

Asymptotics for the partial fractions of the restricted partition generating function I

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May 1, 2014

Abstract

The generating function for $p_N(n)$, the number of partitions of n into at most N parts, may be written as a product of N factors. We find the behavior of coefficients in the partial fraction decomposition of this product as $N \rightarrow \infty$ by applying the saddle-point method, where the saddle-point we need is associated to a zero of the analytically continued dilogarithm. Our main result disproves a conjecture of Rademacher.

1 Introduction

1.1 Rademacher's coefficients

Let $p(n)$ denote the number of partitions of n . The generating function for $p(n)$ is an infinite product and Rademacher, in [Rad73, pp. 292 - 302], obtained a partial fraction decomposition for it

$$\sum_{n=0}^{\infty} p(n)q^n = \prod_{j=1}^{\infty} \frac{1}{1-q^j} = \sum_{\substack{0 \leq h < k \\ (h,k)=1}} \sum_{\ell=1}^{\infty} \frac{C_{hkl}(\infty)}{(q - e^{2\pi i h/k})^\ell} \quad (|q| < 1) \quad (1.1)$$

by using his famous exact formula for $p(n)$. The coefficients $C_{hkl}(\infty)$ are given explicitly in [Rad73, Eq. (130.6)] with, for example,

$$C_{011}(\infty) = -\frac{6}{25} - \frac{12\sqrt{3}}{125\pi}, \quad C_{012}(\infty) = \frac{144}{1225} + \frac{5616\sqrt{3}}{42875\pi}.$$

In this notation, C_{011} is the coefficient of $(q-1)^{-1}$ and C_{012} the coefficient of $(q-1)^{-2}$. Truncating the infinite product in (1.1) gives the generating function for $p_N(n)$, the number of partitions of n into at most N parts, and its partial fraction decomposition may be written as

$$\sum_{n=0}^{\infty} p_N(n)q^n = \prod_{j=1}^N \frac{1}{1-q^j} = \sum_{\substack{0 \leq h < k \leq N \\ (h,k)=1}} \sum_{\ell=1}^{\lfloor N/k \rfloor} \frac{C_{hkl}(N)}{(q - e^{2\pi i h/k})^\ell}. \quad (1.2)$$

Comparing (1.1) and (1.2), Rademacher conjectured in [Rad73, p. 302] that

$$C_{hkl}(N) \rightarrow C_{hkl}(\infty) \quad \text{as} \quad N \rightarrow \infty. \quad (1.3)$$

Investigations in [And03], [DG02], [Mun08] were inconclusive, but Sills and Zeilberger in [SZ13] developed recursive formulas for $C_{hkl}(N)$ and gave convincing numerical evidence that $C_{hkl}(N) \not\rightarrow C_{hkl}(\infty)$. They saw that the points $(N, C_{01\ell}(N))$ start to trace curves oscillating with periods approaching 32 and with amplitude growing exponentially. Their conjecture [SZ13, Conj. 2.1] is that this is the true description.

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2010 *Mathematics Subject Classification*. 11P82, 41A60

Key words and phrases. Restricted partitions, partial fraction decomposition, saddle-point method, dilogarithm.

Support for this project was provided by a PSC-CUNY Award, jointly funded by The Professional Staff Congress and The City University of New York.

In [O'S12] we found relatively simple, explicit formulas for Rademacher's coefficients $C_{hkl}(N)$, linking them to formulas of Sylvester [Syl82] and Glaisher [Gla09]. For example [O'S12, Eq. (2.12)] is

$$C_{01\ell}(N) = \frac{(-1)^N (\ell-1)!}{N!} \sum_{j_0+j_1+j_2+\dots+j_N=N-\ell} \left\{ \begin{matrix} \ell+j_0 \\ \ell \end{matrix} \right\} \frac{B_{j_1} B_{j_2} \dots B_{j_N}}{(\ell-1+j_0)!} \frac{1^{j_1} 2^{j_2} \dots N^{j_N}}{j_1! j_2! \dots j_N!}$$

where B_j is the j th Bernoulli number and $\left\{ \begin{matrix} n \\ m \end{matrix} \right\}$ the Stirling number denoting the number of ways to partition a set of size n into m non-empty subsets. Also in [O'S12], based on an earlier stage of the work in this paper, the exact asymptotic behavior of $C_{011}(N)$ was conjectured. This requires the solution $w_0 \approx 0.916 - 0.182i$ to

$$\text{Li}_2(w) - 2\pi i \log(w) = 0 \quad (1.4)$$

where Li_2 denotes the dilogarithm. (It may be seen that w_0 is a zero of the dilogarithm on a non-principal branch, see Section 2.3.) Set $z_0 := 1 + \log(1 - w_0)/(2\pi i)$ so that

$$w_0 = 1 - e^{2\pi i z_0}, \quad 1/2 < \text{Re}(z_0) < 3/2. \quad (1.5)$$

Conjecture 1.1. [O'S12, Sect. 6] We have¹

$$C_{011}(N) = \text{Re} \left[(-2z_0 e^{-\pi i z_0}) \frac{w_0^{-N}}{N^2} \right] + O \left(\frac{|w_0|^{-N}}{N^3} \right). \quad (1.6)$$

Equivalently, we may present (1.6) more explicitly as

$$C_{011}(N) = \frac{e^{NU}}{N^2} \left(\alpha \sin(\beta + NV) + O \left(\frac{1}{N} \right) \right) \quad (1.7)$$

for

$$U := -\log |w_0| \approx 0.0680762, \quad V := \arg(1/w_0) \approx 0.196576 \quad (1.8)$$

and $\alpha = |-2iz_0 e^{-\pi i z_0}| \approx 5.39532$, $\beta = \arg(-2iz_0 e^{-\pi i z_0}) \approx 1.21367$. This implies the period of $C_{011}(N)$ is $2\pi/V \approx 31.9631$. As we will see, the numbers w_0 and z_0 control the asymptotics for all of the Rademacher coefficients that we examine.

1.2 Main results

Write the Farey fractions of order N in $[0, 1)$ as

$$\mathcal{F}_N := \left\{ h/k : 1 \leq k \leq N, 0 \leq h < k, (h, k) = 1 \right\}. \quad (1.9)$$

Our first result is a kind of averaged version of Conjecture 1.1, with $C_{011}(N)$ replaced by

$$C_{011}(N) + C_{121}(N) + \dots + C_{(99)(100)1}(N) = \sum_{h/k \in \mathcal{F}_{100}} C_{hkl}(N).$$

Theorem 1.2. For an absolute implied constant

$$\sum_{h/k \in \mathcal{F}_{100}} C_{hkl}(N) = \text{Re} \left[(-2z_0 e^{-\pi i z_0}) \frac{w_0^{-N}}{N^2} \right] + O \left(\frac{|w_0|^{-N}}{N^3} \right). \quad (1.10)$$

This has the following consequence.

Corollary 1.3. There exists a pair (h, k) with $h < k \leq 100$ such that $\lim_{N \rightarrow \infty} C_{hkl}(N)$ does not exist. Hence Rademacher's conjecture that $C_{hkl}(N) \rightarrow C_{hkl}(\infty)$ as $N \rightarrow \infty$ is false.

Proof. Expressing the right side of (1.10) as in (1.7), we see that this side cannot have a limit as $N \rightarrow \infty$ since $\alpha \neq 0$, $U > 0$ and $\beta + NV$ comes within $1/10$ of $\pi/2$, say, infinitely often since $V < 1/5$. But the left side of (1.10) is a finite sum, so Rademacher's conjecture implies that its limit as $N \rightarrow \infty$ exists. The corollary follows. \square

¹This statement is equivalent to Conjecture 6.2 in [O'S12] where z_0 and w_0 are replaced by their conjugates.

Theorem 1.2 is the $\ell = m = 1$ case of the next result where we extend the right side of (1.10) to include the first m terms of the asymptotic expansion and generalize $C_{011}(N)$ to $C_{01\ell}(N)$.

Theorem 1.4. *There are explicit coefficients $c_{\ell,0}, c_{\ell,1}, \dots$ so that*

$$C_{01\ell}(N) + \sum_{0 < h/k \in \mathcal{F}_{100}} \sum_{j=1}^{\ell} (e^{2\pi i h/k} - 1)^{\ell-j} C_{h k j}(N) = \operatorname{Re} \left[\frac{w_0^{-N}}{N^{\ell+1}} \left(c_{\ell,0} + \frac{c_{\ell,1}}{N} + \dots + \frac{c_{\ell,m-1}}{N^{m-1}} \right) \right] + O \left(\frac{|w_0|^{-N}}{N^{\ell+m+1}} \right) \quad (1.11)$$

where $c_{\ell,0} = -2z_0 e^{-\pi i z_0} (2\pi i z_0)^{\ell-1}$ and the implied constant depends only on ℓ and m .

See (5.41) for the next coefficient $c_{\ell,1}$. Numerically, it looks like the sum over $0 < h/k \in \mathcal{F}_{100}$ on the left of (1.11) is much smaller than $C_{01\ell}(N)$, so it is natural to generalize Conjecture 1.1 to:

Conjecture 1.5. *For the coefficients $c_{\ell,0}, c_{\ell,1}, \dots$ of Theorem 1.4,*

$$C_{01\ell}(N) = \operatorname{Re} \left[\frac{w_0^{-N}}{N^{\ell+1}} \left(c_{\ell,0} + \frac{c_{\ell,1}}{N} + \dots + \frac{c_{\ell,m-1}}{N^{m-1}} \right) \right] + O \left(\frac{|w_0|^{-N}}{N^{\ell+m+1}} \right). \quad (1.12)$$

Numerical evidence for Conjecture 1.5 is given in Section 6 and the asymptotics of the next cases, $C_{121}(N)$ and $C_{131}(N)$, are also discussed there. The following subsection outlines how the proofs of Theorems 1.2 and 1.4 are constructed.

As this work was being completed, I was contacted by Drmota and Gerhold who provided me with their paper [DG]. They have given an independent disproof of Rademacher's conjecture by combining a Mellin transform approach with the saddle-point method to obtain the asymptotics of $C_{01\ell}(N)$. Their main result is equivalent to Conjecture 1.5 in the case $m = 1$ though with a weaker error term. Combining their techniques with ours should lead to improved asymptotics and a better understanding of all the Rademacher coefficients.

1.3 Method of proof

We have from [O'S12, Eq. (2.1)] that

$$C_{h k \ell}(N) = 2\pi i \operatorname{Res}_{z=h/k} \frac{e^{2\pi i z} (e^{2\pi i z} - e^{2\pi i h/k})^{\ell-1}}{(1 - e^{2\pi i 1z})(1 - e^{2\pi i 2z}) \dots (1 - e^{2\pi i N z})}. \quad (1.13)$$

The right of (1.13) may be expressed in terms of the simpler function

$$Q(z; N, \sigma) := \frac{e^{2\pi i \sigma z}}{(1 - e^{2\pi i 1z})(1 - e^{2\pi i 2z}) \dots (1 - e^{2\pi i N z})} \quad (1.14)$$

and we write

$$Q_{h k \sigma}(N) := 2\pi i \operatorname{Res}_{z=h/k} Q(z; N, \sigma). \quad (1.15)$$

Expanding the numerator on the right of (1.13) then produces

$$C_{h k \ell}(N) = \sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-e^{2\pi i h/k})^{\ell-\sigma} Q_{h k \sigma}(N). \quad (1.16)$$

The numbers $Q_{h k \sigma}(N)$ are slightly easier to work with than $C_{h k \ell}(N)$, though of course for $\ell = 1$ we have $C_{h k 1}(N) = Q_{h k 1}(N)$. Each $Q_{h k \sigma}(N)$ is a component of the Sylvester wave W_k , as described in Section 6.2, and expressions such as $Q(z; N, \sigma)$ and $Q_{h k \sigma}(N)$ appear when counting lattice points in a polytope dilated by a factor $-\sigma > 0$, see [BDR02, Thm. 1] and [BGK01]. We may also invert (1.16) to get

$$Q_{h k \sigma}(N) = \sum_{\ell=1}^{\sigma} \binom{\sigma-1}{\ell-1} (e^{2\pi i h/k})^{\sigma-\ell} C_{h k \ell}(N). \quad (1.17)$$

As a function of z , $Q(z; N, \sigma)$ is meromorphic of period 1 when $\sigma \in \mathbb{Z}$. Fixing a positive integer σ and summing all the residues then leads to the key identity on which Theorem 1.4 is based:

$$\sum_{h/k \in \mathcal{F}_N} Q_{hk\sigma}(N) = 0 \quad \text{for} \quad N(N+1)/2 > \sigma. \quad (1.18)$$

There is a large contribution to the left of (1.18) from $Q_{01\sigma}(N)$ as well as other $Q_{hk\sigma}(N)$ with k small, corresponding to high-order poles of $Q(z; N, \sigma)$. Balancing that are contributions from coefficients $Q_{hk\sigma}(N)$ with k large, corresponding to simple poles. Put

$$\mathcal{A}(N) := \left\{ h/k : \frac{N}{2} < k \leq N, h = 1 \text{ or } h = k-1 \right\} \subseteq \mathcal{F}_N \quad (1.19)$$

and decompose (1.18) into

$$\sum_{h/k \in \mathcal{F}_{100}} Q_{hk\sigma}(N) + \sum_{h/k \in \mathcal{F}_N - (\mathcal{F}_{100} \cup \mathcal{A}(N))} Q_{hk\sigma}(N) + \sum_{h/k \in \mathcal{A}(N)} Q_{hk\sigma}(N) = 0.$$

The reason we focus on the subset $\mathcal{A}(N)$ is given in the next section, but it may already be noticed that, numerically,

$$C_{011}(N) \approx -\mathcal{A}_1(N, 1) \quad \text{as} \quad N \rightarrow \infty \quad (1.20)$$

for

$$\mathcal{A}_1(N, \sigma) := \sum_{h/k \in \mathcal{A}(N)} Q_{hk\sigma}(N). \quad (1.21)$$

Computing the residues of the simple poles lets us describe (1.21) more explicitly as

$$\mathcal{A}_1(N, \sigma) = \text{Im} \sum_{\frac{N}{2} < k \leq N} \frac{2(-1)^k}{k^2} \exp \left(\frac{i\pi}{2} \left[\frac{-N^2 - N + 4\sigma}{k} + 3N \right] \right) \Pi_{N-k}^{-1}(1/k) \quad (1.22)$$

where we write

$$\Pi_m(\theta) := \prod_{j=1}^m 2 \sin(\pi j \theta) \quad (1.23)$$

with $\Pi_0(\theta) := 1$, following Sudler's notation in [Sud64] except that we don't take the absolute value. The main part of the proof of Theorem 1.4 then consists of establishing the following two results. Recall w_0 and z_0 from (1.5).

Theorem 1.6. *With $b_0 = 2z_0 e^{-\pi i z_0}$ and explicit $b_1(\sigma), b_2(\sigma), \dots$ depending on $\sigma \in \mathbb{R}$ we have*

$$\mathcal{A}_1(N, \sigma) = \text{Re} \left[\frac{w_0^{-N}}{N^2} \left(b_0 + \frac{b_1(\sigma)}{N} + \dots + \frac{b_{m-1}(\sigma)}{N^{m-1}} \right) \right] + O \left(\frac{|w_0|^{-N}}{N^{m+2}} \right)$$

for an implied constant depending only on σ and m .

Theorem 1.7. *There exists $W < U := -\log |w_0| \approx 0.068076$ so that*

$$\sum_{h/k \in \mathcal{F}_N - (\mathcal{F}_{100} \cup \mathcal{A}(N))} Q_{hk\sigma}(N) = O(e^{WN})$$

for an implied constant depending only on σ . We may take $W = 0.055$.

The proof of Theorem 1.6 is carried out as follows. In Section 2 we explain the origin of the sum $\mathcal{A}_1(N, \sigma)$ in (1.22) and also give some results on the dilogarithm we will need. Section 3 is quite technical and includes estimates of the sine product $\Pi_m(h/k)$ using Euler-Maclaurin summation, where the number of terms required is proportional to k and N . The sum $\mathcal{A}_1(N, \sigma)$ is replaced by an integral in Section 4, and in Section 5 the saddle-point method is introduced and applied. The required saddle-point is z_0 and with work of Wojdylo [Woj06], we explicitly get the full asymptotic expansion of $\mathcal{A}_1(N, \sigma)$. This proves Theorem 1.6.

See Section 6 for a summary of the proof of Theorem 1.7. The bounds required for $Q_{hk\sigma}(N)$ in this proof can be obtained directly in most cases, but three families also require saddle-point arguments, with these saddle-points corresponding to further zeros of the dilogarithm on other branches. The details are carried out in the companion paper [O'Sa].

Linear combinations of Theorems 1.6 and 1.7 then give Theorem 1.4 in Section 5.4. In Section 6 we also discuss extensions and generalizations of our results and applications to the restricted partition function and Sylvester waves.

2 Preliminary material

2.1 The residues of $Q(z; N, \sigma)$

For $Q(z; N, \sigma)$ defined in (1.14) with $\sigma \in \mathbb{C}$, we clearly have

$$\overline{Q(\bar{z}; N, \sigma)} = Q(-z; N, \bar{\sigma}), \quad (2.1)$$

$$Q(-z; N, \sigma) = (-1)^N Q(z; N, N(N+1)/2 - \sigma) \quad (2.2)$$

and, if $\sigma \in \mathbb{Z}$,

$$Q(z+1; N, \sigma) = Q(z; N, \sigma). \quad (2.3)$$

As a function of z , $Q(z; N, \sigma)$ is meromorphic with all poles contained in \mathbb{Q} . More precisely, the set of poles of $Q(z; N, \sigma)$ in $[0, 1)$ equals \mathcal{F}_N , the Farey fractions of order N in $[0, 1)$.

Theorem 2.1. For $N \in \mathbb{Z}_{\geq 1}$ and $\sigma \in \mathbb{Z}$

$$2\pi i \sum_{h/k \in \mathcal{F}_N} \operatorname{Res}_{z=h/k} Q(z; N, \sigma) = \begin{cases} -p_N(-\sigma) & \text{if } \sigma \leq 0 \\ 0 & \text{if } 0 < \sigma < N(N+1)/2 \\ (-1)^N p_N(\sigma - N(N+1)/2) & \text{if } N(N+1)/2 \leq \sigma. \end{cases} \quad (2.4)$$

Proof. We have

$$\sum_{n=0}^{\infty} p_N(n) e^{2\pi i n z} = \prod_{j=1}^N \frac{1}{1 - e^{2\pi i j z}} \quad (2.5)$$

and since $p_N(n) \leq p(n) \leq 2^{n-1}$, the number of ordered partitions of n , we see the left side of (2.5) is absolutely convergent for $\operatorname{Im}(z)$ large enough. (Better bounds for $p_N(n)$, $p(n)$ imply absolute convergence for $\operatorname{Im}(z) > 0$. See for example [Pri09], employing the dilogarithm.) Hence, for $\operatorname{Im}(w)$ large enough,

$$\int_w^{w+1} Q(z; N, \sigma) dz = \begin{cases} 0 & \text{if } \sigma > 0 \\ p_N(-\sigma) & \text{if } \sigma \leq 0. \end{cases} \quad (2.6)$$

Let \mathcal{R} be the rectangle in \mathbb{C} with upper corners $w, w+1$ and lower corners $v, v+1$ where $\operatorname{Im}(v) < 0$. Integrating around \mathcal{R} in a positive direction and choosing $\operatorname{Re}(w) = \operatorname{Re}(v)$ between 0 and the next pole to the left,

$$\int_{\mathcal{R}} Q(z; N, \sigma) dz = 2\pi i \sum_{h/k \in \mathcal{F}_N} \operatorname{Res}_{z=h/k} Q(z; N, \sigma). \quad (2.7)$$

The integral along the top of \mathcal{R} is -1 times (2.6). The integral along the bottom can be made arbitrarily small by letting $\operatorname{Im}(v) \rightarrow -\infty$ provided $\sigma < N(N+1)/2$ and the integrals along the vertical sides cancel with (2.3). If $\sigma \geq N(N+1)/2$ then use (2.2). This completes the proof. \square

Theorem 2.1 for negative integer σ is a restatement of a special case of Sylvester's Theorem. See for example [O'S12, Sect. 4].

Each $h/k \in \mathcal{F}_N$ is a pole of $Q(z; N, \sigma)$ of order $s = \lfloor N/k \rfloor$. Equivalently, h/k is a pole of order s exactly when

$$\frac{N}{s+1} < k \leq \frac{N}{s}. \quad (2.8)$$

Thus $2\pi i Q(z; N, \sigma)$ has one pole of order N in $[0, 1)$ at $h/k = 0/1$ with residue $Q_{01\sigma}(N)$. The next highest order pole has order $\lfloor N/2 \rfloor$ at $h/k = 1/2$ with residue $Q_{12\sigma}(N)$. By (2.8), h/k is a simple pole when $N/2 < k \leq N$ and the residues of the simple poles of $Q(z; N, \sigma)$ may be computed quite easily.

