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Evaluation of Integrals Required in Scattering Theory: II. Exchange Type Integrals

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This work concludes the presentation of methods for evaluation of integrals required in electron–atom scattering using an analytic basis set. Methods are presented for the calculation of exchange integrals between spherical Bessel functions and exponential functions. For reasons of relative speed and applicability, six different methods are presented. Features of each are discussed and a scheme is described for selecting the most desirable method for a given case.

I. INTRODUCTION AND DEFINITIONS

Techniques for the inclusion of many-particle effects in calculations of bound-state properties of atoms have received extensive development, use, and success [1]. Application of these methods to calculations of electron-atom scattering is of considerable interest and is possible with reasonable expenditure of effort. We have extended a many-body variational technique to permit the calculation of correlation corrections to the reactance matrix R for electron-atom systems of arbitrary size [2]. Since the method utilizes an analytical basis set, this requires the inclusion of analytic functions which can describe a scattered electron asymptotically. For this purpose we have selected the specific forms:

$$S_a(r, \theta, \phi) = N_a{}^S j_{l_a}(k_a r)\, Y_{l_a m_a}(\theta, \phi), \tag{1}$$

$$C_a(r, \theta, \phi) = N_a{}^C \left[j_{l_a+1}(k_a r) + \frac{l_a + 1}{k_a r}\, j_{l_a+2}(k_a r) \right] Y_{l_a m_a}(\theta, \phi), \tag{2}$$

which have, respectively, sine-like and cosine-like behavior at large r. Here $j_l(kr)$ is the spherical Bessel function of the first kind. The linear combination in Eq. (2) is selected to approximate the spherical Bessel function of the second kind, the

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Neumann function, at large r, while remaining bounded at the origin [3]. Functions of this type for each (k_a, l_a) channel available in the system are added to the usual basis of Slater-type orbitals:

$$\eta_a(r, \theta, \phi) = N_a r^{n_a-1} e^{-\zeta_a r} Y_{l_a m_a}(\theta, \phi). \tag{3}$$

The evaluation of all matrix elements required in scattering calculations requires combinations of six basic types of integrals:

$$G(\lambda; p \mid k, \alpha) = \int_0^\infty dr\, j_\lambda(kr)\, r^{p-\lambda} e^{-\alpha r}, \tag{4}$$

$$H(\lambda, \mu; p \mid k_1, k_2, \alpha) = \int_0^\infty dr\, j_\lambda(k_1 r)\, j_\mu(k_2 r)\, r^{p-\lambda-\mu} e^{-\alpha r}, \tag{5}$$

$$I(\lambda, \mu; p \mid k_1, k_2) = \int_0^\infty dr\, j_\lambda(k_1 r)\, j_\mu(k_2 r)\, r^{p-\lambda-\mu}, \tag{6}$$

$$V(\lambda, \mu; p, q \mid k_1, k_2, \alpha) = \int_0^\infty dr\, j_\lambda(k_1 r)\, j_\mu(k_2 r)\, A_p(\alpha, r)\, r^{q-\lambda-\mu}, \tag{7}$$

$$W(\lambda; p, q \mid k, \alpha, \beta) = \int_0^\infty dr\, j_\lambda(kr)\, A_p(\alpha, r)\, r^{q-\lambda} e^{-\beta r}, \tag{8}$$

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) = \int_0^\infty dr_1\, j_\lambda(k_1 r_1)\, r_1^{p-\lambda} e^{-\alpha r_1} \int_{r_1}^\infty dr_2\, j_\mu(k_2 r_2)\, r_2^{q-\mu} e^{-\beta r_2}. \tag{9}$$

In Eqs. (4)–(9), λ, μ, p, and q are nonnegative integers; k_1 and k_2 are nonnegative and real; and the real parts of α and β are positive. The auxiliary function $A_p(\alpha, r)$ in Eqs. (7) and (8) is defined by

$$A_p(\alpha, r) = \int_r^\infty ds\, s^p e^{-\alpha s}. \tag{10}$$

In paper I of this series [4] we have described methods for the evaluation of G, H, I, V, and W integrals. The purpose of the present work is to explain procedures for the evaluation of X integrals as well as to indicate some additional techniques for G, H, and I integrals. Some techniques for evaluating these integrals have also been discussed by Harris and Michels [5]. For X integrals, both α and β are real.

The nature of the X integrals has made their evaluation particularly difficult. Due to its form, the integrand can be wildly oscillatory in two dimensions. This definitely precludes direct application of a quadrature technique since for very reasonable values of the parameters, the number of points required is quite prohibitive. Furthermore, recurrence formulas frequently introduce tremendous

losses of significance and series expansions have small and difficult-to-determine regions of convergence. The result of these considerations has been that, in order to assure uniform minimal accuracy with greatest efficiency, it has been necessary to employ one of six different techniques for the evaluation of X integrals depending on the values of the eight parameters λ, μ, p, q, k_1, k_2, α, and β.

It is convenient in deriving the six methods to introduce some further definitions. We define the core function

$$\chi(\lambda, p, k, \alpha \mid r) = j_\lambda(kr)\, r^{p-\lambda} e^{-\alpha r}, \tag{11}$$

in terms of which the X integral is expressed as

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) = \int_0^\infty dr_1 \int_{r_1}^\infty dr_2\, \chi(\lambda, p, k_1, \alpha \mid r_1)\, \chi(\mu, q, k_2, \beta \mid r_2). \tag{12}$$

At the same time we introduce the complementary integral Z, defined by

$$Z(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) = \int_0^\infty dr_1 \int_0^{r_1} dr_2\, \chi(\lambda, p, k_1, \alpha \mid r_1)\, \chi(\mu, q, k_2, \beta \mid r_2), \tag{13}$$

and since

$$\int_0^\infty dr_1 \int_{r_1}^\infty dr_2 = \int_0^\infty dr_2 \int_0^{r_2} dr_1,$$

we see that the relationship between X and Z is

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) = Z(\mu, \lambda; q, p \mid k_2, k_1, \beta, \alpha). \tag{14}$$

The rest of this paper is organized as follows. In Section II we derive each of the six methods for evaluation of X integrals. Section III contains a discussion of our studies of numerical accuracy and speed as functions of the eight parameters of X for the six methods. We present also an algorithm for selection of the optimum method for a specified λ, μ, p, q, k_1, k_2, α, and β. Our summary conclusions are given in Section IV. The appendices include discussion of additional techniques for the evaluation of G, H, and I integrals in addition to those presented in paper I as well as some of the algebraic detail required in the evaluation of the X integrals.

Our work on these integrals benefitted greatly from discussions with Professor F. E. Harris, which we wish to acknowledge here. Our analysis started from the basis of methods recently published by Harris and Michels [5]. Throughout this work we have relied heavily on the reference work on mathematical functions prepared by the U. S. National Bureau of Standards [6]. In most cases our notation follows theirs. Formulas from this handbook will be referenced here by the notation HMF followed by the referenced equation number.

II. Derivation of Six Methods

A. *Degenerate Case*: *XDEG*

There is one case in which the calculation of X integrals becomes trivial. The sum of X and Z is

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) + Z(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) = G(\lambda; p \mid k_1, \alpha)\, G(\mu; q \mid k_2, \beta). \tag{15}$$

From Eq. (14) it is seen that if $\lambda = \mu$, $p = q$, $k_1 = k_2$, and $\alpha = \beta$, then $X = Z$. Thus Eq. (15) reduces in that case to

$$X(\lambda, \lambda; p, p \mid k_1, k_1, \alpha, \alpha) = \tfrac{1}{2}[G(\lambda; p \mid k_1, \alpha)]^2; \tag{16}$$

so in this important special case, Eq. (16) gives a simple formula for the evaluation of X.

