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An Error Functional Expansion for N-Dimensional Quadrature with an Integrand Function Singular at a Point *

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Abstract. Let If be the integral of $f(\vec{x})$ over an N-dimensional hypercube and $Q^{(m)}f$ be the approximation to If obtained by subdividing the hypercube into m^N equal subhypercubes and applying the same quadrature rule Q to each. In order to extrapolate efficiently for If on the basis of several different approximations $Q^{(m_i)}f$, it is necessary to know the form of the error functional $Q^{(m)}f - If$ as an expansion in m. When $f(\vec{x})$ has a singularity, the conventional form (with inverse even powers of m) is not usually valid. In this paper we derive the expansion in the case in which $f(\vec{x})$ has the form

$$f(\vec{x}) = r^{\alpha}\varphi(\vec{\theta})h(r)g(\vec{x}), \qquad \alpha > -N,$$

the only singularity being at the origin, a vertex of the unit hypercube of integration. Here $(r, \vec{\theta})$ represents the hyperspherical coordinates of $(\vec{x})$. It is shown that for this integrand the error function expansion includes only terms $A_{\alpha+N+t}/m^{\alpha+N+t}$, B_t/m^t, $C_{\alpha+N+t} \ln m/m^{\alpha+N+t}$, $t = 1, 2, \ldots$. The coefficients depend only on the integrand function $f(\vec{x})$ and the quadrature rule Q. For several easily recognizable classes of integrand function and for most familiar quadrature rules some of these coefficients are zero. An analogous expansion for the error functional with integrand function $F(\vec{x}) = \ln rf(\vec{x})$ is also derived.

1. Introduction. When the integrand function has singularities within the hypercube of integration or on its boundary, the use of standard quadrature methods may be very inefficient. The purpose of this paper is to provide an asymptotic expansion for the quadrature error functional which is valid when the integrand function has a particular type of singularity, specified below. This expansion may be used as a basis for extrapolation methods for integration of functions having this type of singularity in the same way as the Euler-Maclaurin expansion is used as a basis for Romberg integration.

We now specify precisely the sort of singularity in the integrand function to which the expansions to be derived apply.

First, the singularity must be located at a vertex of the hypercube of integration; and the integrand function must be analytic throughout this hypercube except at this one vertex. For convenience, we define the coordinate system so that the hypercube is $0 \leqslant x_i \leqslant 1$, $i = 1, 2, \ldots, N$, and the singular point is the origin.

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Second, setting

$$r^2 = x_1^2 + x_2^2 + \ldots + x_N^2 \tag{1.1}$$

the singularity may have one of various allowable forms. These include

$$r^\alpha,\ r^\alpha \varphi(\vec{\theta}),\ r^\alpha \ln r,\ r^\alpha \ln r \varphi(\vec{\theta}), \qquad \alpha > -N, \tag{1.2}$$

where $(r, \vec{\theta})$ is the point $(\vec{x})$ expressed in hyperspherical coordinates. It may also be any linear sum of any allowable form. A less obvious two-dimensional example is $(\lambda x + \mu y)^\alpha$, $\lambda\mu > 0$ as this may be expressed in the form $r^\alpha(\lambda \cos\theta + \mu \sin\theta)^\alpha$.

In order to be quite specific, we note some singularities to which the expansions derived below do *not* apply. These include

$$x_i^\alpha,\ \ln x_i,\ x_i^\alpha x_j^\beta \ln x_k, \qquad \alpha, \beta \neq \text{integer}, \tag{1.3}$$

for which similar expansions exist, based trivially on one-dimensional expansions given in Lyness and Ninham [10]. Also not allowed are combinations of (1.2) and (1.3), for example

$$x_1^\alpha r^\beta,\ \ln x_1 r^\beta \ln r, \qquad \alpha, \beta/2 \neq \text{integer}. \tag{1.4}$$

For these, there is experimental evidence that an expansion exists, but no proof is known to the author.

There are many other types of singularities, such as line singularities and curved line singularities. The expansions derived in this paper apply only to the narrow class of singularities exemplified in (1.2) above.

The use of extrapolation (or Richardson's h^2 extrapolation) or the deferred approach to the limit occurs in many branches of mathematics. A particular implementation to one-dimensional quadrature is known as Romberg integration [2]. An immediate modification of Romberg integration to a two-dimensional square may be based on the two-dimensional product midpoint trapezoidal rule

$$Q^{(m)}f = \frac{1}{m^2} \sum_{j=0}^{m-1} \sum_{k=0}^{m-1} f\left(\frac{2j+1}{m}, \frac{2k+1}{m}\right). \tag{1.5}$$

This is an approximation, based on m^2 evenly distributed function values, to a definite integral

$$If = \int_0^1 \int_0^1 f(x, y)\, dx\, dy. \tag{1.6}$$

If $f(x, y)$, unlike the integrand functions to be discussed in this paper, is analytic in x and y throughout the domain of integration, then a trivial modification of the classical Euler-Maclaurin expansion is valid. This is

$$Q^{(m)}f - If = \frac{B_2}{m^2} + \frac{B_4}{m^4} + \ldots + \frac{B_{2p-2}}{m^{2p-2}} + O(m^{-2p}). \tag{1.7}$$

Since B_{2q} is independent of m, this can be used as the basis of an extrapolation technique. A linear combination

$$\sum \lambda_i Q^{(m_i)} f \tag{1.8}$$

may be formed in such a way as to eliminate the early terms in the resulting expansion.

This technique is described in some detail in the literature.

An essential ingredient of Romberg integration is the existence and validity of expansion (1.7). As mentioned above, this depends on the nature of the integrand function $f(x, y)$ and is valid only if $f(x, y)$ is sufficiently smooth. If the expansion on which the Romberg integration is based does not exist, the results such as (1.8) should not be expected to be particularly accurate. They would reflect only the accuracy of the individual approximations $Q^{(m_i)}f$ and little would be gained by constructing the linear combination.

The only other expansions of this type known to the author are for one-dimensional integrands such as

$$f(x) = x^{\alpha}(1 - x)^{\beta}h(x), \tag{1.9}$$

where $h(x)$ is analytic. In this case

$$\begin{aligned} Q^{(m)}f - \int_0^1 f(x)\,dx \sim{}& \frac{A_{\alpha+1}}{m^{\alpha+1}} + \frac{A_{\alpha+2}}{m^{\alpha+2}} + \frac{A_{\alpha+3}}{m^{\alpha+3}} + \dots \\ &+ \frac{A'_{\beta+1}}{m^{\beta+1}} + \frac{A'_{\beta+2}}{m^{\beta+2}} + \frac{A'_{\beta+3}}{m^{\beta+3}} \dots, \end{aligned} \tag{1.10}$$

the remainder term being of the same order as the first omitted term. A similar expansion for $f(x) = \log x\, x^{\alpha}(1 - x)^{\beta}h(x)$ may be obtained by differentiating with respect to α. Details of the proofs are given in Navot [12] or Lyness and Ninham [10]. A straigh forward iterative use of this expansion leads to corresponding expansions for N-dimensional integrand functions having singularities of type (1.3) above. In this paper we are concerned with singularities of type (1.2) above.

The principal result of this paper is Theorem 5.14. This provides a wide variety of expansions and may be applied when the quadrature rule is $Q^{(m)}$ given by (1.5) and the integrand function,

$$f(x, y) = r^{\alpha}\varphi(\theta)h(r)g(x, y), \qquad \alpha > -2, \tag{1.11}$$

is analytic, except at the origin. In this case, Theorem 5.14 gives

$$\begin{aligned} Q^{(m)}f - If \sim{}& \frac{A_{\alpha+2}}{m^{\alpha+2}} + \frac{A_{\alpha+3}}{m^{\alpha+3}} + \frac{A_{\alpha+4}}{m^{\alpha+4}} + \dots + \frac{C_{\alpha+2}}{m^{\alpha+2}} \ln m \\ &+ \frac{C_{\alpha+3}}{m^{\alpha+3}} \ln m + \frac{C_{\alpha+4}}{m^{\alpha+4}} \ln m + \dots + \frac{B_2}{m^2} + \frac{B_4}{m^4} + \dots, \end{aligned} \tag{1.12}$$

the order of the remainder term being that of one of the first omitted terms in this expansion.

The key result of this paper is Theorem 4.17, which gives the corresponding expansion when the integrand function is a homogeneous function. The earlier sections lead up to this result. Standard properties of the N-dimensional Euler-Maclaurin expansion are described in Section 2, and homogeneous functions are defined and some of their elementary properties are noted in Section 3.

Sections 5 and 6 comprise applications of Theorem 4.17 to provide the expansion for integrands with $r^{\alpha}\varphi(\vec{\theta})$ singularities such as (1.11) above, and the corresponding expansion for integrands with $\log r \cdot r^{\alpha}\varphi(\vec{\theta})$ singularities. Finally, in Section 8 there is a brief discussion of possible applications.

The presentation is general so far as the choice of quadrature rule is concerned. Q may stand for any N-dimensional rule, such as (1.5) above with $m = 1$, or a higher degree rule such as one of those to be found in Stroud [14]. For certain rules some of the coefficients in (1.12) above are zero, and these are specified at each stage. In addition, coefficients may be zero because of some property of a particular integrand function. This is discussed in Section 7. Another feature (see Theorem 4.22) is that an indeterminate function value which may occur at the singularity may be replaced by zero; and with a single minor modification, all expansions are rigorously valid.

