

Analysis of Series and Products.

Part 2: The Trapezoidal Rule

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August 11, 2020

Abstract

Following on from our recent investigation of series and products using the Euler–Maclaurin formula, we show how the trapezoidal rule can be used to obtain the same asymptotic expansions and can also produce exact transformations into equivalent series with different convergence properties.

1 Introduction.

In a recent article [9], henceforth referred to as “Part 1,” we investigated applications of the Euler–Maclaurin formula in analyzing the behavior of infinite series and products. Specifically, if $S(x)$ is a function expressed as a series, we are concerned with the behavior as $x \rightarrow \infty$, where this cannot be obtained by elementary means. As an example, we looked at Poisson’s series

$$S(x) = \sum_{j=1}^{\infty} e^{-j^2/x^2}. \quad (1)$$

Using the Euler–Maclaurin formula, we were able to show that

$$S(x) - \frac{x\sqrt{\pi}}{2} + \frac{1}{2} \rightarrow 0 \quad \text{as } x \rightarrow \infty,$$

and also that the magnitude of the left-hand side decreases exponentially as x increases. However, we did not retrieve the full form of Poisson’s 1823

result [7, p. 420]

$$S(x) = \frac{x\sqrt{\pi}}{2} - \frac{1}{2} + x\sqrt{\pi} \sum_{j=1}^{\infty} e^{-(j\pi x)^2}, \quad x > 0. \quad (2)$$

As further examples, we also considered

$$T(x) = \sum_{j=1}^{\infty} e^{-j^3/x^3}, \quad x > 0, \quad \text{and} \quad F(x) = \sum_{j=1}^{\infty} \ln(1 - e^{-j^2/x^2}). \quad (3)$$

The first of these is motivated by the fact that even summands tend to make matters easier (so we decided to investigate a similar-looking series with an odd function in the summand), and the second originates from the infinite product

$$G(x) = \exp[F(x)] = \prod_{j=1}^{\infty} (1 - e^{-j^2/x^2}),$$

which originates from a method for modelling heat flow through walls (see the supplemental material for Part 1). In this sequel article, we will investigate an alternative method that is slightly more complicated than the Euler–Maclaurin formula, but significantly more powerful: the trapezoidal rule. Using this, we will see that Poisson’s result (2) can be retrieved in full, and (somewhat remarkably) an exact transformation with similar properties can be obtained for $F(x)$.

2 The trapezoidal rule.

The composite trapezoidal rule for the real line may be obtained by starting with a finite interval $[-a, a]$ and dividing this into $2n$ subintervals each of width $\Delta s = a/n$. Given a function h , we then approximate the area under the graph of $h(s)$ on each subinterval using a trapezoid. The area of one such trapezoid is

$$A_j = \frac{\Delta s}{2} [h((j-1)\Delta s) + h(j\Delta s)],$$

and summing over j leads to the result

$$\begin{aligned} \int_{-a}^a h(s) ds &= \frac{\Delta s}{2} \sum_{j=1-n}^n [h((j-1)\Delta s) + h(j\Delta s)] + E \\ &= \Delta s \left[\frac{h(-a) + h(a)}{2} + \sum_{j=1-n}^{n-1} h(j\Delta s) \right] + E, \end{aligned}$$

where E is the error, which generally disappears as $\Delta s \rightarrow 0$. Taking the limit $n \rightarrow \infty$ while keeping Δs fixed (assuming that $h(\pm a) \rightarrow 0$ as $a \rightarrow \infty$, and that the integral exists in this limit), we find that the rule for the whole real line is

$$\int_{-\infty}^{\infty} h(s) ds = \Delta s \sum_{j=-\infty}^{\infty} h(j\Delta s) + E. \quad (4)$$

So, much like the Euler–Maclaurin formula, the trapezoidal rule relates a sum to an integral involving the same function. As a simple example we can set $h(s) = e^{-s^2}$ and $\Delta s = 1/x$ to immediately retrieve the first two terms in (2). The issue now is to determine the error E . One approach is to return to the Euler–Maclaurin formula (see [8, §3.3] for example), but this simply reproduces results we already have. We will employ an alternative method based on contour integration, which can yield more information, especially in cases where E decreases exponentially with Δs (see [10] for a comprehensive survey of these). The idea dates back to paper from the late nineteenth century by Georg Landsberg [3], where it was used to derive (2). Later it was used “in reverse” by Alan Turing [11], as a means of proving that a certain integral representation of the Riemann zeta function can be computed very precisely using a series.

We begin by setting up an integral that will evaluate to the series in question in an appropriate limit. Let Ω be the anticlockwise oriented rectangular contour with vertices at $\pm(Q + \frac{1}{2}) + iu$ and $\pm(Q + \frac{1}{2}) - iv$ for $u, v > 0$ (see Figure 1). Then, provided f is analytic inside Ω , the residue theorem shows that

$$\begin{aligned} \int_{\Omega} \frac{f(s; x)}{e^{2\pi i s} - 1} ds &= 2\pi i \sum_{j=-Q}^Q f(j; x) \lim_{s \rightarrow j} \frac{s - j}{e^{2\pi i s} - 1} \\ &= \sum_{j=-Q}^Q f(j; x). \end{aligned} \quad (5)$$

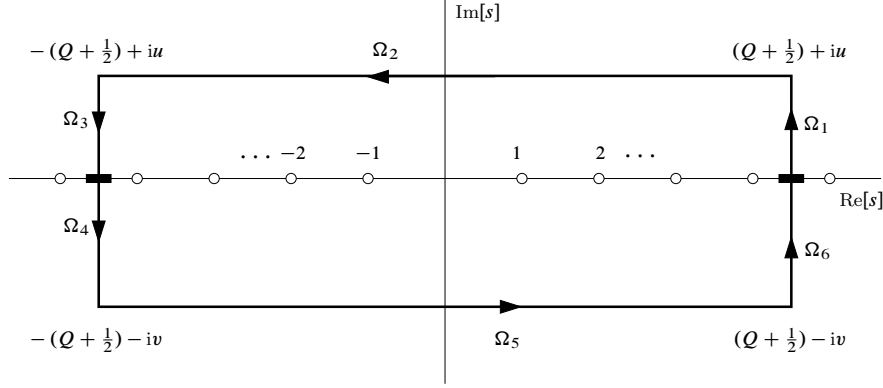


Figure 1: The closed contour Ω , consisting of the straight sections $\Omega_1, \dots, \Omega_6$. The black bars denote the divisions between Ω_1 and Ω_6 and between Ω_3 and Ω_4 at $s = \pm(Q + \frac{1}{2})$.