B. *First Infinite Series*: *XSER*1

Define

$$y(\mu, q, k_2, \beta \mid r) = \int_r^\infty ds\, \chi(\mu, q, k_2, \beta \mid s). \tag{17}$$

Then using (HMF, 10.1.2) for the power series expansion of $j_n(z)$,

$$j_n(z) = z^n \sum_{m=0}^{\infty} \frac{(-1)^m z^{2m}}{(2m)!!\,(2n + 2m + 1)!!}, \tag{18}$$

the function y is expressed as

$$y(\mu, q, k_2, \beta \mid r) = \sum_{m=0}^{\infty} \frac{(-1)^m k_2^{\mu+2m}}{(2m)!!\,(2\mu + 2m + 1)!!} A_{q+2m}(\beta, r). \tag{19}$$

Substitution of this result into X gives

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) = \int_0^\infty dr\, \chi(\lambda, p, k_1, \alpha \mid r)\, y(\mu, q, k_2, \beta \mid r) \tag{20}$$

$$= \sum_{m=0}^{\infty} \frac{(-1)^m k_2^{\mu+2m}}{(2m)!!\,(2\mu + 2m + 1)!!} W(\lambda; q + 2m, p \mid k_1, \beta, \alpha). \tag{21}$$

This result can be expressed in the form

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) = c(\mu, k_2) \sum_{m=0}^{\infty} d_m W_{2m}, \tag{22}$$

where

$$\begin{aligned} c(\mu, k_2) &= k_2^{\mu}/(2\mu + 1)!!, \\ d_m &= (-1)^m k_2^{2m}/(2m)!! \, [2\mu + 3]_{2m}, \end{aligned} \tag{23}$$

and

$$W_{2m} = W(\lambda; q + 2m, p \mid k_1, \beta, \alpha). \tag{25}$$

Here $[a]_{2m}$ is defined by

$$[a]_{2m} = a(a + 2)(a + 4) \cdots [a + 2(m - 1)], \qquad [a]_0 = 1. \tag{26}$$

This series converges for $k_2 < \beta$. However, while in this case $\lim_{m\to\infty} [d_m W_{2m}] \to 0$, we find that d_m becomes vanishingly small while W_{2m} grows very large. The resulting computational difficulties can be overcome by redefining

$$\begin{aligned} d_m' &= (\beta/k_2)^{2m} \, d_m, \\ W_m' &= (k_2/\beta)^m \, W_m, \end{aligned} \tag{27}$$

such that

$$d_m W_{2m} = d_m' W_{2m}'.$$

Successive terms in the series can then be obtained easily as follows:

$$\begin{aligned} d_0' &= 1, \\ d_m' &= (-\beta/2m)[\beta/(2\mu + 2m + 1)] \, d_{m-1}', \qquad m > 0, \end{aligned} \tag{28}$$

$$\begin{aligned} W_0' &= W(\lambda; q, p \mid k_1, \beta, \alpha), \\ W_m' &= [G_m' + (q + m)(k_2/\beta) \, W_{m-1}']/\beta, \qquad m > 0, \end{aligned} \tag{29}$$

where

$$G_m' = (k_2/\beta)^m \, G(\lambda; p + q + m \mid k_1, \alpha + \beta) \tag{30}$$

and Eq. (29) is obtained from Eq. (I-61).

Using Eq. (48) of Paper I, the G_m' are obtained from

$$\begin{aligned} G_0' &= G(\lambda; p + q \mid k_1, \alpha + \beta), \\ G_1' &= (k_2/\beta) \, G(\lambda; p + q + 1 \mid k_1, \alpha + \beta), \\ G_m' &= [(p + q + m - 1)(2\lambda + 2 - p - q - m)(k_2/\beta)^2 \, G_{m-2}' \\ &\quad + 2(\alpha + \beta)(p + q + m - \lambda - 1)(k_2/\beta) \, G_{m-1}']/[(\alpha + \beta)^2 + k_1^2], \qquad m > 1. \end{aligned} \tag{31}$$

Thus after obtaining the starting values of Eqs. (29) and (31), G_0', G_1', and W_0', by the methods of paper I, successive terms in the series of Eq. (22) are obtained recursively. The number of operations required at each step in m may seem larger than desirable, but is quite reasonable in view of the complexity of X.

C. *Second Infinite Series: XSER2*

Define

$$g(\lambda, p, k_1, \alpha \mid r) = e^{\alpha r} \int_0^r ds\, \chi(\lambda, p, k_1, \alpha \mid s). \tag{32}$$

Expanding $e^{\alpha(r-s)}$ in its power series and also expanding $(k_1 s)^{-\lambda} j_\lambda(k_1 s)$ by (HMF, 10.1.2) leads to

$$g(\lambda, p, k_1, \alpha \mid r) = k_1^{\lambda} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^n k_1^{2n} \alpha^m r^{p+m+2n+1}}{(2n)!!\,(2\lambda + 2n + 1)!!\, m!} \int_0^1 ds\, s^{p+2n}(1 - s)^m \tag{33}$$

after transformation of the limits of the integral from $(0, r)$ to $(0, 1)$. Then on recognizing that the integral remaining in Eq. (33) is the Beta function, $B(p + 2n + 1, m + 1)$, and using (HMF, 6.2.1) to evaluate it, g reduces to

$$g(\lambda, p, k_1, \alpha \mid r) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^n k^{\lambda+2n} \alpha^m (p + 2n)!}{(2n)!!\,(2\lambda + 2n + 1)!!\,(p + m + 2n + 1)!} r^{p+m+2n+1}, \tag{34}$$

which may be rewritten

$$g(\lambda, p, k_1, \alpha \mid r) = \sum_{n=0}^{\infty} \left\{ \sum_{m=0}^{[n/2]} \frac{(-1)^m k_1^{\lambda+2m} \alpha^{n-2m} (p + 2m)!}{(2m)!!\,(2\lambda + 2m + 1)!!\,(p + n + 1)!} \right\} r^{p+n+1}, \tag{35}$$

where the sum on m terminates with the largest integer less than or equal to $n/2$. It is convenient to express Eq. (35) in the form

$$g(\lambda, p, k_1, \alpha \mid r) = \frac{c(\lambda, k_1)}{p + 1} \sum_{n=0}^{\infty} d_n \frac{\alpha^n}{(p + 2)_n} r^{p+n+1}, \tag{36}$$

where $c(\lambda, k_1)$ is defined in Eq. (23),

$$d_n = \sum_{m=0}^{[n/2]} t_m, \tag{37}$$

$$t_m = \frac{(-1)^m (p + 1)_{2m}}{(2m)!!\,[2\lambda + 3]_{2m}} \left(\frac{k_1}{\alpha}\right)^{2m}, \tag{38}$$

and $(a)_n$ is Pockhammer's Symbol, (HMF, 6.1.22), defined by:

$$(a)_n = a(a+1)(a+2)\cdots(a+n-1); \qquad (a)_0 = 1. \tag{39}$$

In terms of g, X is defined as:

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) = \int_0^\infty dr\, \chi(\mu, q, k_2, \alpha+\beta \mid r)\, g(\lambda, p, k_1, \alpha \mid r) \tag{40}$$

using Eqs. (14) and (32). On substituting Eq. (36):

$$\begin{aligned} &X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) \\ &\quad = \frac{c(\lambda, k_1)}{p+1} \sum_{n=0}^{\infty} d_n \frac{\alpha^n}{(p+2)_n} \int_0^\infty dr\, \chi(\mu, p+q+n+1, k_2, \alpha+\beta \mid r) \\ &\quad = \frac{c(\lambda, k_1)}{p+1} \sum_{n=0}^{\infty} d_n \frac{\alpha^n}{(p+2)_n} G(\mu; p+q+n+1 \mid k_2, \alpha+\beta) \qquad (41) \\ &\quad = \frac{c(\lambda, k_1)}{p+1} \sum_{n=0}^{\infty} d_n G_n \qquad (42) \end{aligned}$$

where:

$$G_n = \frac{\alpha^n}{(p+2)_n} G(\mu; p+q+n+1 \mid k_2, \alpha+\beta). \tag{43}$$

