Analysis of Series and Products. Part 1: The Euler–Maclaurin Formula

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Abstract

We explore the applications of the Euler–Maclaurin formula in analyzing functions expressed as infinite series and products. Three illustrative examples show the difficulties that may be encountered and the means by which these can be overcome.

1 Introduction.

A seemingly elementary but rarely discussed problem in mathematics is the following: Given a function $S(x)$ expressed as an infinite series, find the value of the limit

$$\lim_{x\to\infty} S(x)$$

(or perhaps the limit as $x \to 0$). Better still, find an asymptotic expansion for $S(x)$. Exact summation is rarely a practical option, as there are relatively few series for which closed-form expressions are known, and few tools for deriving such formulae. Moreover, the limit $x \to \infty$ may not commute with the implicit limit as the number of terms tends to infinity. For example, if

$$S(x) = \sum_{j=1}^{\infty} \mathrm{e}^{-j^2/x^2} = \lim_{N\to\infty} \sum_{j=1}^{N} \mathrm{e}^{-j^2/x^2}, \tag{1}$$

what can we say about the behavior of $S(x)$ as $x \to \infty$? We would like something more insightful than “It diverges!” For this very simple case

Jacobi's imaginary transformation for theta functions [14, p. 476] gives the exact result

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

Jacobi first published this formula in 1828 [4], but he credits it to Poisson, who found it five years earlier [10, p. 420]. If x is large, then (2) can be used to approximate $S(x)$ as a linear function, with an error proportional to $x\mathrm{e}^{-(\pi x)^2}$. In contrast, (1) is useful for computation when x is small, but inefficient when x is large because many terms are needed in order to obtain an accurate result.

In this article, we show how the Euler–Maclaurin formula can be used to analyze series that contain a large (or small) parameter. This approach works by relating the series to an integral, and before attempting a problem of this type, one should ask the following question: "If the summation symbol were to be replaced by an integral, could the integral be evaluated exactly?" It is likely that progress can be made if the answer is "Yes." The same method can sometimes be applied to infinite products. Thus, if

$$G(x) = \prod_{j=1}^{\infty} g(j; x),$$

where $g(j; x) > 0$ for $j \in \mathbb{N}$ and $g(j, x) \to 1$ as $j \to \infty$, then taking logarithms yields

$$\ln G(x) = \sum_{j=1}^{\infty} \ln g(j; x).$$

Therefore we may treat the product as a series, and take exponentials to obtain a final result.

After reviewing the derivation of the Euler–Maclaurin formula in Section 2, we apply it to three examples in Section 3: first Poisson's series (1), then a series with a summand containing an odd function, with no symmetry about $j = 0$, and finally a more challenging example derived from an infinite product, featuring a logarithm in the summand. In each case, we obtain an asymptotic approximation that produces accurate results for parameter regimes in which the convergence of the original series is very slow.

2 The Euler–Maclaurin Formula.

The Euler–Maclaurin formula is a standard result [5, Chapter 14],[11, Section 3.3], though its use in asymptotically expanding infinite series is somewhat obscure. Perhaps the first mathematician to apply it in this way was Niels Erik Nørlund, around 1924 [8, Chapter 4]. Today it is probably fair to class Nørlund's idea as *well known amongst those to whom it is well known.*[1] To see how the Euler–Maclaurin formula operates, it is useful to begin by reviewing a brief derivation, for which we largely follow [2]. Let n_0 and n_1 be integers with $n_1 > n_0$, and consider the integral

$$\int_{n_0}^{n_1} f(s;x)\,\mathrm{d}s = \sum_{j=n_0}^{n_1-1} \int_j^{j+1} f(s;x)\,\mathrm{d}s.$$

For each term in the sum on the right-hand side, write $f(s;x) = 1 \times f(s;x)$ and integrate by parts, using the antiderivative

$$\int 1\,\mathrm{d}s = s - j - \tfrac{1}{2}. \tag{3}$$

In this way, we find that

$$\int_{n_0}^{n_1} f(s;x)\,\mathrm{d}s = \sum_{j=n_0}^{n_1-1} \left\{ \Big[\big(s-j-\tfrac{1}{2}\big) f(s;x) \Big]_j^{j+1} - \int_j^{j+1} \big(s-j-\tfrac{1}{2}\big) f'(s;x)\,\mathrm{d}s \right\},$$

and then by evaluating the boundary terms and rearranging, we obtain

$$\sum_{j=n_0}^{n_1} f(j;x) = \int_{n_0}^{n_1} f(s;x)\,\mathrm{d}s + \frac{f(n_0;x)+f(n_1;x)}{2} + \sum_{j=n_0}^{n_1-1} \int_j^{j+1} \big(s-j-\tfrac{1}{2}\big) f'(s;x)\,\mathrm{d}s. \tag{4}$$

