

# The Legendre Series and a Quadrature Formula for Its Coefficients

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Received July 17, 1973

A quadrature formula which may be used to evaluate the coefficients of the Legendre series is presented. The formula is of more general interest in that it is a quadrature for a Legendre polynomial weight function. An example demonstrates the usefulness of this formula which is also relevant to the finite range Distorted Waves Born Approximation method in nuclear physics.

## I. INTRODUCTION

The Legendre series expresses a function  $f(x)$ , where  $-1 \leq x \leq 1$ , as an infinite series of Legendre polynomials [1]

$$f(x) = \sum_{K=0}^{\infty} (K + \frac{1}{2}) g_K P_K(x). \tag{1}$$

Such an expansion is possible if it is assumed that the infinite series converges uniformly on the interval  $[-1, 1]$  to the sum  $f(x)$ . The conditions to be satisfied by  $f(x)$  to ensure uniform convergence are discussed by Hobson [1], and for the purposes of the present work it is assumed that these conditions are fulfilled.

The Legendre polynomials form a system of polynomials which are mutually orthogonal with respect to the weight function  $p(x) = 1$ , on the interval  $[-1, 1]$ , i.e.,

$$\begin{aligned} \int_{-1}^{+1} P_m(x) P_n(x) dx &= 0 & m \neq n \\ &= \frac{2}{2n + 1} & m = n. \end{aligned} \tag{2}$$

An expression for the expansion coefficients of Eq. (1) follows from this property upon multiplying through by  $P_n(x)$  and integrating over the interval  $[-1, 1]$ , whence

$$g_K = \int_{-1}^{+1} f(x) P_K(x) dx. \tag{3}$$

These coefficients have definite values no matter how the function  $f(x)$  is defined provided that it is summable in the interval  $[-1, 1]$ .

There are several branches of physics where the expansion of Eq. (1) is advantageous [2, 3]. This advantage, however, is hampered by the need to evaluate a series of integrals of the type (3) and the problem may become acute if  $f(x)$  is a nonanalytic function, in which case the integrals need to be performed numerically. An example of the latter case occurs in calculations for certain types of nuclear reactions [4, 5] where the finite range Distorted Waves Born Approximation method, in the formulation of Austern *et al.* [3] is used. This method relies upon the Legendre series expansion of (1) at each point of a two dimensional grid and as a consequence, a significant proportion of computing time is spent in calculating the coefficients of Eq. (3). Here the problem of calculating the  $g_K$  coefficients is investigated. In particular, the present work derives a quadrature formula to evaluate the integral of Eq. (3). This formula is both powerful and convenient and also suitable when an explicit analytic form for  $f(x)$  is not known. The accomplishment of this aim is facilitated by noting another property of the Legendre polynomials, namely, that their roots are all real, distinct, and lie in the interval  $[-1, 1]$ .

## II. THE QUADRATURE FORMULA

It will be observed that the integrand of the r.h.s. of Eq. (3) consists of two components: the polynomial  $P_K(x)$  and the function  $f(x)$  which is either analytic or numerically calculable at points on the interval  $[-1, 1]$ . In seeking to represent the integral of Eq. (3) by a suitable quadrature sum it is sensible to choose the polynomial  $P_K(x)$  as the weight function  $p(x)$ . However,  $P_K(x)$  has  $K$  real roots  $a_1, a_2, \dots, a_K$  in this interval and changes sign at each of these nodes, thus the usual theorems on quadrature formulas [6, 7], which hold only when the weight function  $p(x) \geq 0$ , as is the case for Gaussian quadrature ( $p(x) = 1$ ), or Chebyshev quadrature ( $p(x) = 1/\sqrt{1-x^2}$ ), for example, do not apply.

This difficulty may be overcome if V. I. Krylov's suggestion [8, 9] is followed. An interpolating polynomial,  $S(x)$ , of degree less than  $K$ , is constructed for  $f(x)$ . This polynomial is based on the functional values at the nodes

$$S(a_j) = f(a_j), \quad j = 1, 2, \dots, K$$

and

$$f(x) = S(x) + r(x) \tag{4}$$

where  $r(x)$  is the remainder of the interpolation. If the polynomial  $\Omega(x)$  is defined as

$$\Omega(x) = (x - a_1)(x - a_2) \dots (x - a_K), \tag{5}$$

then this remainder may be represented as [6]

$$r(x) = \Omega(x) f(a_1, a_2, \dots, a_K, x) \quad (6)$$

where  $f(a_1, a_2, \dots, a_K, x)$  is the divided difference corresponding to the nodes  $a_1, a_2, \dots, a_K, x$ . Substituting for  $f(x)$  on the r.h.s. of Eq. (3) it follows that

$$\int_{-1}^{+1} P_K(x) f(x) dx = \int_{-1}^{+1} P_K(x) S(x) dx + \int_{-1}^{+1} P_K(x) \Omega(x) f(a_1, \dots, a_K, x) dx. \quad (7)$$