Successive terms of this series can be obtained as follows:

$$\begin{aligned} d_0 &= t_0 \\ d_{2n+1} &= d_{2n}, \qquad n \geqslant 0 \\ d_{2n} &= d_{2n-1} + t_n, \qquad n > 0 \end{aligned} \tag{44}$$

$$\begin{aligned} t_0 &= 1 \\ t_m &= -\frac{p+2m-1}{2m} \frac{p+2m}{2\lambda+2m+1} \frac{k_1^2}{\alpha^2} t_{m-1}, \qquad m > 0 \end{aligned} \tag{45}$$

$$\begin{aligned} G_{-1} &= \frac{p+1}{\alpha} G(\mu; p+q \mid k_2, \alpha+\beta) \\ G_0 &= G(\mu; p+q+1 \mid k_2, \alpha+\beta) \\ G_n &= \left[\frac{p+q+n}{p+n} \frac{2\mu+1-p-q-n}{p+n+1} \alpha^2 G_{n-2} \right. \\ &\quad \left. + 2(\alpha+\beta) \frac{p+q+n-\mu}{p+n+1} \alpha G_{n-1}\right] \Big/ [(\alpha+\beta)^2 + k_2^2], \qquad n > 0 \end{aligned} \tag{46}$$

This technique is found to be appropriate for $k_1 \leqslant \alpha$. However, for $k_1 > \alpha$, d_n becomes large rapidly with increasing n. In this case, it is advantageous to define:

$$\begin{aligned} d_n' &= (\alpha/k_1)^n \, d_n \\ t_m' &= (\alpha/k_1)^{2m} \, t_m \\ G_n' &= (k_1/\alpha)^n \, G_n \end{aligned} \tag{47}$$

such that $d_n' G_n' = d_n G_n$. Equations (44)–(46) then become

$$\begin{aligned} d_0' &= t_0', \\ d_{2n+1}' &= (\alpha/k_1) \, d_{2n}', \qquad n \geqslant 0, \\ d_{2n}' &= (\alpha/k_1) \, d_{2n-1}' + t_n', \qquad n > 0, \end{aligned} \tag{48}$$

$$t_0' = 1,$$

$$t_m' = -\frac{p + 2m - 1}{2m} \frac{p + 2m}{2\lambda + 2m + 1} t_{m-1}', \qquad m > 0, \tag{49}$$

$$\begin{aligned} G_{-1}' &= \frac{p+1}{k_1} G(\mu; p + q \mid k_2, \alpha + \beta), \\ G_0' &= G(\mu; p + q + 1 \mid k_2, \alpha + \beta), \\ G_n' &= \left[\frac{p+q+n}{p+n} \frac{2\mu + 1 - p - q - n}{p+n+1} k_1^2 G_{n-2}' \right. \\ &\quad \left. + 2(\alpha+\beta) \frac{p+q+n-\mu}{p+n+1} k_1 G_{n-1}'\right] \Big/ [(\alpha+\beta)^2 + k_2^2], \qquad n > 0. \end{aligned} \tag{50}$$

D. *Finite Sum Formula: XSUM*

The integral y defined in Eq. (17) can also be evaluated by using the trigonometric expansion of the spherical Bessel function (HMF, 10.1.8) which can be expressed in the form

$$j_n(z) = \frac{1}{z} \operatorname{Im} \left\{ e^{iz} (-i)^n \sum_{m=0}^{n} i^m \frac{(n+m)!}{m!\,(n-m)!} \frac{1}{(2z)^m} \right\}. \tag{51}$$

Substituting this in Eq. (17) leads to

$$y(\mu, q, k_2, \beta \mid r) = \frac{(-i)^\mu}{k_2} \operatorname{Im} \left\{ \sum_{n=0}^{\mu} i^n \frac{\mu + n!}{n!\,(\mu - n)!\,(2k_2)^n} A_{q-\mu-n-1}(\beta - ik_2, r) \right\} \tag{52}$$

for $q > 2\mu$. Substituting into Eq. (20) gives for this case

$$X(\lambda, \mu; p, q \mid k_k, k_2, \alpha, \beta)$$

$$= \frac{(-i)^\mu}{k_2} \operatorname{Im} \left\{ \sum_{n=0}^{\mu} \frac{i^n(\mu + n)!}{n!\,(\mu - n)!\,(2k_2)^n} W(\lambda; q - \mu - n - 1, p \mid k_1, \beta - ik_2, \alpha) \right\} \tag{53}$$

for the case $q > 2\mu$. And using Eqs. (60) and (61) of paper I gives

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)$$

$$= \frac{(-i)^\mu}{k_2} \operatorname{Im} \left\{ \sum_{n=0}^{\mu} \frac{i^n(\mu + n)!}{n!\,(\mu - n)!\,(2k_2)^n} \sum_{m=0}^{q-\mu-n-1} \frac{(q - \mu - n - 1)!}{m!\,(\beta - ik_2)^{q-\mu-n-m}} \right.$$

$$\left. \times\, G(\lambda; p + m \mid k_1, \alpha + \beta - ik_2) \right\}, \qquad q > 2\mu. \tag{54}$$

The order of these two finite sums can be reversed and the terms in the outer sum added in the inverse order. This is shown diagrammatically in Fig. 1 where it is easily seen that the same area is covered. This leads to

$$X(\lambda, \mu, p, q \mid k_1, k_2, \alpha, \beta) = \frac{(-i)^\mu}{k_2} \operatorname{Im} \left\{ \sum_{n=0}^{q-\mu-1} d_n f_n G_{q-\mu-1-n} \right\}, \qquad q > 2\mu, \tag{55}$$

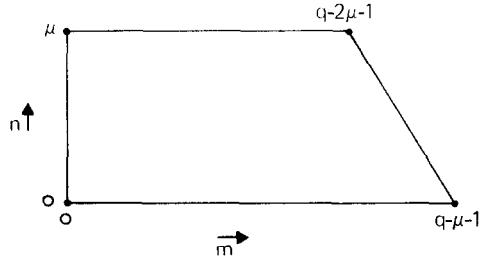

FIG. 1. Terms included in the XSUM method. All terms contained within the diagram must be included. The order is not significant.

where

$$d_n = \sum_{m=0}^{\min(\mu, n)} t_m, \tag{56}$$

$$f_n = (q - \mu - 1)!\,(\beta + ik_2)^{n+1}/(q - \mu - 1 - n)!\,(\beta^2 + k_2^2)^{n+1}, \tag{57}$$

$$G_{q-\mu-1-n} = G(\lambda; p + q - \mu - 1 - n \mid k_1, \alpha + \beta - ik_2), \tag{58}$$

and

$$t_m = (\mu + m)!\,(q - \mu - 1 - m)!\,(k_2 + i\beta)^m/m!\,(\mu - m)!\,(q - \mu - 1)!\,(2k_2)^m. \tag{59}$$

Successive terms in this sum are obtained from

$$t_0 = 1,$$
$$t_m = \frac{\mu + m}{m}\,\frac{\mu - m + 1}{q - \mu - m}\,\frac{k_2 + i\beta}{2k_2}\,t_{m-1}, \qquad m > 0, \tag{60}$$

$$d_0 = t_0,$$
$$d_n = \begin{cases} d_{n-1} + t_n, & 0 < n \leqslant \mu, \\ d_{n-1}, & \mu < n, \end{cases} \tag{61}$$

$$f_0 = (\beta + ik_2)/(\beta^2 + k_2^2),$$
$$f_n = [(q - \mu - n)(\beta + ik_2)/(\beta^2 + k_2^2)]\,f_{n-1}, \qquad n > 0. \tag{62}$$

Complex G integrals from G_0 to $G_{q-\mu-1}$ can be obtained from Eq. (48) of paper I.

