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Accurate Evaluation of an Integral Involving the Product of Two Bessel Functions and a Gaussian

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The integral to be evaluated is of the form

$$G(L) = \int_0^R K_1 K_2 r^2 j_L(K_1 r)\, j_L(K_2 r)\, e^{-r^2/a^2}\, dr,$$

where R and a are real, and the wave numbers K_1 and K_2 can be complex. The js are spherical Bessel functions. Our method makes use of a recursion relation between $G(L)$, $G(L+1)$, and $G(L-1)$, together with the values of G for $L=0$ and $L=-1$. The latter are expressed in terms of error integrals of complex argument and are evaluated numerically with high accuracy by means of a continued fraction. Four methods are presented for calculating G at integer values of L. One consists of solving analytically the inhomogeneous finite difference recursion equation in terms of sums from 0 to L and from $L+1$ to ∞ of quantities which involve the two linearly independent spherical Bessel functions of argument $z_3 = (K_1 a)(K_2 a)/2i$. The other three methods consist in numerically evaluating the recursion relation, either upwards in L, starting with the known values $G(0)$ and $G(-1)$, or downwards in L, either starting with two G values taken equal to zero, or following a method described by Olver. The method of Olver is found to be the one generally most useful, in that it gives a reliable estimate of the truncation error. Accuracies of twelve significant digits are usually achieved, on a computer (IBM 3081) using 16 bit words, as is demonstrated from the comparison of the four methods in numerical examples. The computing time is much less than the methods involving radial mesh sums, by factors of 5 or more, depending on the values of $K_1 R$ and $K_2 R$.

I. INTRODUCTION

The integral examined in the present study is of the form

$$G(L) = \int_0^R f_1(r)\, V(r)\, f_2(r)\, dr, \tag{1.1}$$

where

$$f_i(r) = K_i r j_L(K_i r), \qquad i = 1, 2 \tag{1.2}$$

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and

$$V(r) = \exp(-r^2/a^2).$$

For the case that the limit of integration R is infinite the result for G is known analytically, and the value of the integral is easily computed. For finite values of R a good method for evaluating G does not seem to exist in the literature. Integrals for finite values of R of the type of (1.1) do occur frequently in the solution of scattering problems. For example, in the Kapur Peierls method [1], where the f_i's are Gamow states, or in other methods where the f's are chosen arbitrarily [2], and in still other cases [3, 4] where the f's are spherical Bessel functions of real wave numbers K_i such that the f's vanish at R.

What motivated the present investigation was the formulation of scattering theory in terms of a basis of Sturmian functions [5] (of positive energy). This method avoids the need of the $i\varepsilon$ in the Green's functions since it incorporates the scattering boundary conditions ab initio, leads to a rapidly converging expansion [6] for the scattering T-matrix, and also provides a separable representations of the T operator and of the nonlocalities in the optical potential [6]. A particularly simple set of Sturmian functions are Bessel functions of the type (1.2), in which the K_i's are complex such that the f_i's have the same outgoing wave boundary condition as the scattered wave at the matching radius R. Beyond this distance only Coulomb potentials are assumed to be present, and if the logarithmic derivative of the f_i's is set equal to that of the outgoing physical Coulomb wave, then Coulomb potentials can be included in the scattering problem without loss of the good convergence properties.

The coefficients of the expansion of the scattering wave in terms of a set of basis functions f_i (such as the Sturmians) are obtained by solving a set of algeraic equations, which involve matrix elements of the type of Eq. (1.1). Since the f's can be strongly oscillatory, and since there may be many such matrix elements, the evaluation of the integrals by a numerical summation over a radial mesh in the interval from 0 to R may not be very practical or accurate. Hence the desirability for an alternative method to evaluate integrals of this type. One such method is given in the present study. It consists of deriving an inhomogeneous three term recursion relation between the G's, and showing how the solution to these equations can be obtained with high accuracy.

A Bessel function basis of the type (1.2) is useful because the L-behaviour of these functions is similar to that of the physical scattering functions being expanded. In addition the Bessel functions, being closely related to plane waves, facilitate the transformation from one center of mass to another [4]. Such a transformation occurs in the description of rearrangement reactions, and hence the use of the Sturmian–Bessel basis can simplify the evaluation of the complicated six dimensional integrals enormously [7]. An alternate set of Sturmian basis functions can also be constructed with Chebyshev polynomials [8] rather than Bessel functions. The advantage of these polynomials is that the potential in the matrix elements

(1.1) can be of a general form, provided it is easily expandable in powers of r. In this case the matrix elements can be evaluated rapidly and accurately, without the need of methods of the type developed in the present paper. So far the Chebyshev–Sturmian method has been used only in the evaluation of Sturmian eigenfunctions and eigenvalues for a Woods–Saxon-like nonhermitian potential [8].

Methods to evaluate integrals of the type of Eq. (1.1) by means of recursion relations have been developed by many authors. One of the oldest [9] involves Coulomb functions and was later generalized by Baur *et al.* [10] and by Raynal [11]. For the relativistic Coulomb case Wright and co-workers [12] have described a method which was developed further by Rost [13]. Other methods involving matrix series were given by Onley and collaborators [14]. A recursion for integrals of the type (1.1) in which the potential is of the form $r^a \exp(br)$ has recently been developed by Hirschorn [15], using a matrix recursion technique developed by Wright and collaborators [16]. This method, in which the values L of the two Bessel functions need not be assumed to be equal, would be suitable for generalizing the results developed in the present paper to potentials other than those of Gaussian form.

Numerical solutions to the recurrence relation will be obtained by means of four different methods, between which comparisons are made. Since the recursion relation has three terms, two values of the solution have to be prescribed so as to render it unique. In the method given by Olver [17] the two input values are for $L=0$ and $L=L_{\mathrm{MAX}}$. The value at $L=0$ can be calculated by noting that the integral $G(0)$ can be related to a combination of error functions of complex argument. The latter can be evaluated in terms of a rapidly converging continuous fraction, or by a method given by Gautschi [18]. At L_{MAX} the value of G is set equal to zero. This last condition introduces an error which can be accurately estimated in Olver's method, and thus a suitable value of L_{MAX} can be obtained. A second method makes use of an exact analytical solution of the recurrence relation which is given in the present study. It involves sums over Bessel-related functions which, however, are not as easily evaluated as the recursion relation itself. It gives the most accurate results, and is used for comparison purposes. A third method consists in evaluating the recursion relation downward in L, starting from L_{MAX} and setting both $G(L_{\mathrm{MAX}})$ and $G(L_{\mathrm{MAX}}+1)$ equal to zero. This method is similar to the procedure given by Miller [19]. This method is simpler than Olver's, but has the disadvatage that the truncation error is not known in advance. An advantage is that it can provide an independent check on the error function method for $L=0$. A fourth method consists in carrying the recursion relation upwards in L, starting with the values of G at $L=-1$ and $L=0$, which are known since both $G(-1)$ and $G(0)$ can be obtained from a combination of error functions. This method becomes unstable when $G(L)$ starts to decrease with increasing L. This occurs whenever the turning points for either one of the two Bessel functions in the integrand of (1.1) are less than the upper limit of integration R, i.e., for L larger than either $K_1 R$ or $K_2 R$. For values of L smaller than the above values, the upward recursion method is the fastest and most accurate.

