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Note

Two Series Representations of the Integral $\int_0^\infty \exp[-s(\psi + y \cos \psi - z \sin \psi)]\, d\psi$

Many problems that arise in transport theory for the motion of charged particles involve the calculation of integrals of exponential type. Three independent parameters appear in the integral considered. Two analytic series equivalent to the integral are presented, one of which, involving Bessel functions, is related to a Kapteyn series. Numerical calculations have been performed over a wide range of parameter values and compared with various quadrature routines. The analytic series proved generally more accurate and efficient.

1. Introduction

The integral defined by

$$I(y, z, s) = \int_0^\infty \exp[-s(\psi + y \cos \psi - z \sin \psi)]\, d\psi, \tag{1}$$

where $s > 0$, $y, z \in \mathbb{R}$, has arisen in a recent paper on transport theory for charged particles in electric and magnetic fields [1]. The integral (1) is proportional to the distribution function of test particles that are subject to magnetic and electric fields and suffer loss by collision with particles in a host medium. A simple analytical expansion of (1) is sought in order to ascertain the effect of the magnetic and electric fields on the velocity distribution. For example, when the electric field is absent, parameters y and z are zero. Then

$$I(0, 0, s) = s^{-1}, \tag{2}$$

and the velocity distribution of particles is Maxwellian.

When y only is zero, the integral

$$I(0, z, s) = \int_0^\infty \exp[-s(\psi - z \sin \psi)]\, d\psi \tag{3}$$

can be expressed in two alternative series forms [2]. They are

$$I(0, z, s) = s^{-1} + \sum_{m=1}^{\infty} \frac{z^{2m} s^{2m-1}}{(s^2 + 2^2)(s^2 + 4^2) \cdots (s^2 + 4m^2)} + \sum_{m=1}^{\infty} \frac{z^{2m-1} s^{2m-1}}{(s^2 + 1^2)(s^2 + 3^2) \cdots (s^2 + (2m-1)^2)}, \qquad s > 0, \quad z \in \mathbb{R}, \tag{4}$$

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$$= s^{-1} + 2s \sum_{n=1}^{\infty} J_n(nz)/(n^2+s^2), \qquad s>0, \quad |z|<1. \tag{5}$$

Expression (5) is an example of a *Kapteyn series* $\sum_{n=0}^{\infty} a_n J_n(nz)$ [2] in which J_n is the Bessel function of the first kind of order n and the a_n are constants. In this paper we obtain corresponding series for (1) in which the three parameters y, z, s are non-zero.

2. Series Representations

Analogous to (4) we have, equivalent to (1)

$$I(y,z,s) = s^{-1} + (I(0,r,s) - s^{-1})\,e^{-s\varepsilon} + \sum_{m=1}^{\infty} (-1)^m\, r^m s^m K_m/m!, \tag{6}$$

where

$$r = (y^2+z^2)^{1/2}, \qquad \varepsilon = \tan^{-1}(y/z), \qquad -\pi/2 < \varepsilon < \pi/2, \tag{7}$$

$$K_0 = s^{-1}(1-e^{-s\varepsilon}), \qquad K_1 = (s\sin\varepsilon - \cos\varepsilon + e^{-s\varepsilon})/(s^2+1), \tag{8}$$

and where K_m satisfies the recurrence relation

$$f_m = \sin^{m-1}\varepsilon\ (s\sin\varepsilon - m\cos\varepsilon)/(s^2+m^2) + m(m-1)f_{m-2}/(s^2+m^2), \tag{9}$$

valid for $s>0$, $r \in \mathbb{R}$. We will refer to (6) as the algebraic series. The alternative series representation of (1) analogous to (5) is

$$I(y,z,s) = \Big\{ s^{-1} + 2\sum_{n=1}^{\infty} [\{s\cos(n(\varepsilon - y)) + n\sin(n(\varepsilon - y))\}/(s^2+n^2)]\,J_n(nr) \Big\}\, e^{-sy}, \tag{10}$$

valid for $s>0$, $|r|<1$. We will refer to (10) as the Bessel series.