In reducing the first integral of the r.h.s. to a quadrature sum the usual practice would be to introduce the Lagrangian form of the interpolating polynomial

$$S(x) = \sum_{j=1}^K \frac{\Omega(x)}{(x - a_j) \Omega'(a_j)} f(a_j) \quad (8)$$

which, in the present case, noting that

$$P_K(x) = \frac{(2K)!}{2^K(K!)^2} \Omega(x) \quad (9)$$

becomes

$$S(x) = \sum_{j=1}^K \frac{P_K(x)}{(x - a_j) P_K'(a_j)} f(a_j). \quad (10)$$

Substituting (10) into the first term of (7) would then lead to a quadrature sum whose coefficients may be evaluated with the aid of the Christoffel–Darboux identity, which, for Legendre polynomials states that:

$$\sum_{m=0}^n \frac{2m+1}{2} P_m(x) P_m(y) = \frac{n+1}{2} \frac{P_{n+1}(x) P_n(y) - P_n(x) P_{n+1}(y)}{x - y}. \quad (11)$$

In the case under consideration however, since  $S(x)$  is a polynomial of order  $\leq K - 1$ , it follows from the property

$$\int_{-1}^{+1} x^m P_K(x) dx = 0, \quad m < K$$

that the first integral of Eq. (7) is identically zero.

In the second term of Eq. (7) the new weight function is defined as

$$\rho(x) = P_K(x) \Omega(x) \quad (12)$$

This weight function is always positive on the interval  $[-1, 1]$  since both polynomials  $P_K(x)$  and  $\Omega(x)$  change sign at each of the nodes  $a_1, \dots, a_K$ . The

theorems concerning quadratures for positive weight functions therefore apply [9]. In particular, an interpolatory quadrature formula of the maximum degree of precision is sought, such that

$$\int_{-1}^{+1} \rho(x) f(a_1, \dots, a_K, x) dx \approx \sum_{k=1}^n \beta_k f(a_1, \dots, a_K, x_k). \tag{13}$$

This quadrature formula is exact for polynomials of degree  $\leq 2n - 1$ , or, since the divided difference  $f(a_1, \dots, a_K, x)$  is a polynomial of degree  $K$  less than  $f(x)$ , (13) will be exact when  $f(x)$  is a polynomial of degree  $\leq 2n + K - 1$ .

The coefficients of the quadrature (13) are then given by

$$\beta_k = \int_{-1}^{+1} \rho(x) \frac{\omega(x)}{(x - x_k) \omega'(x_k)} dx \tag{14}$$

where

$$\omega(x) = (x - x_1)(x - x_2) \dots (x - x_n). \tag{15}$$

Whether such a quadrature formula may be constructed rests upon whether there exists a unique set of polynomials  $\Pi_n(x) = b_n \omega(x)$  (with  $b_n$  a constant) orthogonal, with respect to the weight function  $\rho(x)$ , to all polynomials of degree  $< n$  in the interval  $[-1, 1]$ , i.e.,

$$\int_{-1}^{+1} \rho(x) \Pi_n(x) \Pi_s(x) dx = 0 \quad \text{for } s < n. \tag{16}$$

Since  $\rho(x) \geq 0$  in this interval, a polynomial  $\Pi_n(x)$ , whose roots  $x_k, k = 1, 2, \dots, n$ , are all real, distinct, and lie in the interval  $[-1, 1]$ , may indeed be constructed. In constructing this polynomial  $\Pi_n(x)$  both Krylov and Kopal [10] suggest solving a determinantal equation. From a calculational point of view not only is this procedure cumbersome, but it is also subject to severe round-off error effects as the size of the determinant increases. In the following, a more straight forward method of obtaining the quadrature coefficients of Eq. (14) is described.

Using Eqs. (4) and (6) the divided difference  $f(a_1, \dots, a_K, x_k)$  on the r.h.s. of (13) may be replaced by

$$f(a_1, \dots, a_K, x_k) = \frac{f(x_k) - S(x_k)}{\Omega(x_k)} \tag{17}$$

if none of the nodes  $x_k$  coincides with  $a_1, \dots, a_K$ . So that Eq. (13) becomes

$$\int_{-1}^{+1} \rho(x) f(a_1, \dots, a_K, x) dx \approx \sum_{k=1}^n B_k [f(x_k) - S(x_k)] \tag{18}$$

and

$$B_k = \frac{1}{\Omega(x_k)} \int_{-1}^{+1} P_K(x) \Omega(x) \frac{\omega(x)}{(x - x_k) \omega'(x_k)} dx \tag{19}$$

or using Eq. (9)

$$B_k = \frac{1}{P_K(x_k)} \int_{-1}^{+1} [P_K(x)]^2 \frac{\omega(x)}{(x - x_k) \omega'(x_k)} dx. \tag{20}$$

