The Euler-Maclaurin Functional for Functions with a Quasi-Step Discontinuity

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1. Introduction. Following previous extensions, [1], [2], of the form assumed by the Euler-Maclaurin functional

$$E\{f\}_a \equiv \sum_{\nu=1}^{n-1} f\left(\frac{\nu + a}{n}\right) - n \int_0^1 f(x)\, dx; \qquad 0 < a \leqq 1, \tag{1}$$

for functions $f(x)$ with integrable branch, logarithmic and both branch and logarithmic singularities at $x = 0$, consideration is now given to this functional for functions $f(x, \alpha)$ which depend on a parameter α in such a manner that for $\alpha = 0$ we have

$$\operatorname*{Lim}_{0<x\to 0} f(x, 0) = f(0, 0) + C \tag{2}$$

where $C \neq 0$ is a numerical constant. For functions $f(x, \alpha)$ of this type it is generally true that for small values of α their derivatives with respect to x oscillate strongly in the vicinity of $x = 0$, the peaks of the successive derivatives being proportional to successive negative powers of α. Obviously, therefore, when n in (1) is related to α so that $n\alpha$ is of the order of unity, or less, the negative powers of $n\alpha$ in the ordinary Euler-Maclaurin asymptotic series may render it useless for the numerical evaluation of the integral or sum in (1) since it may diverge from the beginning of the series.

Of the various possible quasi-step discontinuities, we consider here that introduced by the function $\tan^{-1} \frac{x}{\alpha}$, which is perhaps the simplest analytically. The subsequent discussion and examples will show that some other types of quasi-step discontinuities may be treated similarly.

2. Derivation of the Required Formula. Let

$$f(x, \alpha) = g(x) \tan^{-1} \frac{x}{\alpha}; \qquad \alpha > 0. \tag{3}$$

where $g(x)$ is an arbitrary real continuous function, with continuous derivatives up to the order $2m$, at $0 \leqq x \leqq 1$. Setting

$$g(x) = P_{2m-1}(x) + Q_{2m}(x);$$

$$P_{2m-1}(x) = \sum_{k=0}^{2m-1} \frac{g^{(k)}(0)}{k!} x^k, \qquad Q_{2m}(x) = \int_0^x \frac{g^{(2m)}(\tau)}{(2m-1)!} (x - \tau)^{2m-1}\, d\tau$$

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and $x = y/n$, we have by an analysis similar to that leading to equation (4) in [1]

$$
\begin{aligned}
E\{f\}_a &\equiv \sum_{\nu=0}^{n-1} f\left(\frac{\nu + a}{n}, \alpha\right) - n \int_0^1 f(x, \alpha)\, dx \\
&= \sum_{\mu=1}^{2m-1} \frac{B_\mu(a)}{\mu!} \left(\frac{1}{n}\right)^{\mu-1} f^{(\mu-1)}(1, \alpha) + \sum_{k=0}^{2m-2} C_k(a, n\alpha) \left(\frac{1}{n}\right)^k \frac{g^{(k)}(0)}{k!} + \rho_{2m}.
\end{aligned} \tag{4}
$$

In (4) $B_\mu(a)$ is Bernoulli's polynomial of degree μ while

$$
\begin{aligned}
C_k(a, n\alpha) &\equiv a^k \tan^{-1} \frac{a}{n\alpha} - \int_0^1 y^k \tan^{-1} \frac{y}{n\alpha}\, dy - \sum_{\mu=1}^{2m} \frac{B_\mu(a)}{\mu!} \frac{d^{\mu-1}}{dy^{\mu-1}} \\
&\quad \cdot \left[y^k \tan^{-1} \frac{y}{n\alpha} \right]_{y=1} + \int_1^\infty \frac{\bar{B}_{2m}(a - y)}{(2m)!} \frac{d^{2m}}{dy^{2m}} \left(y^k \tan^{-1} \frac{n\alpha}{y} \right) dy,
\end{aligned} \tag{5}
$$