Proposition 2.2. For $N/2 < k \leq N$

$$Q_{hk\sigma}(N) = \frac{(-1)^{k+1}}{k^2} \exp\left(\frac{-\pi i h(N^2 + N - 4\sigma)}{2k}\right) \times \exp\left(\frac{\pi i}{2}(2Nh + N + h + k - hk)\right) \prod_{j=1}^{N-k} \frac{1}{2 \sin(\pi j h/k)}.$$

Proof. With (1.13), write

$$Q_{hk\sigma}(N) = \operatorname{Res}_{z=h/k} \frac{2\pi i e^{2\pi i \sigma z}}{[(1 - e^{2\pi i z}) \cdots (1 - e^{2\pi i (k-1)z})] (1 - e^{2\pi i k z}) [(1 - e^{2\pi i (k+1)z}) \cdots (1 - e^{2\pi i N z})]}.$$

Then

$$\operatorname{Res}_{z=h/k} \frac{1}{1 - e^{2\pi i k z}} = \frac{-1}{2\pi i k}.$$

Also

$$(1 - \zeta)(1 - \zeta^2) \cdots (1 - \zeta^{k-1}) = k \quad (2.9)$$

for $\zeta = e^{2\pi i h/k}$ a primitive k th root of unity, by [O'S12, Lemma 4.4] for example. Hence

$$Q_{hk\sigma}(N) = \frac{-e^{2\pi i \sigma h/k}}{k^2} \prod_{j=k+1}^N \frac{1}{1 - e^{2\pi i j h/k}} = \frac{-e^{2\pi i \sigma h/k}}{k^2} \prod_{j=1}^{N-k} \frac{1}{1 - e^{2\pi i j h/k}}. \quad (2.10)$$

A straightforward calculation shows

$$\prod_{j=1}^m \frac{1}{1 - e^{2\pi i j h/k}} = \exp\left(\frac{\pi i m}{2} \left(1 - \frac{h}{k}(m+1)\right)\right) \prod_{j=1}^m \frac{1}{2 \sin(\pi j h/k)} \quad (2.11)$$

and combining this with (2.10) and simplifying completes the proof. \square

2.2 Products of sines

Recall our notation (1.23). Then for integers $k > h \geq 1$ with $(h, k) = 1$

$$\prod_m^{-1}(h/k) = \prod_{j=1}^m \frac{1}{2 \sin(\pi j h/k)} \quad (0 \leq m < k) \quad (2.12)$$

is a real number. For example,

$$\prod_{k-1}^{-1}(h/k) = (-1)^{(h-1)(k-1)/2} \frac{1}{k} \quad (2.13)$$

follows from setting $m = k - 1$ in (2.11) and using (2.9).

With Proposition 2.2 we see that

$$|Q_{hk\sigma}(N)| = \left| \prod_{N-k}^{-1}(h/k) \right| / k^2 \quad (N/2 < k \leq N, \sigma \in \mathbb{R})$$

and so the size of $Q_{hk\sigma}(N)$ is controlled by the sine product $\prod_m^{-1}(h/k)$ for $m = N - k$. As m varies we need to know how big $\prod_m^{-1}(h/k)$ can be. For example, if $h = 1$ and k is large then the first terms

$$\frac{1}{2 \sin(\pi 1/k)} \approx \frac{k}{2\pi}, \quad \frac{1}{2 \sin(\pi 2/k)} \approx \frac{k}{4\pi}, \quad \dots$$

are all greater than 1. The maximum is reached with

$$\frac{1}{2 \sin(\pi 1/k)} \times \frac{1}{2 \sin(\pi 2/k)} \times \cdots \times \frac{1}{2 \sin(\pi (k/6)/k)} = \prod_{k/6}^{-1}(1/k) \quad (2.14)$$

since after that the factors become less than 1. If $h = 2$, the maximum value of $\prod_m^{-1}(2/k)$ is reached for $m = k/12$ and this value is approximately the square root of (2.14). For other values of h the maximum of the product does not become as large because values greater than 1 are multiplied by more values less than 1. An exception is when $h = (k - 1)/2$ since here again large products can build up. We illustrate this with Figure 1 which graphs

$$\Psi(h/k) := \max_{0 \leq m < k} \left\{ \frac{1}{k} \left| \log \left| \prod_m(h/k) \right| \right| \right\}. \quad (2.15)$$

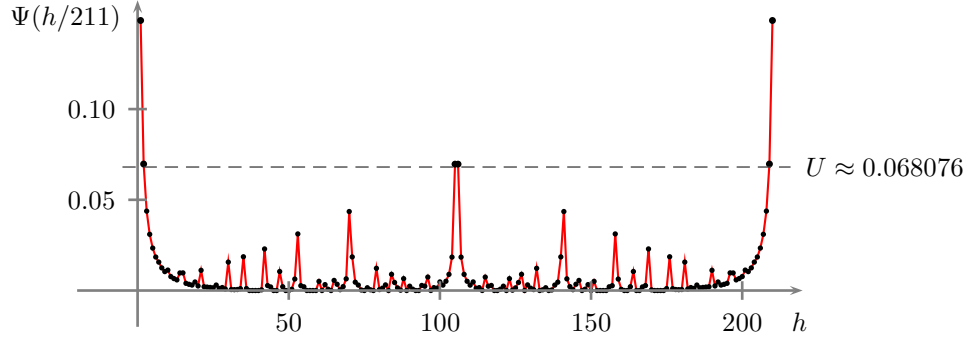


Figure 1: $\Psi(h/k)$ for $1 \leq h < k$ and $k = 211$

for $1 \leq h < k$ with k prime and equalling 211. We see that the largest values of $\Psi(h/k)$ are for $h \in \{1, 2, (k-1)/2\}$ (and symmetrically $h \in \{k-1, k-2, (k+1)/2\}$) with exactly these values greater than $U \approx 0.068076$. These observations are made precise in Section 6.1.

So, among the simple poles of $Q_N(1, z)$, Figure 1 leads us to expect that the largest contribution to the left of (1.18) should be from the sum $\mathcal{A}_1(N, \sigma)$ as defined in (1.21).

With (2.1) and (2.3) we obtain the identity

$$2\pi i \operatorname{Res}_{z=1-h/k} Q(z; N, \sigma) = \overline{2\pi i \operatorname{Res}_{z=h/k} Q(z; N, \bar{\sigma})}.$$

Therefore, assuming $\sigma \in \mathbb{R}$ from now on,

$$\begin{aligned} \mathcal{A}_1(N, \sigma) &:= 2\pi i \sum_{h/k \in \mathcal{A}(N)} \operatorname{Res}_{z=h/k} Q(z; N, \sigma) \\ &= 2\operatorname{Re} \left[2\pi i \sum_{\frac{N}{2} < k \leq N} \operatorname{Res}_{z=1/k} Q(z; N, \sigma) \right]. \end{aligned}$$

So setting $h = 1$ in Proposition 2.2 and simplifying yields (1.22).

2.3 The dilogarithm

We assemble here some of the properties of the dilogarithm we will need. See for example [Max03], [Zag07] for more details. Initially defined as

$$\operatorname{Li}_2(z) := \sum_{n=1}^{\infty} \frac{z^n}{n^2} \quad \text{for } |z| \leq 1, \quad (2.16)$$

the dilogarithm has an analytic continuation given by

$$- \int_{C(z)} \log(1-u) \frac{du}{u} \quad (2.17)$$

where the contour of integration $C(z)$ is a path from 0 to $z \in \mathbb{C}$. This makes the dilogarithm a multi-valued holomorphic function with a branch point at 1 (and off the principal branch another branch point at 0). We let $\operatorname{Li}_2(z)$ denote the dilogarithm on its principal branch so that $\operatorname{Li}_2(z)$ is a single-valued holomorphic function on $\mathbb{C} - [1, \infty)$.

For $z \in \mathbb{C}$ we have the functional equations

$$\operatorname{Li}_2(1/z) = -\operatorname{Li}_2(z) - \operatorname{Li}_2(1) - \frac{1}{2} \log^2(-z) \quad z \notin [0, \infty), \quad (2.18)$$

$$\operatorname{Li}_2(1-z) = -\operatorname{Li}_2(z) + \operatorname{Li}_2(1) - \log(z) \log(1-z) \quad z \notin (-\infty, 0] \cup [1, \infty) \quad (2.19)$$

from [Max03, Eqs. (3.2), (3.3)], where we mean the principal branch of the logarithm on $\mathbb{C} - (-\infty, 0]$. Replacing z by $e^{2\pi iz}$ gives us two further versions of (2.18) and (2.19):

- For $m \in \mathbb{Z}$ and $m < \operatorname{Re}(z) < m + 1$

$$\operatorname{Li}_2(e^{-2\pi iz}) = -\operatorname{Li}_2(e^{2\pi iz}) + 2\pi^2(z^2 - (2m+1)z + m^2 + m + 1/6). \quad (2.20)$$

- Let $(-i\infty, m]$ denote the vertical line in \mathbb{C} made up of all points with real part $m \in \mathbb{Z}$ and imaginary part at most 0. Then for $m - 1/2 < \operatorname{Re}(z) < m + 1/2$ and $z \notin (-i\infty, m]$

$$\operatorname{Li}_2(e^{2\pi iz}) = -\operatorname{Li}_2(1 - e^{2\pi iz}) + \operatorname{Li}_2(1) - 2\pi i(z - m) \log(1 - e^{2\pi iz}). \quad (2.21)$$

We may describe $\operatorname{Li}_2(z)$ for z on the unit circle as

$$\operatorname{Re}(\operatorname{Li}_2(e^{2\pi ix})) = \sum_{n=1}^{\infty} \frac{\cos(2\pi nx)}{n^2} = \pi^2 B_2(x - [x]) \quad (x \in \mathbb{R}), \quad (2.22)$$

$$\operatorname{Im}(\operatorname{Li}_2(e^{2\pi ix})) = \sum_{n=1}^{\infty} \frac{\sin(2\pi nx)}{n^2} = \operatorname{Cl}_2(2\pi x) \quad (x \in \mathbb{R}) \quad (2.23)$$

where $B_2(x) := x^2 - x + 1/6$ is the second Bernoulli polynomial and

$$\operatorname{Cl}_2(\theta) := -\int_0^\theta \log|2 \sin(x/2)| dx \quad (\theta \in \mathbb{R}) \quad (2.24)$$

is Clausen's integral. Note that $\operatorname{Li}_2(1) = \zeta(2) = \pi^2/6$.

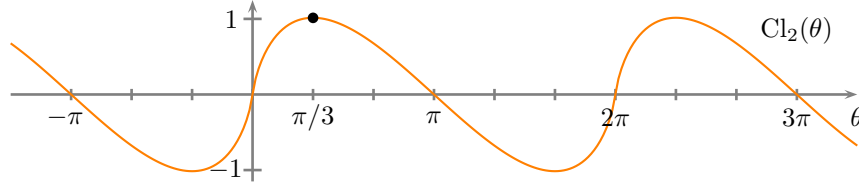


Figure 2: Clausen's integral

The graph of $\operatorname{Cl}_2(\theta)$ is shown in Figure 2. It is an odd function with period 2π and maximum value $\operatorname{Cl}_2(\pi/3) \approx 1.0149416$ indicated. Since, with (2.23),

$$\begin{aligned} \operatorname{Cl}_2(\theta) &= (\operatorname{Li}_2(e^{i\theta}) - \overline{\operatorname{Li}_2(e^{i\theta})}) / (2i) \\ &= (\operatorname{Li}_2(e^{i\theta}) - \operatorname{Li}_2(e^{-i\theta})) / (2i), \end{aligned} \quad (2.25)$$

we may use (2.25) to obtain the analytic continuation of $\operatorname{Cl}_2(\theta)$ to $\theta \in \mathbb{C}$ with $0 < \operatorname{Re}(\theta) < 2\pi$ for example. Another approach to this continuation combines (2.22) and (2.23) to get, for $m \leq z \leq m + 1, m \in \mathbb{Z}$,

$$\operatorname{Cl}_2(2\pi z) = -i \operatorname{Li}_2(e^{2\pi iz}) + i\pi^2(z^2 - (2m+1)z + m^2 + m + 1/6). \quad (2.26)$$

Then the right of (2.26) gives the continuation of $\operatorname{Cl}_2(2\pi z)$ to $z \in \mathbb{C}$ with $m < \operatorname{Re}(z) < m + 1$.

As z crosses the branch cuts the dilogarithm enters new branches. From [Max03, Sect. 3], the value of the analytically continued dilogarithm is always given by

$$\operatorname{Li}_2(z) + 4\pi^2 A + 2\pi i B \log(z) \quad (2.27)$$

for some $A, B \in \mathbb{Z}$. For example, the simplest way to get to a branch corresponding to (2.27) is to circle $z = 1$ once in the negative direction, then circle $z = 0$ in the positive direction A times and circle $z = 1$ in the negative direction $B - 1$ times (using the opposite directions if A or B is negative).

Zeros of the analytically continued dilogarithm will play a key role in our asymptotic calculations and in [O'Sb] we have made a study of them all. When the continued dilogarithm takes the form (2.27) with $B = 0$, there will be a zero if and only if $A \geq 0$ and, for each such A , the zero will be unique and lie on the real line. The cases we will require have $B \neq 0$. In these cases there are no real zeros so we may avoid the branch cuts and look for solutions to

$$\operatorname{Li}_2(z) + 4\pi^2 A + 2\pi i B \log(z) = 0 \quad (z \in \mathbb{C}, z \notin (-\infty, 0] \cup [1, \infty), A, B \in \mathbb{Z}). \quad (2.28)$$

Theorem 2.3. [O'Sb] For nonzero $B \in \mathbb{Z}$, (2.28) has solutions if and only if $-|B|/2 < A \leq |B|/2$. For such a pair A, B the solution z is unique. This unique solution, $w(A, B)$, may be found to arbitrary precision using Newton's method.

Sketch of proof. By considering the two curves where the real part and the imaginary part of (2.27) vanish, it can be shown that they intersect if and only if $-|B|/2 < A \leq |B|/2$. It can also be shown that $w(A, B)$ is close to $e^{2\pi i A/B}$ and from this starting point (the case $A = 0$ needs an adjustment) Newton's method will always converge to $w(A, B)$. Further details will appear in the forthcoming paper [O'Sb]. \square

By conjugating (2.28) it is clear that

$$w(A, -B) = \overline{w(A, B)}.$$

So for nonzero B the first zeros are $w(0, 1)$ and its conjugate $w(0, -1)$. We have

$$w(0, -1) \approx 0.9161978162 - 0.1824588972i$$

and this zero was denoted by w_0 in Section 1. The next few zeros are

$$\begin{aligned} w(0, -2) &\approx 0.9684820460 - 0.1095311065i \\ w(1, -2) &\approx -0.9943069304 - 0.0648889318i \\ w(-1, -3) &\approx -0.5459030969 + 0.8812307423i \\ w(0, -3) &\approx 0.9832603795 - 0.0777596389i \\ w(1, -3) &\approx -0.4594734813 - 0.8485350380i \end{aligned}$$

where $w(0, -2)$ and $w(1, -3)$ will be required in Section 6.

Define

$$p_d(z) := \frac{-\text{Li}_2(e^{2\pi iz}) + \text{Li}_2(1) + 4\pi^2 d}{2\pi iz}, \quad (2.29)$$

a single-valued holomorphic function away from the branch cuts $(-i\infty, n]$ for $n \in \mathbb{Z}$. In Section 5 we will require the solution of $p'_0(z) = 0$ (and in [O'Sa] solutions to $p'_d(z) = 0$ more generally).

Theorem 2.4. Fix integers m and d with $-|m|/2 < d \leq |m|/2$. Then there is a unique solution to $p'_d(z) = 0$ for $z \in \mathbb{C}$ with $m - 1/2 < \text{Re}(z) < m + 1/2$ and $z \notin (-i\infty, m]$. Denoting this solution by z^* , it is given by

$$z^* = m + \frac{\log(1 - w(d, -m))}{2\pi i} \quad (2.30)$$

and satisfies

$$p_d(z^*) = \log(w(d, -m)). \quad (2.31)$$

Proof. Note that

$$\frac{d}{dz} \text{Li}_2(e^{2\pi iz}) = -2\pi i \log(1 - e^{2\pi iz})$$

for z not on any of the vertical lines $(-i\infty, n]$, $n \in \mathbb{Z}$. So

$$\begin{aligned} p_d(z) + zp'_d(z) &= \frac{d}{dz} (zp_d(z)) \\ &= \frac{d}{dz} \left(\frac{\text{Li}_2(1) + 4\pi^2 d}{2\pi i} - \frac{\text{Li}_2(e^{2\pi iz})}{2\pi i} \right) = \log(1 - e^{2\pi iz}) \end{aligned}$$

and hence

$$p'_d(z) = -\frac{1}{z} (p_d(z) - \log(1 - e^{2\pi iz})). \quad (2.32)$$

Similarly

$$p''_d(z) = -\frac{1}{z} \left(2p'_d(z) + \frac{2\pi i \cdot e^{2\pi iz}}{1 - e^{2\pi iz}} \right). \quad (2.33)$$

With (2.29) we may expand (2.32) into

$$2\pi iz^2 p'_d(z) = \text{Li}_2(e^{2\pi iz}) - \text{Li}_2(1) - 4\pi^2 d + 2\pi iz \log(1 - e^{2\pi iz}). \quad (2.34)$$

Applying the functional equation (2.21) to (2.34) implies

$$2\pi iz^2 p'_d(z) = -\text{Li}_2(1 - e^{2\pi iz}) - 4\pi^2 d + 2\pi im \log(1 - e^{2\pi iz})$$

for $m - 1/2 < \text{Re}(z) < m + 1/2$. Letting $w = 1 - e^{2\pi iz}$, we are now looking for solutions to the equation

$$\text{Li}_2(w) + 4\pi^2 d - 2\pi im \log(w) = 0 \quad (2.35)$$

and Theorem 2.3 gives the unique solution as $w(d, -m)$ when $-|m|/2 < d \leq |m|/2$. The formula (2.30) follows and then (2.32) implies (2.31). \square

3 Estimates for the sine product $\prod_m^{-1}(h/k)$

Sudler in [Sud64] approximates $\prod_m(\theta)$ using the first term of the Euler-Maclaurin summation formula and finds that the $\theta \in (0, 1)$ that maximizes $|\prod_m(\theta)|$ is approximately x_0/m where $x_0 \approx 0.791227$ is the x value in $(0, 1)$ where $\frac{d}{dx}(\text{Cl}_2(2\pi x)/(2\pi x))$ vanishes. Wright in [Wri64] uses more terms in the summation to get more detailed results, as do Freiman and Halberstam in [FH88]. We use similar techniques in the next subsection but require arbitrarily many terms of the summation formula.

3.1 Euler-Maclaurin summation

We need to estimate the size of $\prod_m(\theta)$ accurately and also replace it with a continuous (and later holomorphic) function of m .