Here and henceforth, the prime symbol indicates differentiation with respect to the first argument. Now the factor $s - j - \frac{1}{2}$ is the periodic extension of the function $P_1(s) = s - \frac{1}{2}$ from the interval $[0,1)$ to the real line, except at

[1] Credit for this excellent description, which applies to many of the more esoteric mathematical techniques, goes to the late Fritz Ursell [1].

integer values for s where the former takes different values in adjacent terms. However, changing the value of an integrand at isolated points has no effect, so if we write

$$P_1(s) = s - \lfloor s \rfloor - \tfrac{1}{2}, \quad -\infty < s < \infty, \tag{5}$$

where $\lfloor \cdot \rfloor$ means "round down," then the second sum in (4) can be evaluated to yield

$$\sum_{j=n_0}^{n_1} f(j;x) = \int_{n_0}^{n_1} f(s;x)\,\mathrm{d}s + \frac{f(n_0;x)+f(n_1;x)}{2} + \int_{n_0}^{n_1} P_1(s) f'(s;x)\,\mathrm{d}s. \tag{6}$$

This is the first order Euler–Maclaurin formula.

Further formulae are obtained using integration by parts, differentiating f' and integrating P_1. The required antiderivatives are chosen to be continuous, so that boundary terms can only occur at $s = n_0$ or $s = n_1$, and not at the intermediate points $s = n_0 + 1, n_0 + 2, \ldots, n_1 - 1$. We begin by writing

$$P_j(s) = j \int_0^s P_{j-1}(w)\,\mathrm{d}w + c_j, \quad j = 2, 3, \ldots, \tag{7}$$

where the factor j multiplying the integral is included for later convenience. A consequence of this definition is that P_2 is continuous, P_3 is once differentiable, P_4 is twice differentiable, and so on. Now P_2 inherits the 1-periodicity of P_1, because

$$P_2(a+1) - P_2(a) = 2 \int_a^{a+1} P_1(w)\,\mathrm{d}w$$

for any real number a, and the integral of P_1 over one period is zero. (This can easily be deduced from the plot in Figure 1.) For $0 \le s < 1$, we have

$$P_2(s) = 2 \int_0^s \left(w - \tfrac{1}{2}\right) \mathrm{d}w + c_2 = s^2 - s + c_2,$$

and values elsewhere are determined by periodic repetition. It follows that $P_2(s)$ is bounded for $s \in \mathbb{R}$, and since this property turns out to be useful, we will choose the constants c_j so that the functions $P_3, P_4, \ldots$ are also periodic (and therefore bounded). To achieve this, we simply need to ensure that the integral of each function over one period is zero, i.e.,

$$\int_0^1 P_j(w)\,\mathrm{d}w = 0, \quad j = 1, 2, \ldots\ . \tag{8}$$

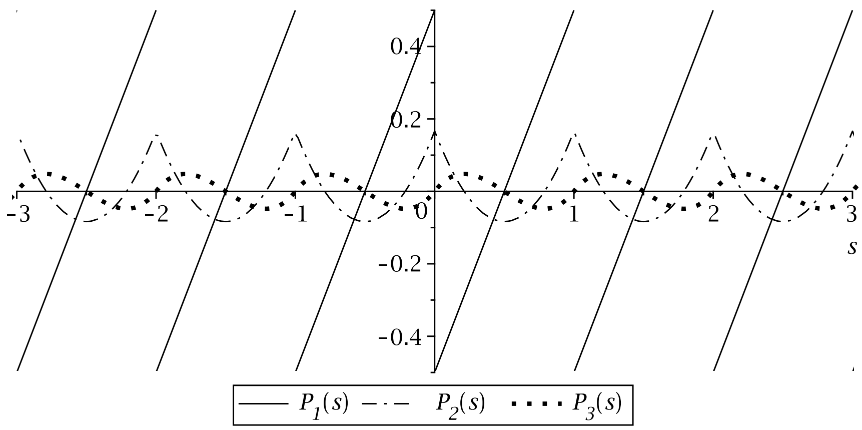

Figure 1: The functions $P_1(s)$, $P_2(s)$, and $P_3(s)$ for $-3 \leq s \leq 3$.

It then follows that $c_2 = \frac{1}{6}$, and in general (using (7)),

$$c_j = -j \int_0^1 \int_0^s P_{j-1}(w)\,\mathrm{d}w\,\mathrm{d}s.$$

The functions that evolve through this process are periodic extensions of the Bernoulli polynomials [9, §24]; indeed,

$$P_j(s) = B_j(s - \lfloor s \rfloor).$$

Graphs of $P_1(s)$, $P_2(s)$, and $P_3(s)$ are shown in Figure 1.