where $\bar{B}_{2m}(y)$ is the periodic Bernoullian function of order $2m$. $C_k(a, n\alpha)$ is independent of $m(k \leqq 2m - 1)$ and for $a = \frac{1}{2}$ or $a = 1$, which are mainly of practical interest, is readily transformed into

$$
\begin{aligned}
&(-)^p \frac{(n\alpha)^{2p+1}}{2p + 1} \left[-\log n\alpha + \frac{1}{2p + 1} \right] \\
&\quad + (-)^p \int_0^{n\alpha} y^{2p} \tfrac{1}{2} \{\psi(a + iy) + \psi(a - iy)\}\, dy \\
&\quad + \begin{cases} -B_1(a) \dfrac{\pi}{2}; & \text{for } p = 0 \\ \displaystyle\sum_{\mu=0}^{p-1} (-)^\mu \frac{B_{2p-2\mu}(a)}{2p - 2\mu} \frac{(n\alpha)^{2\mu+1}}{2\mu + 1}; & \text{for } p = 1, 2, \cdots m - 1 \end{cases}
\end{aligned} \tag{6}
$$

when $k = 2p$; $p = 0, 1, \cdots m - 1$, and into

$$
\begin{aligned}
&-(-)^p \frac{(n\alpha)^{2p+2}}{2p + 2} \frac{\pi}{2} + (-)^p \int_0^{n\alpha} y^{2p+1} \frac{1}{2i} \{\psi(a + iy) - \psi(a - iy)\}\, dy \\
&\qquad - \frac{B_{2p+2}(a)}{2p + 2} \frac{\pi}{2} + (-)^p B_1(a) \frac{(n\alpha)^{2p+1}}{2p + 1}
\end{aligned} \tag{7}
$$

when $k = 2p + 1$; $p = 0, 1, \cdots m - 1$. $\psi(z)$ is the logarithmic derivative of the Gamma function. The remainder ρ_{2m} is given by

$$
\rho_{2m} = \left(\frac{1}{n}\right)^{2m-1} C_{2m-1}(a, n\alpha) \frac{g^{(2m-1)}(0)}{(2m - 1)!} + \sum_{k=0}^{2m} \varepsilon_k \tag{8}
$$

where

$$
\begin{aligned}
\varepsilon_k &= -\left(\frac{1}{n}\right)^{2m-1} \frac{g^{(k)}(0)}{k!} \int_1^\infty \frac{\bar{B}_{2m}(a - nx) - B_{2m}(a)}{(2m)!} \frac{d^{2m}}{dx^{2m}} \\
&\quad \cdot \left(x^k \tan^{-1} \frac{\alpha}{x} \right) dx; \qquad k = 0, 1, \cdots 2m - 2,
\end{aligned} \tag{9a}
$$

$$
\begin{aligned}
\varepsilon_{2m-1} &= -\left(\frac{1}{n}\right)^{2m-1} \frac{g^{(2m-1)}(0)}{(2m - 1)!} \\
&\quad \cdot \left\{ \int_1^\infty \frac{\bar{B}_{2m}(a - nx) - B_{2m}(a)}{(2m)!} \frac{d^{2m}}{dx^{2m}} \left(x^{2m-1} \tan^{-1} \frac{\alpha}{x} \right) dx - \frac{B_{2m}(a)}{2m} \frac{\pi}{2} \right\},
\end{aligned} \tag{9b}
$$

$$\varepsilon_{2m} = -\left(\frac{1}{n}\right)^{2m-1} \int_0^1 \frac{\bar{B}_{2m}(a - nx) - B_{2m}(a)}{(2m)!} \frac{d^{2m}}{dx^{2m}} \cdot \left\{ \int_0^x \frac{g^{(2m)}(\tau)}{(2m-1)!} (x - \tau)^{2m-1} \tan^{-1} \frac{x}{\alpha}\, d\tau \right\} dx. \tag{9c}$$

In some cases to be discussed soon, the term containing $C_{2m-1}(a, n\alpha)$ should be deleted from ρ_{2m} and lumped together with the other terms of this type.