Now consider the individual sections of the contour Ω . On the lower edge, the factor $e^{2\pi v}$ appears in the denominator of the integrand, so if v is chosen to be sufficiently large then the contribution from Ω_5 will be exponentially small. To achieve the same effect on the upper edge, we observe that

$$\frac{f(s; x)}{e^{2\pi is} - 1} = f(s; x) \left(\frac{e^{2\pi is}}{e^{2\pi is} - 1} - 1 \right), \quad (6)$$

and hence

$$\lim_{Q \rightarrow \infty} \int_{\Omega_{1,2,3}} \frac{f(s; x)}{e^{2\pi is} - 1} ds = \lim_{Q \rightarrow \infty} \int_{\Omega_{1,2,3}} \frac{f(s; x)}{1 - e^{-2\pi is}} ds + \int_{-\infty}^{\infty} f(s; x) ds.$$

Here we have introduced the shorthand notation $\Omega_{1,2,3}$ to mean the union of the three sections Ω_1, Ω_2 , and Ω_3 . Combining this with (5), we then have

$$\sum_{j=-\infty}^{\infty} f(j; x) = \int_{-\infty}^{\infty} f(s; x) ds + H + V, \quad (7)$$

where H and V represent the contributions from the horizontal and vertical components of Ω , respectively. That is,

$$H = \lim_{Q \rightarrow \infty} \left[\int_{\Omega_2} \frac{f(s; x)}{1 - e^{-2\pi is}} ds + \int_{\Omega_5} \frac{f(s; x)}{e^{2\pi is} - 1} ds \right] \quad (8)$$

and

$$V = \lim_{Q \rightarrow \infty} \left[\int_{\Omega_{1,3}} \frac{f(s; x)}{1 - e^{-2\pi is}} ds + \int_{\Omega_{4,6}} \frac{f(s; x)}{e^{2\pi is} - 1} ds \right]. \quad (9)$$

Next, we simplify our expression for H . Parametrizing Ω_2 and Ω_5 by writing $s = w + iu$ and $s = w - iv$ (and noting that Ω_2 is traversed from right to left), we obtain

$$H = \int_{-\infty}^{\infty} \frac{f(w + iu; x)}{e^{2\pi(u-iw)} - 1} dw + \int_{-\infty}^{\infty} \frac{f(w - iv; x)}{e^{2\pi(v+iw)} - 1} dw. \quad (10)$$

Up to this point, we have allowed for the possibility that u and v might take different values. This may be useful for complex series, but if the summand $f(s; x)$ is real for real s then the Schwarz reflection principle [6, Theorem 10.4] applies, i.e.,

$$f(\bar{s}; x) = \bar{f}(s; x), \quad (11)$$

where the overbar denotes a complex conjugate. Crucially, this means the singularity structure of f is symmetric about the real axis. In this case, setting $v = u$ makes the integrals in (10) into mutual complex conjugates, meaning that

$$H = 2 \operatorname{Re} \int_{-\infty}^{\infty} \frac{f(w + iu; x)}{e^{2\pi(u-iw)} - 1} dw. \quad (12)$$

Even in this reduced form, it is usually difficult to evaluate H directly. However, it may be possible to proceed using the fact that $|e^{2\pi(u-iw)}| > 1$, and so

$$H = 2 \sum_{j=1}^{\infty} e^{-2\pi ju} \operatorname{Re} \int_{-\infty}^{\infty} f(w + iu; x) e^{2\pi i j w} dw. \quad (13)$$

Generally, the integral in (13) is easier to evaluate than the integral in (12). Failing this, a useful bound can be obtained by noting that

$$|H| < \frac{2}{e^{2\pi u} - 1} \int_{-\infty}^{\infty} |f(w + iu; x)| dw. \quad (14)$$

The factor $e^{2\pi u}$ appearing in the denominator will often facilitate a proof that H is exponentially small.

Finally, we must consider V . Again assuming that the Schwarz reflection principle (11) holds and setting $v = u$, we parametrize the contours in (9) by

writing $s = \pm(Q + \frac{1}{2}) \pm iw$. In this way, we find that

$$V = -2 \lim_{Q \rightarrow \infty} \int_0^u \operatorname{Im} \left[f(Q + \frac{1}{2} + iw; x) - f(-Q - \frac{1}{2} + iw; x) \right] \frac{dw}{1 + e^{2\pi w}}. \quad (15)$$

For most series of practical interest, $f(s; x) \rightarrow 0$ as $s \rightarrow \infty$, at least in the vicinity of the real line, and we aim to use this to show that $V = 0$. A simple strategy is to find an upper bound for the modulus of the term in square brackets. That is, we write

$$M(Q) = \max_{0 \leq w \leq u} \left| \operatorname{Im} \left[f(Q + \frac{1}{2} + iw; x) - f(-Q - \frac{1}{2} + iw; x) \right] \right|,$$

and observe that

$$\begin{aligned} |V| &\leq 2 \lim_{Q \rightarrow \infty} M(Q) \int_0^u \frac{dw}{1 + e^{2\pi w}} \\ &\leq \frac{1}{\pi} \lim_{Q \rightarrow \infty} M(Q), \end{aligned}$$

having replaced the denominator with $e^{2\pi w}$ to reach the last line. It then remains to show that $M(Q) \rightarrow 0$ as $Q \rightarrow \infty$; the method for achieving this will depend upon the particular form of the function f .

A variation of the above analysis allows us to deal with sums in which the index ranges over the natural numbers. The analogue of (4) for this case is

$$\int_0^\infty h(s) ds = \Delta s \left[\frac{h(0)}{2} + \sum_{j=1}^\infty h(j\Delta s) \right] + E,$$

where once again, E represents an error that will disappear as $\Delta s \rightarrow 0$. To obtain additional terms and a bound for the error, we use a contour integral similar to the left-hand side of (5) but with the path now as shown in Figure 2. Assuming $f(s; x)$ is analytic inside the contour, the residue theorem yields

$$\int_\Lambda \frac{f(s; x)}{e^{2\pi is} - 1} ds = \sum_{j=1}^Q f(j; x). \quad (16)$$

As before, the exponential in the denominator will prove useful in showing that the integral along the lower edge is small for large v , and we use (6) to rewrite the contributions from the upper half-plane in the form

$$\int_{\Lambda_{1,2,3}} \frac{f(s; x)}{e^{2\pi is} - 1} ds = \int_{\Lambda_{1,2,3}} \frac{f(s; x)}{1 - e^{-2\pi is}} ds - \int_{\Lambda_{1,2,3}} f(s; x) ds. \quad (17)$$

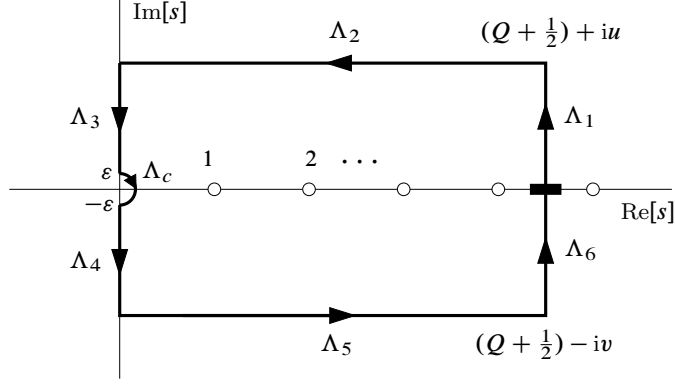


Figure 2: The closed contour Λ , consisting of the straight sections $\Lambda_1, \dots, \Lambda_6$ and the semi-circle Λ_c . The black bar denotes the division between Λ_6 and Λ_1 at $s = Q + \frac{1}{2}$.

