\sqrt{\pi}, 10/\sqrt{\pi})$.

Table 1 shows an example of how Theorem 1.5 approximates $R(s;\alpha,\beta)$ for $s = 1/2+600i$ and $\alpha/\beta = 3$ (so that $\lambda = \sqrt{3}$). The right side of (1.21) for different values of N may be compared with the left side which is displayed in the bottom row. Each decimal is correct to the accuracy shown. Table 2 shows a similar result at $s = -2 + 600i$, outside the critical strip. All the calculations in this paper were carried out using Mathematica. Section 7 contains further examples.

N	Theorem 1.5	
1	$-0.3478598947 + 0.4289646591i$	
3	$-0.3478754856 + 0.4059859119i$	
5	$-0.3479331346 + 0.4059929975i$	
	$-0.3479331128 + 0.4059931509i$	R

Table 2: The approximations of Theorem 1.5 to $R = R(-2 + 600i; 30/\sqrt{\pi}, 10/\sqrt{\pi})$.

2 The method of Riemann and Siegel

2.1 Initial set-up

The notation I will always denote a finite interval in $\mathbb{R}$. The well-known families of polynomials we require are those of Bernoulli and Hermite, with generating functions

$$\frac{te^{xt}}{e^t-1} = \sum_{n=0}^{\infty} B_n(x)\frac{t^n}{n!}, \qquad e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}, \tag{2.1}$$

respectively. Both $B_n(x)$ and $H_n(x)$ have degree n; the coefficients of $B_n(x)$ are rational and those of $H_n(x)$ are integral. For $t > 0$ we will also need the power series expansion

$$w(z,s) := \exp\left((s-1)\log\left(1+\frac{z}{\sqrt{t}}\right) - i\sqrt{t}z + i\frac{z^2}{2}\right) \tag{2.2}$$

$$= \sum_{k=0}^{\infty} a_k(s)\cdot z^k \qquad (|z| < \sqrt{t}). \tag{2.3}$$

The coefficients $a_k(s)$ were given recursively by Siegel as we saw in (1.9). We write them in terms of De Moivre polynomials in Proposition 4.8. The next result generalizes Theorem 1.3.

Theorem 2.1. *Recall the notation* (1.20). *Let s be any complex number in the vertical strip described by $\sigma \in I$ and $t \geqslant 2\pi$. Then for all $\alpha, \beta \in \mathbb{R}_{\geqslant 1}$ with $t = 2\pi\alpha\beta$ we have*

$$\zeta(s) = \sum_{n \leqslant \alpha} \frac{1}{n^s} + \chi(s) \sum_{n \leqslant \beta} \frac{1}{n^{1-s}} + (-1)^{\lfloor \alpha \rfloor \lfloor \beta \rfloor} \frac{(2\pi)^s e^{\pi i s/2}}{\Gamma(s)(e^{2\pi i s}-1)} \left(\frac{2\pi}{t}\right)^{1/4} \lambda^{1/2-s}$$
$$\times \exp\left(\frac{\pi i}{2}\Big[2a\beta - 2b\alpha + a^2\lambda^{-2} - b^2\lambda^2\Big]\right) \exp\left(\left(\frac{s}{2}-\frac{1}{4}\right)\log\frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8}\right)$$
$$\times \sum_{k=0}^{N-1} a_k(s) \sum_{r=0}^{k} \binom{k}{r} G^{(r)}(a\lambda^{-1} + b\lambda; \lambda^2) \frac{e^{\pi i(k-3r)/4}}{2^{k-r}(2\pi)^{r/2}} H_{k-r}(\omega_\lambda) + O\left(\frac{\lambda^{1-\sigma} t^{-\sigma/2}}{t^{N/6}}\right) \quad (2.4)$$

with

$$\omega_\lambda := e^{-\pi i/4}\sqrt{\pi/2}(a\lambda^{-1} - b\lambda).$$

The implied constant depends only on $N \in \mathbb{Z}_{\geqslant 0}$, I and λ. If $\lambda \geqslant 1$ then the implied constant is independent of λ.

The proof is given in this section and follows the main lines of Siegel's work in [Sie32, pp. 278-285]. See also [Tit86, Chap. 4] and [Edw74, Chap. 7]. For any $m \in \mathbb{Z}_{\geqslant 1}$ we begin, as in [Sie32, Eq. (8)], with

$$\zeta(s) = \sum_{n=1}^{m} \frac{1}{n^s} + \frac{(2\pi)^s e^{\pi i s/2}}{\Gamma(s)(e^{2\pi i s}-1)} \int_C \frac{z^{s-1}e^{-2\pi i m z}}{e^{2\pi i z}-1}\, dz. \quad (2.5)$$

The contour C starts at $-i\infty$ (with $\arg z = -\pi/2$), moves up the imaginary axis, circles close to 0 and then returns to $-i\infty$ (with $\arg z = 3\pi/2$) as displayed in Figure 1. Formula (2.5) is valid for all $s \in \mathbb{C}$ and shows that $\zeta(s)$ is holomorphic everywhere, except for a pole at $s = 1$, since $1/(\Gamma(s)(e^{2\pi i s}-1))$ has poles exactly for $s \in \mathbb{Z}_{\geqslant 1}$ and $\int_C$ has zeros for $s \in \mathbb{Z}_{\geqslant 2}$. The asymptotics of (2.5) as $t \to \infty$ are obtained with the saddle-point method. The idea (see for example [Olv74, Chap. 4], [PS97], [O'S19]) is to move the path of integration so that the main contribution to the integral in (2.5) comes from the neighborhood of the saddle-point of the integrand – where its derivative with respect to z is zero. For simplicity we just find the saddle-point of the numerator $z^{s-1}e^{-2\pi i m z}$. It is the value

$$\xi := \frac{s-1}{2\pi i m} = \frac{t}{2\pi m} + \frac{1-\sigma}{2\pi m} i \quad (2.6)$$

and so we need to move C so that it passes close to ξ. A short calculation similar to (2.14), (2.15) shows that

$$z^{s-1}e^{-2\pi i m z} = \xi^{s-1}e^{-2\pi i m \xi} \exp\left(\frac{2\pi^2 m^2}{s-1}(z-\xi)^2 + O\big((z-\xi)^3\big)\right) \quad (2.7)$$

for z close to ξ. Then

$$\mathrm{Re}\left(\frac{2\pi^2 m^2}{s-1}(z-\xi)^2\right) = \frac{2\pi^2 m^2}{|s-1|}|z-\xi|^2 \cos(2\arg(z-\xi) - \arg(s-1))$$

and so the directions in which (2.7) is decreasing the fastest, as z moves away from ξ, are when the cosine is -1. For $\arg(s-1)$ close to $\pi/2$ this corresponds to $\arg(z-\xi)$ close to $3\pi/4$ and $-\pi/4$.

The poles of the integrand in (2.5) occur at integers j with residues essentially j^{s-1}. This means that moving C to pass through ξ will add a sum of the form $\sum_{j \leqslant t/(2\pi m)} j^{s-1}$, giving the desired second part of the approximate functional equation.

As in the statement of the theorem, we choose $\alpha, \beta \in \mathbb{R}_{\geqslant 1}$ with $t = 2\pi\alpha\beta$. Let $m = \lfloor \alpha \rfloor$. Then

$$\xi \approx \frac{t}{2\pi m} \approx \frac{t}{2\pi\alpha} = \beta \quad (2.8)$$

and, following Riemann, we will use β as our base point instead of ξ. Similarly to Siegel we introduce the abbreviations

$$\varepsilon := e^{3\pi i/4}, \qquad g(z) := \frac{z^{s-1}e^{-2\pi imz}}{e^{2\pi iz}-1}.$$

The contour of integration C in (2.5) is moved to a new contour C_β that encloses exactly the integers from $-\lfloor\beta\rfloor$ to $\lfloor\beta\rfloor$ and passes through β in the desired direction of steepest descent ε. As shown in Figure 1, C_β is made with five lines. The first, L_0, is the vertical line ending at $\beta-\varepsilon\beta/2$ and then L_1 goes from $\beta-\varepsilon\beta/2$ to

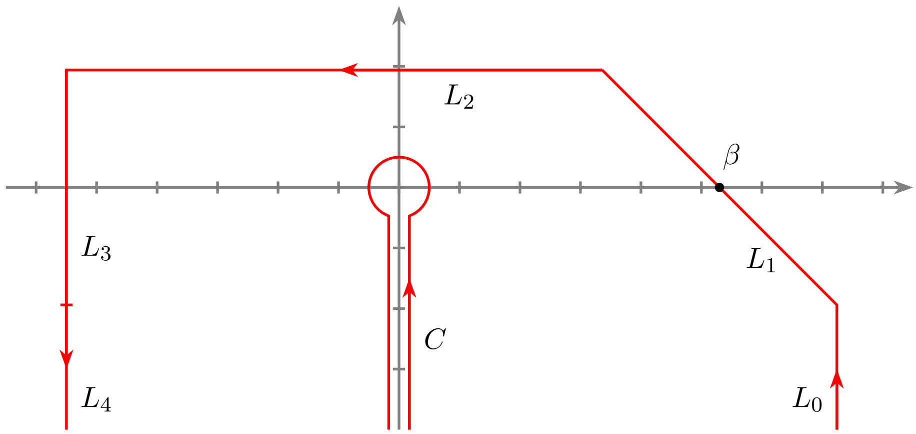

Figure 1: Contours of integration C and $C_\beta = L_0 \cup L_1 \cup \cdots \cup L_4$

$\beta+\varepsilon\beta/2$. We require L_1 to cross the real line in the open interval $(\lfloor\beta\rfloor, \lfloor\beta\rfloor+1)$; this requires moving the path slightly to the right when $\beta\in\mathbb{Z}$. The horizontal line L_2 continues until its real part reaches $-\lfloor\beta\rfloor-1/2$. The vertical lines L_3 and L_4 complete the contour with L_3 finishing, and L_4 starting, level with where L_0 finishes. This is at the imaginary value $-\beta i/(2\sqrt{2})$.

Then

$$\int_C g(z)\,dz = (e^{\pi is}-1)\sum_{n=1}^{\lfloor\beta\rfloor}\frac{1}{n^{1-s}} + \int_{C_\beta} g(z)\,dz$$

and hence

$$\zeta(s) = \sum_{n\leqslant\alpha}\frac{1}{n^s} + \chi(s)\sum_{n\leqslant\beta}\frac{1}{n^{1-s}} + \frac{(2\pi)^s e^{\pi is/2}}{\Gamma(s)(e^{2\pi is}-1)}\int_{C_\beta} g(z)\,dz. \tag{2.9}$$

Proposition 2.2. *For $\alpha,\beta\geqslant 1$ and $\sigma\in I$, we have*

$$\int_{C_\beta} g(z)\,dz = \int_{L_1} g(z)\,dz + O\Big(e^{-t/100}\Big). \tag{2.10}$$

The implied constant depends only on I.

Proof. For the numerator of $g(z)$,

$$\left|z^{s-1}e^{-2\pi imz}\right| = |z|^{\sigma-1}e^{2\pi my - t\arg z}.$$

Our first claim is that

$$\left|z^{s-1}e^{-2\pi imz}\right| \leqslant |z|^{\sigma-1}\times\begin{cases} e^{-t/8} & \text{if } z\in L_2\cup L_3\cup L_4,\\ e^{-t/20} & \text{if } z\in L_0 \text{ and } 10\leqslant\alpha,\\ e^{\pi|y|} & \text{if } z\in L_0 \text{ and } 1\leqslant\alpha\leqslant 10.\end{cases} \tag{2.11}$$

For $z\in L_2\cup L_3\cup L_4$,

$$y\leqslant\frac{\beta}{2\sqrt{2}} \qquad\text{and}\qquad \arg z\geqslant \arctan\left(\frac{1}{2\sqrt{2}-1}\right) > \frac{1}{2\sqrt{2}}+\frac{1}{8}.$$

Hence
$$\left|z^{s-1}e^{-2\pi imz}\right| \leqslant |z|^{\sigma-1}\exp\left(\frac{2\pi\alpha\beta}{2\sqrt{2}} - \frac{t}{2\sqrt{2}} - \frac{t}{8}\right) = |z|^{\sigma-1}e^{-t/8}.$$
With $z \in L_0$ we have
$$y \leqslant -\frac{\beta}{2\sqrt{2}} \qquad \text{and} \qquad \arg z = -\arctan\left(\frac{|y|}{\beta(1+1/(2\sqrt{2}))}\right)$$
so that
$$\left|z^{s-1}e^{-2\pi imz}\right| \leqslant |z|^{\sigma-1}\exp\left(-2\pi\lfloor\alpha\rfloor|y| + \frac{t|y|}{\beta(1+1/(2\sqrt{2}))}\right). \tag{2.12}$$
If $\alpha \geqslant 10$ then replacing $\lfloor\alpha\rfloor$ by $\alpha - 1$ in (2.12) shows
$$\begin{aligned}\left|z^{s-1}e^{-2\pi imz}\right| &\leqslant |z|^{\sigma-1}\exp\left(-t\frac{|y|}{\beta}\left[\frac{1}{1+2\sqrt{2}} - \frac{1}{\alpha}\right]\right)\\ &\leqslant |z|^{\sigma-1}\exp\left(-\frac{t}{2\sqrt{2}}\left[\frac{1}{1+2\sqrt{2}} - \frac{1}{\alpha}\right]\right) < |z|^{\sigma-1}e^{-t/20}.\end{aligned} \tag{2.13}$$
If $1 \leqslant \alpha \leqslant 10$ then writing $2\pi\alpha$ for t/β in (2.12) shows
$$\left|z^{s-1}e^{-2\pi imz}\right| \leqslant |z|^{\sigma-1}\exp\left(2\pi|y|\left[-\lfloor\alpha\rfloor + \frac{\alpha}{1+1/(2\sqrt{2})}\right]\right) < |z|^{\sigma-1}e^{\pi|y|}.$$
This completes the verification of the claim (2.11).

For the denominator of $g(z)$:
$$\begin{aligned}|e^{2\pi iz} - 1|^{-1} &\leqslant (1 - e^{-\pi\beta/\sqrt{2}})^{-1} \leqslant (1 - e^{-\pi/\sqrt{2}})^{-1} < 2 \qquad \text{for} \qquad z \in L_2,\\ |e^{2\pi iz} - 1|^{-1} &= (1 + e^{-2\pi y})^{-1} < 1 \qquad \text{for} \qquad z \in L_3.\end{aligned}$$
Hence, for z in $L_2 \cup L_3$ we have that $g(z) \ll \beta^{\sigma-1}e^{-t/8}$. Therefore
$$\int_{L_2\cup L_3} g(z)\,dz \ll \beta^{\sigma}e^{-t/8} \ll t^{\sigma}e^{-t/8} \ll e^{-t/20}.$$

For z in $L_0 \cup L_4$ we have
$$|z| < 4|y| \qquad \text{and} \qquad |e^{2\pi iz} - 1|^{-1} < 2e^{-2\pi|y|}.$$
Therefore
$$\int_{L_4} g(z)\,dz \ll e^{-t/20}\int_{1/(2\sqrt{2})}^{\infty} e^{-2\pi y}y^{\sigma-1}\,dy \ll e^{-t/20},$$
and we obtain the same bound for $\int_{L_0} g(z)\,dz$ when $10 \leqslant \alpha$. In the final case with $1 \leqslant \alpha \leqslant 10$,
$$\int_{L_0} g(z)\,dz \ll \int_{\beta/(2\sqrt{2})}^{\infty} e^{-\pi y}y^{\sigma-1}\,dy \ll \int_{t/(40\sqrt{2}\pi)}^{\infty} e^{-2\pi y/3}\,dy \ll e^{-t/100}. \qquad \square$$

2.2 The saddle-point method

The work in this paper grew out of the project [O'S19] which aimed to clarify some aspects of the saddle-point method, as elegantly formulated by Perron in 1917. The paper [PS97] documents that this method originated with Riemann, and it is remarkable that one of his first applications was to finding the asymptotic expansion for the difficult case of $\zeta(s)$.

In simpler applications of the saddle-point method, such as [O'S19, Cor. 1.4], the part of the integrand containing the growing parameter N is expanded into the form $\exp(Nc(z-\xi)^2)$ times a power series in z about the fixed saddle-point ξ. The behaviour of the integral for z close to ξ will control the asymptotics. Our case is more difficult as the saddle-point (2.6) is not fixed and changes with the parameters s and α. Adding to the complications, it is inconvenient to expand the numerator of $g(z)$ about ξ and we expand about the nearby point β instead:

$$z^{s-1}e^{-2\pi imz} = \beta^{s-1}e^{-2\pi im\beta}\exp\left(-2\pi im(z-\beta)+(s-1)\log\left(1+\frac{z-\beta}{\beta}\right)\right). \tag{2.14}$$

The argument of exp above may be developed as

$$-2\pi im(z-\beta)-(s-1)\sum_{j=1}^{\infty}\frac{(-1)^j}{j}\left(\frac{z-\beta}{\beta}\right)^j. \tag{2.15}$$

When z is close to β we find (2.15) is

$$\begin{aligned}&\left(\frac{\sigma-1+it}{\beta}-2\pi im\right)(z-\beta)+\frac{1-\sigma-it}{2}\left(\frac{z-\beta}{\beta}\right)^2+O\left(\left(\frac{z-\beta}{\beta}\right)^3\right)\\ &=\left[i\left(\frac{t}{\beta}-2\pi m\right)(z-\beta)-\frac{it}{2\beta^2}(z-\beta)^2\right]+(\sigma-1)\left(\frac{z-\beta}{\beta}\right)-\frac{\sigma-1}{2}\left(\frac{z-\beta}{\beta}\right)^2+O\left(\left(\frac{z-\beta}{\beta}\right)^3\right).\end{aligned} \tag{2.16}$$

For β large, the piece

$$\left[i\left(\frac{t}{\beta}-2\pi m\right)(z-\beta)-\frac{it}{2\beta^2}(z-\beta)^2\right]=2\pi i(\alpha-m)(z-\beta)-\pi i\frac{\alpha}{\beta}(z-\beta)^2$$

of (2.16) will be biggest. Therefore we separate it out and, recalling (2.2), write

$$z^{s-1}e^{-2\pi imz} = \beta^{s-1}e^{-2\pi im\beta}\exp\left(-\pi i\frac{\alpha}{\beta}(z-\beta)^2+2\pi i(\alpha-m)(z-\beta)\right)w\left(\frac{\sqrt{t}}{\beta}(z-\beta),s\right).$$

Since $\alpha/\beta=\lambda^2$ and $\sqrt{t}/\beta=\sqrt{2\pi}\lambda$, we obtain

$$\int_{L_1} g(z)\,dz = \beta^{s-1}e^{-2\pi im\beta}\int_{L_1}\frac{\exp\left(-\pi i\lambda^2(z-\beta)^2+2\pi ia(z-\beta)\right)}{e^{2\pi iz}-1}w\left(\sqrt{2\pi}\lambda(z-\beta),s\right)dz. \tag{2.17}$$

The next step is to replace $w(z,s)$ by the first terms in its expansion (2.3). The tail of this power series has the presentation

$$r_n(z,s) := \sum_{k=n}^{\infty}a_k(s)z^k = \frac{z^n}{2\pi i}\int_{\mathcal{C}}\frac{w(u,s)}{u^n(u-z)}\,du, \tag{2.18}$$

with $\mathcal{C}$ a curve inside the disc $|u|<\sqrt{t}$ which encircles 0 and z in the positive direction. Siegel bounded $r_n(z,s)$ precisely and for completeness we include his proof [Sie32, pp. 281-282] since all the error bounds depend on it.

