

## EULER–MACLAURIN EXPANSIONS FOR INTEGRALS WITH ARBITRARY ALGEBRAIC ENDPOINT SINGULARITIES

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ABSTRACT. In this paper, we provide the Euler–Maclaurin expansions for (off-set) trapezoidal rule approximations of the divergent finite-range integrals  $\int_a^b f(x) dx$ , where  $f \in C^\infty(a, b)$  but can have arbitrary algebraic singularities at one or both endpoints. We assume that  $f(x)$  has asymptotic expansions of the general forms

$$f(x) \sim K(x-a)^{-1} + \sum_{s=0}^{\infty} c_s(x-a)^{\gamma_s} \quad \text{as } x \rightarrow a+,$$

$$f(x) \sim L(b-x)^{-1} + \sum_{s=0}^{\infty} d_s(b-x)^{\delta_s} \quad \text{as } x \rightarrow b-,$$

where  $K, L$ , and  $c_s, d_s$ ,  $s = 0, 1, \dots$ , are some constants,  $|K| + |L| \neq 0$ , and  $\gamma_s$  and  $\delta_s$  are distinct, arbitrary and, in general, complex, and different from  $-1$ , and satisfy

$$\Re \gamma_0 \leq \Re \gamma_1 \leq \dots, \quad \lim_{s \rightarrow \infty} \Re \gamma_s = +\infty; \quad \Re \delta_0 \leq \Re \delta_1 \leq \dots, \quad \lim_{s \rightarrow \infty} \Re \delta_s = +\infty.$$

Hence the integral  $\int_a^b f(x) dx$  exists in the sense of Hadamard finite part. The results we obtain in this work extend some of the results in [A. Sidi, *Numer. Math.* 98 (2004), pp. 371–387] that pertain to the cases in which  $K = L = 0$ . They are expressed in very simple terms based only on the asymptotic expansions of  $f(x)$  as  $x \rightarrow a+$  and  $x \rightarrow b-$ . With  $h = (b-a)/n$ , where  $n$  is a positive integer, one of these results reads

$$h \sum_{i=1}^{n-1} f(a+ih) \sim I[f] + K(C - \log h) + \sum_{\substack{s=0 \\ \gamma_s \notin \{2,4,\dots\}}}^{\infty} c_s \zeta(-\gamma_s) h^{\gamma_s+1}$$

$$+ L(C - \log h) + \sum_{\substack{s=0 \\ \delta_s \notin \{2,4,\dots\}}}^{\infty} d_s \zeta(-\delta_s) h^{\delta_s+1} \quad \text{as } h \rightarrow 0,$$

where  $I[f]$  is the Hadamard finite part of  $\int_a^b f(x) dx$ ,  $C$  is Euler's constant and  $\zeta(z)$  is the Riemann Zeta function. We illustrate the results with an example.

Received by the editor November 16, 2010 and, in revised form, April 17, 2011.

2010 *Mathematics Subject Classification.* Primary 30E15, 40A25, 41A60, 65B15, 65D30.

*Key words and phrases.* Euler–Maclaurin expansions, trapezoidal rule, endpoint singularities, Hadamard finite part, asymptotic expansions.

This research was supported in part by the United States–Israel Binational Science Foundation grant no. 2008399.

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1. INTRODUCTION

In this work, we provide the Euler–Maclaurin expansions for (offset) trapezoidal rule approximations of the divergent finite-range integrals  $\int_a^b f(x) dx$ , where the integrands  $f(x)$  have arbitrary algebraic singularities at  $x = a$  and  $x = b$ . Specifically, we assume that  $f(x)$  has the following properties:

- (1)  $f \in C^\infty(a, b)$  and has the asymptotic expansions

$$(1.1) \quad \begin{aligned} f(x) &\sim K(x-a)^{-1} + \sum_{s=0}^{\infty} c_s(x-a)^{\gamma_s} \quad \text{as } x \rightarrow a+, \\ f(x) &\sim L(b-x)^{-1} + \sum_{s=0}^{\infty} d_s(b-x)^{\delta_s} \quad \text{as } x \rightarrow b-, \end{aligned}$$

where  $K, L$ , and  $c_s, d_s$  are constants,  $|K| + |L| \neq 0$ , and  $\gamma_s$  and  $\delta_s$  are distinct, arbitrary and, in general, complex, and satisfy

$$(1.2) \quad \begin{aligned} \gamma_s &\neq -1; \quad \Re\gamma_0 \leq \Re\gamma_1 \leq \Re\gamma_2 \leq \dots; \quad \lim_{s \rightarrow \infty} \Re\gamma_s = +\infty, \\ \delta_s &\neq -1; \quad \Re\delta_0 \leq \Re\delta_1 \leq \Re\delta_2 \leq \dots; \quad \lim_{s \rightarrow \infty} \Re\delta_s = +\infty. \end{aligned}$$

Here,  $\Re z$  stands for the real part of  $z$ .<sup>1</sup> (We state at this point that this assumption generalizes that in Sidi [15], where  $K = L = 0$ . We will come back to this point later.)

Note that, in case  $f(x) = (x-a)^{-p}g_a(x) = (b-x)^{-q}g_b(x)$ , where  $p$  and  $q$  are positive integers,  $g_a \in C^\infty[a, b]$  and  $g_b \in C^\infty(a, b]$ , and  $g_a(x)$  and  $g_b(x)$  have full Taylor series about  $x = a$  and  $x = b$ , respectively, the  $\gamma_s$  and the  $\delta_s$  are, respectively,

$$-p, -p + 1, \dots, -3, -2, 0, 1, 2, \dots, \quad \text{and} \quad -q, -q + 1, \dots, -3, -2, 0, 1, 2, \dots,$$

and we have

$$K = \frac{g_a^{(p-1)}(a)}{(p-1)!} \quad \text{and} \quad L = (-1)^{q-1} \frac{g_b^{(q-1)}(b)}{(q-1)!}.$$

- (2) By (1.1), we mean that, for every  $r$ , such that  $\Re\gamma_r \geq -1$ ,

$$(1.3) \quad \begin{aligned} f(x) - \left[ K(x-a)^{-1} + \sum_{s=0}^{r-1} c_s(x-a)^{\gamma_s} \right] &= O((x-a)^{\gamma_r}) \quad \text{as } x \rightarrow a+, \\ f(x) - \left[ L(b-x)^{-1} + \sum_{s=0}^{r-1} d_s(b-x)^{\delta_s} \right] &= O((b-x)^{\delta_r}) \quad \text{as } x \rightarrow b-. \end{aligned}$$

This is consistent with (1.2).