Some care must now be taken with limits. Since there is a pole at the origin (unless it should happen that $f(0; x) = 0$), we cannot let $\varepsilon \rightarrow 0$ in (17). However, the last integral does not possess this singularity, so

$$\lim_{Q \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} \int_{\Lambda_{1,2,3}} f(s; x) ds = - \int_0^\infty f(s; x) ds. \quad (18)$$

Therefore, letting $Q \rightarrow \infty$ in (16) yields

$$\sum_{j=1}^{\infty} f(j; x) = \int_0^\infty f(s; x) ds + H + R + L, \quad (19)$$

where H , R , and L denote contributions from the horizontal, left, and right edges of Λ , respectively. That is,

$$H = \lim_{Q \rightarrow \infty} \left[\int_{\Lambda_2} \frac{f(s; x)}{1 - e^{-2\pi i s}} ds + \int_{\Lambda_5} \frac{f(s; x)}{e^{2\pi i s} - 1} ds \right], \quad (20)$$

$$R = \lim_{Q \rightarrow \infty} \left[\int_{\Lambda_1} \frac{f(s; x)}{1 - e^{-2\pi i s}} ds + \int_{\Lambda_6} \frac{f(s; x)}{e^{2\pi i s} - 1} ds \right], \quad (21)$$

and

$$L = \lim_{\varepsilon \rightarrow 0} \left[\int_{\Lambda_3} \frac{f(s; x)}{1 - e^{-2\pi i s}} ds + \int_{\Lambda_{4,c}} \frac{f(s; x)}{e^{2\pi i s} - 1} ds \right]. \quad (22)$$

The first of these can be treated following the procedure used in the previous case; one need only change the lower limit of integration to zero in (10) and (12)–(14) to obtain the relevant equations. Similarly, the contributions from the right edges of Λ and Ω are the same. Therefore, if $f(s; x)$ is real for positive real s , then a simplified form for R is given by (15) with the second term inside the square brackets omitted. However, the location of left edge is now fixed, so we must deal with L in some other way. Parametrizing Λ_3 , Λ_4 , and Λ_c by writing $s = iw$, $s = -iw$, and $s = \varepsilon e^{i\theta}$, we find that

$$L = i \lim_{\varepsilon \rightarrow 0} \left[\int_{\varepsilon}^u \frac{f(iw; x)}{e^{2\pi w} - 1} dw - \int_{\varepsilon}^v \frac{f(-iw; x)}{e^{2\pi w} - 1} dw - \int_{-\pi/2}^{\pi/2} \frac{\varepsilon e^{i\theta} f(\varepsilon e^{i\theta}; x)}{\exp(2\pi i \varepsilon e^{i\theta}) - 1} d\theta \right]. \quad (23)$$

If $f(s; x)$ is analytic at $s = 0$, then the limit $\varepsilon \rightarrow 0$ commutes with the last integral. The first two terms can also be simplified if $f(s; x)$ is real for real positive s . Setting $v = u$ then leads to the result

$$L = -2 \int_0^u \frac{\text{Im}[f(iw; x)]}{e^{2\pi w} - 1} dw - \frac{f(0; x)}{2}. \quad (24)$$

The remaining integral in (24) must be evaluated exactly, or at least approximated, in order to gain an useful expansion for the series. One possibility is to use a Maclaurin series. Thus, if

$$f(s; x) = \sum_{j=0}^{\infty} a_j(x) s^j, \quad (25)$$

then

$$L = -\frac{a_0(x)}{2} + 2 \sum_{j=1}^{\infty} a_{2j-1}(x) (-1)^j \int_0^u \frac{w^{2j-1}}{e^{2\pi w} - 1} dw. \quad (26)$$

In principle, further progress can be made using repeated integration by parts, because it follows from [4, equations (7.1) and (7.2)] that

$$\text{Li}_0(e^{-2\pi w}) = \frac{1}{e^{2\pi w} - 1} \quad \text{and} \quad \frac{d}{dw} \text{Li}_n(e^{-2\pi w}) = -2\pi \text{Li}_{n-1}(e^{-2\pi w}),$$

where $\text{Li}_n(\cdot)$ represents the polylogarithm of order n . However, the resulting expressions are complicated and unlikely to be useful. Alternatively, if it

is possible to let $u \rightarrow \infty$, we may use the much simpler result [2, equation 3.411(2)]

$$\int_0^\infty \frac{w^{2j-1}}{e^{2\pi w} - 1} dw = (-1)^{j+1} \frac{B_{2j}}{4^j}, \quad j = 1, 2, \dots, \quad (27)$$

where B_j represents a Bernoulli number. However, a word of caution is in order here. To reach (26) from (25), we interchanged an infinite series with an integration, and this procedure may not be formally valid if the integral is improper. The effect of this can be observed from the fact that replacing u with infinity in (26) and using (27) yields

$$L = -\frac{a_0(x)}{2} - \sum_{j=1}^{\infty} a_{2j-1}(x) \frac{B_{2j}}{2^j}. \quad (28)$$

Since the coefficient function $a_{2j-1}(x)$ is arbitrary at this point, we cannot say for certain whether the series on the right-hand side is convergent, but in most cases it will be divergent, because the magnitude $|B_{2j}|$ grows *very* rapidly with j . Nevertheless, using a finite number of terms may produce a useful asymptotic representation for L , as we will see in our second example.

3 Examples.

We now apply the trapezoidal rule to the three example series from Part 1; that is $S(x)$ from (1) and then $T(x)$ and $F(x)$ from (3). In each case, x is a positive parameter, and the initial form of the series converges rapidly for small values. We seek alternative forms of the series that provide accurate values for large x .

3.1 Even summand.

For the simple case of Poisson's series $S(x)$, we begin by writing

$$f(s; x) = e^{-s^2/x^2}. \quad (29)$$

As in Part 1, we take advantage of the fact that the summand is an even function, writing

$$S(x) = \frac{1}{2} \left(-1 + \sum_{j=-\infty}^{\infty} e^{-j^2/x^2} \right). \quad (30)$$

We then use (29) in (7) to obtain

$$2S(x) + 1 = x\sqrt{\pi} + H + V, \quad (31)$$

where now

$$H = 2 \operatorname{Re} \int_{-\infty}^{\infty} \frac{e^{-(w+iu)^2/x^2}}{e^{2\pi(u-iw)} - 1} dw \quad (32)$$

and

$$V = 4 \lim_{Q \rightarrow \infty} e^{-(Q+1/2)^2/x^2} \int_0^u \sin((2Q+1)w/x^2) \frac{e^{w^2/x^2}}{1 + e^{2\pi w}} dw. \quad (33)$$

The integral in (32) can be evaluated using (13). We find that

$$\begin{aligned} H &= 2 \sum_{j=1}^{\infty} e^{-2\pi j u} \operatorname{Re} \int_{-\infty}^{\infty} e^{-(w+iu)^2/x^2} e^{2\pi i j w} dw \\ &= 2x\sqrt{\pi} \sum_{j=1}^{\infty} e^{-(j\pi x)^2}, \end{aligned}$$

having used the substitution $w = t + i(\pi j x^2 - u)$. In view of this, we can choose any finite value for u . For example, with $u = 1$ we have

$$|V| \leq 4 \lim_{Q \rightarrow \infty} e^{-(Q+1/2)^2/x^2} \int_0^1 \frac{e^{w^2/x^2}}{1 + e^{2\pi w}} dw,$$

which clearly shows that $V = 0$. Rearranging (31) now yields (2).