3. Derivation of the Series

On making the substitutions (7), integral (1) may be transformed, putting $\psi - \varepsilon = \theta$ into

$$I(y,z,s) = e^{-s\varepsilon} \int_{-\varepsilon}^{\infty} e^{-s(\theta - r\sin\theta)}\,d\theta, \tag{11}$$

which is similar in form to (3) except for the non-zero lower limit.

To establish (6) expand (11) in the form

$$I(y, z, s) = e^{-s\varepsilon} \sum_{m=0}^{\infty} \frac{r^m s^m}{m!} \int_{-\varepsilon}^{\infty} e^{-s\theta} \sin^m \theta \, d\theta. \tag{12}$$

Next divide the range of integration from $-\varepsilon$ to 0 and 0 to ∞. For the infinite range we have already [2]

$$\int_0^{\infty} e^{-s\theta} \sin^{2m} \theta \, d\theta = \frac{(2m)!}{s(s^2+2^2)(s^2+4^2)\cdots(s^2+4m^2)}, \tag{13}$$

$$\int_0^{\infty} e^{-s\theta} \sin^{2m-1} \theta \, d\theta = \frac{(2m-1)!}{(s^2+1^2)(s^2+3^2)\cdots(s^2+(2m-1)^2)}, \tag{14}$$

from which, incidentally, (4) may be verified. The contribution to I from the finite range of integration leads directly to the third term in (6).

To establish (10) we utilise a result in [2], namely,

$$(1 - r\cos\theta)^{-1} = 1 + 2 \sum_{n=1}^{\infty} J_n(nr) \cos n\phi, \qquad |r| < 1, \tag{15}$$

where

$$\phi = \theta - r \sin \theta. \tag{16}$$

On multiplying (15) by $e^{-s\phi}$ and integrating with respect to ϕ from a to ∞, we obtain

$$\int_{-\varepsilon}^{\infty} e^{-s(\theta - r\sin\theta)} \, d\theta = s^{-1} e^{s(\varepsilon - y)} + 2 \sum_{n=1}^{\infty} J_n(nr) \int_a^{\infty} e^{-s\phi} \cos n\phi \, d\phi, \tag{17}$$

where

$$a = -\varepsilon + r \sin \varepsilon. \tag{18}$$

Straightforward evaluation of the integral on the right hand side of (17) completes the proof. On setting $y = \varepsilon = a = 0$ in (17) we recover result (5).

4. Comparison of the Series with Numerical Quadrature

It is not necessarily true that series expressions can be evaluated more swiftly and accurately than numerical quadrature. In order to determine the best choice, calculations have been performed both for the series and various equivalent quadrature routines over a wide range of parameter values. All computations were carried out on an ICL 1904S machine at the University of Strathclyde, using ALGOL 68. We consider the simpler problem (3) before the general case (1).

(a) *Two Parameter Problem;* $y = 0$, $10^{-3} < z, s < 10^3$

Subject to the practical restriction $sz < 150$ to prevent overflow, calculations were made over the range given above at all orders of magnitude from 10^{-3} to 10^3 for s and z. The target relative accuracy was 10^{-10}. A measure of efficiency of each calculation is the number of terms in the series, or number of function evaluations of the quadrature routine, needed to reach the target accuracy. This is displayed under the NT columns in Table I for each method used. In any given parameter range the *worst* result is displayed. For example the algebraic series required at most 4 terms over the range $z = 10^{-3}, 10^{-2}, 10^{-1}$, $s = 10^{-3}$, compared with 88 terms at most over the range $z = 1, 10, 10^2$, $s = 1$. Where no entry appears in an NT column the target accuracy was not reached in the permitted number of terms. In this case under the SF column the number of reliable significant figures that agree with at least one other method is shown.

For the algebraic series (4), provided that $z \leqslant 10^{-1}$ the NT value increased only slowly through six orders of magnitude for s. For large z however the NT value rises rapidly as s increases. The Bessel series (5) is limited by the convergence requirement $|z| < 1$. The elegance of the series masks the fact that $J_n(nz)$ needs to be known accurately. The Bessel function satisfies the recurrence relation [3]

$$f_{n+1}(Nz) - (2n/Nz)f_n(Nz) + f_{n-1}(Nz) = 0, \qquad n = 1, 2, \ldots, \tag{19}$$