2. The N-dimensional Euler-Maclaurin Expansion. In this section we collect together some standard results about the Euler-Maclaurin expansion for N-dimensional quadrature rules. The region of integration is, in all cases, the N-dimensional hypercube $0 \leqslant |x_i| \leqslant 1$, $i = 1, 2, \ldots, N$; and we define

$$If = \int_0^1 \int_0^1 \cdots \int_0^1 f(\vec{x})\, d^N x. \tag{2.1}$$

The symbol $d^N x$ is used for $dx_1 dx_2 \ldots dx_N$ throughout.

An N-dimensional quadrature rule Q is an approximation to this integral of the form

$$Qf = \sum_{j=1}^{\nu} a_j f(\vec{x}_j), \qquad \sum_{j=1}^{\nu} a_j = 1. \tag{2.2}$$

Such a rule is termed *symmetric* when it is invariant under reflections about $x_i = 1/2$, $i = 1, 2, \ldots, N$, and is termed *fully symmetric* when it is invariant under all linear transformations which transform the hypercube into itself. It is of *polynomial degree* d when

$$Qf = If \quad \text{for all } f \in \pi_d, \tag{2.3}$$

where π_d is the set of polynomials of degree d or less. It is of *trigonometric degree* d_T when

$$Qf = If \quad \text{for all } f \in T_{d_T}, \tag{2.4}$$

where T_d is the set of trigonometric polynomials of unit period of degree d or less.

The m^N copy of the rule Q given by (2.2) is

$$\begin{aligned}(m \times Q)f \equiv Q^{(m)}f = &\sum_{k_1=0}^{m-1} \sum_{k_2=0}^{m-1} \cdots \\ &\sum_{k_N=0}^{m-1} \sum_{j=1}^{\nu} \frac{a_j}{m^N} f\left(\frac{x_{1,j} + k_1}{m}, \frac{x_{2,j} + k_2}{m}, \ldots, \frac{x_{N,j} + k_N}{m}\right).\end{aligned} \tag{2.5}$$

This is the sum of function values obtained by subdividing the unit hypercube into m^N equal hypercubes of side $1/m$ and applying a properly scaled version of Q to each. When Q is (fully) symmetric, then $Q^{(m)}$ is (fully) symmetric and when Q is of polynomial degree d, $Q^{(m)}$ is also of polynomial degree d. When Q is of trigonometric degree d, then $Q^{(m)}$ is of trigonometric degree $d' = (m + 1)d - 1$.

The Euler-Maclaurin expansion for $Q^{(m)}f - If$ has been discussed by Lyness [8], Baker and Hodgson [1], and Lyness and McHugh [11]. The fundamental result stated below is a simple consequence of several results given in those papers.

THEOREM 2.6. *Let Qf and $Q^{(m)}f$ be defined by* (2.2) *and* (2.5) *above. Let $f(\vec{x})$ be a function, all of whose derivative functions $f^{(r_1,r_2,\ldots,r_N)}(\vec{x})$ whose total order satisfies $r_1 + r_2 + \ldots + r_N \leqslant p$ are integrable over the unit hypercube. Then*

$$Q^{(m)}f - If = \sum_{s=1}^{l-1} \frac{B_s}{m^s} + R_l(Q^{(m)}; f), \qquad N \leqslant l \leqslant p,$$

where B_s depends on Q and $f(\vec{x})$ but not on m and

$$R_l(Q^{(m)}; f) = O(m^{-l}) \quad \text{as } m \longrightarrow \infty. \tag{2.7}$$

The coefficients B_s have the explicit form

$$B_s = \sum_{\Sigma t_i = s} c_{t_1,t_2,\ldots,t_N}(Q) \int_0^1 \int_0^1 \cdots \int_0^1 f^{(t_1,t_2,\ldots,t_N)}(\vec{x})\, d^N x, \tag{2.8}$$

where the sum includes all sets of nonnegative integers $t_1, t_2, \ldots, t_N$ whose sum is precisely s. The coefficients $c(Q)$ may be obtained by applying the rule Q to a product of Bernoulli polynomials $B_q(x)$. Thus,

$$c_{t_1,t_2,\ldots,t_N}(Q) = Q\varphi \tag{2.9}$$

with

$$\varphi(\vec{x}) = \frac{B_{t_1}(x_1)}{t_1!} \frac{B_{t_2}(x_2)}{t_2!} \cdots \frac{B_{t_N}(x_N)}{t_N!}. \tag{2.10}$$

The remainder term R_l may be expressed in the form

$$R_l(Q^{(m)}; f) = \frac{1}{m^N} \sum_{\Sigma t_i = l} \int_0^1 \int_0^1 \cdots \int_0^1 h_{t_1,t_2,\ldots,t_N}(Q^{(m)}; m\vec{x}) \cdot f^{(t_1,t_2,\ldots,t_N)}(\vec{x})\, d^N x, \qquad N \leqslant l \leqslant p. \tag{2.11}$$

The kernel functions are discussed in Lyness and McHugh [11] where it is shown that

$$\int_0^1 \int_0^1 \cdots \int_0^1 h_{t_1,t_2,\ldots,t_N}(Q^{(m)}; m\vec{x}) d^N x = c_{t_1,t_2,\ldots,t_N}(Q). \tag{2.12}$$

One property of these kernel functions, which is required in Section 4, is that they are periodic with period 1 in each argument x_i. The remainder term (2.11) may be replaced by the asymptotic relation

$$R_l(Q^{(m)}; f) = \frac{B_l}{m^l} + o(m^{-l}). \tag{2.13}$$

The explicit form of (2.9) enables us to determine some properties of the coefficients $c(Q)$ from properties of the Bernoulli polynomials. When Q is a symmetric rule, and $\varphi(\vec{x})$ is antisymmetric under reflection about any $x = 1/2$, then $Q\varphi = 0$. When q is odd, $B_q(x) = -B_q(1-x)$ and so is antisymmetric. Thus, it follows from (2.9) that

$$c_{t_1,t_2,\ldots,t_N}(Q) = 0 \quad \text{any } t_i \text{ odd}, \ Q \text{ symmetric}, \tag{2.14}$$

and from (2.8) we obtain

(2.15) $$B_s = 0, \quad s \text{ odd}, \; Q \text{ symmetric}.$$

A similar kind of result holds for rules Q of specified polynomial degree $d(Q)$. The function $\varphi(\vec{x})$ in (2.10) is of polynomial degree $t_1 + t_2 + \ldots + t_N$. Thus

(2.16) $$c_{t_1,t_2,\ldots,t_N}(Q) = Q\varphi = I\varphi, \qquad t_1 + t_2 + t_N \leqslant d(Q).$$

However, since

(2.17) $$\int_0^1 B_q(x)\,dx = 0, \qquad q = 1, 2, 3, \ldots,$$

it follows that

(2.18) $$c_{t_1,t_2,\ldots,t_N}(Q) = 0, \qquad 0 < t_1 + t_2 + \ldots + t_N \leqslant d(Q);$$

and (2.8) gives

(2.19) $$B_s = 0, \qquad s = 1, 2, \ldots, d(Q).$$

3. Elementary Properties of Homogeneous Functions. In this section we define homogeneous functions, demonstrate some of their elementary properties and establish some notation for subsequent use. A familiar definition is the following:

Definition 3.1. A function $f(x_1, x_2, \ldots, x_N)$ is homogeneous with respect to the origin of degree γ if

(3.1) $$f(\lambda x_1, \lambda x_2, \ldots, \lambda x_N) \equiv \lambda^\gamma f(x_1, x_2, \ldots, x_N)$$

for all $\vec{x}$ other than $\vec{x} = \vec{0}$ and for all λ. For a function expressed in hyperspherical coordinates $(r, \vec{\theta})$, the corresponding definition is

(3.2) $$f(\lambda r, \vec{\theta}) \equiv \lambda^\gamma f(r, \vec{\theta}), \qquad r \neq 0.$$

For notational convenience in what follows, a subscript γ attached to a function denotes that it is a homogeneous function of degree γ. (The notation $f_\gamma^{(p,q)}(x, y)$ refers to the (p, q) partial derivative of the homogeneous function $f_\gamma(x, y)$.) We now collect together some elementary properties of homogeneous functions. These are trivial consequences of the defining property (3.1).

(i) The function $f(\vec{x}) = 0$ is homogeneous of all degrees.

(ii) A function $\varphi(\vec{\theta})$ is homogeneous of degree zero.

(iii) The function $(f_\gamma(\vec{x}))^\alpha (f_\delta(\vec{x}))^\beta$ is homogeneous of degree $\gamma\alpha + \delta\beta$.

(iv) The function $|f_\gamma(\vec{x})|$ is homogeneous of degree γ.

(v) The partial derivative function $f_\gamma^{(q_1,q_2,\ldots,q_N)}(\vec{x})$ is a homogeneous function of degree $\gamma - q_1 - q_2 - \ldots - q_N$.

We are concerned with certain integration properties. As a preliminary we define certain regions.