Lemma 2.3. *For $n\in\mathbb{Z}_{\geqslant 0}$, $\sigma\in I$ and $t>0$ we have the estimates*

$$r_n(z,s)=O\left(\frac{|z|^n}{t^{n/6}}\right) \qquad \textit{for} \qquad 1\leqslant n\leqslant\frac{27}{50}t,\ |z|\leqslant\frac{20}{21}\left(\frac{2n\sqrt{t}}{5}\right)^{1/3}, \tag{2.19}$$

$$r_n(z,s)=O\left(e^{14|z|^2/29}\right) \qquad \textit{for} \qquad |z|\leqslant\sqrt{t}/2. \tag{2.20}$$

The implied constants depend only on I and n.

Proof. With (2.2),

$$\log w(u,s) = (\sigma-1)\log\left(1+\frac{u}{\sqrt{t}}\right) + iu^2\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k+2}\left(\frac{u}{\sqrt{t}}\right)^k.$$

Therefore, in the circle $|u| \leqslant 3\sqrt{t}/5$ we have

$$\operatorname{Re}(\log w(u,s)) \leqslant |\sigma-1|\log\frac{8}{5} + \frac{5|u|^3}{6\sqrt{t}}. \tag{2.21}$$

In (2.18) let $|z| \leqslant 4\sqrt{t}/7$ and let $\mathcal{C}$ be a circle around $u=0$ with a radius ρ_n satisfying

$$\frac{21}{20}|z| \leqslant \rho_n \leqslant \frac{3}{5}\sqrt{t}. \tag{2.22}$$

Then (2.18), (2.21), (2.22) imply the estimate

$$r_n(z,s) = O\left(|z|^n\rho_n^{-n}\exp\left(\frac{5}{6\sqrt{t}}\rho_n^3\right)\right). \tag{2.23}$$

For $n \geqslant 1$, the function $\rho^{-n}e^{5\rho^3/(6\sqrt{t})}$ of ρ reaches its minimum $\left(\frac{5e}{2n\sqrt{t}}\right)^{n/3}$ for $\left(\frac{2n\sqrt{t}}{5}\right)^{1/3}$. According to (2.22), the choice $\rho_n = \rho$ is admissible if

$$\frac{21}{20}|z| \leqslant \left(\frac{2n\sqrt{t}}{5}\right)^{1/3} \leqslant \frac{3}{5}\sqrt{t}.$$

Consequently we obtain (2.19). For $n \geqslant 0$ and $|z| \leqslant 4\sqrt{t}/7$, the choice $\rho_n = 21|z|/20$ is also admissible according to (2.22); from this we obtain (2.20). □

2.3 Error estimates

If we replace $w(\cdot,s)$ in (2.17) by the first n terms of its expansion (2.3) then the error involves the integral

$$J_n(s;\alpha,\beta) := \int_{L_1}\frac{\exp\bigl(-\pi i\lambda^2(z-\beta)^2+2\pi ia(z-\beta)\bigr)}{e^{2\pi iz}-1}r_n\Bigl(\sqrt{2\pi}\lambda(z-\beta),s\Bigr)\,dz. \tag{2.24}$$

Proposition 2.4. *Suppose $\sigma \in I$, $t>0$ and $n \in \mathbb{Z}_{\geqslant 0}$. Then we have*

$$J_n(s;\alpha,\beta) = O\Bigl(t^{-n/6}\Bigr) \tag{2.25}$$

for an implied constant depending only on I, n and λ. If $\lambda \geqslant 1$ then the implied constant does not depend on λ.

Proof. Recall that L_1 is usually a straight line from $\beta-\varepsilon\beta/2$ to $\beta+\varepsilon\beta/2$. However, when β is close to $\lfloor\beta\rfloor$ or $\lfloor\beta\rfloor+1$ we will adjust the path slightly to avoid the denominator in (2.24) becoming too small. The next lemma has a straightforward proof that is omitted.

Lemma 2.5. *Suppose $\delta>0$ and $z\in\mathbb{C}$. If $|z-m|\geqslant\delta$ for all $m\in\mathbb{Z}$ then, for an absolute implied constant,*

$$(e^{2\pi iz}-1)^{-1} = O\bigl(1+\delta^{-1}\bigr).$$

The proof of the proposition breaks into four cases.

Case I: $\lambda \leqslant 1$ and $1/100 \leqslant b \leqslant 99/100$. For these values of b we may take L_1 to be a straight line. The part of the integrand $(e^{2\pi iz}-1)^{-1}$ in (2.24) is absolutely bounded as we may apply Lemma 2.5 with $\delta = 1/(100\sqrt{2})$.

Writing $z = \beta + \varepsilon v/(\sqrt{2\pi}\lambda)$ shows that

$$J_n(s;\alpha,\beta) = \frac{\varepsilon}{\sqrt{2\pi}\lambda}\int_{-\sqrt{t}/2}^{\sqrt{t}/2} \frac{\exp\left(-v^2/2 + \sqrt{2\pi}i\varepsilon a v/\lambda\right)}{e^{2\pi i(\beta+\varepsilon v/(\sqrt{2\pi}\lambda))} - 1} r_n(\varepsilon v, s)\, dv \tag{2.26}$$

and the integrand is bounded by a constant times

$$\exp\left(-v^2/2 + \sqrt{2\pi}|v|/\lambda\right)|r_n(\varepsilon v, s)|. \tag{2.27}$$

Using (2.20) we have

$$J_n(s;\alpha,\beta) \ll \int_0^{\sqrt{t}/2} \exp\left(-\frac{v^2}{58} + \frac{\sqrt{2\pi}}{\lambda}v\right) dv = O(1) \tag{2.28}$$

with an implied constant depending on n and λ. If $n = 0$ then (2.28) gives the correct bound (2.25).

Now we fix $n \in \mathbb{Z}_{\geqslant 1}$. Assume $t \geqslant 50n/27$ so that we may also use (2.19). Let

$$\mu := \frac{20}{21}(2n\sqrt{t}/5)^{1/3},$$

and applying the bounds (2.19) and (2.20) to (2.27) shows

$$\begin{aligned} J_n(s;\alpha,\beta) &\ll t^{-n/6}\int_0^{\mu} \exp\left(-\frac{v^2}{2} + \frac{\sqrt{2\pi}}{\lambda}v\right) v^n\, dv + \int_{\mu}^{\sqrt{t}/2} \exp\left(-\frac{v^2}{58} + \frac{\sqrt{2\pi}}{\lambda}v\right) dv \\ &\ll t^{-n/6}\int_0^{\infty} \exp\left(-\frac{v^2}{3}\right) v^n\, dv + \int_{\mu}^{\infty} \exp\left(-\frac{v^2}{59}\right) dv \\ &\ll t^{-n/6} + e^{-\mu^2/60} = O(t^{-n/6}) \qquad \text{for} \qquad t \geqslant 50n/27. \end{aligned} \tag{2.29}$$

By (2.28) we have

$$J_n(s;\alpha,\beta) = O(1) \qquad \text{for} \qquad 0 < t < 50n/27. \tag{2.30}$$

Combining (2.29) and (2.30) gives the desired bound (2.25).

Case II: $\lambda \leqslant 1$ and $0 \leqslant b \leqslant 1/100$ or $99/100 \leqslant b < 1$. For these values of b we let L_1 be the usual path of integration except that we replace the segment between $\beta - \varepsilon/50$ and $\beta + \varepsilon/50$ with a semicircular arc of radius $1/50$ about β. If $0 \leqslant b \leqslant 1/100$ we need the upper arc traversed in a counter-clockwise direction. For $99/100 \leqslant b < 1$ we need the lower arc traversed in a clockwise direction. We focus on the former case from here and it is shown in Figure 2. The other case is similar.

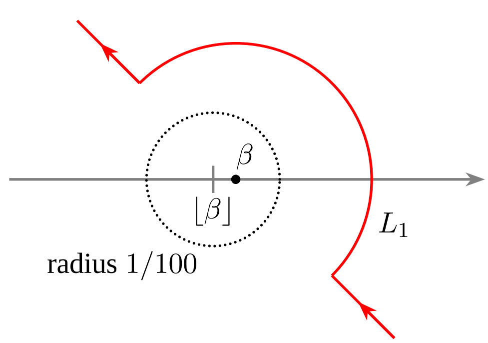

Figure 2: Adjusting the contour of integration L_1 near $\lfloor\beta\rfloor$ in Case II

Since the circle of radius $1/100$ about $\lfloor\beta\rfloor$ is contained in the circle of radius $1/50$ about β we see that $z \in L_1$ satisfies Lemma 2.5 with $\delta = 1/100$. Therefore $(e^{2\pi i z} - 1)^{-1}$ is absolutely bounded and the work of Case I shows the correct bound for the part of J_n given by the integral on the straight lines.

Let $J_n(s;\alpha,\beta)_{\mathcal{A}}$ be the remaining part of J_n given by the integral over the arc:

$$J_n(s;\alpha,\beta)_{\mathcal{A}} = \int_{\mathcal{A}} \frac{\exp\bigl(-\pi i\lambda^2 w^2 + 2\pi i a w\bigr)}{e^{2\pi i(\beta+w)}-1} r_n\Bigl(\sqrt{2\pi}\lambda w, s\Bigr)\, dw \tag{2.31}$$

where $\mathcal{A}$ is given by w with $|w| = 1/50$ and $-\pi/4 \leqslant \arg w \leqslant 3\pi/4$. The integrand is bounded by a constant times

$$\exp\bigl(\pi\lambda^2/50^2 + 2\pi/50\bigr)\Bigl|r_n\Bigl(\sqrt{2\pi}\lambda w, s\Bigr)\Bigr|$$

Using (2.20) we have

$$J_n(s;\alpha,\beta)_{\mathcal{A}} \ll \int_{\mathcal{A}} \exp\biggl(14\Bigl|\sqrt{2\pi}\lambda w\Bigr|^2/29\biggr)\, |dw| = O(1) \tag{2.32}$$

with an implied constant depending on n and λ. If $n=0$ then (2.32) gives the correct bound for (2.25).

Now we fix $n \in \mathbb{Z}_{\geqslant 1}$. Assume $t \geqslant 50n/27$ so that, by (2.19),

$$J_n(s;\alpha,\beta)_{\mathcal{A}} \ll \int_{\mathcal{A}} \Bigl|r_n\Bigl(\sqrt{2\pi}\lambda w, s\Bigr)\Bigr|\, |dw| \ll \left(\frac{\sqrt{2\pi}\lambda}{50}\right)^n t^{-n/6} = O\Bigl(t^{-n/6}\Bigr)$$

provided that $\sqrt{2\pi}\lambda/50 \leqslant \mu$. (Recall μ defined before (2.29).) But this last condition is true if $t > 1.4\times 10^{-7}$. Hence

$$J_n(s;\alpha,\beta)_{\mathcal{A}} = O\Bigl(t^{-n/6}\Bigr) \qquad \text{for} \qquad t \geqslant 50n/27 \tag{2.33}$$

and by (2.32)

$$J_n(s;\alpha,\beta)_{\mathcal{A}} = O(1) \qquad \text{for} \qquad 0 < t < 50n/27. \tag{2.34}$$

The estimates (2.33) and (2.34) complete the proof of (2.25) in this case.

Case III: $\lambda \geqslant 1$ and $1/(100\lambda) \leqslant b \leqslant 99/(100\lambda)$. This is similar to Case I, though we are more careful in showing the λ dependence. The integration path L_1 is straight with no adjustments. For $z \in L_1$, the part of the integrand $(e^{2\pi i z}-1)^{-1}$ in (2.24) is bounded by an absolute constant times $1+\lambda$ as we may apply Lemma 2.5 with $\delta = 1/(100\sqrt{2}\lambda)$.

As in (2.26) and (2.27), it may be seen that $J_n(s;\alpha,\beta)$ is bounded by an absolute constant times

$$\frac{1+\lambda}{\lambda} \int_0^{\sqrt{t}/2} \exp\Bigl(-v^2/2 + \sqrt{2\pi}|v|/\lambda\Bigr)|r_n(\varepsilon v, s)|\, dv. \tag{2.35}$$

As (2.35) is decreasing in λ, we may take $\lambda = 1$ in our bounds and the error will not depend on λ. The arguments of Case I now go through unchanged.

Case IV: $\lambda \geqslant 1$ and $0 \leqslant b \leqslant 1/(100\lambda)$ or $99/(100\lambda) \leqslant b < 1$. Similarly to Case II, L_1 is the usual path of integration except that we replace the segment between $\beta - \varepsilon/(50\lambda)$ and $\beta + \varepsilon/(50\lambda)$ with a semicircular arc of radius $1/(50\lambda)$ about β. As in Case II, we may focus on the situation with $0 \leqslant b \leqslant 1/(100\lambda)$.

Since the circle of radius $1/(100\lambda)$ about $\lfloor\beta\rfloor$ is contained in the circle of radius $1/(50\lambda)$ about β we see that $z \in L_1$ satisfies Lemma 2.5 with $\delta = 1/(100\lambda)$. Therefore $(e^{2\pi i z}-1)^{-1}$ is bounded by an absolute constant times $1+\lambda$ and the work of Case III shows the correct bound for the part of J_n given by the integral on the straight lines. Let $J_n(s;\alpha,\beta)_{\mathcal{A}}$ be the remaining part of J_n given by the integral over the arc:

$$J_n(s;\alpha,\beta)_{\mathcal{A}} = \frac{1}{\lambda}\int_{\mathcal{A}} \frac{\exp\bigl(-\pi i w^2 + 2\pi i a w/\lambda\bigr)}{e^{2\pi i(\beta+w/\lambda)}-1} r_n\Bigl(\sqrt{2\pi}w, s\Bigr)\, dw \tag{2.36}$$

where $\mathcal{A}$ was already defined for (2.31) and given by w with $|w| = 1/50$ and $-\pi/4 \leqslant \arg w \leqslant 3\pi/4$. Hence, $J_n(s;\alpha,\beta)_{\mathcal{A}}$ is bounded by an absolute constant times

$$\frac{1+\lambda}{\lambda}\int_{\mathcal{A}} \exp\left(\frac{\pi}{50^2} + \frac{2\pi}{50\lambda}\right)\Bigl|r_n\Bigl(\sqrt{2\pi}w, s\Bigr)\Bigr|\, dw. \tag{2.37}$$

Then (2.37) is decreasing in λ and so we may reuse the estimates of Case II with $\lambda = 1$ to bound $J_n(s;\alpha,\beta)_{\mathcal{A}}$ as in (2.33) and (2.34). □

With (2.17), (2.24) and Proposition 2.4, we have shown that

$$\int_{L_1} g(z)\,dz = \beta^{s-1} e^{-2\pi i m\beta} \sum_{k=0}^{N-1} a_k(s)(2\pi)^{k/2}\lambda^k \times \int_{L_1} \frac{\exp\big(-\pi i\lambda^2(z-\beta)^2 + 2\pi i a(z-\beta)\big)}{e^{2\pi i z}-1}(z-\beta)^k\,dz + O\Big(\beta^{\sigma-1}t^{-N/6}\Big) \tag{2.38}$$

for $\sigma \in I$, $t > 0$ and $\lambda > 0$, with an implied constant depending only on I, $N \in \mathbb{Z}_{\geqslant 0}$ and λ when $\lambda < 1$.

The last step in rearranging our expressions for $\int_{L_1} g(z)\,dz$ is to extend the line of integration on the right of (2.38) to infinity in both directions. Let L^- be the line from $\beta - \varepsilon\infty$ to $\beta - \varepsilon\beta/2$ and let L^+ be the line from $\beta + \varepsilon\beta/2$ to $\beta + \varepsilon\infty$.

Lemma 2.6. *For $\sigma \in I$, $t \geqslant 1$ and $N \in \mathbb{Z}_{\geqslant 0}$ we have*

$$\sum_{k=0}^{N-1} a_k(s)(2\pi)^{k/2}\lambda^k \int_{L^-\cup L^+} \frac{\exp\big(-\pi i\lambda^2(z-\beta)^2 + 2\pi i a(z-\beta)\big)}{e^{2\pi i z}-1}(z-\beta)^k\,dz = O\Big(e^{-t/16}\Big). \tag{2.39}$$

The implied constant depends only on I, N and λ. If $\lambda \geqslant 1$ then the implied constant is independent of λ.