3. Discussion of Formula (4) and the Numerical Evaluation of the Coefficients $C_k(a, n\alpha)$. The asymptotic summation formula (4), which is an error formula for the approximate evaluation of an integral by summation or the approximate evaluation of a finite sum by integration, is valid for all non-negative values of α and integer values of n. Its main use and advantage over the ordinary EM asymptotic summation formula is when $n\alpha$ remains bounded, or is of a smaller order than n, as $n \to \infty$, or when n is relatively large, and fixed, and $\alpha \to 0$. In these cases, as pointed out before, the remainder in the ordinary EM formula may absolutely increase with m even for small values of m. On the other hand, when $n\alpha$ is of the order of n as $n \to \infty$, the accuracy yielded by the ordinary EM summation formula and by (4) (after deleting the term containing $C_{2m-1}(a, n\alpha)$ from the remainder ρ_{2m} and lumping it with the correction terms) is of the same order, $(1/n)^{2m-1}$, as will be shown in the following section where ρ_{2m} is estimated. Practically, however, the ordinary EM summation formula should be preferred in that case since the coefficients $B_\mu(a)$; $\mu = 1, 2, \cdots 2m - 1$, which depend only on a, are more conveniently available than the coefficients $C_k(a, n\alpha)$; $k = 0, 1, \cdots 2m - 1$. The evaluation of $C_k(a, n\alpha)$ from equations (6) and (7) for $a = \frac{1}{2}$ and $a = 1$ is straightforward except for the integrals. The author is not aware that these integrals have been tabulated but rapidly convergent series expansions are readily available for them. Thus, for $0 < n\alpha \leqq 1$ we have

$$\begin{aligned}
&(-)^p \int_0^{n\alpha} y^{2p} \tfrac{1}{2}\{\psi(a + iy) + \psi(a - iy)\}\, dy \\
&= (-)^p \int_0^{n\alpha} y^{2p} \frac{1}{2}\left\{-\frac{1}{a + iy} - \frac{1}{a - iy}\right\} dy \\
&\qquad + (-)^p \int_0^{n\alpha} y^{2p} \tfrac{1}{2}\{\psi(1 + a + iy) + \psi(1 + a - iy)\}\, dy \\
&= a^{2p} \left\{ \sum_{\mu=0}^{p-1} \frac{(-)^\mu}{2\mu + 1} \left(\frac{n\alpha}{a}\right)^{2\mu+1} - \tan^{-1} \frac{n\alpha}{a} \right\} \\
&\qquad + (-)^p (n\alpha)^{2p+1} \sum_{\mu=0}^{\infty} (-)^\mu \frac{\psi^{(2\mu)}(1 + a)}{(2\mu)!} \frac{(n\alpha)^{2\mu}}{2p + 2\mu + 1}
\end{aligned} \tag{10}$$

and

$$(-)^p \int_0^{n\alpha} y^{2p+1} \frac{1}{2i} \{\psi(a+iy) - \psi(a-iy)\}\, dy$$

$$= (-)^p \int_0^{n\alpha} y^{2p+1} \frac{1}{2i} \left\{-\frac{1}{a+iy} + \frac{1}{a-iy}\right\} dy$$

$$+ (-)^p \int_0^{n\alpha} y^{2p+1} \frac{1}{2i} \{\psi(1+a+iy) - \psi(1+a-iy)\}\, dy \tag{11}$$

$$= a^{2p+1} \left\{\sum_{\mu=0}^{p} \frac{(-)^\mu}{2\mu+1} \left(\frac{n\alpha}{a}\right)^{2\mu+1} - \tan^{-1} \frac{n\alpha}{a}\right\}$$

$$+ (-)^p (n\alpha)^{2p+3} \sum_{\mu=0}^{\infty} (-)^\mu \frac{\psi^{(2\mu+1)}(1+a)}{(2\mu+1)!} \frac{(n\alpha)^{2\mu}}{2p+2\mu+3}.$$