Definition 3.3. The region $L[a, b)$, $0 \leqslant a < b$, is defined by

(3.3) $$L[a, b) = \left\{ (x_1, x_2, \ldots, x_N) \mid a \leqslant \max_i(x_i) < b;\ 0 \leqslant \min_i(x_i) \right\}.$$

In one dimension this is simply the semiopen interval $[a, b)$. In N dimensions when $a = 0$, this is a hypercube of side b. When $a \neq 0$, this is the region obtained by removing a hypercube of side a from the inner corner of a hypercube of side b. In two dimensions the shape is that of a letter L. Clearly,

$$L[a, b) \cup L[b, c) = L[a, c), \qquad a \leqslant b \leqslant c. \tag{3.4}$$

In complete accordance with this definition we define

$$L[a, \infty) = \left\{(x_1, x_2, \ldots, x_N) | a \leqslant \max_i(x_i);\ 0 \leqslant \min_i(x_i)\right\}. \tag{3.5}$$

Thus, $L[0, \infty)$ includes the whole of the first quadrant and $L[a, \infty)$ includes the part of the first quadrant not lying in the hypercube $L[0, a)$. In the sequel we make use of the properties

$$L[1, \infty) = \bigcup_{k=0}^{\infty} L[m^k, m^{k+1}), \qquad m > 1, \tag{3.6}$$

and

$$L[0, 1) = \bigcup_{k=0}^{\infty} L[m^{-k-1}, m^{-k}) \cup (\vec{0}), \qquad m > 1. \tag{3.7}$$

THEOREM 3.8. *Let $f_\gamma(\vec{x})$ be a homogeneous function of degree γ and be analytic in a region $L[a, b)$ for some b and a satisfying $b > a > 0$. Then*

(i) $\int_{L[0,1)} f_\gamma(\vec{x}) d^N x$ *exists when* $\gamma > -N$.

(ii) $\int_{L[1,\infty)} f_\gamma(\vec{x}) d^N x$ *exists when* $\gamma < -N$.

(iii) $\int_{L[1,m)} f_\gamma(\vec{x}) d^N x = (m^{\gamma+N} - 1) \int_{L[0,1)} f_\gamma(\vec{x}) d^N x,\ \gamma > -N$.

(iv) $\int_{L[1,m)} f_\gamma(\vec{x}) d^N x = -(m^{\gamma+N} - 1) \int_{L[1,\infty)} f_\gamma(\vec{x}) d^N x,\ \ \gamma < -N$.

(v) $\int_{L[1,m)} f_{-N}(\vec{x}) d^N x = (\ln m/\ln 2) \int_{L[1,2)} f_{-N}(\vec{x}) d^N x$.

The first two parts of this theorem may be verified using elementary analysis. Essentially, a homogeneous function of degree $\gamma \leqslant -N$ becomes infinite at the origin at a rate too rapid for the function to be integrable there, while if $\gamma \geqslant -N$, it does not decay for large r sufficiently rapidly to be integrable over the infinite part of the first quadrant. The proofs of parts (iii) and (iv) are based on the identity

$$\int_{L[a,b)} f_\gamma(\vec{x}) d^N x = m^{-\gamma-N} \int_{L[ma,mb)} f_\gamma(\vec{x}) d^N x, \tag{3.9}$$

which follows from a change of variable $\vec{x}' = m\vec{x}$ together with the defining property of a homogeneous function $f_\gamma(\vec{x}') = m^\gamma f_\gamma(\vec{x})$. Setting $a = 1$ and $b = m$ in (3.9) and iterating gives

$$\int_{L[m^k, m^{k+1})} f_\gamma(\vec{x}) d^N x = (m^{\gamma+N})^k \int_{L[1,m)} f_\gamma(\vec{x}) d^N x. \tag{3.10}$$

In view of (3.6)

$$\int_{L[1,\infty)} f_\gamma(\vec{x}) d^N x = \sum_{k=0}^{\infty} \int_{L[m^k, m^{k+1})} f_\gamma(\vec{x}) d^N x \tag{3.11}$$

and substituting (3.10) into (3.11) leads to the result stated in part (iv) of the theorem. The other parts are proved in a similar and equally simple manner.

In Section 4 we shall make specific use of parts (iii), (iv) and (v) of this theorem. These will be applied to functions $f_\gamma^{(t_1, t_2, \ldots, t_N)}(\vec{x})$ which are partial derivatives of the homogeneous function $f_\gamma(\vec{x})$. For subsequent convenience we state here the precise result required in the notation which we shall employ. This is

$$\int_{L[1,m)} f_\gamma^{(t_1,t_2,\ldots,t_N)}(\vec{x})d^N x$$

(3.12)
$$= -(m^{(\gamma+N-t_1-t_2-\cdots-t_N)} - 1)I_\gamma^{(t_1,t_2,\ldots,t_N)}, \quad \sum t_i \neq \gamma + N,$$

$$\int_{L[1,m)} f_\gamma^{(t_1,t_2,\ldots,t_N)}(\vec{x})d^N x = \ln m K_\gamma^{(t_1,t_2,\ldots,t_N)}, \quad \sum t_i = \gamma + N,$$

where I_γ and K_γ are integrals which do not depend on m and are defined by

(3.13)
$$I_\gamma^{(t_1,t_2,\ldots,t_N)} = -\int_{L[0,1)} f_\gamma^{(t_1,t_2,\ldots,t_N)}(\vec{x})d^N x, \quad \sum t_i < \gamma + N,$$
$$= \int_{L[1,\infty)} f_\gamma^{(t_1,t_2,\ldots,t_N)}(\vec{x})d^N x, \quad \sum t_i > \gamma + N,$$

(3.14)
$$K_\gamma^{(t_1,t_2,\ldots,t_N)} = \frac{1}{\ln 2}\int_{L[1,2)} f_\gamma^{(t_1,t_2,\ldots,t_N)}(\vec{x})d^N x.$$

4. The Error Functional Expansion for a Homogeneous Function. In this section we derive an asymptotic expansion for the error functional

(4.1)
$$Q^{(m)}f_\gamma - If_\gamma,$$

where $f_\gamma(\vec{x})$ is a homogeneous function of degree γ whose only singularity is at the origin; $Q^{(m)}f$ is the m^N-copy (2.5) of the general N-dimensional rule (2.2). The main results appear in Theorems 4.17 and 4.22 below. In this derivation we make use of some of the properties of homogeneous functions mentioned in Section 3, and the Euler-Maclaurin expansion for $Q^{(m)}f$ derived in Section 2. We assume pro tem that $Q^{(1)}f$ does not require an indeterminate function value at the origin. Later in this section we show that the results hold if $f_\gamma(\vec{0})$ is replaced by zero (thus ignoring the singularity).

The first stage of this derivation consists of applying the property

(4.2)
$$f_\gamma(\vec{x}/m) = m^{-\gamma}f_\gamma(\vec{x})$$

to reexpress the error functional (4.1). To this end we introduce the notation

(4.3)
$$I(k_1, k_2, \ldots, k_N)f = \int_{k_1}^{k_1+1}\int_{k_2}^{k_2+1}\cdots\int_{k_N}^{k_N+1} f(\vec{x})d^N x$$

and

(4.4)
$$Q(k_1, k_2, \ldots, k_N)f = \sum_{j=1}^{\nu} a_j f(x_{1,j} + k_1, x_{2,j} + k_2, \ldots, x_{N,j} + k_N)$$

to denote the exact integral over the hypercube $k_i < x_i < k_i + 1$ $(i = 1, 2, \ldots, N)$ and the approximation to this integral using the rule $Q^{(1)}$ (or Q). It follows by straightforward manipulation that

(4.5)
$$If_\gamma = \int_0^1\int_0^1\cdots\int_0^1 f_\gamma(\vec{x})d^N x = \frac{1}{m^{\gamma+N}}\int_0^m\int_0^m\cdots\int_0^m f_\gamma(\vec{x})d^N x$$
$$= \frac{1}{m^{\gamma+N}}If_\gamma + \frac{1}{m^{\gamma+N}}\sum_{k_1=0}^{m-1}\sum_{k_2=0}^{m-1}\cdots\sum_{k_N=0}^{m-1}{}^{*}\, I(k_1, k_2, \ldots, k_N)f_\gamma,$$

the asterisk on the summation symbol indicating that the term with all $k_i = 0$ is to be omitted. In a precisely similar manner we find

$$Q^{(m)}f_\gamma = \frac{1}{m^{\gamma+N}} Qf_\gamma + \frac{1}{m^{\gamma+N}} \sum_{k_1=0}^{m-1} \sum_{k_2=0}^{m-1} \cdots \sum_{k_N=0}^{m-1}{}^{*}\, Q(k_1, k_2, \ldots, k_N) f_\gamma, \tag{4.6}$$

and taking the difference between (4.5) and (4.6) gives

$$\begin{aligned} Q^{(m)}f_\gamma - If_\gamma = {} & \frac{1}{m^{\gamma+N}} (Qf_\gamma - If_\gamma) + \frac{1}{m^{\gamma+N}} \sum_{k_1=0}^{m-1} \sum_{k_2=0}^{m-1} \\ & \cdots \sum_{k_N=0}^{m-1}{}^{*} (Q(k_1, k_2, \ldots, k_N) f_\gamma - I(k_1, k_2, \ldots, k_N) f_\gamma). \end{aligned} \tag{4.7}$$

Since the only singularity of $f_\gamma(\vec{x})$ is at the origin, each term other than the first here contains an error functional for the rule Qf over a hypercube within which the function is analytic. Consequently, the second stage of this proof consists of replacing each of these $m^N - 1$ error functionals by the Euler-Maclaurin expansion (2.6). Since each term in (2.6) involves an integral over the appropriate integration domain in which kernel functions are periodic with period 1, the result of the summation over k_i is to provide an integral over the (L shaped) domain $L[1, m)$ defined in Section 3. Thus,

$$\begin{aligned} Q^{(m)}f_\gamma - If_\gamma = {} & \frac{1}{m^{\gamma+N}} (Qf_\gamma - If_\gamma) \\ & + \frac{1}{m^{\gamma+N}} \sum_{s=1}^{l-1} \sum_{\Sigma t_i = s} c_{t_1, t_2, \ldots, t_N}(Q) \int_{L[1,m)} f^{(t_1, t_2, \ldots, t_N)}(\vec{x}) d^N x \\ & + \frac{1}{m^{\gamma+N}} \sum_{\Sigma t_i = l} \int_{L[1,m)} h_{t_1, t_2, \ldots, t_N}(Q, \vec{x}) f^{(t_1, t_2, \ldots, t_N)}(\vec{x}) d^N x, \\ & \qquad l \geq N. \end{aligned} \tag{4.8}$$