Proof. We first note that for $z \in L^- \cup L^+$ it is true that

$$|\mathrm{Im} z| \geqslant \frac{\beta}{2\sqrt{2}} = \frac{\sqrt{t}}{2\sqrt{2}\cdot\sqrt{2\pi}\lambda} \geqslant \frac{1}{4\sqrt{\pi}\lambda}.$$

Hence by Lemma 2.5, $(e^{2\pi i z}-1)^{-1} = O(1+\lambda)$ for an absolute implied constant. Next we see by using (2.20) with $z = 1/2$ that

$$a_k(s) = (r_k(z,s) - r_{k+1}(z,s))z^{-k} = O(1) \tag{2.40}$$

(where this implied constant depends on k and I).

With the change of variables $z = \beta + \varepsilon v/(\sqrt{2\pi}\lambda)$ that we used in (2.26), the left side of (2.39) equals

$$\sum_{k=0}^{N-1} a_k(s)\frac{\varepsilon}{\sqrt{2\pi}\lambda}\int_{(-\infty,-\sqrt{t}/2]\cup[\sqrt{t}/2,\infty)} \frac{\exp\big(-v^2/2 + \sqrt{2\pi}i\varepsilon a v/\lambda\big)}{e^{2\pi i(\beta+\varepsilon v/(\sqrt{2\pi}\lambda))}-1}(\varepsilon v)^k\,dv$$

and this is bounded by an absolute constant times

$$\sum_{k=0}^{N-1} |a_k(s)|\frac{1+\lambda}{\lambda}\int_{\sqrt{t}/2}^{\infty} \exp\Big(-v^2/2 + \sqrt{2\pi}v/\lambda\Big)v^k\,dv. \tag{2.41}$$

Then (2.41) is

$$\ll \int_{\sqrt{t}/2}^{\infty} \exp\big(-v^2/3\big)\,dv \ll \exp\Big(-(\sqrt{t}/2)^2/4\Big)$$

as required. The implied constant in (2.39) is independent of λ for $\lambda \geqslant 1$ because (2.41) is decreasing in λ. □

2.4 Relating the integral to $G(u;\tau)$

Proof of Theorem 2.1. It follows from Lemma 2.6 that (2.38) is true with the path of integration L_1 extended to infinity. If we replace z by $z + \lfloor\beta\rfloor$ in the integral in (2.38) then it is easy to see that the path of integration may now be taken as any infinite straight line crossing the real line in the interval $(0,1)$ and in the direction of ε. As before, we use $0 \nwarrow 1$ to denote this path.

Then combining this with (2.9) and Proposition 2.2 gives

$$\zeta(s) = \sum_{n\leqslant\alpha} n^{-s} + \chi(s)\sum_{n\leqslant\beta} n^{s-1} + \frac{(2\pi)^s e^{\pi is/2}}{\Gamma(s)(e^{2\pi is}-1)}\beta^{s-1}e^{-2\pi im\beta}\sum_{k=0}^{N-1} a_k(s)(2\pi)^{k/2}\lambda^k$$
$$\times \int_{0\nwarrow 1} \frac{\exp\bigl(-\pi i\lambda^2(z-b)^2 + 2\pi i a(z-b)\bigr)}{e^{2\pi iz}-1}(z-b)^k\,dz + O\left(\frac{\beta^{\sigma-1}t^{1/2-\sigma}}{t^{N/6}}\right). \quad (2.42)$$

For the error, we used that

$$\frac{(2\pi)^s e^{\pi is/2}}{\Gamma(s)(e^{2\pi is}-1)} = O\Bigl(t^{1/2-\sigma}\Bigr)$$

for $\sigma\in I$ and $t\geqslant 2\pi$ by Stirling's formula or Proposition 4.7. Writing the error in (2.42) in terms of λ gives the error stated in (2.4).

The integral in (2.42) may be expressed in terms of $G(u;\tau)$. It is simpler to relate the integral directly to the Mordell integral $\Upsilon(u;\tau)$ in (1.15), but this would obscure the symmetry in $s\leftrightarrow 1-s$, $\alpha\leftrightarrow\beta$ we wish to exploit. The integral in (2.42) is $k!(2\pi i)^{-k}$ times the coefficient of u^k in

$$\int_{0\nwarrow 1} \frac{\exp\bigl(-\pi i\lambda^2(z-b)^2 + 2\pi i a(z-b)\bigr)}{e^{2\pi iz}-1}\exp\bigl(2\pi i(z-b)u\bigr)\,dz$$
$$= \lambda^{-1/2}\exp\left(-\pi i\left(b^2\lambda^2+\frac{1}{8}\right)\right)\exp\left(\frac{\pi i}{2}\Bigl(\frac{a}{\lambda}-b\lambda+\frac{u}{\lambda}\Bigr)^2\right)G\Bigl(\frac{a}{\lambda}+b\lambda+\frac{u}{\lambda};\lambda^2\Bigr). \quad (2.43)$$

It follows from the right identity in (2.1) that

$$e^{-c^2(u+q)^2} = e^{-c^2q^2}\sum_{n=0}^{\infty} H_n(cq)\frac{(-c)^n u^n}{n!}.$$

Expanding the exponential factor on the right of (2.43) using this, with $c = e^{-\pi i/4}\sqrt{\pi/2}$ and $q = a/\lambda - b\lambda$, produces

$$\exp\left(\frac{\pi i}{2}\Bigl(\frac{a}{\lambda}-b\lambda+\frac{u}{\lambda}\Bigr)^2\right) = \exp\left(\frac{\pi i}{2}(a\lambda^{-1}-b\lambda)^2\right)\sum_{n=0}^{\infty} H_n(\omega_\lambda)\Bigl(\frac{\pi}{2}\Bigr)^{n/2}\Bigl(\frac{\varepsilon}{\lambda}\Bigr)^n\frac{u^n}{n!}.$$

Combining this with the Taylor expansion of $G\bigl(a/\lambda+b\lambda+u/\lambda;\lambda^2\bigr)$ shows the integral in (2.42) equals

$$\frac{1}{(2\pi i)^k}\lambda^{-1/2-k}\exp\left(-\pi i\left(b^2\lambda^2+\frac{1}{8}\right)\right)\exp\left(\frac{\pi i}{2}(a\lambda^{-1}-b\lambda)^2\right)$$
$$\times\sum_{r=0}^{k}\binom{k}{r}G^{(r)}\bigl(a\lambda^{-1}+b\lambda;\lambda^2\bigr)H_{k-r}(\omega_\lambda)\Bigl(\frac{\pi}{2}\Bigr)^{(k-r)/2}\varepsilon^{k-r}. \quad (2.44)$$

Put (2.44) into (2.42) and the final step, to get the formula into the form we want, uses the identities

$$\frac{\beta^{s-1}}{\lambda^{1/2}} = \Bigl(\frac{2\pi}{t}\Bigr)^{1/4}\exp\left(\Bigl(\frac{s}{2}-\frac{1}{4}\Bigr)\log\frac{t}{2\pi}\right)\lambda^{1/2-s} \quad (2.45)$$

and

$$\exp\left(-2\pi im\beta-\pi i\left(b^2\lambda^2+\frac{1}{8}\right)\right)\exp\left(\frac{\pi i}{2}(a\lambda^{-1}-b\lambda)^2\right)$$
$$= (-1)^{\lfloor\alpha\rfloor\lfloor\beta\rfloor}\exp\left(\frac{\pi i}{2}\Bigl[2a\beta-2b\alpha+a^2\lambda^{-2}-b^2\lambda^2\Bigr]\right)\exp\left(-\frac{it}{2}-\frac{i\pi}{8}\right). \quad (2.46)$$

Equation (2.45) follows from $\beta^2 = t/(2\pi\lambda^2)$. Also $m=\lfloor\alpha\rfloor$, $\pi i\alpha\beta = it/2$ and the equalities

$$1 = e^{2\pi i\lfloor\alpha\rfloor\lfloor\beta\rfloor} = e^{2\pi i(\alpha-a)(\beta-b)} = e^{2\pi i(\alpha\beta-\alpha b-a\beta+ab)},$$
$$(-1)^{\lfloor\alpha\rfloor\lfloor\beta\rfloor} = e^{\pi i(\alpha-a)(\beta-b)} = e^{\pi i(\alpha\beta-\alpha b-a\beta+ab)}$$

show (2.46). This completes the proof of Theorem 2.1. □

3 The Mordell integral $\Upsilon(u;\tau)$

3.1 Relations

For $u,\tau \in \mathbb{C}$ with $\mathrm{Re}(\tau) > 0$, recall our definition from (1.15)

$$\Upsilon(u;\tau) := \int_{0 \nwarrow 1} \frac{e^{-\pi i \tau z^2 + 2\pi i u z}}{e^{2\pi i z} - 1}\, dz. \tag{3.1}$$

This type of integral was studied in detail by Mordell [Mor33] with earlier work by Kronecker, Lerch, Ramanujan and Riemann; see the references in the introduction of [CR15]. The method of Riemann for $\tau = 1$, described in [Sie32, Sect. 1], easily extends to give

$$\Upsilon(u+1;\tau) = \Upsilon(u;\tau) + \tau^{-1/2} e^{\pi i (u^2/\tau + 3/4)}, \tag{3.2}$$

$$\Upsilon(u+\tau;\tau) = e^{\pi i(\tau+2u)}(\Upsilon(u;\tau) - 1). \tag{3.3}$$

Applying these relations repeatedly yields the following result.

Proposition 3.1. *Suppose* $u,\tau \in \mathbb{C}$ *with* $\mathrm{Re}(\tau) > 0$. *Then for all* $m,n \in \mathbb{Z}_{\geqslant 0}$

$$\Upsilon(u+m;\tau) = \Upsilon(u;\tau) + e^{3\pi i/4}\tau^{-1/2} \sum_{j=0}^{m-1} e^{\pi i (j+u)^2/\tau}, \tag{3.4}$$

$$\Upsilon(u+n\tau;\tau) = e^{\pi i n(n\tau+2u)}\Upsilon(u;\tau) - e^{\pi i (n\tau+u)^2/\tau} \sum_{j=0}^{n-1} e^{-\pi i (j\tau+u)^2/\tau}. \tag{3.5}$$

This allows us to compute $\Upsilon(u;\tau)$ explicitly for τ a positive rational. If $n\tau = m$ for $m,n \in \mathbb{Z}_{\geqslant 1}$ then equating (3.4) and (3.5) shows, as in [Deu67, Sect. 1],

$$\left(e^{\pi i n(m+2u)} - 1\right)\Upsilon\left(u;\frac{m}{n}\right) = e^{3\pi i/4}\frac{\sqrt{n}}{\sqrt{m}} \sum_{j=0}^{m-1} e^{\pi i (j+u)^2 n/m} + e^{\pi i (m+u)^2 n/m} \sum_{j=0}^{n-1} e^{-\pi i (j+nu/m)^2 m/n}. \tag{3.6}$$

The right side of (3.6) is left essentially unchanged if m and n are interchanged, u is replaced by nu/m, and everything is conjugated. Precisely, we have

$$\overline{\left(e^{\pi i m(n+2n\overline{u}/m)} - 1\right)\Upsilon\left(\frac{n\overline{u}}{m};\frac{n}{m}\right)} = e^{-3\pi i/4}\frac{\sqrt{m}}{\sqrt{n}} e^{-\pi i (m+u)^2 n/m}\left(e^{\pi i n(m+2u)} - 1\right)\Upsilon\left(u;\frac{m}{n}\right).$$

Simplifying this shows

$$\begin{aligned}\overline{\Upsilon\left(\frac{n\overline{u}}{m};\frac{n}{m}\right)} &= -e^{-3\pi i/4}\frac{\sqrt{m}}{\sqrt{n}} e^{-\pi i (m+u)^2 n/m} e^{\pi i n(m+2u)}\Upsilon\left(u;\frac{m}{n}\right)\\ &= \frac{\sqrt{m}}{\sqrt{n}} e^{-\pi i (nu^2/m - 1/4)}\Upsilon\left(u;\frac{m}{n}\right).\end{aligned} \tag{3.7}$$

As in (1.16), set

$$G(u;\tau) := \tau^{1/4}\exp\left(-\frac{\pi i u^2}{2} + \frac{\pi i}{8}\right)\Upsilon\left(\sqrt{\tau}\cdot u;\tau\right). \tag{3.8}$$

This definition gives the simplest possible transformation under $\tau \to 1/\tau$, as we see next.

Proposition 3.2. *For all* $u,\tau \in \mathbb{C}$ *with* $\mathrm{Re}(\tau) > 0$ *we have*

$$\Upsilon(u/\tau;1/\tau) = \sqrt{\tau} e^{\pi i (u^2/\tau - 1/4)}\overline{\Upsilon(\overline{u};\overline{\tau})}, \tag{3.9}$$

$$G(u;1/\tau) = \overline{G(\overline{u};\overline{\tau})}, \tag{3.10}$$

$$G^{(k)}(u;1/\tau) = \overline{G^{(k)}(\overline{u};\overline{\tau})}, \qquad (k \in \mathbb{Z}_{\geqslant 0}). \tag{3.11}$$

Proof. We obtain (3.9) from (3.7) for all $u \in \mathbb{C}$ and all $\tau \in \mathbb{Q}_{>0}$. Since both sides of (3.9) are holomorphic functions of τ for $\mathrm{Re}(\tau) > 0$, it follows that (3.9) extends to all these values of τ. Then (3.10) follows directly from (3.9). Differentiating (3.10) with respect to u provides (3.11). $\square$

3.2 Examples

Let

$$\theta_k(u) := u^2/2 - \sqrt{k}u - k/2 - 1/8. \tag{3.12}$$

For all $m, n \in \mathbb{Z}_{\geqslant 1}$ we have from (3.6) and (3.8) that

$$\begin{aligned} G\Big(u; \frac{m}{n}\Big) = & \frac{1}{2i\sin(\pi(\sqrt{mn}u + mn/2))} \\ & \times \Bigg[\Big(\frac{m}{n}\Big)^{1/4} \exp\Big(-\pi i\theta_{mn}(u)\Big) \sum_{j=0}^{n-1} \exp\Big(-\pi i j\Big[2u\sqrt{\frac{m}{n}} + j\frac{m}{n}\Big]\Big) \\ & - \Big(\frac{m}{n}\Big)^{-1/4} \exp\Big(\pi i\theta_{mn}(u)\Big) \sum_{j=0}^{m-1} \exp\Big(\pi i j\Big[2u\sqrt{\frac{n}{m}} + j\frac{n}{m}\Big]\Big)\Bigg]. \end{aligned} \tag{3.13}$$

If u makes $\sqrt{mn}u + mn/2$ an integer, then the denominator $\sin(\pi(\sqrt{mn}u + mn/2))$ is zero. Since $G(u; m/n)$ is a holomorphic function of u, it follows that the numerator in (3.13) must also be zero. For these values of u, $G(u; m/n)$ may be found by taking limits. The numerator being zero in these cases also gives instances of Gauss sum reciprocity as mentioned by Siegel in [Sie32] and shown in [Deu67].

In the simplest case of $\tau = 1$ we know by (3.10) that $G(u;1) = \overline{G(\overline{u};1)}$ and so $G(u;1)$ is real-valued when $u \in \mathbb{R}$. Then (3.13) implies

$$G(u;1) = -\frac{1}{2i\sin(\pi(u+1/2))}\Big(e^{\pi i\theta_1(u)} - e^{-\pi i\theta_1(u)}\Big) = -\frac{\sin(\pi\theta_1(u))}{\sin(\pi(u+1/2))}.$$

This may also be written as

$$G(u;1) = -\frac{\sin(\pi(u^2/2 - u - 5/8))}{\sin(\pi(u+1/2))} = \frac{\cos(\pi(u^2/2 - u - 1/8))}{\cos(\pi u)}. \tag{3.14}$$

For $\tau = 2, 3$ we find

$$G(u;2) = \frac{-1}{2i\sin(\sqrt{2}\pi u)}\Big[2^{1/4}e^{-\pi i\theta_2(u)} - 2^{-1/4}e^{\pi i\theta_2(u)}\Big(1 + ie^{\sqrt{2}\pi i u}\Big)\Big], \tag{3.15}$$

$$G(u;3) = \frac{-1}{2i\cos(\sqrt{3}\pi u)}\Big[3^{1/4}e^{-\pi i\theta_3(u)} - 3^{-1/4}e^{\pi i\theta_3(u)}\Big(1 + e^{\pi i(2u/\sqrt{3}+1/3)} + e^{\pi i(4u/\sqrt{3}+4/3)}\Big)\Big].$$

3.3 Analytic continuation and Zwegers' $h(u;\tau)$

The results in this subsection will not be needed in the rest of the paper, though they establish an interesting connection. In his thesis [Zwe02], [BFOR17, Chap. 8], Zwegers puts the mock theta functions of Ramanujan into a modular framework. His Appell-Lerch series $\mu(z_1, z_2; \tau)$, see [Zwe02, Sect. 1.3], is a two-variable Jacobi form of weight $1/2$, except that a term containing

$$h(u;\tau) := \int_{-\infty}^{\infty} \frac{e^{\pi i\tau y^2 + 2\pi u y}}{\cosh(\pi y)}\, dy \qquad (u \in \mathbb{C},\ \mathrm{Im}(\tau) > 0) \tag{3.16}$$

appears in its modular transformations. Zwegers then shows that, by adding a non-holomorphic component, μ may be completed into a Jacobi form that transforms correctly. The mock theta functions can then be expressed in terms of μ, as in [BFOR17, Appendix A].

The function $h(u;\tau)$ also appears in [Zwe02, Sect. 1.5] as the period integral of a weight $3/2$ unary theta function. Ramanujan wrote $h(u;\tau)$ in terms of a partial theta function; see [CR15, Thm. 2.1]. Thus, $h(u;\tau)$ has many interesting connections to modular and mock modular forms. We see next that $h(u;\tau)$ and $\Upsilon(u;\tau)$ are closely related.