Now $P_1(s)$ is antisymmetric about $s = \frac{1}{2}$, which means $P_2(s)$ is symmetric. It then follows that $P_3(s)$ is antisymmetric except possibly for a constant vertical shift. However, (8) can only hold if the vertical shift is absent, so $P_3(\frac{1}{2}) = 0$ and $P_3(0) = -P_3(1)$. By periodicity $P_3(0) = P_3(1)$, and this is only possible if $P_3(0) = c_3 = 0$. The alternating pattern of symmetry and antisymmetry continues throughout the sequence, meaning that $c_{2j+1} = 0$,

$$P_{2j-1}(n + \tfrac{1}{2}) = 0, \quad \text{and} \quad P_{2j+1}(n) = 0,$$

for all integers n and natural numbers j. In view of the last result, it is conventional to apply an even number of integrations by parts to the last term in (6). In this way, we arrive at the general Euler–Maclaurin formula

$$\sum_{j=n_0}^{n_1} f(j;x) = \int_{n_0}^{n_1} f(s;x)\,\mathrm{d}s + \frac{f(n_0;x)+f(n_1;x)}{2} + \sum_{j=1}^{m} \frac{B_{2j}}{(2j)!}\big[f^{(2j-1)}(n_1;x) - f^{(2j-1)}(n_0;x)\big] + \Delta_m, \quad (9)$$

where

$$\Delta_m = \int_{n_0}^{n_1} \frac{P_{2m+1}(s)}{(2m+1)!}\, f^{(2m+1)}(s;x)\,\mathrm{d}s.$$

Here we have used the fact that $P_{2j}(n) = B_{2j}$, the $2j$th Bernoulli number, for $j \geq 0$ and any integer n [3, Section 9.6]. The usual strategy for employing (9) to asymptotically expand a series is to evaluate the integral on the right-hand side exactly, and prove that Δ_m is of smaller magnitude than the other terms. Often this last step can be achieved by making an appropriate substitution to remove the dependence upon x from f and then using the bound [6]

$$\left| \frac{P_{2m+1}(s)}{(2m+1)!} \right| < \frac{2}{(2\pi)^{2m+1}}. \quad (10)$$

If (as is often the case) $f(s;x) = f(w)$ where $w = s/x$, then

$$\Delta_m = x^{-2m} \int_{n_0/x}^{n_1/x} \frac{P_{2m+1}(xw)}{(2m+1)!}\, f^{(2m+1)}(w)\,\mathrm{d}w, \quad (11)$$

and hence

$$|\Delta_m| \leq \frac{1}{\pi(2\pi x)^{-2m}} \int_{n_0/x}^{n_1/x} \left| f^{(2m+1)}(w) \right| \mathrm{d}w. \quad (12)$$

It is difficult to determine how the integral in (12) behaves as m increases, so the error is usually estimated by considering the next term that would appear in the finite series on the right-hand side of (9), if m were to be increased. However, there are situations in which this series disappears entirely. For example, if $f(s;x)$ is symmetric about $s = n_0$ (or n_1), then all its odd derivatives will vanish at this point. Alternatively, if n_0 and n_1 are extended to $\pm\infty$, and the resulting series and integrals are convergent, then in most problems of practical interest f and its derivatives will vanish in these limits. Should the series disappear from the right-hand side of (9), m may be chosen arbitrarily, and the error caused by discarding Δ_m is then exponentially small. This phenomenon has previously been observed in [13] and (in the context of analyzing infinite series) [12].

3 Examples.

We now consider three example series. Each contains a positive parameter x, and converges rapidly when this is small. We will derive asymptotic approximations that provide accurate results for large x. The first two examples are relatively straightforward, and the last is much more difficult.

3.1 Even summand.

For our introductory example, we consider the series $S(x)$ given in (1). We begin by setting

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

Clearly, it will be easier to evaluate the relevant integral in (9) if we apply the Euler–Maclaurin formula starting at $s = 0$, rather than $s = 1$. In addition, since $f(s;x)$ is an even function, we have $f^{(2j-1)}(0) = 0$. Thus, substituting into (9), taking $n_0 = 0$, and letting $n_1 \to \infty$, we find that

$$\sum_{j=0}^{\infty} \mathrm{e}^{-j^2/x^2} = \int_0^{\infty} \mathrm{e}^{-s^2/x^2}\,\mathrm{d}s + \frac{1}{2} + \Delta_m, \tag{13}$$

where

$$\Delta_m = \int_0^{\infty} \frac{P_{2m+1}(s)}{(2m+1)!} \left(\frac{\mathrm{d}}{\mathrm{d}s}\right)^{2m+1} \mathrm{e}^{-s^2/x^2}\,\mathrm{d}s. \tag{14}$$

Evaluating the integral in (13) then yields the first two terms in (2). For (14), we may write $w = s/x$ and then use (10) as in (11) and (12) to show that $\Delta_m = O(x^{-2m})$. Since m may be chosen arbitrarily, it follows that the error committed in discarding this term is asymptotically smaller than any algebraic power of x. This is in agreement with Poisson's result (which implies that Δ_m decreases exponentially as $x \to \infty$), but we have not succeeded in making further progress towards (2) from (14).