TABLE I

Comparison of Numerical Methods: Two Parameter Problem

		Series		Quadrature							
		Algebraic	Bessel	Legendre 1		Legendre 2		Laguerre		Patterson	
Integration range →					$[0, 2\pi]$		$[0, e]$		$[0, \infty)$		$[0, e]$
Maximum no. terms →				64		64		48		255	
$z = 10^{\gamma}$	$s = 10^{\delta}$										
range of γ	δ	NT	NT	NT	SF	NT	SF	NT	SF	NT	SF
$[-3, -1]$	-3	4	5	16			4		4		4
$[0, 3]$	-3	9	—	64			1		0		2
$[-3, -1]$	-2	4	6	16			5		3		3
$[0, 3]$	-2	21	—	64			0		0		1
$[-3, -1]$	-1	5	8	16			4		2	255	
$[0, 3]$	-1	87	—		4		0		0		0
$[-3, -1]$	0	6	10	32		64		48		127	
$[0, 2]$	0	88	—		4		0		1		2
$[-3, -1]$	1	8	12	64		32		16		63	
$[0, 1]$	1	87	—	64		64		48		63	
$[-3, -1]$	2	8	12		9	32		8		63	
0	2	61	—	64		64			8		9
$[-3, -1]$	3	8	12		0	64		16		63	

for each fixed N. Three-term homogeneous recurrence relations have been considered in [4] from which we deduce that $J_n(Nz)$ may be computed by backwards recursion when

$$\beta = (Nz/2n)^2 \ll 1, \tag{20}$$

or by recursion in either direction when $\beta \gg 1$. For $n \geqslant N$ and $z \leqslant 1$ (20) is reasonably satisfied so each $J_n(Nz)$ was computed by backwards recursion from a sufficiently large index m. A normalising condition [3, Eq. 9.1.46]

$$1 = J_0(x) + 2J_2(x) + 2J_4(x) + \cdots \tag{21}$$

was used to scale the computed functions correctly. The calculations were repeated by advancing m until successive answers for $J_n(Nz)$ reached the desired accuracy. As a check test values obtained in this way were compared with tabular entries in [3]. For $z \leqslant 10^{-1}$ convergence was rapid and comparable with the algebraic series, seen in Table I. At $z \simeq 1$, however, $J_n(nz) = O(10^{-1})$ for all n and convergence was too slow for practical use, as might have been expected.

Integral (3) contains an integrand of the form $\exp(-sg(\psi))$, where

$$g(\psi) = \psi - z \sin \psi. \tag{22}$$

For $z < 1$ $g(\psi)$ is monotonic increasing from zero; hence the integrand is an exponentially decreasing function of ψ. At $z = 1$, $\delta g/\delta\psi = 0$ when $\psi = 2n\pi$, n integer, and the integrand is non-increasing. For $z > 1$ $g(\psi)$ is stationary when

$$\cos \psi = z^{-1}. \tag{23}$$

In this case there will be intervals of ψ over which the integrand becomes an exponentially *increasing* function, interlaced with exponentially decreasing behaviour. For $z \gg 1$ these oscillations persist until $\psi \simeq z/2\pi$, and will be made sharper by increasing s. We anticipate that numerical quadrature will be least accurate in this range.

Three routines were chosen from the system library [5]. The Gauss–Laguerre rule was suitable for the semi-infinite range of integration whilst the Gauss–Legendre 2 and Patterson interlaced rules used a finite range. After some experimentation the end point $e = z + 30/s$ was used, at which the integrand in (3) is $O(\exp(-30))$. A check was made upon the resulting residual error by repeating the quadrature over $[e, 2e]$. Seen in Table I these rules gave similar results. They are comparable with the algebraic series in the range $z = 10^{-3} - 10^{-1}$, $s = 10^2$, 10^3; everywhere else they are poorer. End point e varied from 3×10^{-2} for large s to 3×10^4 for small s, where the oscillatory nature of the integrand at high z eluded the routines.