The radii of convergence of the series in (10) and (11) are $1 + a$ and the numerical values of the coefficients may be obtained from tables [3] of $\psi^{(\mu)}(x)$ ($\mu = 0, 1, 2, \cdots$) or with the aid of a table [4] of Riemann's zeta function $\zeta(s) \equiv \zeta(s, 1)$, use being also made of the functional relation

$$\zeta(s, \tfrac{1}{2}) = (2^s - 1) \cdot \zeta(s, 1).$$

For $1 < n\alpha \leqq 2$ we have to add

$$(1+a)^{2p} \left\{\sum_{\mu=0}^{p-1} \frac{(-)^\mu}{2\mu+1} \left(\frac{n\alpha}{1+a}\right)^{2\mu+1} - \tan^{-1} \frac{n\alpha}{1+a}\right\} \tag{12a}$$

and

$$(1+a)^{2p+1} \left\{\sum_{\mu=0}^{p} \frac{(-)^\mu}{2\mu+1} \left(\frac{n\alpha}{1+a}\right)^{2\mu+1} - \tan^{-1} \frac{n\alpha}{1+a}\right\} \tag{12b}$$

to (10) and (11) respectively, and to replace $\psi^{(\mu)}(1 + a)/\mu!$ in the series in these equations by $\psi^{(\mu)}(2 + a)/\mu!$ which is related to it by

$$\frac{\psi^{(\mu)}(2+a)}{\mu!} = \frac{(-)^\mu}{(1+a)^\mu} + \frac{\psi^{(\mu)}(1+a)}{\mu!}; \qquad \mu = 0, 1, \cdots \tag{13}$$

The radii of convergence of the new series are $2 + a$. The evaluation of the integrals defining $C_k(a, n\alpha)$ may theoretically be carried out in this way for any value of $n\alpha$, and their asymptotic behavior as $n\alpha$ increases may thus be established.

4. Estimation of the Remainder ρ_{2m}. Not very sharp but generally sufficiently good bounds, valid for $a = \frac{1}{2}$ and $a = 1$ and easily obtained from equations (9), are the following:

$$|\varepsilon_k| = \left(\frac{1}{n}\right)^{2m-1} \theta_k\, \alpha^{k+1} \frac{|B_{2m}(a) g^{(k)}(0)|}{2m(k+1)!}; \tag{14a}$$

$$0 < \theta_k < 1, k = 0, 1, \cdots 2m - 1.$$

$$|\varepsilon_{2m-1}| \leqq \left(\frac{1}{n}\right)^{2m-1} \left(\frac{\theta_{2m-1}\, \alpha^{2m}}{2m} + \frac{\pi}{2}\right) \frac{|B_{2m}(a) g^{(2m-1)}(0)|}{(2m)!}; \quad 0 < \theta_{2m-1} < 1. \tag{14b}$$

$$|\varepsilon_{2m}| \leqq \left(\frac{1}{n}\right)^{2m-1} \theta_{2m} \left\{\frac{\pi}{2} + N_a\, \alpha \left(2m + \frac{1}{2m-1}\right)\right\} \frac{|B_{2m}(a) g^{(2m)}(\xi)|}{(2m)!}, \tag{14c}$$

$$0 < \theta_{2m} < 1; \qquad N_{1/2} = 3, \qquad N_1 = 2; \qquad 0 \leqq \xi \leqq 1.$$

Equations (14) provide an upper bound for $\sum_{k=0}^{2m} \varepsilon_k$. Hence, referring to equation (8), we see that except for the first term in it, ρ_{2m} decreases as $(1/n)^{2m-1}$ for a fixed m.

