Physics 116A Winter 2006

## Bernoulli numbers and the Euler-Maclaurin summation formula

In this note, I shall motivate the origin of the Euler-Maclaurin summation formula. I will also explain why the coefficients on the right hand side of this formula involve the Bernoulli numbers.

First, we define the Bernoulli numbers  $B_{2n}$ . These arise in the Taylor series expansions of  $x \coth(x)$  and  $x \cot(x)$  about x = 0.\* It is convenient to define the normalization of the Bernoulli numbers via the Taylor expansion of  $(x/2) \coth(x/2)$  as follows:

$$\frac{x}{2} \coth\left(\frac{x}{2}\right) = \sum_{k=0}^{\infty} B_{2k} \frac{x^{2k}}{(2k)!}, \qquad |x| < 2\pi.$$
 (1)

This formula only defines Bernoulli numbers with even non-negative indices. The more common definition is based on the observation that

$$\frac{x}{2}\left[\coth\left(\frac{x}{2}\right) - 1\right] = \frac{x}{e^x - 1} \tag{2}$$

is an identity.<sup>†</sup> Then,

$$\frac{x}{e^x - 1} = \sum_{k=0}^{\infty} B_k \frac{x^k}{k!} \,, \qquad |x| < 2\pi \,.$$

defines all the Bernoulli numbers with non-negative indices. Comparing the above formulae, it follows that  $B_1 = -\frac{1}{2}$  and  $B_{2k+1} = 0$  for  $k = 1, 2, 3, \ldots$  For the remainder of this note, we will only be concerned with Bernoulli numbers of the form  $B_{2k}$ , for non-negative integers k. For the record, we list the first six  $B_{2k}$  here:

$$B_0 = 1$$
,  $B_2 = \frac{1}{6}$ ,  $B_4 = -\frac{1}{30}$ ,  $B_6 = \frac{1}{42}$ ,  $B_8 = -\frac{1}{30}$ ,  $B_{10} = \frac{5}{66}$ , etc.

In general, the signs alternate beginning with  $B_2$ , so that

$$B_{2k} = (-1)^{k+1} |B_{2k}|, \quad \text{for } k = 1, 2, 3, \dots$$

<sup>\*</sup>As  $x \to 0$ , both  $\coth(x)$  and  $\cot(x)$  behave as 1/x; hence we multiply by x in order to have a function with a finite limit as  $x \to 0$ .

<sup>&</sup>lt;sup>†</sup>To prove this, recall that  $\coth(x) = \cosh(x)/\sinh(x)$  where  $\cosh(x) \equiv \frac{1}{2}(e^x + e^{-x})$  and  $\sinh(x) \equiv \frac{1}{2}(e^x - e^{-x})$ .

Given the Taylor series for  $x \coth(x)$  [expanded about x = 0], one can immediately obtain the Taylor series for  $x \cot x$  by using  $x \cot(x) = ix \coth(ix)$ . By using the following hyperbolic and trigonometric identities:

$$\tanh(x) = 2 \coth(2x) - \coth(x), \qquad \tan(x) = \cot(x) - 2 \cot(2x),$$
  
$$\operatorname{csch}(2x) = \coth(x) - \coth(2x), \qquad \operatorname{csc}(2x) = \cot(x) - \cot(2x),$$

one finds that the Taylor expansions about x=0 for  $\cot(x)$ ,  $\tan(x)$ ,  $\csc(x)$  and the corresponding hyperbolic functions all involve the Bernoulli numbers. Note that there are no similar identities for  $\operatorname{sech}(x)$  and  $\operatorname{sec}(x)$  in terms of  $\coth(x)$  and  $\cot(x)$ , respectively. Hence, the Taylor expansions about x=0 of these two functions do not involve the Bernoulli numbers.