The Christoffel–Darboux identity is now invoked and writing  $y = x_k$  in Eq. (11) yields

$$\sum_{m=0}^{n-1} \frac{2m + 1}{2} P_m(x) P_m(x_k) = - \frac{n + 1}{2} \frac{P_n(x) P_{n+1}(x_k)}{x - x_k}$$

if  $x_k$  is a root of  $P_n(x)$ . Multiplying through by  $[P_K(x)]^2$  and integrating over the interval  $[-1, 1]$ , noting that [11]

$$\int_{-1}^{+1} P_K(x) P_K(x) P_m(x) dx = \frac{2}{2m + 1} [C(KKm; 000)]^2 \tag{21}$$

where  $C(j_1 j_2 j_3; 000)$  is the Clebsch–Gordan coefficient as defined by Rose [12] leads to the expression

$$\begin{aligned} & \sum_{m=0(2)}^{n-1 \leq 2K} P_m(x_k) [C(KKm; 000)]^2 \\ &= - \frac{n + 1}{2} P_{n+1}(x_k) \int_{-1}^{+1} [P_K(x)]^2 \frac{P_n(x)}{(x - x_k)} dx \end{aligned} \tag{22}$$

where the summation index on the l.h.s. increments by two units in the range 0 to  $2K$  as required by the Clebsch–Gordan coefficient. Comparing Eqs. (22) and (20) it is seen that upon choosing the roots of the polynomial  $\omega(x)$  to be those of  $P_n(x)$ , i.e.

$$P_n(x) = \frac{(2n)!}{2^n (n!)^2} \omega(x) \tag{23}$$

the system of orthogonal polynomials satisfying condition (16) is that of the Legendre polynomials. This is made more obvious by observing that the Legendre polynomials possess an addition theorem [12]

$$P_s(x) P_t(x) = \sum_q P_q(x) [C(stq; 000)]^2 \tag{24}$$

(with  $|s - t| \leq q \leq s + t$ , such that  $s + t + q$  is even) the use of which enables the result of Eq. (21) to be derived.

The existence of a polynomial  $\Pi_n(x) = P_n(x)$  satisfying the orthogonality condition of Eq. (16) and possessing roots  $x_k, k = 1, 2, \dots, n$  which are all real, distinct, and lie on the interval  $[-1, 1]$  ensures the existence of the quadrature formula of Eq. (18).

Combining Eqs. (3), (7) and (18) and remembering that the first term on the r.h.s. of Eq. (7) is zero the required quadrature formula may now be written down:

$$g_K = \int_{-1}^{+1} f(x) P_K(x) dx \tag{25}$$

$$= \sum_{k=1}^n B_k [f(x_k) - S(x_k)]$$

where, using Eq. (22) in Eq. (20) after noting the assumption of Eq. (23), the expression for the quadrature coefficient becomes

$$B_k = - \frac{2}{n + 1} \frac{1}{P_K(x_k) P_{n+1}(x_k) P_n'(x_k)} \sum_{m=0(2)}^{n-1 \leq 2K} P_m(x_k) [C(KKm; 000)]^2. \tag{26}$$

The algebraic degree of precision [9] of the interpolatory quadrature formula of Eq. (25) is  $2n + K - 1$ ; that is, the quadrature formula is exact when  $f(x)$  is a polynomial of degree  $\leq 2n + K - 1$ . The maximum degree of precision of this formula is attained when  $n$  takes its maximum allowable value, namely,  $n = 2K + 1$ .

### III. COMPUTATIONAL FORM

When programming the quadrature formula of Eq. (25) for a computer a more convenient form may be used.

Noting that

$$P_s'(x) = \frac{s}{1 - x^2} [P_{s-1}(x) - xP_s(x)] \tag{27}$$

and also the recurrence relation

$$(s + 1) P_{s+1}(x) = (2s + 1) xP_s(x) - sP_{s-1}(x) \tag{28}$$

then, if  $P_n'(x_k)$  and  $(n+1)P_{n+1}(x_k)$  in the denominator of Eq. (26) are replaced by their equivalents according to Eqs. (27) and (28), Eq. (26) becomes

$$B_k = \frac{2(1-x_k^2)}{P_K(x_k)[nP_{n-1}(x_k)]^2} \sum_{m=0(2)}^{n-1 \leq 2K} P_m(x_k)[C(KKm; 000)]^2. \quad (29)$$

A useful expression for the interpolating polynomial  $S(x)$  is obtained from Eq. (10) using the relation (27):

$$S(x) = \sum_{j=1}^K \frac{P_K(x)}{(x-a_j)} \frac{(1-a_j^2)}{KP_{K-1}(a_j)} f(a_j)$$

Therefore, a form of the quadrature formula of Eq. (25) which is suitable for use on a computer is

$$\begin{aligned} g_K &= \int_{-1}^{+1} f(x) P_K(x) dx \\ &= \sum_{k=1}^n B_k \left[ f(x_k) - \sum_{j=1}^K A_{kj} f(a_j) \right] \end{aligned} \quad (30)$$

where the coefficient  $B_k$  is given by Eq. (29) and the coefficient  $A_{kj}$  by

$$A_{kj} = \frac{P_K(x_k)}{(x_k - a_j)} \frac{(1 - a_j^2)}{KP_{K-1}(a_j)} \quad (31)$$

Also, since  $P_s(-x) = (-1)^s P_s(x)$ , it follows from Eqs. (29) and (31) that

$$B_{n-k+1} = (-1)^K B_k \quad (32)$$

and

$$A_{n-k+1, K-j+1} = A_{kj}. \quad (33)$$

Clearly, both sets of coefficients need to be evaluated once only. There is one proviso regarding the use of Eq. (29). When  $K$  is odd and  $n = 2K + 1$  then  $P_K(x)$  and  $P_n(x)$  have a root in common at  $x = 0$ . Consequently an alternative expression to that of Eq. (17) has to be used [9]. However, calculation showed that the summation of Eq. (29) always gave a value of the order of the limit of accuracy whenever this case arose and therefore the coefficient  $B_k$  was assumed to be zero.