Let $\rho(z) := \log((\sin z)/z)$, a holomorphic function for $|z| < \pi$ that satisfies $\rho(-z) = \rho(z)$. Also

$$\cot(\pi z) = \frac{1}{\pi z} + \rho'(\pi z) \quad (3.1)$$

and so

$$\cot^{(k)}(\pi z) = \frac{(-1)^k k!}{(\pi z)^{k+1}} + \rho^{(k+1)}(\pi z). \quad (3.2)$$

Proposition 3.1. *For $m, L \in \mathbb{Z}_{\geq 1}$ and $-1/m < \theta < 1/m$ with $\theta \neq 0$ we have*

$$\begin{aligned} \prod_m(\theta) &= \left(\frac{\theta}{|\theta|}\right)^m \left(\frac{2\sin(\pi m\theta)}{\theta}\right)^{1/2} \exp\left(-\frac{\text{Cl}_2(2\pi m\theta)}{2\pi\theta}\right) \\ &\quad \times \exp\left(\sum_{\ell=1}^{L-1} \frac{B_{2\ell}}{(2\ell)!} (\pi\theta)^{2\ell-1} \cot^{(2\ell-2)}(\pi m\theta)\right) \exp(T_L(m, \theta)) \end{aligned} \quad (3.3)$$

for

$$T_L(m, \theta) := (\pi\theta)^{2L} \int_0^m \frac{B_{2L} - B_{2L}(x - \lfloor x \rfloor)}{(2L)!} \rho^{(2L)}(\pi x\theta) dx + \int_0^\infty \frac{B_{2L} - B_{2L}(x - \lfloor x \rfloor)}{2L(x+m)^{2L}} dx.$$

Proof. Write

$$\begin{aligned} \prod_m(\theta) &= (2\pi\theta)^m m! \prod_{j=1}^m \frac{\sin(\pi j\theta)}{\pi j\theta} \\ &= (2\pi\theta)^m m! \prod_{j=1}^m \exp(\rho(\pi j\theta)) = (2\pi\theta)^m m! \exp\left(\sum_{j=1}^m \rho(\pi j\theta)\right). \end{aligned} \quad (3.4)$$

With Euler-Maclaurin summation, as in [Rad73, Chap. 2] or [Olv74, p. 285], we obtain for $|\theta| < 1/m$,

$$\begin{aligned} \sum_{j=1}^m \rho(\pi j \theta) &= \int_0^m \rho(\pi x \theta) dx + \frac{1}{2} (\rho(\pi m \theta) - \rho(\pi 0 \theta)) \\ &\quad + \sum_{\ell=1}^{L-1} \frac{B_{2\ell}}{(2\ell)!} (\pi \theta)^{2\ell-1} \left\{ \rho^{(2\ell-1)}(\pi m \theta) - \rho^{(2\ell-1)}(\pi 0 \theta) \right\} + R_L(m, \theta) \end{aligned} \quad (3.5)$$

where $L \geq 1$ and

$$R_L(m, \theta) := (\pi \theta)^{2L} \int_0^m \frac{B_{2L} - B_{2L}(x - \lfloor x \rfloor)}{(2L)!} \rho^{(2L)}(\pi x \theta) dx. \quad (3.6)$$

The integral in (3.5) may be evaluated using (2.24) to get

$$\int_0^m \rho(\pi x \theta) dx = -m \log |2\pi m \theta| + m - \frac{\text{Cl}_2(2\pi m \theta)}{2\pi \theta} \quad (\theta \neq 0)$$

and therefore

$$\begin{aligned} \Pi_m(\theta) &= \left(\frac{\theta e}{|\theta| m} \right)^m m! \left(\frac{\sin(\pi m \theta)}{\pi m \theta} \right)^{1/2} \exp \left(-\frac{\text{Cl}_2(2\pi m \theta)}{2\pi \theta} \right) \\ &\quad \times \exp \left(\sum_{\ell=1}^{L-1} \frac{B_{2\ell}}{(2\ell)!} (\pi \theta)^{2\ell-1} \rho^{(2\ell-1)}(\pi m \theta) \right) \exp(R_L(m, \theta)). \end{aligned} \quad (3.7)$$

Stirling's formula is

$$\log \Gamma(m) = (m - \frac{1}{2}) \log m - m + \frac{1}{2} \log 2\pi + \sum_{\ell=1}^{L-1} \frac{B_{2\ell}}{2\ell(2\ell-1)m^{2\ell-1}} + S_L(m) \quad (3.8)$$

with

$$S_L(m) := \int_0^\infty \frac{B_{2L} - B_{2L}(x - \lfloor x \rfloor)}{2L(x+m)^{2L}} dx \quad (3.9)$$

as in [Olv74, (4.03) p. 294]. Hence

$$\left(\frac{e}{m} \right)^m m! = \left(\frac{e}{m} \right)^m m \Gamma(m) = (2\pi m)^{1/2} \exp \left(\sum_{\ell=1}^{L-1} \frac{B_{2\ell}}{2\ell(2\ell-1)m^{2\ell-1}} \right) \exp(S_L(m)). \quad (3.10)$$

Putting (3.10) into (3.7), recombining the two sums with (3.2), and setting $T_L(m, \theta) := R_L(m, \theta) + S_L(m)$ completes the proof. \square

3.2 Derivatives of the cotangent

We next examine the cotangent function and its derivatives in detail. For all $z \in \mathbb{C}$,

$$\cot(\pi z) = i + \frac{2i}{e^{2\pi i z} - 1} = -i - \frac{2i}{e^{-2\pi i z} - 1}. \quad (3.11)$$

For $k \geq 1$, by induction,

$$\cot^{(k)}(z) = (-1)^k (2i)^{k+1} \sum_{r=1}^{k+1} (r-1)! \left\{ \begin{matrix} k+1 \\ r \end{matrix} \right\} \frac{1}{(e^{2iz} - 1)^r}, \quad (3.12)$$

$$= (-1)^k (-2i)^{k+1} \sum_{r=1}^{k+1} (r-1)! \left\{ \begin{matrix} k+1 \\ r \end{matrix} \right\} \frac{1}{(e^{-2iz} - 1)^r}. \quad (3.13)$$

As in [GKP94, Chap. 6] these Stirling numbers satisfy the relations

$$\left\{ \begin{matrix} k \\ r-1 \end{matrix} \right\} + r \left\{ \begin{matrix} k \\ r \end{matrix} \right\} = \left\{ \begin{matrix} k+1 \\ r \end{matrix} \right\}, \quad \sum_{r=0}^k \left\{ \begin{matrix} k \\ r \end{matrix} \right\} x(x-1) \cdots (x-r+1) = x^k. \quad (3.14)$$

For $k \geq 0$, $\cot^{(k)}(\pi z)$ is clearly holomorphic in \mathbb{C} except for poles when $z \in \mathbb{Z}$.

Lemma 3.2. For $c > 0$ and $k \in \mathbb{Z}_{\geq 0}$

$$\sum_{\ell=1}^{\infty} \ell^k e^{-c\ell} \leq k! \left(\frac{2}{c}\right)^{k+1}.$$

Proof. The result follows by comparing the series to the integral

$$\int_0^{\infty} x^k e^{-cx} dx = \frac{\Gamma(k+1)}{c^{k+1}} = \frac{k!}{c^{k+1}}. \quad \square$$

Theorem 3.3. For all nonzero $z \in \mathbb{C}$ with $-1/2 \leq \operatorname{Re}(z) \leq 1/2$ we have

$$\left| \cot^{(k)}(\pi z) \right| \leq \delta_{0,k} + 20 \frac{k!}{\pi^{k+1}} \left(\frac{1}{|z|^{k+1}} + 8^{k+1} \right) e^{-\pi|y|}. \quad (3.15)$$

Also, for all $z \in \mathbb{C}$ with $|y| \geq 1$,

$$\left| \cot^{(k)}(\pi z) \right| \leq \delta_{0,k} + \frac{k!}{\pi^{k+1}} \left(\frac{4.01}{|y|} \right)^{k+1} e^{-\pi|y|}. \quad (3.16)$$

Proof. By [Rad73, (11.1)] and (3.1)

$$-\rho'(w) = \sum_{r=1}^{\infty} \frac{2^{2r} |B_{2r}|}{(2r)!} w^{2r-1} \quad (|w| < \pi) \quad (3.17)$$

so that all the coefficients of $-\rho'(w)$ are positive. Hence, with $|w| < \pi$ and the bound

$$\frac{|B_{2n}|}{(2n)!} \leq \frac{\pi^2}{3(2\pi)^{2n}} \quad (3.18)$$

from [Rad73, (9.6)], we have

$$|\rho'(w)| \leq -\rho'(|w|) \leq \frac{\pi}{3} \sum_{r=1}^{\infty} \left(\frac{|w|}{\pi} \right)^{2r-1} \leq \frac{\pi}{3} \sum_{r=0}^{\infty} \left(\frac{|w|}{\pi} \right)^r \leq \frac{\pi}{3(1 - |w|/\pi)}.$$

Letting $f(t) := \frac{\pi}{3(1 - t/\pi)}$ we see that

$$f^{(k)}(t) = \frac{k!}{3\pi^{k-1}(1 - t/\pi)^{k+1}}.$$

Since the power series coefficients of f are greater than the corresponding power series coefficients of $-\rho'$, and all coefficients are positive, it follows that the coefficients of $f^{(k)}$ are greater than the corresponding coefficients of $-\rho^{(k+1)}$. Therefore

$$\left| \rho^{(k+1)}(w) \right| \leq \frac{k!}{3\pi^{k-1}(1 - |w|/\pi)^{k+1}} \quad (k \geq 0, |w| < \pi). \quad (3.19)$$

With (3.2) and (3.19) we have proved that

$$\left| \cot^{(k)}(\pi z) \right| \leq \frac{\pi^2}{3} \frac{k!}{\pi^{k+1}} \left(\frac{1}{|z|^{k+1}} + \frac{1}{(1 - |z|)^{k+1}} \right) \quad (|z| < 1). \quad (3.20)$$

Next we assume $y \neq 0$. Formulas (3.11), (3.12) and (3.13) imply

$$\begin{aligned} \left| \cot^{(k)}(\pi z) \right| &\leq \delta_{0,k} + 2^{k+1} \sum_{r=1}^{k+1} (r-1)! \left\{ \begin{matrix} k+1 \\ r \end{matrix} \right\} \frac{e^{-2\pi|y|r}}{(1 - e^{-2\pi|y|})^r} \\ &\leq \delta_{0,k} + \frac{2^{k+1}}{(1 - e^{-2\pi|y|})^{k+1}} \sum_{r=1}^{k+1} r^k e^{-2\pi|y|r} \\ &\leq \delta_{0,k} + \left(\frac{2}{1 - e^{-2\pi|y|}} \right)^{k+1} e^{-\pi|y|} \sum_{r=1}^{k+1} r^k e^{-\pi|y|r} \end{aligned} \quad (3.21)$$

where we used that $(r-1)! \left\{ \frac{k+1}{r} \right\} \leq r^k$ which follows from the relation on the right of (3.14) with $x = r$. Lemma 3.2 applied to (3.21) shows

$$\left| \cot^{(k)}(\pi z) \right| \leq \delta_{0,k} + k! \left(\frac{4}{\pi|y|(1-e^{-2\pi|y|})} \right)^{k+1} e^{-\pi|y|} \quad (y \neq 0). \quad (3.22)$$

Then (3.15) in the statement of the theorem follows by combining (3.20) for $|y| \leq 0.55$ and (3.22) for $|y| \geq 0.55$. Finally, (3.16) follows from (3.22). \square

3.3 Initial estimates for $\prod_m^{-1}(h/k)$

Stirling's formula implies

$$2\sqrt{n} \left(\frac{n}{e} \right)^n < n! < 3\sqrt{n} \left(\frac{n}{e} \right)^n \quad (n \in \mathbb{Z}_{\geq 1})$$

and it follows that

$$(n-1)! < 3(n/e)^n. \quad (3.23)$$

Since $|B_{2n}(x - \lfloor x \rfloor)| \leq |B_{2n}|$ as in [Olv74, Thm 1.1, p. 283], we see that $B_{2n} - B_{2n}(x - \lfloor x \rfloor)$ has the same sign as B_{2n} if it's non-zero. Therefore the terms in (3.8) alternate in sign and it follows that ([Olv74, (4.05) p. 294])

$$|S_L(m)| \leq \frac{|B_{2L}|}{2L(2L-1)m^{2L-1}}. \quad (3.24)$$

Employing (3.18) and (3.23) in (3.24) gives

$$|S_L(m)| \leq \frac{\pi}{6} \frac{(2L-2)!}{(2\pi m)^{2L-1}} < \frac{\pi}{2} \left(\frac{2L-1}{2\pi e m} \right)^{2L-1} \quad (L, m \in \mathbb{Z}_{\geq 1}). \quad (3.25)$$

Lemma 3.4. For $m, L \in \mathbb{Z}_{\geq 1}$ and $-1/m < \theta < 1/m$ we have

$$|R_L(m, \theta)| \leq \frac{\pi^3}{3} \left(\frac{(2L-1)|\theta|}{2\pi e(1-m|\theta|)} \right)^{2L-1}. \quad (3.26)$$

Proof. With (3.6), (3.18) and the inequality $|B_{2n} - B_{2n}(x - \lfloor x \rfloor)| \leq 2|B_{2n}|$ we have

$$\begin{aligned} |R_L(m, \theta)| &\leq \frac{2\pi^2}{3(2\pi)^{2L}} (\pi|\theta|)^{2L} \int_0^m \left| \rho^{(2L)}(\pi x \theta) \right| dx \\ &= \frac{\pi}{3} \left(\frac{|\theta|}{2} \right)^{2L-1} \left| \rho^{(2L-1)}(\pi m \theta) \right|. \end{aligned}$$

Then applying (3.19) shows

$$|R_L(m, \theta)| \leq \frac{\pi^3}{9} (2L-2)! \left(\frac{|\theta|}{2\pi(1-m|\theta|)} \right)^{2L-1}. \quad (3.27)$$

The result follows with (3.23). \square

We now concentrate on the case where $\theta = h/k$ for relatively prime integers $k > h \geq 1$. We think of h, k as fixed with integer m varying in the range $1 \leq m < k/h$.

Lemma 3.5. For $1 \leq m < k/h$ we have

$$|T_1(m, h/k)| \leq \pi^2 h/18 + 1/12. \quad (3.28)$$

Proof. Note that since m is an integer

$$1 \leq m < k/h \implies h \leq mh \leq k-1. \quad (3.29)$$

Consequently $1/(1-mh/k) \leq k$ and using this in (3.27) gives a bound for R_1 . Bound S_1 with (3.24). \square

Define

$$c(h) := \frac{h^{1/2}}{2} \exp(\pi^2 h/18 + 1/6). \quad (3.30)$$

(We increased $1/12$ in (3.28) to $1/6$ to ensure $c(h) > 1$ for $h \geq 1$, as needed in Proposition 3.9.) The next result gives us our initial estimate for $\prod_m^{-1}(h/k)$.

Proposition 3.6. *For $1 \leq m < k/h$*

$$\prod_m^{-1}(h/k) \leq c(h) \exp\left(\frac{k}{2\pi h} \text{Cl}_2(2\pi m h/k)\right).$$

Proof. Combining Lemma 3.5 with Proposition 3.1 shows

$$\prod_m^{-1}(h/k) \leq \left(\frac{h}{2k \sin(\pi m h/k)}\right)^{1/2} \exp(\pi^2 h/18 + 1/12) \exp\left(\frac{k}{2\pi h} \text{Cl}_2(2\pi m h/k)\right). \quad (3.31)$$

Note the simple inequality

$$1 \leq \frac{x}{\sin x} \leq \frac{\pi}{2} \quad (-\pi/2 \leq x \leq \pi/2) \quad (3.32)$$

and hence

$$1 \leq \frac{1}{\sin x} \leq \frac{1}{\sin \varepsilon} \leq \frac{\pi}{2\varepsilon} \quad \text{for} \quad 0 \leq \varepsilon \leq x \leq \pi - \varepsilon.$$

It follows from (3.29) that $\pi/k \leq \pi m h/k \leq \pi - \pi/k$ and so

$$\frac{h}{2k \sin(\pi m h/k)} \leq \frac{h}{4} \quad (1 \leq m < k/h). \quad (3.33)$$

Inequalities (3.31) and (3.33) complete the proof. \square

Proposition 3.6 implies that

$$\prod_m^{-1}(h/k) \leq c(h) \quad \text{for} \quad k/2h \leq m < k/h, \quad (3.34)$$

since $\text{Cl}_2(\theta) \leq 0$ for $\pi \leq \theta \leq 2\pi$. For the rest of this subsection we focus on m in the range $1 \leq m \leq k/2h$. Our next goal is to show that for m near the end points of this range the product $\prod_m^{-1}(h/k)$ is also quite small - see Figure 3. We first develop a simpler version of the bound in Proposition 3.6.

Lemma 3.7. *For $0 \leq \theta \leq \pi$ we have*

$$\text{Cl}_2(\theta) \leq \theta - \theta \log \theta + \theta^3/54, \quad (3.35)$$

$$\text{Cl}_2(\pi - \theta) \leq \theta \log 2. \quad (3.36)$$

Proof. Integrate (3.17) twice and use (2.24) to show that, for $0 \leq \theta \leq \pi$,

$$\begin{aligned} \text{Cl}_2(\theta) &= \theta - \theta \log \theta + \sum_{n=1}^{\infty} \frac{|B_{2n}|}{2n(2n+1)!} \theta^{2n+1} \\ &\leq \theta - \theta \log \theta + \theta^3 \frac{\pi^2}{3} \sum_{n=1}^{\infty} \frac{\theta^{2n-2}}{2n(2n+1)(2\pi)^{2n}}. \end{aligned}$$

The series above is bounded by

$$\sum_{n=1}^{\infty} \frac{\pi^{2n-2}}{2n(2n+1)(2\pi)^{2n}} = \frac{1}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{2n(2n+1)4^n} < \frac{1}{24\pi^2} \sum_{n=0}^{\infty} 4^{-n}$$

and (3.35) follows.

Put $f(\theta) := \theta \log 2 - \text{Cl}_2(\pi - \theta)$. Then $f'(\theta) = -\log \sin((\pi - \theta)/2) \geq 0$ and so $f(\theta)$ is increasing on $[0, \pi]$ and therefore $f(\theta) \geq f(0) = 0$, proving (3.36). \square

Lemma 3.8. For $1 \leq m \leq k/2h$ we have

$$\prod_m^{-1}(h/k) < c(h) \left(\frac{k}{mh} \right)^m, \quad (3.37)$$

$$\prod_m^{-1}(h/k) < c(h) 2^{k/(2h) - m}. \quad (3.38)$$

Proof. From Proposition 3.6 and (3.35),

$$\begin{aligned} \prod_m^{-1}(h/k) &\leq c(h) \exp \left(m \left(1 - \log(2\pi mh/k) + (2\pi mh/k)^2 / 54 \right) \right) \\ &\leq c(h) \exp \left(m \left(1 + \log(k/(2\pi mh)) + \pi^2 / 54 \right) \right) \\ &= c(h) \left(\frac{e}{2\pi} e^{\pi^2/54} \frac{k}{mh} \right)^m < c(h) \left(\frac{k}{mh} \right)^m. \end{aligned}$$

Similarly, Proposition 3.6 and (3.36) give (3.38). \square

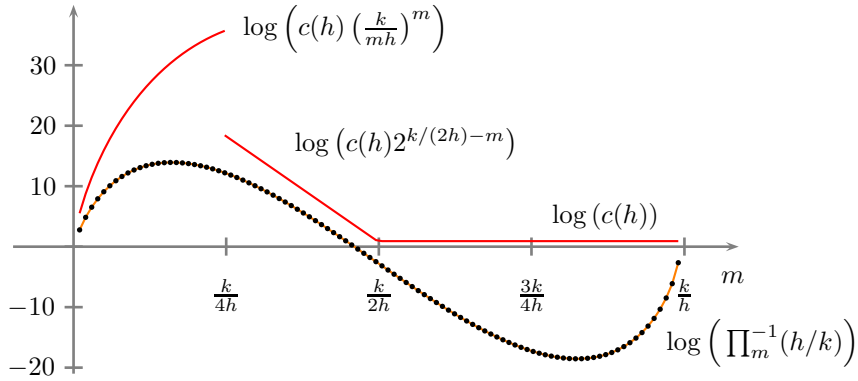


Figure 3: Bounds for $\prod_m^{-1}(h/k)$ with $1 \leq m < k/h$ and $h = 2, k = 201$

Define $g(x) := x \log(1/x)$. Then g is an increasing function on $[0, 1/e]$ with $g(0) = 0$ and $g(1/e) = 1/e$.

Proposition 3.9. Let $W > 0$. For δ satisfying $0 < \delta \leq 1/e$ and $\delta \log(1/\delta) \leq W$ we have

$$\prod_m^{-1}(h/k) \leq c(h) \exp \left(\frac{kW}{h} \right) \quad \text{for} \quad 0 \leq \frac{mh}{k} \leq \delta \quad \text{and} \quad \frac{1}{2} - \delta \leq \frac{mh}{k} < 1.$$

Proof. The result is true for $m = 0$ since $\prod_0^{-1}(h/k) = 1 < c(h)$. For $0 < \frac{mh}{k} \leq \delta$, starting with (3.37),

$$\begin{aligned} \prod_m^{-1}(h/k) &\leq c(h) \left(\frac{k}{mh} \right)^m \\ &= c(h) \exp \left(\frac{k}{h} g \left(\frac{mh}{k} \right) \right) \\ &\leq c(h) \exp \left(\frac{k}{h} g(\delta) \right) \\ &\leq c(h) \exp \left(\frac{k}{h} W \right) \end{aligned}$$

since $g(\delta) \leq W$. For $\frac{1}{2} \leq \frac{mh}{k} < 1$ we have already seen in (3.34) that $\prod_m^{-1}(h/k) \leq c(h)$. For $\frac{1}{2} - \delta \leq \frac{mh}{k} \leq \frac{1}{2}$

we have, starting with (3.38),

$$\begin{aligned}
\Pi_m^{-1}(h/k) &\leq c(h) \exp \left(\log 2 \frac{k}{2\pi h} \left(\pi - \frac{2\pi mh}{k} \right) \right) \\
&\leq c(h) \exp \left(\log 2 \frac{k}{2\pi h} \cdot 2\pi\delta \right) \\
&\leq c(h) \exp \left(\frac{k}{h} g(\delta) \right) \\
&\leq c(h) \exp \left(\frac{k}{h} W \right).
\end{aligned}$$

□

Lemma 3.10. For $1 \leq L$ and $1 \leq m \leq k/2h$ we have

$$|T_L(m, h/k)| \leq \frac{\pi^3}{2} \left(\frac{2L-1}{2\pi em} \right)^{2L-1}.$$

Proof. Combine the bounds (3.25), (3.26) and use

$$\frac{h/k}{1 - mh/k} = \frac{1}{m(k/(mh) - 1)} \leq \frac{1}{m}.$$

□

3.4 Controlling the error term

We have seen with Proposition 3.1 that for $1 \leq m < k/h$

$$\begin{aligned}
\Pi_m^{-1}(h/k) &= \left(\frac{h}{2k \sin(\pi mh/k)} \right)^{1/2} \exp \left(\frac{k}{2\pi h} \text{Cl}_2(2\pi mh/k) \right) \\
&\times \exp \left(- \sum_{\ell=1}^{L-1} \frac{B_{2\ell}}{(2\ell)!} \left(\frac{\pi h}{k} \right)^{2\ell-1} \cot^{(2\ell-2)} \left(\frac{\pi mh}{k} \right) \right) \exp(-T_L(m, h/k)). \quad (3.39)
\end{aligned}$$

For L large, what is the effect of removing the factor $\exp(-T_L(m, h/k))$ above? Our bound on $T_L(m, h/k)$ from Lemma 3.10 is poor for m small but gets much better when $m > (2L-1)/(2\pi e)$. Proposition 3.9 proves that $\Pi_m^{-1}(h/k)$ is small for small m , so we may assume $m > \delta k/h$ for a fixed $\delta > 0$. As m increases we have $\Pi_m^{-1}(h/k)$ getting bigger and the bound from Lemma 3.10 getting smaller. Our goal in this subsection is to choose an integer L (depending on a large parameter s where $0 < h < k \leq s$) so that these competing bounds produce a small enough error.