In Section 2 the recurrence formula is derived; in Section 3 the evaluation of $G(0)$ and $G(-1)$ is described in terms of error functions and their continued fraction expressions. In Section 4 the analytic solution is presented; in Section 5 numerical applications of the various methods are made and the numerical accuracy achieved is examined.

2. The Recurrence Relations

The integral to be evaluated is

$$G(L, K_1, K_2, R, a) = \int_0^R f_L(K_1 r) \exp(-r^2/a^2) f_L(K_2 r)\, dr, \tag{2.1}$$

where

$$f_L(z) = z j_L(z). \tag{2.2}$$

The j's are spherical Bessel functions, [20], the K's are real or complex, and R and a are real.

The gaussian form of the potential was dictated by the simplicity of the corresponding recursion relation which is

$$G(L-1) - [(4L+2)/(K_1 a K_2 a)]\, G(L) - G(L+1) = X(L) \exp(-R^2/a^2), \tag{2.3a}$$

where

$$X(L) = (2L+1)\, R j_L(K_1 R)\, j_L(K_2 r). \tag{2.3b}$$

This result follows from the recursion relation between products of spherical Bessel functions

$$\begin{aligned} &f_{L-1}(z_1) f_{L-1}(z_2) - f_{L+1}(z_1) f_{L+1}(z_2) \\ &\quad = [(2L+1)/K_1 K_2]\, d/dr[f_L(z_1) f_L(z_2)/r], \end{aligned} \tag{2.4}$$

where z_1 and z_2 are complex arguments. Multiplying both sides of Eq. (2.4) with a general potential $V(r)$, integrating over r from 0 to R, and integrating by parts the right hand side of the equation, one obtains

$$\begin{aligned} G(L-1) - G(L+1) = {} & [(2L+1)/(K_1 K_2 r)]\, V(r) f_L(K_1 r) f_L(K_2 r)\big|_0^R \\ & - [(2L+1)/K_1 K_2] \int_0^R f_L(K_1 r) f_L(K_2 r) \left(\frac{1}{r}\frac{dV}{dr}\right) dr. \end{aligned} \tag{2.5}$$

The only from which V can have so that the expression $r^{-1}\,dV/dr$ in the integral is proportional to V itself, is for a gaussian radial dependence $\exp(\lambda r^2)$. For the present application it is chosen to be of the form

$$V(r) = \exp(-r^2/a^2) \tag{2.6}$$

and as a result one obtains Eq. (2.3) which is the basic recurrence relation used in the numerical applications in Section 5.

The homogeneous part of the recurrence relation (2.3) (obtained by setting the right-hand side equal to zero) is satisfied by the two linearly independent Bessel functions of the type [20]

$$\bar{f}_L(z_3) = i^{L+1} z_3\, j_L(z_3), \tag{2.7}$$

$$\bar{q}_L(z_3) = i^{L+1} z_3 [\, y_L(z_3) + i j_L(z_3)], \tag{2.8}$$

where

$$z_3 = K_1 a K_2 a/2i. \tag{2.9}$$

Through this observation one can obtain an anlytical expression for $G(L)$ in terms of $\bar{f}_L$ and $\bar{q}_L$, as is discussed in Section 4.

For the case that the two L-values of the Bessel functions in the integral are not the same, a general expression to evaluate such an integral has not been found. However, the particular integral

$$G_n(L, K_1, K_2, R, a) = \int_0^R f_L(K_1 r)\, r^n \exp(-r^2/a^2)\, f_{L-n}(K_2 r)\, dr \tag{2.10}$$

can be evaluated by relating these G_n's to the integral G described above (i.e., the case when $n = 0$). The desired relations are obtained by starting from the recursion relation

$$\begin{aligned} r^{n-m-1}[K_1 f_{n-1}(z_1)\, f_m(z_2) - K_2 f_n(z_1)\, f_m(z_2)] \\ = d/dr[r^{n-m-1} f_n(z_1)\, f_m(z_2)]. \end{aligned} \tag{2.11}$$

When n is set equal to m, this expression does not reduce to Eq. (2.4), unless, in addition, the relation

$$z(f_{n+1} + f_{n-1}) = (2n+1) f_n \tag{2.12}$$

is used.

Multiplying both sides of Eq. (2.1) by the gaussian potential of Eq. (2.6), integrating over r from 0 to R, again doing an integration by parts, then setting $m = n - 1$ and finally denoting n as L, one obtains

$$\begin{aligned} (2/a^2)\, G_1(L) = & -f_L(K_1 R)\, f_{L-1}(K_2 R) \exp(-R^2/a^2) \\ & + K_1 G(L-1) - K_2 G(L). \end{aligned} \tag{2.13}$$

Repeating the same procedure but setting $m = n - 2$, one obtains

$$(2/a^2)\, G_2(L) = -f_L(K_1 R)\, f_{L-2}(K_2 R)\, R \exp(-R^2/a^2) + K_1 G_1(L-1) - K_2 G_1(L) \tag{2.14}$$

and so forth. The above results show that the basic quantities needed for the evaluation of the G_n's are the G's, which are obtained numerically in Section 5. Setting $n = m = L$ does not appear to yield a useful result. In the next section the case $L = 0$ and $L = -1$ will be discussed.