5. A Numerical Example. As a simple application of formula (4) we shall evaluate numerically the integral

$$(15)\qquad I = \frac{1}{2}\int_{-1}^{1} \tan^{-1}\frac{1+t}{\alpha}\tan^{-1}\frac{1-t}{\alpha}\,dt = \int_0^1 \tan^{-1}\frac{2-x}{\alpha}\tan^{-1}\frac{x}{\alpha}\,dx, \qquad \alpha = 10^{-3},$$

by the trapezoidal rule with $n = 10$. The approximating sum to eight decimals yields

$$(16)\qquad \frac{1}{n}\sum_{\nu=1}^{n-1} \tan^{-1}\frac{2n-\nu}{n\alpha}\tan^{-1}\frac{\nu}{n\alpha} + \frac{1}{2n}\left(\tan^{-1}\frac{1}{\alpha}\right)^2 = 2.33846010.$$

Since all the odd derivatives of the integrand at $x = 1$ vanish, the first two correction terms are

$$(17)\qquad \begin{aligned} -\frac{1}{n}\, C_0(1, n\alpha)\tan^{-1}\frac{2}{\alpha} &= 0.11543535 \\ \left(\frac{1}{n}\right)^2 C_1(1, n\alpha)\,\frac{\alpha}{2^2+\alpha^2} &= -0.00000031. \end{aligned}$$

The approximate value 2.45389514 of I thus obtained checks well (disregarding rounding errors) with its exact value to the same number of decimals computed from

$$(18)\qquad \begin{aligned} I &= \int_0^1 \left\{\frac{\pi}{2} - \frac{\alpha}{2-x} + \frac{1}{3}\frac{\alpha^3}{(2-x)^3} - \cdots\right\}\tan^{-1}\frac{x}{\alpha}\,dx = \left(\frac{\pi}{2}\right)^2 \\ &\quad - \left(\frac{\pi}{2} - \frac{\alpha}{2}\right)\alpha\log\frac{1}{\alpha} - (1 + \log 2)\left(\frac{\pi}{2} - \frac{\alpha}{2}\right)\alpha + O(\alpha^3) = 2.45389513 \end{aligned}$$

6. Integrands with a Different Type of Quasi-Step Discontinuity. We shall now determine the correction terms in evaluating by the tangent-trapezoidal rule ($a = \frac{1}{2}$) or trapezoidal rule ($a = 1$) integrals of the form

$$(19)\qquad I = \int_0^1 g(x)\tan^{-1}\frac{\sin\frac{\pi}{2}x}{\alpha}\,dx$$

where $g(x)$ is an odd function of $\sin\frac{\pi}{2}x$ and α is a positive parameter. The quasi-step discontinuity at $x = 0$ (which occurs here not in the integrand but in some odd derivative of it) is introduced by a different function, $\tan^{-1}\frac{\sin(\pi x/2)}{\alpha}$, from that investigated previously. The vanishing of all the odd derivatives of the integrand at both $x = 0$ and $x = 1$ shows, as is well known [5], that the ordinary Euler-Maclaurin summation formula is unable to provide correction terms since all of them vanish. Special methods are therefore required. Furthermore, the periodicity of the integrand calls for a comparison with the methods of Luke [6] and Davis [7], especially when $n\alpha$ is less than unity. This will be made later.

Writing

$$f(x,\alpha) = f_1\left(x, \frac{2}{\pi}\alpha\right) + f_2(x,\alpha) \tag{20}$$

where

$$f(x) = g(x)\tan^{-1}\frac{\sin\frac{\pi}{2}x}{\alpha};$$

$$f_1\left(x,\frac{2}{\pi}\alpha\right) = g(x)\tan^{-1}\frac{\pi}{2\alpha}x, \qquad f_2(x,\alpha) = g(x)\tan^{-1}\frac{\alpha\left(\sin\frac{\pi}{2}x - \frac{\pi}{2}x\right)}{\alpha^2 + \frac{\pi}{2}x\sin\frac{\pi}{2}x} \tag{21}$$

we see that $f_1\left(x, \frac{2}{\pi}\alpha\right)$ is of the form of (3) while $f_2(x, \alpha)$ can be expanded into a double series (which in the interval $0 \leqq x \leqq 1$ converges absolutely and uniformly for all positive values of α)

$$\begin{aligned} f_2(x,\alpha) &= g(x)\{W - \tfrac{1}{3}W^3 + \tfrac{1}{5}W^5 - \cdots\} \\ &= g(x)\{U(1 - V + V^2 - \cdots) - \tfrac{1}{3}U^3(1 - 3V + 6V^2 - \cdots) \\ &\qquad + \tfrac{1}{5}U^5(1 - 5V + 15V^2 - \cdots) - \cdots\} \end{aligned} \tag{22}$$