We first give some preliminary results that shall be required in Proposition 3.12 below. Given $\Delta > 0$, we will need real numbers $r \in [0, 1]$ that satisfy both the inequalities

$$\frac{1}{e^{r+1}} \left(1 + r \log \frac{r}{2\pi} \right) \leq \Delta \log \frac{1}{\Delta}, \quad (3.40)$$

$$\frac{r}{e^{r+1}} \leq 2\pi e \Delta. \quad (3.41)$$

Note that the left side of (3.40) is a decreasing continuous function of $r \in [0, 1]$, decreasing from the value $1/e$ to become negative at $r = 1$. The left side of (3.41) is increasing and continuous from 0 at $r = 0$ to $1/e^2$ at $r = 1$. Therefore, there exist $r_1 = r_1(\Delta)$, $r_2 = r_2(\Delta)$ so that

$$\frac{1}{e^{r_1+1}} \left(1 + r_1 \log \frac{r_1}{2\pi} \right) = \Delta \log \frac{1}{\Delta}, \quad (3.42)$$

$$\frac{r_2}{e^{r_2+1}} = 2\pi e \Delta \quad (3.43)$$

where we assume

$$\Delta \leq \frac{1}{2\pi e^3} \approx 0.0079$$

so that (3.43) has a solution. If $r_1 \leq r_2$ then the set of all $r \in [0, 1]$ satisfying both (3.40) and (3.41) is the interval $[r_1, r_2]$. Calculations displayed in Table 1 show that $r_1(\Delta) < r_2(\Delta)$ for $0.0048 \leq \Delta \leq 0.0079$.

Δ	$\Delta \log 1/\Delta$	$r_1(\Delta)$	$r_2(\Delta)$	R_Δ
0.0079	0.0382	0.276	0.924	51.9
0.007	0.0347	0.282	0.581	72.6
0.006	0.0307	0.288	0.427	130.7
0.005	0.0265	0.295	0.320	665.2
0.00477	0.0255	0.297	0.298	11701.6

Table 1: Some values for Δ and related quantities.

Suppose $u > 0$ and $L - 1/2 = \pi e \Delta \cdot u$. If $0.0048 \leq \Delta \leq 0.0079$ then we can find r satisfying both (3.40) and (3.41) such that

$$2L - 1 = \frac{r}{e^{r+1}} u \quad (3.44)$$

since we may take $r = r_2(\Delta)$. We next show that (3.44) still has a solution $r \in [r_1, r_2]$ if we replace L by the integer $\lfloor \pi e \Delta \cdot u \rfloor$. All this requires is that r_1 and r_2 are far enough apart. Define R_Δ as

$$R_\Delta := 3 / \left(\frac{r_2}{e^{r_2+1}} - \frac{r_1}{e^{r_1+1}} \right) \quad (r_1 < r_2).$$

Lemma 3.11. *Given Δ satisfying $0.0048 \leq \Delta \leq 0.0079$, suppose $u \in \mathbb{R}$ satisfies $u \geq R_\Delta$. Set $L := \lfloor \pi e \Delta \cdot u \rfloor$. Then*

$$2L - 1 = \frac{r}{e^{r+1}} u \quad (3.45)$$

for r satisfying both (3.40) and (3.41).

Proof. Since, as we have seen, r/e^{r+1} increases from 0 to $1/e^2$ with $r \in [0, 1]$, we may use (3.45) to define r . From the definitions of L and r_2 we obtain

$$u \frac{r_2}{2e^{r_2+1}} - 1 < L \leq u \frac{r_2}{e^{r_2+1}}$$

and hence

$$u \frac{r_2}{e^{r_2+1}} - 3 < 2L - 1 \leq u \frac{r_2}{e^{r_2+1}} - 1. \quad (3.46)$$

The right inequality in (3.46) implies that $r < r_2$. Also $u \geq R_\Delta$ implies

$$u \frac{r_1}{e^{r_1+1}} \leq u \frac{r_2}{e^{r_2+1}} - 3$$

so that the left inequality in (3.46) implies that $r_1 < r$. Then $r \in [r_1, r_2]$ implies r satisfies (3.40) and (3.41) as required. \square

Proposition 3.12. *Suppose Δ and W satisfy $0.0048 \leq \Delta \leq 0.0079$ and $\Delta \log 1/\Delta \leq W$. For the integers h, k, s and m we require*

$$0 < h < k \leq s, \quad R_\Delta \leq s/h, \quad \Delta s/h \leq m \leq k/(2h).$$

Then for $L := \lfloor \pi e \Delta \cdot s/h \rfloor$ we have

$$\left| \prod_m^{-1}(h/k) T_L(m, h/k) \right| \leq (\pi^3/2) c(h) \cdot e^{sW/h}, \quad (3.47)$$

$$|T_L(m, h/k)| \leq \pi^3/2. \quad (3.48)$$

Proof. We write $2L - 1 = \beta s/h$ for some $\beta = r/e^{r+1}$ and r satisfying both (3.40) and (3.41) by Lemma 3.11. With the bounds from Lemmas 3.8 and 3.10 we have

$$\left| \prod_m^{-1}(h/k) T_L(m, h/k) \right| \leq c(h) \left(\frac{k}{mh} \right)^m \frac{\pi^3}{2} \left(\frac{\beta s}{2\pi e m h} \right)^{\beta s/h}. \quad (3.49)$$

Taking the h/s power of both sides, we see that (3.47) follows if we can establish that

$$\left(\frac{s}{mh} \right)^{mh/s} \left(\frac{\beta s}{2\pi e m h} \right)^\beta \leq e^W$$

or equivalently, for $t = s/(mh)$ and $2 < t \leq 1/\Delta$, that

$$t^{\beta+1/t} \left(\frac{\beta}{2\pi e} \right)^\beta \leq e^W. \quad (3.50)$$

We see that $t^{\beta+1/t}$ has maxima on the interval $(0, 1/\Delta]$ at $t = 1/\Delta$ and $t = e^{r+1}$. To prove (3.50) we therefore just need to verify it at $t = 1/\Delta$ and $t = e^{r+1}$.

Since $(1/\Delta)^\Delta \leq e^W$ by the definition of Δ and

$$\frac{\beta}{2\pi e \Delta} \leq 1 \quad (3.51)$$

by (3.41) we see that (3.50) is true for $t = 1/\Delta$. Next, a short calculation shows that, for $t = e^{r+1}$,

$$\log \left(t^{\beta+1/t} \left(\frac{\beta}{2\pi e} \right)^\beta \right) = \frac{1}{e^{r+1}} \left(1 + r \log \frac{r}{2\pi} \right).$$

Therefore (3.40) implies that (3.50) is true for $t = e^{r+1}$. We have proved (3.47).

We also have

$$|T_L(m, h/k)| \leq \frac{\pi^3}{2} \left(\frac{\beta s}{2\pi e m h} \right)^{\beta s/h} \leq \frac{\pi^3}{2} \left(\frac{\beta}{2\pi e \Delta} \right)^{\beta s/h} \leq \frac{\pi^3}{2}$$

using (3.51). This proves the inequality (3.48). \square

As a numerical check of Proposition 3.12, take for example $\Delta = 0.006$, $W = 0.031$, $s = 500$ and $h = 1$. Then $L = \lfloor \pi e \Delta s/h \rfloor = 25$ and we require $3 \leq m \leq k/2 \leq 500/2$. For these m and k we find

$$\begin{aligned} \max_{m,k} \left| \prod_{m=1}^{-1} (1/k) T_{25}(m, 1/k) \right| &\approx 144.7 < 8.54 \times 10^7 \approx (\pi^3/2) c(1) \cdot e^{500W/1}, \\ \max_{m,k} |T_{25}(m, 1/k)| &\approx 0.002 < 15.5 \approx \pi^3/2. \end{aligned} \quad (3.52)$$

(The maximum of the bound on the right of (3.49) is 8.22×10^6 , closer to the right side of (3.52).) Similarly, with the same Δ , W and s , take $h = 3$ so that $L = 8$ and $1 \leq m \leq k/6 \leq 500/6$. For these m and k we find

$$\begin{aligned} \max_{m,k} \left| \prod_{m=1}^{-1} (3/k) T_8(m, 3/k) \right| &\approx 0.133 < 1.4 \times 10^4 \approx (\pi^3/2) c(3) \cdot e^{500W/3}, \\ \max_{m,k} |T_8(m, 3/k)| &\approx 0.005 < 15.5 \approx \pi^3/2. \end{aligned}$$

Since the bounds for $T_L(m, h/k)$ used in the proof of Proposition 3.12 (coming from Lemma 3.10) are independent of h/k , a short verification shows the following generalization of Proposition 3.12, needed in [O'Sa].

Corollary 3.13. *Let W, Δ, s, h, k, m and L be as in Proposition 3.12. Suppose also that $0 < u/v \leq h/k$. Then*

$$\left| \prod_{m=1}^{-1} (h/k) T_L(m, u/v) \right| \leq (\pi^3/2) c(h) \cdot e^{sW/h}, \quad (3.53)$$

$$|T_L(m, u/v)| \leq \pi^3/2. \quad (3.54)$$

Proposition 3.14. *For W, Δ, s, h, k, m and L as in Proposition 3.12 we have*

$$\begin{aligned} \prod_{m=1}^{-1} (h/k) &= \left(\frac{h}{2k \sin(\pi m h/k)} \right)^{1/2} \exp \left(\frac{k}{2\pi h} \text{Cl}_2(2\pi m h/k) \right) \\ &\times \exp \left(- \sum_{\ell=1}^{L-1} \frac{B_{2\ell}}{(2\ell)!} \left(\frac{\pi h}{k} \right)^{2\ell-1} \cot^{(2\ell-2)} \left(\frac{\pi m h}{k} \right) \right) + O(e^{sW/h}) \end{aligned} \quad (3.55)$$

for an implied constant depending only on h .

Proof. With (3.39) we see that (3.55) follows if we can prove

$$\prod_m^{-1}(h/k) = \prod_m^{-1}(h/k) \exp(T_L(m, h/k)) + O\left(e^{sW/h}\right).$$

For any $\kappa > 0$, say, note that the simple inequality

$$|e^x - 1| \leq |x| \frac{e^\kappa - 1}{\kappa} \quad \text{for } x \in (-\infty, \kappa] \quad (3.56)$$

follows from the fact that $(e^x - 1)/x$ is positive and increasing. Then, using Proposition 3.12,

$$\begin{aligned} \left| \prod_m^{-1}(h/k) [\exp(T_L(m, h/k)) - 1] \right| &\leq \left| \prod_m^{-1}(h/k) T_L(m, h/k) \right| \frac{e^{\pi^3/2} - 1}{\pi^3/2} \\ &\leq (e^{\pi^3/2} - 1) c(h) e^{sW/h}. \end{aligned} \quad \square$$

Remark 3.15. The requirement $\Delta s/h \leq m$ in Propositions 3.12 and 3.14 is essential since the bound we are using from Lemma 3.10,

$$|T_L(m, h/k)| \leq \frac{\pi^3}{2} \left(\frac{2L-1}{2\pi em} \right)^{2L-1},$$

worsens dramatically for

$$2L-1 \approx 2\pi e \Delta s/h > 2\pi em.$$

See inequality (3.51).

4 Expressing $\mathcal{A}_1(N, \sigma)$ as an integral

4.1 First results for $\mathcal{A}_1(N, \sigma)$

Rewrite (1.22) more in terms of N/k as

$$\begin{aligned} \mathcal{A}_1(N, \sigma) = \text{Im} \sum_{\frac{N}{2} < k \leq N} \frac{2(-1)^k}{k^2} \exp\left(N \left[\frac{i\pi}{2} \left(-\frac{N}{k} + 3 \right) \right]\right) \\ \times \exp\left(-\frac{i\pi}{2} \frac{N}{k}\right) \exp\left(\frac{1}{N} \left[2i\pi\sigma \frac{N}{k} \right]\right) \prod_{N-k}^{-1}(1/k) \end{aligned} \quad (4.1)$$

and define

$$g_\ell(z) := -\frac{B_{2\ell}}{(2\ell)!} (\pi z)^{2\ell-1} \cot^{(2\ell-2)}(\pi z). \quad (4.2)$$

Theorem 4.1 (Sine product approximation). *Fix $W > 0$. Let Δ be in the range $0.0048 \leq \Delta \leq 0.0079$ and set $\alpha := \Delta\pi e$. Suppose δ and δ' satisfy*

$$\frac{\Delta}{1-\Delta} < \delta \leq \frac{1}{e}, \quad 0 < \delta' \leq \frac{1}{e} \quad \text{and} \quad \delta \log 1/\delta, \quad \delta' \log 1/\delta' \leq W. \quad (4.3)$$

Then for all $N \geq R_\Delta$ we have

$$\prod_{N-k}^{-1}(1/k) = O(e^{WN}) \quad \text{for} \quad \frac{N}{k} \in [1, 1+\delta] \cup [3/2 - \delta', 2] \quad (4.4)$$

and

$$\begin{aligned} \prod_{N-k}^{-1}(1/k) &= \left(\frac{N/k}{2N \sin(\pi(N/k - 1))} \right)^{1/2} \exp\left(\frac{N}{2\pi N/k} \text{Cl}_2(2\pi N/k) \right) \\ &\times \exp\left(\sum_{\ell=1}^{L-1} \frac{g_\ell(N/k)}{N^{2\ell-1}} \right) + O(e^{WN}) \quad \text{for} \quad \frac{N}{k} \in (1+\delta, 3/2 - \delta') \end{aligned} \quad (4.5)$$

with $L = \lfloor \alpha \cdot N \rfloor$. The implied constants in (4.4), (4.5) are absolute.

Proof. The bound (4.4) follows directly from Proposition 3.9 with $m = N - k$ and $h = 1$. Next, in Proposition 3.14, we set $s = N$ and again $m = N - k$ and $h = 1$. The condition $\Delta \log 1/\Delta \leq W$ we need for that result follows from (4.3) since $\Delta < \Delta/(1 - \Delta) < \delta$ and $\Delta \log 1/\Delta$ is increasing. We also see from Table 1 in Section 3.4 that our choice of $\Delta \in [0.0048, 0.0079]$ ensures R_Δ is finite. The condition on m in Proposition 3.14 is equivalent to

$$1 + \frac{\Delta}{1 - \Delta} \leq \frac{N}{k} \leq \frac{3}{2}.$$

So (4.5) follows from Proposition 3.14 if $\Delta/(1 - \Delta) < \delta$, as we assumed. \square

We will later fix some of the parameters in Theorem 4.1:

Corollary 4.2. *Let $W = 0.05$ and $\alpha = 0.006\pi e \approx 0.0512$. Then for all $N \geq 131$ we have that (4.4), (4.5) hold when $L = \lfloor \alpha \cdot N \rfloor$ and*

$$0.0061 \leq \delta, \delta' \leq 0.01. \quad (4.6)$$

It follows from (4.1) and Theorem 4.1 that

$$\begin{aligned} \mathcal{A}_1(N, \sigma) = \text{Im} \sum_{k : \frac{N}{k} \in (1+\delta, \frac{3}{2}-\delta')} \frac{2(-1)^k}{k^2} \exp \left(N \left[\frac{\text{Cl}_2(2\pi N/k)}{2\pi N/k} + \frac{i\pi}{2} \left(-\frac{N}{k} + 3 \right) \right] \right) \\ \times \left(\frac{N/k}{2N \sin(\pi(N/k - 1))} \right)^{1/2} \exp \left(-\frac{i\pi N}{2k} \right) \exp \left(\frac{1}{N} \left[2i\pi\sigma \frac{N}{k} \right] + \sum_{\ell=1}^{L-1} \frac{g_\ell(N/k)}{N^{2\ell-1}} \right) + O(e^{WN}). \end{aligned} \quad (4.7)$$

To describe this concisely we use the notation, with $z \in (1, 2)$ to begin,

$$r(z) := \frac{\text{Cl}_2(2\pi z)}{2\pi z} + \frac{\pi i}{2}(-z + 3), \quad (4.8)$$

$$q(z) := \left(\frac{z}{2 \sin(\pi(z - 1))} \right)^{1/2} \exp(-i\pi z/2), \quad (4.9)$$

$$v(z; N, \sigma) := \frac{2\pi i \sigma z}{N} + \sum_{\ell=1}^{L-1} \frac{g_\ell(z)}{N^{2\ell-1}}, \quad (L = \lfloor \alpha \cdot N \rfloor). \quad (4.10)$$

(If we need to show the dependence of $v(z; N, \sigma)$ on α we may write $v(z; N, \sigma, \alpha)$.) For $z = z(N, k) := N/k$, set

$$\mathcal{A}_2(N, \sigma) := \frac{2}{N^{1/2}} \text{Im} \sum_{k : z \in (1+\delta, \frac{3}{2}-\delta')} \frac{(-1)^k}{k^2} \exp(N \cdot r(z)) q(z) \exp(v(z; N, \sigma))$$

and (4.7) now implies that for $\sigma \in \mathbb{R}$ and an absolute implied constant

$$\mathcal{A}_2(N, \sigma) = \mathcal{A}_1(N, \sigma) + O(e^{WN}). \quad (4.11)$$

We wish to replace the sum defining $\mathcal{A}_2(N, \sigma)$ with an integral. Our goal in the rest of this section is to prove the following, (with $\alpha = 0.006\pi e$ as in Corollary 4.2).

Theorem 4.3. *For $W = 0.05$ and an implied constant depending only on σ , we have*

$$\mathcal{A}_2(N, \sigma) = \frac{2}{N^{3/2}} \text{Im} \int_{1.01}^{1.49} \exp(N[r(z) - \pi i/z]) q(z) \exp(v(z; N, \sigma)) dz + O(e^{WN}).$$

In the next subsections we develop properties of $r(z)$, $q(z)$ and $v(z; N, \sigma)$ considered as functions of $z = x + iy$ in a vertical strip in \mathbb{C} .

4.2 Properties of $v(z; N, \sigma)$ and $q(z)$

Lemma 4.4. *Suppose $\beta, \gamma > 0$ satisfy $\beta\gamma < 1$. Then given any $N, d \geq 1$ we have*

$$\sum_{j=d}^{\lfloor N \cdot \beta \rfloor} \left(\frac{\gamma j}{N} \right)^j = O\left(\frac{1}{N^d} \right)$$

for an implied constant depending only on β, γ and d .

Proof. Note that, as j varies, $(\frac{\gamma j}{N})^j$ decreases for $1 \leq j \leq N/(e\gamma)$ and increases for $j \geq N/(e\gamma)$. Consequently, for $d+1 \leq j \leq \lfloor N \cdot \beta \rfloor$,

$$\begin{aligned} \left(\frac{\gamma j}{N}\right)^j &\leq \max \left\{ \left(\frac{\gamma(d+1)}{N}\right)^{(d+1)}, \left(\frac{\gamma N\beta}{N}\right)^{\lfloor N \cdot \beta \rfloor} \right\} \\ &\ll \max \left\{ N^{-d-1}, (\beta\gamma)^{\lfloor N \cdot \beta \rfloor} \right\} \\ &\ll N^{-d-1} \end{aligned}$$

since $\beta\gamma < 1$ implies $(\beta\gamma)^{\lfloor N \cdot \beta \rfloor}$ decays exponentially with N . Thus

$$\sum_{j=d}^{\lfloor N \cdot \beta \rfloor} \left(\frac{\gamma j}{N}\right)^j \ll \left(\frac{\gamma d}{N}\right)^d + (\lfloor N \cdot \beta \rfloor - d) \frac{1}{N^{d+1}} \ll \frac{1}{N^d}$$

as we wanted. \square

Proposition 4.5. Suppose $1/2 \leq \operatorname{Re}(z) \leq 3/2$ and $|z - 1| \geq \varepsilon > 0$. Also assume that

$$\max \left\{ 1 + \frac{1}{\varepsilon}, 16 \right\} < \frac{\pi e}{\alpha}. \quad (4.12)$$

Then, for an implied constant depending only on ε, α and d ,

$$\sum_{\ell=d}^{L-1} \frac{g_\ell(z)}{N^{2\ell-1}} \ll \frac{1}{N^{2d-1}} e^{-\pi|y|} \quad (d \geq 2, L = \lfloor \alpha \cdot N \rfloor). \quad (4.13)$$

Proof. We have

$$\begin{aligned} \frac{g_\ell(z)}{N^{2\ell-1}} &\ll \frac{|B_{2\ell}|}{(2\ell)!} \left(\frac{\pi|z|}{N}\right)^{2\ell-1} \left| \cot^{(2\ell-2)}(\pi z) \right| \\ &\ll \left(\frac{|z|}{2N}\right)^{2\ell-1} \left| \cot^{(2\ell-2)}(\pi z) \right| \end{aligned}$$

using (3.18). Suppose $\ell \geq 2$ and write $z = 1 + w$. Then (3.15) from Theorem 3.3 and (3.23) show

$$\frac{g_\ell(z)}{N^{2\ell-1}} \ll \left(\frac{|z|(2\ell-1)}{2\pi e N}\right)^{2\ell-1} \left(\frac{1}{|w|^{2\ell-1}} + 8^{2\ell-1}\right) e^{-\pi|y|}. \quad (4.14)$$

Since $|z|/|w| \leq (1 + |w|)/|w| \leq 1 + 1/\varepsilon$ and also $8|z| < 16$ if $|y| \leq 1$, we see that

$$e^{\pi|y|} \sum_{\ell=d}^{L-1} \frac{g_\ell(z)}{N^{2\ell-1}} \ll \sum_{\ell=2d-1}^{2L} \left(\frac{1 + \frac{1}{\varepsilon}}{2\pi e} \frac{\ell}{N}\right)^\ell + \sum_{\ell=2d-1}^{2L} \left(\frac{16}{2\pi e} \frac{\ell}{N}\right)^\ell$$

and the proposition follows in this case with an application of Lemma 4.4, using assumption (4.12). The $|y| \geq 1$ case is similar, employing (3.16) from Theorem 3.3. \square

It is now convenient to fix the choice of constants in Corollary 4.2 for the rest of this section. We note that condition (4.12) in Proposition 4.5 is met for $\varepsilon = 0.0061$ and $\alpha = 0.006\pi e$:

$$\max \left\{ 1 + \frac{1}{\varepsilon}, 16 \right\} \approx \max \{164.9, 16\} = 164.9 < 166.\bar{6} = \frac{\pi e}{\alpha}. \quad (4.15)$$

We have therefore shown the next result.