3. Expressions for $G(0)$ and $G(-1)$ in Terms of Continued Fractions

For the case that L is 0 or -1 the functions $f_L(z)$ are equal to $\sin z$ or $\cos z$, respectively, and the G's have the form

$$G(0) = \int_0^R \sin(K_1 r) \exp(-r^2/a^2) \sin(K_2 r)\, dr,$$

$$G(-1) = \int_0^R \cos(K_1 r) \exp(-r^2/a^2) \cos(K_2 r)\, dr.$$

By expressing the product of the two sines or the two cosines in terms of a sum of two cosines, one obtains

$$G(-1) \pm G(0) = I(K_\mp, R, a), \tag{3.1}$$

where

$$K_\mp = K_1 \mp K_2 \tag{3.2}$$

and where

$$I(K, R, a) = \int_0^R \cos(Kr) \exp(-r^2/a^2)\, dr. \tag{3.3}$$

By making further use of the definition of the error function $\operatorname{erf}(z)$, given by Eq. (7.1.1) in [20], one finds

$$I(K, R, a) = (a\pi^{1/2}/4) \exp[-(aK/2)^2] \times [\operatorname{erf}(R/a - iaK/2) + \operatorname{erf}(R/a + iaK/2)]. \tag{3.4}$$

This result is equivalent to Eq. (3.322) in Ref. [21]. If the argument z of the error

function is in absolute value smaller than 2 or 3, the series expansion given by Eq. (7.1.5) of [20],

$$(\pi^{1/2}/2)\,\mathrm{erf}(z) = z \sum_{n=0}^{\infty} (-z^2)^n/[n!(2n+1)] \tag{3.5}$$

is useful since it converges rapidly with good accuracy. Otherwise one can make use of the connection of the erf(z) with erf $c(z)$ (their sum is unity) and express erf $c(z)$ in terms of the continued fraction

$$C(z) = \frac{1}{z+}\,\frac{1/2}{z+}\,\frac{1}{z+}\,\frac{3/2}{z+}\,\frac{2}{z+}\cdots \tag{3.6}$$

as given by Eq. (7.1.14) of [20]. The requirement for the validity of this connection is that the real part of z be positive, which requires

$$2(R/a)^2 > |\mathrm{Im}(K_1 \pm K_2)R|. \tag{3.7}$$

The connection is

$$\exp(z^2)\,\mathrm{erf}(z) = \exp(z^2) - \pi^{-1/2} C(z). \tag{3.8}$$

The final expression, which is convenient for numerical evaluation, is obtained by combining Eqs. (3.4) and (3.8). The result is

$$\begin{aligned} I(K, R, a) = {} & (a/2)\,\pi^{1/2} \exp(-aK^2/4) \\ & - (a/4) \exp(-R^2/a^2)[\exp(iKR)\, C(R/a - iaK/2) \\ & + \exp(-iKR)\, C(R/a + iaK/2)]. \end{aligned} \tag{3.9}$$

Inserting Eq. (3.9) into (3.1) and solving for the G's one obtains

$$G(-1) = N\cos(z_3) - (a/4)\exp(-R^2/a^2)(u_- + u_+)/2, \tag{3.10a}$$

$$G(0) = iN\sin(z_3) - (a/4)\exp(-R^2/a^2)(u_- - u_+)/2, \tag{3.10b}$$

where z_3 is defined in Eq. (2.9), where

$$N = (a/2)\,\pi^{1/2} \exp[-a^2(K_1^2 + K_2^2)/4] \tag{3.11}$$

and where

$$\begin{aligned} u_\pm = {} & \exp(iK_\pm R)\, C(R/a - iaK_\pm/2) \\ & + \exp(-iK_\pm R)\, C(R/a + iaK_\pm/2). \end{aligned} \tag{3.12}$$

These are the results needed in Sections 4 and 5.

4. Analytic Expression for $G(L)$

The basic idea for obtaining an analytical expression for $G(L)$ is to treat the recurrence relation (2.3) as a second order finite difference equation in L, where the $X(L)$ is the inhomogeneous driving term. The two independent solutions of the homogeneous parts of the difference equations are the functions $\bar{f}_L(z_3)$ and $\bar{q}_L(z_3)$, defined in Eqs. (2.7)–(2.9), and the effect of the inhomogeneous term is taken into account by the method of variation of parameters [22].

The first step consists in separating $G(L)$ into a part $\bar{G}(L)$ which is the solution of the homogeneous recurrence relation, plus a remainder which takes into account the effect of the inhomogeneous term

$$G(L, K_1, K_2, R, a) = \bar{G}(L, K_1, K_2, a) + \exp(-R^2/a^2)\, \mathcal{G}(L, K_1, K_2, R, a). \tag{4.1}$$

Both G and $\bar{G}$ go to zero as L tends to infinity because the f's in the respective integrands become very small in the radial region where $\exp(-r^2/a^2)$ is significant. Since $\bar{G}(L)$ is the solution of the homogeneous recursion equation (Eq. (2.3a) with $X(L)=0$), it is of the form $A\bar{f}_L + B\bar{q}_L$. However, B must vanish because $\bar{G}$ goes to zero as L goes to infinity, while $\bar{q}_L$ goes to infinity. By matching $\bar{G}(0)$ to the limit of $G(0)$ as $R \to \infty$, we find that $A = N$, with N given by Eq. (3.11). Thus, the result for $\bar{G}$ is the well-known expression

$$\bar{G}(L, K_1, K_2, a) \equiv \int_0^\infty f_L(K_1 r)\, e^{-r^2/a^2} f_L(K_2 r)\, dr = (a/2)\, \pi^{1/2}\, e^{-a^2(K_1^2 + K_2^2)/4}\, i^{L+1} f_L(K_1 a K_2 a/2i). \tag{4.2}$$

An analytical expression for $\mathcal{G}(L)$ will now be derived from the recursion relation which it obeys. The recurrence relation for $\mathcal{G}(L)$ is obtained by inserting Eq. (4.1) into (2.3) and cancelling the gaussian on both sides. The result is

$$\mathcal{G}(L-1) + i[(2L+1)/z_3]\, \mathcal{G}(L) - \mathcal{G}(L+1) = X(L), \tag{4.3}$$

where z_3 and X are defined in Eq. (2.9), and (2.3b), respectively. The values of $\mathcal{G}(-1)$ and $\mathcal{G}(0)$ are obtained from the coefficients of $\exp(-R^2/a^2)$ in Eqs. (3.10). The result is

$$\mathcal{G}(-1) = -(a/4)(u_- + u_+)/2, \tag{4.4a}$$

$$\mathcal{G}(0) = -(a/4)(u_- - u_+)/2, \tag{4.4b}$$

where the u's are known from Eq. (3.12).