E. *Contour Integral Method: XCI*

Direct numerical quadrature is not in general of value for the calculation of X integrals. However, as shown by Harris and Michels [5] for special values of the parameters, if X is transformed into a contour integral in the complex plane such that a nonoscillatory integrand is obtained, then numerical quadrature is feasible. Such a transformation may be effected by using the Poisson integral representation of $j_n(z)$ (HMF, 10.1.13),

$$j_n(z) = \frac{z^n}{2^{n+1}n!}\int_{-1}^{1} e^{izt}(1 - t^2)^n\,dt. \tag{63}$$

When substituted in Eq. (17), this gives

$$y(\mu, q, k_2, \beta \mid r) = \frac{{k_2}^\mu}{2^{\mu+1}\mu!}\int_{-1}^{1} dt(1 - t^2)^\mu\,A_q(\beta - ik_2 t, r). \tag{64}$$

Integration is carried out by numerical quadrature along a contour path in the complex plane, selected to avoid the possible pole at the origin. A good choice is a path in the complex plane which connects the limits of the integral using only an angular integration at constant radius. This is shown in Fig. 2 where the path of Eq. (64) is indicated as Γ_1 and the desired path at constant radius is shown

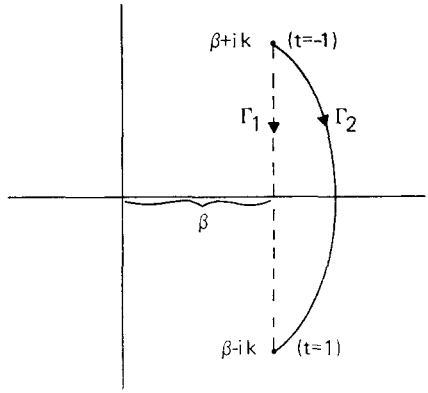

FIG. 2. Contours for XCI method. The path Γ_2 is at constant distance from the origin.

as Γ_2. Using the transformation $\rho e^{i\phi} = \beta - ikt$, Eq. (64) may be expressed in the form

$$y(\mu, q, k_2, \beta \mid r) = \frac{\rho^{\mu+1}}{2\mu!\, k_2^{\mu+1}} \int_{-\phi_1}^{\phi_1} d\phi\, e^{i(\mu+1)\phi}(\rho \cos\phi - \beta)^{\mu} A_q(\rho e^{i\phi}, r), \quad (65)$$

where

$$\begin{aligned} \rho^2 &= \beta^2 + k_2^2, \\ \phi_1 &= \tan^{-1}(k_2/\beta). \end{aligned} \quad (66)$$

Substitution of this expression into Eq. (20) for X leads to

$$X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)$$

$$= \frac{\rho^{\mu+1}}{2\mu!\, k_2^{\mu+1}} \int_{-\phi_1}^{\phi_1} d\phi\, e^{i(\mu+1)\phi}(\rho \cos\phi - \beta)^{\mu} W(\lambda; q, p \mid k_1, \rho e^{i\phi}, \alpha). \quad (67)$$

A special case of this formula was derived by Harris and Michels [5]. This integral is evaluated by numerical quadrature with W obtained by recurrence as in the first infinite series.

F. *Recurrence Procedure*: *XREC*

The last of the methods used to evaluate X integrals utilizes a series of recurrence relations. These all follow from properties of $j_n(z)$ and relate X integrals with the same k_1, k_2, α, and β but differing values of λ, μ, p, and q. The procedure used here is based on a series of three-term recurrence relations in which only μ and q

vary. These relations are shown diagrammatically in Fig. 3. The equations and their derivation are given in Appendix A. It is also shown in Appendix A that the same relations are applicable to Z integrals if the sign of each term in H is reversed.

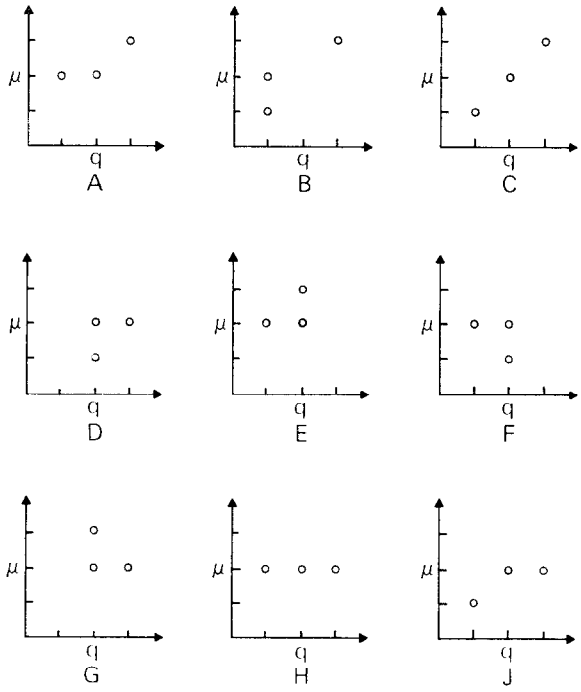

FIG. 3. Diagrams defining recurrence relations used in the XREC method. Small circles denote parameter values connected by a recurrence relation.

Using the recurrence relations in μ and q for both X and Z, which are represented by Fig. 3, the recurrence procedure shown in Fig. 4 is constructed. As shown there, this procedure starts with $Z(0, 0; 0, 0 \mid k_2, k_1, \beta, \alpha)$. This integral is obtained most rapidly and accurately by the second infinite series XSER2, which is found to converge satisfactorily for X and/or Z in the case $\lambda = \mu = p = q = 0$. In the second step of the procedure a special formula is employed for $Z(0, 1; 0, 1 \mid k_2, k_1, \beta, \alpha)$. This formula follows from the relation represented by diagram C of Fig. 3 and derived in Appendix B in the form

$$k_1 Z(0, 1; 0, 1 \mid k_2, k_1, \beta, \alpha) = -\alpha Z(0, 0; 0, 0 \mid k_2, k_1, \beta, \alpha) + \tan^{-1}(k_2/\beta)/k_2 - H(0, 0; 0 \mid k_2, k_1, \alpha + \beta), \tag{68}$$

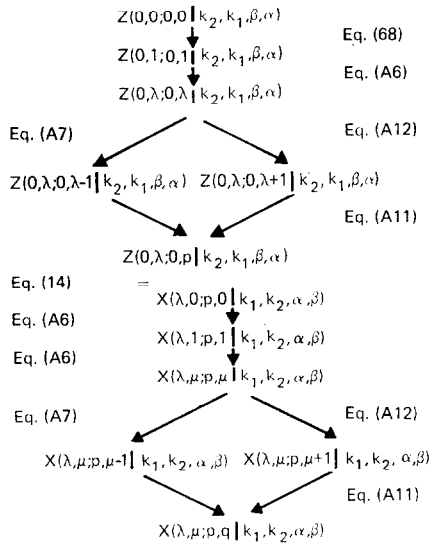

FIG. 4. Schematic representation of the recurrence procedure for obtaining $X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)$.

where

$$H(0, 0; 0 \mid k_2, k_1, \alpha + \beta) = \frac{1}{2k_1k_2}\left[(k_1 + k_2)\tan^{-1}\left(\frac{k_1 + k_2}{\alpha + \beta}\right) - (k_1 - k_2)\tan^{-1}\left(\frac{k_1 - k_2}{\alpha + \beta}\right)\right] - \frac{\alpha + \beta}{4k_1k_2}\ln\left[\frac{(\alpha + \beta)^2 + (k_1 + k_2)^2}{(\alpha + \beta)^2 + (k_1 - k_2)^2}\right]. \tag{69}$$