Lemma 3.3. *We have*

$$\Upsilon(u;\tau) = e^{\pi i(u-1/2-\tau/4)} \int_{-\infty}^{\infty} \frac{e^{\pi i\tau y^2+\pi y(\tau-2u+1)}}{e^{\pi y}+e^{-\pi y}}\,dy \tag{3.17}$$

for all u, τ *with*

$$\mathrm{Re}(\tau)>0, \quad \mathrm{Im}(\tau)>0 \quad \textit{and} \quad \frac{\mathrm{Re}(\tau)-\mathrm{Im}(\tau)}{2} < \mathrm{Re}(u) < 1+\frac{\mathrm{Re}(\tau)-\mathrm{Im}(\tau)}{2}. \tag{3.18}$$

Proof. We wish to rotate the line of integration $0 \nwarrow 1$ in (1.15) and make it vertical, passing through $1/2$. For large $Y>0$ we replace the line of integration from $1/2$ to $1/2-Y+iY$ by the lines from $1/2$ to $1/2+iY$ and $1/2+iY$ to $1/2-Y+iY$. To bound the integral on the horizontal segment

$$\mathfrak{I}_Y := \int_{1/2+iY}^{1/2-Y+iY} \frac{e^{-\pi i\tau z^2+2\pi iuz}}{e^{2\pi iz}-1}\,dz,$$

we let $z=x+iY$ and find

$$\mathfrak{I}_Y \ll \int_{1/2-Y}^{1/2} \frac{\exp\big(2\pi\big[\mathrm{Re}(\tau)xY+\mathrm{Im}(\tau)(x^2-Y^2)/2-\mathrm{Re}(u)Y-\mathrm{Im}(u)x\big]\big)}{e^{-2\pi Y}-1}\,dx.$$

For $\mathrm{Im}(\tau)>0$ we have $\mathrm{Im}(\tau)(x^2-Y^2) \leqslant \mathrm{Im}(\tau)(1/4-Y)$, and so obtain

$$\begin{aligned}\mathfrak{I}_Y &\ll \exp\Big(-\pi Y(2\mathrm{Re}(u)+\mathrm{Im}(\tau))\Big)\int_{1/2-Y}^{1/2} \exp(2\pi x[\mathrm{Re}(\tau)Y-\mathrm{Im}(u)])\,dx \\ &\ll \exp\Big(-\pi Y(2\mathrm{Re}(u)+\mathrm{Im}(\tau)-\mathrm{Re}(\tau))\Big).\end{aligned} \tag{3.19}$$

The line of integration from $1/2+Y-iY$ to $1/2$ is also replaced by horizontal and vertical lines. A similar argument shows that the horizontal integral satisfies

$$\mathfrak{I}_{-Y} := \int_{1/2+Y-iY}^{1/2-iY} \frac{e^{-\pi i\tau z^2+2\pi iuz}}{e^{2\pi iz}-1}\,dz \ll \exp\Big(-\pi Y(-2\mathrm{Re}(u)+2-\mathrm{Im}(\tau)+\mathrm{Re}(\tau))\Big). \tag{3.20}$$

Therefore, as $Y\to\infty$, the bounds (3.19), (3.20) imply that $\mathfrak{I}_Y\to 0$ and $\mathfrak{I}_{-Y}\to 0$ if the inequalities on the right of (3.18) are satisfied. This completes the proof. $\square$

Hence

$$\Upsilon(u;\tau) = \frac{1}{2}e^{\pi i(u-1/2-\tau/4)}h\Big(\frac{\tau}{2}-u+\frac{1}{2};\tau\Big), \tag{3.21}$$

initially for all u and τ satisfying (3.18). By analytically continuing both sides in u we see that (3.21) becomes true for all $u\in\mathbb{C}$ when $\mathrm{Re}(\tau), \mathrm{Im}(\tau)>0$. Therefore (3.17) and (3.21) give the analytic continuation of $\Upsilon(u;\tau)$ to all τ with $\mathrm{Im}(\tau)>0$ (and (3.21) gives the analytic continuation of $h(u;\tau)$ to all τ with $\mathrm{Re}(\tau)>0$).

Conjugating both sides of (3.17) shows that, for all $u\in\mathbb{C}$ and all τ with $\mathrm{Im}(\overline{\tau})>0$, we have

$$\overline{\Upsilon(\overline{u};\overline{\tau})} = e^{\pi i(\tau-2u+1)}\Upsilon(u-\tau;-\tau). \tag{3.22}$$

Rearranging and simplifying with (3.3) shows, for $\mathrm{Im}(\tau)>0$,

$$\Upsilon(u;\tau) = 1-\overline{\Upsilon(\overline{u};-\overline{\tau})}. \tag{3.23}$$

Since $\Upsilon(u;\tau)$ exists for $\mathrm{Re}(\tau)>0$, the relation (3.23) provides the continuation of $\Upsilon(u;\tau)$ to all τ with $\mathrm{Re}(\tau)<0$. In this way we have extended the definition of $\Upsilon(u;\tau)$ to all $u\in\mathbb{C}$ and all $\tau\in\mathbb{C}$ except for τ on the negative imaginary axis: $(-\infty,0]i$. It follows that (3.23) is valid for all τ outside $(-\infty,0]i$. Numerically, the values of $\Upsilon(u;\tau)$ for τ on each side of $(-\infty,0]i$ do not match, so we may take it as a branch cut. We have shown:

Proposition 3.4. *For each $u \in \mathbb{C}$, the function $\Upsilon(u;\tau)$ defined in* (3.1) *is an analytic function of τ when $\mathrm{Re}(\tau) > 0$. With* (3.16) *and* (3.21) *we obtain the analytic continuation to $\mathrm{Im}(\tau) > 0$. Then* (3.23) *gives the continuation to $\mathrm{Re}(\tau) < 0$.*

Combining (3.22) with (3.9) shows

$$e^{\pi i(\tau-2u+1)}\Upsilon(u-\tau;-\tau) = \frac{1}{\sqrt{\tau}}e^{-\pi i(u^2/\tau-1/4)}\Upsilon(u/\tau;1/\tau) \qquad (\mathrm{Re}(\tau)>0).$$

This is also

$$\Upsilon(-u/\tau;-1/\tau) = \sqrt{-\tau}e^{-\pi i(u^2/\tau+2u+\tau-3/4)}\Upsilon(u+\tau;\tau) \qquad (\mathrm{Re}(\tau)<0). \tag{3.24}$$

For $\mathrm{Re}(\tau) < 0$ and $\mathrm{Im}(\tau) > 0$ we have the equality of principal square roots $\sqrt{-\tau} = e^{-\pi i/4}\sqrt{-i\tau}$. Putting this into (3.24) gives

$$\Upsilon(-u/\tau;-1/\tau) = \sqrt{-i\tau}e^{-\pi i(u^2/\tau+2u+\tau-1/2)}\Upsilon(u+\tau;\tau) \tag{3.25}$$

which by analytic continuation in τ is valid for all τ outside of the negative imaginary axis. Translating (3.25) into a relation for $h(z;\tau)$ by (3.21), with $z = u + \tau/2 - 1/2$ and using $h(-z;\tau) = h(z;\tau)$, shows

$$h(z/\tau;-1/\tau) = \sqrt{-i\tau}e^{-\pi i z^2/\tau}h(z;\tau) \tag{3.26}$$

which is part (5) of [Zwe02, Prop. 1.2]. Therefore we have given another proof of (3.26) which is proved in [Zwe02] with the Fourier transform. Alternatively, starting with (3.26) and using (3.22), we may give another proof of Proposition 3.2.

Parts (1) and (2) of [Zwe02, Prop. 1.2] are equivalent to (3.2), (3.3). Part (6) translates into the following interesting identity. For all $u \in \mathbb{C}$ and initially for all τ with $\mathrm{Im}(\tau) > 0$

$$\Upsilon(u;\tau) - \Upsilon\left(u+\frac{1}{2};\tau+1\right) = \frac{1}{\sqrt{\tau+1}}\exp\left(\pi i\left[\frac{4u^2-4u-\tau}{4(\tau+1)}\right]\right)\cdot\Upsilon\left(\frac{2u+\tau}{2(\tau+1)};\frac{\tau}{\tau+1}\right).$$

3.4 Bounds for Υ and G

The proof of our main theorem will require these next estimates.

Proposition 3.5. *For all $u, \tau \in \mathbb{R}$ with $0 < \tau \leqslant 1$ we have*

$$\tau^{k/2}\Upsilon^{(k)}(u;\tau) \ll \tau^{-1/2}(1+|u|)\left(1+\frac{1+|u|^k}{\tau^{k/2}}\right)$$

for an implied constant depending only on $k \in \mathbb{Z}_{\geqslant 0}$.

Proof. Suppose that $u = x + m$ with $0 \leqslant x < 1$ and $m \in \mathbb{Z}$. If $m \geqslant 0$, then differentiating (3.4) k times implies

$$\Upsilon^{(k)}(u;\tau) = \Upsilon^{(k)}(x;\tau) + e^{3\pi i/4}\tau^{-1/2}\sum_{j=0}^{m-1}\frac{d^k}{dx^k}e^{\pi i(j+x)^2/\tau}.$$

The right-hand terms may be evaluated with the identity

$$\frac{d^k}{dx^k}e^{-c^2(x+q)^2} = \Big[(-c)^k H_k(c(x+q))\Big]e^{-c^2(x+q)^2} \tag{3.27}$$

and $c = e^{-\pi i/4}\sqrt{\pi/\tau}$, $q = j$. Hence

$$\Upsilon^{(k)}(u;\tau) - \Upsilon^{(k)}(x;\tau) = \tau^{-1/2}\sum_{j=0}^{m-1}e^{3\pi i(k+1)/4}\left(\frac{\pi}{\tau}\right)^{k/2}H_k\left(e^{-\pi i/4}\frac{\sqrt{\pi}}{\sqrt{\tau}}(x+j)\right)e^{\pi i(j+x)^2/\tau} \tag{3.28}$$

$$\ll \tau^{-k/2-1/2}\sum_{j=0}^{m-1}\left(1+\frac{(j+1)^k}{\tau^{k/2}}\right)$$

$$\ll \tau^{-k/2-1/2}(1+|u|)\left(1+\frac{(1+|u|)^k}{\tau^{k/2}}\right). \tag{3.29}$$

We find the same bound when $u = x + m$ with $m \leqslant 0$. This reduces the question to estimating $\Upsilon^{(k)}(u;\tau)$ for $0 \leqslant u < 1$.

Differentiating (1.15) inside the integral is valid and writing $z = 1/2 + \varepsilon t$ then shows

$$\Upsilon^{(k)}(u;\tau) = -\varepsilon(\pi i)^k e^{\pi i(u-\tau/4)} \int_{\mathbb{R}} \frac{\exp\big(-\pi\tau t^2 + \pi i\varepsilon(2u-\tau)t\big)}{e^{2\pi i\varepsilon t}+1}(1+2\varepsilon t)^k \, dt. \tag{3.30}$$

It is straightforward to see that

$$\frac{1}{|e^{2\pi i\varepsilon t}+1|} < \begin{cases} 2e^{\sqrt{2}\pi t} & \text{if} \quad t \leqslant 0, \\ 2 & \text{if} \quad t \geqslant 0. \end{cases} \tag{3.31}$$

We have

$$\Upsilon^{(k)}(u;\tau) \ll \int_{\mathbb{R}} \exp\left(-\pi\tau t^2 + \frac{\pi\tau t}{\sqrt{2}}\right) \frac{\exp\big(-\sqrt{2}\pi u t\big)}{|e^{2\pi i\varepsilon t}+1|}(1+|t|^k)\, dt. \tag{3.32}$$

If we now assume that $0 \leqslant u \leqslant 1$, then the middle fraction in (3.32) is at most 2 by (3.31). Changing variables we obtain

$$\Upsilon^{(k)}(u;\tau) \ll \int_{\mathbb{R}} \exp\left(-\pi v^2 + \frac{\pi\sqrt{\tau} v}{\sqrt{2}}\right)\left(1 + \frac{|v|^k}{\tau^{k/2}}\right)\frac{dv}{\tau^{1/2}}$$

and this is $\ll \tau^{-1/2}(1+\tau^{-k/2})$ when $\tau \leqslant 1$. Using this last bound for $\Upsilon^{(k)}(x;\tau)$ in (3.29) and simplifying completes the proof. ☐

Theorem 3.6. *For all $u, \tau \in \mathbb{R}$ with $\tau > 0$ we have*

$$G^{(k)}(u;\tau) \ll \begin{cases} \tau^{-1/4}\big(1+\tau^{1/2}|u|\big)\big(1+\tau^{-k/2}+|u|^k\big) & \textit{if} \quad \tau \leqslant 1, \\ \tau^{1/4}\big(1+\tau^{-1/2}|u|\big)\big(1+\tau^{k/2}+|u|^k\big) & \textit{if} \quad \tau \geqslant 1 \end{cases} \tag{3.33}$$

for an implied constant depending only on $k \in \mathbb{Z}_{\geqslant 0}$.

Proof. From the definition (1.16) and (3.27) we have

$$G^{(k)}(u;\tau) := \tau^{1/4} e^{\pi i/8} \sum_{j=0}^{k} \binom{k}{j} \frac{d^j}{du^j} \exp\left(-\frac{\pi i u^2}{2}\right) \cdot \frac{d^{k-j}}{du^{k-j}} \Upsilon(\sqrt{\tau} u;\tau)$$
$$= \tau^{1/4} \exp\left(-\frac{\pi i u^2}{2} + \frac{\pi i}{8}\right) \sum_{j=0}^{k} \binom{k}{j} e^{5\pi i j/4} \left(\frac{\pi}{2}\right)^{j/2} H_j\left(e^{\pi i/4}\frac{\sqrt{\pi}}{\sqrt{2}} u\right) \cdot \tau^{(k-j)/2}\Upsilon^{(k-j)}(\sqrt{\tau}u;\tau). \tag{3.34}$$

Then, using Proposition 3.5,

$$G^{(k)}(u;\tau) \ll \tau^{-1/4} \sum_{j=0}^{k} (1+|u|^j)\Big(1+\tau^{1/2}|u|\Big)\Big(1+\tau^{(j-k)/2}+|u|^{k-j}\Big)$$
$$\ll \tau^{-1/4}\Big(1+\tau^{1/2}|u|\Big)\Big(1+\tau^{-k/2}+|u|^k\Big) \tag{3.35}$$

for $\tau \leqslant 1$. When $\tau \geqslant 1$, the relation (3.11) combined with (3.35) finishes the proof of (3.33). ☐

Corollary 3.7. *For $\lambda > 0$ and a, b satisfying $0 \leqslant a, b \leqslant 1$ we have*

$$G^{(k)}(a\lambda^{-1} + b\lambda; \lambda^2) = O\Big(\lambda^{k+1/2} + \lambda^{-k-1/2}\Big)$$

for an implied constant depending only on $k \in \mathbb{Z}_{\geqslant 0}$.

3.5 Linear independence

The next result will be needed in the proof of Theorem 6.1.

Proposition 3.8. *Let τ with $\mathrm{Re}(\tau) > 0$ be fixed. The functions of u in the set*

$$\Big\{G(u;\tau),\ G^{(1)}(u;\tau),\ G^{(2)}(u;\tau),\ \dots,\ G^{(m)}(u;\tau)\Big\}$$

are linearly independent for any $m \in \mathbb{Z}_{\geqslant 0}$. (The $m = 0$ case is saying that, for each τ, $G(u;\tau)$ is never identically 0 as a function of u.)