3.2 A summand without symmetry.

We now consider the series

$$T(x) = \sum_{j=1}^{\infty} \mathrm{e}^{-j^3/x^3}, \quad x > 0. \tag{15}$$

As before, the corresponding integral is easier to evaluate if its lower limit is zero; indeed the substitution $w = s^3/x^3$ shows that

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

where $\Gamma(\cdot)$ represents the Gamma function [9, Chapter 5], and we have used the identity $z\Gamma(z) = \Gamma(z+1)$. Therefore we apply the Euler–Maclaurin formula with $n_0 = 0$, rather than $n_0 = 1$. Letting $n_1 \to \infty$ and writing

$$f(s;x) = \mathrm{e}^{-s^3/x^3}$$

in (9), we find that

$$T(x) = x\Gamma\left(\tfrac{4}{3}\right) - \frac{1}{2} - \sum_{j=1}^{m} \frac{B_{2j}}{(2j)!} f^{(2j-1)}(0;x) + \Delta_m, \tag{16}$$

where

$$\Delta_m = \int_0^\infty \frac{P_{2m+1}(s)}{(2m+1)!}\left(\frac{\mathrm{d}}{\mathrm{d}s}\right)^{2m+1} \mathrm{e}^{-s^3/x^3}\,\mathrm{d}s.$$

Next, we look to simplify the finite sum in (16), by finding an explicit value for the derivative. To achieve this, we write the exponential as a Maclaurin series and then differentiate repeatedly. In this way, we find that

$$\begin{aligned} f^{(k)}(s;x) &= \sum_{p=0}^{\infty} \frac{(-1)^p}{x^{3p}p!}\left(\frac{\mathrm{d}}{\mathrm{d}s}\right)^k s^{3p} \\ &= \sum_{p=\lceil k/3\rceil}^{\infty} \frac{(-1)^p}{x^{3p}p!}(3p)(3p-1)\cdots(3p-k+1)s^{3p-k}, \end{aligned}$$

where $\lceil\cdot\rceil$ means "round up." In the last line, the lower limit for the series is determined by noting that differentiating once eliminates one term, differentiating four times eliminates two terms, etc. A nonzero value at $s = 0$ can only occur if k is divisible by three, in which case

$$f^{(k)}(0;x) = \frac{(-1)^{k/3}k!}{x^k(k/3)!}.$$

Therefore the summand in (16) evaluates to zero unless $2j - 1 = 6p - 3$ (i.e., an odd multiple of 3) for some $p \in \mathbb{N}$. We can then perform further integrations by parts in the error term Δ_m, stopping at the last step before a nonzero boundary term occurs. However, a simpler approach is to base the error estimate on the first (nonzero) term omitted from the series; that is,

$$T(x) = x\Gamma\left(\tfrac{4}{3}\right) - \frac{1}{2} + \frac{1}{2}\sum_{p=1}^{r} \frac{B_{6p-2}}{(2p-1)!(3p-1)x^{6p-3}} + O(x^{-6r-3}). \tag{17}$$

This is an asymptotic representation of T; the series will diverge if the upper limit r is extended to infinity. Nevertheless, very accurate results can be obtained using a finite number of terms. Generally, for a given x, the best available approximation occurs when r is chosen so that the terms included in the series decrease monotonically in magnitude, but subsequent terms do not [7, Chapter 1]. In the particular case of (17), the terms initially decrease fairly rapidly in magnitude, after which the summand remains small for a sequence of p values. For example, if $x = 2.5$, the magnitude of the terms decreases monotonically up to $p = 6$, at which point (17) yields $T(2.5) \approx 1.731915773$, which has nine correct digits. Similar approximations may be obtained by taking r to have any value in the range $3, \ldots, 9$. Increasing the upper limit beyond $r = 9$ causes the approximation to deteriorate.