Using these first two Z integrals, Eq. (A6) can be used to obtain $Z(0, \lambda; 0, \lambda \mid k_2, k_1, \beta, \alpha)$. Figure 3H can then be used to recur either upward or downward in p to obtain $Z(0, \lambda; 0, p \mid k_2, k_1, \beta, \alpha)$ providing that first either $Z(0, \lambda; 0, \lambda - 1 \mid k_2, k_1, \beta, \alpha)$ or $Z(0, \lambda; 0, \lambda + 1 \mid k_2, k_1, \beta, \alpha)$ has been found. These follow from Fig. 3D and Fig. 3J, respectively, except in the special case $\lambda = 0, p > 0$. In that case, a special formula for Z is used:

$$Z(0, 0; 0, 1 \mid k_2, k_1, \beta, \alpha) = \left\{\tan^{-1}(k_2/\beta) - 1/2\tan^{-1}\left(\frac{k_1 + k_2}{\alpha + \beta}\right) + 1/2\tan^{-1}\left(\frac{k_1 - k_2}{\alpha + \beta}\right) + \frac{\alpha}{4k_1}\ln\left[\frac{(\alpha + \beta)^2 + (k_1 - k_2)^2}{(\alpha + \beta)^2 + (k_1 + k_2)^2}\right]\right\}\Big/[(\alpha^2 + k_1^2)k_2]. \tag{70}$$

This is also derived in Appendix B.

At this point Eq. (14) is used to give

$$X(\lambda, 0; p, 0 \mid k_1, k_2, \alpha, \beta) = Z(0, \lambda; 0, p \mid k_2, k_1, \beta, \alpha). \tag{71}$$

The same procedure is then followed in μ and q for X integrals as was employed in λ and p for Z integrals. Thus, $X(\lambda, 1; p, 1 \mid k_1, k_2, \alpha, \beta)$ is obtained from Fig. 3C in the special case $q = 1$. Then Fig. 3C gives $X(\lambda, \mu; p, \mu \mid k_1, k_2, \alpha, \beta)$. From this integral, Fig. 3H gives $X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)$ after the starting points $X(\lambda, \mu; p, \mu - 1 \mid k_1, k_2, \alpha, \beta)$ or $X(\lambda, \mu; p, \mu + 1 \mid k_1, k_2, \alpha, \beta)$ are obtained from Fig. 3D or Fig. 3J, respectively. Again in the special case $\mu = 0$, $q > 0$, a specific formula is required for the starting point. It is easily shown that

$$X(\lambda, 0; p, 1 \mid k_1, k_2, \alpha, \beta) = \operatorname{Im}\left\{\frac{1}{\beta - ik_2} G(\lambda; p \mid k_1, \alpha + \beta - ik_2)\right\}/k_2. \tag{72}$$

Thus, in principle, any X integral can be obtained by this recurrence prescription though the process is quite lengthy and tedious and requires the calculation of numerous H integrals along the way.

III. Numerical Considerations: Choice of Method

Exhaustive calculations of X integrals were performed with each of the methods to determine accuracy and computation time as functions of the eight parameters. Most of these tests were carried out in the BASIC language on the CALL/360 computer terminal system. This made possible such techniques as effortless repetition of identical calculations in single and double precision. It was also possible with this approach to examine details of each of the methods in order to understand their regions of applicability and rates of convergence. For example, it was found that in certain special cases, the second infinite series has a zero for every fourth term in the sum. Knowledge of this sort of detail has made it possible greatly to improve the performance of programs for these algorithms. The accuracy of a specific X integral was determined by observing the number of digits in agreement between single and double precision calculations or between calculations by two independent methods. In addition, use was made of the fact that any desired X integral can be obtained very easily from the corresponding Z integral by the simple transformation of Eq. (15). Thus, each of the methods could be used either for X or for Z. Using these techniques we determined ranges of the parameters for which each of the methods will give results accurate to not less than eight significant digits for the parameter range:

$$0 \leqslant \lambda, \quad \mu \leqslant 5,$$
$$0 \leqslant p, \quad q \leqslant 20,$$
$$0 \leqslant k_1, k_2 \leqslant 2.0,$$
$$0.1 \leqslant \alpha, \quad \beta \leqslant 20.0.$$

Since the X integral depends in a complex way on eight parameters, it is difficult to obtain a clear concept of its analytical behavior. Some general observations can be made, however, and are of value in examining the applicability of each of the methods. First it is clear that the integrand is oscillatory in each of the two integration variables. Furthermore, this behavior becomes more pronounced as α and β become smaller relative to k_1 and k_2, respectively, and as λ and μ increase. Thus, one would expect to have greater difficulty in evaluating X for small α and β and large λ and μ. This is borne out by our experience. It is also of value to realize that the character of the X integral function is closely tied to the surfaces $p = 2\lambda$ and $q = 2\mu$. It was shown in paper I that G integrals are rational functions for $p > 2\lambda$ and transcendental for $p \leqslant 2\lambda$. The same pattern holds for X integrals with the result that X is most easily calculated for both $p > 2\lambda$ and $q > 2\mu$; while if either $p > 2\lambda$ or $q > 2\mu$, X is better behaved than when both p and q are small relative to 2λ and 2μ.

Our aim has been to determine a means for calculating a general set of X integrals to specified accuracy with minimum computational time. In this process the parameter space was split into four regions as follows:

$$\text{I: } p \leqslant 2\lambda \text{ and } q \leqslant 2\mu, \qquad \text{A: } \alpha \leqslant k_1 \text{ and } \beta \leqslant k_2,$$
$$\text{II: } p > 2\lambda \text{ or } q > 2\mu, \qquad \text{B: } \alpha > k_1 \text{ or } \beta > k_2.$$

Tests were carried out in each region on all methods applicable in that region. The most rapid was used first to calculate as many integrals as possible. The second most rapid method was then utilized on as many of the remaining integrals as possible. Continuing in this way an algorithm was developed to determine which method to utilize for a given set of parameters. The most difficult cases are those in region IA in which $k_1 \cong k_2$ with α and β much smaller than k_1 and k_2 and with λ and μ large. Fortunately, these X integrals, when normalized, are also relatively quite small and will be of lesser significance in a calculation.

The considerations about the individual methods which were used in this process are the following: XDEG is the quickest and most accurate method. Since in this method the X integral reduces to a G integral and methods have been presented for the accurate calculation of any G integral [4], there is never a question of accuracy. XDEG is used whenever applicable, i.e., when $\lambda = \mu, p = q, k_1 = k_2$, and $\alpha = \beta$.

XSER1 is the second most rapid method for calculating X. This series converges when $k_2 < \beta$. Thus, it can be applied to calculate Z instead of X when $k_1 < \alpha$. It is found to become inaccurate as the number of terms required for convergence increases. Thus, XSER1 should not be used for k_2 larger than some threshold value which we have taken to be 0.6β.

XSUM applies when $q > 2\mu$ in an X integral or likewise when $p > 2\lambda$ in Z The sum is found to be accurate for X only when k_2 is greater than some threshold value. The minimum value of k_2 has been taken to be 0.1 in our calculations. XSUM is comparable in time to XSER1 and is used when applicable after XSER1 in preference.