At this point the value of l is at our disposal, except that it should be greater than $N - 1$. We now set a value of l to be greater than $\gamma + N$. The reason for doing this is that the terms in the final summation over t contain integrals which are then dominated by homogeneous functions of degree less than $-N$. Thus, in these terms each integral over $L[1, m)$ may be replaced by the difference of the corresponding integral over $L[1, \infty)$ and the corresponding integral over $L[m, \infty)$. The third stage of this proof consists of doing this; at the same time we employ (3.12) to replace the integrals over $L[1, m)$ by terms involving expressions (3.13) and (3.14). The result of doing this and carrying some minor rearrangement of the terms obtained in this way is as follows:

$$Q^{(m)}f_\gamma - If_\gamma = \frac{A_{N+\gamma}}{m^{N+\gamma}} + \sum_{s=1}^{l-1} \frac{B_{\gamma,s}}{m^s} + \frac{C_{N+\gamma}}{m^{N+\gamma}} \ln m + R_l^{(m)} f_\gamma, \qquad l > \gamma + N. \tag{4.9}$$

Here

$$\begin{aligned} A_{N+\gamma} = {} & Qf_\gamma - If_\gamma + \sum_{s=1}^{l-1} \sum_{\Sigma t_i = s} c_{t_1, t_2, \ldots, t_N}(Q) I_\gamma^{(t_1, t_2, \ldots, t_N)} (1 - \delta_{s-\gamma-N}) \\ & + \sum_{\Sigma t_i = l} \int_{L[1,\infty)} h_{t_1, t_2, \ldots, t_N}(Q, \vec{x}) f_\gamma^{(t_1, t_2, \ldots, t_N)}(\vec{x}) d^N x, \end{aligned} \tag{4.10}$$

$$
\begin{aligned}
B_{\gamma,s} &= -\sum_{\Sigma t_i = s} c_{t_1,t_2,\ldots,t_N}(Q) I_\gamma^{(t_1,t_2,\ldots,t_N)}, \qquad s \neq \gamma + N,\\
&= 0, \qquad s = \gamma + N,
\end{aligned} \tag{4.11}
$$

$$
\begin{aligned}
C_{N+\gamma} &= 0, \qquad \gamma + N \neq \text{integer},\\
&= \sum_{\Sigma t_i = s} c_{t_1,t_2,\ldots,t_N}(Q) K_\gamma^{(t_1,t_2,\ldots,t_N)}, \qquad \gamma + N = s \geqslant 1,
\end{aligned} \tag{4.12}
$$

and

$$
R_l^{(m)} f_\gamma = -\frac{1}{m^{\gamma+N}} \sum_{\Sigma t_i = l} \int_{L[m,\infty)} h_{t_1,t_2,\ldots,t_N}(Q, \vec{x}) f_\gamma^{(t_1,t_2,\ldots,t_N)}(\vec{x}) d^N x, \qquad l > \gamma + N. \tag{4.13}
$$

The restriction $l > \gamma + N$ is required only to obtain this expansion in this form with this particular remainder term. Naturally, terms of any order in m in (4.9) may be included in the remainder term if one wishes, and the order of the new remainder term appropriately adjusted.

The coefficient $A_{N+\gamma}$ is independent of the value of l used to compute (4.10) so long as $l > \gamma + N$. Using integration by parts, expression (4.10) may be manipulated into many different forms. One of these is identical with (4.10) except that l is replaced by $l + 1$. The term $(1 - \delta_{s-\gamma-N})$ in (4.10) indicates that, when γ is an integer, the term in the summation with $s = \gamma + N$ is omitted. Similarly, when γ is an integer the term $B_{\gamma,\gamma+N}/m^{\gamma+N}$ drops out, but is replaced by a term $C_{\gamma+N} \ln m/m^{\gamma+N}$ which would not otherwise occur.

The coefficients $A_{\gamma+N}$, $B_{\gamma,s}$ and $C_{N+\gamma}$ are evidently independent of m. To establish an asymptotic expansion it remains to show that the remainder term (4.13) is of the correct order.

LEMMA 4.14. *The remainder term* $R_l^{(m)} f_\gamma = O(m^{-l})$, $l > \gamma + N$.

Proof. It follows from Theorem 3.8(iv) that if $\varphi_\delta(\vec{x})$ is a homogeneous function of degree $\delta < -N$, then

$$
\begin{aligned}
\int_{L[m,\infty)} \varphi_\delta(\vec{x}) d^N x &= \int_{L[1,\infty)} \varphi_\delta(\vec{x}) d^N x - \int_{L[1,m)} \varphi_\delta(\vec{x}) d^N x\\
&= m^{\delta+N} \int_{L[1,\infty)} \varphi_\delta(\vec{x}) d^N x
\end{aligned} \tag{4.15}
$$

and so is of order $m^{\delta+N}$. The kernel functions in (4.13) are bounded, so

$$
|R_l^{(m)} f_\gamma| \leqslant \frac{K}{m^{\gamma+N}} \sum_{\Sigma t_i = l} \int_{L[m,\infty)} |f_\gamma^{(t_1,t_2,\ldots,t_N)}(\vec{x})| d^N x. \tag{4.16}
$$

This involves a finite sum (independent of m) of integrals, each of whose integrands is a homogeneous function of degree $\delta = \gamma - l$. In view of (4.15) each integral is of order $m^{\delta+N} = m^{\gamma+N-l}$ and so the right-hand side of (4.13) is of order m^{-l} as stated in Lemma 4.14. Lemma 4.14 establishes the following theorem.

THEOREM 4.17. *Let $Q^{(m)}f$ given by* (2.5) *be the m^N copy version of Qf given by* (2.2) *which approximates If given by* (2.1). *Let $f_\gamma(\vec{x})$ be a homogeneous function of degree γ which is analytic within the hypercube $0 \leqslant x_i \leqslant 1$, $i = 1, 2, \ldots, N$, except possibly at the origin. Then*

$$Q^{(m)}f_\gamma - If_\gamma = \frac{A_{N+\gamma}}{m^{N+\gamma}} + \sum_{s=1}^{l-1} \frac{B_{\gamma,s}}{m^s} + \frac{C_{N+\gamma} \ln m}{m^{N+\gamma}} + R_l^{(m)}f_\gamma, \qquad l > N + \gamma, \tag{4.17}$$

where the coefficients $A_{N+\gamma}$, $B_{\gamma,s}$ and $C_{N+\gamma}$, given by (4.10), (4.11), *and* (4.12), *are independent of m and $R_l^{(m)}f_\gamma$ given by* (4.13) *is of order $O(m^{-l})$.*

There are certain special cases in which some of the coefficients are zero. Thus, if $f_\gamma(\vec{x})$ is a polynomial (in which case γ is a nonnegative integer which coincides with the degree of this polynomial) then

$$A_{\gamma+N} = C_{\gamma+N} = 0 \qquad (f_\gamma(\vec{x}) \text{ polynomial}). \tag{4.18}$$

These results are evident from the results of Section 2. However, they follow from (4.10) and (4.12) directly. The first reduces to an identity. The second involves partial derivatives of order greater than the degree of the polynomial.

There are two results which correspond to (2.15) and (2.19) for the Euler-Maclaurin series. If Q is a symmetric rule, then applying (2.14) to (4.11) and (4.12) gives

$$\begin{aligned} B_{\gamma,s} &= 0, \qquad s \text{ odd}, \ Q \text{ symmetric}, \\ C_{\gamma+N} &= 0, \qquad \gamma + N \text{ odd}, \ Q \text{ symmetric}. \end{aligned} \tag{4.19}$$

If Q is a rule of polynomial degree $d(Q)$, then applying (2.18) to (4.11) and (4.12) gives

$$\begin{aligned} B_{\gamma,s} &= 0, \qquad s \leqslant d(Q), \\ C_{\gamma+N} &= 0, \qquad \gamma + N \leqslant d(Q). \end{aligned} \tag{4.20}$$

Up to this point we have assumed that the quadrature rule does not require a function value at the origin. Many familiar quadrature rules, such as the product end-point trapezoidal rule and N-dimensional versions of Simpson's rule do require function values at the origin. This function value $f_\gamma(\vec{0})$ is zero when $\gamma > 0$ but may be indeterminate when $\gamma \leqslant 0$. We now show that the theory given above applies with one minor modification if the function value at the origin is consistently ignored. To this end we define a new "rule".

Definition 4.21.

$$\bar{Q}f = Qf - w_0 f(\vec{0}), \qquad \bar{Q}^{[m]}f = Q^{(m)}f - w_0 f(\vec{0})/m^N. \tag{4.21}$$

Here w_0 is the weight assigned by Qf to the function value $f(\vec{0})$ at the origin, and $\bar{Q}^{[m]}f$ is the result obtained by the rule $Q^{(m)}$ when this function value is replaced by zero.