3.3 A summand with a real singularity.

As a more challenging example, we now consider a series that originates from the infinite product

$$G(x) = \prod_{j=1}^{\infty}\left(1 - \mathrm{e}^{-j^2/x^2}\right).$$

Expressions of this type appear in the study of heat transfer through walls; see the supplemental material and references therein. Taking logarithms yields

$$F(x) = \ln G(x) = \sum_{j=1}^{\infty} \ln\left(1 - \mathrm{e}^{-j^2/x^2}\right), \tag{18}$$

and we aim to determine the behavior of $F(x)$ for large x. We begin by writing

$$f(s;x) = \ln\left(1 - \mathrm{e}^{-s^2/x^2}\right).$$

Although this is an even function, it is not defined at the origin, and this presents some problems. However, $f(s;x)$ does have the property that odd-ordered derivatives vanish at $s = 0$, and we can take advantage of this as follows. We start with the first order Euler–Maclaurin formula (6), letting $n_1 \to \infty$ and setting $n_0 = 1$; that is,

$$F(x) = \int_1^\infty f(s;x)\,\mathrm{d}s + \frac{f(1;x)}{2} + \int_1^\infty P_1(s) f'(s;x)\,\mathrm{d}s. \tag{19}$$

As in the two previous examples, the first integral on the right-hand side is easier to evaluate if the lower limit is replaced by zero. Thus, expanding the logarithm as a Taylor series, we find that

$$\begin{aligned}\int_0^\infty \ln\bigl(1 - \mathrm{e}^{-s^2/x^2}\bigr)\,\mathrm{d}s &= -\sum_{j=1}^\infty \frac{1}{j}\int_0^\infty \mathrm{e}^{-js^2/x^2}\,\mathrm{d}s \\ &= -\frac{x\sqrt{\pi}}{2}\,\zeta\bigl(\tfrac{3}{2}\bigr),\end{aligned} \tag{20}$$

having used the substitution $w = s\sqrt{j}/x$. Here, $\zeta(\cdot)$ represents the Riemann zeta function [9, Chapter 25], that is

$$\zeta(x) = \sum_{j=1}^\infty \frac{1}{j^x}, \quad x > 1. \tag{21}$$

In view of (20), we rewrite (19) in the form

$$F(x) = -\frac{x\sqrt{\pi}}{2}\,\zeta\bigl(\tfrac{3}{2}\bigr) - \int_0^1 f(s;x)\,\mathrm{d}s + \frac{f(1;x)}{2} + \int_1^\infty P_1(s) f'(s;x)\,\mathrm{d}s. \tag{22}$$

It is now desirable to “join” the remaining two integrals, but the singularity at the origin prevents integration by parts using (3). To overcome this, we introduce the regularized function

$$\hat{f}(s;x) = \ln\bigl(1 - \mathrm{e}^{-s^2/x^2}\bigr) - \ln\bigl(s^2/x^2\bigr).$$

This has no singularity at the origin; in fact it is not difficult to show that $\hat{f}(0;x) = 0$. In addition, $\hat{f}'(s;x) \to 0$ as $s \to \infty$, so we can replace f with $\hat{f}$ in (22) provided we add the correction term

$$C = -\int_0^1 \ln\bigl(s^2/x^2\bigr)\,\mathrm{d}s + \frac{\ln\bigl(1/x^2\bigr)}{2} + 2\int_1^\infty \frac{P_1(s)}{s}\,\mathrm{d}s. \tag{23}$$

The first integral that appears here is elementary. For the second, we use (5) to obtain

$$\int_1^\infty \frac{P_1(s)}{s}\,\mathrm{d}s = \lim_{N\to\infty}\sum_{j=1}^{N}\int_j^{j+1}\frac{s-j-\frac{1}{2}}{s}\,\mathrm{d}s$$
$$= \lim_{N\to\infty}\Big[N-\sum_{j=1}^{N}\big(j+\tfrac{1}{2}\big)\big(\ln(j+1)-\ln j\big)\Big].$$

The above series can be made partially telescopic by rearranging the summand; thus

$$\big(j+\tfrac{1}{2}\big)\big(\ln(j+1)-\ln j\big) = (j+1)\ln(j+1) - j\ln j - \tfrac{1}{2}\big(\ln(j+1)+\ln j\big),$$

which leads us to

$$\int_1^\infty \frac{P_1(s)}{s}\,\mathrm{d}s = \lim_{N\to\infty}\big[N-(N+\tfrac{1}{2})\ln(N+1)+\ln(N!)\big].$$