Corollary 4.6. With $\delta, \delta' \in [0.0061, 0.01]$ and $z \in \mathbb{C}$ such that $1 + \delta \leq \operatorname{Re}(z) \leq 3/2 - \delta'$ we have

$$v(z; N, \sigma) = \frac{2\pi i \sigma z}{N} + \sum_{\ell=1}^{d-1} \frac{g_\ell(z)}{N^{2\ell-1}} + O\left(\frac{1}{N^{2d-1}}\right)$$

for $2 \leq d \leq L = \lfloor 0.006\pi e \cdot N \rfloor$ and an implied constant depending only on d .

Inequality (4.15) holds because the bounds obtained for $g_\ell(z)$ in the above proof of Proposition 4.5 are similar to those obtained for $T_L(m, h/k)$ in Lemma 3.10. In particular, for $z = N/k$ and $m = N - k$, (4.14) implies

$$\frac{g_\ell(N/k)}{N^{2\ell-1}} \ll \left(\frac{2\ell-1}{2\pi em} \right)^{2\ell-1} + \left(\frac{16(2\ell-1)}{2\pi eN} \right)^{2\ell-1}.$$

We see that condition (4.12) is equivalent to

$$\frac{2\ell-1}{2\pi em}, \quad \frac{16(2\ell-1)}{2\pi eN} < 1 \quad (4.16)$$

when $z = N/k$. The requirement $\Delta s/h \leq m$, see Remark 3.15, is in place in Theorem 4.1 with $s = N$ and $h = 1$ so that $\Delta N \leq m$. Hence

$$2L - 1 \approx 2\pi e \Delta N < 2\pi em$$

and

$$\frac{2\ell-1}{2\pi em} < \frac{2L-1}{2\pi em} < 1, \quad \frac{16(2\ell-1)}{2\pi eN} < \frac{16(2L-1)}{2\pi eN} < 16\Delta.$$

Recall that $\Delta \leq 0.0079$ so that $16\Delta < 1$. Therefore $\Delta N \leq m$ and $16\Delta < 1$ imply (4.16) and (4.15).

Proposition 4.7. *The functions $q(z)$ and $v(z; N, \sigma)$ are holomorphic in z for $1 < \operatorname{Re}(z) < 3/2$. In the box with $1 + \delta \leq \operatorname{Re}(z) \leq 3/2 - \delta'$ and $-1 \leq \operatorname{Im}(z) \leq 1$,*

$$q(z), \quad \exp(v(z; N, \sigma)) \ll 1$$

for an implied constant depending only on $\sigma \in \mathbb{R}$.

Proof. Check that for $w \in \mathbb{C}$,

$$-\pi/2 < \arg(\sin(\pi w)) < \pi/2 \quad \text{for } 0 < \operatorname{Re}(w) < 1.$$

Consequently, $-\pi < \arg(z/\sin(\pi(z-1))) < \pi$ for $1 < \operatorname{Re}(z) < 3/2$ and so $q(z)$ is holomorphic in this strip. Also $v_C(z; N, \sigma)$ is holomorphic here since the only poles of $g_\ell(z)$ are at $z \in \mathbb{Z}$.

Finally, $q(z)$ is clearly bounded on the compact box, as is $\exp(v(z; N, \sigma))$ by Corollary 4.6. \square

4.3 Properties of $r(z)$

We defined $r(z)$ in (4.8) for $1 < z < 2$. Use (2.26) to extend it as

$$r(z) = \frac{\operatorname{Li}_2(e^{2\pi iz})}{2\pi iz} + \frac{13\pi i}{12z},$$

now holomorphic in the strip $1 < \operatorname{Re}(z) < 2$. Adding a parameter j , we get

$$r(z) + \frac{\pi i j}{z} = \frac{1}{2\pi iz} \left[-\operatorname{Li}_2(1) + \operatorname{Li}_2(e^{2\pi iz}) - 2\pi^2(j+1) \right]. \quad (4.17)$$

From (2.20) we obtain the identity

$$\frac{\operatorname{Li}_2(e^{2\pi iz})}{2\pi iz} = \frac{-\operatorname{Li}_2(e^{-2\pi iz})}{2\pi iz} - \pi i(z-3) - \frac{13\pi i}{6z} \quad (1 < \operatorname{Re}(z) < 2)$$

and substituting in (4.17) produces the alternate expression, valid only for $1 < \operatorname{Re}(z) < 2$,

$$r(z) + \frac{\pi i j}{z} = -\pi i(z-3) + \frac{1}{2\pi iz} \left[\operatorname{Li}_2(1) - \operatorname{Li}_2(e^{-2\pi iz}) - 2\pi^2(j-1) \right]. \quad (4.18)$$

Lemma 4.8. *Consider $\operatorname{Im}(\operatorname{Li}_2(e^{2\pi iz}))$ as a function of $y \in \mathbb{R}$. It is positive and decreasing for fixed $x \in (0, 1/2)$ and negative and increasing for fixed $x \in (1/2, 1)$.*

Proof. We have

$$\frac{d}{dy} \operatorname{Im}(\operatorname{Li}_2(e^{2\pi iz})) = \operatorname{Im}\left(\frac{d}{dy} \operatorname{Li}_2(e^{2\pi iz})\right) = 2\pi \arg(1 - e^{2\pi iz}).$$

Clearly this derivative is negative for $x \in (0, 1/2)$ and positive for $x \in (1/2, 1)$. Also, we have

$$\lim_{y \rightarrow \infty} \operatorname{Im}(\operatorname{Li}_2(e^{2\pi iz})) = \operatorname{Im}(\operatorname{Li}_2(0)) = 0$$

implying the function decreases or increases to zero. \square

Lemma 4.9. For $y \geq 0$ we have $|\operatorname{Li}_2(e^{2\pi iz})| \leq \operatorname{Li}_2(1)$.

Proof. With $y \geq 0$ we have $|e^{2\pi iz}| \leq 1$ and

$$|\operatorname{Li}_2(e^{2\pi iz})| = \left| \sum_{m=1}^{\infty} \frac{e^{2\pi imz}}{m^2} \right| \leq \sum_{m=1}^{\infty} \frac{1}{m^2} = \operatorname{Li}_2(1). \quad \square$$

Theorem 4.10. The function $r(z)$ is holomorphic for $1 < \operatorname{Re}(z) < 3/2$. In this strip, for $j \in \mathbb{R}$,

$$\operatorname{Re}\left(r(z) + \frac{\pi ij}{z}\right) \leq \frac{1}{2\pi|z|^2} \left(x \operatorname{Cl}_2(2\pi x) + \pi^2|y| \left[\frac{1}{3} + 2(j+1) \right] \right) \quad (y \geq 0) \quad (4.19)$$

$$\operatorname{Re}\left(r(z) + \frac{\pi ij}{z}\right) \leq \frac{1}{2\pi|z|^2} \left(x \operatorname{Cl}_2(2\pi x) + \pi^2|y| \left[\frac{1}{3} - 2j \right] \right) \quad (y \leq 0). \quad (4.20)$$

Proof. With (4.17), we see that $r(z)$ is actually holomorphic for all $z \in \mathbb{C}$ away from the vertical branch cuts $(-i\infty, n]$, $n \in \mathbb{Z}$. Let $z = x + iy$. Equation (4.17) implies

$$\operatorname{Re}\left(r(z) + \frac{\pi ij}{z}\right) = y \left(\frac{\operatorname{Li}_2(1) - \operatorname{Re}(\operatorname{Li}_2(e^{2\pi iz})) + 2\pi^2(j+1)}{2\pi|z|^2} \right) + \frac{x \operatorname{Im}(\operatorname{Li}_2(e^{2\pi iz}))}{2\pi|z|^2}. \quad (4.21)$$

For $y \geq 0$ we have

$$\operatorname{Im}(\operatorname{Li}_2(e^{2\pi iz})) \leq \operatorname{Im}(\operatorname{Li}_2(e^{2\pi ix})) = \operatorname{Cl}_2(2\pi x) \quad (4.22)$$

by Lemma 4.8. Also, using Lemma 4.9,

$$\begin{aligned} \operatorname{Li}_2(1) - \operatorname{Re}(\operatorname{Li}_2(e^{2\pi iz})) + 2\pi^2(j+1) &\leq 2\operatorname{Li}_2(1) + 2\pi^2(j+1) \\ &= \pi^2[1/3 + 2(j+1)] \end{aligned} \quad (4.23)$$

and (4.19) follows from (4.21), (4.22) and (4.23).

Equation (4.18) implies

$$\operatorname{Re}\left(r(z) + \frac{\pi ij}{z}\right) = \pi y - y \left(\frac{\operatorname{Li}_2(1) - \operatorname{Re}(\operatorname{Li}_2(e^{-2\pi iz})) - 2\pi^2(j-1)}{2\pi|z|^2} \right) - \frac{x \operatorname{Im}(\operatorname{Li}_2(e^{-2\pi iz}))}{2\pi|z|^2}. \quad (4.24)$$

For $y \leq 0$ we have

$$-x \operatorname{Im}(\operatorname{Li}_2(e^{-2\pi iz})) \leq -x \operatorname{Im}(\operatorname{Li}_2(e^{-2\pi ix})) = -x \operatorname{Cl}_2(-2\pi x) = x \operatorname{Cl}_2(2\pi x) \quad (4.25)$$

by Lemma 4.8. Then Lemma 4.9 shows

$$\begin{aligned} \operatorname{Li}_2(1) - \operatorname{Re}(\operatorname{Li}_2(e^{-2\pi iz})) - 2\pi^2(j-1) &\leq 2\operatorname{Li}_2(1) - 2\pi^2(j-1) \\ &= \pi^2[1/3 - 2(j-1)] \end{aligned} \quad (4.26)$$

and writing

$$\pi y = -\pi|y| = \frac{\pi^2|y| \cdot (-2)|z|^2}{2\pi|z|^2} \leq \frac{1}{2\pi|z|^2} \pi^2|y|(-2) \quad (4.27)$$

we see that (4.20) follows from (4.24) - (4.27). \square

4.4 Contour integrals

Recall that $1/(2i \sin(\pi z))$ has poles exactly at $z = m \in \mathbb{Z}$. Each such pole is simple with residue $(-1)^m/(2\pi i)$. By the calculus of residues, see for example [Olv74, p. 300],

$$\sum_{k=a}^b (-1)^k \varphi(k) = \int_C \frac{\varphi(z)}{2i \sin(\pi z)} dz \quad (4.28)$$

for $\varphi(z)$ a holomorphic function and C a positively oriented closed contour surrounding the interval $[a, b]$ and not surrounding any integers outside this interval. Next, let $a, b \in \mathbb{Z}$ so that $0 < a < b$. With a change of variables in (4.28) we obtain

$$\sum_{k=a}^b \frac{(-1)^k}{k^2} \varphi(N/k) = -\frac{1}{N} \int_C \frac{\varphi(z)}{2i \sin(\pi N/z)} dz \quad (4.29)$$

for C now surrounding $\{N/k \mid a \leq k \leq b\}$.

With (4.29), we have

$$\mathcal{A}_2(N, \sigma) = -\frac{2}{N^{3/2}} \operatorname{Im} \int_C \exp(N \cdot r(z)) \frac{q(z)}{2i \sin(\pi N/z)} \exp(v(z; N, \sigma)) dz \quad (4.30)$$

where we may take C to be a positively oriented rectangle with left and right vertical sides

$$C_L := \{1 + \delta + iy : |y| \leq 1/N^2\}, \quad C_R := \{3/2 - \delta' + iy : |y| \leq 1/N^2\}$$

and with corresponding horizontal sides C^+ , C^- with imaginary parts $1/N^2$ and $-1/N^2$, respectively as shown in Figure 4. Recall that we have some flexibility with δ, δ' and are free to choose them in $[0.0061, 0.01]$.

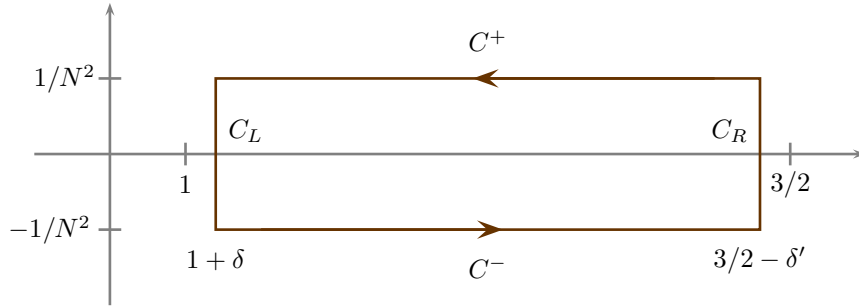


Figure 4: The rectangle $C = C^+ \cup C_L \cup C^- \cup C_R$

So that the path of integration in (4.30) passes midway between the poles of $1/\sin(\pi N/z)$, we require

$$1 + \delta = \frac{N}{b + 1/2}, \quad 3/2 - \delta' = \frac{N}{a - 1/2} \quad \text{for } a, b \in \mathbb{Z}, \quad \delta, \delta' \in [0.0061, 0.01]. \quad (4.31)$$

The relation in (4.31) implies

$$\frac{d\delta}{db} = -\frac{N}{(b + 1/2)^2} = -\frac{(1 + \delta)^2}{N}$$

so that changing b by 1 corresponds to changing δ by $\approx 1/N$. Similarly for a and δ' . Thus, by adjusting δ and δ' , we can ensure that (4.31) is true for N sufficiently large.

Proposition 4.11. *With δ, δ' chosen as in (4.31) we have*

$$\mathcal{A}_2(N, \sigma) = -\frac{2}{N^{3/2}} \operatorname{Im} \int_{C^+ \cup C^-} \exp(N \cdot r(z)) \frac{q(z)}{2i \sin(\pi N/z)} \exp(v(z; N, \sigma)) dz + O(e^{WN})$$

for $W = 0.05$ and an implied constant depending only on σ .

Proof. The proposition follows from (4.30) if we can show $\int_{C_L \cup C_R} = O(e^{WN})$. Note that for z on the left vertical side we have $|\pi N/z - \pi(b + 1/2)| < 1/N$ and similarly on the right vertical side. Since $|\sin(\pi(b + 1/2))| = 1$ it follows that for large N

$$\frac{1}{2i \sin(\pi N/z)} \ll 1 \quad (z \in C_L \cup C_R). \quad (4.32)$$

Proposition 4.7 implies

$$q(z) \exp(v(z; N, \sigma)) \ll 1 \quad (z \in C_L \cup C_R). \quad (4.33)$$

Theorem 4.10 with $j = 0$ implies

$$\operatorname{Re}(r(z)) < \frac{1}{2\pi} \left(x \operatorname{Cl}_2(2\pi x) + \frac{3\pi^2}{N^2} \right) \quad (z \in C_L \cup C_R)$$

and we have, using Lemma 3.7 for example,

$$\operatorname{Cl}_2(2\pi x) < 0.24 \quad \text{if } 1 \leq x \leq 1.01, \quad \operatorname{Cl}_2(2\pi x) < 0.05 \quad \text{if } 1.49 \leq x \leq 1.5. \quad (4.34)$$

Therefore

$$\operatorname{Re}(r(z)) < \frac{1}{2\pi} \left(1.01 \times 0.24 + \frac{3\pi^2}{N^2} \right) < 0.05 \quad (z \in C_L, N \geq 25). \quad (4.35)$$

We obtain (4.35) for $z \in C_R$ in the same way. Consequently

$$\exp(N \cdot r(z)) \ll \exp(0.05N) \quad (z \in C_L \cup C_R). \quad (4.36)$$

The proposition now follows from the bounds (4.32), (4.33) and (4.36). \square

We note for future reference that

$$x \operatorname{Cl}_2(2\pi x)/(2\pi) < 0.04 \quad (x \in [1, 1.01] \cup [1.49, 1.5]). \quad (4.37)$$

4.5 Integrating over C^+ and C^-

For the integral $\int_{C^+ \cup C^-}$ in Proposition 4.11, we consider separately \int_{C^+} and \int_{C^-} . Now

$$\frac{1}{2i \sin(\pi N/z)} = \frac{e^{-\pi i N/z}}{1 - e^{-2\pi i N/z}} = \sum_{j < 0, \text{ odd}} e^{\pi i j N/z} \quad (\operatorname{Im}(z) > 0) \quad (4.38)$$

so that

$$\int_{C^+} = \sum_{j < 0, \text{ odd}} \int_{C^+} \exp(N[r(z) + \pi i j/z]) q(z) \exp(v(z; N, \sigma)) dz. \quad (4.39)$$

Similarly,

$$\frac{1}{2i \sin(\pi N/z)} = \frac{e^{\pi i N/z}}{e^{2\pi i N/z} - 1} = - \sum_{j > 0, \text{ odd}} e^{\pi i j N/z} \quad (\operatorname{Im}(z) < 0)$$

and

$$\int_{C^-} = - \sum_{j > 0, \text{ odd}} \int_{C^-} \exp(N[r(z) + \pi i j/z]) q(z) \exp(v(z; N, \sigma)) dz. \quad (4.40)$$

The contributions to (4.39), (4.40) when $|j| > N^2$ are next shown to be negligible.

Lemma 4.12. For $N \geq 2$ and $m \geq 0$,

$$\operatorname{Re} \left(r(z) + \frac{\pi i(-N^2 - 1 - m)}{z} \right) \leq -\frac{m}{N^2} \quad (z \in C^+) \quad (4.41)$$

$$\operatorname{Re} \left(r(z) + \frac{\pi i(N^2 + 1 + m)}{z} \right) \leq -\frac{m}{N^2} \quad (z \in C^-). \quad (4.42)$$

Proof. With $z \in C^+$ and $j = -N^2 - 1 - m$, Theorem 4.10 implies

$$\operatorname{Re} \left(r(z) + \frac{\pi i(-N^2 - 1 - m)}{z} \right) \leq \frac{1}{2\pi|z|^2} \left(x \operatorname{Cl}_2(2\pi x) + \frac{\pi^2}{N^2} \left[\frac{1}{3} - 2N^2 - 2m \right] \right). \quad (4.43)$$

Since $1 < |z|^2 < 3$ and $x \operatorname{Cl}_2(2\pi x) \leq 3 \operatorname{Cl}_2(\pi/3)/2$, we see that (4.43) implies (4.41). The proof of (4.42) is similar. \square

With Proposition 4.7 and (4.41) it follows that

$$\begin{aligned} \sum_{j < -N^2, \text{ odd}} \int_{C^+} \exp(N[r(z) + \pi i j/z]) q(z) \exp(v(z; N, \sigma)) dz \\ \ll \sum_{j < -N^2} \int_{C^+} \exp(N \operatorname{Re}[r(z) + \pi i j/z]) dz \ll \sum_{m \geq 0} \int_{C^+} \exp(N(-m/N^2)) dz \end{aligned}$$

and this last is bounded by

$$\sum_{m \geq 0} e^{-m/N} = \frac{1}{1 - e^{-1/N}} = O(N).$$

The same is true for $j > N^2$ on C^- and therefore the total contribution to (4.39) and (4.40) from terms with $|j| > N^2$ is $O(N)$.