3.2 A summand without symmetry.

We now consider the series $T(x)$ from (3). To apply the trapezoidal rule here we must use (19), because the index clearly cannot be extended to $-\infty$ in a manner similar to (30). The necessary integral is given in Part 1; we have

$$\int_0^{\infty} e^{-s^3/x^3} ds = x\Gamma\left(\frac{4}{3}\right), \quad x > 0,$$

where $\Gamma(\cdot)$ represents the Gamma function [5, Chapter 5]. Consequently (19) yields

$$T(x) = x\Gamma\left(\frac{4}{3}\right) + H + R + L, \quad (34)$$

with

$$H = 2 \operatorname{Re} \int_0^\infty \frac{e^{-(w+iu)^3/x^3}}{e^{2\pi(u-iw)} - 1} dw, \quad (35)$$

$$R = 2 \lim_{Q \rightarrow \infty} e^{-(Q+1/2)^3/x^3} \int_0^u e^{3w^2(Q+1/2)/x^3} \sin\left(\frac{3w(Q + \frac{1}{2})^2 - w^3}{x^3}\right) \frac{dw}{1 + e^{2\pi w}}, \quad (36)$$

and

$$L = -\frac{1}{2} - 2 \int_0^u \frac{\sin(w^3/x^3)}{e^{2\pi w} - 1} dw. \quad (37)$$

Now

$$|H| < \frac{2}{e^{2\pi u} - 1} \int_0^\infty e^{-(w^3-3wu^2)/x^3} dw,$$

and this can be bounded by setting $u = x$ and then writing $w = xt$. In this way, we find that

$$|H| < \frac{2x}{e^{2\pi x} - 1} \int_0^\infty e^{3t-t^3} dt.$$

The remaining integral does not depend on x . It can be bounded by splitting the integration path at $t = 2$. To the left of this point the integrand is bounded above by e^2 , and to the right we have $3t - t^3 < -t$. Therefore

$$|H| < \frac{2x}{e^{2\pi x} - 1} (2e^2 + e^{-2}).$$

Clearly this term is exponentially small for large x . For R we observe that the magnitude of the integrand (with $u = x$) is bounded above by $e^{3(Q+1/2)/x} e^{-2\pi w}$. Taking the limit $Q \rightarrow \infty$ then shows that $R = 0$. Finally, consider L . We can derive an asymptotic expansion by writing the sine function as a Maclaurin series. Repeating the calculation for the specific case of (37) turns out to be slightly easier than using the general formulae (25) and (28). Thus, we have the exact result

$$L = -\frac{1}{2} + 2 \sum_{p=1}^{\infty} \frac{(-1)^p}{(2p-1)! x^{6p-3}} \int_0^x \frac{w^{6p-3}}{e^{2\pi w} - 1} dw,$$

and since we are aiming to find an approximation of $T(x)$ for large x , we may extend the upper limit to infinity to make the integration straightforward at

the cost of causing the series to diverge. In this way, we obtain the asymptotic formula

$$L = -\frac{1}{2} + \frac{1}{2} \sum_{p=1}^r \frac{B_{6p-2}}{(2p-1)!(3p-1)x^{6p-3}} + O(x^{-6r-3}),$$

having used (27). Using this in (34), we find that

$$T(x) = x\Gamma\left(\frac{4}{3}\right) - \frac{1}{2} + \frac{1}{2} \sum_{p=1}^r \frac{B_{6p-2}}{(2p-1)!(3p-1)x^{6p-3}} + O(x^{-6r-3}), \quad (38)$$

which is the expansion we found in Part 1.

3.3 A summand with a real singularity.

Finally, we tackle the series $F(x)$ from (3). To apply the trapezoidal rule in this case, we must overcome several technical difficulties associated with complex logarithms. This calculation will lead us into some of the darker recesses of the complex plane; anyone who shivers at the mention of a branch cut should probably stop reading now. To avoid any ambiguity, we will use the convention that $\ln(\cdot)$ represents the real natural logarithm (which exists only for positive real arguments), whereas

$$\log z = \ln |z| + i \arg z$$

is defined for $z \in \mathbb{C} \setminus \{0\}$ up to an additive factor $2j\pi i$, $j \in \mathbb{Z}$. Now, let

$$f(s; x) = \log(1 - e^{-s^2/x^2}). \quad (39)$$

Clearly there is a branch point at the origin in the s -plane. We place the cut on the negative real axis and choose a branch so that $f(s; x)$ is real for positive real s . Expanding the exponential as a Maclaurin series shows that

$$f(s; x) = \log(s^2/x^2) + \log\left(1 + \sum_{j=1}^{\infty} \frac{(-1)^j}{(j+1)!} (s/x)^{2j}\right). \quad (40)$$

The imaginary part of (39), which is the argument of the complex quantity $1 - e^{-s^2/x^2}$, must vary continuously within the cut plane. Therefore, if s moves from the positive real axis to the negative real axis, traversing a semicircle

centered at the origin, $\pm 2\pi$ is added to the imaginary part of f with the sign depending on the orientation of the path. Consequently, a continuous branch of $f(s; x)$ that vanishes as $s \rightarrow +\infty$ cannot vanish as $s \rightarrow -\infty$. This causes enormous complications if we extend the summation to include negative indices as we did for Poisson's series $S(x)$. Instead we follow the approach used for $T(x)$, integrating around the contour Λ (Figure 2), so that we need not be concerned with the behavior of $f(s; x)$ in the left half of the s -plane. In the right half-plane, there are branch points at $s = s_j^\pm$, where

$$s_j^\pm = x\sqrt{2j\pi}e^{\pm i\pi/4} = x\sqrt{j\pi}(1 \pm i), \quad j = 1, 2, \dots \quad (41)$$

We place branch cuts on the lines $s = s_j^\pm \pm iw$, $w > 0$, and initially assume that neither u nor v exceeds $x\sqrt{\pi}$ so that all points s_j^\pm lie outside the contour Λ and therefore do not interfere with the calculation. Since the configuration of singularities is symmetric about the real axis, it is natural to set $u = v$, after which the Schwarz reflection principle (11) applies for $s \in \Lambda$.