XSER2 requires about the same length of time as XSER1. However, it has not been possible to determine a precise region of convergence for this series. In fact, if precautions are taken in the handling of very large and very small numbers, this series is found to converge in the case $\lambda = \mu = p = q = 0$ for all values of the parameters k_1, k_2, α, and β. However, the number of terms required for a specified accuracy becomes very large in some cases and, consequently, the method becomes rather slow. Moreover, as the values of λ, μ, p, and q increase the number of terms increases rapidly, the sum becomes numerically less accurate, and the series fails to converge with increasing frequency. In practice, though this series often provides a very rapid and accurate means of calculating X, its value is seriously diminished by the vagueness concerning its region of convergence. Experience in a great many calculations of X integrals with this series has shown that speed and accuracy improve as α and β become larger relative to k_1 and as λ, μ, p, and q decrease. Exact values of these parameters which may be used to obtain specified accuracy must be determined empirically. XSER2 is used when the previous methods are not applicable for cases in which experience has shown the method to be reliable.

XCI is about 1/2 to one order of magnitude slower than XSER1 when a sixteen point Gaussian quadrature formula is used. The method is quite generally applicable, though as α and β become small relative to k_1 and k_2, particularly when $k_1 \cong k_2$, more points are required to yield consistent accuracy. XCI is used when none of the above methods will work, unless α and β are very small.

XREC is the last choice because it is extremely slow. In general, it requires ten to twenty times as much computing time as XSER1. It is used only when none of the other methods will produce reliable results. This is mainly in region IA when $\alpha \ll k_1$, $\beta \ll k_2$, and $k_1 \cong k_2$. Even XREC becomes less accurate as these conditions become more pronounced but, as mentioned earlier, these values tend to represent a very small contribution in an actual scattering calculation. We were not able to derive a method for calculating X integrals which improves in accuracy and speed as α and β decrease in value. This would clearly be of considerable value.

The properties of the six methods listed above can be combined in an algorithm to select one of the methods for a given set of the eight parameters. This algorithm is presented in block diagram form as Fig. 5. This lists clearly the criteria used,

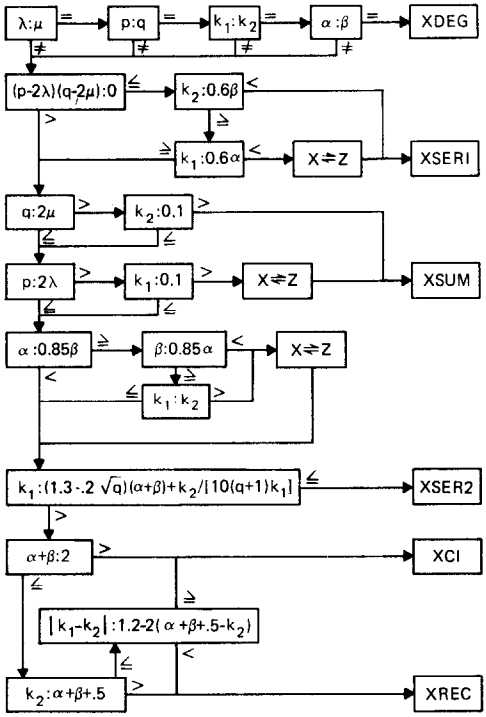

FIG. 5. Algorithm to select among the six methods of calculating an X integral.

the order in which the choice is made, and in which cases the result is obtained through X and which through Z. The switch from Z back to X in these cases is always accurate and represents the transformation of Eq. (15). This algorithm was tested exhaustively over a grid of reasonable mesh size in each of the eight parameters. In each case X was calculated by the method indicated by Fig. 5 and also by XCI using a 64 point quadrature formula. A table was produced giving the numbers of integrals calculated by each method and the number and details of all cases in which the two results differed by more than 10^{-10}. These results are summarized in Table I for the four regions indicated above. The average time for calculation of an X integral was found to be 0.038 sec on an IBM 360/91 computer system in calculations of over 10^5 X integrals.

TABLE I

Results of Tests of Selection Algorithm Shown in Fig. 5.[a]

	IA	IB	IIA	IIB
XDEG	135	144	120	128
XSUM	0	0	18592	26224
XSER1	0	18828	0	21696
XSER2	5969	3645	2184	1232
XCI	1231	63	0	0
XREC	2385	0	224	0
Total	9720	22680	22120	49280
Average time	0.056	0.037	0.038	0.035

[a] Number of integrals done by each method in each region and average time in seconds per integral.

IV. Summary

The methods presented above are useful for the rapid and accurate calculation of X integrals. In the only case in which difficulty still is encountered, the case $\alpha \ll k_1$, $\beta \ll k_2$, with $k_1 \cong k_2$, the values after normalization are orders of magnitude smaller than more accurate X integrals. So it is felt this is not a major obstacle. However, these integrals do require more time for evaluation. Thus, it would be of interest to have an additional means for evaluation of X which would improve in speed and accuracy as cases move further into this region.

A program which embodies the techniques described in this paper has been employed very successfully in calculations of e^-–H and e^-–He elastic scattering [7].

We have not taken into account here any advantage gained when an entire set of integrals can be obtained by a single recurrence procedure. The integrals required in our practical calculations have varying exponent parameters α and β as well as powers of r. In general, the computational disadvantage of the recurrence procedure XREC appeared to outweigh any possible saving from producing several integrals at once.

Since the completion of our work, a new method for computing the integrals considered here has been published by Ramaker [8]. A detailed comparison of this method with those considered here for X integrals has not yet been carried out.

APPENDIX A

The recurrence relations for X integrals are derived from the properties of $j_n(z)$. Using the derivative formula for the spherical Bessel function (HMF, 10.1.24)

$$(1/z)(d/dz)[z^{-n+1}j_{n-1}(z)] = -z^{-n}j_n(z) \tag{A1}$$

in an integration by parts of y gives

$$\begin{aligned} &y(\mu, q, k_2, \beta \mid r) \\ &\quad = (1/k_2)\,\chi(\mu - 1, q - 1, k_2, \beta \mid r) - (\beta/k_2)\,y(\mu - 1, q - 1, k_2, \beta \mid r) \\ &\qquad + \left[\frac{q-1}{k_2}\,y(\mu - 1, q - 2, k_2, \beta \mid r)\right]_{q>1}, \end{aligned} \tag{A2}$$

where the term in brackets is present only if q is greater than 1. Substituting this in X gives the first recurrence relation

$$\begin{aligned} &k_2X(\lambda, \mu; p, q + 1 \mid k_1, k_2, \alpha, \beta) + \beta X(\lambda, \mu - 1; p, q \mid k_1, k_2, \alpha, \beta) \\ &\quad - H(\lambda, \mu - 1; p + q \mid k_1, k_2, \alpha + \beta) \\ &\quad - [qX(\lambda, \mu - 1; p, q - 1 \mid k_1, k_2, \alpha, \beta)]_{q>0} = 0 \end{aligned} \tag{A3}$$

Figure 3A represents this relationship. A second recurrence relation follows from the usual recurrence relation for $j_n(z)$ (HMF, 10.1.19)

$$zj_{n-1}(z) + zj_{n+1}(z) = (2n + 1)\,j_n(z) \tag{A4}$$

which leads to

$$\begin{aligned} &k_2X(\lambda, \mu - 1; p, q - 1 \mid k_1, k_2, \alpha, \beta) + k_2X(\lambda, \mu + 1; p, q + 1 \mid k_1, k_2, \alpha, \beta) \\ &\quad - (2\mu + 1)\,X(\lambda, \mu; p, q - 1 \mid k_1, k_2, \alpha, \beta) = 0. \end{aligned} \tag{A5}$$