Integral (3) may be re-expressed over a finite range. From the definition

$$I_n = \int_{(n-1)\pi}^{n\pi} \exp[-s(\psi - z \sin \psi)]\, d\psi, \tag{24}$$

a straightforward calculation leads to

$$I_{n+2} = e^{-2\pi s} I_n, \tag{25}$$

from which

$$I(0, z, s) = (1 - e^{-2\pi s})^{-1} \int_0^{2\pi} \exp[-s(\psi - z\sin\psi)]\,d\psi. \tag{26}$$

Integral (26) was computed by the Gauss–Legendre method again and denoted by Legendre 1 in Table I. Though the results are clearly superior to the other quadrature results the algebraic series still shows the best overall performance, which should be used at least throughout the displayed parameter range. However, where the product $zs = O(10^2)$ or higher, the required number of terms approaches 100 for high accuracy and its reliability may be questioned.

(b) *Three Parameter Problem;* $10^{-3} \leqslant y, z, s \leqslant 10^3$

The methods of calculation generally follow those in (a), subject to the practical constraint $sr < 150$. In Table II the results are summarised and we see a similar pattern of comparison to that in Table I. The Gauss–Legendre 1 routine remains the most accurate quadrature except for large s. In turn Legendre 1 does not match either the algebraic or Bessel series. For $z \leqslant 10^{-1}$ these series are comparable except for high s where Bessel has the edge. Overall the algebraic series (6) still has the best performance although caution must again be exercised as to the reliability of the results at high NT values.

Integral (1) can be put into an equivalent form

$$I(y, z, s) = (1 - e^{-2\pi s})^{-1} \int_0^{2\pi} \exp[-s(\psi + y\cos\psi - z\sin\psi)]\,d\psi, \tag{27}$$

analogous to (26). No special problems arise with Bessel series (10) but in the algebraic series (6) the K_m terms are obtained from the second order inhomogeneous recurrence relation (9), which raises the question of computational stability. It was necessary to examine the growth rates of the complementary and particular solutions, identify the required quantities K_m, and seek the recursive direction for which the K_m growth rate dominates other unwanted solutions. Stability in a given direction will depend upon the values of parameters s and ε and upon the running integer variable m. The simple stability criterion developed for three-term homogeneous relations [4] may be extended to this case also.

From (6) and (12) we see that

$$K_m = e^{-s\varepsilon} \int_0^{\varepsilon} e^{s\theta} \sin^m\theta\,d\theta, \tag{28}$$

TABLE II

Comparison of Numerical Methods: Three Parameter Problem

			Series			Quadrature							
			Algebraic		Bessel	Legendre 1		Legendre 2		Laguerre		Patterson	
Integration range →							$[0, 2\pi]$		$[0, e]$		$[0, \infty)$		$[0, e]$
Maximum no. terms →			100[a]			64		64		48		255	
$y = 10^{\beta}$ range of β	$z = 10^{\gamma}$ range of γ	$s = 10^{\delta}$ δ	NT[b]	SF	NT	NT	SF	NT	SF	NT	SF	NT	SF
[−3, −1] [0, 3]	[−3, −1]	−3	6 19		9 —	16	6		4 0		4 0		4 1
	[0, 3]		10 20		— —	64	3		1 0		0 0		2 0
[−3, −1] [0, 3]	[−3, −1]	−2	7 22		10 —	16	9		4 0		3 0		3 1
	[0, 3]		54 53		— —		9 9		0 0		0 0		1 0
[−3, −1] [0, 3]	[−3, −1]	−1	9 87		11 —	32	4		4 0		2 0	255	0
	[0, 3]		87		— —		3 1		0 0		0 0		0 0
[−3, −1] [0, 2]	[−3, −1]	0	13 88		11 —	32	2	64	0	48	0	127	0
	[0, 2]		88		— —		4 2		0 0		1 0		2 0
[−3, −1] [0, 1]	[−3, −1]	1	22 87		14 —		9 3	32	0	16	0	63 255	
	[0, 1]		87		— —		4 1		1 0		1 0		8 4
[−3, −1] 0	[−3, −1]	2	59	4	14 —		2 9	64	8	16	9	63	8
	0			3 0	— —		9 0	64	8		9 0	63	8
[−3, −1]	[−3, −1]	3	—		14		0	64			8		9

[a] For K_m and $I(0, r, s)$ separately in (6).
[b] Combined total.