One property of the Bernoulli numbers will be important in what follows. We will need to know the behavior of the  $B_{2k}$  as k becomes very large. We can determine this by using the famous connection between the Bernoulli numbers and the Riemann zeta function:

$$|B_{2k}| = \frac{2(2k)! \zeta(2k)}{(2\pi)^{2k}}, \tag{3}$$

where  $\zeta(2k) \equiv \sum_{n=0}^{\infty} (1/(2k)^n)$ . Note that  $\lim_{k\to\infty} \zeta(2k) = 1$ , since in this limit only the first term in the series (which is equal to one) survives. Hence, using this result in eq. (3) and employing Stirling's approximation for (2k)!,

$$(2k)! \simeq (4\pi k)^{1/2} (2k)^{2k} e^{-2k}, \quad \text{as } k \to \infty,$$

we end up with

$$|B_{2k}| \simeq 4(\pi k)^{1/2} \left(\frac{k}{\pi e}\right)^{2k}$$
, as  $k \to \infty$ . (4)

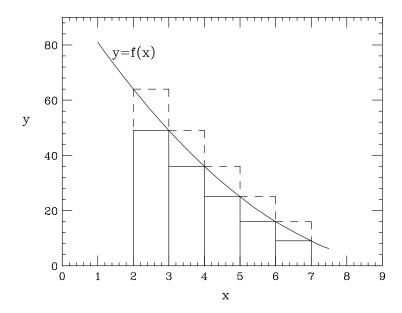
With this background, we are now ready to introduce the Euler-Maclaurin summation formula.§ This formula arises in the following context. Suppose we wish to numerically approximate an integral of the form:

$$I \equiv \int_{k}^{k+n} f(x)dx,$$

where k is an integer and n is a positive integer. The simplest possible approximation to the integral corresponds to dividing up the interval  $k \leq x \leq k + n$  in units of one, and estimating the value of the integral by computing the area of all the rectangles of unit length that approximate the area under the curve. We illustrate this procedure with the following graph at the top of the next page.

<sup>&</sup>lt;sup>‡</sup>Instead, they require the introduction of a new type of numbers called the Euler numbers. The explicit definition of the Euler numbers was given at the end of the handout on the Riemann zeta function. We will not need the Euler numbers in this note.

<sup>§</sup>This presentation is inspired by Jon Mathews and R.L. Walker, *Mathematical Methods of Physics*, Chapter 13.



Here, one can either compute the area bounded by the rectangles indicated by the solid lines or by the rectangles indicated by the dashed lines. (In this particular example, k = 2 and n = 5.) The former underestimates the area under the curve y = f(x), while the latter overestimates this area. That is,  $I_1 < I < I_2$  where

$$I_1 = f(k+1) + f(k+2) + \dots + f(k+n),$$
  

$$I_2 = f(k) + f(k+1) + \dots + f(k+n-1).$$
 (5)

The trapezoidal rule for numerical integration takes the average of  $I_1$  and  $I_2$ . So, we shall make the approximation  $I = \frac{1}{2}(I_1 + I_2)$ , which we can write as:

$$\int_{k}^{k+n} f(x) dx \approx \frac{1}{2} [f(k) + f(k+n)] + \sum_{j=1}^{n-1} f(k+j).$$

The Euler-Maclaurin sum formula arises when we attempt to convert the above result into an exact formula. That is, we seek to determine an expression,  $\mathcal{R}$ , such that:

$$\int_{k}^{k+n} f(x) dx = \frac{1}{2} [f(k) + f(k+n)] + \sum_{m=1}^{n-1} f(k+m) + \mathcal{R}.$$
 (6)

I will show you a sophisticated, yet simple, method for determining  $\mathcal{R}$ . You should be forewarned that this method is slick and will gloss over some subtleties that I will mention later. The trick is to introduce two operators called D and E. These operators  $act\ on^{\P}$  a function f(x) and have very simple definitions:

$$Df(k) \equiv f'(k), \qquad Ef(k) \equiv f(k+1), \qquad (7)$$

<sup>¶</sup>By  $act\ on$ , I mean that D and E operate on functions. You can think of D and E as little machines. You feed these machines a function and they will spit out a new function.

where as usual,  $f'(k) \equiv (df/dx)_{x=k}$ . With this notation, eq. (6) reads:

$$\int_{k}^{k+n} f(x) dx = \left[\frac{1}{2} + E + E^{2} + \dots + E^{n-1} + \frac{1}{2}E^{n}\right] f(k) + \mathcal{R},$$

since, e.g.,  $E^2f(k) = E \cdot Ef(k) = Ef(k+1) = f(k+2)$ , etc. Now, for the slick part. We shall write:

$$\frac{1}{2} + E + E^{2} + \dots + E^{n-1} + \frac{1}{2}E^{n} = 1 + E + E^{2} + \dots + E^{n-1} - \frac{1}{2}(1 - E^{n})$$