The solution of the inhomogeneous difference Eq. (4.3) by the method of variation of parameters [22] (or oscullating parameters, as it is also called), con-

sists in expanding $\mathcal{G}$ in terms of the two linearly independent solutions of the homogeneous equations, $\bar{f}$ and $\bar{q}$.

$$\mathcal{G}(L) = A_L \bar{f}_L(z_3) + B_L \bar{q}_L(z_3). \tag{4.5}$$

Inserting Eq. (4.5) into Eq. (4.3), making use of the homogeneous recursion relation satisfied by the $\bar{f}$'s and $\bar{q}$'s and further imposing the oscullating condition on the coefficients A and B,

$$(A_L - A_{L+1})\bar{f}_{L+1} + (B_L - B_{L+1})\bar{q}_{L+1} = 0 \tag{4.6}$$

one obtains the result

$$(A_{L-1} - A_L)\bar{f}_{L-1} + (B_{L-1} - B_L)\bar{q}_{L-1} = X(L). \tag{4.7}$$

The general solution of Eqs. (4.6) and (4.7) is

$$A_L = A_0 - \sum_{l=1}^{L} X_l \bar{q}_l / \bar{d}_l, \tag{4.8a}$$

$$B_L = B_0 + \sum_{l=1}^{L} X_l \bar{f}_l / \bar{d}_l \tag{4.8b}$$

with

$$\bar{d}_l = \bar{q}_l(z_3)\,\bar{f}_{l-1}(z_3) - \bar{f}_l(z_3)\,\bar{q}_{l-1}(z_3) = i(-)^{l+1}. \tag{4.9}$$

The quantities A_0 and B_0 are still arbitrary constants which express the fact that one can add to the solution of the inhomogeneous equation an arbitrary amount of solutions of the homogeneous equation. (For $L = 0$ the sums in the two expressions above are to be set to zero.)

The constants A_0 and B_0 are determined from the boundary conditions as follows. For large values of L the quantity $\mathcal{G}_L$ should become very small since both G and $\bar{G}$ become small. Since $\bar{q}_L$ increases with L, the coefficient B_L has to decrease with L faster than $\bar{q}_L$ increases. This can be accomplished by setting B_0 equal to the negative of the sum S,

$$-B_0 \equiv S = \sum_{l=1}^{\infty} X_l \bar{f}_l / \bar{d}_l. \tag{4.10}$$

On the other hand, A_0 and B_0 can both be evaluated in terms of $\mathcal{G}_0$ and $\mathcal{G}_{-1}$, given by Eq. (4.4), and by taking into account Eq. (4.7). Making explicit use of the functions $\bar{f}$ and $\bar{q}$ listed in Table I, one obtains the result

$$A_0 = (\mathcal{G}_{-1} - X_0 + \mathcal{G}_0)\exp(iz_3), \tag{4.11}$$

$$B_0 = (\mathcal{G}_{-1} - X_0)\sin(z_3) + i\mathcal{G}_0 \cos(z_3). \tag{4.12}$$

TABLE I

Functions $\bar{f}_L, \bar{q}_L$[a]

L	$\bar{f}_L(z)$	$\bar{q}_L(z)$
-1	$\cos(z)$	$i\exp(-iz)$
0	$i\sin(z)$	$-i\exp(-iz)$
1	$\cos(z)-\sin(z)/z$	$(i+1/z)\exp(-iz)$

[a] Defined by Eqs. (2.7) and (2.8), respectively. They obey $y_{L-1}-y_{L+1}+iy_L(2L+1)/z=0$, where $y\equiv\bar{f}$ or $\bar{q}$.

Since S has to be the negative of B_0, the result (4.11) implies the existence of an identity between error integrals and sums over Bessel functions

$$(\mathscr{G}_{-1}-X_0)\sin(z_3)+i\mathscr{G}_0\cos(z_3)=-S. \tag{4.13}$$

The validity of this identity is confirmed by numerical calculation, as is discussed in Section 5. By combining the results of Eqs. (4.2), (4.10)–(4.13), one obtains the final answer.

$$\begin{aligned} G(L)=\Bigg\{&\frac{a}{2}\pi^{1/2}\exp[-a^2(K_1^2+K_2^2)/4] \\ &+(\mathscr{G}_{-1}-X_0+\mathscr{G}_0)\exp(-iz_3-R^2/a^2)\Bigg\}\bar{f}_L(z_3) \\ &-e^{-R^2/a^2}\Bigg\{\bar{f}_L(z_3)\Bigg[\sum_{l=1}^{L}X_l\bar{q}_l(z_3)/\bar{d}_l\Bigg] \\ &+\bar{q}_L(z_3)\Bigg[\sum_{l=L+1}^{\infty}X_l\bar{f}_l(z_3)/\bar{d}_l\Bigg]\Bigg\}. \end{aligned} \tag{4.14}$$

In the above, X_L is defined in Eq. (4.5); the u's needed in the definition of the $\mathscr{G}$'s according to Eqs. (4.4) are given in Eq. (3.12); the $\bar{q}$'s, $\bar{f}$'s, and $\bar{d}$'s are defined in Eqs. (2.7), (2.8), and (4.11), respectively; z_3 is given by Eq. (2.9). When $L=0$ the sum from $l=1$ to L is replaced by zero and the sum form $L+1$ to ∞ is replaced by $-B_0$, given by Eq. (4.12). Combining the various terms one regains Eq. (3.10b).

5. Numerical Accuracy

In this section the various methods for evaluating the recursion relation (2.3) will be applied to numerical examples. In particular, it will be shown that Olver's method is very well suited because it gives a very reliable estimate of the truncation error, and it works well under general conditions.

In Olver's method [17] the solutions $G(L)$ of Eq. (2.3) are calculated for a range of L's between 0 and an upper value P, so that $G(0)$ is equal to a known value. For this purpose a value of L larger than P is chosen, denoted as N, at which $G(N)$ is set equal to zero. A method is given for choosing N so that the values of G in the interval from $L=0$ to $L=P$ have a truncation error which is smaller than a prescribed value. Further details are given in the Appendix 2.

The value $G(0)$ needed as input for Olver's method is calculated by expressing it as a combination of complex error functions, and evaluating each error function by a continued fraction, as is described in Section 3. The evaluation of the continued fraction $C(z)$ is carried out by means of a method developed by Steed [23] and applied by Barnett *et al.* [24] and also by Rawitscher and Rasmussen [25]. This method employs a recursion technique involving powers of z^{-2} which is terminated when an accuracy parameter ε_c has been satisfied, as is described further in Appendix 1. It has been verified in previous applications of the method [25], that the accuracy delivered by the algorithm is indeed better than what is prescribed by the parameter ε_0. A value of 10^{-13} is assigned to this parameter in the present application. All calculations are carried out in double precision on an IBM 3081, which carries between 16 and 17 significant decimal figures in each step of the calculation.

The Bessel functions provide an important input into the calculation and it is their accuracy which ultimately limits the accuracy of the final result as will be shown. Bessel functions are needed for the evaluation of the inhomogeneous terms $X(L)$, as well as for the analytic solution. The former requires $j_L(KR)$ and the latter $j_L(z_3)$ and $y_L(z_3)$, where $z_3 = K_1 a K_2 a/(2i)$. Two methods are used for evaluating the Bessel functions, depending on how large the argument is compared to L. When $|z| < L$, the expansion of $j_L(z)$ in polynomials of $(1/z)$ times $\exp(\pm iz)$ is employed, following Eq. (10.1.10) of [20]. When $|z| > L$, then j_L is calculated from a downward recursion relation which is started at a value of L_{MAX}, which can be as large as 160. What dictates the choice of L_{MAX} are the overflow–underflow problems of the computer, as well as the requires accuracy criteria. The method for determining the latter is verfied by a procedure given by W. Kahan, as described on p. 52 of a paper by Gautschi [18].

