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Evaluation of Atomic Scattering Integrals by Numerical Techniques

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Integrals needed in calculations of electron scattering off atoms are solved. The basis functions consist of Slater-type functions to describe the bound-like character of the wavefunction, and spherical Bessel functions of the first and second kind for the free particle portion. A damping factor is used with the latter Bessel function to insure proper behavior at the origin. With integral representations of the Bessel functions, numerical techniques are developed to obtain all one- and two-electron integrals.

INTRODUCTION

Theories of electron scattering off atoms and molecules entail an expansion of the total wavefunction in terms of bound state functions and a scattering function which displays an appropriate asymptotic behavior. In particular

$$\Psi = \sum_n \mathcal{A}\{\Phi_n(1, 2,..., n)\, \chi_n(n+1)\}, \tag{1}$$

where $\mathcal{A}$ is the antisymmetrizer, may be considered as well as wavefunctions containing additional terms which account for the bound-like character. Whatever the choice, solutions for the basic integrals which arise will be solved in this paper. Here

$$\mathscr{H}^0\Phi_n = E_n{}^0\Phi_n \qquad (n = 1, 2,...) \tag{2}$$

are the solutions of the target state, and

$$\mathscr{H}\Psi = E\Psi \tag{2'}$$

is Schrödinger's equation for the scattering problem, where

$$\mathscr{H} = \mathscr{H}^0 + V(n+1) - \tfrac{1}{2}\nabla^2_{n+1},$$

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$V(n+1)$ is the potential interaction between the scattering electron and the target, and $E = E_n^0 + \frac{1}{2}k_n^2$. The scattering function is expanded in terms of partial waves

$$\chi_n = \sum_{l=0}^{\infty} d_l \frac{G_l(kr)}{kr} P_l(\cos\theta) \tag{3}$$

which obey the boundary condition $G_l(0) = 0$ and have the asymptotic dependence

$$G_l(kr) \xrightarrow{r\to\infty} kr[j_l(kr) + \tan\eta_l y_l(kr)]. \tag{4}$$

The asymptotic solutions are Bessel functions of the first and second kind. The approximation

$$G_l(r) = \sum_{m=1}^{N} g_m r^m e^{-\alpha_m r} + kr[j_l(kr) + \tan\eta_l F_{2l+1}(cr)\, y_l(kr)], \tag{5}$$

with

$$F_s(cr) = (1 - e^{-cr})^s,$$

has been used by a number of authors [1] to insure proper behavior both at the origin and for large r.

To simplify the integrals required for electron scattering, Armstead [2] proposed the functional form

$$\phi_l(kr) = \left[j_{l+1}(kr) + \frac{l+1}{kr} j_{l+2}(kr)\right] \tag{6}$$

to replace $F_{2l+1} y_l$ in Eq. (5).

An advantage of ϕ_l is that it remains finite as $r \to 0$ without the complication of a damping factor, and the integrals require only the Bessel functions j_l. Also as $r \to \infty$

$$\phi_l(kr) \to -\frac{\cos(kr - (l/2)\,\pi)}{kr}, \tag{7}$$

which yields the correct asymptotic form of y_l.

However, because ϕ_l is not a solution of Bessel's equation, accurate approximations to G_l require many bound-like functions to simulate y_l in the region beyond the vanishing of the potential and before y_l achieves its cosine dependence. This is seen by substituting ϕ_l into Schrödinger's equation for $V = 0$.

$$\mathscr{L}_l\phi_l = \frac{(4l^2 + 8l + 2)}{(kr)^3} j_{l+2}(kr) \xrightarrow{r\to\infty} -\frac{\sin(kr - (l/2)\,\pi)}{(kr)^4}, \tag{8}$$

where

$$\mathscr{L}_l = \frac{1}{r}\frac{d^2}{dr^2}r - \frac{l(l+1)}{r^2} + k^2, \tag{9}$$

whereas

$$\mathscr{L}_l F_{2l+1} kry_l \to \mathscr{L}_l kry_l = 0 \tag{10}$$

if c is chosen such that $F_{2l+1} \to 1$ when the potential becomes vanishingly small. The right hand side of Differential Eq. (8) approaches zero as $(kr)^{-4}$. As the incident energy (and also k) decreases, larger values of r must be attained before $\mathscr{L}_l\phi_l$ becomes vanishingly small, and consequently, bound-like functions must be employed to construct the free-particle portion of the wavefunction.

To circumvent this problem, asymptotic forms which are solutions of Schrödinger's equation when $V = 0$ (Eq. (9)) are employed in this paper. Although the number of integral types increases as well as difficulty in their evaluation, the author feels that the proper asymptotic form, which is attained just outside the influence of the potential region, will reduce the number of terms in the approximation to G_l. Inclusion of the damping factor with y_l in Eq. (5) increases the complexity of the recursion relations for analytical evaluation to the extent that up to six dimensional arrays must be formed. This dilemma led to examination of numerical techniques based on integral representations because (i) they can be used routinely throughout the entire formulation, thereby reducing the possibility of errors in the coding of the integrals, and (ii) these techniques can be used to check the faster analytical methods as they are coded.