The next step is to substitute (39) into (19). It should be noted that (19) depends on (18), which remains valid because the singularity of $f(s; x)$ at the origin is integrable. In this way, we find that

$$F(x) = -\frac{x\sqrt{\pi}}{2} \zeta\left(\frac{3}{2}\right) + H + R + L, \quad (42)$$

where $\zeta(\cdot)$ represents the Riemann zeta function [5, Chapter 25]. In (42), H , R , and L are the contributions from the horizontal, right, and left edges of the contour, given by (20)–(22), respectively, and we have used the fact that

$$\int_0^\infty \ln(1 - e^{-s^2/x^2}) ds = -\frac{x\sqrt{\pi}}{2} \zeta\left(\frac{3}{2}\right),$$

which was derived in Part 1. Our strategy for evaluating the remaining terms in (42) is to allow the contour to expand vertically as well as horizontally in the limit $Q \rightarrow \infty$. It is then possible to evaluate H exactly, by summing the contributions from the branch cuts emanating from the singularities at $s = s_j^+$. We can also evaluate L exactly, though it is necessary to return to (23) in order to achieve this; (24) is not valid here because $f(0; x)$ does not exist. However, we must first find an appropriate value for u , by considering the contribution from the right edge of Λ . A simplified expression for this is given by (15) with the second term in the square bracket omitted (see Section

2); thus

$$R = -2 \lim_{Q \rightarrow \infty} \int_0^u \operatorname{Im} \left[f \left(Q + \frac{1}{2} + iw; x \right) \right] \frac{dw}{1 + e^{2\pi w}}.$$

On the path of integration, the imaginary part of f is the argument of the complex quantity

$$1 - e^{-(Q+1/2+iw)^2/x^2} = 1 - e^{(w^2 - (Q+1/2)^2 - iw(2Q+1))/x^2},$$

which clearly lies in the right half-plane if $w < Q + \frac{1}{2}$. Moreover, since $f(s; x)$ is real for positive real s (so that the argument is zero), a continuous branch can only be maintained by using the principal value (with imaginary part in the interval $(-\pi, \pi]$) whenever w satisfies this inequality. Since the upper bound for w is u , a natural choice is to set $u = Q$. The argument can then be determined using the inverse sine function; thus

$$R = -2 \lim_{Q \rightarrow \infty} \int_0^Q \arcsin \left(\frac{e^{(w^2 - (Q+1/2)^2)/x^2} \sin(w(2Q+1)/x^2)}{|1 - e^{(w^2 - (Q+1/2)^2 - iw(2Q+1))/x^2}|} \right) \frac{dw}{1 + e^{2\pi w}}.$$

Then, by maximizing the modulus of the argument to the inverse sine function, we find that

$$\begin{aligned} |R| &\leq 2 \lim_{Q \rightarrow \infty} \arcsin \left(\frac{e^{(Q^2 - (Q+1/2)^2)/x^2}}{1 - e^{(Q^2 - (Q+1/2)^2)/x^2}} \right) \int_0^\infty \frac{dw}{e^{2\pi w}} \\ &\leq \frac{1}{\pi} \lim_{Q \rightarrow \infty} \arcsin \left(\frac{e^{-(Q+1/4)/x^2}}{1 - e^{-(Q+1/4)/x^2}} \right) \\ &= 0. \end{aligned} \tag{43}$$

Next consider L . Unlike the corresponding integral for $T(x)$ (which is (37)), this contribution depends on Q , because we are expanding the contour vertically as well as horizontally. Therefore (23) becomes

$$L = \lim_{Q \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} \left[-2 \int_\varepsilon^Q \frac{\operatorname{Im}[f(iw; x)]}{e^{2\pi w} - 1} dw - \int_{-\pi/2}^{\pi/2} \frac{i\varepsilon e^{i\theta} f(\varepsilon e^{i\theta}; x)}{\exp(2\pi i \varepsilon e^{i\theta}) - 1} d\theta \right].$$

To determine $f(iw; x)$, we begin by observing that the argument of $1 - e^{-(iw)^2/x^2}$ is fixed for $w > 0$. Then, if we allow s to traverse a small circular arc from $s = \varepsilon$ to $s = \varepsilon e^{i\pi/2}$, (40) shows that the argument varies continuously from zero to π . Therefore $\operatorname{Im}[f(iw; x)] = \pi$ in the above expression for L . For the

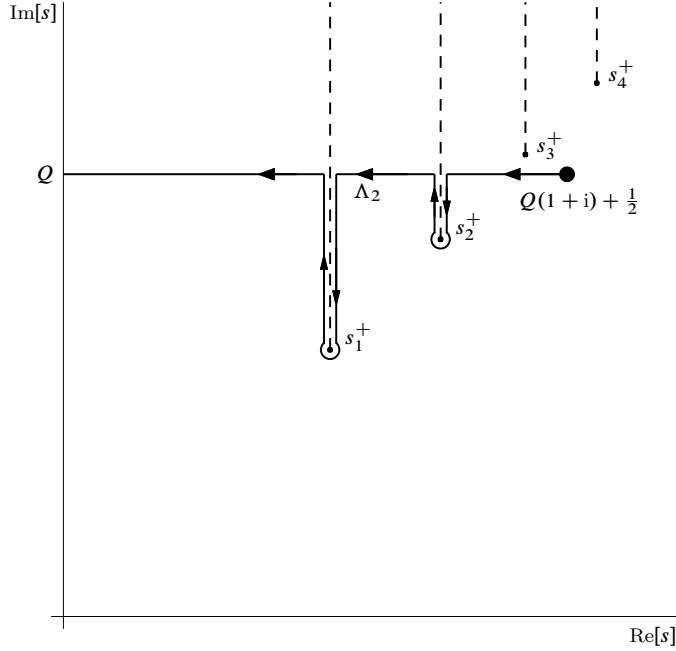


Figure 3: The deformed contour Λ_2 , with $x\sqrt{3\pi} > Q > x\sqrt{2\pi}$. The dashed lines represent branch cuts.

second integral, we expand the integrand as a series in ε using (40), retaining only those terms that do not vanish as $\varepsilon \rightarrow 0$. The result is that

$$L = - \lim_{Q \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} \left[2\pi \int_{\varepsilon}^Q \frac{dw}{e^{2\pi w} - 1} + \frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} \log(\varepsilon^2 e^{2i\theta}/x^2) d\theta \right]. \quad (44)$$

After evaluating the integrals and taking the two limits, we arrive at the result

$$L = \ln(2\pi x). \quad (45)$$

Finally, consider H . Applying the Schwarz reflection principle (11), we find that

$$H = 2 \operatorname{Re} \int_{\Lambda_2} \frac{f(s; x)}{1 - e^{-2\pi i s}} ds. \quad (46)$$