The variable z_3 is mainly imaginary when the values of K are mainly real, as is the case in the present numerical examples. The corresponding Bessel functions are proportional to $\exp\{\pm \mathrm{Im}(z_3)\}$ which can become very large for large values of K_1 and K_2, and hence can produce underflow and overflow errors. This happens for the IBM 3081 machine when $|\mathrm{Im}(z_3)| > 174.6$. In this case, to prevent the overflows from occurring the anlytic calculation is bypassed when

$$|\mathrm{Im}(K_1 a K_2 a/2i)| > 150. \tag{5.1}$$

The numerical sample calculations are performed for values of K_1, K_2, a, and R which occur in the Sturmian treatment [5, 6] of 21.6 MeV deuterons scattering from a nickel target in the presence of Coulomb potentials. The values of K depend

on the value of L and R, the present choice corresponding to a value of $L=9$ and $R=12$ fm. This means that the turning point of the corresponding Bessel functions occurs at a value of r less than R, i.e., the recursion relation (2.3) can be solved in the upward direction as long as L stays below 9. However, to test the method, values of L as high as 20 are included in the calculation. The values of KR actually used are listed in Table II, and also, for comparison purposes, what would have been the values of KR for $L=0$ and $R=12$ fm. The values of the parameters a and R, and the various combinations which describe the numerical cases, are listed in Table III.

The procedure used to determine the accuracy achieved in the calculation will be described in what follows. One set of values of G, denoted as G_D, is obtained by solving the recursion relations downward in L, starting with two consecutive values where G is set to zero. The value of L for which $G(L)$ and $G(L+1)$ are set to zero, which is denoted as L_D, is chosen as large as possible so as to prevent under- and overflow errors. The result for $L=0$ ($G_D(0)$) is compared with the value $G_A(0)$ obtained by means of the continued fraction expression and the ratio $G_A(0)/G_D(0)$ is printed out. The deviation from unity is listed in Table IV in the columns A–D in the row for $L=0$. In all cases the agreement was good to seven significant figures or better. The values of G_D for values of L larger than zero are renormalized by this ratio, so as to increase their accuracy, and are then compared with the other methods in Table IV. The analytic expression was also evaluated for values of L [illegible] L_A. The result is indicated with the letter A, and the comparison of the number of significant figures for which agreement with other methods is obtained (regardless of the power of 10 by which the answer is multiplied) is listed in Table IV. The corresponding values of L_A and L_D are listed in Table V.

TABLE II

Sturmian Values of K_iR[a]

	$L=0$		$L=9$	
i	Real	Imaginary	Real	Imaginary
1	3.1269	−0.2066	13.4879	−1.3634
2	6.2480	−0.4314	16.5087	−1.4543
3	9.3491	−0.7043	19.7885	−0.9653
13	39.2762	−0.4124	52.5570	−0.2428
24	73.8287	−0.1920	87.4540	−0.1411
First zero	3.1416		13.9158	

[a] These values of K_iR are obtained by matching the Sturmian–Bessel functions $f_i(r)$, defined in Eq. (1.2), to the corresponding Coulomb functions at $R=12$ fm and the angular momentum L of 0 or 9. The latter correspond to 21.6 MeV deuterons (lab energy) indicent on the nucleus of nickel.

TABLE III

Parameters and Notation[a]

Case	K_1R	K_2R[b]	Case	R (fm)	a (fm)
1	13	16	a	12	4
2	13	52	b	6	4
3	13	87	c	4	4
4	52	87			
5	13	1			

KR Values

Abbreviated	Full	
KR	Real	Imaginary
13	13.4879	−1.3634
16	16.5087	−1.4543
52	52.5570	−0.2428
87	87.4540	−0.1411
1	1.3953	0

[a] For example, Case 4b means that the values of K_1R; K_2R; R; a are $52.5570 - 0.2428i$; $87.4540 - 0.1411i$; 6 fm, 4 fm.

[b] These are abbreviated values for K_iR. The explicit values are given in the bottom half of the table.

The recursion relation was also evaluated upwards in L, starting with $L = -1$ and $L = 0$. The recursion of the G's upwards in L, Eq. (2.3), generates severe cancellation erros when the value of G starts to decrease rapidly with L. This happens when the turning point of either $j_L(K_1r)$ or $j_L(K_2r)$ falls outside of the interval 0–R, since then the value of j_L rapidly decreases with L in that interval. (The turning point r_T is given approximately by $Kr_T \approx L$.) Accodingly the upwards recursions relation, is stopped at an L_U which is the largest integer less than either $|K_1R|$ or $|K_2R|$.

From the comparison of the agreement between the three methods, one can deduce which of them is the most accurate. For example, for Case 1a the methods A and D have approximately the same accuracy, which is larger than that for U; for Cases 1b and c A and U are more accurate than D, and so forth. The value deemed most accurate from the type of comparison described above is then used for the accuracy test of Olver's method, which is described in Table V. The method picked for the comparison is indicated by the letters A or D, and the results from Olver's method are denoted by O. The entries listed under the label L_{MAX} are the values of L_A and L_D and for Olver's case it is the value of L_N. For methods A or D the value of the absolute error is estimated from the comparison of the G_A and G_D values at $L = 0$, and the error for O's method is taken from Eq. (A8) in the Appendix. The values of $G(L)$ obtained by the various methods are listed in Table V. The last

TABLE IV

Accuracy for $G(L)$[a]

Case[b] / L	1a			1b			1c		
	A–D[c]	U–D[c]	A–U[c]	A–D	U–D	A–U	A–D	U–D	A–U
0	⩾	—	—	10	—	—	7	—	—
5	⩾	⩾	⩾	10	11	⩾	7	7	⩾
10	⩾	12	12	10	10	14	7	7	⩾
15	⩾			11			6		
20	13			7			3		

Case / L	2a			2b	3a			3b
	A–D	U–D	A–U	U–D	A–D	U–D	A–U	U–D
0	⩾	—	—	⩾	⩾	—	—	⩾
5	⩾	⩾	⩾	⩾	11	⩾	11	⩾
10	⩾	⩾	⩾	13	12	⩾	12	⩾
15	12				11			
20	11				9			

Case / L	4a	4b	5a	5b
	U–D	U–D	A–D	A–D
0	12	13	>	12
5	11	13	>	10
10	12	13	11	8
15	12	13	3	4
20	13	13	3	—

[a] The entries in the table represent the number of significant digits for which relative agreement between any two of the three methods is obtained. For example, the two numbers $0.2467279(-4)$ and $0.2467189(-4)$ are in agreement o the fourth significant figure, i.e., $0.2467(-4)$, and the entry of 4 would be placed into the table. The exponent of 10 is -4 in this example. The symbol ⩾ indicates that the agreement is better or equal to the 14 significant figures printed out. The entries for the lines $L=0$ indicate the agreement between the downward recursion relation and the error integral-continued fraction methods for $L=0$.