The point at which the proof breaks down in this section is in Eq. (4.6). This can be rectified if the left-hand side is altered to $\bar{Q}^{[m]}f$ and the term Qf_γ on the right-hand side is altered to $\bar{Q}f_\gamma$. That is, in the subdivision into m^N hypercubes, the function value at the origin occurs only in one of these hypercubes; and replacing it by zero affects only one element on the right-hand side, in the manner stated.

The rest of the proof of Theorem 4.17 is virtually unaffected by this change. The only alterations required are that in the left-hand side of Eqs. (4.7) to (4.9), $Q^{(m)}f$ is replaced by $\bar{Q}^{[m]}f$ and on the right-hand sides the term $(Qf_\gamma - If_\gamma)$ is replaced by $(\bar{Q}f_\gamma - If_\gamma)$. This leads to a different coefficient $A_{N+\gamma}$ in (4.9); it is necessary to replace $A_{N+\gamma}$ in (4.9) and (4.17) by $\bar{A}_{N+\gamma}$ which coincides with (4.10) except that $Qf_\gamma - If_\gamma$ is replaced by $\bar{Q}f_\gamma - If$ on the right-hand side. The coefficients $B_{\gamma,s}$ and $C_{N+\gamma}$ are unaltered, and so are the properties (4.19) and (4.20). We state the result of ignoring the singularity as a theorem.

THEOREM 4.22. *In the notation of Theorem* 4.17, *defining* $\bar{Q}^{[m]}f$ *by* (4.21),

$$\bar{Q}^{[m]}f_\gamma - If_\gamma = \frac{\bar{A}_{N+\gamma}}{m^{N+\gamma}} + \sum_{s=1}^{l-1} \frac{B_{\gamma,s}}{m^s} + \frac{C_{N+\gamma}\ln m}{m^{N+\gamma}} + R_l^{(m)}f_\gamma, \qquad l > N+\gamma,$$

where the coefficients $B_{\gamma,s}$ *and* $C_{N+\gamma}$ *coincide with those in* (4.17), $R_l^{(m)}f_\gamma$ *is of order* $O(m^{-l})$ *and*

$$\bar{A}_{N+\gamma} = A_{N+\gamma} + \bar{Q}f_\gamma - Qf_\gamma = A_{N+\gamma} - w_0 f(\vec{0}). \tag{4.23}$$

The only further result which requires comment is (4.18). The corresponding result in the case in which a function value at the origin is ignored is

$$\bar{A}_{\gamma+N} = 0, \qquad \gamma > 0 \quad (f_\gamma(\vec{x}) \text{ polynomial}). \tag{4.24}$$

For the constant function $f(\vec{x}) = K$, we have $A_N = 0$ while $\bar{A}_N = -w_0 f(\vec{0})$.

5. The Error Functional for Integrand Functions with $r^\alpha\varphi(\vec{\theta})$ Singularities. Theorems 4.17 and 2.6 provide asymptotic expansions for the error functional of two types of integrand functions. Clearly, these may be used to provide corresponding asymptotic expansions for any other integrand functions which may be expressed as a linear sum of these special types of integrand functions. In this section we treat a class of integrand functions, essentially ones having an $r^\alpha\varphi(\vec{\theta})$ singularity, where

$$r^2 = x_1^2 + x_2^2 + \ldots + x_N^2 \tag{5.1}$$

and $(r, \theta_2, \theta_3, \ldots, \theta_N)$ abbreviated to $(r, \vec{\theta})$ represents the point $(\vec{x})$ in a hyperspherical coordinate system.

Definition 5.2. $f(\vec{x}) \in H_\alpha^{(N)}$ if

$$f(\vec{x}) = r^\alpha \varphi(\vec{\theta}) h(r) g(\vec{x}), \tag{5.2}$$

where

(i) $f(\vec{x})$ is integrable over the unit hypercube $0 \leqslant x_i \leqslant 1$;

(ii) $\varphi(\vec{\theta})$ is analytic in $\theta_2, \theta_3, \ldots, \theta_N$ for all values of these variables for which the point $(1, \vec{\theta})$ lies within the closed unit hypercube;

(iii) $h(r)$ is analytic for $0 \leqslant r \leqslant \sqrt{N}$;

(iv) $g(\vec{x})$ is analytic in each variable x_i in the closed unit hypercube.

In two dimensions we have $r^2 = x^2 + y^2$ and $\theta = \arctan(y/x)$ and condition (ii) is simply

(ii) $\varphi(\theta)$ is analytic in the interval $0 \leqslant \theta \leqslant \pi/2$.

We note that condition (i) need not restrict α to be greater than $-N$. For example, the two-dimensional function $r^{-4}x^3$ belongs to $H_\alpha^{(2)}$ with $\alpha = -1$ since $r^{-4}x^3 = r^{-1}\cos^3\theta$ which is clearly integrable. One of the main effects of conditions (ii) and (iv) is to exclude line singularities which pass through the hypercube. Thus, $f(x, y) = (\lambda x + \mu y)^\beta$ with β not a nonnegative integer is excluded when $\lambda\mu \leqslant 0$ but included when $\beta > -2$ and $\lambda\mu > 0$. In either case $f(x, y)$ may be expressed in the form $r^\beta(\lambda\cos\theta + \mu\sin\theta)^\beta$ and condition (ii) leads to these conditions on λ and μ.

LEMMA 5.3. *When $f(\vec{x}) \in H_\alpha^{(N)}$, it may be expressed in the form*

$$f(\vec{x}) = f_\alpha(\vec{x}) + f_{\alpha+1}(\vec{x}) + \ldots + f_{\alpha+p-1}(\vec{x}) + g_{\alpha+p}(\vec{x}) \tag{5.3}$$

where

(i) *$f_{\alpha+j}(\vec{x})$ is a homogeneous function of degree $\alpha + j$ and is analytic within the unit hypercube except at the origin;*

(ii) *$g_{\alpha+p}(\vec{x})$ together with all its partial derivatives of order n are integrable over the unit hypercube when*

$$n \leqslant \alpha + p + N. \tag{5.4}$$

The proof is elementary. One need only expand $h(r)$ and $g(\vec{x})$ in multivariate Taylor expansions about the origin. Setting

$$h(r) = \sum_{j=0}^{p-1} b_j r^j + H_p(r), \tag{5.5}$$

$$g(\vec{x}) = \sum_{j=0}^{p-1} g_j(\vec{x}) + G_p(\vec{x}), \tag{5.6}$$

with

$$b_j = h^{(j)}(0)/j!, \tag{5.7}$$

$$g_j(\vec{x}) = \left(\sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i}\right)^j \frac{g(\vec{x})}{j!}\Bigg|_{\vec{x}=0}, \tag{5.8}$$

we find explicitly

$$f_{\alpha+t}(\vec{x}) = r^\alpha \varphi(\vec{\theta}) \sum_{j=0}^{t} b_j r^j g_{t-j}(\vec{x}) \tag{5.9}$$

and

$$g_{\alpha+p}(\vec{x}) = r^\alpha \varphi(\vec{\theta}) \sum_{j=0}^{p} H_j(r) G_{p-j}(\vec{x}). \tag{5.10}$$

Since r^α, $\varphi(\vec{\theta})$, r^j, and $g_{t-j}(\vec{x})$ are homogeneous functions of degrees α, 0, j, and $t - j$, respectively, the expression on the right-hand side of (5.9) is a homogeneous function of degree $\alpha + t$. The function $g_{\alpha+p}(\vec{x})$ given by (5.10) is a sum of functions whose behavior at the origin has the form $r^\alpha\varphi(\theta)r^j x_1^{t_1} x_2^{t_2} \ldots x_N^{t_N}$, where $\Sigma\, t_i = p - j$ and each of these separately satisfy condition (ii). This establishes Lemma 5.3.

We now proceed to use this lemma in conjunction with Theorems 4.17 and 2.6 to establish Theorem 5.14 below. It follows from (5.3) that

$$Q^{(m)}f - If = \sum_{t=0}^{p-1} (Q^{(m)}f_{\alpha+t} - If_{\alpha+t}) + Q^{(m)}g_{\alpha+p} - Ig_{\alpha+p}. \tag{5.11}$$

Theorem 4.17 provides an expansion for each of the p expressions in the summation over index t. Applying Theorem 2.6 to the function $g_{\alpha+p}(\vec{x})$, taking into account condition (ii) of Lemma 5.3, one obtains

$$Q^{(m)}g_{\alpha+p} - Ig_{\alpha+p} = \sum_{s=1}^{l-1} \frac{\widetilde{B}_{\alpha+p,s}}{m^s} + O(m^{-l}), \qquad N \leqslant l < \alpha + p + N, \tag{5.12}$$

with

$$\widetilde{B}_{\alpha+p,s} = \sum_{\Sigma t_i = s} c_{t_1,t_2,\ldots,t_N}(Q) \int_0^1 \int_0^1 \cdots \int_0^1 g_{\alpha+p}^{(t_1,t_2,\ldots,t_N)}(\vec{x}) d^N x. \tag{5.13}$$

Substituting (4.17) and (5.12) into (5.11) leads to the following theorem.