In the above derivations the  $n$  zeros of the Legendre polynomial  $P_n(x)$  are assumed to be labelled according to the usual definition

$$-1 < x_1 < x_2, \dots, x_{n-1} < x_n < 1. \quad (34)$$

They may be obtained by Newton's method, as discussed by Davis and Rabinowitz [13] using the inequality derived by Szegő [14], here written as

$$\cos \left[ \frac{j_{0,n-k+1}}{[(n + 1/2)^2 + (c/4)]} \right] > x_k > \cos \left[ \frac{j_{0,n-k+1}}{n + 1/2} \right], \quad k = 1, 2, \dots, n \quad (35)$$

where  $c = 1 - [2/\pi]^2$  and  $j_{0,i}$  is the  $i$ th zero of the Bessel function  $J_0(x)$ . The values of  $j_{0,i}$  are obtainable from tables [15, 16]. It should be pointed out in this context that the relations (22.16.7) of [17] define  $x_{n-k+1}$  not  $x_k$ .

Standard computer subroutines are available to calculate the Clebsch-Gordan coefficient [18, 19] or the associated  $3 - j$  symbol [20]. Alternatively, an explicit expression for  $[C(KK m; 000)]^2$  may be obtained upon writing  $m = 2s$  and using Eq. (3.32) of Rose [12]:

$$[C(KK 2s; 000)]^2 = \frac{4s + 1}{[2(K + s) + 1]} \frac{[2(K - s)]!}{[2(K + s)]!} \left[ \frac{(K + s)! (2s)!}{(K - s)! (s!)^2} \right]^2$$

A recurrence relation in  $s$  follows from this expression upon taking the ratio of  $[C(KK 2s + 2; 000)]^2$  to  $[C(KK 2s; 000)]^2$ .

The present calculations obtained the zeros of (34) by terminating Newton's method when the correction was less than  $10^{-24}$  and the coefficients of the quadrature (30) were then computed from Eqs. (29) and (31). The zeros and coefficients required to evaluate  $g_K$  for  $K = 1$  to 9 are given in Table I. In this table  $B(k)$  corresponds to the coefficient  $B_{n-k+1}$  and is tabulated for the positive interval  $[0, 1]$  for  $x_k$ . When  $K$  is odd the coefficient  $B_{K+1}$ , which is zero, is omitted from the table. For each  $B(k)$  of the table there is a series of entries  $A(k, j)$ ,  $j = 1, \dots, K$  each entry corresponding to the coefficient  $A_{n-k+1, K-j+1}$ . An extensive table of these coefficients is given in [21].

#### IV. AN EXAMPLE

As an example of the application of the quadrature formula derived above, consider the integral obtained if  $f(x) = e^x$  in Eq. (3)

$$I_K = \int_{-1}^{+1} e^x P_K(x) dx \quad (36)$$

From the Bateman manuscripts [22]

$$\begin{aligned} I_K(y) &= \int_{-1}^{+1} e^{-ixy} P_K(x) dx \\ &= (-1)^K i^K (2\pi)^{1/2} y^{-1/2} J_{K+1/2}(y) \end{aligned}$$