- (3) For each  $k = 1, 2, \dots$ , the  $k$ th derivative of  $f(x)$  also has asymptotic expansions as  $x \rightarrow a+$  and  $x \rightarrow b-$  that are obtained by differentiating those in (1.1) term by term.

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<sup>1</sup>We can write the expansions in (1.1) in the “simpler” form

$$f(x) \sim \sum_{s=0}^{\infty} c_s(x-a)^{\gamma_s} \quad \text{as } x \rightarrow a+, \quad f(x) \sim \sum_{s=0}^{\infty} d_s(b-x)^{\delta_s} \quad \text{as } x \rightarrow b-,$$

ordering the  $\gamma_s$  and the  $\delta_s$  as in (1.2), and allowing now one of the  $\gamma_s$  and/or one of the  $\delta_s$  to be equal to  $-1$ . However, this complicates the statements of our results. Therefore, we have chosen to separate these two exponents as in (1.1).

The following are consequences of (1.2):

- (i) There are only finitely many  $\gamma_s$  and only finitely many  $\delta_s$  having the same real parts; consequently,  $\Re\gamma_s < \Re\gamma_{s+1}$  and  $\Re\delta_{s'} < \Re\delta_{s'+1}$  for infinitely many values of the indices  $s$  and  $s'$ .
- (ii) The sequences  $\{(x-a)^{\gamma_s}\}_{s=0}^\infty$  along with  $(x-a)^{-1}$  and  $\{(b-x)^{\delta_s}\}_{s=0}^\infty$  along with  $(b-x)^{-1}$  are asymptotic scales as  $x \rightarrow a+$  and  $x \rightarrow b-$ , respectively, in the following sense: For each  $s = 0, 1, \dots$ ,

$$\lim_{x \rightarrow a+} \left| \frac{(x-a)^{\gamma_{s+1}}}{(x-a)^{\gamma_s}} \right| = \begin{cases} 1 & \text{if } \Re\gamma_s = \Re\gamma_{s+1}, \\ 0 & \text{if } \Re\gamma_s < \Re\gamma_{s+1}, \end{cases}$$

$$\lim_{x \rightarrow b-} \left| \frac{(b-x)^{\delta_{s+1}}}{(b-x)^{\delta_s}} \right| = \begin{cases} 1 & \text{if } \Re\delta_s = \Re\delta_{s+1}, \\ 0 & \text{if } \Re\delta_s < \Re\delta_{s+1}. \end{cases}$$

- (iii) The integral  $\int_a^b f(x) dx$  does not exist in the ordinary sense, because  $f(x)$  is not integrable through either  $x = a$  or  $x = b$  or both, since either  $K \neq 0$  or  $L \neq 0$  or both. It does exist in the sense of the *Hadamard finite part*, however.<sup>2</sup> [When  $K = L = 0$ ,  $\int_a^b f(x) dx$  exists in the ordinary sense if  $\Re\gamma_0 > -1$  and  $\Re\delta_0 > -1$ . Otherwise, it exists in the sense of the Hadamard finite part.] The Hadamard finite part of  $\int_a^b f(x) dx$  is defined as follows: Let the integers  $\mu$  and  $\nu$  be such that

$$\Re\gamma_{\mu-1} \leq -1 < \Re\gamma_\mu, \quad \Re\delta_{\nu-1} \leq -1 < \Re\delta_\nu.$$

Define also

$$(1.4) \quad \begin{aligned} \phi_\mu(x) &:= f(x) - \left[ K(x-a)^{-1} + \sum_{s=0}^{\mu-1} c_s (x-a)^{\gamma_s} \right], \\ \psi_\nu(x) &:= f(x) - \left[ L(b-x)^{-1} + \sum_{s=0}^{\nu-1} d_s (b-x)^{\delta_s} \right]. \end{aligned}$$

Then, for arbitrary  $t \in (a, b)$ ,

$$(1.5) \quad \begin{aligned} \int_a^b f(x) dx &= K \log(t-a) + \sum_{s=0}^{\mu-1} c_s \frac{(t-a)^{\gamma_s+1}}{\gamma_s+1} + \int_a^t \phi_\mu(x) dx \\ &\quad + L \log(b-t) + \sum_{s=0}^{\nu-1} d_s \frac{(b-t)^{\delta_s+1}}{\delta_s+1} + \int_t^b \psi_\nu(x) dx, \end{aligned}$$

Here the integrals of  $\phi_\mu(x)$  and  $\psi_\nu(x)$  exist in the ordinary sense, as is clear from the way we have chosen  $\mu$  and  $\nu$ .

In Sidi [15], we derived, among other results, the Euler–Maclaurin expansions for (offset) trapezoidal rule approximations of finite-range integrals  $\int_a^b f(x) dx$ , where

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<sup>2</sup>The usual notation for Hadamard finite part integrals is  $\int_a^b f(x) dx$ . For simplicity, in this work, we use  $\int_a^b f(x) dx$  to denote both ordinary and Hadamard finite part integrals. For the definition and properties of Hadamard finite part integrals, see Davis and Rabinowitz [3, pp. 11–14] or Evans [4] or Kythe and Schäferkötter [5], for example. These integrals have most of the properties of regular integrals and some properties that are quite unusual. For example, they are invariant with respect to translation, but they are not invariant under a scaling of the variable of integration.

$f(x)$  is as described above, except that  $K = L = 0$  in (1.1).<sup>3</sup> Thus, in a sense, the present work completes the treatment of [15] with respect to such  $f(x)$ . In connection with these generalized Euler–Maclaurin expansions, we mention that the results of [15] were later used in Sidi [16], [18], and [17], in conjunction with some singular variable transformations, to “optimize” the accuracy of the trapezoidal rule approximations for finite-range integrals with algebraic endpoint singularities.