THEOREM 5.14. *Let $Q^{(m)}f$ given by* (2.5) *be the m^N copy version of Qf given by* (2.2) *which approximates If given by* (2.1). *Let $f(\vec{x}) \in H_\alpha^{(N)}$ defined in* (5.2). *Then*

$$Q^{(m)}f - If = \sum_{t=0}^{p-1} \frac{A_{\alpha+N+t}}{m^{\alpha+N+t}} + \sum_{s=1}^{l-1} \frac{B_s}{m^s} + O(m^{-l}), \tag{5.14}$$
$$N \leqslant l < \alpha + N + p, \ \alpha \neq \text{integer}$$

and

$$Q^{(m)}f - If = \sum_{s=1}^{l-1} \frac{A_s + B_s}{m^s} + \sum_{s=1}^{l-1} \frac{C_s}{m^s} \ln m + O(m^{-l} \ln m), \qquad l \geqslant N, \ \alpha = \text{integer}. \tag{5.15}$$

The coefficients $A_{N+\alpha+t}$ and $C_{N+\alpha+t}$ are given by (4.10) and (4.12) and

$$B_s = \sum_{t=0}^{p-1} B_{\alpha+t,s} + \widetilde{B}_{\alpha+p,s}, \tag{5.16}$$

where $B_{\alpha+t,s}$ is given by (4.11) and $\widetilde{B}_{\alpha+p,s}$ by (5.13).

The case in which the function value at the origin is replaced by zero is precisely analogous.

THEOREM 5.17. *In the notation of Theorem* 5.14, *let $\bar{Q}^{[m]}f$ be defined by* (4.21). *Then Theorem* 5.14 *is valid when $Q^{(m)}f$ is replaced by $\bar{Q}^{[m]}f$ so long as coefficients A_γ are replaced by $\bar{A}_\gamma$ defined by* (4.23).

Contrary to appearance, the value of B_s is independent of the value of p used in (5.16). B_s has an integral representation which displays its independence of p. We demonstrate this only in the two-dimensional case when α is not an integer. The expansion of $f^{(t,r)}(x, y)$ corresponding to (5.3) may be written in the form

$$f^{(t,r)}(x, y) = \sum_{w=0}^{\overline{w}} f_{\alpha+w}^{(t,r)}(x, y) + \sum_{w=\overline{w}+1}^{p-1} f_{\alpha+w}^{(t,r)}(x, y) + g_{\alpha+p}^{(t,r)}(x, y), \tag{5.18}$$

where $t + r - \alpha - 3 < \overline{w} < t + r - \alpha - 2$. The first sum is composed of functions which are integrable over $L[1, \infty)$ but not over $L[0, 1)$ while the rest of the terms have the opposite property. Reference to (3.13), (4.11), and (5.13) leads to the integral representation

$$B_s = \sum_{t=0}^{s} c_{t,s-t}(Q)\left[-\int_{L[1,\infty)} \theta_{t,s-t}(x, y)\, dx\, dy + \int_{L[0,1)} (f^{(t,s-t)}(x, y) - \theta_{t,s-t}(x, y))\, dx\, dy\right]. \tag{5.19}$$

Here

$$\theta_{t,s-t}(x, y) = \sum_{w=0}^{\overline{w}} f_{\alpha+w}^{(t,s-t)}(x, y), \qquad \overline{w} = [s - \alpha - 2]. \tag{5.20}$$

In words, the situation is that for functions without singularities the coefficient B_s coincides with (5.19) with $\theta_{t,s-t}(x, y) = 0$. In cases where the integrand function has unintegrable singularity, homogeneous functions involving the singularity are "subtracted out" and integrated instead over the domain $L[1, \infty)$ (with a sign reversal).

The coefficients A_s, B_s and C_s which occur in the error functional expansions (5.14) and (5.15) depend on the quadrature rule Q and the integrand function $f(\vec{x})$. So far as the quadrature rule is concerned, the results about the vanishing of some of the coefficients are straightforward. Reference to (5.16), (4.19), (4.20), (2.15), and (2.19) show that if Q is a symmetric rule

$$B_s = C_s = 0, \qquad s \text{ odd}, \ Q \text{ symmetric}, \tag{5.21}$$

and that if Q is of polynomial degree $d(Q)$

$$B_s = C_s = 0, \qquad s \leqslant d(Q). \tag{5.22}$$

Other coefficients $A_{\alpha+t+N}$ and $C_{\alpha+t+N}$ may vanish for certain integrand functions. This is discussed in Section 7.

6. The Error Functional for Integrand Functions with $\ln r \cdot r^\alpha \varphi(\theta)$ **Singularities.** In this section we derive the corresponding expansion for $Q^{(m)}F - IF$ where

$$F(\vec{x}) = \ln r \cdot r^\alpha \varphi(\theta) h(r) g(\vec{x}) = \frac{\partial}{\partial \alpha} f(\vec{x}) \tag{6.1}$$

and, as before,

$$f(\vec{x}) = r^\alpha \varphi(\theta) h(r) g(\vec{x}) \tag{6.2}$$

is an element of $H_\alpha^{(N)}$. This is most easily accomplished by treating the coefficients in (5.14) as functions of the variable α and differentiating with respect to α. When α is not an integer this is trivial. The result is

THEOREM 6.3. *When α is not an integer,*

$$Q^{(m)}F - IF = \sum_{t=0}^{p-1} \frac{\partial A_{\alpha+N+t}/\partial \alpha}{m^{\alpha+N+t}} - \sum_{t=0}^{p-1} \frac{A_{\alpha+N+t} \ln m}{m^{\alpha+N+t}} + \sum_{s=0}^{l-1} \frac{\partial B_s/\partial \alpha}{m^s} + O(m^{-l}), \qquad N \leqslant l < d + N + p, \ \alpha \neq \textit{integer}. \tag{6.3}$$

The rest of this section is devoted to deriving the result which corresponds to 6.3 in the case in which α is an integer. In this case the same approach may be used, but is more difficult to implement. In order to differentiate with respect to α, one requires an expansion whose coefficients treated as functions of α are differentiable at the value of α of interest. Expansion (5.15), unlike (5.14), is not such an expansion.

In Section 4, two separate expressions for $Q^{(m)}f_\gamma - If_\gamma$ are given, one valid when γ is not an integer and the other when γ is an integer. While these expressions are convenient for direct applications, this dichotomy is aesthetically unsatisfactory. When one considers a one parameter family of homogeneous functions, such as $f_\gamma = r^\gamma$, one does not expect any abrupt change in the value of $Q^{(m)}f_\gamma - If_\gamma$ as the value of γ passes through each integer value. Indeed, as we shall show, there is no abrupt change. The right-hand side of (4.17) is a limiting form of the right-hand side of (4.17) as γ approaches an integer either from above or below.

When γ is not an integer, the expansion (4.17) involves terms

$$\frac{A_{N+\gamma}}{m^{N+\gamma}} \quad \text{and} \quad \frac{B_{\gamma,s}}{m^s} \quad \text{and} \quad R_l^{(m)}f_\gamma,$$

the coefficients being given explicitly by (4.10), (4.11), and (4.13). So long as γ does not become an integer these expressions, which involve the integrals $I_\gamma^{(t_1,t_2,\ldots,t_N)}$ defined in (3.13), vary in a continuous manner. But as γ passes through the integer $n - N$, the definition of $I_\gamma^{(t_1,t_2,\ldots,t_N)}$ where $\Sigma t_i = n$ alters abruptly from an integral over domain $L[1, \infty)$ to an integral over domain $L[0, 1)$, either becoming divergent at $\gamma = n - N$.

To investigate the expansion near $\gamma = n - N$, we remove terms involving $I_\gamma^{(t_1,t_2,\ldots,t_N)}$, $\Sigma t_i = n$ from $A_{N+\gamma}$ and $B_{\gamma,s}$ and treat them separately. We use parts (iii) and (iv) of Theorem 3.8 to express these integrals in terms of an integral over $L[1, 2)$. This involves some elementary manipulation, in the course of which it becomes convenient to define

$$(6.4)\qquad \begin{aligned} A^*_{\gamma+N} &= A_{\gamma+N} - \sum_{\Sigma t_i=n} c_{t_1,t_2,\ldots,t_N}(Q) I_\gamma^{(t_1,t_2,\ldots,t_N)}, \qquad && \gamma \neq n - N, \\ A^*_{\gamma+N} &= A_{\gamma+N}, && \gamma = n - N, \end{aligned}$$

$$(6.5)\qquad C^*_{\gamma+N} = \sum_{\Sigma t_i=n} c_{t_1,t_2,\ldots,t_N}(Q) K_\gamma^{(t_1,t_2,\ldots,t_N)}.$$

The functions $A^*_{\gamma+N}$ and $C^*_{\gamma+N}$, unlike $A_{\gamma+N}$ and $C_{\gamma+N}$ defined by (4.10) and (4.12), vary continuously with γ as γ passes through the integer value $\gamma = n - N$ and coincide with $A_{\gamma+N}$ and $C_{\gamma+N}$ when $\gamma = n - N$. The result is the following:

THEOREM 6.6. *When $\gamma = n - N + \epsilon$ with $|\epsilon| < 1$ and $n < l$,*

$$(6.6)\qquad Q^{(m)}f_\gamma - If_\gamma = \frac{A^*_{\gamma+N}}{m^{\gamma+N}} + \sum_{s=1;s\neq n}^{l-1} \frac{B_{\gamma,s}}{m^s} + \varphi(m,n,\epsilon) \ln 2\, C^*_{\gamma+N} + R_l^{(m)}f_\gamma$$

with

$$(6.7)\qquad \varphi(m,n,\epsilon) = \left(\frac{1}{m^{n+\epsilon}} - \frac{1}{m^n}\right)\bigg/(1 - 2^\epsilon), \qquad \epsilon \neq 0,$$

$$(6.8)\qquad \varphi(m,n,0) = \ln m/(m^n \ln 2).$$

The function $\varphi(m, n, \epsilon)$ is analytic in ϵ and

$$\frac{\partial}{\partial\epsilon}\varphi(m, n, 0) = -\frac{\ln m}{2m^n} - \frac{(\ln m)^2}{2m^n \ln 2}. \tag{6.9}$$

The form (6.6) of expansion (4.17) has the advantage that all coefficients vary continuously with γ over the range $n - N - 1 < \gamma < n - N + 1$ which includes the integer value $\gamma = n - N$. Using (6.7) or (6.8), (6.6) reduces to (4.17) whether or not γ is an integer.