Proof of Theorem 4.3. With Proposition 4.11 and the above arguments we have shown

$$\begin{aligned} \mathcal{A}_2(N, \sigma) = -\frac{2}{N^{3/2}} \operatorname{Im} \left[\sum_{-N^2 \leq j < 0, j \text{ odd}} \int_{C^+} \exp(N[r(z) + \pi i j/z]) q(z) \exp(v(z; N, \sigma)) dz \right. \\ \left. - \sum_{0 < j \leq N^2, j \text{ odd}} \int_{C^-} \exp(N[r(z) + \pi i j/z]) q(z) \exp(v(z; N, \sigma)) dz \right] + O(e^{WN}). \quad (4.44) \end{aligned}$$

We claim that all terms in (4.44) are $O(e^{0.04N})$ except the $j = -1$ term.

Let D^+ be the three lines which, when added to C^+ , make a rectangle with top side having imaginary part 1. Orient D^+ so that it has the same starting and ending points as C^+ . Since the integrand in (4.44) is holomorphic here we see that $\int_{C^+} = \int_{D^+}$. We have $q(z) \exp(v(z; N, \sigma)) \ll 1$ for $z \in D^+$ by Proposition 4.7. On the vertical sides of D^+ we have

$$\operatorname{Re} \left(r(z) + \frac{\pi i j}{z} \right) < \frac{x \operatorname{Cl}_2(2\pi x)}{2\pi} < 0.04$$

by Theorem 4.10 and (4.37) if $j < -1$. On the horizontal side of D^+ , with $y = 1$, Theorem 4.10 implies

$$\operatorname{Re} \left(r(z) + \frac{\pi i j}{z} \right) \leq \frac{1}{2\pi|z|^2} \left(\frac{3 \operatorname{Cl}_2(\pi/3)}{2} + \pi^2 \left[\frac{1}{3} + 2(j+1) \right] \right) < 0$$

if $j < -1$. Hence, for each integer j with $-N^2 \leq j < -1$, the integral in (4.44) over C^+ is $O(e^{0.04N})$. We will see later that the integral with $j = -1$ cannot be bounded by $O(e^{0.04N})$.

Similarly, the integral in (4.44) over C^- is $O(e^{0.04N})$, this time for all odd j with $0 < j \leq N^2$. Hence

$$\mathcal{A}_2(N, \sigma) = -\frac{2}{N^{3/2}} \operatorname{Im} \int_{C^+} \exp(N[r(z) + \pi i(-1)/z]) q(z) \exp(v(z; N, \sigma)) dz + O(e^{WN}).$$

We may change the path of integration from C^+ to $[1.01, 1.49]$. By (4.33), (4.36) this introduces an error of size $O(e^{WN})$. \square

5 Asymptotics for $\mathcal{A}_1(N, \sigma)$

5.1 The saddle-point method

Define

$$p(z) := -\left(r(z) - \frac{\pi i}{z}\right) = \frac{\text{Li}_2(1) - \text{Li}_2(e^{2\pi i z})}{2\pi i z}, \quad (5.1)$$

$$\mathcal{A}_3(N, \sigma) := \frac{2}{N^{3/2}} \text{Im} \int_{1.01}^{1.49} e^{-N \cdot p(z)} q(z) \cdot \exp(v(z; N, \sigma)) dz. \quad (5.2)$$

Then $p(z)$ is the $d = 0$ case of the function $p_d(z)$ we met earlier in (2.29). We have established with (4.11) and Theorem 4.3 that, for $W = 0.05$,

$$\mathcal{A}_1(N, \sigma) = \mathcal{A}_3(N, \sigma) + O(e^{WN}). \quad (5.3)$$

The form of (5.2) allows us to find its asymptotic expansion by the saddle-point method. We state a simpler version of [Olv74, Theorem 7.1, p. 127] that is all we need:

Theorem 5.1 (Saddle-point method). *Let \mathcal{P} be a finite polygonal path in \mathbb{C} with $p(z)$, $q(z)$ holomorphic functions in a neighborhood of \mathcal{P} . Assume p , q and \mathcal{P} are independent of a parameter $N > 0$. Suppose $p'(z)$ has a simple zero at a non-corner point $z_0 \in \mathcal{P}$ with $\text{Re}(p(z) - p(z_0)) > 0$ for $z \in \mathcal{P}$ except at $z = z_0$. Then there exist explicit numbers a_{2s} depending on p , q , z_0 and \mathcal{P} so that we have*

$$\int_{\mathcal{P}} e^{-N \cdot p(z)} q(z) dz = 2e^{-N \cdot p(z_0)} \left(\sum_{s=0}^{S-1} \Gamma(s+1/2) \frac{a_{2s}}{N^{s+1/2}} + O\left(\frac{1}{N^{S+1/2}}\right) \right) \quad (5.4)$$

for S an arbitrary positive integer and an implied constant independent of N .

We need to set up some notation to describe the numbers a_{2s} . Write the power series for p and q near z_0 as

$$p(z) = p(z_0) + p_0(z - z_0)^2 + p_1(z - z_0)^3 + \dots, \quad (5.5)$$

$$q(z) = q_0 + q_1(z - z_0) + q_2(z - z_0)^2 + \dots. \quad (5.6)$$

(We have $p_0 \neq 0$ by our assumption that $p'(z)$ has a simple zero at z_0 . For simplicity we also assume that $q_0 \neq 0$. This corresponds to the case $(\mu, \lambda) = (2, 1)$ in [Olv74] and the case $(\mu, \alpha) = (2, 1)$ in [Woj06].) Choose $\omega \in \mathbb{C}$ giving the direction of the path \mathcal{P} through z_0 : near z_0 , \mathcal{P} looks like $z = z_0 + \omega t$ for small $t \in \mathbb{R}$ increasing. Note that the condition $\text{Re}(p(z) - p(z_0)) > 0$ implies $\text{Re}(\omega^2 p_0) > 0$.

We also need the *partial ordinary Bell polynomials*, see [Com74, p. 136], defined as

$$\hat{B}_{i,j}(p_1, p_2, p_3, \dots) := \sum_{\substack{1\ell_1+2\ell_2+3\ell_3+\dots=i \\ \ell_1+\ell_2+\ell_3+\dots=j}} \frac{j!}{\ell_1! \ell_2! \ell_3! \dots} p_1^{\ell_1} p_2^{\ell_2} p_3^{\ell_3} \dots \quad (5.7)$$

where the sum is over all possible $\ell_1, \ell_2, \ell_3, \dots \in \mathbb{Z}_{\geq 0}$. They satisfy, for example,

$$(p_1 x + p_2 x^2 + \dots)^j = \sum_{i=j}^{\infty} \hat{B}_{i,j}(p_1, p_2, \dots) x^i \quad (5.8)$$

and are related to the usual partial Bell polynomials by $\hat{B}_{i,j}(p_1, p_2, \dots) = j! B_{i,j}(1!p_1, 2!p_2, \dots)/i!$. The numbers a_{2s} in Theorem 5.1 may be found by complicated manipulations of the series (5.5) and (5.6), see [Olv74, pp. 85-86, 121-127]. Wojdylo in [Woj06, Theorem 1.1] found an explicit formula for them. Adapted to the saddle-point method, a special case of his result is

$$a_{2s} = \frac{\omega}{2(\omega^2 p_0)^{1/2}} \sum_{i=0}^{2s} q_{2s-i} \sum_{j=0}^i p_0^{-s-j} \binom{-s-1/2}{j} \hat{B}_{i,j}(p_1, p_2, \dots) \quad (5.9)$$

where we must choose the square root $(\omega^2 p_0)^{1/2}$ in (5.9) so that $\operatorname{Re}((\omega^2 p_0)^{1/2}) > 0$. Note that

$$\frac{\omega}{(\omega^2 p_0)^{1/2}} = \pm \frac{1}{(p_0)^{1/2}},$$

so we see that the dependence of each a_{2s} on the path \mathcal{P} just involves a sign, corresponding to the direction of the path through the saddle-point. The first cases are

$$a_0 = \frac{\omega}{2(\omega^2 p_0)^{1/2}} q_0, \quad a_2 = \frac{\omega}{2(\omega^2 p_0)^{1/2}} \left(\frac{q_2}{p_0} - \frac{3}{2} \frac{p_1 q_1 + p_2 q_0}{p_0^2} + \frac{15}{8} \frac{p_1^2 q_0}{p_0^3} \right), \quad (5.10)$$

agreeing with [Olv74, p. 127]. For \mathcal{P} , p and z_0 fixed and q possibly varying in (5.4) we write $a_{2s}(q)$ in what follows.

5.2 A path through the saddle-point

To apply Theorem 5.1 to $\mathcal{A}_3(N, \sigma)$ in (5.2), we need to find the saddle-point for $p(z)$. By Theorem 2.4, the unique solution to $p'(z) = 0$ for $1/2 < \operatorname{Re}(z) < 3/2$ is given by the z_0 we met earlier in (1.5).

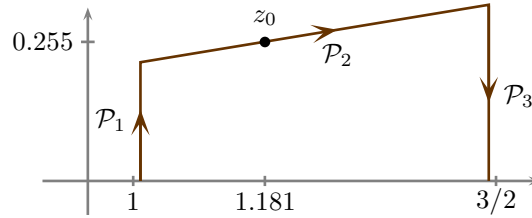


Figure 5: The path $\mathcal{P} = \mathcal{P}_1 \cup \mathcal{P}_2 \cup \mathcal{P}_3$ through z_0

Now we replace the path $[1.01, 1.49]$ in (5.2) with a path through z_0 . We noted in Section 2.3 that z_0 may be found to arbitrary precision, and later we will set the parameter v to be

$$v = \operatorname{Im}(z_0)/\operatorname{Re}(z_0) \approx 0.216279, \quad (5.11)$$

but we only require for the results below that $0.21 \leq v \leq 0.22$.

Write $c := 1 + iv$. Let \mathcal{P}_1 be the vertical path from 1.01 to $1.01c$, \mathcal{P}_2 the line from $1.01c$ to $1.49c$:

$$\mathcal{P}_2 = \{ct \mid 1.01 \leq t \leq 1.49\}, \quad (5.12)$$

and let \mathcal{P}_3 be the vertical path from $1.49c$ to 1.49 . So the path $\mathcal{P} := \mathcal{P}_1 \cup \mathcal{P}_2 \cup \mathcal{P}_3$ goes from 1.01 to 1.49 and when v is given by (5.11) it passes through z_0 as in Figure 5. Our goal in this subsection is to prove the following.

Theorem 5.2. *For the path \mathcal{P} above, passing through the saddle point z_0 , we have $\operatorname{Re}(p(z) - p(z_0)) > 0$ for $z \in \mathcal{P}$ except at $z = z_0$.*

This is exactly the requirement of Theorem 5.1 and it seems apparent from Figure 6. We prove Theorem 5.2 by approximating $\operatorname{Re}(p(z))$ and its derivatives by the first terms in their series expansions and reducing the issue to a finite computation. The path \mathcal{P} is chosen to make this argument easier and does not use the line of steepest descent.

Generalizing to $p_d(z)$, we examine $\operatorname{Re}(p_d(z))$ for z on the ray $z = ct$ for $c = 1 + iv$ with $v > 0$. We also write

$$c = \rho e^{i\theta} \quad (0 < \rho, 0 < \theta < \pi/2).$$

Then, using (2.16) since $|e^{2\pi iz}| \leq 1$ when $\operatorname{Im}(z) \geq 0$,

$$\begin{aligned} \operatorname{Re}[p_d(ct)] &= \operatorname{Re} \left[\frac{-i(\operatorname{Li}_2(1) + 4\pi^2 d)e^{-i\theta}}{2\pi \rho t} + \frac{ie^{-i\theta}}{2\pi \rho t} \sum_{m=1}^{\infty} \frac{e^{-2\pi mvt} e^{2\pi imt}}{m^2} \right] \\ &= \frac{1}{2t} \left(\frac{-\pi(24d+1)\sin\theta}{6\rho} - \frac{1}{\pi\rho} \sum_{m=1}^{\infty} \frac{e^{-2\pi mvt} \sin(2\pi mt - \theta)}{m^2} \right). \end{aligned} \quad (5.13)$$

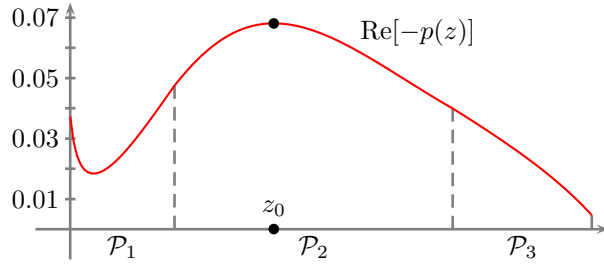


Figure 6: Graph of $\text{Re}[-p(z)]$ for $z \in \mathcal{P}$

Similarly, employing (2.32), (2.33)

$$\frac{d}{dt}\text{Re}[p_d(ct)] = \text{Re}[cp'_d(ct)] = -\frac{1}{t} \left(\text{Re}[p_d(ct)] + \sum_{m=1}^{\infty} \frac{e^{-2\pi mvt} \cos(2\pi mt)}{m} \right) \quad (5.14)$$

$$\frac{d^2}{dt^2}\text{Re}[p_d(ct)] = \text{Re}[c^2 p''_d(ct)] = -\frac{2}{t} \left(\text{Re}[cp'_d(ct)] - \pi\rho \sum_{m=1}^{\infty} e^{-2\pi mvt} \sin(2\pi mt + \theta) \right). \quad (5.15)$$

We may bound the tails of these series:

$$\left| \sum_{m=L}^{\infty} \frac{e^{-2\pi mvt}}{m^k} \right| \leq \frac{e^{-2L\pi vt}}{L^k(1 - e^{-2\pi vt})}.$$

Collecting the first $L - 1$ terms in (5.13), (5.14) and (5.15) we obtain

$$\frac{d^2}{dt^2}\text{Re}[p_d(ct)] = R_2(L; t) + R_2^*(L; t)$$

(with the subscript 2 indicating the second derivative) for

$$\begin{aligned} R_2(L; t) &:= -\frac{\pi(24d+1)\sin\theta}{6\rho t^3} + \sum_{m=1}^{L-1} \left(A_m(t) \cos(2\pi mt) + B_m(t) \sin(2\pi mt) \right), \\ A_m(t) &:= e^{-2\pi mvt} \left(\frac{2}{mt^2} + \sin\theta \left(\frac{2\pi\rho}{t} + \frac{1}{m^2\pi\rho t^3} \right) \right), \\ B_m(t) &:= e^{-2\pi mvt} \cos\theta \left(\frac{2\pi\rho}{t} - \frac{1}{m^2\pi\rho t^3} \right) \end{aligned}$$

and

$$|R_2^*(L; t)| \leq E_2(L; t) := \frac{e^{-2\pi Lvt}}{1 - e^{-2\pi vt}} \left(\frac{1}{\pi\rho L^2 t^3} + \frac{2}{L t^2} + \frac{2\pi\rho}{t} \right).$$

We see that $E_2(L; t)$ is a decreasing function of L and t . We have $A_m(t)$ a positive and decreasing function of t . Also $B_m(t)$ is a positive and decreasing function of t when $t > \frac{\sqrt{3}}{\sqrt{2\pi\rho m}}$.

Let $v_1 = 0.21$ and $v_2 = 0.22$. Writing $\rho_1 e^{i\theta_1} = 1 + iv_1$ and $\rho_2 e^{i\theta_2} = 1 + iv_2$ we have

$$1 < \rho_1 \leq \rho \leq \rho_2, \quad 0 < \theta_1 \leq \theta \leq \theta_2 < \pi/2.$$

For v in the interval $[v_1, v_2]$, we may bound $A_m(t)$, $B_m(t)$ and $E_2(L; t)$ from above and below by replacing v, ρ and θ appropriately by v_j, ρ_j and $\theta_j, j = 1, 2$. For example

$$0 < A_m^-(t) \leq A_m(t) \leq A_m^+(t) \quad (v \in [v_1, v_2])$$

with

$$\begin{aligned} A_m^-(t) &:= e^{-2\pi m v_2 t} \left(\frac{2}{mt^2} + \sin\theta_1 \left(\frac{2\pi\rho_1}{t} + \frac{1}{m^2\pi\rho_2 t^3} \right) \right), \\ A_m^+(t) &:= e^{-2\pi m v_1 t} \left(\frac{2}{mt^2} + \sin\theta_2 \left(\frac{2\pi\rho_2}{t} + \frac{1}{m^2\pi\rho_1 t^3} \right) \right) \end{aligned}$$

and similarly write $0 < B_m^-(t) \leq B_m(t) \leq B_m^+(t)$ and $0 < E_2^-(L; t) \leq E_2(L; t) \leq E_2^+(L; t)$.

Lemma 5.3. Let $c = 1 + iv$ with $0.21 \leq v \leq 0.22$. Then $\frac{d^2}{dt^2} \operatorname{Re}[p(ct)] > 0$ for $t \in [1, 5/4]$.

Proof. Break up $[1, 5/4]$ into n equal segments $[x_{j-1}, x_j]$. Then

$$\frac{d^2}{dt^2} \operatorname{Re}[p(ct)] \geq \min_{1 \leq j \leq n} \left(\left(\min_{t \in [x_{j-1}, x_j]} R_2(L; t) \right) - E_2^+(L; x_{j-1}) \right). \quad (5.16)$$

Let $t = x_{j,m}^*$ correspond to the minimum value of $\cos(2\pi mt)$ for $t \in [x_{j-1}, x_j]$ (so that $x_{j,m}^*$ equals x_{j-1} , x_j or a local minimum $k/2m$ for k odd). Similarly, let $t = x_{j,m}^{**}$ correspond to the minimum value of $\sin(2\pi mt)$ for $t \in [x_{j-1}, x_j]$. Then

$$\min_{t \in [x_{j-1}, x_j]} R_2(L; t) \geq -\frac{\pi \sin \theta_2}{6\rho_1 x_{j-1}^3} + \sum_{m=1}^{L-1} \left(A_m^-(x_j) \cos(2\pi m x_{j,m}^*) + B_m^-(x_j) \sin(2\pi m x_{j,m}^{**}) \right) \quad (5.17)$$

where we must replace $A_m^-(x_j)$ in (5.17) by $A_m^+(x_{j-1})$ if $\cos(2\pi m x_{j,m}^*) < 0$ and replace $B_m^-(x_j)$ in (5.17) by $B_m^+(x_{j-1})$ if $\sin(2\pi m x_{j,m}^{**}) < 0$.

A computation using (5.16) and (5.17) with $L = 3$ and $n = 2$ for example shows $\frac{d^2}{dt^2} \operatorname{Re}[p(ct)] > 0.12$. \square

We may analyze the first derivative in a similar way. We have

$$\frac{d}{dt} \operatorname{Re}[p_d(ct)] = R_1(L; t) + R_1^*(L; t)$$

for

$$R_1(L; t) := \frac{\pi(24d+1) \sin \theta}{12\rho t^2} + \sum_{m=1}^{L-1} \left(-C_m(t) \cos(2\pi mt) + D_m(t) \sin(2\pi mt) \right),$$

$$C_m(t) := e^{-2\pi mvt} \left(\frac{1}{mt} + \frac{\sin \theta}{m^2 2\pi \rho t^2} \right), \quad D_m(t) := e^{-2\pi mvt} \frac{\cos \theta}{m^2 2\pi \rho t^2}$$

and

$$|R_1^*(L; t)| \leq E_1(L; t) := \frac{e^{-2\pi Lvt}}{1 - e^{-2\pi vt}} \left(\frac{1}{2\pi \rho L^2 t^2} + \frac{1}{Lt} \right).$$

We see that $E_1(L; t)$ is a decreasing function of L and t . Also $C_m(t)$ and $D_m(t)$ are positive and decreasing functions of t .

Lemma 5.4. Let $c = 1 + iv$ with $0.21 \leq v \leq 0.22$. Then $\frac{d}{dt} \operatorname{Re}[p(ct)] > 0$ for $t \in [5/4, 3/2]$.

Proof. Break $[5/4, 3/2]$ into n equal segments and, as in the proof of Lemma 5.3, bound $\frac{d}{dt} \operatorname{Re}[p(ct)]$ from below on each piece. Taking $n = 2$ and $L = 3$ shows $\frac{d}{dt} \operatorname{Re}[p(ct)] > 0.03$ for example. \square

Corollary 5.5. Let $c = 1 + iv$ with $0.21 \leq v \leq 0.22$. There is a unique solution to $\frac{d}{dt} \operatorname{Re}[p(ct)] = 0$ for $t \in [1, 3/2]$ that we label as t_0 . We then have $\operatorname{Re}[p(ct) - p(ct_0)] > 0$ for $t \in [1, 3/2]$ except at $t = t_0$.

Proof. Check that $\frac{d}{dt} \operatorname{Re}[p(ct)] < 0$ when $t = 1$ and $\frac{d}{dt} \operatorname{Re}[p(ct)] > 0$ when $t = 5/4$. By Lemma 5.3 we see that $\frac{d}{dt} \operatorname{Re}[p(ct)]$ is strictly increasing for $t \in [1, 5/4]$. It necessarily has a unique zero that we label t_0 . By Lemma 5.4, $\frac{d}{dt} \operatorname{Re}[p(ct)]$ remains > 0 for $t \in [5/4, 3/2]$. Hence $\operatorname{Re}[p(ct) - p(ct_0)]$ is strictly decreasing on $[1, t_0)$ and strictly increasing on $(t_0, 3/2]$ as required. \square

Before the proof of Theorem 5.2, we need a result similar to Lemma 4.8 to let us find bounds on $\mathcal{P}_1 \cup \mathcal{P}_3$.