where

$$W = \frac{\alpha\left(\sin\frac{\pi}{2}x - \frac{\pi}{2}x\right)}{\alpha^2 + \frac{\pi}{2}x\sin\frac{\pi}{2}x},$$

$$V = \frac{\frac{\pi}{2}x\left(\sin\frac{\pi}{2}x - \frac{\pi}{2}x\right)}{\alpha^2 + \left(\frac{\pi}{2}x\right)^2}, \qquad U = \frac{\alpha\left(\sin\frac{\pi}{2}x - \frac{\pi}{2}x\right)}{\alpha^2 + \left(\frac{\pi}{2}x\right)^2}. \tag{23}$$

To evaluate the Euler-Maclaurin functional $E\{f_2\}_a$ to an accuracy at which terms only up to, say, n^{-3} are retained, we write

$$E\{f_2\}_a = E\{gU\}_a + E\{-gUV\}_a + E\{gUS_{1,2} + gT_3\}_a \tag{24}$$

where

$$S_{1,2} = V^2 - V^3 + \cdots; \qquad T_3 = -\tfrac{1}{3}W^3 + \tfrac{1}{5}W^5 - \cdots \tag{25}$$

For the first two terms of (24) we have from (4)

$$\begin{aligned} E\{gU\}_a &= -\alpha\frac{\partial}{\partial\alpha}E\left\{g\cdot\frac{\sin\frac{\pi}{2}x - \frac{\pi}{2}x}{\frac{\pi}{2}x}\cdot\tan^{-1}\frac{\pi}{2\alpha}x\right\}_a = \alpha\frac{\partial}{\partial\alpha}C_3\left(a, \frac{2}{\pi}n\alpha\right) \\ &\quad\cdot\left(\frac{1}{n}\right)^3\frac{g'(0)}{3!}\left(\frac{\pi}{2}\right)^2 + \sum_{\mu=1,2,4}\frac{B_\mu(a)}{\mu!}\left(\frac{1}{n}\right)^{\mu-1}\frac{d^{\mu-1}}{dx^{\mu-1}}[gU]_{x=1} + \delta_{6,1} \end{aligned} \tag{26}$$

and

$$(27)\quad \begin{aligned} E\{-gUV\}_a &= \alpha \frac{\partial}{\partial\alpha^2}\frac{\partial}{\partial\alpha} E\left\{-g \cdot \left(\sin\frac{\pi}{2}x - \frac{\pi}{2}x\right)^2 \cdot \tan^{-1}\frac{\pi}{2\alpha}x\right\}_a \\ &= \sum_{\mu=1,2,4} \frac{B_\mu(a)}{\mu!}\left(\frac{1}{n}\right)^{\mu-1}\frac{d^{\mu-1}}{dx^{\mu-1}}[-gUV]_{x=1} + \delta_{6,2} \end{aligned}$$

while for the third term of (24) we have from the ordinary Euler-Maclaurin formula [1]

$$(28)\quad E\{gUS_{1,2} + gT_3\}_a = \sum_{\mu=1,2,4}\frac{B_\mu(a)}{\mu!}\left(\frac{1}{n}\right)^{\mu-1}\frac{d^{\mu-1}}{dx^{\mu-1}}[gUS_{1,2} + gT_3]_{x=1} + R_6 .$$

$\delta_{6,1}$, $\delta_{6,2}$ and R_6 are of an order of magnitude not larger than n^{-5} and can readily be estimated.