TABLE I

Zeros of  $P_K(x)$  and the coefficients  $A$  and  $B$

K = 1	1 0.0	2 0.92843488366357351734
K = 2	1 0.57735026918962576451	3 0.82720131506976499319
K = 3	1 0.77459666924148337704	4 0.68729290481168547015
2 0.0	5 0.51524863635815409197	
K = 4	1 0.86113631159405257522	6 0.31911236892788976044
2 0.33998104358485626480	7 0.10805494870734366207	
K = 5	1 0.90617984593866399280	K = 15
2 0.53846531010568309104	1 0.98799251802048542849	
3 0.0	2 0.93727339240070590431	
K = 6	1 0.93246951420315202781	3 0.84820658341042721620
2 0.66120538646626451366	4 0.72441773136017004742	
3 0.23861918608319690863	5 0.57097217260853884754	
K = 7	1 0.94910791234275852453	6 0.39415134707756336990
2 0.74153118559939443966	7 0.20119409399743452230	
3 0.40584515137739716691	8 0.0	
4 0.0	K = 16	
K = 8	1 0.96028585649753623168	1 0.98940093459164993260
2 0.79666647741362673959	2 0.94457502307323257608	
3 0.52553240991632898582	3 0.86563120238783174388	
4 0.18343464249564980494	4 0.75540440835500303390	
K = 9	1 0.96816023950762608984	5 0.61787624440264374845
2 0.83603110732663579430	6 0.45801677765722738634	
3 0.61337143270059039731	7 0.28160355077925891323	
4 0.32425342340380892904	8 0.09501250983763744018	
5 0.0	K = 17	
K = 10	1 0.97390652851717172008	1 0.990575475314441733568
2 0.86506336668898451073	2 0.95067552176876776122	
3 0.67940956829902440623	3 0.88023915372698590212	
4 0.43339539412924719080	4 0.78151400389680140693	
5 0.14887433898163121088	5 0.65767115921669076585	
K = 11	1 0.97822865814605699280	6 0.51269053708647696789
2 0.88706259976809529908	7 0.35123176345387631530	
3 0.73015200557404932409	8 0.17848418149584785585	
4 0.51909612920681181593	9 0.0	
5 0.26954315595234497233	K = 18	
6 0.0	1 0.99156516842093094673	
K = 12	2 0.95582394957139775518	
1 0.98156063424671925069	3 0.89260246649755573921	
2 0.90411725637047485668	4 0.80370495897252311568	
3 0.76990267419430468704	5 0.69168704306035320787	
4 0.58731795428661744730	6 0.55977083107394753461	
5 0.36783149899818019375	7 0.41175116146284264604	
6 0.12523340851146891547	8 0.25188622569150550959	
K = 13	9 0.08477501304173530124	
1 0.98418305471858814947	K = 19	
2 0.9175989922297796521	1 0.99240684384358440319	
3 0.80157009073330991279	2 0.96020615213483003085	
4 0.64234933944034022064	3 0.90315590361481790164	
5 0.44849275103644685288	4 0.82271465653714282498	
6 0.23045831595513479407	5 0.72096617733522937862	
7 0.0	6 0.60054530466168102347	
K = 14	7 0.46457074137596094572	
1 0.98628380869681233884	8 0.31656409996362983199	
	9 0.16035664564022537587	
	10 0.0	
	G ( K = 1 )	
	B ( 1 ) = 0.43033148291193520946	
	A ( 1, 1 ) = 1.00000000000000000000	
	G ( K = 2 )	
	B ( 1 ) = 0.17336955879860923364	
	A ( 1, 1 ) = 1.28477476698035188970	
	A ( 1, 2 ) = -0.28477476698035188972	

TABLE I (continued)

B(2) = -0.03114733657638701142	A(3, 3) = -0.29418257656614857828
A(2, 1) = 0.96632810170980230845	A(3, 4) = 0.13086652365008291340
A(2, 2) = 0.03367189829019769155	A(3, 5) = -0.03582467835900840115
B(3) = -0.20444444444444444444	B(4) = C.01077524955290485054
A(3, 1) = 0.50000000000000000000	A(4, 1) = -0.01737511482038365922
A(3, 2) = 0.50000000000000000000	A(4, 2) = 0.98319245719591542711
	A(4, 3) = 0.04747460293018780393
	A(4, 4) = -0.01801076758337027064
	A(4, 5) = 0.00471882227765069882
G(K = 3)	B(5) = C.09073179928244358242
B(1) = 0.09241898582591524077	A(5, 1) = -0.07893273853672301521
A(1, 1) = 1.36331804743588993530	A(5, 2) = 0.52920346553879694739
A(1, 2) = -0.50134304878604899864	A(5, 3) = 0.68312011138334680549
A(1, 3) = 0.13802500135015906331	A(5, 4) = -0.17613175381596981462
B(2) = -0.02599447035394214482	A(5, 5) = 0.04274091543054907696
A(2, 1) = 0.93688007143368560027	
A(2, 2) = 0.08355250130592739349	
A(2, 3) = -0.02043257273961299375	
B(3) = -0.16863545134198199213	G(K = 6)
A(3, 1) = 0.34923049115106657217	B(1) = C.02806731220456762455
A(3, 2) = 0.7254828517242929746	A(1, 1) = 1.41747065773342052820
A(3, 3) = -0.12471334632349586963	A(1, 2) = -0.68394826635595722668
	A(1, 3) = 0.43678766214514242525
	A(1, 4) = -0.26631706116895204432
	A(1, 5) = 0.13425203310204338454
	A(1, 6) = -0.03824502545569706698
G(K = 4)	B(2) = -0.01162810429588537739
B(1) = C.05720512906448278117	A(2, 1) = 0.89743990869885357129
A(1, 1) = 1.39433729542762370200	A(2, 2) = 0.15686336212790823367
A(1, 2) = -0.60170328234829880073	A(2, 3) = -0.08732313059661046092
A(1, 3) = 0.28894240169234350903	A(2, 4) = 0.05127978613617810408
A(1, 4) = -0.0815764147166841028	A(2, 5) = -0.02547307888492878457
B(2) = -0.01964433652856423947	A(2, 6) = C.00721375251859933645
A(2, 1) = 0.91834852361951491508	B(3) = -0.05471766387514606106
A(2, 2) = 0.11772345015438751375	A(3, 1) = C.31827163499857001317
A(2, 3) = -0.04965656596976873566	A(3, 2) = 0.89435688414692018559
A(2, 4) = 0.01358459219586630683	A(3, 3) = -0.32875267752607292760
B(3) = -0.10856600036482904587	A(3, 4) = 0.17792225702347936260
A(3, 1) = 0.35647520497230292239	A(3, 5) = -0.08582225301815821890
A(3, 2) = 0.81828205766790789439	A(3, 6) = 0.02402415437525658514
A(3, 3) = -0.23465659943937775340	B(4) = C.01027546568641815243
A(3, 4) = 0.05989933679916693692	A(4, 1) = -0.02102076640666233690
B(4) = C.00908532876617429857	A(4, 2) = 0.97444139439721368317
A(4, 1) = -0.01148658972542175530	A(4, 3) = 0.06710766927124292135
A(4, 2) = 0.99317289570183591041	A(4, 4) = -0.03075409486419330119
A(4, 3) = 0.02351616312321797579	A(4, 5) = 0.01409833723414115592
A(4, 4) = -0.00520246909954413093	A(4, 6) = -0.00387253963174212235
B(5) = C.12383975812547241119	B(5) = C.06026066439805346734
A(5, 1) = -0.09232659844072882091	A(5, 1) = -0.0717576010720709597
A(5, 2) = 0.59232659844072882091	A(5, 2) = 0.49199760229703751257
A(5, 3) = 0.59232659844072882091	A(5, 3) = 0.73514252927989739902
A(5, 4) = -0.09232659844072882091	A(5, 4) = -0.22454417545922460951
	A(5, 5) = C.09431005948648777793
	A(5, 6) = -0.02514841453212598403
G(K = 5)	B(6) = -0.00392149392568375741
B(1) = C.03883444955593843196	A(6, 1) = 0.00261009445837121162
A(1, 1) = 1.40929647901228558730	A(6, 2) = -0.01281875710262328608
A(1, 2) = -0.65391454642438921595	A(6, 3) = 0.9747188556469087058
A(1, 3) = 0.38033417994800689355	A(6, 4) = 0.01735371762427948473
A(1, 4) = -0.18559940649332461786	A(6, 5) = -0.90619254609053956024
A(1, 5) = C.05388329395712135296	A(6, 6) = 0.30157560554554127938
B(2) = -0.01494468950412721684	B(7) = -0.07267236038464839694
A(2, 1) = 0.90607049735692690917	A(7, 1) = C.03543368918328000190
A(2, 2) = 0.14072627284377832476	A(7, 2) = -0.15058580069668520317
A(2, 3) = -0.071549993551730335994	A(7, 3) = 0.61515211151340520126
A(2, 4) = 0.03441258245624714368	A(7, 4) = 0.61515211151340520126
A(2, 5) = -0.00965935910525201788	
B(3) = -0.37502768326371488070	
A(3, 1) = 0.33302153879533550602	
A(3, 2) = 0.86611919247973856000	