Lemma 5.6. Consider $\operatorname{Re}(\operatorname{Li}_2(e^{2\pi iz}))$ as a function of $y \geq 0$. It is positive and decreasing for fixed x with $|x| \leq 1/6$. It is negative and increasing for fixed x with $1/4 \leq |x| \leq 3/4$.

Proof. We have

$$\frac{d}{dy} \operatorname{Re}(\operatorname{Li}_2(e^{2\pi iz})) = \operatorname{Im}(2\pi i \log(1 - e^{2\pi iz})) = 2\pi \log|1 - e^{2\pi iz}|. \quad (5.18)$$

Noting that

$$\begin{aligned} |1 - e^{2\pi iz}| &\leq 1 & (|x| \leq 1/6, y \geq 0), \\ 1 &\leq |1 - e^{2\pi iz}| \leq 2 & (1/4 \leq |x| \leq 3/4, y \geq 0) \end{aligned}$$

shows that the derivative (5.18) is negative for $|x| \leq 1/6$ and positive for $1/4 \leq |x| \leq 3/4$. Also, we have

$$\lim_{y \rightarrow \infty} \operatorname{Re}(\operatorname{Li}_2(e^{2\pi iz})) = \operatorname{Re}(\operatorname{Li}_2(0)) = 0$$

implying the function decreases or increases to zero. \square

Proposition 5.7. For $0.21 \leq v \leq 0.22$ we have $\operatorname{Re}[-p(z)] < 0.06$ for $z \in \mathcal{P}_1 \cup \mathcal{P}_3$.

Proof. We have x fixed as 1.01 on \mathcal{P}_1 and 1.49 on \mathcal{P}_3 . By (4.21) we know

$$\operatorname{Re}[-p(z)] = \frac{f(y) + g(y)}{2\pi|z|^2}$$

for

$$f(y) := y(\operatorname{Li}_2(1) - \operatorname{Re}(\operatorname{Li}_2(e^{2\pi iz}))), \quad g(y) = x \operatorname{Im}(\operatorname{Li}_2(e^{2\pi iz})).$$

If $x = 1.01$ or 1.49 it follows from Lemma 4.8 that $g(y)$ is positive and decreasing. We claim that, for these x values, $f(y)$ is always positive and increasing for $y > 0$.

For $x = 1.01$, Lemma 5.6 tells us that $\operatorname{Re}(\operatorname{Li}_2(e^{2\pi i(x+iy)}))$ is a decreasing function of y . Recalling (2.22), we see it decreases from $\pi^2 B_2(0.01) < \pi^2/6$. Therefore $f(y)$ is positive and increasing for $x = 1.01$.

Next let $x = 1.49$. We have

$$\frac{d}{dy} f(y) = \operatorname{Li}_2(1) - \operatorname{Re}(\operatorname{Li}_2(e^{2\pi iz})) - 2\pi y \log|1 - e^{2\pi iz}|$$

as in (5.18). Lemma 5.6 implies that $-\operatorname{Re}(\operatorname{Li}_2(e^{2\pi iz})) \geq 0$ so that

$$\frac{d}{dy} f(y) \geq \pi^2/6 - 2\pi y \log(1 + e^{-2\pi y}) > 0.$$

Since $f(0) = 0$, we have shown $f(y)$ is positive and increasing for $x = 1.49$.

For $z \in \mathcal{P}_1$, so that $x = 1.01$ and $0 \leq y \leq Y := 1.01 \times 0.22 = 0.2222$,

$$\operatorname{Re}[-p(z)] \leq \begin{cases} (f(Y/2) + g(0))/(2\pi 1.01^2) \approx 0.0558 & y \in [0, Y/2] \\ (f(Y) + g(Y/2))/(2\pi(1.01^2 + (Y/2)^2)) \approx 0.054 & y \in [Y/2, Y]. \end{cases}$$

For $z \in \mathcal{P}_3$, so that $x = 1.49$ and $0 \leq y \leq Y := 1.49 \times 0.22 = 0.3278$,

$$\operatorname{Re}[-p(z)] \leq (f(Y) + g(0))/(2\pi 1.49^2) \approx 0.0462, \quad y \in [0, Y]. \quad \square$$

Proof of Theorem 5.2. Let v be given by (5.11). Then the saddle-point z_0 lies on \mathcal{P}_2 , parameterized in (5.12), and when $t = \operatorname{Re}(z_0)$ we have $ct = z_0$. Then

$$\left. \frac{d}{dt} \operatorname{Re}[p(ct)] \right|_{t=\operatorname{Re}(z_0)} = \operatorname{Re}[cp'(c\operatorname{Re}(z_0))] = \operatorname{Re}[cp'(z_0)] = 0.$$

It follows from Corollary 5.5 that $\operatorname{Re}[p(z) - p(z_0)] > 0$ for $z \in \mathcal{P}_2$ and $z \neq z_0$. We also note that $\operatorname{Re}[-p(z_0)] = U \approx 0.068076$.

For $z \in \mathcal{P}_1 \cup \mathcal{P}_3$, Proposition 5.7 implies $\operatorname{Re}[p(z) - p(z_0)] > -0.06 + 0.068 > 0$. \square

5.3 Asymptotic expansions

In order to apply Theorem 5.1 to (5.2) we need to understand the dependence of $\exp(v(z; N, \sigma))$ on N and remove this dependence from the integral. The result we prove in this subsection is the following.

Proposition 5.8. *For $1.01 \leq \operatorname{Re}(z) \leq 1.49$ and $|\operatorname{Im}(z)| \leq 1$, say, there are holomorphic functions $u_{\sigma,j}(z)$ and $\zeta_d(z; N, \sigma)$ of z so that*

$$\exp(v(z; N, \sigma)) = \sum_{j=0}^{d-1} \frac{u_{\sigma,j}(z)}{N^j} + \zeta_d(z; N, \sigma) \quad \text{for} \quad \zeta_d(z; N, \sigma) = O\left(\frac{1}{N^d}\right)$$

with an implied constant depending only on σ and d where $1 \leq d \leq 2L - 1$ and $L = \lfloor 0.006\pi e \cdot N \rfloor$.

We first establish a general result. Fix $M \in \mathbb{Z}_{\geq 1}$. Suppose we have a function f on the positive integers with the following property. There exist $a_1, \dots, a_{M-1} \in \mathbb{C}$ and $K = K(M) > 0$ so that

$$\left| f(N) - \sum_{i=1}^{M-1} \frac{a_i}{N^i} \right| \leq \frac{K}{N^M} \quad (5.19)$$

for all $N \in \mathbb{Z}_{\geq 1}$. In other words

$$f(N) = \sum_{i=1}^{M-1} \frac{a_i}{N^i} + O\left(\frac{1}{N^M}\right). \quad (5.20)$$

We next show that $\exp(f(N))$ must have a similar expansion to (5.20).

Set $A := |a_1| + |a_2| + \dots + |a_{M-1}|$ and

$$b_j := \sum_{i_1+2i_2+\dots+(M-1)i_{M-1}=j} \frac{a_1^{i_1} a_2^{i_2} \dots a_{M-1}^{i_{M-1}}}{i_1! i_2! \dots i_{M-1}!}. \quad (5.21)$$

Lemma 5.9. *With the above M, f, a_i, K, A and b_j we have*

$$\left| \exp(f(N)) - \sum_{j=0}^{m-1} \frac{b_j}{N^j} \right| \leq \frac{e^{A+K}}{N^m}$$

for any m with $1 \leq m \leq M$ and all $N \in \mathbb{Z}_{\geq 1}$.

Proof. Clearly

$$f(N) = \sum_{i=1}^{M-1} \frac{a_i}{N^i} + \frac{f_M(N)}{N^M}$$

for some $f_M(N)$ with $|f_M(N)| \leq K$. Therefore

$$\exp(f(N)) = \exp\left(\sum_{i=1}^{M-1} \frac{a_i}{N^i}\right) \exp\left(\frac{f_M(N)}{N^M}\right). \quad (5.22)$$

We have

$$\exp\left(\sum_{i=1}^{M-1} \frac{a_i}{N^i}\right) = \left(\sum_{i_1=0}^{\infty} \frac{a_1^{i_1}}{N^{1 \cdot i_1} i_1!}\right) \cdots \left(\sum_{i_{M-1}=0}^{\infty} \frac{a_{M-1}^{i_{M-1}}}{N^{(M-1) \cdot i_{M-1}} i_{M-1}!}\right) = \sum_{j=0}^{\infty} \frac{b_j}{N^j}. \quad (5.23)$$

Note that if we replace the a_i s by their absolute values in (5.21), (5.23) we find

$$\sum_{j=0}^{\infty} \frac{|b_j|}{N^j} \leq \exp\left(\sum_{i=1}^{M-1} \frac{|a_i|}{N^i}\right) \leq e^A \quad (N \in \mathbb{Z}_{\geq 1}), \quad (5.24)$$

and in particular, (5.24) is valid for $N = 1$.

With (5.22), (5.23)

$$\exp(f(N)) = \sum_{j=0}^{m-1} \frac{b_j}{N^j} + \sum_{j=m}^{\infty} \frac{b_j}{N^j} + \left(\sum_{j=0}^{\infty} \frac{b_j}{N^j} \right) \left(\exp\left(\frac{f_M(N)}{N^M}\right) - 1 \right).$$

Recall the inequality (3.56)

$$|e^x - 1| \leq |x| \frac{e^{\kappa} - 1}{\kappa} \quad \text{for } x \in (-\infty, \kappa], \kappa > 0.$$

It follows that

$$\exp\left(\frac{f_M(N)}{N^M}\right) - 1 \leq \frac{f_M(N)}{N^M} \frac{e^K - 1}{K} \leq \frac{e^K - 1}{N^M}. \quad (5.25)$$

Hence

$$\left| \sum_{j=m}^{\infty} \frac{b_j}{N^j} + \left(\sum_{j=0}^{\infty} \frac{b_j}{N^j} \right) \left(\exp\left(\frac{f_M(N)}{N^M}\right) - 1 \right) \right| \leq \frac{e^A}{N^m} + e^A \frac{e^K - 1}{N^M} \leq \frac{e^{A+K}}{N^m},$$

proving the lemma. \square

If (5.19) is valid for every $M \in \mathbb{Z}_{\geq 1}$ then this is an example of an *asymptotic expansion*. It may be written formally as

$$f(N) \sim \sum_{i=1}^{\infty} \frac{a_i}{N^i}$$

where the right side does not necessarily converge. Lemma 5.9 relates the asymptotic expansions of $\exp(f(N))$ and $f(N)$. See also [Olv74, p. 22] for similar exercises.

Proof of Proposition 5.8. Recall from Corollary 4.6 that for $z \in \mathbb{C}$ such that $1.01 \leq \operatorname{Re}(z) \leq 1.49$ we have

$$v(z; N, \sigma) = \frac{2\pi i \sigma z}{N} + \sum_{\ell=1}^{d-1} \frac{g_{\ell}(z)}{N^{2\ell-1}} + O\left(\frac{1}{N^{2d-1}}\right) \quad (5.26)$$

for $2 \leq d \leq L = \lfloor 0.006\pi e \cdot N \rfloor$ and an implied constant, $K(d)$, depending only on d . For $j \in \mathbb{Z}_{\geq 0}$ put

$$u_{\sigma,j}(z) := \sum_{m_1+3m_2+5m_3+\dots=j} \frac{(2\pi i \sigma z + g_1(z))^{m_1}}{m_1!} \frac{g_2(z)^{m_2}}{m_2!} \dots \frac{g_j(z)^{m_j}}{m_j!}, \quad (5.27)$$

with $u_{\sigma,0} = 1$. Apply Lemma 5.9 with $f(N)$ replaced by $v(z; N, \sigma)$ and $a_1 = 2\pi i \sigma z + g_1(z)$, $a_2 = 0, \dots$ and also $b_j = u_{\sigma,j}(z)$. Let $A(\sigma, d)$ be a bound for $|a_1| + \dots + |a_{d-1}|$ for z in the stated range of the proposition. Set

$$\zeta_d(z; N, \sigma) := \exp(v(z; N, \sigma)) - \sum_{j=0}^{d-1} \frac{u_{\sigma,j}(z)}{N^j}.$$

Then $\zeta_d(z; N, \sigma)$ is clearly holomorphic in z and Lemma 5.9 implies $|\zeta_d(z; N, \sigma)| \leq \exp(A(\sigma, d) + K(d))/N^d$ as required. \square

5.4 Proofs of Theorems 1.4 and 1.6

We restate Theorem 1.6 here:

Theorem 1.6. With $b_0 = 2z_0 e^{-\pi i z_0}$ and explicit $b_1(\sigma), b_2(\sigma), \dots$ depending on $\sigma \in \mathbb{R}$ we have

$$\mathcal{A}_1(N, \sigma) = \operatorname{Re} \left[\frac{w_0^{-N}}{N^2} \left(b_0 + \frac{b_1(\sigma)}{N} + \dots + \frac{b_{m-1}(\sigma)}{N^{m-1}} \right) \right] + O\left(\frac{|w_0|^{-N}}{N^{m+2}}\right) \quad (5.28)$$

for an implied constant depending only on σ and m .

Proof. Recall from (2.31) that $e^{-p(z_0)} = w_0^{-1}$. Proposition 5.8 implies

$$\mathcal{A}_3(N, \sigma) = \operatorname{Im} \left[\sum_{j=0}^{d-1} \frac{2}{N^{3/2+j}} \int_{\mathcal{P}} e^{-N \cdot p(z)} \cdot q(z) \cdot u_{\sigma,j}(z) dz + \frac{2}{N^{3/2}} \int_{\mathcal{P}} e^{-N \cdot p(z)} \cdot q(z) \cdot \zeta_d(z; N, \sigma) dz \right] \quad (5.29)$$

where the last term in (5.29) is

$$\ll \frac{1}{N^{3/2}} \int_{\mathcal{P}} \left| e^{-N \cdot p(z)} \right| \cdot 1 \cdot \frac{1}{N^d} dz \ll \frac{1}{N^{d+3/2}} e^{-N \operatorname{Re}(p(z_0))} = \frac{|w_0|^{-N}}{N^{d+3/2}}$$

by Theorem 5.2 and Propositions 4.7 and 5.8. Applying Theorem 5.1 to each integral in the first part of (5.29) we obtain

$$\int_{\mathcal{P}} e^{-N \cdot p(z)} \cdot q(z) \cdot u_{\sigma,j}(z) dz = 2e^{-N p(z_0)} \left(\sum_{s=0}^{S-1} \Gamma(s+1/2) \frac{a_{2s}(q \cdot u_{\sigma,j})}{N^{s+1/2}} + O\left(\frac{1}{N^{S+1/2}}\right) \right). \quad (5.30)$$

The error term in (5.30) corresponds to an error for $\mathcal{A}_3(N, \sigma)$ of size $O(|w_0|^{-N}/N^{s+j+2})$. We choose $S = d$ so that this error is less than $O(|w_0|^{-N}/N^{d+3/2})$ for all $j \geq 0$. Therefore

$$\begin{aligned} \mathcal{A}_3(N, \sigma) &= \operatorname{Im} \left[\sum_{j=0}^{d-1} \frac{4}{N^{j+3/2}} e^{-N \cdot p(z_0)} \sum_{s=0}^{d-1} \frac{\Gamma(s+1/2) a_{2s}(q \cdot u_{\sigma,j})}{N^{s+1/2}} \right] + O\left(\frac{|w_0|^{-N}}{N^{d+3/2}}\right) \\ &= \operatorname{Im} \left[w_0^{-N} \sum_{t=0}^{2d-2} \frac{4}{N^{t+2}} \sum_{s=0}^{\min(t, d-1)} \Gamma(s+1/2) a_{2s}(q \cdot u_{\sigma, t-s}) \right] + O\left(\frac{|w_0|^{-N}}{N^{d+3/2}}\right) \\ &= \operatorname{Re} \left[w_0^{-N} \sum_{t=0}^{d-2} \frac{-4i}{N^{t+2}} \sum_{s=0}^t \Gamma(s+1/2) a_{2s}(q \cdot u_{\sigma, t-s}) \right] + O\left(\frac{|w_0|^{-N}}{N^{d+1}}\right). \end{aligned}$$

Hence, recalling (5.3) and with

$$b_t(\sigma) := -4i \sum_{s=0}^t \Gamma(s+1/2) a_{2s}(q \cdot u_{\sigma, t-s}), \quad (5.31)$$

we obtain (5.28) in the statement of the theorem.

Use the formula for a_0 on the left of (5.10) to get

$$b_0(\sigma) = -4i \Gamma(1/2) a_0(q \cdot u_{\sigma,0}) = -4i \sqrt{\pi} \left(\frac{\omega}{2(\omega^2 p_0)^{1/2}} q_0 \right) \quad (5.32)$$

which is independent of σ . The terms p_0 and q_0 are defined in (5.5), (5.6) so that, using (2.33),

$$p_0 = p''(z_0)/2 = \frac{-\pi i e^{2\pi i z_0}}{z_0 w_0}, \quad q_0^2 = q(z_0)^2 = \frac{i z_0}{w_0}. \quad (5.33)$$

The square of the term in parentheses in (5.32) is therefore

$$\frac{q_0^2}{4p_0} = \frac{-z_0^2}{4\pi e^{2\pi i z_0}}.$$

We may take $\omega = z_0$ since the path \mathcal{P}_2 is a segment of the ray from the origin through z_0 . A numerical check then gives us the correct square root:

$$a_0(q) = \frac{\omega}{2(\omega^2 p_0)^{1/2}} q_0 = \frac{i z_0}{2\sqrt{\pi} e^{\pi i z_0}} \quad (5.34)$$

and the formula $b_0 = 2z_0 e^{-\pi i z_0}$ follows. \square

N	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$\mathcal{A}_1(N, 1)$
200	-33.8689	-32.5734	-32.4829	-32.4681	-32.4692
400	2.17937×10^7	2.16780×10^7	2.16710×10^7	2.16712×10^7	2.16712×10^7
600	1.80284×10^{12}	1.77324×10^{12}	1.77260×10^{12}	1.77255×10^{12}	1.77255×10^{12}
800	-3.72536×10^{18}	-3.71475×10^{18}	-3.71444×10^{18}	-3.71444×10^{18}	-3.71444×10^{18}
1000	-2.58000×10^{23}	-2.54119×10^{23}	-2.54072×10^{23}	-2.54070×10^{23}	-2.54070×10^{23}

Table 2: Theorem 1.6's approximations to $\mathcal{A}_1(N, 1)$.

For example, Table 2 displays how well (5.28) in Theorem 1.6 approximates $\mathcal{A}_1(N, \sigma)$ for $\sigma = 1$ and some values of m and N .

The expansion coefficients $b_t(\sigma)$ may all be written explicitly in terms of w_0 and z_0 . We give $b_1(\sigma)$ next.

Proposition 5.10. *Each $b_t(\sigma)$ is a polynomial in σ of degree t . For $t = 1$ we have*

$$b_1(\sigma) = \frac{4\pi i z_0^2}{e^{\pi i z_0}} \sigma - \frac{w_0}{\pi i e^{3\pi i z_0}} \left(\frac{(2\pi i z_0)^2}{12} - 2\pi i z_0 + 1 \right). \quad (5.35)$$

Proof. Note that $u_{\sigma,j}(z)$ is a polynomial in σ of degree j . Since $a_{2s}(q)$ is linear in its argument, $a_{2s}(c_1 q_1(z) + c_2 q_2(z)) = c_1 a_{2s}(q_1(z)) + c_2 a_{2s}(q_2(z))$, it follows from (5.31) that $b_t(\sigma)$ is a polynomial in σ of degree t .

With $t = 1$, (5.31) implies

$$\begin{aligned} b_1(\sigma) &= -4i\Gamma(1/2)a_0(q \cdot u_{\sigma,1}) - 4i\Gamma(3/2)a_2(q \cdot u_{\sigma,0}) \\ &= -4i\sqrt{\pi} \cdot a_0(q) \cdot u_{\sigma,1}(z_0) - 2i\sqrt{\pi}a_2(q). \end{aligned}$$

Since

$$u_{\sigma,1}(z) = 2\pi i \sigma z + g_1(z) = \frac{\pi i z}{6} \left(12\sigma - \frac{1}{2} + \frac{1}{1 - e^{2\pi i z}} \right)$$

we see that $u_{\sigma,1}(z_0) = \pi i z_0(12\sigma - 1/2 + 1/w_0)/6$. Also (5.10) implies

$$a_2(q) = \frac{a_0(q)}{p_0} \left(\frac{q_2}{q_0} - \frac{3}{2} \frac{p_1}{p_0} \frac{q_1}{q_0} - \frac{3}{2} \frac{p_2}{p_0} + \frac{15}{8} \frac{p_1^2}{p_0^2} \right).$$

Taking derivatives of $q^2(z) = iz/(1 - e^{2\pi i z})$ and evaluating at $z = z_0$ shows that

$$\frac{q_1}{q_0} = -\pi i + \frac{1}{2z_0} + \frac{\pi i}{w_0}, \quad \frac{q_2}{q_0} = -\frac{\pi^2}{2} - \frac{\pi i}{2z_0} + \frac{2\pi^2}{w_0} - \frac{1}{8z_0^2} + \frac{\pi i}{2z_0 w_0} - \frac{3\pi^2}{2w_0^2}.$$

Similarly, recalling p_0 from (5.33) and using (2.32), (2.33) and their generalizations, we have

$$\frac{p_1}{p_0} = -\frac{1}{z_0} + \frac{2\pi i}{3w_0}, \quad \frac{p_2}{p_0} = \frac{\pi^2}{3w_0} + \frac{1}{z_0^2} - \frac{2\pi i}{3z_0 w_0} - \frac{2\pi^2}{3w_0^2}.$$

Putting this all together with $a_0(q)$ from (5.34) and simplifying completes the proof. \square

Assuming Theorem 1.7 – see the summary of its proof in the next section – we may now prove our main result.