As Q is increased, the contour Λ_2 “wraps” around the branch cuts emanating from $s = s_j^+$ (see (41)). This is illustrated in Figure 3. The lowest point on Λ_2 is then fixed by the branch point s_1^+ ; its imaginary part is $x\sqrt{\pi}$. Since there is a factor $e^{-2\pi i s}$ in the denominator of the integrand in (46), we may

conclude that $|H|$ is proportional to $e^{-2\pi^{3/2}x}$ and so decreases exponentially as $x \rightarrow \infty$. Using the values we have obtained for R and L , (42) now reproduces the result calculated using the Euler–Maclaurin formula in Part 1. However, we can go further and determine H exactly by reasoning as follows. Suppose that Q exceeds $x\sqrt{j\pi}$ for some positive integer j . Denoting the diversion around the branch cut emanating from s_j^+ by Λ_j^+ , we find that

$$\int_{\Lambda_j^+} \frac{f(s; x)}{1 - e^{-2\pi is}} ds = \int_{(1+i)x\sqrt{j\pi}}^{x\sqrt{j\pi}+iQ} \frac{f_\ell(s; x)}{1 - e^{-2\pi is}} ds - \int_{(1+i)x\sqrt{j\pi}}^{x\sqrt{j\pi}+iQ} \frac{f_r(s; x)}{1 - e^{-2\pi is}} ds, \quad (47)$$

where the subscripts “ ℓ ” and “ r ” denote evaluation on the left and right faces of the branch cut, respectively. Now the only difference between f_ℓ and f_r is due to the change in argument that occurs as the contour encircles the branch point. This circle is traversed clockwise, and $1 - e^{-s^2/x^2}$ has a simple zero at $s = s_j^+$, so it follows that

$$f_\ell(s; x) = f_r(s; x) - 2\pi i.$$

Consequently, (47) reduces to

$$\int_{\Lambda_j^+} \frac{f(s; x)}{1 - e^{-2\pi is}} ds = 2\pi \int_{x\sqrt{j\pi}}^Q \frac{dw}{1 - e^{2\pi w} e^{-ik_j}}, \quad (48)$$

where

$$k_j = 2\sqrt{j\pi}^{3/2}x,$$

and the substitution $s = x\sqrt{j\pi} + iw$ has been used. In view of (46), only the real part of (48) contributes to H . This avoids any further technicalities involving complex logarithms; indeed

$$\begin{aligned} \operatorname{Re} \int_{\Lambda_j^+} \frac{f(s; x)}{1 - e^{-2\pi is}} ds &= 2\pi \operatorname{Re} \int_{x\sqrt{j\pi}}^Q \frac{dw}{1 - e^{2\pi w} e^{-ik_j}} \\ &= -\operatorname{Re} \left[\log(e^{-2\pi w} - e^{-ik_j}) \right]_{x\sqrt{j\pi}}^Q \\ &= \frac{1}{2} \ln \left(\frac{1 - 2e^{-k_j} \cos k_j + e^{-2k_j}}{1 - 2e^{-2\pi Q} \cos k_j + e^{-4\pi Q}} \right). \end{aligned} \quad (49)$$

The exact value for H is then obtained by taking the limit $Q \rightarrow \infty$ and summing over j (noting the factor 2 in (46)). That is,

$$H = \sum_{j=1}^{\infty} \ln(1 - 2e^{-k_j} \cos k_j + e^{-2k_j}). \quad (50)$$

In this last step, we have implicitly assumed that contributions from the remaining horizontal parts of the contour (i.e., those between the branch cuts, and the sections joining Λ_2 to the vertical edges Λ_1 and Λ_3) disappear as $Q \rightarrow \infty$. In some sense this is obviously true, because the integrand decays exponentially as the contour is moved upwards. This might just be enough to satisfy an applied mathematician, physicist or engineer. However, the distance between adjacent branch points is

$$|s_{j+1}^{\pm} - s_j^{\pm}| = x\sqrt{2\pi}(\sqrt{j+1} - \sqrt{j}),$$

and this tends to zero as j is increased. This means we cannot avoid the appearance of a singularity either on or close to the path of integration as the contour is moved upwards, which might alarm readers of a “pure” disposition. A rigorous proof that the horizontal sections can indeed be disregarded is provided in the supplemental material.

Finally, we piece together all of our results by substituting (43), (45), and (50) into (42). Recalling the definition of F from (3), we arrive at the exact result

$$F(x) = \sum_{j=1}^{\infty} \ln(1 - e^{-j^2/x^2}) = \ln(2\pi x) - \frac{x\sqrt{\pi}}{2} \zeta\left(\frac{3}{2}\right) + \sum_{j=1}^{\infty} \ln\left(1 - 2e^{-2\sqrt{j}\pi^{3/2}x} \cos(2\sqrt{j}\pi^{3/2}x) + e^{-4\sqrt{j}\pi^{3/2}x}\right). \quad (51)$$

All of the terms appearing here are elementary, except the Riemann zeta function, for which we need only the single value

$$\zeta\left(\frac{3}{2}\right) = \sum_{j=1}^{\infty} \frac{1}{j^{3/2}} = 2.612375348685488\dots$$

The series on the right-hand side of (51) converges very rapidly for large x and its value is negligible relative to the other two terms unless x is small. Retaining only the leading contribution to the series results in the three-term approximation

$$\sum_{j=1}^{\infty} \ln(1 - e^{-j^2/x^2}) = \ln(2\pi x) - \frac{x\sqrt{\pi}}{2} \zeta\left(\frac{3}{2}\right) - 2 \cos(2\pi^{3/2}x) e^{-2\pi^{3/2}x} + O(e^{-(2\pi)^{3/2}x}), \quad (52)$$

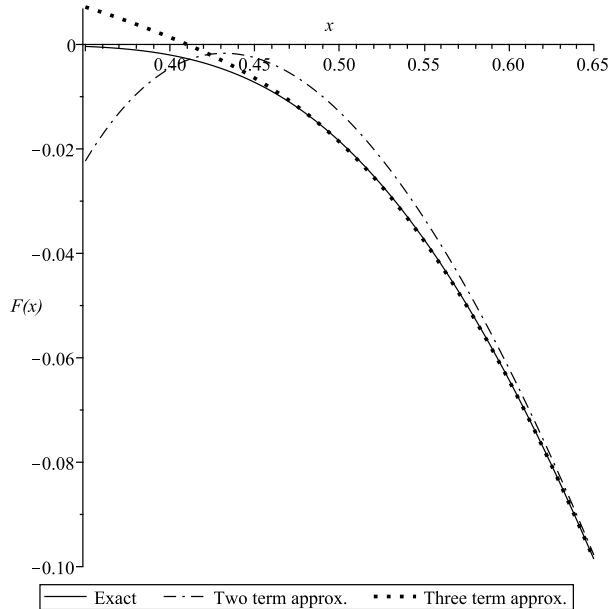


Figure 4: The function $F(x)$, two-term approximation (obtained by discarding the sum from the right-hand side of (51)), and three-term approximation (52).

verifying our earlier prediction that $|H|$ is proportional to $e^{-2\pi^{3/2}x}$, and also confirming that the error in the formula we found in Part 1 is exponentially small. Plots of the function $F(x)$ and the two- and three-term approximations are shown in Figure 4, for $0.35 \leq x \leq 0.65$. The three-term approximation is visually indistinguishable from the exact curve for $x > 0.48$. All three curves are visually indistinguishable for $x > 0.65$.