In the next section, we state the main results of this work. In Section 3, we provide the proofs of these results. In Section 4, we illustrate them with an interesting example treated recently by Brauchart, Hardin, and Saff [2].

Special cases of the problem we treat here have been considered by various authors. The case  $f(x) = (x - a)^\gamma g(x)$ ,  $g \in C^\infty[a, b]$  was first treated in the paper by Navot [10]. Later Navot [11] extended his treatment to the more general case of  $f(x) = (x - a)^\gamma \log(x - a)g(x)$ . [This is achieved by differentiating the Euler–Maclaurin expansion for the integral  $\int_a^b (x - a)^\gamma g(x) dx$  with respect to  $\gamma$ .] Navot’s results were rederived later by Lyness and Ninham [8] using a different method involving generalized functions. The treatment of [8] covers the more general cases of  $f(x) = (x - a)^\gamma (b - x)^\delta g(x)$  and  $f(x) = (x - a)^\gamma \log(x - a)(b - x)^\delta \log(b - x)g(x)$ ,  $g \in C^\infty[a, b]$ . (Actually, these cases can be treated by using Navot’s results as well.) For a brief survey of the relevant results, see also Sidi [14, Appendix D]. Subsequently, in a paper by Ninham [12], Navot’s expansions were shown to hold also for the case in which  $\Re\gamma \leq -1$  and/or  $\Re\delta \leq -1$ , such that  $\gamma$  and  $\delta$  are different from  $-1, -2, \dots$ ; in this case,  $\int_a^b f(x) dx$  is defined as a Hadamard finite part integral. Finally, the remaining case in which  $\gamma$  or  $\delta$  or both are negative integers has been dealt with by Lyness [7] and by Monegato and Lyness [9].

We would like to emphasize that our present results and those in [15] do not follow from the previous works on extensions of Euler–Maclaurin expansions in the presence of endpoint singularities.

Before closing this section, we note that we have assumed that  $f \in C^\infty(a, b)$  only for the sake of simplifying the presentation. We can assume that  $f \in C^k(a, b)$  for some finite  $k$  just as well. The method of proof provided in [15] applies to this case with minor changes.

## 2. MAIN RESULTS

Throughout the remainder of the paper, we use the notation

$$(2.1) \quad I[f] := \int_a^b f(x) dx,$$

whether  $\int_a^b f(x) dx$  exists as an ordinary integral or as a Hadamard finite part integral, and

$$(2.2) \quad \tilde{T}_n[f; \theta] := h \sum_{i=0}^{n-1} f(a + ih + \theta h); \quad h = \frac{b - a}{n}, \quad n = 1, 2, \dots$$

Here  $\tilde{T}_n[f; \theta]$  is the *offset trapezoidal rule* approximation to  $I[f]$ , and  $\theta \in (0, 1)$ . Because  $f \in C^\infty(a, b)$ ,  $\tilde{T}_n[f; \theta]$  with  $\theta \in (0, 1)$  is well defined. Note that  $\tilde{T}_n[f; \frac{1}{2}]$  is

<sup>3</sup>Even though the results of [15] are correct for  $\gamma_s, \delta_s \neq -1$ , they were stated under the condition that  $\gamma_s, \delta_s \neq -1, -2, -3, \dots$ , due to an unfortunate oversight. In this work, we correct this blunder.

simply the midpoint rule approximation to  $I[f]$ . For  $\theta = 1$ , we modify  $\tilde{T}_n[f; \theta]$  and define

$$(2.3) \quad \check{T}_n[f] := h \sum_{i=1}^{n-1} f(a + ih), \quad h = \frac{b-a}{n}, \quad n = 1, 2, \dots$$

By the fact that  $f \in C^\infty(a, b)$ ,  $\check{T}_n[f]$  is always well defined just as  $\tilde{T}_n[f; \theta]$  with  $0 < \theta < 1$ . We also set

$$(2.4) \quad T_n[f] = h \left[ \frac{1}{2}f(a) + \sum_{i=1}^{n-1} f(a + ih) + \frac{1}{2}f(b) \right] = \check{T}_n[f] + \frac{h}{2} [f(a) + f(b)]$$

and

$$(2.5) \quad T'_n[f] = h \sum_{i=1}^{n-1} f(a + ih) + \frac{h}{2} f(b), \quad T_n^*[f] = h \sum_{i=1}^{n-1} f(a + ih) + \frac{h}{2} f(a),$$

when these are defined. Note that  $T_n[f]$  is the standard trapezoidal rule for  $I[f]$ .

Note that the offset trapezoidal rule allows extensions for composite (or  $n$ -panel) Gauss-Legendre or other rules of a higher degree of accuracy, where the  $n$ -panel rules become linear combinations of offset type rules. This provides further motivation for considering the offset trapezoidal rule in our developments.

In our results below,  $\zeta(z, \theta)$  denotes the *generalized Zeta function*, which is defined by the convergent Dirichlet series  $\sum_{k=0}^\infty 1/(k + \theta)^z$  for  $\Re z > 1$  and continued analytically to the whole complex  $z$ -plane, with the exception of  $z = 1$ , where it has a simple pole with residue 1. For  $\theta = 1$ ,  $\zeta(z, 1)$  is simply  $\zeta(z)$ , the *Riemann Zeta function*. At this point, we only note the following relations among the two Zeta functions and the Bernoulli polynomials  $B_j(\theta)$  and the Bernoulli numbers  $B_j$  (see, [13, Chapters 24, 25] or [14, Appendices D, E], for example):

$$(2.6) \quad \begin{aligned} \zeta(-j, \theta) &= -\frac{B_{j+1}(\theta)}{j+1}, \quad j = 0, 1, \dots, \\ B_j(0) &= B_j, \quad j \geq 0; \quad B_1(1) = -B_1; \quad B_j(1) = B_j, \quad j \geq 0, \quad j \neq 1, \\ B_0 &= 1, B_1 = -\frac{1}{2}; \quad B_{2j+1} = 0, \quad B_{2j} \neq 0, \quad j = 1, 2, \dots, \\ \zeta(0) &= -\frac{1}{2}; \quad \zeta(-2j) = 0, \quad \zeta(1-2j) = -\frac{B_{2j}}{2j} \neq 0, \quad j = 1, 2, \dots, \\ B_j(1-\theta) &= (-1)^j B_j(\theta), \quad B_{2j+1}(\frac{1}{2}) = 0, \quad \zeta(-2j, \frac{1}{2}) = 0, \quad j = 0, 1, \dots \end{aligned}$$