We may now consider a one parameter family of homogeneous functions $f_\gamma(\vec{x})$ which is analytic in γ and differentiate expansion (6.6) with respect to γ and then set $\gamma = n - N$. The result is

$$\begin{aligned} Q^{(m)}\frac{\partial}{\partial\gamma}f_\gamma - I\frac{\partial}{\partial\gamma}f_\gamma & \\ &= \frac{\partial A^*_{\gamma+N}/\partial\gamma}{m^{\gamma+N}} + \sum_{s=1;s\neq\gamma+N}^{l-1} \frac{\partial B_{\gamma,s}/\partial\gamma}{m^s} \\ &\quad + \left(-A^*_{\gamma+N} + \frac{\partial}{\partial\gamma}C^*_{\gamma+N} - \frac{\ln 2}{2}C^*_{\gamma+N}\right)\frac{\ln m}{m^{\gamma+N}} \\ &\quad - \frac{C^*_{\gamma+N}}{2}\frac{(\ln m)^2}{m^{\gamma+N}} + \frac{\partial}{\partial\gamma}R_l^{(m)}f_\gamma, \qquad \gamma = \text{integer}. \end{aligned} \tag{6.10}$$

When γ is not an integer, the corresponding expansion is simpler. That expansion may be obtained by differentiating (4.17) and coincides with (6.10) if one removes terms involving $C^*_{\gamma+N}$, removes the restriction on the sum over s and replaces $A^*_{\gamma+N}$ by $A_{\gamma+N}$.

In order to apply (6.10) to obtain the analogue of (6.3), we have to specify more precisely the function f_γ. We treat the functions

$$f_{\alpha+t}(\vec{x}) = r^\alpha\varphi(\vec{\theta})\sum_{j=0}^{t} b_j r^j g_{t-j}(\vec{x}) \tag{6.11}$$

defined in (5.9) which are elements of the expansion (5.3), namely

$$f(\vec{x}) = \sum_{t=0}^{p-1} f_{\alpha+t}(\vec{x}) + g_{\alpha+p}(\vec{x}). \tag{6.12}$$

Setting $\gamma = \alpha + t$, it appears that for functions (6.11) the operators $\partial/\partial\gamma$ and $\partial/\partial\alpha$ are identical. It also follows that

$$F(\vec{x}) = \sum_{t=0}^{p-1} \frac{\partial}{\partial\alpha}f_{\alpha+t}(\vec{x}) + \frac{\partial}{\partial\alpha}g_{\alpha+p}(\vec{x}). \tag{6.13}$$

Operating on each term of this identity with $Q^{(m)} - I$ and applying (6.10) and (2.6) we find:

THEOREM 6.14.

$$Q^{(m)}F - IF = \sum_{t=0}^{p-1} \frac{\partial A^*_{\alpha+t+N}/\partial\alpha}{m^{\alpha+t+N}} + \sum_{s=1}^{l-1} \frac{\partial B_s/\partial\alpha}{m^s}$$

$$(6.14) \qquad + \sum_{t=0}^{p-1} \left(-A^*_{\alpha+t+N} + \frac{\partial}{\partial\alpha} C^*_{\alpha+t+N} - \frac{\ln 2}{2} C^*_{\alpha+t+N} \right) \frac{\ln m}{m^{\alpha+t+N}}$$

$$- \sum_{t=0}^{p-1} \frac{C^*_{\alpha+t+N}}{2} \frac{(\ln m)^2}{m^{\alpha+t+N}} + O(m^{-(\alpha+p+N)}(\ln m)^2),$$

$$N \leqslant l = \alpha + p + N, \ \alpha = \textit{integer}.$$

In precisely the same manner as in the previous section, certain coefficients vanish when Q is symmetric or when Q is of polynomial degree $d(Q)$. Specifically,

$$(6.15) \qquad \partial B_s/\partial\alpha = \partial C^*_s/\partial\alpha = C^*_s = 0, \qquad s \text{ odd}, \ Q \text{ symmetric},$$

$$(6.16) \qquad \partial B_s/\partial\alpha = \partial C^*_s/\partial\alpha = C^*_s = 0, \qquad s \leqslant d(Q).$$

Other coefficients may vanish for certain integrand functions. This is discussed in the next section.

The same technique may be used to derive the corresponding expansion for an integrand function

$$(6.17) \qquad F(x) = (\ln r)^q f(\vec{x})$$

for integer q. All that is necessary is to differentiate either (6.3) or (6.6) $q - 1$ times with respect to α or γ and to collect together like terms. The error functional $Q^{(m)}F - IF$ when F is given by (6.17) contains terms m^{-t} and $m^{-(\alpha+N+t)}(\ln m)^s$, $s = 0, 1, \ldots, s_q$ for $t = 1, 2, \ldots$. When α is not an integer, $s_q = q$. When α is an integer, $s_q = q + 1$.

7. Examples in Which Some Terms in the Expansion Are Zero. In the various expansions derived in this paper, we noted at each stage that if Q is symmetric or if Q is of specified polynomial degree, certain coefficients in the expansion are zero. However, the coefficients depend both on Q and on the integrand function; and there are some easily recognizable forms of integrand function for which certain coefficients vanish. In this section we draw attention to some of these.

As a preliminary, we note that the specification of a given function in form (5.2) is not unique. A two-dimensional example is

$$(7.1) \qquad f(x, y) = r^{-4}x^3 = r^{-1}\sin^3\theta = r^{-2}x^3(x^2 + y^2).$$

Application of Theorem 5.14 to each of these forms gives three apparently different expansions for $Q^{(m)}f - If$. Each of these is correct and each displays many coefficients which are in fact zero. In this case, since $f(x, y)$ is a homogeneous function of degree -1, expansion 4.17 is valid and any expansion obtained from 5.14 contains a whole sequence of terms which are zero.

The derivation of Theorem 5.14 is accomplished in Section 5 by expressing $h(r)g(\vec{x})$ as a multivariate Taylor expansion and collecting together terms of the same degree to form

$$f(\vec{x}) = \sum_{t=0}^{p-1} f_{\alpha+t}(\vec{x}) + g_{\alpha+p}(\vec{x}). \tag{7.2}$$

The coefficients $A_{\alpha+t+N}$ and $C_{\alpha+t+N}$ arise from the component $f_{\alpha+t}(\vec{x})$ and are absent if $f_{\alpha+t}(\vec{x})$ is zero. In the example (7.1) above, all $f_{\alpha+t}(x, y)$ are zero except for $f_{-1}(x, y)$.

Another case in which some terms are absent is one in which the multivariate Taylor expansion is even (or odd) in character. Then $f_{\alpha+t}(\vec{x}) = 0$, t odd (or even), and all terms in expansion 5.14, 6.3, or 6.14 arising from these terms are also zero. We state this result as a theorem.

THEOREM 7.3. *If*

$$h(r)g(\vec{x}) \equiv h(-r)g(-\vec{x}) \quad (or\ h(r)g(\vec{x}) \equiv -h(-r)g(-\vec{x})),$$

then the coefficients in (5.10), (6.3), *and* (6.14) *satisfy*

$$\begin{aligned} A_{\alpha+s+N} &= C_{\alpha+s+N} = \frac{\partial}{\partial\alpha}A_{\alpha+s+N} = A^*_{\alpha+t+N} \\ &= \frac{\partial}{\partial\alpha}A^*_{\alpha+t+N} = C^*_{\alpha+s+N} = \frac{\partial}{\partial\alpha}C^*_{\alpha+s+N} = 0 \quad s\ odd\ (or\ even). \end{aligned} \tag{7.3}$$

Perhaps it should be emphasized that this symmetry is about the origin, while the symmetry in the quadrature rule which causes other coefficients to vanish is about hyperplanes $x_i = ½$ $(i = 1, 2, \ldots, N)$. We also note with regard to (7.3) that only $h(r)g(\vec{x})$ need be symmetric. There is no symmetry condition on the factors $r^\alpha\varphi(\vec{\theta})$.

Another set of circumstances in which coefficients may vanish arises if $f_{\alpha+t}(\vec{x})$ is a polynomial. This can happen only if α is an integer and $\varphi(\vec{\theta})$ is a trigonometric polynomial. When $f_{\alpha+t}(\vec{x})$ is a polynomial, it follows from (4.18) that $A_{\alpha+t+N} = C_{\alpha+t+N} = 0$. Since α is an integer, $A^*_{\alpha+t+N}$ and $C^*_{\alpha+t+N}$ as defined by (6.4) and (6.5) are zero; but neither $(\partial/\partial\alpha)A^*_{\alpha+t+N}$ nor $(\partial/\partial\alpha)C^*_{\alpha+t+N}$ required in (6.10) or (6.14) need be zero.

A trivial example of this occurs when $f(\vec{x})$ has no singularity in which case all $f_{\alpha+t}(\vec{x})$ are polynomials and one recovers the Euler-Maclaurin expansion (2.6).