Transformations for some other, similar, series can be obtained directly from (51). For example if

$$F_2(x) = \sum_{j=1}^{\infty} \ln(1 - e^{-(2j-1)^2/x^2}) \quad \text{and} \quad F_3(x) = \sum_{j=1}^{\infty} \ln(1 + e^{-j^2/x^2}),$$

then (following [1]),

$$F(x) - F(x/2) = \sum_{j=1}^{\infty} \left[\ln(1 - e^{-j^2/x^2}) - \ln(1 - e^{-(2j)^2/x^2}) \right] = F_2(x),$$

and

$$F(\sqrt{2}x) + F_3(\sqrt{2}x) = F(x).$$

It is noted in [1] that both $F_2(x)$ and $F_3(x)$ are approximately linear for large x . This follows directly from (52); indeed

$$F_2(x) \approx \ln(2) - \frac{x\sqrt{\pi}}{4} \zeta\left(\frac{3}{2}\right) \quad \text{and} \quad F_3(x) \approx -\frac{\ln 2}{2} + (2 - \sqrt{2}) \frac{x\sqrt{\pi}}{4} \zeta\left(\frac{3}{2}\right),$$

with exponentially small errors in both cases.

4 Concluding remarks.

We have considered two methods for finding asymptotic expansions of series and products that contain a large (or small) parameter. Of the two, Euler–Maclaurin summation is perhaps slightly simpler, in that it requires fewer exact integrations. On the other hand, the trapezoidal rule also enables us to derive exact relationships between certain series that have opposing convergence properties, in the sense that one series converges rapidly for small x (say) whereas the other converges rapidly for large x .

A final remark concerns series obtained by taking logarithms of infinite products, as in our third example. It should not be thought that the elementary exact integrations that occurred when calculating the contribution from the left edge of the contour Λ (see (44)–(45)) were due to chance, or a contrived (or inspired) choice of example. Since real summands satisfy the Schwarz reflection principle (11), only the imaginary part of f contributes to the integrals in (23). In other words, the logarithm itself disappears, leaving only the argument, which is constant. The same phenomenon facilitated the exact determination of the branch cut contributions at the end of Section 3. Here the difference between the logarithms on opposite faces of the cut is constant, and this leads to the simple integration in (49). Thus the trapezoidal rule offers a very promising general technique for analyzing infinite products.

We leave this subject (for now at least) with a challenge. Is it possible to obtain exact transformations of series whose summand is not an even function, such as $T(x)$ in (3)? The best we could do, using either the Euler–Maclaurin formula or the trapezoid rule, is the asymptotic formula (38). Might there be something even better?

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Analysis of Series and Products: Supplemental Material for Part 2

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August 11, 2020

A daunting proof.

In achieving the exact transformation of the series

$$F(x) = \sum_{j=1}^{\infty} \ln(1 - e^{-j^2/x^2})$$

in the main part of the article, we assumed that

$$\lim_{Q \rightarrow \infty} \int_{\Lambda_2^h} \frac{f(s; x)}{1 - e^{-2\pi is}} ds = 0,$$

where

$$f(s; x) = \log(1 - e^{-s^2/x^2}).$$

The contour Λ_2^h consists of the union of horizontal sections of the contour Λ_2 , which joins the point $s = Q(1 + i) + \frac{1}{2}$ to $s = iQ$, and is diverted around the branch cuts of $f(s; x)$, as shown in Figure 1.

We now present a rigorous proof that this assumption is indeed correct. The first step is to determine a bound for the imaginary part of the complex logarithm. Since the branch is chosen so that $f(s; x)$ is real for positive, real s it follows that the principal value can be used except at points separated from the positive real axis by a branch cut or a curve on which $1 - e^{-s^2/x^2}$ is real and negative. To locate these curves, we simply write $s = \alpha + i\beta$, and we easily find that

$$\alpha^2 - \beta^2 < 0 \quad \text{and} \quad \alpha\beta = j\pi x^2, \quad j \in \mathbb{Z}. \quad (1)$$

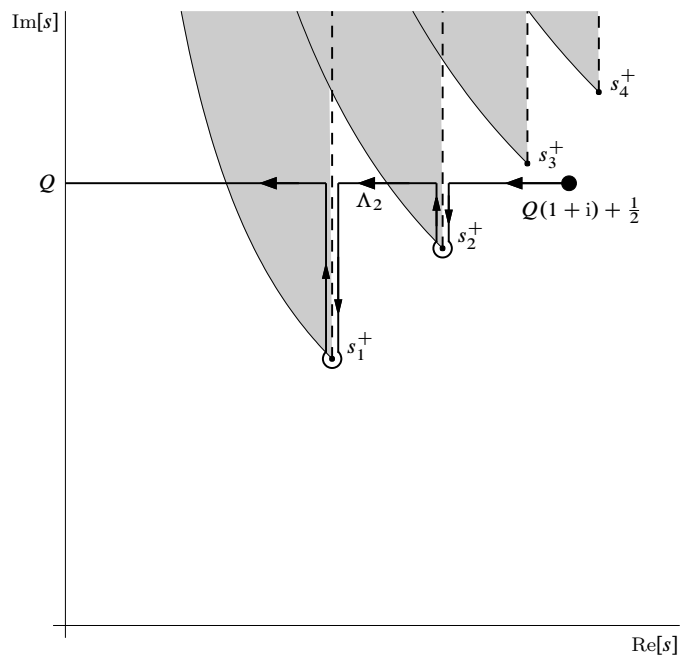


Figure 1: The contour Λ_2 , with $x\sqrt{3\pi} > Q > x\sqrt{2\pi}$. The dashed lines indicate the locations of the branch cuts, and the shaded gray areas are regions in which $\arg(1 - e^{-s^2/x^2})$ may lie outside the interval $(-\pi, \pi]$.

Note that $\alpha = 0$ corresponds to the imaginary axis, which is never crossed. The curves in the upper right quadrant are given by (1) with j , α , and β all positive, and $\beta > \alpha$. In each case, $\alpha = \beta$ corresponds to a branch point, because here we have $s = s_j^+$, where

$$s_j^\pm = x\sqrt{2j\pi}e^{\pm i\pi/4} = x\sqrt{j\pi}(1 \pm i), \quad j = 1, 2, \dots \quad (2)$$

A sketch of the first four curves is shown in Figure 1. Next consider the variation in $\arg(1 - e^{-s^2/x^2})$ as s passes along Λ_2 , moving from right to left and diverting around the branch cuts as illustrated in Figure 1. Before the first cut is reached, the argument must lie in the interval $(-\pi, \pi)$. However, as s climbs along the left face of a branch cut, it crosses at least one of the curves defined in (1). The number of curves crossed is bounded above by the number of branch points s_j^+ whose imaginary part satisfies $\text{Im } s_j^+ \leq Q$, which is the integer part of $Q^2/(x^2\pi)$. Each crossing causes the argument to move from the interval $(p\pi, (p+2)\pi)$ to either $((p+2)\pi, (p+4)\pi)$ or $((p-2)\pi, p\pi)$, for some $p \in \mathbb{Z}$. Each curve is then crossed a second time as s moves horizontally and then down the right face of the next branch cut. Before reaching the next branch point, s must pass back into the unshaded region, so that the argument is again a principal value. Assuming a *worst case* scenario in which the magnitude of the argument increases monotonically as s ascends the left face of a cut gives an upper bound of $\pi + 2Q^2/x^2$.