[b] The parameters for the cases are explained in Table III. The values of L_{MAX} for the A and D calculations are listed in Table V.

[c] A, U, and D stand for the anlytic, upward recursion and downward recursion methods, respectively, as explained in the text. The columns A–D describe the accuracy of the agreement between the A and D methods, for example.

figure printed is already supposed to be unreliable, according to the error estimates listed to the left.

The main result which emerges from Table VI is that Olver's error estimates are very reliable. This can be seen by noting that the last figure printed for each G,

TABLE V

Values of L_{MAX} for the Cases Listed in Table IV

Case	1a	1b	1c	2a	2b	3a	3b	4a	4b	5a	5b
L_A	38	32	32	32	—	32	—	—	—	32	32
L_D	62	62	64	64	62	60	60	106	104	50	50

which should be unreliable according to Olver's prescription, is indeed in disagreement with the more accurate results listed in the line above, while the second to last figure is in agreement with the more accurate results. Case 5a is also interesting. It shows that the absolute errors in the D-method for high L values are much smaller than what is expected from the comparison A–D at $L=0$. The numbers in parenthesis listed for Case 5a are the figures printed out by the computer which should no longer be reliable according to the estimate based on the A–D comparison at $L=0$. Yet, these figures are in agreement with the more accurate 0 result. Thus, while in Olver's method the absolute error, once introduced at $L=L_N$, propagates virtually unchanged to all other L values, in the D-method the absolute error appears to increase as the recursion proceeds downward in L.

The effect of cutting off the integral (2.1) at the upper limit R can be very pronounced. The absolute values of $\bar{G}$ and G are listed in Table VII in order to illustrate the magnitude of this effect. The difference between $\bar{G}$ and G can become

TABLE VI

Absolute Accuracy for $G(L)$

Case 1c
$L=5$

	L_{MAX}[a]	Error[b]	Re $G(5)$[c]	Im $G(5)$
A	32	0.1(−12)?	0.4576545059987	−0.1184469683469
0	39	0.80(−13)	0.4576545059986	−0.1184469683468
0	31	0.25(−10)	0.45765450598	−0.11844696834
0	26	0.20(−9)	0.4576545061	−0.1184469682
0	21	0.10(−6)	0.4576544	−0.1184468
0	16	0.18(−2)	0.458	−0.117

[a] L_{MAX} is the value of L at which truncation to zero is started.

[b] This is the absolute error, which for the first line is obtained from the comparison of the relative errors in Table IV, and if uncertain is followed by a questionmark. For Olver's method the error is calculated from Eqs. (A.8).

[c] The last significant digit printed is the first one which is deemed inaccurate according to the absolute error quoted in the preceding column. No rounding with the digits following it (but not printed) was performed. The number in parenthesis indicate the powers of ten by which the entries are to be multiplied. The parenthesis in Case 5a are discussed in the text.

Table continued

TABLE VI (*continued*)

$L = 15$

	L_{MAX}	Error	Re $G(15)$	Im $G(15)$
A	32	0.1(−12)?	0.24728844216(−2)	−0.459918093136(−1)
0	39	0.12(−12)	0.24728844215(−2)	−0.459918093135(−1)
0	31	0.40(−10)	0.247288440(−2)	−0.4599180931(−1)
0	26	0.31(−9)	0.24728846(−2)	−0.459918091(−1)
0	21	0.18(−6)	0.24727(−2)	−0.459917(−1)

Case 2b

$L = 5$

	L_{MAX}	Error	Re $G(5)$	Im $G(5)$
D	62	0.2(−15)	−0.62891245695030(−2)	0.10258436414620(−1)
0	39	0.20(−18)	−0.62891245695030(−2)	0.10258436414620(−1)
0	31	0.10(−11)	−0.6289124568(−2)	0.10258436414(−1)
0	26	0.20(−4)	−0.6289126(−2)	0.10258436(−1)
0	21	0.14(−5)	−0.6289(−2)	0.10256(−1)
0	16	0.57(−3)	−0.65(−2)	0.107(−1)

$L = 20$

	L_{MAX}	Error	Re $G(20)$	Im $G(20)$
D	62	0.2(−15)	0.5245699829 (−6)	0.660553706739 (−4)
0	39	0.35(−18)	0.5245699829777(−6)	0.66055370673986(−4)
0	31	0.19(−11)	0.524568(−6)	0.66055370(−4)
0	26	0.34(−8)	0.527(−6)	0.66056(−4)

Case 5a

$L = 5$

	L_{MAX}	Error	Re $G(5)$	Im $G(5)$
D	50	0.1(−15)	0.26908495487(764)(−5)	0.12434504051(292)(−5)
A	32	0.1(−15)?	0.26908495487(764)(−5)	0.12434504051(292)(−5)
0	24	0.57(−67)	0.26908495487764(−5)	0.12434504051292 (−5)
0	9	0.50(−17)	0.2690849548787(−5)	0.1243450405125(−5)

$L = 10$

	L_{MAX}	Error	Re $G(10)$	Im $G(10)$
D	50	0.1(−15)	0.27120(967265472)(−11)	−0.721(49374378477)(−12)
A	32	0.1(−15)?	0.27120(965265490)(−11)	−0.721(49374378878)(−12)
0	19	0.90(−43)	0.27120967265472(−11)	−0.72149374378477(−12)

TABLE VII

Order of Magnitude of $\bar{G}$ and G (in fm)

Case / L	1a		1b		1c	
	$\bar{G}$	G	$\bar{G}$	G	$\bar{G}$	G
0	0.2(1)	0.2(1)	0.6(0)	0.8(0)	0.2(0)	0.5(0)
5	0.4(0)	0.4(0)	0.5(0)	0.6(0)	0.2(0)	0.5(0)
10	0.2(−1)	0.2(−1)	0.2(0)	0.3(0)	0.1(0)	0.4(0)
15	0.2(−3)	0.2(−3)	0.6(−1)	0.2(−1)	0.6(−1)	0.5(−1)
20	0.5(−6)	0.5(−7)	0.1(−1)	0.1(−4)	0.3(−1)	0.3(−4)