Our results also involve the *Psi function*, which is defined via  $\psi(z) = \Gamma'(z)/\Gamma(z)$ , where  $\Gamma(z)$  is the *Gamma function*. We note that (see Luke [6, pp. 12-13], for example)

$$(2.7) \quad \begin{aligned} \lim_{n \rightarrow \infty} \left[ \sum_{i=0}^n (i + \theta)^{-1} - \log n \right] &= -\psi(\theta), \\ \lim_{n \rightarrow \infty} \left[ \sum_{k=1}^n \frac{1}{k} - \log n \right] &= C \quad (\text{Euler constant}), \\ \psi(1) &= -C, \quad \psi(\frac{1}{2}) = -C - 2 \log 2. \end{aligned}$$

Here are the main results.

**Theorem 2.1.** *Let  $f(x)$  be as in (1.1)–(1.3). Then, with  $0 < \theta < 1$ , there holds*

$$(2.8) \quad \begin{aligned} \tilde{T}_n[f; \theta] \sim I[f] + K[-\psi(\theta) - \log h] &+ \sum_{s=0}^{\infty} c_s \zeta(-\gamma_s, \theta) h^{\gamma_s+1} \\ &+ L[-\psi(1 - \theta) - \log h] + \sum_{s=0}^{\infty} d_s \zeta(-\delta_s, 1 - \theta) h^{\delta_s+1} \quad \text{as } h \rightarrow 0. \end{aligned}$$

The following corollary is obtained by invoking in Theorem 2.1 the relations given in (2.6).

**Corollary 2.2.** *When  $\theta = \frac{1}{2}$ , the result in (2.8) can be re-expressed as in*

$$(2.9) \quad \begin{aligned} \tilde{T}_n[f; \tfrac{1}{2}] \sim I[f] + (K + L)(C + 2 \log 2 - \log h) \\ + \sum_{\substack{s=0 \\ \gamma_s \notin \{0, 2, 4, \dots\}}}^{\infty} c_s \zeta(-\gamma_s, \tfrac{1}{2}) h^{\gamma_s+1} + \sum_{\substack{s=0 \\ \delta_s \notin \{0, 2, 4, \dots\}}}^{\infty} d_s \zeta(-\delta_s, \tfrac{1}{2}) h^{\delta_s+1} \quad \text{as } h \rightarrow 0. \end{aligned}$$

**Theorem 2.3.** *For  $\tilde{T}_n[f]$ , we have*

$$(2.10) \quad \begin{aligned} \tilde{T}_n[f] \sim I[f] + (K + L)(C - \log h) \\ + \sum_{\substack{s=0 \\ \gamma_s \notin \{2, 4, 6, \dots\}}}^{\infty} c_s \zeta(-\gamma_s) h^{\gamma_s+1} + \sum_{\substack{s=0 \\ \delta_s \notin \{2, 4, 6, \dots\}}}^{\infty} d_s \zeta(-\delta_s) h^{\delta_s+1} \quad \text{as } h \rightarrow 0. \end{aligned}$$

**Remarks.**

- (1) From (1.2), it is obvious that the expansions in (2.8), (2.9), and (2.10) are genuine asymptotic expansions.
- (2) The results in (2.9) and (2.10) imply that the (even) powers  $(x - a)^{2s}$  and  $(b - x)^{2s}$ , even if present in the asymptotic expansions of (1.1), do not contribute to the Euler–Maclaurin expansion of  $\tilde{T}_n[f; \frac{1}{2}]$  when  $s \in \{0, 1, \dots\}$ , and they do not contribute to the Euler–Maclaurin expansion of  $\tilde{T}_n[f]$  when  $s \in \{1, 2, \dots\}$ . Actually, this is caused by the facts that  $\zeta(-2s, \frac{1}{2}) = 0$  for  $s = 0, 1, 2, \dots$ , and  $\zeta(-2s) = 0$  for  $s = 1, 2, \dots$ , [recall (2.6)]. Despite this, we have chosen to emphasize their absence from the relevant summations in (2.9) and (2.10).

3. PROOFS

**3.1. Asymptotic expansion of the sum  $\sum_{i=0}^{n-1} (i + \theta)^{-1}$ .** We begin by stating the classical result on the Euler–Maclaurin expansion for sums. For a proof of this result, we refer the reader to Steffensen [19].

**Theorem 3.1.** *Let  $F(t) \in C^m[r, \infty)$ , where  $r$  is an integer, and let  $\theta \in [0, 1]$  be fixed. Then, for any integer  $n > r$ ,*

$$\sum_{i=r}^{n-1} F(i + \theta) = \int_r^n F(t) dt + \sum_{k=1}^m \frac{B_k(\theta)}{k!} [F^{(k-1)}(n) - F^{(k-1)}(r)] + R_m(n; \theta),$$

where the remainder term  $R_m(n; \theta)$  is given by

$$R_m(n; \theta) = - \int_r^n F^{(m)}(t) \frac{\bar{B}_m(\theta - t)}{m!} dt,$$

where  $\bar{B}_k(x)$  is the periodic Bernoullian function that is the 1-periodic extension of the Bernoulli polynomial  $B_k(x)$ .