Proof. Suppose we have

$$\sum_{j=0}^{m} c_j \tau^{-j/2} G^{(j)}(u;\tau) = 0 \qquad (u \in \mathbb{C}). \tag{3.36}$$

The constants c_j may depend on the fixed τ and it is convenient to include the nonzero factor $\tau^{-j/2}$. Replacing $G(u;\tau)$ with $\Upsilon(\sqrt{\tau}u;\tau)$ using (3.34), and then replacing u by $u/\sqrt{\tau}$ implies

$$\sum_{j=0}^{m} \psi_j(u)\Upsilon^{(j)}(u;\tau) = 0 \qquad (u \in \mathbb{C}) \tag{3.37}$$

for polynomials $\psi_j(u)$. Explicitly, for $0 \leqslant j \leqslant m$, we have

$$\psi_j(u) = \sum_{k=j}^{m} c_k \binom{k}{j} e^{5\pi i(k-j)/4} \Big(\frac{\pi}{2\tau}\Big)^{(k-j)/2} H_{k-j}\Big(e^{\pi i/4}\frac{\sqrt{\pi}}{\sqrt{2\tau}}u\Big).$$

The highest degree term in $H_n(y)$ is $2^n y^n$ by (6.7) and so $\psi_j(u)$ has degree $m - j$ with highest degree term

$$c_m \binom{m}{j} (-\pi i/\tau)^{m-j} \cdot u^{m-j}. \tag{3.38}$$

Since we know (3.2), it is natural to apply the difference operator Δ to (3.37). We have

$$\Delta\Upsilon^{(j)}(u;\tau) := \Upsilon^{(j)}(u+1;\tau) - \Upsilon^{(j)}(u;\tau) = L_j(u)e^{\pi i u^2/\tau}$$

for, using the calculation in (3.28) with $m = 1$,

$$L_j(u) := \tau^{-1/2} e^{3\pi i(j+1)/4} \Big(\frac{\pi}{\tau}\Big)^{j/2} H_j\Big(e^{-\pi i/4}\frac{\sqrt{\pi}}{\sqrt{\tau}}u\Big).$$

Recall that

$$\Delta(f(u)g(u)) = (\Delta f(u)) \cdot g(u) + f(u+1) \cdot (\Delta g(u)),$$

and applying Δ to a polynomial reduces the degree by at least 1. Hence Δ applied to (3.37) implies

$$\sum_{j=0}^{m-1} (\Delta\psi_j(u))\Upsilon^{(j)}(u;\tau) + \sum_{j=0}^{m} \psi_j(u+1)L_j(u)e^{\pi i u^2/\tau} = 0 \tag{3.39}$$

and a second application gives

$$\sum_{j=0}^{m-2} \big(\Delta^2\psi_j(u)\big)\Upsilon^{(j)}(u;\tau) + \sum_{j=0}^{m-1} (\Delta\psi_j(u+1))L_j(u)e^{\pi i u^2/\tau} + \sum_{j=0}^{m} \Delta\Big[\psi_j(u+1)L_j(u)e^{\pi i u^2/\tau}\Big] = 0.$$

After a total of $m + 1$ applications of the difference operator to (3.37), the functions $\Upsilon^{(j)}(u;\tau)$ disappear and we are left with

$$\sum_{k=0}^{m} \sum_{j=0}^{m-k} \Delta^{m-k}\Big[\Big(\Delta^k\psi_j(u+1)\Big)L_j(u)e^{\pi i u^2/\tau}\Big] = 0. \tag{3.40}$$

To expand (3.40), note the easily verified relations

$$\Delta^m(f(u)g(u)) = \sum_{j=0}^{m} \binom{m}{j} \Delta^{m-j}(f(u+j)) \cdot \Delta^j g(u),$$
$$\Delta^m f(u) = \sum_{j=0}^{m} (-1)^{m-j} \binom{m}{j} f(u+j).$$

Define the polynomial $h_{k,j}(u) := \big(\Delta^k \psi_j(u+1)\big) L_j(u)$, and the left side of (3.40) equals

$$\sum_{k=0}^{m} \sum_{j=0}^{m-k} \Delta^{m-k}\Big[h_{k,j}(u) e^{\pi i u^2/\tau}\Big]$$
$$= \sum_{k=0}^{m} \sum_{j=0}^{m-k} \sum_{r=0}^{m-k} \binom{m-k}{r} \Delta^{m-k-r} h_{k,j}(u+r) \cdot \Delta^r e^{\pi i u^2/\tau}$$
$$= e^{\pi i u^2/\tau} \sum_{k=0}^{m} \sum_{j=0}^{m-k} \sum_{r=0}^{m-k} \binom{m-k}{r} \Delta^{m-k-r} h_{k,j}(u+r) \cdot \sum_{\ell=0}^{r} e^{\pi i \ell^2/\tau} (-1)^{r-\ell} \binom{r}{\ell} e^{2\pi i \ell u/\tau}. \quad (3.41)$$

Dividing both sides of (3.40) by $e^{\pi i u^2/\tau}$ implies with (3.41) that

$$\sum_{\ell=0}^{m} \phi_\ell(u) e^{2\pi i \ell u/\tau} = 0 \quad (3.42)$$

for polynomials $\phi_\ell(u)$. Clearly $e^{2\pi i m u/\tau}$ only appears in (3.41) when $k=0$, and so for $\ell = r = m$ in (3.41) we find

$$\phi_m(u) = e^{\pi i m^2/\tau} \sum_{j=0}^{m} \psi_j(u+m+1) L_j(u+m).$$

The degree of $\phi_m(u)$ is m since $\psi_j(u)$ has degree $m-j$ and $L_j(u)$ has degree j. The coefficient of u^m in $\phi_m(u)$ is therefore, using (3.38),

$$e^{\pi i m^2/\tau} \sum_{j=0}^{m} \left[c_m \binom{m}{j} \left(\frac{-\pi i}{\tau}\right)^{m-j} \right] \cdot \left[\tau^{-1/2} e^{3\pi i/4} \left(\frac{2\pi i}{\tau}\right)^{j} \right]$$
$$= c_m \cdot \tau^{-1/2} e^{\pi i (m^2/\tau + 3/4)} \sum_{j=0}^{m} \binom{m}{j} \left(\frac{-\pi i}{\tau}\right)^{m-j} \left(\frac{2\pi i}{\tau}\right)^{j}$$
$$= c_m \cdot \tau^{-1/2} e^{\pi i (m^2/\tau + 3/4)} \left(\frac{\pi i}{\tau}\right)^{m}. \quad (3.43)$$

However, it follows from (3.42) that all the polynomials $\phi_k(u)$ are identically 0. A simple way to see this is to put $u = -i\tau y$ and examine the size of each term as $y \to \infty$. Hence (3.43) is 0 and so $c_m = 0$. Repeating this argument shows that all of the coefficients $c_0, c_1, \dots, c_m$ in (3.36) are 0, as we wanted to prove. □

4 Some series expansions

4.1 The Riemann-Siegel function $\vartheta(s)$

We begin with

Lemma 4.1. *Suppose $s \in \mathbb{C}$ satisfies $\sigma \in I$ and $t \neq 0$. Then for all $k, R \in \mathbb{Z}_{\geqslant 0}$ we have*

$$\frac{1}{(\sigma+it)^k} = \frac{1}{(it)^k} \sum_{r=0}^{R-1} \binom{k+r-1}{r} \left(\frac{-\sigma}{it}\right)^r + O\left(\frac{1}{|t|^{k+R}}\right) \quad (4.1)$$

for an implied constant depending only on I, k and R.

Proof. By Taylor's Theorem and bounding the integral form of the remainder in the usual way, as in (2.18), we have

$$(1+z)^{-k} = \sum_{r=0}^{R-1} \binom{-k}{r} z^r + O(|z|^R) \tag{4.2}$$

for all $z \in \mathbb{C}$ when $|z| \leqslant 1/2$, say. The coefficients of z^r in the sum (4.2) are given by the Generalized Binomial Theorem. With $z = \sigma/(it)$, this proves (4.1) when $|t| \geqslant 2|\sigma|$. If $0 < |t| \leqslant 2|\sigma|$ then

$$\begin{aligned} |t|^{k+R} & \left| \frac{1}{(\sigma+it)^k} - \frac{1}{(it)^k} \sum_{r=0}^{R-1} \binom{k+r-1}{r} \left(\frac{-\sigma}{it}\right)^r \right| \\ & \leqslant |t|^R + \sum_{r=0}^{R-1} \binom{k+r-1}{r} |\sigma|^r |t|^{R-r} \leqslant |2\sigma|^R + \sum_{r=0}^{R-1} \binom{k+r-1}{r} |\sigma|^r |2\sigma|^{R-r} = O(1). \end{aligned}$$

Hence the error in (4.1) is $O(|t|^{-k-R})$ for $0 < |t| \leqslant 2|\sigma|$ as well, completing the proof. □

Hermite and Barnes gave the asymptotics of $\log \Gamma(z+a)$ as $|z| \to \infty$ when $0 \leqslant a \leqslant 1$. These shifted argument results and further improvements are described in [Nem13]. See also [Olv74, Ex. 4.4, p. 295], for example. Our next proposition shows the asymptotics of $\log \Gamma(s)$, for s in any vertical strip, in terms of σ and t. It agrees with the previously mentioned work when $0 \leqslant \sigma \leqslant 1$.

Proposition 4.2. *Suppose $s \in \mathbb{C}$ satisfies $\sigma \in I$ and $t \neq 0$. Then*

$$\log \Gamma(s) = \left(s - \frac{1}{2}\right) \log it - it + \frac{1}{2} \log 2\pi - \sum_{k=1}^{N-1} \left(\frac{i}{t}\right)^k \frac{B_{k+1}(\sigma)}{k(k+1)} + O\left(\frac{1}{|t|^N}\right)$$

for an implied constant depending only on I and $N \in \mathbb{Z}_{\geqslant 1}$.

Proof. Stirling's series as in [Olv74, p. 294] states that for all $s \in \mathbb{C}$ with $s \notin (-\infty, 0]$ we have

$$\log \Gamma(s) - \left(s - \frac{1}{2}\right) \log s + s - \frac{\log 2\pi}{2} = \sum_{n=1}^{M-1} \frac{B_{2n}}{2n(2n-1)} \frac{1}{s^{2n-1}} - \frac{1}{2M} \int_0^\infty \frac{B_{2M}(v - \lfloor v \rfloor)}{(v+s)^{2M}}\, dv \tag{4.3}$$

where $M \in \mathbb{Z}_{\geqslant 1}$. We may replace the last term in (4.3) with $O(1/|t|^{2M-1})$ since

$$\int_0^\infty \frac{|B_{2M}(v - \lfloor v \rfloor)|}{|v+s|^{2M}}\, dv \ll \int_{-\infty}^\infty \frac{1}{((v+\sigma)^2 + t^2)^M}\, dv = \sqrt{\pi} \frac{\Gamma(M - 1/2)}{\Gamma(M)} \frac{1}{|t|^{2M-1}}$$

where the last equality is [GR07, 3.241.4]. With Lemma 4.1 we may write each $1/s^{2n-1}$ term in (4.3) as

$$\frac{1}{s^{2n-1}} = \sum_{r=0}^{R_n - 1} \binom{2n+r-2}{r} \frac{(-i)^{2n-1}(i\sigma)^r}{t^{2n+r-1}} + O\left(\frac{1}{|t|^{2n+R_n-1}}\right).$$

Choosing R_n so that $2n + R_n - 1 = 2M - 1$ we find that the left side of (4.3) equals

$$\begin{aligned} \sum_{n=1}^{M-1} & \frac{B_{2n}}{2n(2n-1)} \sum_{r=0}^{2M-2n-1} \binom{2n+r-2}{r} \frac{(-i)^{2n-1}(i\sigma)^r}{t^{2n+r-1}} + O\left(\frac{1}{|t|^{2M-1}}\right) \\ & = -\sum_{k=1}^{2M-2} \frac{i^k}{t^k} \sum_{n=1}^{\lfloor (k+1)/2 \rfloor} \binom{k-1}{2n-2} \frac{B_{2n}}{2n(2n-1)} \sigma^{k+1-2n} + O\left(\frac{1}{|t|^{2M-1}}\right) \\ & = -\sum_{k=1}^{2M-2} \frac{i^k}{k(k+1)} \left[B_{k+1}(\sigma) + \frac{k+1}{2}\sigma^k - \sigma^{k+1} \right] \frac{1}{t^k} + O\left(\frac{1}{|t|^{2M-1}}\right). \end{aligned}$$

Therefore

$$\log\Gamma(s) = \left(s-\frac{1}{2}\right)\log s - s + \frac{1}{2}\log 2\pi \\ - \sum_{k=1}^{N-1} \frac{i^k}{k(k+1)}\left[B_{k+1}(\sigma) + \frac{k+1}{2}\sigma^k - \sigma^{k+1}\right]\frac{1}{t^k} + O\left(\frac{1}{|t|^N}\right). \quad (4.4)$$

A similar proof to Lemma 4.1 shows that, for $\sigma \in I$ and $t \neq 0$,

$$\log s = \log(it) + \log\left(1+\frac{\sigma}{it}\right) = \log(it) - \sum_{k=1}^{N-1}\frac{(i\sigma)^k}{k\cdot t^k} + O\left(\frac{1}{|t|^N}\right)$$

where the implied constant depends only on $N \in \mathbb{Z}_{\geqslant 1}$ and I. Hence

$$\left(s-\frac{1}{2}\right)\log s = (s-1/2)\log(it) + \sigma + \sum_{k=1}^{N-1}\left(\frac{i}{t}\right)^k\left[\frac{\sigma^k}{2k} - \frac{\sigma^{k+1}}{k(k+1)}\right] + O\left(\frac{1}{|t|^N}\right). \quad (4.5)$$

Inserting (4.5) into (4.4) completes the proof. ☐

Since $-2i\vartheta(s) = (s-1/2)\log\pi + \log\Gamma((1-s)/2) - \log\Gamma(s/2)$ we easily now obtain

Corollary 4.3. *Suppose $s \in \mathbb{C}$ satisfies $\sigma \in I$ and $t \neq 0$. Then*

$$i\vartheta(s) = \left(\frac{s}{2}-\frac{1}{4}\right)\log\frac{|t|}{2\pi} - \frac{it}{2} - \operatorname{sgn}(t)\frac{i\pi}{8} \\ - \sum_{n=1}^{N-1}\left(\frac{2i}{t}\right)^n\left[\frac{B_{n+1}(\sigma/2) + (-1)^{n+1}B_{n+1}((1-\sigma)/2)}{2n(n+1)}\right] + O\left(\frac{1}{|t|^N}\right)$$

for an implied constant depending only on I and $N \in \mathbb{Z}_{\geqslant 1}$.

Corollary 4.4. *Suppose $t \neq 0$. Then*

$$\vartheta(1/2+it) = \frac{t}{2}\log\frac{|t|}{2\pi} - \frac{t}{2} - \operatorname{sgn}(t)\frac{\pi}{8} - \sum_{n=1}^{N-1}\frac{(-4)^{n-1}B_{2n}(1/4)}{(2n-1)n\cdot t^{2n-1}} + O\left(\frac{1}{|t|^{2N-1}}\right)$$

for an implied constant depending only on $N \in \mathbb{Z}_{\geqslant 1}$.

Corollary 4.4 agrees with [Gab79, Satz 4.2.3(b)] as $B_{2n}(1/4) = 2^{-2n}(2^{1-2n}-1)(-1)^{n+1}|B_{2n}|$.

4.2 De Moivre polynomial expansions

The De Moivre polynomials $\mathcal{A}_{i,j}$ give a convenient and explicit way to express the series coefficients we need. They complement the methods of Riemann and Siegel based on generating functions and recursions.

Let $p_1, p_2, p_3, \dots$ be any sequence of complex numbers and consider the formal series $p_1x + p_2x^2 + p_3x^3 + \cdots$. For integers i and j with $j \geqslant 0$, the generating function definition of $\mathcal{A}_{i,j}(p_1,p_2,p_3,\dots)$ is given by

$$\left(p_1x + p_2x^2 + p_3x^3 + \cdots\right)^j = \sum_{i\in\mathbb{Z}}\mathcal{A}_{i,j}(p_1,p_2,p_3,\dots)x^i. \quad (4.6)$$

For $i \geqslant j$ we note that

$$\mathcal{A}_{i,j}(p_1,p_2,p_3,\dots) = \sum_{\substack{1\ell_1+2\ell_2+\cdots+m\ell_m=i \\ \ell_1+\ell_2+\cdots+\ell_m=j}}\binom{j}{\ell_1,\ell_2,\cdots,\ell_m}p_1^{\ell_1}p_2^{\ell_2}\cdots p_m^{\ell_m}, \quad (4.7)$$

for $m = i - j + 1$ where the sum is over all possible $\ell_1, \ell_2, \dots, \ell_m \in \mathbb{Z}_{\geqslant 0}$. Hence $\mathcal{A}_{i,j}(p_1, p_2, p_3, \dots)$ is a polynomial in $p_1, p_2, \dots, p_{i-j+1}$ of homogeneous degree j with positive integer coefficients. For instance,

$$\mathcal{A}_{8,4}(p_1, p_2, p_3, \dots) = p_2^4 + 12p_1 p_2^2 p_3 + 6p_1^2 p_3^2 + 12p_1^2 p_2 p_4 + 4p_1^3 p_5.$$

The paper [O'S] gives a detailed account of these polynomials and their history. They may be expressed in terms of the closely related 'partial Bell polynomials' which are included in the Mathematica system, for example.

Based on the terms in Corollary 4.3 we make the definitions

$$f_n(\sigma) := \frac{B_{n+1}(\sigma/2) + (-1)^{n+1} B_{n+1}((1-\sigma)/2)}{2n(n+1)}, \tag{4.8}$$

$$u_m(\sigma) := (-2)^m \sum_{k=0}^{m} \frac{1}{k!} \mathcal{A}_{m,k}(f_1(\sigma), f_2(\sigma), \dots). \tag{4.9}$$

Then $f_n(\sigma)$ is a polynomial of degree $n+1$ with rational coefficients. Hence, $\mathcal{A}_{m,k}(f_1(\sigma), f_2(\sigma), \dots)$ has degree at most $m+k$. It follows that $u_m(\sigma)$ is a polynomial with rational coefficients. Its degree is exactly $2m$ since it may be checked that the coefficient of σ^{2m} in $u_m(\sigma)$ is $(-1)^m/(4^m m!)$. We have for example $u_0(\sigma) = 1$ and

$$u_1(\sigma) = (-1 + 6\sigma - 6\sigma^2)/24, \qquad u_2(\sigma) = (1 + 36\sigma - 96\sigma^2 + 24\sigma^3 + 36\sigma^4)/1152.$$

The next result requires the finite version of (4.6):

$$\big(p_1 x + p_2 x^2 + \cdots + p_r x^r\big)^j = \sum_{i=j}^{rj} \mathcal{A}_{i,j}(p_1, p_2, \dots, p_r, 0, 0, \dots) x^i. \tag{4.10}$$

Theorem 4.5. *Suppose $s \in \mathbb{C}$ satisfies $\sigma \in I$ and $t \geqslant \epsilon > 0$. Then*

$$\exp\left(\left(\frac{s}{2} - \frac{1}{4}\right) \log \frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8} - i\vartheta(s)\right) = \sum_{m=0}^{L-1} \frac{u_m(\sigma)}{(it)^m} + O\left(\frac{1}{t^L}\right) \tag{4.11}$$

for an implied constant depending only on I, ϵ and $L \in \mathbb{Z}_{\geqslant 0}$.