Now Stirling's series [9, equation 5.11.1] can be written in the form

$$\ln(N!) = \big(N+\tfrac{1}{2}\big)\ln(N+1)-(N+1)+\frac{\ln(2\pi)}{2}+O(N^{-1}),$$

and this shows that

$$\int_1^\infty \frac{P_1(s)}{s}\,\mathrm{d}s = \frac{\ln(2\pi)}{2}-1.$$

Returning to (23), we now find that $C=\ln(2\pi x)$ and then from (22),

$$F(x) = \ln(2\pi x) - \frac{x\sqrt{\pi}}{2}\,\zeta\big(\tfrac{3}{2}\big) + \frac{\hat{f}(1;x)}{2} + \int_1^\infty P_1(s)\hat{f}'(s;x)\,\mathrm{d}s - \int_0^1 \hat{f}(s;x)\,\mathrm{d}s.$$

Integrating once by parts in the last term reduces this to

$$F(x) = \ln(2\pi x) - \frac{x\sqrt{\pi}}{2}\,\zeta\big(\tfrac{3}{2}\big) + \int_0^\infty P_1(s)\hat{f}'(s;x)\,\mathrm{d}s.$$

Having eliminated the singularity at the origin, the next step is to integrate by parts repeatedly. In this way, we find that

$$F(x) = \ln(2\pi x) - \frac{x\sqrt{\pi}}{2}\,\zeta\big(\tfrac{3}{2}\big) + \Delta_m, \tag{24}$$

where

$$\Delta_m = \int_0^\infty \frac{P_{2m+1}(s)}{(2m+1)!} \hat{f}^{\,(2m+1)}(s;x)\,\mathrm{d}s. \tag{25}$$

Note that, since $\hat{f}$ is an even function, no boundary terms are produced in any step (in contrast to the derivation of (9)). However, integrating by parts an even number of times facilitates the use of (10) after making the substitution $w = s/x$. A slightly more complicated bound is required if even indices are permitted [6]. Ultimately, these are minor details; the end result is that Δ_m is asymptotically smaller than any algebraic power of x. This rapid decay can be observed with a simple numerical experiment, computing $F(x)$ directly using (18) and approximating using (24) with $\Delta_m = 0$. Three correct significant figures are obtained if $x \gtrapprox 0.68$, six if $x \gtrapprox 1.3$, and sixteen if $x \gtrapprox 3.2$.

4 Concluding remarks.

We have demonstrated that the Euler–Maclaurin formula provides a simple but powerful means for finding asymptotic expansions of series and products that contain a large (or small) parameter. It takes some creativity to make this work with summands that possess real singularities (such as (18)), but ultimately the techniques used are all based on elementary calculus, and integration by parts in particular. However, we have not retrieved Poisson's full result (2) by this approach. Indeed, it is not clear how information about the precise nature of Δ_m can be obtained from (14) or (25), if this is possible at all. Of course we would be delighted to hear from any readers who can find a way to derive (2) using the Euler–Maclaurin formula. In Part 2 of our article, we will explore an even more powerful approach to the same problem, capable of reproducing Poisson's result and also a corresponding exact transformation for (18).

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Analysis of Series and Products: Supplemental Material for Part 1

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1 Wall d coefficients.

The series

$$F(x) = \sum_{j=1}^{\infty} \ln\bigl(1 - \mathrm{e}^{-j^2/x^2}\bigr), \tag{1}$$

which motivated this study, came to the authors' attention through its appearance in a technique used for modelling heat transfer through building walls, due to climate and other time-varying conditions. Analysis of the flow of heat through a building wall in steady conditions was first undertaken in the nineteenth century. However, with incorporation of large areas of glazed wall into the light-weight fabric of buildings in the post World War II era, some buildings overheated in summer and had unusably cold areas in winter. By the 1960s, attention was turning to time-varying behavior.

The determining relation for wall heat transfer is the Fourier continuity equation (also called the heat equation), that is,

$$\lambda \frac{\partial^2 T}{\partial y^2} = \rho c_p \frac{\partial T}{\partial t}, \tag{2}$$

where λ, ρ, and c_p are the thermal conductivity, density, and specific heat of a layer of the material, with units $\mathrm{W\,m^{-1}K^{-1}}$, $\mathrm{kg\,m^{-3}}$, and $\mathrm{J\,K^{-1}kg^{-1}}$, respectively. We use y to denote position, rather than the customary x, since x has been used with a different meaning in the main body of the article. There are four classes of solution to (2), each corresponding to specific physical conditions, discussed in [3, Chapter 17]. In one of them, y and t appear as the product yt, and in another as a quotient y^2/t. However, y and t appear separately if a slab or series of slabs forming a wall is excited by a sinusoidally varying temperature (with period 24 hours in building applications). The variables y and t also appear separately if a slab or wall has some arbitrary temperature distribution within it, and from time $t = 0$ onwards, the inside and outside temperatures are held at zero. The temperature distribution can then be resolved into a series of orthogonal profiles. The profiles are sinusoidal in wall elements having mass (concrete, insulation, etc.) and linear in the elements modelling convective and radiative exchange inside and outside. Plotted against progressive resistance through the wall, the first mode profile approximates to a single half-wave, the second to two half-waves, etc. The temperature in the jth profile falls everywhere as e^{-t/z_j}, where z_j is its decay time. The largest decay time, z_1, is typically of the order of hours in building applications.