Applying this theorem with  $F(t) = t^{-1}$  and  $r = 1$ , we obtain

$$(3.1) \quad \sum_{i=0}^{n-1} (i + \theta)^{-1} = \theta^{-1} + \log n + \sum_{k=1}^m \frac{B_k(\theta)}{k!} ([-1]_{k-1} n^{-k} - [-1]_{k-1}) + R_m(n; \theta),$$

where

$$R_m(n; \theta) = - \int_1^n [-1]_m t^{-m-1} \frac{\bar{B}_m(\theta - t)}{m!} dt.$$

Here, we have defined

$$[\omega]_0 = 1 \quad \text{and} \quad [\omega]_s = \prod_{i=0}^{s-1} (\omega - i), \quad s = 1, 2, \dots .$$

By the fact that  $\bar{B}_m(x)$  is bounded for all  $x$ , it follows that the integrand in  $R_m(n; \theta)$  is  $O(t^{-m-1})$  as  $t \rightarrow \infty$ . As a result,  $R_m(\infty; \theta)$  exists when  $m \geq 1$ , and

$$R_m(n; \theta) - R_m(\infty; \theta) = \int_n^\infty [-1]_m t^{-m-1} \frac{\bar{B}_m(\theta - t)}{m!} dt = O(n^{-m}) \quad \text{as } n \rightarrow \infty.$$

With the help of this, we can now rewrite (3.1) in the form

$$(3.2) \quad \sum_{i=0}^{n-1} (i + \theta)^{-1} = \log n + S'_m(\theta) + S''_m(\theta),$$

where

$$(3.3) \quad S'_m(\theta) = \theta^{-1} - \sum_{k=1}^m \frac{B_k(\theta)}{k!} [-1]_{k-1} + R_m(\infty; \theta)$$

and

$$(3.4) \quad S''_m(\theta) = \sum_{k=1}^m \frac{B_k(\theta)}{k!} [-1]_{k-1} n^{-k} + O(n^{-m}) \quad \text{as } n \rightarrow \infty.$$

Clearly,  $\lim_{n \rightarrow \infty} S''_m(\theta) = 0$ . Consequently,

$$(3.5) \quad \lim_{n \rightarrow \infty} \left[ \sum_{i=0}^{n-1} (i + \theta)^{-1} - \log n \right] = S'_m(\theta), \quad \text{independently of } m.$$

Now, invoking (2.7), we also realize that  $S'_m(\theta) = -\psi(\theta)$ . Combining this and (3.4) in (3.2), we finally have

$$(3.6) \quad \sum_{i=0}^{n-1} (i + \theta)^{-1} = \log n - \psi(\theta) + \sum_{k=1}^m \frac{B_k(\theta)}{k!} [-1]_{k-1} n^{-k} + O(n^{-m}) \quad \text{as } n \rightarrow \infty.$$

Note that, for  $\theta = 1$ , (3.6) reduces to the well-known result

$$(3.7) \quad \sum_{i=0}^{n-1} (i + 1)^{-1} = \log n + C + \frac{1}{2n} + \sum_{\substack{k=2 \\ k \text{ even}}}^m \frac{B_k}{k!} [-1]_{k-1} n^{-k} + O(n^{-m}) \quad \text{as } n \rightarrow \infty.$$

**3.2. Euler–Maclaurin expansions for the integrals  $\int_a^b (x-a)^\omega dx$  and  $\int_a^b (b-x)^\omega dx$ .** We now consider the Euler–Maclaurin expansions for the integrals of the functions

$$(3.8) \quad u_\omega(x) = (x-a)^\omega \quad \text{and} \quad v_\omega(x) = (b-x)^\omega.$$

Note that  $\int_a^b u_\omega(x) dx$  and  $\int_a^b v_\omega(x) dx$  exist as ordinary integrals when  $\Re\omega > -1$ . Otherwise, they exist as Hadamard finite part integrals. We have

$$(3.9) \quad I[u_\omega] = \frac{(b-a)^{\omega+1}}{(\omega+1)} = I[v_\omega] \quad \text{if } \omega \neq -1, \quad I[u_{-1}] = \log(b-a) = I[v_{-1}].$$

In addition, it is easy to show that, for all  $\omega$  and for  $\theta \in (0, 1)$ ,

$$(3.10) \quad \tilde{T}_n[u_\omega; \theta] = h \sum_{i=0}^{n-1} (ih + \theta h)^\omega \quad \text{and} \quad \tilde{T}_n[v_\omega; \theta] = h \sum_{i=0}^{n-1} (ih + (1-\theta)h)^\omega,$$

so that

$$(3.11) \quad \tilde{T}_n[v_\omega; \theta] = \tilde{T}_n[u_\omega; 1-\theta].$$

In addition,

$$(3.12) \quad \tilde{T}_n[u_\omega] = h \sum_{i=1}^{n-1} (ih)^\omega = \tilde{T}_n[v_\omega],$$

and also

$$(3.13) \quad T'_n[u_\omega] = h \sum_{i=1}^{n-1} (ih)^\omega + \frac{h}{2} (b-a)^\omega = T_n^*[v_\omega].$$

Then we have the following results:

**Theorem 3.2.** *Let  $m$  be a nonnegative integer such that  $m > \Re\omega + 1$ . Then the following are true:*

(1) *For  $\omega \neq -1$  and  $\theta \in (0, 1]$ ,*

$$(3.14a) \quad \begin{aligned} \tilde{T}_n[u_\omega; \theta] &= I[u_\omega] + \zeta(-\omega, \theta) h^{\omega+1} \\ &+ \sum_{k=1}^m \frac{B_k(\theta)}{k!} u_\omega^{(k-1)}(b) h^k + O(h^m) \quad \text{as } h \rightarrow 0, \end{aligned}$$

$$(3.14b) \quad T'_n[u_\omega] = I[u_\omega] + \zeta(-\omega) h^{\omega+1} + \sum_{\substack{k=2 \\ \text{keven}}}^m \frac{B_k}{k!} u_\omega^{(k-1)}(b) h^k + O(h^m) \quad \text{as } h \rightarrow 0.$$

(2) *For  $\omega \neq -1$  and  $\theta \in [0, 1)$ ,*

$$(3.15a) \quad \begin{aligned} \tilde{T}_n[v_\omega; \theta] &= I[v_\omega] + \zeta(-\omega, 1-\theta) h^{\omega+1} \\ &- \sum_{k=1}^m \frac{B_k(\theta)}{k!} v_\omega^{(k-1)}(a) h^k + O(h^m) \quad \text{as } h \rightarrow 0, \end{aligned}$$

$$(3.15b) \quad T_n^*[v_\omega] = I[v_\omega] + \zeta(-\omega) h^{\omega+1} - \sum_{\substack{k=2 \\ \text{keven}}}^m \frac{B_k}{k!} v_\omega^{(k-1)}(a) h^k + O(h^m) \quad \text{as } h \rightarrow 0.$$