The correction terms in evaluating (19) by the tangent-trapezoidal or trapezoidal rule to an accuracy of n^{-4} may therefore be obtained from

$$(29)\quad \begin{aligned} &\int_0^1 f_1\left(x, \frac{2}{\pi}\alpha\right)dx - \frac{1}{n}\sum_{\nu=0}^{n-1} f_1\left(\frac{\nu+a}{n}, \frac{2}{\pi}\alpha\right) + \frac{1}{n}B_1(a) f_1\left(1, \frac{2}{\pi}\alpha\right) \\ &= -\sum_{k=1,3}\left(\frac{1}{n}\right)^{k+1} C_k\left(a, \frac{2}{\pi}n\alpha\right)\frac{g^{(k)}(0)}{k!} - \sum_{\mu=2,4}\left(\frac{1}{n}\right)^{\mu}\frac{B_\mu(a)}{\mu!} f_1^{(\mu-1)}\left(1, \frac{2}{\pi}\alpha\right) - \frac{1}{n}\rho_6 \end{aligned}$$

and

$$(30)\quad \begin{aligned} &\int_0^1 f_2(x,\alpha)\,dx - \frac{1}{n}\sum_{\nu=0}^{n-1} f_2\left(\frac{\nu+a}{n}, \alpha\right) + \frac{1}{n}B_1(a) f_2(1,\alpha) \\ &= -\left(\frac{1}{n}\right)^4 \alpha\frac{\partial}{\partial\alpha} C_3\left(a, \frac{2}{\pi}n\alpha\right)\frac{g'(0)}{3!}\left(\frac{\pi}{2}\right)^2 - \sum_{\mu=2,4}\left(\frac{1}{n}\right)^{\mu}\frac{B_\mu(a)}{\mu!} f_2^{(\mu-1)}(1,\alpha) \\ &\qquad - \frac{1}{n}\left(\delta_{6,1} + \delta_{6,2} + R_6\right) \end{aligned}$$

on adding these equations. We thus obtain

$$(31)\quad \begin{aligned} &\int_0^1 g(x)\tan^{-1}\frac{\sin\frac{\pi}{2}x}{\alpha}\,dx - \frac{1}{n}\sum_{\nu=0}^{n-1} g\left(\frac{\nu+a}{n}\right)\tan^{-1}\frac{\sin\left(\frac{\pi}{2}\cdot\frac{\nu+a}{n}\right)}{\alpha} \\ &\qquad + \frac{1}{n}B_1(a) g(1)\tan^{-1}\frac{1}{\alpha} \\ &= -\sum_{k=1,3}\left(\frac{1}{n}\right)^{k+1} C_k\left(a, \frac{2}{\pi}n\alpha\right)\frac{g^{(k)}(0)}{k!} \\ &\qquad - \left(\frac{1}{n}\right)^4 \alpha\frac{\partial}{\partial\alpha} C_3\left(\alpha, \frac{2}{\pi}n\alpha\right)\frac{g'(0)}{3!}\left(\frac{\pi}{2}\right)^3 + \text{remainder} \end{aligned}$$

where the remainder is of an order not larger than n^{-6}.

As a numerical example we choose

$$g(x) = \sin\frac{\pi}{2}x, \qquad a = 1, \qquad \frac{2}{\pi}\alpha = 10^{-2}, \qquad n = 10.$$

The first three correction terms to nine decimals are

$$-\left(\frac{1}{n}\right)^2 C_1\left(a, \frac{2}{\pi} n\alpha\right)\frac{\pi}{2} = 0.001385560$$

$$\left(\frac{1}{n}\right)^4 C_3\left(a, \frac{2}{\pi} n\alpha\right)\frac{1}{3!}\left(\frac{\pi}{2}\right)^3 = 0.000000837$$

$$-\left(\frac{1}{n}\right)^4 \alpha\frac{\partial}{\partial\alpha} C_3\left(a, \frac{2}{\pi} n\alpha\right)\frac{1}{3!}\left(\frac{\pi}{2}\right)^3 = 0.000000023$$

and their sum is 0.001386420. The exact value of

$$(32)\qquad \int_0^1 \sin\frac{\pi}{2}x\cdot\tan^{-1}\frac{\sin\frac{\pi}{2}x}{\alpha}\,dx - \frac{1}{n}\left\{\sum_{\nu=1}^{n-1}\sin\left(\frac{\pi}{2}\cdot\frac{\nu}{n}\right)\cdot\tan^{-1}\frac{\sin\left(\frac{\pi}{2}\cdot\frac{\nu}{n}\right)}{\alpha} + \frac{1}{2}\tan^{-1}\frac{1}{\alpha}\right\}$$