The values of temperature and heat flow at the outside and inside surface of a slab are related by a four-element slab transfer matrix and the outside and inside values for the whole wall are related by the product of the slab matrices. The elements of the product matrix are functions of $1/z$, and as this increases from zero, each element in the product matrix oscillates about zero. Zero values of each element denote corresponding imposed boundary conditions. The condition of interest here is that $T_{\text{outside}} = T_{\text{inside}} = 0$, and a search has to be made for the sequence of values $z_1, z_2, z_3, \ldots$ that satisfy it. There are four sets of such values and they are discussed in [5].

Consider now a building wall. The inside space is held at zero temperature T_i, the mean outside temperature $T_{o,t=k\delta}$ is known at hourly intervals δ up to time $t = 0$. The inward heat flow q_0 (units $\mathrm{W\,m^{-2}}$) at time $t = 0$ into the internal space can be found from short series of b_k and d_k values — "transfer coefficients" which include values of recent fluxes. The value of the present heat flow is then given by

$$q_0 = \sum_{k=0}^{N} b_k T_{o,k\delta} - \sum_{k=1}^{N} d_k q_{k\delta}. \tag{3}$$

The b_k coefficients have units $\mathrm{W\,m^{-2}\,K^{-1}}$ and describe the heat flow from the wall due to imposition of a triangular temperature pulse of unit height and base 2δ at the other side at the earlier time $k\delta$, but we are not concerned with it here. The d_k values, which are dimensionless, are found from the values of the wall decay times z_j together with the choice of the sampling time δ. The transfer coefficients have the property that the ratio $\sum_{k=0}^{N} b_k / \sum_{k=0}^{N} d_k$ describes the steady state transmittance of the wall, long denoted by U. The U value for single glazing is about $5.8\mathrm{W\,m^{-2}\,K^{-1}}$ (but very dependent on wind speed); walls have lower values and, since the energy crisis of 1973, increasing thicknesses of insulating materials including super-insulation have been incorporated to reduce heat losses, achieving U values as low as $0.15\mathrm{W\,m^{-2}\,K^{-1}}$.

2 The d_k values.

If there is no variation of temperature after time $t = 0$, the expression for heat flow (3) reduces to

$$q_0 = -\sum_{k=1}^{N} d_k q_{k\delta}.$$

The values of the d_k coefficients follow from the decay times z_j and the choice of δ. Their evaluation can be illustrated by supposing that the wall is represented by two lumped capacities with flanking resistances. This structure has two decay times z_1 and z_2 and any net temperature profile in the model can be resolved into two independent components, one decaying as e^{-t/z_1} and the other as e^{-t/z_2}. Suppose that the heat outflow at $t = -2\delta$ is written as $q_{-2} = A + B$. One interval δ later, its value falls to $q_{-1} = A\beta_1 + B\beta_2$, where

$$\beta_j = \mathrm{e}^{-\delta/z_j}.$$

A further interval δ later, the heat outflow is $q_0 = A\beta_1^2 + B\beta_2^2$, which can be expressed in terms of earlier values as

$$q_0 = (\beta_1 + \beta_2)q_{-1} - \beta_1\beta_2 q_{-2}.$$

It is conventional to write $(\beta_1 + \beta_2) = -d_1$ and $\beta_1\beta_2 = +d_2$. This can be generalized to model a wall by an indefinite number of capacities and so a continuous distribution of capacity and resistance. We then have

$$\begin{aligned} +d_0 &= 1 \\ -d_1 &= \beta_1 + \beta_2 + \beta_3 + \beta_4 + \cdots \\ +d_2 &= \beta_1\beta_2 + \beta_1\beta_3 + \beta_1\beta_4 + \beta_2\beta_3 + \beta_2\beta_4 + \cdots \\ -d_4 &= \beta_1\beta_2\beta_3 + \beta_1\beta_2\beta_4 + \cdots \\ &\ \vdots \\ \pm d_N &= \beta_1\beta_2\cdots\beta_N. \end{aligned} \tag{4}$$

Conversely, the coefficients β_j are the solutions of the polynomial

$$d_0\beta^n + d_1\beta^{n-1} + \cdots + d_N = 0.$$

The sum of the d coefficients can be expressed in product form; thus

$$\sum_{k=0}^{N} d_k = \prod_{k=1}^{N}(1 - \beta_k).$$

In most applications, a relatively small number of z_j values, N', say, are needed to compute d_1, and a decreasing number are needed to accurately compute d_2, d_3, etc. The number of z_j values needed to compute d_N and the sum of d_k values, N, is smaller; see [4]. Walls with greater density, thickness, etc. have greater values for z_j, and consequently, larger values for both N' and N.