(3) For  $\omega = -1$  and  $\theta \in (0, 1]$ ,

$$(3.16a) \quad \begin{aligned} \tilde{T}_n[u_{-1}; \theta] &= I[u_{-1}] - [\log h + \psi(\theta)] \\ &+ \sum_{k=1}^m \frac{B_k(\theta)}{k!} u_{-1}^{(k-1)}(b) h^k + O(h^m) \quad \text{as } h \rightarrow 0, \end{aligned}$$

$$(3.16b) \quad T'_n[u_{-1}] = I[u_{-1}] - [\log h - C] + \sum_{\substack{k=2 \\ \text{keven}}}^m \frac{B_k}{k!} u_{-1}^{(k-1)}(b) h^k + O(h^m) \quad \text{as } h \rightarrow 0,$$

(4) For  $\omega = -1$  and  $\theta \in [0, 1)$ ,

$$(3.17a) \quad \begin{aligned} \tilde{T}_n[v_{-1}; \theta] &= I[v_{-1}] - [\log h + \psi(\theta)] \\ &- \sum_{k=1}^m \frac{B_k(\theta)}{k!} v_{-1}^{(k-1)}(b) h^k + O(h^m) \quad \text{as } h \rightarrow 0, \end{aligned}$$

$$(3.17b) \quad T_n^*[v_{-1}] = I[v_{-1}] - [\log h - C] - \sum_{\substack{k=2 \\ \text{keven}}}^m \frac{B_k}{k!} v_{-1}^{(k-1)}(b) h^k + O(h^m) \quad \text{as } h \rightarrow 0.$$

When  $\omega$  is a positive integer and  $m = \omega + 1$ , the  $O(h^m)$  terms in (3.14a), (3.14b), (3.15a), and (3.15b) are all zero.

*Proof.* Parts 1 and 2 are simply Theorems 3.2 and 3.3 in Sidi [15], which are extensions to all complex  $\omega \neq -1$  of the corresponding results by Navot [10], whether  $I[u_\omega]$  and  $I[v_\omega]$  exist in the regular sense or as Hadamard finite part integrals. The proof of parts 3 and 4 can be achieved as follows: We first note that

$$\tilde{T}_n[u_{-1}; \theta] = \sum_{i=0}^{n-1} (i + \theta)^{-1}.$$

Next, we invoke  $n = (b - a)/h$  in (3.6), and make use of the fact that

$$[-1]_{k-1} (b - a)^{-k} = u_{-1}^{(k-1)}(b) = (-1)^{k-1} v_{-1}^{(k-1)}(a).$$

The results in (3.16a) and (3.17a) now follow. The results in (3.16b) and (3.17b) are obtained from those in (3.16a) and (3.17a) by letting in the latter  $\theta = 1$  and  $\theta = 0$ , respectively. □

**3.3. Completion of proofs.** To complete the proof of Theorem 2.1, we define the functions  $\phi_\mu(x)$  and  $\psi_\nu(x)$  exactly as in (1.4), and rewrite these as in

$$(3.18) \quad \begin{aligned} \phi_\mu(x) &:= f(x) - \left[ K u_{-1}(x) + \sum_{s=0}^{\mu-1} c_s u_{\gamma_s}(x) \right], \\ \psi_\nu(x) &:= f(x) - \left[ L v_{-1}(x) + \sum_{s=0}^{\nu-1} d_s v_{\delta_s}(x) \right]. \end{aligned}$$

Next, we split the integral  $I[f] = \int_a^b f(x) dx$  as in

$$I[f] = \int_a^t f(x) dx + \int_t^b f(x) dx, \quad t = a + rh, \quad r = \left\lfloor \frac{n+1}{2} \right\rfloor,$$

and derive the Euler–Maclaurin expansions of the (offset) trapezoidal rule for the integrals

$$\int_a^t f(x) dx = \int_a^t \left[ K u_{-1}(x) + \sum_{s=0}^{\mu-1} c_s u_{\gamma_s}(x) \right] dx + \int_a^t \phi_\mu(x) dx$$

and

$$\int_t^b f(x) dx = \int_t^b \left[ L v_{-1}(x) + \sum_{s=0}^{\nu-1} d_s v_{\delta_s}(x) \right] dx + \int_t^b \psi_\nu(x),$$

exactly as is done in [15], by invoking all four parts of Theorem 3.2. Following this, we sum the two expansions to obtain our main results. [Note that, upon summing the Euler–Maclaurin expansions of the (offset) trapezoidal rules for the two integrals, the contribution from the left of the point  $x = t$  cancels that from the right completely, because the summations involving the  $B_k(\theta)$  and the  $B_k$  in Theorem 3.2 have opposite signs for the  $u_\omega(x)$  and  $v_\omega(x)$ .] We refer the reader to [15] for the details.

#### 4. AN EXAMPLE

The summation

$$(4.1) \quad E_n(p) = 2^{-p} n \sum_{k=1}^{n-1} \left( \sin \frac{k\pi}{n} \right)^{-p}, \quad p \neq 0,$$

is the *Riesz energy* of the  $n$ th roots of unity, and its asymptotic expansions (as  $n \rightarrow \infty$ ) for all values of  $p$  have been derived in [2]. We now show how these results can be obtained in a simple way by applying Theorem 2.3.

First, defining

$$(4.2) \quad f(x) = (\sin \pi x)^{-p},$$

we can express  $E_n(p)$  as in

$$(4.3) \quad E_n(p) = 2^{-p} n^2 \tilde{T}_n[f], \quad \tilde{T}_n[f] = h \sum_{k=1}^{n-1} f(kh), \quad h = \frac{1}{n}.$$

Clearly,  $\tilde{T}_n[f]$  approximates

$$(4.4) \quad I[f] = \int_0^1 f(x) dx,$$

whether this integral exists as a regular integral or is defined in the sense of the Hadamard finite part.