TABLE I (continued)

A( 7, 5) = -0.15058580069668520317  
 A( 7, 6) = 0.03543368918328000190

G ( K = 7 )

B( 1 ) = 0.02122424024946612230  
 A( 1, 1) = 1.42233304349709847510  
 A( 1, 2) = -0.70258290677205722836  
 A( 1, 3) = 0.47342035982259288636  
 A( 1, 4) = -0.31932985950433368549  
 A( 1, 5) = 0.19772777120093266291  
 A( 1, 6) = -0.10011977226845912989  
 A( 1, 7) = 0.02855136402422601935  
 B( 2 ) = -0.00925956286507559473  
 A( 2, 1) = 0.89107535680514417295  
 A( 2, 2) = 0.16867393297246738407  
 A( 2, 3) = -0.09888292822514745778  
 A( 2, 4) = 0.06418196028584161467  
 A( 2, 5) = -0.03912475250771705298  
 A( 2, 6) = 0.01966673685701927233  
 A( 2, 7) = -0.00559030618754793326  
 B( 3 ) = -0.0415787979229446990  
 A( 3, 1) = 0.30816495533952750826  
 A( 3, 2) = 0.91260582589879976161  
 A( 3, 3) = -0.35027065097819548089  
 A( 3, 4) = 0.20911860978719259841  
 A( 3, 5) = -0.12355648691963404875  
 A( 3, 6) = 0.06123814363484917423  
 A( 3, 7) = -0.01730039656253951286  
 B( 4 ) = 0.00920834131314236692  
 A( 4, 1) = -0.02353102676475276602  
 A( 4, 2) = 0.96728547587390995753  
 A( 4, 3) = 0.08270227354047074420  
 A( 4, 4) = -0.04163418683515071042  
 A( 4, 5) = 0.02331022017498750639  
 A( 4, 6) = -0.01129206859538281072  
 A( 4, 7) = 0.00315931260591843905  
 B( 5 ) = 0.05283051788189680589  
 A( 5, 1) = -0.06733844296435779030  
 A( 5, 2) = 0.46741591518451146112  
 A( 5, 3) = 0.76841090585613764098  
 A( 5, 4) = -0.25439586110313136898  
 A( 5, 5) = 0.12989675843154284347  
 A( 5, 6) = -0.06074041384468426791  
 A( 5, 7) = 0.01675113843998148163  
 B( 6 ) = -0.00541269215155540176  
 A( 6, 1) = 0.00419858917669743459  
 A( 6, 2) = -0.02100028261085580045  
 A( 6, 3) = 0.99290437329274493499  
 A( 6, 4) = 0.03372201731744639936  
 A( 6, 5) = -0.01451360031219957517  
 A( 6, 6) = 0.00642351587919436902  
 A( 6, 7) = -0.00173461274293776235  
 B( 7 ) = -0.05827835053610987204  
 A( 7, 1) = 0.03146899419897022379  
 A( 7, 2) = -0.13637570589515180268  
 A( 7, 3) = 0.57308797566764838391  
 A( 7, 4) = 0.66731882810904605490  
 A( 7, 5) = -0.19320507048882344067  
 A( 7, 6) = 0.07816577520872757486  
 A( 7, 7) = -0.02046079680041699411