The 1993 *ASHRAE Handbook of Fundamentals* [1, p26.26] and subsequent editions listed the b_k and d_k values of 41 building walls from lightweight to heavyweight construction (those including at least 300mm of heavy concrete). Coefficients for a further 35 walls are listed in [2].

It is found (see [5] for example) that $(\log_{10}\sum d_k)_{\mathrm{wall}_W}$ is highly correlated with the value of V_W of the wall, where

$$V_W = \sum\sqrt{\frac{c_i r_i}{4\pi\delta}}.$$

Here, c_i is the capacity of layer i of wall W (units $\mathrm{J\,m^{-2}\,K^{-1}}$), the product of its density, specific heat and thickness Y, and r_i is the resistance of layer i (units $\mathrm{m^2\,K\,W^{-1}}$), which is the ratio of thickness and conductivity. Values of V_W generally lie in the range 0.6 to 3.3.

3 The plain slab.

For a plain slab, the decay times are found simply as $z_j = cr/(j\pi)^2$. The component profiles are now strictly sinusoidal; in fact

$$T(y,t) = \sum_{j=1}^{\infty} A_j \sin\left(\frac{j\pi y}{Y}\right) \mathrm{e}^{-t/z_j}, \quad t > 0.$$

It was noted in [3, p. 378] that when $V_{\text{slab}} = \sqrt{cr/(4\pi\delta)}$ exceeds about 1.5, d_1 is an approximately linear function of V_{slab}, d_2 is approximately quadratic, etc. In fact these results follow from Poisson's formula

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

after writing

$$x^2 = cr/(\pi^2\delta) = 4V_{\text{slab}}^2/\pi, \tag{5}$$

and omitting exponentially small terms. Thus, $-d_1 \approx S(x)$, so

$$d_1 \approx \frac{1}{2} - V_{\text{slab}}.$$

Note that there is a typographical error in the corresponding equation in [3] (which is 17.17(a)): the left-hand side should be $-d_1$, not d_1. The approximation for d_2 given in [3, equation 17.17(b)] can then be reproduced by using (4) to observe that, in general,

$$\begin{aligned} d_1^2 &= (\beta_1^2 + \beta_2^2 + \beta_3^2 \cdots) + 2(\beta_1\beta_2 + \beta_1\beta_3 + \beta_2\beta_3 + \cdots) \\ &= \sum_{j=1}^{\infty} \beta_j^2 + 2d_2. \end{aligned}$$

Now squaring β_j is equivalent to replacing δ with 2δ, or V with $V/\sqrt{2}$. Therefore,

$$\left(\frac{1}{2} - V_{\text{slab}}\right)^2 \approx -\left(\frac{1}{2} - \frac{V_{\text{slab}}}{\sqrt{2}}\right) + 2d_2,$$

which rearranges to yield

$$d_2 \approx \frac{1}{2}V_{\text{slab}}^2 - \frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right)V_{\text{slab}} + \frac{3}{8}.$$

The sum of d_k values is related to the series $F(x)$ from (1) via

$$\left(\sum_{k=0}^{\infty} d_k\right)_{\text{slab}} = \prod_{j=1}^{\infty}\bigl(1-\mathrm{e}^{-\delta/z_j}\bigr) = \prod_{j=1}^{\infty}\bigl(1-\mathrm{e}^{-j^2/x^2}\bigr),$$

in view of (5). The product on the right-hand side is then the exponential of $F(x)$. In engineering literature, its value is generally reported as a base 10 logarithm. The values of the physical constants needed for finding d values—conductivity, density, specific heat and radiative and convective transfer coefficients for building materials—cannot generally be determined to high precision, so a relative error of approximately 10^{-3} is generally acceptable. Therefore, for practical purposes, it is sufficient to retain only the logarithmic and linear terms in the approximation obtained at the end of the main article, and then write

$$\begin{aligned}\log_{10}\left(\sum_{k=1}^{\infty} d_k\right)_{\text{slab}} &\approx \log_{10}(\mathrm{e})\bigl[\ln(4\sqrt{\pi}\,V) - \zeta(3/2)V\bigr]\\ &\approx 0.4343\bigl[\ln(7.090V) - 2.612\bigr].\end{aligned}$$

References

[1] ASHRAE (1993). *ASHRAE Handbook*, vol. Fundamentals. Atlanta: American Society of Heating, Refrigerating and Air-Conditioning Engineers.

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