Proof. We first note that for all $z \in \mathbb{C}$ with $|z| \leqslant T$, and with an implied constant depending only on $K \in \mathbb{Z}_{\geqslant 0}$ and T, we have

$$e^z = \sum_{k=0}^{K-1} \frac{z^k}{k!} + O\big(|z|^K\big) \tag{4.12}$$

by Taylor's Theorem with the usual remainder estimates. Choose any $N \geqslant 1$ and set

$$z_t := \left(\frac{s}{2} - \frac{1}{4}\right) \log \frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8} - i\vartheta(s) - \sum_{n=1}^{N-1} \left(\frac{2i}{t}\right)^n f_n(\sigma)$$

for any s satisfying the conditions of the theorem. Then by Corollary 4.3 there is a constant $C_{I,N}$ so that

$$|z_t| \leqslant C_{I,N}/t^N \leqslant C_{I,N}/\epsilon^N.$$

Using (4.12) with $T = C_{I,N}/\epsilon^N$ and $K = 1$ we obtain $e^{z_t} = 1 + O(1/t^N)$, so that

$$\exp\left(\left(\frac{s}{2} - \frac{1}{4}\right) \log \frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8} - i\vartheta(s)\right) = \exp\left(\sum_{n=1}^{N-1} \left(\frac{2i}{t}\right)^n f_n(\sigma)\right) \left(1 + O\left(\frac{1}{t^N}\right)\right) \tag{4.13}$$

$$= \exp\left(\sum_{n=1}^{N-1} \left(\frac{2i}{t}\right)^n f_n(\sigma)\right) + O\left(\frac{1}{t^N}\right). \tag{4.14}$$

When $N = 1$ we mean $1 + O(1/t)$ on the right of (4.13) and (4.14). For $N \geqslant 2$, (4.14) follows from (4.13) by using that

$$\sum_{n=1}^{N-1} \left(\frac{2i}{t}\right)^n f_n(\sigma) = O\left(\frac{1}{t}\right) \quad \implies \quad \exp\left(\sum_{n=1}^{N-1} \left(\frac{2i}{t}\right)^n f_n(\sigma)\right) = O(1). \tag{4.15}$$

It is also true by (4.12) and the left bound in (4.15) that

$$\exp\left(\sum_{n=1}^{N-1} \left(\frac{2i}{t}\right)^n f_n(\sigma)\right) = \sum_{k=0}^{K-1} \frac{1}{k!}\left(\sum_{n=1}^{N-1} \left(\frac{2i}{t}\right)^n f_n(\sigma)\right)^k + O\left(\frac{1}{t^K}\right). \tag{4.16}$$

By (4.10), the sum on the right is

$$\begin{aligned} \sum_{k=0}^{K-1} \frac{1}{k!}\left(\sum_{n=1}^{N-1} \left(\frac{2i}{t}\right)^n f_n(\sigma)\right)^k &= \sum_{k=0}^{K-1} \frac{1}{k!} \sum_{m=k}^{(N-1)k} \mathcal{A}_{m,k}(f_1(\sigma), \dots, f_{N-1}(\sigma), 0, 0, \dots) \left(\frac{2i}{t}\right)^m \\ &= \sum_{m=0}^{(N-1)(K-1)} \left(\frac{-2}{it}\right)^m \times \sum_{k=0}^{\min(m,K-1)} \frac{1}{k!}\mathcal{A}_{m,k}(f_1(\sigma), \dots, f_{N-1}(\sigma), 0, 0, \dots). \end{aligned} \tag{4.17}$$

Recall that $\mathcal{A}_{m,k}(f_1(\sigma), \dots, f_{N-1}(\sigma), 0, 0, \dots)$ just requires the first $m - k + 1$ terms of the sequence $f_1(\sigma), \dots, f_{N-1}(\sigma), 0, 0, \dots$ and so will not use the 0 terms if $m-k+1 \leqslant N-1$. Therefore we may write (4.17) as

$$\sum_{m=0}^{N-2} \left(\frac{-2}{it}\right)^m \times \sum_{k=0}^{m} \frac{1}{k!}\mathcal{A}_{m,k}(f_1(\sigma), f_2(\sigma), \dots) + O\left(\frac{1}{t^{N-1}}\right) \tag{4.18}$$

if $N - 2 \leqslant K - 1$. Assembling (4.14), (4.16) and (4.18) yields

$$\begin{aligned} &\exp\left(\left(\frac{s}{2} - \frac{1}{4}\right) \log \frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8} - i\vartheta(s)\right) \\ &\qquad = \sum_{m=0}^{N-2} \left(\frac{-2}{it}\right)^m \times \sum_{k=0}^{m} \frac{1}{k!}\mathcal{A}_{m,k}(f_1(\sigma), f_2(\sigma), \dots) + O\left(\frac{1}{t^{N-1}}\right) + O\left(\frac{1}{t^{N}}\right) + O\left(\frac{1}{t^{K}}\right) \end{aligned}$$

for $K = N - 1$. Letting $L = N - 1$ in (4.11) completes the proof. ☐

Corollary 4.6. *Suppose $s \in \mathbb{C}$ satisfies $\sigma \in I$ and $t \geqslant \epsilon > 0$. Then*

$$\exp(i\vartheta(s)) = O\left(t^{\sigma/2-1/4}\right), \qquad \exp(-i\vartheta(s)) = O\left(t^{-\sigma/2+1/4}\right) \tag{4.19}$$

for implied constants depending only on I and ϵ.

Proof. By Theorem 4.5 with $L = 1$,

$$\exp\left(\left(\frac{s}{2} - \frac{1}{4}\right) \log \frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8} - i\vartheta(s)\right) = 1 + O\left(\frac{1}{t}\right). \tag{4.20}$$

It follows simply that the reciprocal of the left side has the same bound:

$$\exp\left(-\left(\frac{s}{2} - \frac{1}{4}\right) \log \frac{t}{2\pi} + \frac{it}{2} + \frac{i\pi}{8} + i\vartheta(s)\right) = 1 + O\left(\frac{1}{t}\right). \tag{4.21}$$

Multiplying both sides of (4.21) by $\exp\left(\left(\frac{s}{2} - \frac{1}{4}\right) \log \frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8}\right)$ and bounding gives the left estimate in (4.19). The right estimate is similar, manipulating (4.20). ☐

It should be possible to replace the restriction $t \geqslant \epsilon > 0$ in Theorem 4.5 and Corollary 4.6 with just $t > 0$. This would require a more careful treatment in Proposition 4.2 when $|t| < 1$. Our applications will only require $t \geqslant 2\pi$ in any case.

Set

$$g_n(\sigma) := -\frac{B_{n+1}(\sigma)}{n(n+1)} \qquad \text{and} \qquad \gamma_m(\sigma) := i^m \sum_{k=0}^{m} \frac{1}{k!} \mathcal{A}_{m,k}(g_1(\sigma), g_2(\sigma), \dots)$$

so that, for instance, $\gamma_0(\sigma) = 1$ and

$$\gamma_1(\sigma) = (-1 + 6\sigma - 6\sigma^2)i/12, \qquad \gamma_2(\sigma) = (-1 + 36\sigma - 120\sigma^2 + 120\sigma^3 - 36\sigma^4)/288.$$

Then a similar proof to that of Theorem 4.5, using Proposition 4.2, gives the asymptotics of the Γ function in vertical strips:

Proposition 4.7. *Suppose $s \in \mathbb{C}$ satisfies $\sigma \in I$ and $t \geqslant \epsilon > 0$. Then*

$$\Gamma(s) = \sqrt{2\pi} \exp\left(\frac{\pi i s}{2} - it - \frac{\pi i}{4}\right) t^{s-1/2} \left(\sum_{m=0}^{L-1} \frac{\gamma_m(\sigma)}{t^m} + O\left(\frac{1}{t^L}\right)\right)$$

for an implied constant depending only on I, ϵ and $L \in \mathbb{Z}_{\geqslant 0}$.

The power series coefficients $a_k(s)$ of $w(z,s)$ in (2.2) and (2.3) may also be expressed in terms of De Moivre polynomials. For this we will need the identity

$$\exp\big(u(p_1 x + p_2 x^2 + \dots)\big) = \sum_{n=0}^{\infty} x^n \sum_{k=0}^{n} \mathcal{A}_{n,k}(p_1, p_2, \dots) \frac{u^k}{k!}. \tag{4.22}$$

Define

$$d_{m,r}(\sigma) := \sum_{n=r}^{m} \frac{\mathcal{A}_{n,r}(\frac{1}{3}, -\frac{1}{4}, \frac{1}{5}, \dots)}{r!} \sum_{k=0}^{m-n} \frac{\mathcal{A}_{m-n,k}(1, -\frac{1}{2}, \frac{1}{3}, \dots)}{k!} (\sigma - 1)^k. \tag{4.23}$$

Proposition 4.8. *For all $k \in \mathbb{Z}_{\geqslant 0}$ we have*

$$a_k(s) = \sum_{r=0}^{\lfloor k/3 \rfloor} i^r \cdot d_{k-2r,r}(\sigma) \cdot t^{r-k/2}. \tag{4.24}$$

Proof. Expanding the logarithm in (2.2) into its power series and then employing (4.22) produces

$$\begin{aligned}
w(z,s) &= \exp\left((\sigma-1)\sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j}\left(\frac{z}{\sqrt{t}}\right)^j\right) \exp\left(iz^2 \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j+2}\left(\frac{z}{\sqrt{t}}\right)^j\right) \\
&= \left(\sum_{n=0}^{\infty}\left(\frac{z}{\sqrt{t}}\right)^n \sum_{k=0}^{n} \mathcal{A}_{n,k}(1, -\tfrac{1}{2}, \tfrac{1}{3}, \dots)\frac{(\sigma-1)^k}{k!}\right)\left(\sum_{m=0}^{\infty}\left(\frac{z}{\sqrt{t}}\right)^m \sum_{r=0}^{m} \mathcal{A}_{m,r}(\tfrac{1}{3}, -\tfrac{1}{4}, \tfrac{1}{5}, \dots)\frac{(iz^2)^r}{r!}\right) \\
&= \sum_{h=0}^{\infty}\left(\frac{z}{\sqrt{t}}\right)^h \sum_{r=0}^{h} (iz^2)^r \sum_{m=r}^{h} \frac{\mathcal{A}_{m,r}(\frac{1}{3}, -\frac{1}{4}, \frac{1}{5}, \dots)}{r!} \sum_{k=0}^{h-m} \frac{\mathcal{A}_{h-m,k}(1, -\frac{1}{2}, \frac{1}{3}, \dots)}{k!}(\sigma-1)^k.
\end{aligned}$$

Therefore

$$\begin{aligned}
w(z,s) &= \sum_{h=0}^{\infty} t^{-h/2} \sum_{r=0}^{h} i^r \cdot d_{h,r}(\sigma) \cdot z^{h+2r} \\
&= \sum_{k=0}^{\infty} z^k \sum_{r=0}^{\lfloor k/3 \rfloor} i^r \cdot d_{k-2r,r}(\sigma) \cdot t^{r-k/2}.
\end{aligned}$$

□

For example $a_0(s) = 1$, $a_1(s) = (\sigma - 1)/t^{1/2}$ and

$$a_2(s) = (\sigma^2 - 3\sigma + 2)/(2t), \qquad a_3(s) = (\sigma^3 - 6\sigma^2 + 11\sigma + 2it - 6)/(6t^{3/2}).$$

Siegel gave $a_k(s)$ in terms of the recursion (1.9). The advantage of Proposition 4.8 is that it gives explicit formulas for the coefficients of the powers of t in $a_k(s)$. These formulas will be needed in the next section.

5 Proof of most parts of the main theorem

Our goal in this section is the next result.

Theorem 5.1. *Recall the statement of Theorem 1.5. This statement, with the change that the implied constant in* (1.21) *may also depend on λ when $\lambda < 1$, is true.*

Proof. We begin with Theorem 2.1 and multiply both sides of (2.4) by $e^{i\vartheta(s)}$. Corollary 4.6 gives the estimate $e^{i\vartheta(s)} = O(t^{\sigma/2-1/4})$. It is convenient to abbreviate the inner sum in (2.4) as

$$c_k(\lambda) := \sum_{r=0}^{k} \binom{k}{r} G^{(r)}(a\lambda^{-1} + b\lambda; \lambda^2) \frac{e^{\pi i(k-3r)/4}}{2^{k-r}(2\pi)^{r/2}} H_{k-r}(\omega_\lambda). \tag{5.1}$$

Thus we have shown the following. Let $\sigma \in I$ and $t = 2\pi\alpha\beta$ for real numbers $\alpha, \beta \geqslant 1$. Then for all $N \in \mathbb{Z}_{\geqslant 0}$ we have

$$\begin{aligned} R(s;\alpha,\beta) = e^{i\vartheta(s)}(-1)^{\lfloor\alpha\rfloor\lfloor\beta\rfloor} &\frac{(2\pi)^s e^{\pi i s/2}}{\Gamma(s)(e^{2\pi i s}-1)} \\ &\times \exp\left(\frac{\pi i}{2}\left[2a\beta - 2b\alpha + a^2\lambda^{-2} - b^2\lambda^2\right]\right) \exp\left(\left(\frac{s}{2} - \frac{1}{4}\right)\log\frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8}\right) \\ &\qquad \times \left(\frac{2\pi}{t}\right)^{1/4} \lambda^{1/2-s} \sum_{k=0}^{N-1} a_k(s)\cdot c_k(\lambda) + O\left(\frac{\lambda^{1-\sigma}t^{-1/4}}{t^{N/6}}\right). \end{aligned} \tag{5.2}$$

The implied constant in (5.2) depends only on I, N and λ. If $\lambda \geqslant 1$ then the implied constant is independent of λ. We may simplify the initial terms on the right of (5.2) by noting that

$$e^{-2i\vartheta(s)} = \chi(s) = \frac{(2\pi)^s}{2\cos(\pi s/2)\Gamma(s)}.$$

Then

$$\begin{aligned} e^{i\vartheta(s)}\frac{(2\pi)^s e^{\pi i s/2}}{\Gamma(s)(e^{2\pi i s}-1)} &= e^{i\vartheta(s)}\frac{e^{\pi i s/2}}{(e^{2\pi i s}-1)} 2\cos(\pi s/2) e^{-2i\vartheta(s)} \\ &= e^{-i\vartheta(s)}\frac{e^{\pi i s}+1}{e^{2\pi i s}-1} = \frac{e^{-i\vartheta(s)}}{e^{\pi i s}-1} = -e^{-i\vartheta(s)}\big(1 + O(e^{-\pi t})\big). \end{aligned} \tag{5.3}$$

So replacing the left side of (5.3) with $-e^{-i\vartheta(s)}$ in (5.2) introduces an error of size

$$\left| e^{-i\vartheta(s)} \left(\frac{t}{2\pi}\right)^{(s-1)/2} \lambda^{1/2-s} \sum_{k=0}^{N-1} a_k(s)\cdot c_k(\lambda) \right| e^{-\pi t}. \tag{5.4}$$

By Corollary 4.6, $e^{-i\vartheta(s)} = O(t^{-\sigma/2+1/4})$. We have $a_k(s) = O(1)$ by (2.40). With Corollary 3.7 and the fact that $H_n(x)$ has degree n, it follows from (5.1) that

$$c_k(\lambda) \ll \lambda^{k+1/2} + \lambda^{-k-1/2}. \tag{5.5}$$

Putting these estimates together shows that (5.4) is

$$O\Big(\lambda^{1/2-\sigma}(\lambda^{N-1/2} + \lambda^{-N+1/2})t^{-1/4}e^{-\pi t}\Big).$$

Our results so far have established the next estimate (replacing N with M).

Proposition 5.2. *Let $\sigma \in I$ and $t = 2\pi\alpha\beta$ for real numbers $\alpha, \beta \geqslant 1$. Then for all $M \in \mathbb{Z}_{\geqslant 0}$ we have*

$$R(s;\alpha,\beta) = (-1)^{\lfloor\alpha\rfloor\lfloor\beta\rfloor+1} \exp\left(\frac{\pi i}{2}\Big[2a\beta - 2b\alpha + a^2\lambda^{-2} - b^2\lambda^2\Big]\right)$$
$$\times \exp\left(\left(\frac{s}{2}-\frac{1}{4}\right)\log\frac{t}{2\pi} - \frac{it}{2} - \frac{i\pi}{8} - i\vartheta(s)\right)\left(\frac{2\pi}{t}\right)^{1/4}\lambda^{1/2-s}\sum_{k=0}^{M-1} a_k(s)\cdot c_k(\lambda)$$
$$+ O\left(\frac{\lambda^{1/2-\sigma}}{t^{1/4}}\Big(\lambda^{M-1/2}+\lambda^{-M+1/2}\Big)e^{-\pi t} + \frac{\lambda^{1-\sigma}}{t^{M/6+1/4}}\right). \quad (5.6)$$

The implied constant in (5.6) *depends only on I, M and λ. If $\lambda \geqslant 1$ then the implied constant is independent of λ.*

The proof of Theorem 5.1 continues by inserting (4.11) and (4.24) into (5.6) to obtain the desired asymptotic expansion in decreasing powers of t. An argument similar to the one bounding (5.4) shows that the total error introduced from the error term in (4.11) is

$$O\Big(\lambda^{1/2-\sigma}\Big(\lambda^{M-1/2}+\lambda^{-M+1/2}\Big)t^{-1/4-L}\Big). \quad (5.7)$$

Ignoring the constant and modulus 1 pieces of (5.6) for the moment, we have

$$\frac{\lambda^{1/2-s}}{t^{1/4}}\left(\sum_{m=0}^{L-1}\frac{u_m(\sigma)}{(it)^m}\right)\sum_{k=0}^{M-1}c_k(\lambda)\left(\sum_{j=0}^{\lfloor k/3\rfloor} i^j\cdot d_{k-2j,j}(\sigma)\cdot\frac{1}{t^{k/2-j}}\right)$$
$$= \frac{\lambda^{1/2-s}}{t^{1/4}}\sum_{n=0}^{M+2L-3}\frac{1}{t^{n/2}}\sum_{\substack{m,k,j,\\ 2m+k-2j=n}} c_k(\lambda)\cdot i^{j-m}\cdot d_{k-2j,j}(\sigma)\cdot u_m(\sigma)$$
$$= \frac{\lambda^{1/2-s}}{t^{1/4}}\sum_{n=0}^{M+2L-3}\frac{1}{t^{n/2}}\sum_k c_k(\lambda)\cdot i^{(k-n)/2}\sum_j d_{k-2j,j}(\sigma)\cdot u_{j+(n-k)/2}(\sigma) \quad (5.8)$$

where in the last line we are summing over all k and j such that

$$k \equiv n \bmod 2, \quad 0 \leqslant k \leqslant M-1, \quad 2-2L+n \leqslant k \leqslant 3n, \quad (5.9)$$
$$0 \leqslant j \leqslant k/3, \quad (k-n)/2 \leqslant j \leqslant (k-n)/2 + L - 1. \quad (5.10)$$

The natural ranges of k and j are $0 \leqslant k \leqslant 3n$ and $\max(0,(k-n)/2) \leqslant j \leqslant k/3$, but for large n these ranges become truncated. We may choose N small enough in relation to M and L so that, for $0 \leqslant n \leqslant N-1$, the ranges of k and j are not truncated. This requires

$$M \geqslant 3N+1, \qquad L \geqslant N/2+1. \quad (5.11)$$

The size of the remaining part of the sum (5.8) with $N \leqslant n \leqslant M+2L-3$ is $O(t^{-N/2-1/4})$ in t (see the next lemma) and we also require that the error $O(t^{-M/6-1/4})$ in (5.6) and the error $O(t^{-L-1/4})$ in (5.7) are both less than this. This requires $M \geqslant 3N$ and $L \geqslant N/2$ and so is already ensured by (5.11). Given N, we therefore choose $M = 3N+1$ and $L = \lceil N/2\rceil + 1$.