To obtain the full asymptotic expansion of  $\tilde{T}_n[f]$ , we need  $I[f]$  and we need to analyze  $f(x)$  near  $x = 0$  and  $x = 1$ . First, it is easy to see that

$$(4.5) \quad f(x) = (\pi x)^{-p} \left( \frac{2i\pi x}{\exp(2i\pi x) - 1} \right)^p \exp(i\pi p x).$$

Consequently, we have the convergent expansion

$$(4.6) \quad f(x) = (\pi x)^{-p} \sum_{s=0}^{\infty} \alpha_s(p) x^{2s}, \quad |x| < 1,$$

where the  $\alpha_s(p)$  are defined in terms of the *generalized Bernoulli polynomials*<sup>4</sup> as in

$$(4.7) \quad \alpha_s(p) = (-1)^s \frac{B_{2s}^{(p)}(\frac{1}{2}p)}{(2s)!} (2\pi)^{2s}, \quad s = 0, 1, \dots .$$

By the fact that  $f(1 - x) = f(x)$ , we also have

$$(4.8) \quad f(x) = [\pi(1 - x)]^{-p} \sum_{s=0}^{\infty} \alpha_s(p) (1 - x)^{2s}.$$

Next, because the series expansions of  $f(x)$  about  $x = 0$  and  $x = 1$  begin with the powers  $x^{-p}$  and  $(1 - x)^{-p}$ , respectively,  $I[f]$  exists as a regular integral only for  $\Re p < 1$ . We can derive a series representation for  $I[f]$  when  $\Re p < 1$  as follows: First, we observe that

$$(4.9) \quad I[f] = 2 \int_0^{1/2} f(x) dx,$$

since  $f(1 - x) = f(x)$ . Next, we substitute the expansion given in (4.6) in (4.9), and integrate termwise since this expansion is absolutely and uniformly convergent for  $0 < x < 1$ . This results in the convergent expansion

$$(4.10) \quad I[f] = F(p) = 2\pi^{-p} \sum_{s=0}^{\infty} \alpha_s(p) \frac{(\frac{1}{2})^{2s-p+1}}{2s - p + 1}, \quad \Re p < 1.$$

By making the transformation of variable  $y = \sin(\frac{1}{2}x)$  in (4.9), we can also obtain the closed-form expression

$$(4.11) \quad I[f] = F(p) = \frac{1}{\sqrt{\pi}} \frac{\Gamma(\frac{1}{2} - \frac{1}{2}p)}{\Gamma(1 - \frac{1}{2}p)}, \quad \Re p < 1.$$

For all other values of  $p$  (that is, for  $\Re p \geq 1$ ),  $I[f]$  exists as a Hadamard finite part integral defined as in (1.5). We concentrate on this issue below.

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<sup>4</sup> The generalized Bernoulli polynomials  $B_s^{(\sigma)}(u)$  are defined via (see Luke [6, pp. 18–23] or Andrews, Askey, and Roy [1, p. 615], for example)

$$\left(\frac{t}{e^t - 1}\right)^\sigma e^{ut} = \sum_{s=0}^{\infty} B_s^{(\sigma)}(u) \frac{t^s}{s!}, \quad |t| < 2\pi.$$

$B_s^{(\sigma)}(u)$  is of degree  $s$  in  $u$ .  $B_s^{(\sigma)}(\sigma - u) = (-1)^s B_s^{(\sigma)}(u)$ ; hence  $B_s^{(\sigma)}(\sigma/2) = 0$  for  $s = 1, 3, 5, \dots$ .  $B_s^{(\sigma)}(0)$  are called the generalized Bernoulli numbers and are denoted by  $B_s^{(\sigma)}$ .  $B_s^{(\sigma)}$  is a polynomial in  $\sigma$  of degree  $s$ . Note that  $B_0^{(\sigma)}(u) = B_0^{(\sigma)} = 1$  for all  $\sigma$ . In addition,  $B_s^{(\sigma)}(u) = \sum_{k=0}^s \binom{s}{k} B_{s-k}^{(\sigma)} u^k$ . As a result,  $B_{2s}^{(\sigma)}(\sigma/2)$  is a polynomial in  $\sigma$  of degree  $2s$ .

4.1.  $E_n(p)$  for  $p \neq 1, 3, 5, \dots$ . Now the function  $F(p)$  can be continued analytically to the  $p$ -plane, except for  $p = 1, 3, 5, \dots$ , where it has simple poles. This can be seen in two different ways:

- The  $s$ th term of the series in (4.10) is an analytic function of  $p$ , for all complex  $p \neq 2s + 1$ . This is so because  $\alpha_s(p)$  are entire functions of  $p$ , due to the fact that  $B_{2s}^{(p)}(\frac{1}{2}p)$  is a polynomial in  $p$  of degree  $2s$  (see footnote 4) and  $\pi^{-p}(\frac{1}{2})^{2s-p+1}$  is entire. Therefore, the expansion in (4.10) continues  $F(p)$  analytically to the whole  $p$ -plane, with the exception of  $p = 1, 3, 5, \dots$ , where it has simple poles. In addition, the series in (4.10) is precisely what we obtain when computing  $I[f]$  in the sense of the Hadamard finite part as described in (1.5).
- Because  $\Gamma(z)$  is analytic for all complex  $z$ , except  $z = 0, -1, -2, \dots$ , where it has simple poles, the right-hand side of (4.11) is an analytic function of  $p$  for all complex  $p$ , except  $p = 1, 3, 5, \dots$ , where  $\Gamma(\frac{1}{2} - \frac{1}{2}p)$  has simple poles. [The case  $p = 2, 4, 6, \dots$ , for which  $\Gamma(1 - \frac{1}{2}p)$  has simple poles, has some rather interesting features, and so does the case  $p = -2, -4, -6, \dots$ . We treat these cases separately below.]