$$= \frac{1 - E^{n}}{1 - E} - \frac{1}{2}(1 - E^{n})$$

$$= (E^{n} - 1) \left[ \frac{1}{2} + \frac{1}{E - 1} \right], \tag{8}$$

where we have summed a finite geometric series in the usual way. But, E is an operator, so what does  $(1-E)^{-1}$  mean? The answer is that we are actually using a short-hand notation. When in doubt, a function of an operator is always defined by its Taylor series. For example, in eq. (8),  $(1-E)^{-1} = 1 + E + E^2 + \cdots$ . This is an infinite series, so we should really worry about convergence (what does it mean when you have an infinite convergent series of operators rather than numbers?). For the moment, I will treat these power series expansions as formal objects, and postpone questions of convergence until later.

So, if you are willing to go along with this strategy, then we have the following result:

$$\int_{k}^{k+n} f(x) dx = (E^{n} - 1) \left[ \frac{1}{2} + \frac{1}{E - 1} \right] f(k) + \mathcal{R}.$$
 (9)

Our next step is to consider the Taylor expansion of f(x) about x = k:

$$f(x) = f(k) + \sum_{m=1}^{\infty} \frac{f^{(m)}(k)}{m!} (x - k)^m.$$

Again, we should check for which values of x this series converges, but we will sidestep this issue again. If we set x = k + 1 in the above expansion, we find:

$$f(k+1) = \sum_{m=0}^{\infty} \frac{f^{(m)}(k)}{m!}$$
.

Thus, we can use our operators D and E to rewrite this as

$$Ef(k) = \sum_{m=0}^{\infty} \frac{D^m}{m!} f(k).$$

Note that this formula would be true for any function f, so we can conclude that we have an *operator identity*:

$$E = \sum_{m=0}^{\infty} \frac{D^m}{m!} \,. \tag{10}$$

I hope you recognize the sum on the right hand side of eq. (10). This is the power series expansion of  $e^D$ . Thus, we conclude that

$$E = e^D. (11)$$

Once again, we have introduced a strange new object—the exponential of an operator. As before, this is a formal definition, and you should always think of  $e^D$  as being equal to its Taylor series expansion [eq. (10)].

The final step of our analysis introduces the indefinite integral of f(x). Let us call it g(x):

$$g(x) = \int f(x) dx$$
, or equivalently  $f(x) = \frac{dg(x)}{dx}$ .

In particular, g'(k) = Dg(k) = f(k). The fundamental theorem of calculus then allows us to write:

$$\int_{k}^{k+n} f(x) \, dx = g(k+n) - g(k) = (E^{n} - 1)g(k) \, .$$

Now for the bold move. Since Dg(k) = f(k), we shall write:

$$g(k) = \frac{1}{D}f(k).$$

This will allow us to write

$$\int_{k}^{k+n} f(x) dx = (E^{n} - 1) \frac{1}{D} f(k).$$
 (12)

We now have two different expressions for  $\int_k^{k+n} f(x) dx$  given by eqs. (9) and (12). Since only one of these expressions involves  $\mathcal{R}$ , this means that we can now solve for  $\mathcal{R}$ . Setting eqs. (9) and (12) equal to each other, we obtain:

$$\mathcal{R} = (E^n - 1) \left[ \frac{1}{D} - \frac{1}{2} - \frac{1}{E - 1} \right] f(k)$$
$$= (E^n - 1) \frac{1}{D} \left[ 1 - D \left( \frac{1}{2} + \frac{1}{E - 1} \right) \right] f(k).$$

At this point, we shall substitute  $E = e^D$  [eq. (11)] inside the brackets to obtain

$$\mathcal{R} = (E^n - 1) \frac{1}{D} \left[ 1 - D \left( \frac{1}{2} + \frac{1}{e^D - 1} \right) \right] f(k).$$

Using the identity given by eq. (2), we can write this last result in a very suggestive way:

 $\mathcal{R} = (E^n - 1)\frac{1}{D} \left[ 1 - \frac{D}{2} \coth \frac{D}{2} \right] f(k).$ 

Once again, we have a function of an operator, which we are instructed to interpret as a power series. It is at this point that the Bernoulli numbers enter. Using eq. (1), we can write:

$$\frac{1}{D} \left[ 1 - \frac{D}{2} \coth \frac{D}{2} \right] = -\sum_{m=1}^{\infty} B_{2m} \frac{D^{2m-1}}{(2m)!}.$$
 (13)