from which, because $0 < \varepsilon < \pi/2$, the forward growth rate satisfies

$$K_m/K_{m-1} < \sin\varepsilon. \tag{29}$$

The corresponding growth rate for the complementary functions c_m of (9), on neglecting 1 compared with m for simplicity, is

$$c_{gf} = |c_m/c_{m-1}| \simeq (m^2/(m^2+s^2))^{1/2}. \tag{30}$$

For the particular solution p_m of (9)

$$p_{gf} = |p_m/p_{m-1}| \simeq \sin\varepsilon, \tag{31}$$

unless $m = m_0$, where the inhomogeneous term vanishes if

$$m_0 = s\tan\varepsilon = sy/z. \tag{32}$$

These results suggest that K_m is to be identified with p_m. From (30), (31) and (32) the ratio of growth rates is

$$\alpha = \frac{p_{gf}}{c_{gf}} \simeq \left[\frac{1+(s/m)^2}{1+(s/m_0)^2}\right]^{1/2}. \tag{33}$$

For a given choice of y, z, s, parameter m_0 is fixed. Then p_m will dominate c_m in forward recursion for $m < m_0$ and in backward recursion for $m > m_0$.

The various regimes of behaviour are shown in Table III. We distinguish between "absolute" and "marginal" stability by reserving "A" to mean that the K_m growth rate is at least an order of magnitude greater than the c_m growth rate in the chosen direction, whilst by "M" we mean that the corresponding ratio lies between 1 and 10.

TABLE III

Numerical Stability of Recursion for K_m

				Parameter example		
range of m_0	range of m	range of α	K_m stability	y	z	s
$m_0 \ll 1$	$[1, \tilde{m}]$	$\alpha \leqslant 10^{-1}$	ASB	10^{-1}	10	10^{-1}
$m_0 < 1$	$[1, \tilde{m}]$	$10^{-1} < \alpha \leqslant 1$	MSB	1	1	10^{-1}
	$[m_0, \tilde{m}]$	$\alpha \leqslant 1$	MSB			
$1 < m_0 < \tilde{m}$				10	1	1
	$[1, m_0]$	$1 < \alpha$	MSF			
$\tilde{m} < m_0$	$[1, \tilde{m}]$	$1 < \alpha \leqslant 10$	MSF	10	10^{-1}	10
$\tilde{m} \ll m_0$	$[1, \tilde{m}]$	$\alpha \leqslant 10$	ASF	10^{-1}	10^{-1}	10^3

Key: $\tilde{m} \equiv$ limit of recursion, generally 100; $S \equiv$ stable; $B \equiv$ backwards; $F \equiv$ forwards; $M \equiv$ marginally; $A \equiv$ absolutely.

In full forward recursion from m equals 2 to the maximum desired value $\tilde{m}$, usually 100 in the computations, initial conditions (8) determine subsequent K_m. In full backward recursion from $\tilde{m}-2$ to zero, the starting values $\tilde{m}$, $\tilde{m}-1$ for K_m were obtained from (9) in the form

$$K_m \simeq \sin^{m+1} \varepsilon[(m+2)\cos\varepsilon - s\sin\varepsilon]/(m+2)(m+1). \tag{34}$$

These provisional K_m were normalised finally by the known K_0 and K_1. It is not sufficient to give *arbitrary* starting values because the problem is not linear due to the inhomogeneous term. For the intermediate case $1 < m_0 < \tilde{m}$, K_m is stable when computed *towards* m_0 from below *and* above. Backwards and forwards recursions were matched at m_0, $m_0 - 1$ to give the overall result.

Examples of y, z, s parameter values suitable for each category are given in Table III. The practical restrictions $\varepsilon s, rs < 150$ imply that category ASF is encountered only when $\tilde{m}$ is smaller than 100.

5. Conclusion

The algebraic and Bessel series proved superior to standard quadrature routines over most of the parameter range $10^{-3} \leqslant y, z, s \leqslant 10^3$ that was investigated. Though the two series were comparable in the range $z \leqslant 10^{-1}$, the wider validity of the algebraic series gives it a clear advantage both in the two-parameter form (4) to represent (3) and in the three-parameter form (6) to represent (1).

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R. J. Cole*
Laboratorio di Ingegneria Nucleare dell' Universitá
Bologna, Italy

* Present address: Department of Mathematics, University of Strathclyde, Glasgow, Scotland.