Beside these terms, other terms vanish when the rule is symmetric and when the rule Q is of specified degree. These are B_s, C_s, C^*_s, $(\partial/\partial\alpha)B_s$, $(\partial/\partial\alpha)C^*_s$ both when s is odd and also when $s \leqslant d(Q)$. In the simpler examples, so many terms vanish that the whole appearance of the final series may be quite different from that expected.

As an example, we deal with the very simple function

$$f(x) = h(r)g(\vec{x}). \tag{7.4}$$

Direct application of (5.15) with $\alpha = 0$ gives

$$Q^{(m)}f - If = \sum_{s=1}^{l-1}\frac{A_s}{m^s} + \sum_{s=1}^{l-1}\frac{B_s}{m^s} + \sum_{s=1}^{l-1}\frac{C_s \ln m}{m^s} + O(m^{-l}\ln m). \tag{7.5}$$

However, it is obvious that $f_t(\vec{x})$ is a polynomial when t is even, so the only nonzero terms A_s and C_s are those with $s = t + N$ with t odd. Thus, because of the simple nature of the integrand, we have

$$(7.6)\quad Q^{(m)}f - If = \sum_{s=N;s\,\text{odd}}^{l-1} \frac{A_s}{m^s} + \sum_{s=1}^{l-1} \frac{B_s}{m^s} + \sum_{s=N;s\,\text{odd}}^{l-1} \frac{C_s \ln m}{m^s} + O(m^{-l}\ln m), \qquad N \text{ even},$$

$$(7.7)\quad Q^{(m)}f - If = \sum_{s=N;s\,\text{even}}^{l-1} \frac{A_s}{m^s} + \sum_{s=1}^{l-1} \frac{B_s}{m^s} + \sum_{s=N;s\,\text{even}}^{l-1} \frac{C_s \ln m}{m^s} + O(m^{-l}\ln m), \qquad N \text{ odd}.$$

If Q is a symmetric rule of degree $d(Q)$ then $B_s = C_s$ for all s odd and for $s \leqslant d(Q)$. Applying this to (7.6) and (7.7) gives

$$(7.8)\qquad Q^{(m)}f - If \sim \sum_{s=N;s\,\text{odd}} \frac{A_s}{m^s} + \sum_{s=d+1;s\,\text{even}} \frac{B_s}{m^s}, \qquad N \text{ even},$$

$$(7.9)\qquad Q^{(m)}f - If \sim \sum_{s=N;s\,\text{even}} \frac{A_s}{m^s} + \sum_{s=d+1;s\,\text{even}} \frac{B_s}{m^s} + \sum_{s=N;s\,\text{even}} \frac{C_s \ln m}{m^s}, \qquad N \text{ odd}.$$

The pattern of these expansions may be described as follows. When N is even, apart from some early terms, all inverse powers m^{-s} occur, but no terms $m^{-s} \ln m$. When N is odd, apart from early terms, only even inverse powers m^{-s} and terms $m^{-s} \ln m$ with s even occur.

This result is one of those given in Table 1 which also gives the corresponding results for other very simple forms of integrand function.

One can endlessly pursue sets of conditions for the vanishing of coefficients. We have stated here only some of those which may be easy to recognize from the analytic form of the integrand function.

It is pertinent to remark that it is doubtful that any of the asymptotic expansions converge except in trivial circumstances; and that if one does converge, it may converge to a result which is different from the left-hand side. The corresponding one-dimensional situation is discussed at length in Lyness [9]. There it appears that if the integrand function has a singularity anywhere in the finite complex plane there is no convergence and simple examples of "wrong" convergence are given.

It seems at first sight surprising that these expansions have not been discovered experimentally. One of the reasons may be that there are so many special cases in which different terms drop out of the expansion. By the time one has constructed an example for which the exact integral is known, one is dealing with a special case.

The special case $\alpha = 0$ is described by Table 1. The author was surprised to find this rather bewildering pattern of terms present in the expansion. An experimental approach, in which one has no clear idea about the final pattern and in which one is dealing with nonconvergent expansions, would be extremely difficult to carry out to completion.

TABLE 1

The structure of the error functional expansion for $Q^{(m)}\varphi - I\varphi$, when Q is a symmetric rule of degree d and $\varphi(\vec{x})$ is an N-dimensional integrand function. Here $r = |\vec{x}|$, $h(r)$ is analytic in r and $g(\vec{x})$ is analytic in each component of $\vec{x}$.

$\varphi(\vec{x})$	Set of values of s for which there may may be a nonzero coefficient		
	m^{-s}	$m^{-s} \ln m$	$m^{-s}(\ln m)^2$
$g(\vec{x})$	s even $> d$	$\varnothing$	$\varnothing$
$h(r)g(\vec{x})$ N even	s even $> d$ s odd $> N$	$\varnothing$	$\varnothing$
$h(r)g(\vec{x})$ N odd	s even $> d$ s even $> N$	s even $> \max(N, d)$	$\varnothing$
$\ln r\, g(\vec{x})$	s even $> d$ $s \geqslant N$	s even $\geqslant \max(N, d)$	$\varnothing$
$\ln r\, h(r)g(\vec{x})$ N even	s even $> d$ $s \geqslant N$	s even $\geqslant \max(N, d)$ s odd $> N$	$\varnothing$
$\ln r\, h(r)g(\vec{x})$ N odd	s even $> d$ $s \geqslant N$	s even $> N$	s even $> \max(N, d)$

8. Concluding Remarks. The purpose of this paper is to derive expansions such as those given in Theorem 5.14. The more general question of whether or not numerical quadrature based on extrapolation is more or less efficient than other quadrature methods is one which is separate from the derivation of the expansions, and it is not treated in any detail here. In order only to place these expansions in proper perspective, a few brief remarks are appropriate.

The author believes that the main applications of these expansions will be to N-dimensional integrals whose integrand functions are given analytically and are clearly recognizable as being of the specified form. In particular, the value of α will be known. An integration may be carried out by using a specified quadrature rule Q to evaluate

$$Q^{(m)}f, \qquad m = m_0, m_1, m_2, \ldots, \tag{8.1}$$

and using extrapolation based on the proper expansion to refine the results. The choice of a moderate degree rule such as one of those in Stroud [14] eliminates automatically some of the terms in the expansion. The choice of a sequence m_i which grows as slowly as is convenient is suggested. The sequence $m_j = j + 1$ may be suitable so long as a check on the buildup of round-off error in the extrapolation process is incorporated. A great deal of investigation into methodology is required. For example, a *convenient* extrapolation process (corresponding to Romberg integration) is not available for these expansions (unless the sequence is geometric i.e., $m_{j+1} = km_j$). Which moderate degree rule should be used? And how far should the extrapolation process be taken? And how can the round-off error be controlled? An investigation into these matters would delay and lengthen this paper and has not been carried out.

However, these expansions form a sound analytic basis for recent work on nonlinear methods based on the epsilon algorithm. So long as

$$Q^{(m)}f - If \sim \sum \frac{A_j}{m^{\alpha_j}} + \sum \frac{C_j}{m^{\beta_j}} \ln m \tag{8.2}$$

where α_j and β_j are arbitrary, and the sequence chosen is geometric, for example

$$\{m\} = 1, 2, 4, 8, \ldots, \tag{8.3}$$

then the epsilon algorithm may be used to eliminate terms in the expansion. This is discussed by Kahaner [7] in a one-dimensional context (where a sound analytic basis already exists) and has been developed experimentally with success by Genz [5], [6] and Chisholm, Genz and Rowlands [3].

Any detailed relative evaluation of methods based on the epsilon algorithm and direct extrapolation methods should await a detailed investigation. But the following remarks seem pertinent. First, using the epsilon algorithm, one requires two extrapolations to eliminate a term like A/m^α in (8.2) since both A and α are treated as unknown. The direct method takes advantage of the known value of α and requires only one extrapolation to eliminate this term. Second, the epsilon algorithm requires a geometric sequence like (8.3) while the direct method can be used (with numerical safeguards) with a sequence like

$$\{m\} = 1, 2, 3, 4, \ldots . \tag{8.4}$$

Since, in an N-dimensional quadrature, the number of function evaluations associated with the calculation of $Q^{(m)}f$ is roughly km^N, the circumstance that one may use (8.4) in place of (8.3) may turn out to be a considerable advantage.

The epsilon algorithm though is more general since it may be valid for integrand functions not covered by this paper. Thus, if it is known that the expansion is of form (8.2) but the values of α_j and β_j are not known, then there is no basis for the direct approach, and there is a basis for using the epsilon algorithm.

To the author's knowledge, the work mentioned above is the only published work on these specific problems. However, it is only proper to draw attention to a general method for one-dimensional quadrature due to Stenger [13], whose N-dimensional analogue may be competitive. This consists of transforming a finite interval $[-1, 1]$ into the infinite interval using $w = \tanh x$ and then applying a truncated trapezoidal rule to the transformed integral, giving an approximation of the type

$$\int_0^1 f(x)dx \simeq Q(h; n)f = \sum_{k=-n}^{n} \frac{e^{kh}}{(1 + e^{kh})^2} f\left(\frac{e^{kh}}{1 + e^{kh}}\right). \tag{8.5}$$

A sequence of such approximations $Q(h; n)$ with $h = \lambda n^{-1/2}$ approaches the true integral with an error $O(e^{-cn^{1/2}})$, $c > 0$. Transformations of this type have also been suggested by Takahasi and Mori [15]. No N-dimensional numerical results have been reported.

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