Notice that at this point, we only have non-negative powers of the operator D on the right hand side of eq. (13), which we can easily handle. Thus, we conclude that:

$$\mathcal{R} = \left[ (1 - E^n) \sum_{m=1}^{\infty} B_{2m} \frac{D^{2m-1}}{(2m)!} \right] f(k).$$

We can write out this expression more explicitly by using the definitions of the operators D and E [eq. (7)]:

$$\mathcal{R} = -\sum_{m=1}^{\infty} \frac{B_{2m}}{(2m)!} \left[ f^{(2m-1)}(k+n) - f^{(2m-1)}(k) \right].$$

Inserting this result back into eq. (6) yields the following remarkable formula:

$$\int_{k}^{k+n} f(x) dx = \sum_{m=1}^{n-1} f(k+m) + \frac{1}{2} [f(k) + f(k+n)] - \sum_{m=1}^{\infty} \frac{B_{2m}}{(2m)!} [f^{(2m-1)}(k+n) - f^{(2m-1)}(k)].$$

Notice that this is an *exact* result. Somehow, we have managed to turn a formula that started out as an approximation to an integral into an exact result.

The finite sum  $\sum_{m} f(k+m)$  is also an interesting object, and we can reinterpret the above result as providing a formula for this finite sum. If we write:

$$\sum_{m=1}^{n-1} f(k+m) + \frac{1}{2} [f(k) + f(k+n)] = \sum_{m=1}^{n} f(k+m) - \frac{1}{2} [f(k) + f(k+n)],$$

then we end up with the Euler-Maclaurin summation formula:

$$\sum_{m=1}^{n} f(k+m) = \int_{k}^{k+n} f(x) dx + \frac{1}{2} [f(k) + f(k+n)] + \sum_{m=1}^{\infty} \frac{B_{2m}}{(2m)!} [f^{(2m-1)}(k+n) - f^{(2m-1)}(k)].$$

(14)

It is now time to face up to the question of convergence. The Euler-Maclaurin summation formula as presented here involves an infinite sum. Given the behavior of the Bernoulli numbers  $B_{2m}$  as  $m \to \infty$  [see eq. (4)], it is not surprising to learn that in most cases of interest this is a divergent series. Our derivation has been too slick, in that it ignored questions of convergence. In fact, one can be more careful by replacing all infinite sums encountered above by finite sums plus remainder terms. By carefully keeping track of these remainder terms, one can obtain a more robust version of the Euler-Maclaurin summation formula with a remainder term explicitly included. This derivation is beyond the scope of these notes. You can find (the more conventional) derivation of the Euler-Maclaurin summation formula with remainder term in the textbook by Arfken and Weber, Mathematical Methods for Physicists. For completeness, I shall display the final result here:

$$\sum_{m=1}^{n} f(k+m) = \int_{k}^{k+n} f(x) dx + \frac{1}{2} [f(k) + f(k+n)]$$

$$+ \sum_{m=1}^{p} \frac{B_{2m}}{(2m)!} \left[ f^{(2m-1)}(k+n) - f^{(2m-1)}(k) \right]$$

$$+ \frac{1}{(2p)!} \int_{0}^{1} B_{2p}(x) \sum_{m=0}^{n-1} f^{(2p)}(x+k+m) dx, \qquad (15)$$

where  $B_{2p}(x)$  is the Bernoulli polynomial of order 2p (defined on p. 152 of McQuarrie).

In many applications, the Euler-Maclaurin summation formula provides an asymptotic expansion, in which case the divergent nature of the series in eq. (14) is not problematical. In other cases, the infinite sum turns out to be finite. We shall end this note with a few applications. For our first example, we take  $f(x) = x^p$  and k = 0 in eq. (14). The infinite sum on the right hand side of eq. (14) is in fact finite in this case, since  $f^{(2m-1)}(x) = 0$  for  $2m \ge p + 2$ . Evaluating the derivatives on the right hand side of eq. (14), we can cast the resulting formula into the following form:

$$\sum_{m=1}^{n} m^{p} = \frac{1}{2} n^{p} + \frac{1}{p+1} \sum_{m=0}^{[p/2]} {p+1 \choose 2m} B_{2m} n^{p+1-2m},$$

where [p/2] is the integer part of  $\frac{1}{2}p$ . For example, if p=2 then

$$\sum_{m=1}^{n} m^2 = \frac{1}{3}n^3 + \frac{1}{2}n^2 + \frac{1}{6}n = \frac{1}{6}n(n+1)(2n+1),$$

which reproduces a formula I derived in the first lecture.