to the same number of decimals computed from

$$(33)\qquad \int_0^1 \sin\frac{\pi}{2}x\cdot\tan^{-1}\frac{\sin\frac{\pi}{2}x}{\alpha}\,dx = \sqrt{1+\alpha^2}-\alpha$$

and from a direct computation of

$$\frac{1}{n}\left\{\sum_{\nu=1}^{n-1}\sin\left(\frac{\pi}{2}\cdot\frac{\nu}{n}\right)\cdot\tan^{-1}\frac{\sin\left(\frac{\pi}{2}\cdot\frac{\nu}{n}\right)}{\alpha} + \frac{1}{2}\tan^{-1}\frac{1}{\alpha}\right\}$$

is 0.001386421. The neglected remainder in the correction is thus of an order not larger than the rounding errors.

It is interesting to compare the approximation to (32) given by the correction terms above with some other estimates of it. The point of departure in both [6] and [7] for obtaining such estimates is the Fourier series expansion of the integrand, i.e.

$$(34)\qquad \sin\frac{\pi}{2}x\cdot\tan^{-1}\frac{\sin\frac{\pi}{2}x}{\alpha} = \left\{e^{-\sigma}+\frac{1}{3}e^{-3\sigma}\cos\pi x+\frac{1}{5}e^{-5\sigma}\cos 2\pi x+\cdots\right\} - \left\{e^{-\sigma}\cos\pi x+\frac{1}{3}e^{-3\sigma}\cos 2\pi x+\frac{1}{5}e^{-5\sigma}\cos 3\pi x+\cdots\right\}$$

where

$$(35)\qquad \sigma = \sinh^{-1}\alpha > 0.$$

Observing that

$$(36)\qquad \int_0^1 \cos\mu x\,dx - \frac{1}{n}\left\{\sum_{\nu=1}^{n-1}\cos\mu\pi\frac{\nu}{n}+\frac{1}{2}+\frac{1}{2}\cos\mu\pi\right\} = \begin{cases} -1;\ \mu = 2nk, & k=1,2,\\ 0;\ \text{all other integer values of } \mu \end{cases}$$

we have for (32)

$$\sum_{k=1}^{\infty} \left\{ \frac{e^{-(4nk-1)\sigma}}{4nk - 1} - \frac{e^{-(4nk+1)\sigma}}{4nk + 1} \right\}. \tag{37}$$

To obtain a good approximation to (32) by summing this series, after substituting the numerical values of n and σ, would require quite a large number of terms to be taken. An estimate of (37) following [7] by considering the analytic continuation of

$$\begin{aligned} f(x, \alpha) &= \frac{1}{2i} \sin \frac{\pi}{2} x \cdot \log \frac{\alpha + i \sin (\pi x/2)}{\alpha - i \sin (\pi x/2)} \\ &= \frac{1}{2i} \sin \frac{\pi}{2} x \cdot \log \frac{\sinh \sigma + i \sin (\pi x/2)}{\sinh \sigma - i \sin (\pi x/2)} \end{aligned} \tag{38}$$

in the $z = x + iy$ plane and expressing (37) as a contour integral gives

$$\left\{ \sum_{k=1}^{\infty} \frac{e^{-(4nk-1)\sigma}}{4nk - 1} - \frac{e^{-(4nk+1)\sigma}}{4nk + 1} \right\} \leqq \max_{z \in l_\tau} |f(z, \alpha)| \frac{2 \exp.(-\pi\tau n)}{1 - \exp.(-\pi\tau n)}, \text{for all } 0 < \tau < \frac{2}{\pi} \sigma, \tag{39}$$

where l_τ designates the line $x + i\tau$, $-\infty < x < \infty$. Since $\pi\tau n$ is rather small, this also is not helpful in estimating (32).

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