Proof of Theorem 1.4. Putting $h/k = 0/1$ in (1.16) gives

$$C_{01\ell}(N) = \sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-1)^{\ell-\sigma} Q_{01\sigma}(N).$$

Taking the same linear combination of (1.18) produces

$$\sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-1)^{\ell-\sigma} \sum_{h/k \in \mathcal{F}_N} Q_{hk\sigma}(N) = 0 \quad \text{for} \quad N(N+1)/2 > \ell \quad (5.36)$$

and we partition \mathcal{F}_N into three parts: \mathcal{F}_{100} , $\mathcal{A}(N)$ and the rest. The sum over this third part is $O(e^{WN})$ by Theorem 1.7 implying that (5.36) breaks into

$$C_{01\ell}(N) + \sum_{0 < h/k \in \mathcal{F}_{100}} \sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-1)^{\ell-\sigma} Q_{hk\sigma}(N) + \sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-1)^{\ell-\sigma} \mathcal{A}_1(N, \sigma) = O(e^{WN}). \quad (5.37)$$

Use (1.17) to see that

$$\sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-1)^{\ell-\sigma} Q_{hk\sigma}(N) = \sum_{j=1}^{\ell} (e^{2\pi i h/k} - 1)^{\ell-j} C_{hkj}(N). \quad (5.38)$$

Then (5.38) and Theorem 1.6 let us write (5.37) as

$$\begin{aligned} C_{01\ell}(N) + \sum_{0 < h/k \in \mathcal{F}_{100}} \sum_{j=1}^{\ell} (e^{2\pi i h/k} - 1)^{\ell-j} C_{hkj}(N) \\ = \operatorname{Re} \left[\frac{w_0^{-N}}{N^2} \left(b_{\ell,0}^* + \frac{b_{\ell,1}^*}{N} + \dots + \frac{b_{\ell,m-1}^*}{N^{m-1}} \right) \right] + O\left(\frac{|w_0|^{-N}}{N^{m+2}}\right) \end{aligned} \quad (5.39)$$

for

$$b_{\ell,t}^* := - \sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-1)^{\ell-\sigma} b_t(\sigma).$$

We claim that $b_{\ell,t}^* = 0$ for $0 \leq t \leq \ell-2$ and $b_{\ell,\ell-1}^* = -2z_0 e^{-\pi i z_0} (2\pi i z_0)^{\ell-1}$. To see this, observe that $\mathcal{A}_1(N, \sigma)$ may be replaced in (5.37) by $\mathcal{A}_3(N, \sigma)$, as defined in (5.2), since (5.3) is true. The dependence of $\mathcal{A}_3(N, \sigma)$ on σ comes from the $\exp(v(z; N, \sigma))$ term and we have

$$\begin{aligned} \sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-1)^{\ell-\sigma} \exp(v(z; N, \sigma)) &= \sum_{\sigma=1}^{\ell} \binom{\ell-1}{\sigma-1} (-1)^{\ell-\sigma} \exp(2\pi i z/N)^{\sigma} \exp(v(z; N, 0)) \\ &= [\exp(2\pi i z/N) - 1]^{\ell-1} \exp(v(z; N, 1)) \\ &= \left(\frac{2\pi i z}{N} + \frac{(2\pi i z)^2}{2!N^2} + \dots \right)^{\ell-1} \left(u_{1,0}(z) + \frac{u_{1,1}(z)}{N} + \dots \right) \\ &= \frac{1}{N^{\ell-1}} \left(v_{\ell,0}^*(z) + \frac{v_{\ell,1}^*(z)}{N} + \frac{v_{\ell,2}^*(z)}{N^2} + \dots \right) \end{aligned}$$

where $v_{\ell,0}^*(z) = (2\pi i z)^{\ell-1}$, and in general, employing (5.7), (5.8),

$$v_{\ell,j}^*(z) = \sum_{t=0}^j \hat{B}_{\ell-1+t, \ell-1}(1/1!, 1/2!, 1/3!, \dots) \cdot (2\pi i z)^{\ell-1+t} \cdot u_{1,j-t}(z).$$

Now repeating the proof of Theorem 1.6 with $u_{\sigma,j}$ replaced by $v_{\ell,j}^*$ yields

$$c_{\ell,t} = 4i \sum_{s=0}^t \Gamma(s+1/2) a_{2s}(q \cdot v_{\ell,t-s}^*) \quad (5.40)$$

in the statement of the theorem, with $c_{\ell,0} = -2z_0 e^{-\pi i z_0} (2\pi i z_0)^{\ell-1} = b_{\ell,\ell-1}^*$ as desired. \square

With (5.40) we may compute the coefficients $c_{\ell,t}$ explicitly. For example, similar calculations to those of Proposition 5.10 produce $v_{\ell,1}^*(z) = (2\pi i z)^{\ell} (6\ell + 11/2 + 1/(1 - e^{2\pi i z})) / 12$ and

$$c_{\ell,1} = -\frac{(\ell+1)z_0(2\pi i z_0)^{\ell}}{e^{\pi i z_0}} + \frac{z_0 w_0 (2\pi i z_0)^{\ell}}{e^{3\pi i z_0}} \left(\frac{1}{6} - \frac{\ell+1}{2\pi i z_0} + \frac{\ell(\ell+1)}{(2\pi i z_0)^2} \right). \quad (5.41)$$

6 Further results

6.1 Proof of Theorem 1.7

To prove Theorem 1.7 we first need a general estimate for the sine product $\prod_m^{-1}(h/k)$, without the restriction $0 \leq m < k/h$ that was in place in Section 3. Define the set

$$Z(h, k) := \{(\beta, \gamma) \in \mathbb{Z} \times \mathbb{Z} : 1 \leq |\beta| < k, 1 \leq \gamma < k, \beta h \equiv \gamma \pmod{k}\}.$$

Theorem 6.1. *For all $m, h, k \in \mathbb{Z}$ with $1 \leq h < k$, $(h, k) = 1$ and $0 \leq m < k$ we have*

$$\frac{1}{k} \log \left| \prod_m^{-1}(h/k) \right| = \frac{\text{Cl}_2(2\pi m \gamma_0 h/k)}{2\pi |\beta_0 \gamma_0|} + O\left(\frac{\log k}{\sqrt{k}}\right) \quad (6.1)$$

where (β_0, γ_0) is a pair in $Z(h, k)$ with $|\beta_0 \gamma_0|$ minimal. The implied constant in (6.1) is absolute.

Very briefly, the proof of Theorem 6.1 involves showing, with another application of Euler-Maclaurin summation, that

$$\frac{1}{k} \log \left| \prod_m^{-1}(h/k) \right| = \frac{S(m; h, k)}{2\pi} + O\left(\frac{\log^2 k}{k}\right)$$

for

$$S(m; h, k) := \sum_{(\beta, \gamma) \in Z(h, k)} \frac{\sin(2\pi m \gamma/k)}{\beta \gamma}$$

and then relating $S(m; h, k)$ to Clausen's integral.

Define $D(h, k)$ to be the above minimal value $|\beta_0 \gamma_0|$ in the statement of Theorem 6.1. For example, it is easy to see that

$$D(h, k) = 1 \iff h \equiv \pm 1 \pmod{k}$$

and if $D(h, k) \neq 1$ then

$$D(h, k) = 2 \iff h \text{ or } h^{-1} \equiv \pm 2 \pmod{k}$$

with k necessarily odd. A simple corollary to Theorem 6.1 says there exists an absolute constant τ such that

$$\frac{1}{k} \left| \log \left| \prod_m(h/k) \right| \right| \leq \frac{\text{Cl}_2(\pi/3)}{2\pi D(h, k)} + \tau \frac{\log k}{\sqrt{k}}. \quad (6.2)$$

The second result we need is a general bound for $Q_{hk\sigma}(N)$:

Proposition 6.2. *For $1 \leq k \leq N$, $\sigma \in \mathbb{R}$ and $s := \lfloor N/k \rfloor$*

$$|Q_{hk\sigma}(N)| \leq \frac{3}{k^3} \exp\left(N \frac{2 + \log(1 + 3k/4)}{k} + \frac{|\sigma|}{N}\right) \left| \prod_{N-sk}^{-1}(h/k) \right|.$$

This proposition is proved by expressing $Q_{hk\sigma}(N)$ as the integral of $Q(z; N, \sigma)$ around a small loop circling h/k (recall (1.15)) and bounding the absolute value of $Q(z; N, \sigma)$ on this loop. A refinement of Proposition 6.2, restricting the values of k to $101 \leq k \leq N$, has

$$|Q_{hk\sigma}(N)| \leq \frac{9}{k^3} \exp\left(N \frac{2 + \log(\xi/2 + \xi'k/8)}{k} + \frac{|\sigma|}{N}\right) \left| \prod_{N-sk}^{-1}(h/k) \right| \quad (6.3)$$

for $\xi = 1.00038$ and $\xi' = 1.01041$. Combining (6.2) with (6.3) gives

$$Q_{hk\sigma}(N) \ll \frac{1}{k^3} \exp\left(N \frac{2 + \log(\xi/2 + \xi'k/8)}{k} + \frac{\text{Cl}_2(\pi/3)}{2\pi D(h, k)} \cdot k + \tau \sqrt{N} \log N\right) \quad (6.4)$$

for $k \geq 101$. A straightforward calculation with (6.4) then shows that, when $W > \text{Cl}_2(\pi/3)/(6\pi) \approx 0.0538$, we have

$$Q_{hk\sigma}(N) \ll e^{WN}/k^3 \quad (6.5)$$

for all $h/k \in \mathcal{F}_N - \mathcal{F}_{100}$ except in the cases where

$$\begin{aligned} h &\equiv \pm 1, \pm 2, (k \pm 1)/2 \pmod{k} & \text{and} & & N/2 < k \leq N, \\ \text{or} & & h &\equiv \pm 1 \pmod{k} & \text{and} & & N/3 < k \leq N/2, \end{aligned}$$

corresponding to N large and $D(h, k)$ small. Hence, the three subsets of $\mathcal{F}_N - (\mathcal{F}_{100} \cup \mathcal{A}(N))$ we must consider separately are

$$\begin{aligned} \mathcal{C}(N) &:= \left\{ h/k : \frac{N}{2} < k \leq N, k \text{ odd}, h = 2 \text{ or } h = k - 2 \right\}, \\ \mathcal{D}(N) &:= \left\{ h/k : \frac{N}{2} < k \leq N, k \text{ odd}, h = \frac{k-1}{2} \text{ or } h = \frac{k+1}{2} \right\}, \\ \mathcal{E}(N) &:= \left\{ h/k : \frac{N}{3} < k \leq \frac{N}{2}, h = 1 \text{ or } h = k - 1 \right\} \end{aligned}$$

with $\mathcal{C}(N)$, $\mathcal{D}(N)$ sets of simple poles of $Q(z; N, \sigma)$ and $\mathcal{E}(N)$ a set of double poles.

To describe the asymptotics of the corresponding sums of $Q_{hk\sigma}(N)$ s, recall the dilogarithm zero $w_0 = w(0, -1)$ and its associated saddle-point z_0 given by (1.5). We also need the new saddle-points

$$z_3 := 3 + \log(1 - w(1, -3))/(2\pi i), \quad z_1 := 2 + \log(1 - w(0, -2))/(2\pi i)$$

using the notation of Section 2.3. The proof of Theorem 1.6, giving the asymptotic expansion of $\mathcal{A}_1(N, \sigma)$, extends to cover these three new cases and, for implied constants depending only on σ and m , we obtain

$$\sum_{h/k \in \mathcal{C}(N)} Q_{hk\sigma}(N) = \operatorname{Re} \left[\frac{w(1, -3)^{-N}}{N^2} \left(c_0^* + \frac{c_1^*(\sigma)}{N} + \dots + \frac{c_{m-1}^*(\sigma)}{N^{m-1}} \right) \right] + O \left(\frac{|w(1, -3)|^{-N}}{N^{m+2}} \right), \quad (6.6)$$

$$\sum_{h/k \in \mathcal{D}(N)} Q_{hk\sigma}(N) = \operatorname{Re} \left[\frac{w_0^{-N/2}}{N^2} \left(d_0(\overline{N}) + \frac{d_1(\sigma, \overline{N})}{N} + \dots + \frac{d_{m-1}(\sigma, \overline{N})}{N^{m-1}} \right) \right] + O \left(\frac{|w_0|^{-N/2}}{N^{m+2}} \right), \quad (6.7)$$

$$\sum_{h/k \in \mathcal{E}(N)} Q_{hk\sigma}(N) = \operatorname{Re} \left[\frac{w(0, -2)^{-N}}{N^2} \left(e_0 + \frac{e_1(\sigma)}{N} + \dots + \frac{e_{m-1}(\sigma)}{N^{m-1}} \right) \right] + O \left(\frac{|w(0, -2)|^{-N}}{N^{m+2}} \right) \quad (6.8)$$

where \overline{N} denotes $N \bmod 2$ and the expansion coefficients may be given explicitly; the first ones are

$$c_0^* = -z_3 e^{-\pi i z_3} / 4, \quad d_0(\overline{N}) = z_0 \sqrt{2e^{-\pi i z_0} (e^{-\pi i z_0} + (-1)^N)}, \quad e_0 = -3z_1 e^{-\pi i z_1} / 2.$$

The bounds in (6.6), (6.7) and (6.8) are

$$O(e^{0.0357N}), \quad O(e^{0.0341N}), \quad O(e^{0.0257N})$$

respectively and so, with (6.5), we have completed the summary of the proof of Theorem 1.7. See [O'Sa] for further details.

6.2 Generalizations and conjectures

In Table 3 we give numerical evidence for Conjecture 1.5 in the case $\ell = 1$ by comparing both sides of (1.12) for different values of m . These entries match those of Table 2 since $c_{1,t} = -b_t(1)$. Compare also [O'S12,

N	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$\mathcal{C}_{011}(N)$
400	-2.17937×10^7	-2.16780×10^7	-2.16710×10^7	-2.16712×10^7	-2.16712×10^7
600	-1.80284×10^{12}	-1.77324×10^{12}	-1.77260×10^{12}	-1.77255×10^{12}	-1.77255×10^{12}
800	3.72536×10^{18}	3.71475×10^{18}	3.71444×10^{18}	3.71444×10^{18}	3.71444×10^{18}
1000	2.58000×10^{23}	2.54119×10^{23}	2.54072×10^{23}	2.54070×10^{23}	2.54070×10^{23}

Table 3: Conjecture 1.5's approximations to $\mathcal{C}_{011}(N)$.

Table 1]. Table 4 shows the case $\ell = 4$ of Conjecture 1.5.

N	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$C_{014}(N)$
400	-56.2851	-58.7844	-58.6802	-58.6857	-58.6545
600	-1.52353×10^7	-1.52212×10^7	-1.52136×10^7	-1.52132×10^7	-1.52133×10^7
800	1.44649×10^{12}	1.47247×10^{12}	1.47185×10^{12}	1.47186×10^{12}	1.47186×10^{12}

Table 4: Conjecture 1.5's approximations to $C_{014}(N)$.

The identity (1.18) for $\sigma = 1$ says

$$\sum_{h/k \in \mathcal{F}_N} C_{hkl}(N) = 0 \quad (N \geq 2) \quad (6.9)$$

since $C_{hkl}(N) = Q_{hkl}(N)$. With the proof of Theorem 1.2, we have shown that the largest terms in (6.9) have h/k in \mathcal{F}_{100} and $\mathcal{A}(N)$. The $\ell = 1$ case of Conjecture 1.5 indicates that all the terms with h/k in \mathcal{F}_{100} are relatively small except for $h/k = 0/1$. So we expect

$$C_{011}(N) \sim - \sum_{\substack{N/2 < b \leq N \\ a \equiv \pm 1 \pmod{b}}} C_{ab1}(N), \quad (6.10)$$

i.e. that the asymptotic expansions of both sides of (6.10) are the same.

Can we match up the other terms of (6.9) in the same way? A clue to the asymptotics of $C_{121}(N)$ comes from noticing how closely it matches -1 times (6.7). This lets us expect

$$C_{121}(N) \sim - \sum_{\substack{N/2 < b \leq N, (b,2)=1 \\ a \equiv \pm 2^{-1} \pmod{b}}} C_{ab1}(N). \quad (6.11)$$

Conjecture 6.3. *For the coefficients $d_0(\overline{N})$, $d_1(\sigma, \overline{N})$, \dots of (6.7) and an implied constant depending only on the positive integer m , we have*

$$C_{121}(N) = -\operatorname{Re} \left[\frac{w_0^{-N/2}}{N^2} \left(d_0(\overline{N}) + \frac{d_1(1, \overline{N})}{N} + \dots + \frac{d_{m-1}(1, \overline{N})}{N^{m-1}} \right) \right] + O \left(\frac{|w_0|^{-N/2}}{N^{m+2}} \right).$$

Some numerical evidence for Conjecture 6.3 is given in Table 5. The $m = 1$ case of Conjecture 6.3 appeared already in [O'S12, Conj. 6.3].

N	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$C_{121}(N)$
1000	1.76776×10^9	1.77847×10^9	1.7778×10^9	1.77778×10^9	1.77778×10^9
1001	2.10996×10^9	2.11483×10^9	2.1142×10^9	2.11418×10^9	2.11418×10^9

Table 5: Conjecture 6.3's approximations to $C_{121}(N)$.

Continuing the pattern from (6.10), (6.11) we guess that

$$C_{131}(N) + C_{231}(N) \sim - \sum_{\substack{N/2 < b \leq N, (b,3)=1 \\ a \equiv \pm 3^{-1} \pmod{b}}} C_{ab1}(N) \quad (6.12)$$

and indeed numerical evidence seems to support this. With more work, the techniques we have developed to prove Theorem 1.6 and (6.7) should give the asymptotic expansion of the right side of (6.12).

We finally list some further interesting directions for investigation:

- (i) Rademacher's original conjecture (1.3) has been disproved, but what is the correct conjecture? As discussed in [O'S12, Sect. 6], for each triple hkl there seems to be some initial agreement between $C_{hkl}(\infty)$ and the coefficients $C_{hkl}(N)$ for small N .

- (ii) Each Rademacher coefficient $C_{hk\ell}(N)$ is a linear combination of the numbers $Q_{hk\sigma}(N)$ for $1 \leq \sigma \leq \ell$, as we have seen. For σ negative, on the other hand, combinations of $Q_{hk\sigma}(N)$ produce the restricted partition function: with $\sigma = -n$ in Theorem 2.1 we obtain Sylvester's result

$$p_N(n) = \sum_{k=1}^N \left[\sum_{0 \leq h < k, (h,k)=1} -Q_{hk(-n)}(N) \right]. \quad (6.13)$$

The inner sum in brackets is Sylvester's k th wave [Syl82], which may be denoted as $W_k(N, n)$. See also [O'S12, Sect. 4], for example. The techniques we have developed in this paper should allow quantification of how well (or poorly) the first waves $W_1(N, n), W_2(N, n), \dots$ approximate $p_N(n)$ as N and possibly n tend to infinity. This ties in to work of Szekeres in [Sze51] who found asymptotic formulas for $p_N(n)$ when $n \geq 0.135N^2$ by using the first wave, $W_1(N, n)$, in the decomposition (6.13). He extended this result in [Sze53], removing the restriction $n \geq 0.135N^2$, by using a different approach that incorporated the saddle-point method.

- (iii) If we replace the product $\prod_{j=1}^N 1/(1 - q^j)$ in (1.2) with a different product and examine the coefficients in its partial fraction decomposition as the number of factors goes to infinity, can we obtain results similar to Theorem 1.4? For example, following Sylvester's general theory in [Syl82], we may replace the sequence $1, 2, 3, \dots$ with any sequence a_1, a_2, a_3, \dots of possibly repeating positive integers and study the partial fractions of

$$\prod_{j=1}^N \frac{1}{1 - q^{a_j}} \quad (6.14)$$

as $N \rightarrow \infty$. The coefficient of q^n in (6.14) is now the number of solutions in nonnegative integers x_i to $a_1x_1 + \dots + a_Nx_N = n$, expressed by Sylvester as a sum of waves.

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