Lemma 5.3. *We have*

$$\frac{\lambda^{1/2-s}}{t^{1/4}}\sum_{n=N}^{3N+2\lceil N/2\rceil}\frac{1}{t^{n/2}}\sum_k c_k(\lambda)\cdot i^{(k-n)/2}\sum_j d_{k-2j,j}(\sigma)\cdot u_{j+(n-k)/2}(\sigma)$$
$$= O\left(\frac{\lambda^{1/2-\sigma}}{t^{N/2+1/4}}\Big(\lambda^{3N+1/2}+\lambda^{-3N-1/2}\Big)\right) \quad (5.12)$$

where the indices k and j sum over the ranges (5.9) *and* (5.10) *for $M = 3N+1$ and $L = \lceil N/2\rceil + 1$. The implied constant depends only on N and I.*

Proof. By (5.9), the largest k appearing in the sum is $3N$. Therefore $c_k(\lambda)$ is always $\ll \lambda^{3N+1/2}+\lambda^{-3N-1/2}$ with (5.5). The other bounds are clear. $\square$

For $n \equiv k \bmod 2$ let

$$q_{n,k}(\sigma) := \sum_{j=\max(0,(k-n)/2)}^{\lfloor k/3 \rfloor} d_{k-2j,j}(\sigma) \cdot u_{j+(n-k)/2}(\sigma). \tag{5.13}$$

With the definitions (4.23) and (4.9) it is clear that $q_{n,k}(\sigma)$ is a polynomial in σ with rational coefficients. Since $d_{m,r}(\sigma)$ has degree $m-r$ and $u_m(\sigma)$ has degree $2m$ it follows that $q_{n,k}(\sigma)$ has degree at most n.

For our choice of M and L, the error in (5.12) is larger then the error terms in (5.6) and (5.7). Therefore we have shown that

$$\begin{aligned} R(s;\alpha,\beta) = (-1)^{\lfloor\alpha\rfloor\lfloor\beta\rfloor+1} \exp\left(\frac{\pi i}{2}\left[2a\beta - 2b\alpha + a^2\lambda^{-2} - b^2\lambda^2\right]\right)(2\pi)^{1/4} \\ \times \frac{\lambda^{1/2-s}}{t^{1/4}} \sum_{n=0}^{N-1} \frac{1}{t^{n/2}} \sum_{\substack{0\leqslant k\leqslant 3n \\ k\equiv n \bmod 2}} i^{(k-n)/2} q_{n,k}(\sigma) \sum_{r=0}^{k} \binom{k}{r} G^{(r)}(a\lambda^{-1}+b\lambda;\lambda^2) \frac{e^{\pi i(k-3r)/4}}{2^{k-r}(2\pi)^{r/2}} H_{k-r}(\omega_\lambda) \\ + O\left(\frac{\lambda^{1/2-\sigma}}{t^{N/2+1/4}}\left(\lambda^{3N+1/2}+\lambda^{-3N-1/2}\right)\right). \end{aligned} \tag{5.14}$$

The sums over k and r in (5.14), after interchanging, are

$$\sum_{r=0}^{3n} \frac{G^{(r)}(a\lambda^{-1}+b\lambda;\lambda^2)}{(2\pi)^{r/2}} e^{\pi i(n-3r)/4} \sum_{\substack{r\leqslant k\leqslant 3n \\ k\equiv n \bmod 2}} \binom{k}{r} \frac{(-1)^{(n-k)/2}}{2^{k-r}} \cdot q_{n,k}(\sigma) \cdot H_{k-r}(\omega_\lambda).$$

Recall that $\omega_\lambda = e^{-\pi i/4}\sqrt{\frac{\pi}{2}}(a\lambda^{-1}-b\lambda)$. Write the inner piece as

$$P_{n,3n-r}(x,\sigma) := e^{\pi i(n-3r)/4} \sum_{\substack{r\leqslant k\leqslant 3n \\ k\equiv n \bmod 2}} \binom{k}{r} \frac{(-1)^{(n-k)/2}}{2^{k-r}} \cdot q_{n,k}(\sigma) \cdot H_{k-r}\left(e^{-\pi i/4}x\right).$$

Then

$$P_{n,k}(x,\sigma) = e^{3\pi i k/4} \sum_{\ell=0}^{\lfloor k/2 \rfloor} \binom{3n-2\ell}{3n-k} \frac{(-1)^{n+\ell}}{2^{k-2\ell}} \cdot q_{n,3n-2\ell}(\sigma) \cdot H_{k-2\ell}\left(e^{-\pi i/4}x\right). \tag{5.15}$$

Clearly $P_{n,k}(x,\sigma)$ is a polynomial in x and σ with degree at most k in x. A short calculation finds that the coefficient of x^k is $i^k\binom{3n}{k}/((-3)^n n!)$ and so the degree is exactly k. The complete construction of $P_{n,k}(x,\sigma)$ is repeated for convenience in (6.1). This finishes the proof of Theorem 5.1. $\square$

If $\lambda < 1$ then the implied constant in Theorem 5.1 may have extra λ dependence; this can be traced back to Proposition 2.4. We will use the symmetry (1.19) to fix this issue in the next section and complete the proof of Theorem 1.5.

6 The polynomials $P_{n,k}(x,\sigma)$

6.1 A functional equation

Recall the Bernoulli, Hermite and De Moivre polynomials from (2.1) and (4.6). Assembling our results, we may give a complete description of $P_{n,k}(x,\sigma)$ in terms of these polynomials as follows. In (4.8), (4.9) and

(4.23) we defined

$$f_n(\sigma) := \frac{B_{n+1}(\sigma/2) + (-1)^{n+1} B_{n+1}((1-\sigma)/2)}{2n(n+1)}, \tag{6.1a}$$

$$u_m(\sigma) := (-2)^m \sum_{k=0}^{m} \frac{1}{k!} \mathcal{A}_{m,k}(f_1(\sigma), f_2(\sigma), \dots), \tag{6.1b}$$

$$d_{m,r}(\sigma) := \sum_{n=r}^{m} \frac{\mathcal{A}_{n,r}(\frac{1}{3}, -\frac{1}{4}, \frac{1}{5}, \dots)}{r!} \sum_{k=0}^{m-n} \frac{\mathcal{A}_{m-n,k}(1, -\frac{1}{2}, \frac{1}{3}, \dots)}{k!} (\sigma-1)^k. \tag{6.1c}$$

Rearranging (5.13) we may set

$$q_{n,3n-2\ell}(\sigma) := \sum_{m=\max(0,\ell-n)}^{\lfloor \ell/3 \rfloor} u_m(\sigma) \cdot d_{n-2m,n-\ell+m}(\sigma) \tag{6.1d}$$

for $0 \leqslant \ell \leqslant \lfloor 3n/2 \rfloor$. Then as we saw with (5.15),

$$P_{n,k}(x,\sigma) = e^{3\pi i k/4} \sum_{\ell=0}^{\lfloor k/2 \rfloor} \binom{3n-2\ell}{3n-k} \frac{(-1)^{n+\ell}}{2^{k-2\ell}} \cdot q_{n,3n-2\ell}(\sigma) \cdot H_{k-2\ell}\Big(e^{-\pi i/4} x\Big). \tag{6.1e}$$

We next show that the polynomials $P_{n,k}(x,\sigma)$ obey a functional equation as $\sigma \to 1-\sigma$. It seems difficult to prove this directly with (6.1); our proof is based on Theorem 5.1.

Theorem 6.1. *For all $x, \sigma \in \mathbb{R}$ and all $n, k \in \mathbb{Z}$ with $0 \leqslant k \leqslant 3n$ we have*

$$P_{n,k}(x,\sigma) = \overline{P_{n,k}(-x, 1-\sigma)}.$$

Proof. Recall that $R(s;\alpha,\beta)$ is unchanged under the transformation $\mathcal{T}$ given in (1.25). All the components of the right side of (1.21), except for possibly $P_{n,k}$, are also unchanged under $\mathcal{T}$. For example

$$\begin{aligned} \mathcal{T}(\lambda^{1/2-s}) &= \overline{(1/\lambda)^{1/2-(1-\overline{s})}} &= \lambda^{1/2-s}, \\ \mathcal{T}G^{(r)}(a\lambda^{-1}+b\lambda;\lambda^2) &= \overline{G^{(r)}(b\lambda+a\lambda^{-1};\lambda^{-2})} &= G^{(r)}(a\lambda^{-1}+b\lambda;\lambda^2) \end{aligned}$$

using (3.11). Hence, by Theorem 5.1 we obtain

$$\sum_{n=0}^{N-1} \frac{1}{t^{n/2}} \sum_{r=0}^{3n} \frac{G^{(r)}(a\lambda^{-1}+b\lambda;\lambda^2)}{(2\pi)^{r/2}} \times \left[P_{n,3n-r}\left(\frac{\sqrt{\pi}}{\sqrt{2}}(a\lambda^{-1}-b\lambda),\sigma\right) - \overline{P_{n,3n-r}\left(\frac{\sqrt{\pi}}{\sqrt{2}}(b\lambda-a\lambda^{-1}),1-\sigma\right)} \right] = O\left(\frac{1}{t^{N/2}}\right) \tag{6.2}$$

where the implied constant depends on $N \in \mathbb{Z}_{\geqslant 0}$ and also on λ and σ which we assume are fixed. We choose λ such that λ^2 is a rational u/v with $(u,v)=1$. If we think of α varying then we have the dependent relations

$$\beta = \frac{v}{u}\alpha, \quad t = 2\pi\frac{v}{u}\alpha^2, \quad a = \alpha - \lfloor \alpha \rfloor, \quad b = \frac{v}{u}\alpha - \left\lfloor \frac{v}{u}\alpha \right\rfloor. \tag{6.3}$$

Suppose $\alpha = \alpha_0$ has the corresponding a and b values a_0 and b_0, respectively. Then clearly $\alpha = \alpha_0 + u$ will have the same a and b values. Hence, for t taking values in the sequence $2\pi\frac{v}{u}(\alpha_0+ku)^2$ for integers k, the inner sum in (6.2) is unchanged with $a = a_0$ and $b = b_0$. By letting k, and hence t, become arbitrarily large we obtain

$$\sum_{r=0}^{3n} \frac{G^{(r)}(a\lambda^{-1}+b\lambda;\lambda^2)}{(2\pi)^{r/2}} \left[P_{n,3n-r}\left(\frac{\sqrt{\pi}}{\sqrt{2}}(a\lambda^{-1}-b\lambda),\sigma\right) - \overline{P_{n,3n-r}\left(\frac{\sqrt{\pi}}{\sqrt{2}}(b\lambda-a\lambda^{-1}),1-\sigma\right)} \right] = 0$$

for $a = a_0$ and $b = b_0$ and $n \leqslant N-1$. This follows since we may first show that the coefficient of $1/t^0$ must be 0. Then the coefficient of $1/t^{1/2}$ must be 0, etc. (If asymptotic expansions exist then they are unique.)

Let

$$f(\alpha) := a\lambda^{-1} + b\lambda, \qquad g(\alpha) := a\lambda^{-1} - b\lambda,$$

where a and b depend on α as in (6.3). As we already saw, $f(\alpha)$ and $g(\alpha)$ both have period u. The next result shows which values they can take and we omit its elementary proof.

Lemma 6.2. *For $f(\alpha)$ and $g(\alpha)$ as defined above:*

(i) The function $g(\alpha)$ is constant on $u+v-1$ non-empty intervals $[x_j, x_{j+1})$ which partition $[0,u)$.

(ii) The values $g(\alpha)$ takes are

$$\frac{\ell}{\sqrt{uv}} \quad \text{for integers } \ell \text{ with} \quad 1-u \leqslant \ell \leqslant v-1. \tag{6.4}$$

(iii) On each interval $[x_j, x_{j+1})$ where $g(\alpha)$ is constant, the graph of $f(\alpha)$ is a line of slope $2/\lambda$.

Fix x as one of the $g(\alpha)$ values in (6.4). By part (iii) of the lemma we have

$$\sum_{r=0}^{3n} \frac{G^{(r)}(w;\lambda^2)}{(2\pi)^{r/2}} \left[P_{n,3n-r}\left(\frac{\sqrt{\pi}}{\sqrt{2}}x, \sigma\right) - \overline{P_{n,3n-r}\left(-\frac{\sqrt{\pi}}{\sqrt{2}}x, 1-\sigma\right)} \right] = 0 \tag{6.5}$$

for w in some non-empty interval. Since each $G^{(r)}(w;\lambda^2)$ is a holomorphic function of w, it follows that (6.5) is true for all $w \in \mathbb{C}$.

The linear independence of the derivatives of G shown in Proposition 3.8 implies that

$$P_{n,k}\left(\frac{\sqrt{\pi}}{\sqrt{2}}x, \sigma\right) - \overline{P_{n,k}\left(-\frac{\sqrt{\pi}}{\sqrt{2}}x, 1-\sigma\right)} \tag{6.6}$$

is 0 for every k with $0 \leqslant k \leqslant 3n$. Hence the numbers (6.4) give $u+v-1$ distinct zeros of the polynomial (6.6) in x. It has degree at most $3n$ in x. Returning to our choice of $\lambda^2 = u/v$, we may choose a reduced fraction so that $u+v-1 > 3n$. This gives too many zeros and so (6.6) is identically zero as required. □

Proof of Theorem 1.5. By Theorem 5.1, we know that Theorem 1.5 is true for $\lambda \geqslant 1$, so assume that $\lambda < 1$. Then by (1.19) we have $R(s;\alpha,\beta) = \overline{R(1-\overline{s};\beta,\alpha)}$. We may apply Theorem 5.1 to $R(1-\overline{s};\beta,\alpha)$ and obtain an error that is independent of λ. All the components of the right side of (1.21) are invariant under the transformation $\mathcal{T}$ in (1.25), including the $P_{n,k}$ term by Theorem 6.1. In this way we obtain Theorem 1.5 when $\lambda < 1$. This completes our proof of the main theorem. □

6.2 Formulas for the coefficients

With the well-known formula for Hermite polynomials

$$H_n(x) = n! \sum_{j=0}^{\lfloor n/2 \rfloor} \frac{(-1)^j}{j!(n-2j)!}(2x)^{n-2j} \tag{6.7}$$

we obtain from (5.15)

$$\begin{aligned} P_{n,k}(x,\sigma) &= \sum_{\ell=0}^{\lfloor k/2 \rfloor} \frac{(3n-2\ell)!}{(3n-k)!} \frac{(-1)^{n+\ell}}{2^{k-2\ell}} \cdot q_{n,3n-2\ell}(\sigma) \sum_{m=\ell}^{\lfloor k/2 \rfloor} \frac{(-1)^{m-\ell} i^{k+m} (2x)^{k-2m}}{(m-\ell)!(k-2m)!} \\ &= \frac{(-1)^n}{(3n-k)!} \sum_{m=0}^{\lfloor k/2 \rfloor} \frac{i^{k+m} x^{k-2m}}{(-4)^m (k-2m)!} \sum_{\ell=0}^{m} 4^\ell \frac{(3n-2\ell)!}{(m-\ell)!} \cdot q_{n,3n-2\ell}(\sigma). \end{aligned}$$

For $0 \leqslant m \leqslant \lfloor 3n/2 \rfloor$ put

$$s_{n,m}(\sigma) := \sum_{\ell=0}^{m} 4^{\ell} \frac{(3n-2\ell)!}{(m-\ell)!} \cdot q_{n,3n-2\ell}(\sigma) \tag{6.8}$$

so that

$$P_{n,k}(x,\sigma) = \frac{(-1)^n i^k}{(3n-k)!} \sum_{m=0}^{\lfloor k/2 \rfloor} \frac{s_{n,m}(\sigma)}{(4i)^m} \frac{x^{k-2m}}{(k-2m)!}. \tag{6.9}$$

An easy calculation with (6.9) gives the next result, showing how Theorem 6.1 may be interpreted at the level of the coefficients of $P_{n,k}(x,\sigma)$.

Lemma 6.3. *Let n be in $\mathbb{Z}_{\geqslant 0}$. For all integers k with $0 \leqslant k \leqslant 3n$, we have $P_{n,k}(x,\sigma) = \overline{P_{n,k}(-x,1-\sigma)}$ if and only if*

$$s_{n,m}(\sigma) = (-1)^m s_{n,m}(1-\sigma)$$

for all integers m satisfying $0 \leqslant m \leqslant \lfloor 3n/2 \rfloor$.