Our second application is the derivation of the asymptotic series for  $\ln n!$  as  $n \to \infty$ . Here, we take  $f(x) = \ln x$ , with k = 1 and  $n \to n - 1$  in eq. (14). The integral in eq. (14) is easily computed:

$$\int_{1}^{n} \ln x \, dx = n \ln n - n + 1 \,,$$

and the derivatives  $f^{(2m-1)}(x)$  are given by:

$$f^{(2m-1)}(x) = \frac{(2m-2)!}{x^{2k-1}}, \qquad m = 1, 2, 3, \dots$$

Noting that the summation on the left hand side of eq. (14) takes the following form:

$$\sum_{m=1}^{n-1} \ln(1+m) = \ln 1 + \ln 2 + \dots + \ln n = \ln(1 \cdot 2 \cdot 3 \cdot \dots \cdot n) = \ln n!$$

we can write eq. (14) as

$$\ln n! = (n + \frac{1}{2}) \ln n - n + C + \sum_{m=1}^{\infty} \frac{B_{2m}}{2m(2m-1)} \frac{1}{n^{2m-1}}, \tag{16}$$

where the constant C represents all the remaining terms of eq. (14) that are independent of n:

$$C = 1 - \sum_{m=1}^{\infty} \frac{B_{2m}}{2m(2m-1)}.$$
 (17)

Unfortunately, due to the asymptotic behavior of  $B_{2m}$  as  $m \to \infty$  [eq. (4)], the sum in eq. (17) is divergent. However, this is not surprising since we are using the form of the Euler-Maclaurin summation formula without the remainder term. If we would have included the remainder term, the summations on the right hand sides of eqs. (16) and (17) would have been finite sums. In addition, we would have included the n-independent part of the remainder term in the definition of C above. In this case, the resulting expression for C would have been perfectly well-defined and finite. In fact, one can analyze that resulting form for C and evaluate this constant. However, this requires a number of additional tricks that lie beyond the scope of these notes. Finally, the n-dependent part of the remainder term would appear in eq. (16). By examining its form [c.f. eq. (15)], one can prove that the remainder term is of  $\mathcal{O}(1/n^{2p})$ . This means that eq. (16) is indeed an asymptotic expansion as  $n \to \infty$ .

Here we shall take the simpler approach. Namely, we shall simply assume that eq. (16) is an asymptotic expansion as  $n \to \infty$ . Comparing this result with Stirling's approximation, we conclude that  $C = \ln 2\pi$ . Thus, eq. (16) now reads:

$$\ln n! \sim (n + \frac{1}{2}) \ln n - n + \ln 2\pi + \sum_{m=1}^{\infty} \frac{B_{2m}}{2m(2m-1)} \frac{1}{n^{2m-1}}, \qquad n \to \infty.$$
 (18)

This is called Stirling's asymptotic series. Although the proof given here strictly applies only for the case of positive integer n, there is a generalization of this derivation that can yield the full asymptotic series for  $\ln \Gamma(x+1)$  for any real number  $x \to \infty$ . Not surprisingly, the resulting asymptotic series is identical to eq. (18) with n replaced by x.

For our third example, we choose f(x) = 1/x, with k = 1 and  $n \to n-1$  in eq. (14). Again, the integral and (2m-1)-fold derivatives are easily computed:

$$\int_{1}^{n} \frac{dx}{x} = \ln n, \qquad f^{(2m-1)}(x) = -\frac{(2m-1)!}{x^{2m}}.$$

Thus,

$$\sum_{m=1}^{n} \frac{1}{m} = \ln n + C + \frac{1}{2n} - \sum_{m=1}^{\infty} \frac{B_{2m}}{2m} \frac{1}{n^{2m}},$$
 (19)

where

$$C = \frac{1}{2} + \sum_{m=1}^{\infty} \frac{B_{2m}}{2m} \,.$$

Once again, C appears to be divergent. However, as in the previous example, a more careful analysis including the remainder term would produce a finite expression for C and prove that eq. (19) is an asymptotic series. Thus, if we proceed under this assumption, we can compute the constant C by taking the  $n \to \infty$  limit of eq. (19):

$$C = \lim_{n \to \infty} \left( \sum_{m=1}^{n} \frac{1}{m} - \ln n \right) = \gamma.$$
 (20)

We recognize this limit as Euler's constant. Thus, we have derived the following asymptotic series:

$$\sum_{m=1}^{n} \frac{1}{m} \sim \ln n + \gamma + \frac{1}{2n} - \sum_{m=1}^{\infty} \frac{B_{2m}}{2m} \frac{1}{n^{2m}}, \qquad n \to \infty.$$

By the way, we can turn this equation around and use it for an accurate numerical computation of  $\gamma$ .