G ( K = 8 )

B( 1 ) = 0.01660789874996872997  
 A( 1, 1) = 1.42540729732629568690

A( 1, 2) = -0.71482908076187983750  
 A( 1, 3) = 0.49830558968244363064  
 A( 1, 4) = -0.35669370208774844294  
 A( 1, 5) = 0.24522961718707419123  
 A( 1, 6) = -0.15284767079465230459  
 A( 1, 7) = 0.07755625393042198335  
 A( 1, 8) = -0.02212830448195490714  
 B( 2 ) = -0.00752801748235510054  
 A( 2, 1) = 0.88620165390376500184  
 A( 2, 2) = 0.17763572503805655645  
 A( 2, 3) = -0.10757965550401473313  
 A( 2, 4) = 0.07406096905971343791  
 A( 2, 5) = -0.05010324817787766794  
 A( 2, 6) = 0.030982592987819549549  
 A( 2, 7) = -0.01565664207078216136  
 A( 2, 8) = 0.00445860476318461075  
 B( 3 ) = -0.03262319750636844342  
 A( 3, 1) = 0.30081892231597195412  
 A( 3, 2) = 0.92518958321584118765  
 A( 3, 3) = -0.36443019743212451192  
 A( 3, 4) = 0.23047757539066256572  
 A( 3, 5) = -0.1509840844411805126  
 A( 3, 6) = 0.09195366588751272598  
 A( 3, 7) = -0.04610907622392356771  
 A( 3, 8) = 0.01308361129017769741  
 B( 4 ) = 0.00808755127756999034  
 A( 4, 1) = -0.02537979753721420340  
 A( 4, 2) = 0.96147549967839349776  
 A( 4, 3) = 0.09514846227635061826  
 A( 4, 4) = -0.05059499128204320325  
 A( 4, 5) = 0.03135899530942950913  
 A( 4, 6) = -0.01863457546797541071  
 A( 4, 7) = 0.00923134724987616363  
 A( 4, 8) = -0.00260494022703697141  
 B( 5 ) = 0.04193487329118270605  
 A( 5, 1) = -0.06436572852429457908  
 A( 5, 2) = 0.4499611509162127445  
 A( 5, 3) = 0.79128650021011178599  
 A( 5, 4) = -0.27392065703099303667  
 A( 5, 5) = 0.1544332684884289353  
 A( 5, 6) = -0.0883692315078935080  
 A( 5, 7) = 0.04300410838082083383  
 A( 5, 8) = -0.01203877765061982124  
 B( 6 ) = -0.00580168617147591930  
 A( 6, 1) = 0.00528156244158594721  
 A( 6, 2) = -0.02672975845867725958  
 A( 6, 3) = 0.9881820778297931889  
 A( 6, 4) = 0.04788368967552319353  
 A( 6, 5) = -0.02264820687837785558  
 A( 6, 6) = 0.01222291282701305925  
 A( 6, 7) = -0.00579720290872574625  
 A( 6, 8) = 0.00160492547258472452  
 B( 7 ) = -0.04729653073607258670  
 A( 7, 1) = 0.0290133606642748167  
 A( 7, 2) = -0.12737888407475033738  
 A( 7, 3) = 0.54421594131429954388  
 A( 7, 4) = 0.702330583327314441670  
 A( 7, 5) = -0.22041603611497598549  
 A( 7, 6) = 0.10819080493655918576  
 A( 7, 7) = -0.04942857717899208854  
 A( 7, 8) = 0.013473527124117878341  
 B( 8 ) = 0.00208541145853801285  
 A( 8, 1) = -0.00094829032057303659  
 A( 8, 2) = 0.00385077654183427630



writing  $y = \lambda z$ , the multiplication theorem [23] may be applied to the Bessel function  $J_{n+1/2}(y)$ . This theorem states that

$$J_\nu(\lambda z) = \lambda^\nu \sum_{k=0}^{\infty} \frac{J_{\nu+k}(z)}{k!} \left[ \frac{1 - \lambda^2}{2} \cdot z \right]^k$$

given that  $\nu = K + 1/2$ ,  $\lambda = i$  and  $z = 1$  an expression for the integral of Eq. (36) is obtained

$$I_K = 2 \sum_{k=0}^{\infty} \frac{j_{K+k}(1)}{k!}. \quad (37)$$

The Spherical Bessel function

$$j_n(z) = \left[ \frac{\pi}{2z} \right]^{1/2} \cdot J_{n+1/2}(z)$$

may be calculated by a method which is a slight modification of that due to J. C. P. Miller as discussed in [17].