In view of the above, the Hadamard finite part of  $I[f]$  for  $\Re p \geq 1, p \neq 1, 3, 5, \dots$ , is simply the analytic continuation of  $F(p)$ . Thus, we have both

$$(4.12) \quad I[f] = F(p) = 2\pi^{-p} \sum_{s=0}^{\infty} \alpha_s(p) \frac{(\frac{1}{2})^{2s-p+1}}{2s-p+1}, \quad p \neq 1, 3, 5, \dots,$$

and

$$(4.13) \quad I[f] = F(p) = \frac{1}{\sqrt{\pi}} \frac{\Gamma(\frac{1}{2} - \frac{1}{2}p)}{\Gamma(1 - \frac{1}{2}p)}, \quad p \neq 1, 3, 5, \dots$$

Since the convergent expansions in (4.6) and (4.8) are also asymptotic as  $x \rightarrow 0$  and  $x \rightarrow 1$ , respectively, we can apply Theorem 2.3. In case  $p \neq 1, 3, 5, \dots$ , we have  $K = L = 0$ , and  $\gamma_s = \delta_s = 2s - p$  and  $c_s = d_s = \pi^{-p}\alpha_s(p)$ ,  $s = 0, 1, \dots$ . Therefore, Theorem 2.3 gives

$$(4.14) \quad \check{T}_n[f] \sim F(p) + 2\pi^{-p} \sum_{\substack{s=0 \\ 2s-p \notin \{2,4,6,\dots\}}}^{\infty} \alpha_s(p)\zeta(p-2s)h^{2s-p+1} \quad \text{as } h \rightarrow 0.$$

Thus,

$$(4.15) \quad E_n(p) \sim 2^{-p}F(p)n^2 + 2(2\pi)^{-p} \sum_{\substack{s=0 \\ 2s-p \notin \{2,4,6,\dots\}}}^{\infty} \alpha_s(p)\zeta(p-2s)n^{p-2s+1} \quad \text{as } n \rightarrow \infty.$$

The cases  $p = \pm 2m, m = 1, 2, \dots$ , are rather unusual, and they are treated in detail in [2]. For completeness, we turn briefly to these cases next.

- When  $p = 2m, 1/\Gamma(1 - \frac{1}{2}p) = 0$  and hence  $I[f] = F(2m) = 0$ . In addition,  $\zeta(p - 2s) = 0$  for  $s > m$  by (2.6). The results in (4.14) and (4.15) now become, respectively,

$$(4.16) \quad \check{T}_n[f] = 2\pi^{-p} \sum_{s=0}^m \alpha_s(p)\zeta(p-2s)h^{2s-p+1} + O(h^\mu) \quad \text{as } h \rightarrow 0, \quad \forall \mu > 0$$

and

$$(4.17) \quad E_n(p) = 2(2\pi)^{-p} \sum_{s=0}^m \alpha_s(p) \zeta(p-2s) n^{p-2s+1} + O(n^{-\mu}), \quad \text{as } n \rightarrow \infty, \quad \forall \mu > 0.$$

- When  $p = -2m$ , by (4.13), we have

$$(4.18) \quad I[f] = F(-2m) = 2^{-2m} \binom{2m}{m}.$$

In addition, the infinite series in (4.14) is empty since  $\zeta(p-2s) = 0$  for  $s = 0, 1, \dots$ . Thus, (4.14) gives

$$\check{T}_n[f] = F(p) + O(h^\mu), \quad \text{as } h \rightarrow 0, \quad \forall \mu > 0.$$

Actually, we have exactly

$$(4.19) \quad \check{T}_n[f] = F(p) \quad \text{for } n > m.$$

We can see this as follows: First, because  $f(0) = f(1) = 0$ , we have  $\check{T}_n[f] = T_n[f]$ , where  $T_n[f]$  is the standard trapezoidal rule approximation for  $I[f]$  defined as in (2.4). Next,  $f(x) = (\sin \pi x)^{2m}$  is a trigonometric polynomial of the form

$$f(x) = \sum_{j=0}^m u_j \cos(2\pi jx).$$

Therefore,  $T_n[f] = I[f]$  when  $n > m$ . This proves (4.19). As a result, (4.15) becomes

$$(4.20) \quad E_n(p) = \binom{2m}{m} n^2, \quad \text{for } n > m.$$

4.2.  $E_n(p)$  for  $p = 1, 3, 5, \dots$ . Let  $p = 2m + 1$ ,  $m = 0, 1, \dots$ . In this case,  $I[f]$  can be computed in the sense of the Hadamard finite part precisely as described in (1.5). We start by rewriting (4.6) and (4.8) in the form

$$(4.21) \quad f(x) = \pi^{-p} \left[ \alpha_m(p) x^{-1} + \sum_{\substack{s=0 \\ s \neq m}}^{\infty} \alpha_s(p) x^{2s-p} \right]$$

and

$$(4.22) \quad f(x) = \pi^{-p} \left[ \alpha_m(p) (1-x)^{-1} + \sum_{\substack{s=0 \\ s \neq m}}^{\infty} \alpha_s(p) (1-x)^{2s-p} \right].$$

Next, we substitute (4.21) in the expansion in (4.9) and integrate termwise in the sense of the Hadamard finite part since this expansion is absolutely and uniformly convergent for  $0 < x < 1$ . We obtain the convergent expansion

$$(4.23) \quad I[f] = 2\pi^{-p} \left[ \alpha_m(p) \log\left(\frac{1}{2}\right) + \sum_{\substack{s=0 \\ s \neq m}}^{\infty} \alpha_s(p) \frac{\left(\frac{1}{2}\right)^{2s-p+1}}{2s-p+1} \right] \equiv G_m.$$

For a simple and more explicit representation of  $G_m$ , see [2].

The asymptotic expansion of  $\check{T}_n[f]$  can be obtained by applying Theorem 2.3 with (4.21) and (4.22). We have

$$(4.24) \quad \check{T}_n[f] \sim G_m + 2\pi^{-p} \left[ \alpha_m(p) (C - \log h) + \sum_{\substack{s=0 \\ s \neq m}}^{\infty} \alpha_s(p) \zeta(p-2s) h^{2s-p+1} \right] \quad \text{as } h \rightarrow 0.$$

Thus,

$$(4.25) \quad E_n(p) \sim 2^{-p} G_m n^2 + 2(2\pi)^{-p} \left[ \alpha_m(p) (C + \log n) n^2 + \sum_{\substack{s=0 \\ s \neq m}}^{\infty} \alpha_s(p) \zeta(p-2s) n^{p-2s+1} \right] \quad \text{as } n \rightarrow \infty.$$

#### ACKNOWLEDGEMENT

The author would like to thank Professor Edward B. Saff for a conversation concerning the paper [2], which motivated this paper.

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