Case / L	2a		2b	3a	3b
	$\bar{G}$	G	G	G	G
0	0.7(−18)	0.2(−4)	0.2(−1)	0.3(−4)	0.1(−1)
5	0.5(−18)	0.4(−4)	0.1(−1)	0.1(−4)	0.4(−2)
10	0.2(−18)	0.5(−4)	0.2(−1)	0.3(−4)	0.1(−1)
15	0.3(−19)	0.1(−4)	0.5(−2)	0.4(−5)	0.2(−2)
20	0.4(−20)	0.2(−6)	0.7(−4)	0.3(−7)	0.2(−4)

Case / L	4a	4b	5a		5b	
	G	G	$\bar{G}$	G	$\bar{G}$	G
0	0.4(−5)	0.4(−2)	0.3(−1)	0.3(−1)	0.2(−6)	0.1(0)
5	0.1(−4)	0.1(−2)	0.3(−5)	0.3(−5)	0.6(−8)	0.7(−4)
10	0.1(−4)	0.3(−2)	0.3(−11)	0.3(−11)	0.4(−11)	0.3(−9)
15	0.1(−4)	0.4(−2)	0.3(−18)	0.5(−19)	0.4(−15)	0.1(−16)
20	0.1(−4)	0.7(−2)	0.5(−26)	0.3(−28)	0.7(−20)	0.7(−26)

particularly pronounced when the integrand is very oscillatory, as is the case when the wave numbers K are large compared to a^{-1}. In this case the negative parts of the integrand nearly cancel the positive parts, but the cancellation is interrupted at the upper limit of integration R for the last oscillation lobe. Depending on where this lobe occurs, G can thus be substantially larger than $\bar{G}$, as can be seen for Case 2a. Under these conditions G will also vary nonmonotonically for successive values of L, depending on how the last noncancelled lobe is placed relative to R. This effect will not be large if R is substantially larger than a, since then the factor $\exp(-r^2/a^2)$ will be quite small at the upper limit of the integral, and G will be very close to $\bar{G}$, as is true, for example, for Case 1a.

6. Summary and Conclusions

The integral $G(L)$ of the product of two spherical Bessel functions $j_L(K_1 r)$ and $j_L(K_2 r)$ times $r^2 \exp(-r^2/a^2)$ over a finite radial range from 0 to R can be evaluated

by using a simple recursion relation, Eq. (2.3), between $G(L)$, $G(L+1)$, and $G(L+2)$. The inhomogeneous terms $X(L)$ of this recursion relation arise from the upper limit of integration R.

A second ingredient needed for the calculation of $G(L)$ is the evaluation of an error function of complex argument in terms of which $G(0)$ and $G(-1)$ can be expressed. A continued fraction expression exists in the literature for the latter, which converges better the more oscillatory is the integrand in $G(L)$, i.e., the more difficult it would be to evaluate $G(L)$ by a radial mesh summation technique. The recursion relation is solved both analytically and numerically by means of various algorithms. The comparison of the numerical results (Tables IV and V) allows one to establish the accuracy of the methods, relative accuracies of one part in 10^7 being easily achieved. The recursion algorithm of Olver [17] was found to be particularly stable and to give rise to reliable absolute error estimates (Table V).

The analytical solution is obtained by treating the recurrence relation as a finite difference equation [22]. The homogeneous part of the equation gives rise to two independent solutions, $\bar{f}_L(z_3)$ and $\bar{q}_L(z_3)$ where $z_3 = K_1 a K_2 a/2i$. The inhomogeneous recurrence relation is then solved in terms of sums over l from 0 to L and from $L+1$ to ∞, a technique which is reminiscent of the use of Green's functions for the solution of inhomogeneous differential equations. In this process an identity emerges (Eq. (4.13)), between one of the sums from 1 to ∞ and a certain combination between $G(0)$ and $G(-1)$. This identity has been verified to hold numerically to a large degree of accuracy.

If the values of $K_1 R$ and $K_2 R$ and $K_2 R$ are both less than L_U, then the values of $G(L)$ for $L = 0, 1, 2, \ldots, L_U$ are all of the same order of magnitude and can be calculated directly from the upward recurrence relation starting from the values $G(-1)$ and $G(0)$ without loss of accuracy. The latter are calculated reliably from the continued fraction representation of the error functions. This method is found to be the fastest, and generally the most accurate, of the various methods examined. The case of the Sturmian Bessel functions [5] is particularly suitable for the use of the upward recursion technique, because the turning points of these functions always occur within the range of the integral for G.

The computing time for the 20 L-values of G used in the numerical examples given, is approximately 0.03 to 0.04 sec for the analytical method, 0.01 to 0.02 sec for the down recursion, and less than 0.01 sec for the up-recursion, on the IBM 3081 computer, used in double precision. Olver's method is comparable in complexity to the down recursion method, and hence should require comparable execution times.

In summary, the indefinite integral (2.1) of the product of two Bessel functions and a gaussian has been found to obey a simple inhomogeneous three point recursion relation. An analytical solution for this finite difference equation has been given, and several numerical methods for evaluating the recursion have been examined. The method of Olver was found to give very reliable absolute error estimates, and hence the accuracy of the result is determined by the accuracy with which the required input Bessel functions can be obtained.

The existence of a method to evaluate such integrals now opens up the possibility of solving a set of coupled channel equations to high accuracy, by the use of a Sturmian expansion technique [5, 6], provided that the coupling potentials can be expressed in terms of a few Gaussians.

Recursion relations for potentials for the form $r^a \exp(-b/r)$ have been obtained [15], and hence a generalization of the present numerical method to this case is feasible. However, these recursion relations are more involved than the one for the Gaussian potential, and a numerical accuracy analysis has as yet not been carried out.

APPENDIX A1: Calculation of a Continued Fraction

The method employed here is the one developed by Steed [23], at the University of Manchester in 1967. This method employs a recursion technique involving powers of $(1/z)^2$, with a number of terms N chosen such that when the difference between the Nth and $(N-1)$th approximants to the continued fraction, together with that of the $(N-2)$th and $(N-1)$th approximants becomes less than the imposed accuracy parameter ε_c, then the recursion is terminated. The error in the continued fraction then becomes less than ε_c. This has been verified during an application [25] of Steed's algorithm to the evaluation of the exponential integral by means of the continued fraction given by Eq. (5.1.22) in [20]. Comparison of

TABLE IA

Number of Terms N in the Evaluation of $\mathrm{erf}(z)^a$ so as to Achieve Accuracy ε_c

z \ ε_c	10^{-8}	10^{-13}
0.05	3	5
0.2	5	7
0.5	7	10
1.4	14	19
1.5	31	68
2.0	20	42
3.0	12	24
4.0	10	17
$3.0+3.0i$	10	19
5.0	8	14

[a] When $|z|^2 < 2$ the power series of Eq. (3.5) is used. For $|z|^2 > 2$ the Steed method for evaluating the continued fraction in Eq. (3.6) is used, as is described in the text.

the answer with numerical results given in [20] for the sine and cosine integrals, where they are listed to 10 places, shows that the error parameter ε_c is reliable, i.e., the error in the continued fraction is somewhat less than the value of ε_c. A comparison with the value of the erf(z) for complex z, given in Table 7.9 of [20], showed perfect agreement to all the six figures listed. The function $C(z)$ defined in Eq. (3.9), is calculated by the continued fraction method described above when $|z^2| > 2$.