This equation is shown diagrammatically as Fig. 3B. Equations (A3) and (A5) may be combined to give the two relations:

$$\begin{aligned} &[qk_2X(\lambda, \mu - 1; p, q - 1 \mid k_1, k_2, \alpha, \beta)]_{q>0} - (2\mu + 1)\,\beta X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) \\ &\quad + (q - 2\mu - 1)\,k_2X(\lambda, \mu + 1; p, q + 1 \mid k_1, k_2, \alpha, \beta) \\ &\quad + (2\mu + 1)\,H(\lambda, \mu; p + q \mid k_1, k_2, \alpha, \beta) = 0, \end{aligned} \tag{A6}$$

and

$$\begin{aligned} &k_2X(\lambda, \mu - 1; p, q \mid k_1, k_2, \alpha, \beta) + (q - 2\mu)\,X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta) \\ &\quad - \beta X(\lambda, \mu; p, q + 1 \mid k_1, k_2, \alpha, \beta) + H(\lambda, \mu; p + q + 1 \mid k_1, k_2, \alpha + \beta) = 0, \end{aligned} \tag{A7}$$

corresponding to Figs. 3C and 3D, respectively. These four equations may be further combined to yield the relations of Figs. 3E, 3F, and 3G as the following forms:

$$\begin{aligned}&[q\beta X(\lambda, \mu; p, q-1 \mid k_1, k_2, \alpha, \beta)] - (\beta^2 + k_2^2)\, X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)\\ &\quad - (q - 2\mu - 2)\, k_2 X(\lambda; \mu + 1; p, q \mid k_1, k_2, \alpha, \beta)\\ &\quad + \beta H(\lambda, \mu; p + q \mid k_1, k_2, \alpha + \beta)\\ &\quad - k_2 H(\lambda, \mu + 1; p + q + 1 \mid k_1, k_2, \alpha + \beta) = 0, \end{aligned} \tag{A8}$$

$$\begin{aligned}&(q - 2\mu - 1)\, q\beta X(\lambda, \mu; p, q-1 \mid k_1, k_2, \alpha, \beta)\\ &\quad + (\beta^2 + k_2^2)\, k_2 X(\lambda, \mu - 1; p, q \mid k_1, k_2, \alpha, \beta)\\ &\quad + [(q - 2\mu)\, k_2^2 - q\beta^2]\, X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)\\ &\quad + q\beta H(\lambda, \mu; p + q \mid k_1, k_2, \alpha + \beta)\\ &\quad - \beta k_2 H(\lambda, \mu - 1, p + q \mid k_1, k_2, \alpha + \beta)\\ &\quad + k_2^2 H(\lambda, \mu; p + q + 1 \mid k_1, k_2, \alpha + \beta) = 0, \end{aligned} \tag{A9}$$

and

$$\begin{aligned}&[(q - 2\mu - 1)\, k_2^2 - (q + 1)\, \beta^2]\, X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)\\ &\quad + (\beta^2 + k_2^2)\, \beta X(\lambda, \mu; p, q + 1 \mid k_1, k_2, \alpha, \beta)\\ &\quad + (q - 2\mu - 1)(q - 2\mu - 2)\, k_2 X(\lambda, \mu + 1; p, q \mid k_1, k_2, \alpha, \beta)\\ &\quad + (q - 2\mu - 1)\, k_2 H(\lambda, \mu + 1; p + q + 1 \mid k_1, k_2, \alpha + \beta)\\ &\quad - \beta^2 H(\lambda, \mu; p + q + 1 \mid k_1, k_2, \alpha + \beta)\\ &\quad + \beta k_2 H(\lambda, \mu + 1; p + q + 2 \mid k_1, k_2, \alpha + \beta) = 0. \end{aligned} \tag{A10}$$

Next, Eqs. (A7) and (A9) or alternatively Eqs. (A8) and (A10) may be combined to produce

$$\begin{aligned}&(q - 2\mu - 1)\, q\beta X(\lambda, \mu; p, q-1 \mid k_1, k_2, \alpha, \beta)\\ &\quad - 2(q - \mu)\, \beta^2 X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)\\ &\quad + (\beta^2 + k_2^2)\, \beta X(\lambda, \mu; p, q + 1 \mid k_1, k_2, \alpha, \beta)\\ &\quad - \beta k_2 H(\lambda, \mu - 1; p + q \mid k_1, k_2, \alpha + \beta)\\ &\quad + q\beta H(\lambda, \mu; p + q \mid k_1, k_2, \alpha + \beta)\\ &\quad - \beta^2 H(\lambda, \mu; p + q + 1 \mid k_1, k_2, \alpha + \beta) = 0 \end{aligned} \tag{A11}$$

corresponding to Fig. 3H.

The last relation needed in the recurrence procedure is the one which corresponds to Fig. 3J. By combining Eqs. (A7) and (A8) this equation is obtained as

$$qk_2X(\lambda, \mu - 1; p, q - 1 \mid k_1, k_2, \alpha, \beta) + (q - 2\mu)\,\beta X(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)$$
$$- (\beta^2 + k_2^2)\,X(\lambda, \mu; p, q + 1 \mid k_1, k_2, \alpha, \beta)$$
$$+ k_2 H(\lambda, \mu - 1; p + q \mid k_1, k_2, \alpha + \beta)$$
$$+ \beta H(\lambda, \mu; p + q + 1 \mid k_1, k_2, \alpha + \beta) = 0. \tag{A12}$$

These same relationships may be applied to Z integrals simply by replacing X with Z and changing the sign of each term in H. This may be shown as follows. By substituting Eq. (15) for X into Eq. (A3) and using recurrence relations between G integrals given in paper I we obtain

$$qZ(\lambda, \mu; p, q - 1 \mid k_1, k_2, \alpha, \beta) - \beta Z(\lambda, \mu; p, q \mid k_1, k_2, \alpha, \beta)$$
$$- k_2 Z(\lambda, \mu + 1; p, q + 1 \mid k_1, k_2, \alpha, \beta)$$
$$- H(\lambda, \mu; p + q \mid k_1, k_2, \alpha + \beta) = 0, \tag{A13}$$

which corresponds to Fig. 3A for Z integrals. The recurrence relation for $j_n(z)$, Eq. (A4), leads to exactly the same relation for Z as given for X in Eq. (A5). Combining these two relations for Z, as done above, for X gives the same set of equations with the sole exception that the sign preceding each term in H has now been reversed.

Appendix B

Equations (68) and (69) are derived starting from the version of Eq. (A6) which applies to Z integrals in the case $\lambda = \mu = p = q = 0$:

$$k_1 Z(0, 1; 0, 1 \mid k_2, k_1, \beta, \alpha)$$
$$= -\alpha Z(0, 0; 0, 0 \mid k_2, k_1, \beta, \alpha) - H(0, 0; 0 \mid k_1, k_2, \alpha + \beta)$$
$$+ \lim_{q \to 0} [qk_1 Z(0, -1; p, q - 1 \mid k_2, k_1, \beta, \alpha)]. \tag{B1}$$

The last term in Eq. (B1) is simply $G(0; 0 \mid k_2, \beta)$ and thus Eq. (68) follows by using Eq. (45) of paper I to evaluate this integral.