For large orders

$$J_\nu(z) \approx \frac{1}{(2\pi\nu)^{1/2}} \left[ \frac{ez}{2\nu} \right]^\nu$$

or

$$j_n(z) \approx \left[ \frac{e}{2} \right]^{1/2} \frac{(ez)^n}{(2n+1)^{n+1}}. \quad (38)$$

This last equation is used to obtain the first two values of a sequence  $F_{N+1}$  and  $F_N$  and subsequent values down to  $N = 0$  are obtained by downward recurrence using the same recurrence relation as that for  $j_n(z)$

$$F_{N-1}(z) = \frac{2N+1}{z} \cdot F_N(z) - F_{N+1}(z).$$

Then

$$j_n(z) = p \cdot F_n$$

where the normalisation factor  $p = 1/\sqrt{\sigma}$ , with

$$\sigma = \sum_{k=0}^{N+1} (2k+1) F_k^2.$$

Choosing  $N = 69$  the values of  $j_n(1)$  for  $0 \leq n \leq 65$  obtained by this procedure agree to twenty-three significant figures with those of the more elaborate algorithm of Mechel [24].

Table II compares the result of the quadrature (30) when  $f(x) = e^x$  and  $n = 2K + 1$  with the correct value  $I_K$  given by Eq. (37).  $I_K$  is calculated by truncating the summation of (37) when the last term of the series attains a magnitude of  $10^{-24}$  relative to that of the first term. Less than 15 terms are required to achieve this for  $1 \leq K \leq 18$ . Also shown in Table II is the ratio  $g_K/I_K$ . The case  $K = 0$ , for which Gaussian quadrature is applicable, is not shown. All calculations used 26 decimals (double precision arithmetic), and in view of the above discussion, errors of the order of several units in the 23rd figure are to be expected. The algebraic degree of precision of the quadrature formula is  $5K + 1$  which accounts for the sharp improvement of the quadrature over the first few  $K$  values. As  $K$  approaches 18 however, the quality of the agreement deteriorates, the reason being the increasing figure losses in forming the terms in square brackets of Eq. (30). For  $K = 18$  for example, this means that a polynomial of order 17 is a good representation of  $e^x$  for the interval  $-1 \leq x \leq 1$  to a high order of accuracy.

TABLE II  
Quadrature vs correct value<sup>a</sup>

$K$	$I_K$	$g_K$	$g_K/I_K$
1	0.73575888234288464319D+00	0.73536214416085346382D+00	0.99946077690456438410D+00
2	0.14312574025894898419D+00	0.14312562825294747746D+00	0.9999921742936452879D+00
3	0.20130181048139722233D-01	0.20130181036288472460D-01	0.9999999941126958847D+00
4	0.22144729219709285610D-02	0.22144729219703332102D-02	0.9999999999973115460D+00
5	0.19992475040136518371D-03	0.19992475040136516726D-03	0.999999999999591773D+00
6	0.15300667555911540247D-04	0.15300667555911540245D-04	0.99999999999999990D+00
7	0.10160721745151604956D-05	0.10160721745151604955D-05	0.999999999999999988D+00
8	0.59584938184132812696D-07	0.59584938184132812311D-07	0.999999999999999935D+00
9	0.31282253849026797972D-08	0.31282253849026810665D-08	0.10000000000000004058D+01
10	0.1486558709818964822D-09	0.1486558709818983507D-09	0.1000000000000000153835D+01
11	0.64520942828522845732D-11	0.64520942828534830274D-11	0.10000000000000001857466D+01
12	0.25770247629400303916D-12	0.25770247629241370751D-12	0.99999999999383268772D+00
13	0.95323755022085941660D-14	0.95323755014994154872D-14	0.99999999992560315331D+00
14	0.32833773437099667849D-15	0.32833773445179673167D-15	0.100000000002460882339D+01
15	0.10581205449690489847D-16	0.10581204670945520248D-16	0.9999999264030007485D+00
16	0.32036543059149321927D-18	0.32036394799183549617D-18	0.99999937216092577229D+00
17	0.91462461712136115250D-20	0.9146235537186830725D-20	0.99999949296160590138D+00
18	0.24702459901681589390D-21	0.24639750676536672591D-21	0.997461411779423969249D+00

<sup>a</sup> The notation  $D + n$  indicates that the entry is to be multiplied by 10 raised to the power  $+n$ .

ACKNOWLEDGMENTS

The present work found its guidance in V. I. Krylov's book, cited as reference [9]. The author gratefully acknowledges Prof. Dr. F. Beck's encouragement of this research, as well as the sponsorship of the GSI, Darmstadt, which also funded the computations. The latter were performed on the TELEFUNKEN TR-440 at the GMD, Darmstadt, and were much facilitated by the helpfulness of the staff.

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