Now consider the integral along Λ_2^h (the contributions from the faces of the branch cuts have already been included, and so are not important here). Writing $s = w + iQ$ and

$$Z(w; Q) = 1 - \exp[-(w + iQ)^2/x^2],$$

we find that

$$\int_{\Lambda_2^h} \frac{f(s; x)}{1 - e^{-2\pi is}} ds = - \int_0^{Q+1/2} \frac{\ln |Z(w; Q)| + i \arg Z(w; Q)}{1 - e^{2\pi(Q-iw)}} dw. \quad (3)$$

Multiplying the bound for the imaginary part of the numerator by the path length, we see that

$$\left| \int_0^{Q+1/2} \frac{\arg Z(w; Q)}{1 - e^{2\pi(Q-iw)}} dw \right| < \frac{(\pi + 2(Q/x)^2)(Q + \frac{1}{2})}{e^{2\pi Q} - 1},$$

which shows that this term vanishes as $Q \rightarrow \infty$. For the remaining term, we note that $\ln |Z|$ is continuous in (3) unless it should happen that

$Q = x\sqrt{j\pi}$ for some natural number j , in which case there is a singularity at $w = Q$. However, this singularity is logarithmic and therefore integrable. To proceed, we seek simple bounds for the magnitude of $\ln |Z|$. This may be achieved by replacing $|Z|$ with a larger value or a smaller value for $|Z| > 1$ or $|Z| < 1$, respectively. Now,

$$|Z(w; Q)|^2 = 1 + e^{2(Q^2-w^2)/x^2} - 2e^{(Q^2-w^2)/x^2} \cos(2Qw/x^2),$$

and therefore

$$(1 - e^{(Q^2-w^2)/x^2})^2 \leq |Z(w; Q)|^2 \leq (1 + e^{(Q^2-w^2)/x^2})^2, \quad (4)$$

but it is difficult to determine which bound should be used throughout the path in (3). Clearly $|Z| > 1$ when $e^{(Q^2-w^2)/x^2} > 2$, so we define

$$w_0 = \sqrt{Q^2 - x^2 \ln 2};$$

since we are to take the limit $Q \rightarrow \infty$, we may assume that $Q^2 > x^2 \ln 2$. Then

$$\left| \int_0^{w_0} \frac{\ln |Z(w; Q)|}{1 - e^{2\pi(Q-iw)}} dw \right| \leq \frac{\sqrt{Q^2 - x^2 \ln 2}}{e^{2\pi Q} - 1} \ln(1 + e^{Q^2/x^2}) \quad (5)$$

$$\leq \frac{\sqrt{Q^2 - x^2 \ln 2}}{e^{2\pi Q} - 1} \left[\frac{Q^2}{x^2} + \ln(1 + e^{-Q^2/x^2}) \right], \quad (6)$$

which vanishes as $Q \rightarrow \infty$. On the remaining part of the path, from $w = w_0$ to $w = Q + \frac{1}{2}$, we can achieve a bound on the magnitude of $\ln |Z|$ by adding together the bounds from (4). That is, it must be the case that

$$|\ln |Z(w; Q)|| \leq \left| \ln |1 - e^{(Q^2-w^2)/x^2}| \right| + \ln(1 + e^{(Q^2-w^2)/x^2}).$$

The second term on the right-hand side has no singularities, and is maximized by taking $w = w_0$. The argument used in (5)–(6) can be applied to show that its contribution to the integral vanishes in the limit $Q \rightarrow \infty$. For the final term, we split the path again, to resolve the modulus signs. Thus

$$\left| \ln |1 - e^{(Q^2-w^2)/x^2}| \right| = \begin{cases} -\ln(e^{(Q^2-w^2)/x^2} - 1) & \text{if } w_0 \leq w \leq Q, \\ -\ln(1 - e^{(Q^2-w^2)/x^2}) & \text{if } w > Q, \end{cases}$$

from which it follows that

$$\begin{aligned} & \left| \int_{w_0}^{Q+1/2} \ln \left| 1 - e^{(Q^2-w^2)/x^2} \right| \frac{dw}{1 - e^{2\pi(Q-iw)}} \right| \\ & \leq \frac{1}{e^{2\pi Q} - 1} \left| \int_{w_0-Q}^0 \ln(e^{-t(t+2Q)/x^2} - 1) dt + \int_0^{1/2} \ln(1 - e^{-t(t+2Q)/x^2}) dt \right|. \end{aligned} \quad (7)$$

In the first integral on the right-hand side, the exponent lies between zero and $\ln 2$ so that the argument to the logarithm is positive and bounded above by 1. A simplified bound may be obtained by minimizing $t + 2Q$, replacing this with $w_0 + Q$. We then integrate by parts to remove the singularity at $t = 0$. In this way, we find that

$$\left| \int_{w_0-Q}^0 \ln(e^{-t(t+2Q)/x^2} - 1) dt \right| \leq \left| \int_{w_0-Q}^0 \ln(e^{-t(w_0+Q)/x^2} - 1) dt \right| \quad (8)$$

$$\leq \frac{w_0 + Q}{x^2} \left| \int_{w_0-Q}^0 \frac{t dt}{1 - e^{t(w_0+Q)/x^2}} \right|. \quad (9)$$

Using elementary calculus, it is not difficult to show that the function $r(t) = t/(1 - e^{at})$ is monotonic, and $r(0) = -1/a$. Since $a = (w_0 + Q)/x^2 > 0$ in (9), we also have $r(t) \rightarrow -\infty$ as $t \rightarrow -\infty$. Therefore the maximum modulus of the integrand must occur at $t = w_0 - Q$. Multiplying the maximum modulus by the path length and simplifying, we eventually obtain the bound

$$\left| \int_{w_0-Q}^0 \ln(e^{-t(t+2Q)/x^2} - 1) dt \right| < 2(Q - w_0) \ln 2 = \frac{2(x \ln 2)^2}{w_0 + Q}.$$

The same process can be applied to the second integral in (7). In this case we replace $t + 2Q$ with $2Q$, and after integrating by parts, the maximum modulus for the integrand must occur at $t = 0$. The final result is that

$$\left| \int_0^{1/2} \ln(1 - e^{-t(t+2Q)/x^2}) dt \right| \leq \frac{1}{2} \left[1 - \ln(1 - e^{-Q/x^2}) \right].$$

This shows that the term in square brackets in (7) remains bounded as $Q \rightarrow \infty$, which completes the proof.

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