The evaluation of the H integral to give Eq. (69) presents somewhat greater difficulty. By definition,

$$H(0, 0; 0 \mid k_1, k_2, \alpha) = \int_0^\infty j_0(k_1 r)\, j_0(k_2 r)\, e^{-\alpha r}\, dr. \tag{B2}$$

Using the Poisson integral representation for $j_n(z)$ (HMF, 10.1.13) leads to

$$H(0, 0; 0 \mid k_1, k_2, \alpha) = \frac{1}{4}\int_{-1}^{1} ds \int_{-1}^{1} dt \int_{0}^{\infty} dr \exp\{-[\alpha - i(k_1 s + k_2 t)]\, r\} \quad \text{(B3)}$$

$$= \frac{1}{4}\int_{-1}^{1} ds \int_{-1}^{1} dt \frac{1}{\alpha - i(k_1 s + k_2 t)}. \quad \text{(B4)}$$

The substitution $\zeta = \alpha - i(k_1 s + k_2 t) = \rho e^{i\phi}$ may then be employed. The integrand is analytic everywhere except at $\zeta = 0$. A contour must be selected which avoids the singularity and simplifies the integral as much as possible. For the inner integration (on t) the path is broken into two sections, one at constant ϕ and the second at constant ρ. This results in

$$H(0, 0; 0 \mid k_1, k_2, \alpha) = \frac{1}{4k_2}\int_{-1}^{1} ds \left\{\frac{i}{2} \ln\left[\frac{\alpha^2 + (k_1 s + k_2)^2}{\alpha^2 + (k_1 s - k_2)^2}\right]\right.$$
$$\left. - \tan^{-1}\left[\frac{k_1 s - k_2}{\alpha}\right] + \tan^{-1}\left[\frac{k_1 s + k_2}{\alpha}\right]\right\}. \quad \text{(B5)}$$

It is seen at this point that the imaginary term is an odd function of s and, thus, its contribution vanishes over the symmetric limits. The remaining terms can be combined in the form

$$H(0, 0; 0 \mid k_1, k_2, \alpha) = \frac{1}{2k_1 k_2}\int_{k_2 - k_1}^{k_2 + k_1} du \tan^{-1}\left(\frac{u}{\alpha}\right). \quad \text{(B6)}$$

Integrating this function produces the expression given as Eq. (69).

The derivation of Eq. (70) follows mainly from the application of results presented in paper I. From Eq. (15),

$$Z(0, 0; 0, 1 \mid k_2, k_1, \beta, \alpha) = G(0; 0 \mid k_2, \beta)\, G(0; 1 \mid k_1, \alpha)$$
$$- X(0, 0; 0, 1 \mid k_2, k_1, \beta, \alpha), \quad \text{(B7)}$$

where

$$G(0; 0 \mid k_2, \beta) = (1/k_2) \tan^{-1}(k_2/\beta) \quad \text{(B8)}$$

and

$$G(0; 1 \mid k_1, \alpha) = 1/(\alpha^2 + k_1^2), \quad \text{(B9)}$$

from Eqs. (45) and (42) of paper I, respectively. Also from Eq. (53) of this paper and Eq. (60) of paper I,

$$X(0, 0; 0, 1 \mid k_2, k_1, \beta, \alpha) = \operatorname{Im}\left\{\frac{1}{k_1} W(0; 0, 0 \mid k_2, \alpha - ik_1, \beta)\right\} \quad \text{(B10)}$$

$$= \frac{1}{k_1} \operatorname{Im}\left\{\frac{1}{\alpha - ik_1} G(0; 0 \mid k_2, \alpha + \beta - ik_1)\right\}. \quad \text{(B11)}$$

This is expressed in terms of a hypergeometric function through Eq. (67) of I which may then be evaluated through (HMF, 15.1.4) to give

$$X(0, 0; 0, 1 \mid k_2, k_1, \beta, \alpha) = \frac{1}{2k_1k_2} \operatorname{Im}\left\{\frac{i}{\alpha - ik_1} \ln\left[\frac{\alpha + \beta - ik_1 - ik_2}{\alpha + \beta - ik_1 + ik_2}\right]\right\}. \quad \text{(B12)}$$

The imaginary part of this final expression may be combined with Eqs. (B7)–(B9) to give Eq. (70).

Appendix C

During the course of the development of techniques for evaluating X and during further testing of G, H, and I integrals subsequent to the publication of paper I, other methods were found for G, H, and I integrals. In the case of H and I, these other techniques have proved superior to those previously described and are being employed in our calculations. The method of paper I for G integral is still being used though an additional method is presented here for completeness.

The new method for G and H integrals is analogous to XCI and follows also from the Poisson integral representation of $j_n(z)$. Substitution of Eq. (63) into Eq. (4) leads to

$$\begin{aligned} G(\lambda; p \mid k_1\alpha) &= \frac{{k_1}^\lambda}{2^{\lambda+1}\lambda!} \int_{-1}^{1} dt(1 - t^2)^\lambda \int_0^\infty dr\, e^{-(\alpha - ik_1t)r} r^p \\ &= \frac{{k_1}^\lambda}{2^{\lambda+1}\lambda!} \int_{-1}^{1} dt(1 - t^2)^\lambda \frac{p!}{(\alpha - ik_1t)^{p+1}}. \end{aligned} \quad \text{(C1)}$$

Transformation to a contour at constant distance from the origin in the complex plane as used in XCI and some rearrangement of terms yields the form

$$G(\lambda; p \mid k_1, \alpha) = \frac{p!\,\rho^{2\lambda - p}}{\lambda!\,{k_1}^{\lambda+1}} \int_0^\Phi d\phi \cos[(\rho - \lambda)\,\phi] \left(\cos\phi - \frac{\alpha}{\rho}\right)^\lambda, \quad \text{(C2)}$$

where

$$\begin{aligned} \rho^2 &= \alpha^2 + {k_1}^2, \\ \Phi &= \tan^{-1}(k_1/\alpha). \end{aligned} \quad \text{(C3)}$$

The same technique applied to the spherical Bessel function $j_\mu(k_1r)$ in H produces the result

$$\begin{aligned} H(\lambda, \mu; p \mid k_1, k_2, \alpha) = \frac{\rho^{\mu+1}}{\mu!\,{k_2}^{\mu+1}} \int_0^\Phi d\phi[\rho\cos\phi - \alpha]^\mu \\ \times \{\cos[(\mu + 1)\,\phi] \operatorname{Re}[G(\lambda; p \mid k_1, \rho e^{-i\phi})] \\ + \sin[(\mu + 1)\,\phi] \operatorname{Im}[G(\lambda; p \mid k_1, \rho e^{-i\phi})]\}, \end{aligned} \quad \text{(C4)}$$

where use has been made of the relations

$$\begin{aligned} \mathrm{Re}[G(\lambda; p \mid k, z)] &= \mathrm{Re}[G(\lambda; p \mid k, z^*)], \\ \mathrm{Im}[G(\lambda; p \mid k, z)] &= -\mathrm{Im}[G(\lambda; p \mid k, z^*)]. \end{aligned} \tag{C5}$$

An alternative formula for H may be obtained by using the Poisson integral representation for both $j_\lambda(k_1 r)$ and $j_\mu(k_2 r)$ in the definition of H. The resulting expression was found to be less useful than Eq. (C4). In our work, H integrals are calculated either by Eq. (C4) or by the finite sum method presented in paper I. Numerical quadrature of Eq. (C4) with a 16 point Gauss formula is found to be sufficiently accurate and rapid for all cases where the finite sum formula is not applicable. The recurrence method for H integrals described in paper I is always slower.

Two complementary formulas have been employed for the calculation of I integrals. One or the other of these is found to be rapid and accurate for every case and always superior to considering I as the limit of H as α goes to zero as proposed in paper I. The basic formula is given as Eq. (A10) of paper I. This formula is valid for $k_1 < k_2$. Thus, of course, the same formula may be utilized for the case $k_1 > k_2$ by interchanging k_1 with k_2 and λ with μ.

If the two k values are far apart so that the ratio k_1/k_2 is not close to 1, then the usual infinite series for ${}_2F_1(a, b; c; z)$, (HMF, 15.1.1), will converge rapidly. We have found this the most efficient way to calculate I when k_1/k_2 is not close to 1. For $k_1/k_2 \sim 1$, (HMF, 15.3.11) may be used to give a series expansion for ${}_2F_1(a, b; c; z)$ which converges more rapidly as the ratio approaches 1. This method is entirely complementary to the previous case: Whenever the first expansion decreases in efficiency, the second improves. The two formulas cover all cases very well.

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