When $|z|^2 > 2$ the continued fraction is expressed in terms of the error function according to Eq. (3.8), and the latter is evaluated by the power series, Eq. (3.5). The sum is stopped when the nth term is Eq. (3.5) becomes less than ε_c. The number of terms N, needed in either the power series or in the recursion relations of the continued fraction, so as to get various accuracies ε_c are listed in Table IA. All calculations are carried out in double precision on a IBM 3081 computer.

APPENDIX A2: OLVER'S METHOD FOR SOLVING AN INHOMOGENEOUS FINITE DIFFERENCE EQUATION

The formulae used for Olver's method [17] will be briefly described in what follows.

The functions y_L to be calculated for $L = 0, 1, 2, \ldots, P$ with a given accuracy obey the inhomogeneous recursion relations

$$a_L y_{L-1} - b_L y_L + c_L y_{L+1} = d_L, \tag{A1}$$

where in the present application

$$\begin{aligned} a_L &= 1; \qquad c_L = -1, \\ b_L &= (4L+2)/(k_1 k_2 a^2), \\ d_L &= X_L \exp(-R^2/a^2). \end{aligned} \tag{A2}$$

According to the accuracy desired for the function $y_0, y_1, \ldots, y_P$, a maximum value of L is chosen (denoted as N) and the $N-1$ equations (A1) for $L = 1, 2, \ldots, N-1$ are solved for $y_1^{(N)}, y_2^{(N)}, \ldots, y_{N-1}^{(N)}$ under the assumption that $y_0 = e_0$ is known and $y_N^{(N)} = 0$.

For this purpose one needs the quantities p_L for $L = 0, 1, 2, \ldots, L_{\mathrm{MAX}}$ which satisfy the homogeneous recursion relation

$$a_L p_{L-1} - b_L p_L + c_L p_{L+1} = 0 \tag{A3}$$

and which are such that

$$p_0 = 0, \qquad p_1 = 1. \tag{A4}$$

The p's are linear combinations of two independent solutions of Eq. (A3), which for our present application is

$$p_L = i(\bar{q}_0 \bar{f}_L - \bar{f}_0 \bar{q}_L). \tag{A5}$$

The p's are calculated either from Eq. (A5), with the $\bar{q}$'s and f's obtained independently in terms of spherical Bessel functions of argument z_3, or by upward recursion of Eq. (A3), using for starting values (A4). The first method is more accurate, but the second method is much preferable since it does not require knowledge of the $\bar{f}$'s. Both methods were used in the present application.

Next the quantities e_L are needed for $L = 0, 1, ..., L_{\mathrm{MAX}}$. They obey the recursion relation

$$e_L = (a_L e_{L-1} - d_L p_L)/c_L,$$
$$L = 1, 2, ..., L_{\mathrm{MAX}},$$

with

$$e_0 = G(0), \tag{A6a}$$

assumed as known. For our case the recursion relation is

$$e_L = -e_{L-1} + X_L p_L \exp(-R^2/a^2). \tag{A6b}$$

To evaluate the truncation error $y_N = 0$, the sums E_N are calculated

$$E_N = \sum_{r=N}^{\infty} r_r/(p_r p_{r+1}). \tag{A7}$$

For numerical applications the upper limit of the sum is truncated at the value L_{MAX} which is chosen as described in Appendix A3. The truncation error of the functions y is then given by [17, Eq. (5.01)],

$$y_L^{(N)} - y_L^{(\infty)} = p_L E_N \tag{A8}$$

and the functions $y^{(N)}$ are evaluated by backward recursion of the equation

$$y_L^{(N)} = (e_L + p_L y_{L+1}^{(N)})/p_{L+1},$$
$$L = N-1, N-2, ..., 1 \tag{A9}$$

with $y_N^{(N)} = 0$.

APPENDIX A3: Evaluation of the Bessel Functions

As is indicated in Section 5, two methods for calculating $j_L(z)$ are employed according to how large z is compared to L. If $|z|^2 > (L-6)L$ Eq. (10.1.10) of [20]

is used. In this case the turning point occurs for values of the argument of j_L less than z, and the expression of j_L in terms of polynomials in $(1/z)$ times $\exp(\pm iz)$ will not lead to loss of accuracy due to cancellations. The condition $|z|^2 > (L-6)L$ is imposed somewhat arbitrarily. If it is not satisfied, then the Bessel functions are evaluated by a downward recursion starting a L_{MAX} and $L_{\mathrm{MAX}}+1$. At these values of L the Bessel function are evaluated by the analytic series expansion in powers of $(\frac{1}{2}z^2)$, Eq. (10.1.2) of [20], and the series is stopped either when the square of the last term in the series is less than 10^{-13} or when the number of terms exceeds 25. Should neither of these two conditions be fulfilled, then the initial values of the Bessel functions at L_{MAX} are inaccurate. The downward recursion is nevertheless carried out, and the accuracy of the resulting Bessel functions is investigated for the L's at which the functions are actually used. The accuracy test used is the one given by W. Kahan, as described on p. 52 of a 1967 paper by Gautschi [18]. In the present application sufficiently good accuracies for the Bessel functions have been achieved for those values of L for which they are needed.

The value of L_{MAX} is chosen as follows. If $|\frac{1}{2}z|^2$ is less than 160, L_{MAX} is set equal to $|\frac{1}{2}z|^2$ or to L whichever is larger and the power series expansion converges well after 25 terms. Otherwise, L_{MAX} is set equal to $2|z|$ and the power series will have an error remaining. The normalization factor of thepower series, which should have the value $z^L/(2L+1)!!$, is instead set equal to $\exp(-70)$ for L_{MAX}, and $z \times \{\exp(-70)\}/(2L+3)$ for $L_{\mathrm{MAX}}+1$. This is dictated by the requirement that the product of two Bessel functions, which occurs in the calculation of Y, will not [illegible] for large values of L. The recursion relation is then started from $L_{\mathrm{MAX}}+1$ downward through all L's to $L=0$. The required normalization of the Bessel functions at all L values is subsequently determined by comparison of $j_0(z)$ thus obtained with $\sin(z)/z$, calculated separately, and the normalization factor is stored for a final renormalization of all the quantities which are needed in the calculations of the recurrence relation.

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