Theorem 6.1 and Lemma 6.3 show in particular that $s_{n,m}(1/2) = 0$ for m odd. Hence m may be assumed to be even in (6.9) when $\sigma = 1/2$. We obtain

$$P_{n,k}(x,1/2) = \frac{(-1)^n i^k}{(3n-k)!} \sum_{m=0}^{\lfloor k/4 \rfloor} (-1)^m \frac{s_{n,2m}(1/2)}{16^m} \frac{x^{k-4m}}{(k-4m)!}. \tag{6.10}$$

In the case $x = 0$ we see that $P_{n,k}(0,1/2)$ is zero if $k \not\equiv 0 \bmod 4$. This explains why only every fourth derivative appears in the classical Riemann-Siegel formulas (1.11), (1.24).

The coefficients of the highest powers of x in $P_{n,k}(x,\sigma)$ may be computed explicitly:

$$x^k: \quad \frac{(-1)^n i^k}{3^n n!}\binom{3n}{k}, \tag{6.11a}$$

$$x^{k-2}: \quad \frac{(-1)^n i^{k-1}}{3^{n-1}(n-1)!}\binom{3n-2}{k-2}(\sigma-1/2), \tag{6.11b}$$

$$x^{k-4}: \quad \frac{(-1)^n i^k}{3^{n-2}(n-2)!}\binom{3n-4}{k-4}\left[\frac{3n-1}{20} - \frac{1}{2}(\sigma-1/2)^2\right], \tag{6.11c}$$

$$x^{k-6}: \quad \frac{(-1)^n i^{k-1}}{3^{n-2}(n-2)!}\binom{3n-6}{k-6}(\sigma-1/2)\left[\frac{9n^2-20n+9}{20} - \frac{n-2}{2}(\sigma-1/2)^2\right]. \tag{6.11d}$$

The general pattern continues with the next coefficient

$$x^{k-8}: \quad \frac{(-1)^n i^k}{3^{n-3}(n-3)!}\binom{3n-8}{k-8} \times \left[\frac{63n^2-141n+31}{5600}(3n-5) - \frac{9n^2-28n+23}{40}(\sigma-1/2)^2 + \frac{n-3}{8}(\sigma-1/2)^4\right]. \tag{6.11e}$$

These calculations use (6.9), (6.8) and (6.1). Finding $d_{m,r}(\sigma)$ involves the De Moivre polynomials and we used the explicit expressions for $\mathcal{A}_{r,r}$, $\mathcal{A}_{r+1,r}$, $\mathcal{A}_{r+2,r}$ and so on, given in [O'S, Sect. 2]. The algebra to obtain the coefficients in (6.11) was carried out with Mathematica.

7 Examples and numerical work

7.1 The case $\alpha = 2\beta$

The classical case of the Riemann-Siegel formula has the lengths of the partial sums equal, so that $\alpha = \beta$ and $\lambda = 1$. In Theorem 1.5, the next simplest case has the length of one partial sum twice the other:

$$\alpha = 2\beta \quad \implies \quad \lambda = \sqrt{2}, \quad \alpha = \sqrt{\frac{t}{\pi}}, \quad \beta = \frac{1}{2}\sqrt{\frac{t}{\pi}}.$$

With a and b the fractional parts of 2β and β we obtain

$$R(s;2\beta,\beta) = (-1)^{\lfloor 2\beta\rfloor\lfloor\beta\rfloor+1}\exp\bigl(\pi i(a\beta-2b\beta+a^2/4-b^2)\bigr)$$
$$\times\left(\frac{2\pi}{t}\right)^{1/4}\sum_{n=0}^{N-1}\frac{2^{1/4-s/2}}{t^{n/2}}\left[\sum_{r=0}^{3n}\frac{G^{(r)}(a/\sqrt{2}+\sqrt{2}b;2)}{(2\pi)^{r/2}}\cdot P_{n,3n-r}\bigl(\sqrt{\pi}(a/2-b),\sigma\bigr)\right]$$
$$+O\left(\frac{2^{(1-\sigma+3N)/2}}{t^{N/2+1/4}}\right). \quad (7.1)$$

As we saw in (3.15), with $\theta_2(u) := u^2/2-\sqrt{2}u-9/8$,

$$G(u;2) = \frac{-1}{2i\sin(\sqrt{2}\pi u)}\Bigl[2^{1/4}e^{-\pi i\theta_2(u)}-2^{-1/4}e^{\pi i\theta_2(u)}\Bigl(1+ie^{\sqrt{2}\pi iu}\Bigr)\Bigr].$$

It is easy to see that the polynomials $P_{n,3n-r}(x,\sigma)$ in (7.1) are only evaluated at $x=0$ if $b\in[0,1/2)$ and at $x=-\sqrt{\pi}/2$ if $b\in[1/2,1)$. This corresponds to Lemma 6.2 with $u=2$ and $v=1$. Examples of (7.1) for $s=3/4+400i$ and different values of N are displayed in Table 3, correct to the accuracy shown.

N	Theorem 1.5	
1	$0.11628656704+0.031020387\,22i$	
3	$0.11503659264+0.03134163666i$	
5	$0.11503572670+0.03134146229i$	
	$0.11503572550+0.03134146183i$	R

Table 3: The approximations of Theorem 1.5 to $R=R(3/4+400i;20/\sqrt{\pi},10/\sqrt{\pi})$.

7.2 An example with increasing λ

Suppose we take $\alpha=t^c$ in Theorem 1.5 for some $c>1/2$. Then

$$\beta=\frac{t}{2\pi\alpha}=\frac{t^{1-c}}{2\pi}, \qquad \lambda=\sqrt{\frac{\alpha}{\beta}}=\sqrt{2\pi}\,t^{c-1/2}.$$

The error term in (1.21) is $O(t^{-(c-1/2)(\sigma-1/2)+N(3c-2)-1/2})$ and so we require $c<2/3$ for this to decrease with N. If we take $c=5/8$, for example, then Theorem 1.5 gives

$$R(s;t^{5/8},t^{3/8}/(2\pi)) = e^{\pi iA(t)}(2\pi)^{3/4-s}t^{-1/8-s/4}$$
$$\times\sum_{n=0}^{N-1}\frac{1}{t^{n/2}}\left[\sum_{r=0}^{3n}\frac{G^{(r)}(\frac{a}{\sqrt{2\pi}}t^{-1/8}+b\sqrt{2\pi}t^{1/8};2\pi t^{1/4})}{(2\pi)^{r/2}}\cdot P_{n,3n-r}\Bigl(\frac{a}{2}t^{-1/8}-b\pi t^{1/8},\sigma\Bigr)\right]$$
$$+O\left(\frac{1}{t^{(N+1+\sigma)/8}}\right) \quad (7.2)$$

for

$$A(t) := \lfloor t^{5/8}\rfloor\lfloor t^{3/8}/(2\pi)\rfloor+1+at^{5/8}-b\frac{t^{3/8}}{2\pi}+\frac{a^2}{4\pi}t^{-1/4}-b^2\pi t^{1/4}$$

and a, b the fractional parts of $t^{5/8}$, $t^{3/8}/(2\pi)$. The derivatives of G in (7.2) may be expressed in terms of Hermite polynomials and derivatives of Υ as in (3.34). Then the derivatives of Υ can be computed with (3.30). Table 4 shows each side of (7.2) when $s=1/2+256i$.

It is natural to consider the difference $R(s;\alpha,\beta)-R(s;\alpha',\beta')$, as the $\zeta(s)$ terms cancel. With $\alpha=t^{5/8}$ as above and $\alpha'=t^{5/8}/2$ we may obtain the asymptotics of

$$e^{i\vartheta(s)}\Biggl(\sum_{\frac{t^{5/8}}{2}<n\leqslant t^{5/8}}\frac{1}{n^s}\Biggr)-e^{i\vartheta(1-s)}\Biggl(\sum_{\frac{t^{3/8}}{2\pi}<n\leqslant\frac{t^{3/8}}{\pi}}\frac{1}{n^{1-s}}\Biggr),$$

for example, with (7.2) minus a similar expression.

N	Theorem 1.5	
1	$-0.12120812956 + 0.00884587559i$	
2	$-0.12075592244 + 0.00789494686i$	
4	$-0.12074208191 + 0.00787729724i$	
	$-0.12074212743 + 0.00787728177i$	R

Table 4: The approximations of Theorem 1.5 to $R = R(1/2 + 256i; 32, 4/\pi)$.

7.3 On the line $\mathrm{Re}(s) = 1$

When $\sigma = 1$ there are some simplifications in the definition of $P_{n,k}(x, \sigma)$ in (6.1). With basic properties of Bernoulli polynomials we find

$$f_n(1) = \frac{B_{n+1}}{n(n+1)2^{n+1}}.$$

Also, for $d_{m,r}(1)$ in (6.1c), only the $k = 0$ term can be non-zero. Then $\mathcal{A}_{m-n,0}(1, -\frac{1}{2}, \frac{1}{3}, \dots)$ is zero unless $n = m$. Therefore

$$d_{m,r}(1) = \mathcal{A}_{m,r}(\tfrac{1}{3}, -\tfrac{1}{4}, \tfrac{1}{5}, \dots)/r!.$$

With this, the first polynomials $P_{n,k}(x, 1)$ for $0 \leqslant k \leqslant 3n$ are $P_{0,0}(x, 1) = 1$ and

$$P_{1,0}(x,1) = -\tfrac{1}{3}, \quad P_{1,1}(x,1) = -ix, \quad P_{1,2}(x,1) = x^2 - \tfrac{i}{2}, \quad P_{1,3}(x,1) = \tfrac{i}{3}x^3 + \tfrac{1}{2}x.$$

For $n = 2$ we have

$$\begin{gathered} P_{2,0}(x,1) = \tfrac{1}{18}, \quad P_{2,1}(x,1) = \tfrac{i}{3}x, \quad P_{2,2}(x,1) = -\tfrac{5}{6}x^2 + \tfrac{i}{6}, \quad P_{2,3}(x,1) = -\tfrac{10i}{9}x^3 - \tfrac{2}{3}x, \\ P_{2,4}(x,1) = \tfrac{5}{6}x^4 - ix^2 + \tfrac{1}{8}, \quad P_{2,5}(x,1) = \tfrac{i}{3}x^5 + \tfrac{2}{3}x^3 + \tfrac{i}{4}x, \\ P_{2,6}(x,1) = -\tfrac{1}{18}x^6 + \tfrac{i}{6}x^4 - \tfrac{1}{8}x^2 + \tfrac{i}{8}. \end{gathered} \tag{7.3}$$

For example, taking $\sigma = 1$, $t = 600$ and $\alpha/\beta = 5/3$ in Theorem 1.5 gives the results in Table 5.

N	Theorem 1.5	
1	$0.07827091811 - 0.076570008324i$	
3	$0.07798494014 - 0.076932555693i$	
5	$0.07798504883 - 0.07693266047i$	
	$0.07798504890 - 0.07693266040i$	R

Table 5: The approximations of Theorem 1.5 to $R = R(1 + 600i; \sqrt{500/\pi}, \sqrt{180/\pi})$.

7.4 On the critical line

For $\sigma = 1/2$ we have already seen with (6.10) that the polynomials $P_{n,k}(x, \sigma)$ take a simpler form; only coefficients of powers of x that are congruent to $k \bmod 4$ can be non-zero. For example, $P_{0,0}(x, 1/2) = 1$ and

$$P_{1,0}(x,1/2) = -\tfrac{1}{3}, \quad P_{1,1}(x,1/2) = -ix, \quad P_{1,2}(x,1/2) = x^2, \quad P_{1,3}(x,1/2) = \tfrac{i}{3}x^3. \tag{7.4}$$

Of course, (7.4) is a special case of (1.23). For $n = 2$ we have

$$\begin{gathered} P_{2,0}(x,1/2) = \tfrac{1}{18}, \quad P_{2,1}(x,1/2) = \tfrac{i}{3}x, \quad P_{2,2}(x,1/2) = -\tfrac{5}{6}x^2, \quad P_{2,3}(x,1/2) = -\tfrac{10i}{9}x^3, \\ P_{2,4}(x,1/2) = \tfrac{5}{6}x^4 + \tfrac{1}{4}, \quad P_{2,5}(x,1/2) = \tfrac{i}{3}x^5 + \tfrac{i}{2}x, \quad P_{2,6}(x,1/2) = -\tfrac{1}{18}x^6 - \tfrac{1}{4}x^2. \end{gathered} \tag{7.5}$$

We give a more detailed numerical example in Table 6 for $s = 1/2 + 800i$ and $\alpha/\beta = 4$.

N	Theorem 1.5	
1	$-0.07966764263636 - 0.07373504930114i$	
3	$-0.07957371736089 - 0.07351910859701i$	
5	$-0.07957365182034 - 0.07351897839664i$	
7	$-0.07957365178158 - 0.07351897825965i$	
	$-0.07957365178152 - 0.07351897825948i$	R

Table 6: The approximations of Theorem 1.5 to $R = R(1/2 + 800i; 40/\sqrt{\pi}, 10/\sqrt{\pi})$.

Specializing (6.11) to $\sigma = 1/2$, and extending the calculation to x^{k-12}, shows that the highest degree terms in $P_{n,k}(x, 1/2)$ are

$$\begin{aligned}\frac{P_{n,k}(x,1/2)}{(-1)^n i^k} &= \binom{3n}{k}\frac{x^k}{3^n n!} + \binom{3n-4}{k-4}\frac{3n-1}{20}\frac{x^{k-4}}{3^{n-2}(n-2)!} \\ &\quad + \binom{3n-8}{k-8}\frac{63n^2-141n+31}{5600}(3n-5)\frac{x^{k-8}}{3^{n-3}(n-3)!} \\ &\quad + \binom{3n-12}{k-12}\frac{567n^4-4374n^3+10968n^2-9621n+1280}{112000}(n-3)\frac{x^{k-12}}{3^{n-4}(n-4)!} + \cdots . \qquad (7.6)\end{aligned}$$

The formulas in (7.6) only make sense for n large enough. For $P_{n,k}(x, 1/2)$ to contain x^{k-12} for instance, we need $k \geqslant 12$ and hence $n \geqslant 4$. It may be verified that the coefficient of x^{k-12} in (7.6) is always positive for these n and k. Similarly, the higher powers of x in (7.6) always have positive coefficients. Combining these calculations with (6.10), we have proved:

Proposition 7.1. *The terms in $P_{n,k}(x, 1/2)/((-1)^n i^k)$ may only contain powers of x of the form x^{k-4m} for $0 \leqslant m \leqslant k/4$. For these m values, the coefficients of x^{k-4m} are always positive if $0 \leqslant m \leqslant 3$.*

To examine this positivity further, let $S_{n,k}$ be the set of all the coefficients of x^{k-4m} for $0 \leqslant m \leqslant k/4$ in $P_{n,k}(x, 1/2)/((-1)^n i^k)$. Let S_n be the union of these $S_{n,k}$ for k in the range $0 \leqslant k \leqslant 3n$. Then further computations show that all the elements of S_n are positive for $0 \leqslant n \leqslant 50$. It seems likely that this positivity continues for all n. This would also imply that the sign pattern for $C_n(a)$ we see in (1.11) continues for all n, with positive coefficients for n even and negative coefficients for n odd. The signs of the coefficients of $P_{n,k}(x, \sigma)$ also appear to obey predictable patterns, at least for σ not too far from $1/2$.

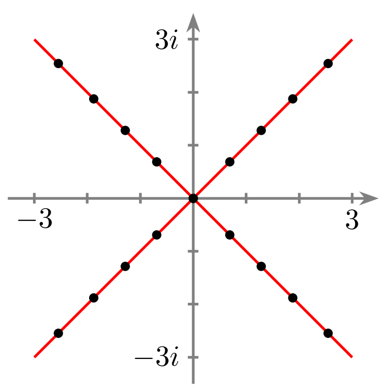

Figure 3: The zeros of $P_{6,18}(x, 1/2)$

Another interesting aspect of $P_{n,k}(x, 1/2)$ is that, in all the cases we have examined, its zeros are on the lines bisecting the quadrants and are nearly evenly spaced. Figure 3 shows the zeros of

$$P_{6,18}(x, 1/2) = -\tfrac{1}{524880}x^{18} - \tfrac{17}{38880}x^{14} - \tfrac{18889}{907200}x^{10} - \tfrac{367}{1920}x^6 - \tfrac{5}{32}x^2.$$

For σ near $1/2$ the zeros of $P_{n,k}(x, \sigma)$ appear to have a similar distribution.

7.5 Conclusion

We have shown that the Riemann-Siegel formula and the Hardy-Littlewood approximate functional equation are special cases of a shared natural generalization in Theorem 1.5. The classical Riemann-Siegel coefficients $C_n(a)$ are given in our reformulation by

$$C_n(a) = \sum_{r=0}^{3n} \frac{G^{(r)}(2a;1)}{(2\pi)^{r/2}} \cdot P_{n,3n-r}(0,1/2) \tag{7.7}$$

as is seen by comparing (1.10) with (1.24). In the wider context of Theorem 1.5, we need the more general Mordell integral $G(u;\tau)$, and the constant terms $P_{n,k}(0,1/2)$ in (7.7) are replaced with the polynomials $P_{n,k}(x,\sigma)$ in x and σ. The remarkable properties of Mordell integrals have attracted many authors, as we have seen in Sections 3.1, 3.3. The key symmetry of $G(u;\tau)$ as $\tau \to 1/\tau$ is related through Theorem 1.5 to the functional equation of $\zeta(s)$. The polynomials $P_{n,k}(x,\sigma)$ inherit a functional equation from $\zeta(s)$, (Theorem 6.1), and as noted above they also seem to inherit interesting zeros.

In future work we will examine these components $G(u;\tau)$ and $P_{n,k}(x,\sigma)$ in greater detail. Also a natural extension of the techniques in this paper is to Dirichlet L-functions $L(s,\chi)$. This would generalize the treatments in [Sie43] and [Deu67].

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