Many other finite series, summed from m=1 to n, can be expressed in the form of an asymptotic series as  $n\to\infty$ . I will leave it to you as an exercise to work out the asymptotic series for:

$$\sum_{m=1}^{n} \frac{1}{m^p} \sim \zeta(p) + \frac{1}{n^p} \left[ \frac{n}{1-p} + \frac{1}{2} + \mathcal{O}\left(\frac{1}{n}\right) \right], \qquad n \to \infty,$$

where p > 1 and  $\zeta(p)$  is the Riemann zeta function. The  $\mathcal{O}(1/n)$  term above can be expressed in terms of an asymptotic series with coefficients proportional to the Bernoulli numbers, using the same techniques employed above.

In our final example, we choose  $f(x) = (\ln x)/x$ , with k = 1 and  $n \to n - 1$ . It follows that

$$\sum_{m=1}^{n} \frac{\ln m}{m} \sim \int_{1}^{n} \frac{\ln x}{x} dx + C + \frac{\ln n}{2n} + \mathcal{O}\left(\frac{\ln n}{n^{2}}\right)$$

$$\sim C + \frac{1}{2} \ln^{2} n + \frac{\ln n}{2n} + \mathcal{O}\left(\frac{\ln n}{n^{2}}\right), \tag{21}$$

where C represents the n-independent pieces of eq. (14), and the  $\mathcal{O}(\ln n/n^2)$  remainder corresponds to a sum with Bernoulli number coefficients (which we do not write out explicitly here). Thus,

$$C = \lim_{n \to \infty} \left( \sum_{m=1}^{n} \frac{\ln m}{m} - \frac{1}{2} \ln^2 n \right) . \tag{22}$$

This result can be used to evaluate the sum

$$S \equiv \sum_{n=1}^{\infty} (-1)^n \frac{\ln n}{n} \,.$$

Consider the sum  $S_{2N}$  made up of the first 2N terms of the above series. We can write:

$$S_{2N} = \sum_{n=1}^{2N} (-1)^n \frac{\ln n}{n} = -\sum_{n=1}^{2N} \frac{\ln n}{n} + 2\sum_{n=1}^{N} \frac{\ln 2n}{2n}$$
$$= -\sum_{n=1}^{2N} \frac{\ln n}{n} + \sum_{n=1}^{N} \frac{\ln n}{n} + \ln 2\sum_{n=1}^{N} \frac{1}{n},$$
(23)

where we have used  $\ln(2n) = \ln n + \ln 2$  in obtaining the second line of eq. (23). However, eqs. (21) and (22) and eqs. (19) and (20) imply respectively that:

$$\sum_{n=1}^{N} \frac{\ln n}{n} = C + \frac{1}{2} \ln^2 N + \mathcal{O}\left(\frac{1}{N}\right), \qquad \sum_{n=1}^{N} \frac{1}{n} = \gamma + \ln N + \mathcal{O}\left(\frac{1}{N}\right).$$

Inserting these result into eq. (23), the constant C drops out, and we find:

$$S_{2N} = -\frac{1}{2}\ln^2(2N) + \frac{1}{2}\ln^2 N + \ln 2(\gamma + \ln N) + \mathcal{O}\left(\frac{1}{N}\right)$$
$$= \ln 2(\gamma - \frac{1}{2}\ln 2) + \mathcal{O}\left(\frac{1}{N}\right).$$

Taking the limit of  $N \to \infty$ , we obtain the desired sum  $S = \lim_{N \to \infty} S_{2N}$ :

$$\sum_{n=1}^{\infty} (-1)^n \frac{\ln n}{n} = \ln 2 \left( \gamma - \frac{1}{2} \ln 2 \right) .$$

This result (the n = 1 term does not contribute to the sum) was previously noted in the Riemann zeta function handout.