The basic types of integrals [3] needed for the linear variational procedures of Kohn, Hulthén, and Feshbach and Rubinow [4] have already been set forth for more restricted cases using the approximation Eq. (6), and they are essentially the same as needed here. The following five one-electron integrals

$$\int_0^\infty dr\, r^p e^{-\alpha r} \mathscr{J}_l(h, r) \qquad (p \geqslant -l), \tag{11}$$

$$\int_0^\infty dr\, r^p e^{-\alpha r} \mathscr{J}_l(h, r)\, \mathscr{K}_m(k, r) \qquad (p \geqslant -l - m), \tag{12}$$

and four two-electron integrals

$$\int_0^\infty dr\, r^p e^{-\alpha r} \mathscr{J}_l(h, r) \int_r^\infty dv\, v^q e^{-\beta v} \mathscr{K}_m(k, v) \tag{13}$$

arise, where $p \geqslant -l$, $q \geqslant -m$, and $\mathscr{J}_l$ and $\mathscr{K}_m$ are $j_\mu(hr)$ and/or $F_{2\mu+1}(cr)\, y_\mu(kr)$ for $\mu = l$ and m.

Integral representations of the Poisson type [5]

$$j_l(z) = \frac{z^l}{2^l l!} \int_0^1 d\eta\, (1 - \eta^2)^l \cos(z\eta) \tag{14}$$

and

$$y_l(z) = \frac{z^l}{2^l l!} \left\{ \int_0^1 d\eta\, (1 - \eta^2)^l \sin(z\eta) - \int_0^\infty d\xi\, e^{-z\xi}(1 + \xi^2)^l \right\} \tag{15}$$

give rise to integrands containing Fourier and Laplace transforms and variations of these transforms over the part of the infinite interval after integration over r has been performed. The resulting integrands are polynomial-like, and consequently, Gauss-Quadrature can be applied. In all, nine types of integrals will be evaluated. In subsequent sections the variables η (and $\bar{\eta}$) and ξ (and $\bar{\xi}$) will be reserved for integration on the intervals [0, 1] and [0, ∞] respectively. Modified weighting factors ω and ρ introduced with Integrals I and II for transformations $\eta = (1 + x)/2$ and $\xi = (1 + x)/(1 - x)$ to the Legendre interval are used consistently throughout this paper. For convenience the following coefficients are defined:

$$a_l(h) = \frac{h^l}{2^l l!}, \tag{16}$$

and

$$b_\mu{}^s = \binom{s}{\mu} (-1)^\mu. \tag{17}$$

In the presentation upper case Latin letters will be used to define the integrals and upper case script letters will be used to denote their corresponding integrands. The sine and cosine Fourier transforms encountered are

$$\begin{aligned} C_p(\alpha, h) &= \int_0^\infty dr\, r^p e^{-\alpha r} \cos(hr) \\ &= p! \left[\frac{\alpha}{\alpha^2 + h^2}\right]^{p+1} \sum_{m=0}^{[(p+1)/2]} (-1)^m \binom{p+1}{2m} \left(\frac{h}{\alpha}\right)^{2m} \end{aligned} \tag{18}$$

and

$$\begin{aligned} S_p(\alpha, h) &= \int_0^\infty dr\, r^p e^{-\alpha r} \sin(hr) \\ &= p! \left[\frac{\alpha}{\alpha^2 + h^2}\right]^{p+1} \sum_{m=0}^{[p/2]} (-1)^m \binom{p+1}{2m+1} \left(\frac{h}{\alpha}\right)^{2m+1}. \end{aligned} \tag{19}$$

These sums are polynomials in h of degree $2[(p + 1)/2]$ and $2[p/2] + 1$ respectively, modified by the damping factor $(\alpha^2 + h^2)^{-p-1}$ which doesn't significantly alter the near polynomial character of these transforms over small ranges of h. In practice ht will appear in place of h were t is ξ or η.

One-Electron Integrals

Integral I

That

$$\begin{aligned} A_l^n(\alpha, h) &= \int_0^\infty dr\, r^n e^{-\alpha r} j_l(hr) \\ &= a_l(h) \int_0^1 d\eta\, (1 - \eta^2)^l\, C_{n+l}(\alpha, h\eta) \end{aligned} \tag{20}$$

with $n \geqslant l$ can be obtained directly by use of Eq. (14) and integration over r. Since the Fourier cosine transform is nearly a polynomial in η, the integrand of Eq. (20) is well represented by a polynomial of order $N = l + 2[(n + l + 1)/2]$. With the transformation $\eta = (1 + x)/2$, the Gauss–Legendre quadrature becomes

$$A_l^n = h^l \sum_{i=1}^{N} \omega_i^l C_{n+l}(\alpha, h\eta_i), \tag{21}$$

where the weighting factors

$$\omega_i^l = w_i \frac{(1 - \eta_i^2)^l}{2^{l+1} l!} \tag{22}$$

are related to w_i and x_i, the weights and zeros respectively of order N. Throughout this paper this definition of ω_i^l and the relationship between η_i and x_i will be retained.

Integral II

$$\begin{aligned} B_l^n(\alpha, h, c) &= \int_0^\infty dr\, r^n e^{-\alpha r} y_l(hr)\, F_{2l+1}(cr) \\ &= a_l(h) \left\{ \int_0^1 d\eta\, (1 - \eta^2)^l\, \mathscr{B}_{n+l}^{(1)2l+1}(\alpha, h\eta, c) \right. \\ &\qquad \left. - \int_0^\infty d\xi\, (1 + \xi^2)^l\, \mathscr{B}_{n+l}^{(2)2l+1}(\alpha + h\xi, c) \right\} \end{aligned} \tag{23}$$

with $n \geqslant -l$, where

$$\mathscr{B}_p^{(1)s}(a, h, c) = \int_0^\infty dr\, r^p e^{-ar} \sin(hr)\, F_s(cr)$$
$$= \sum_{\mu=0}^{s} b_\mu{}^s S_p(a + \mu c, h) \tag{24}$$

is a sum of Fourier sine transforms, and

$$\mathscr{B}_p^{(2)s}(a, c) = \int_0^\infty dr\, r^p e^{-ar} F_s(cr)$$
$$= p! \sum_{\mu=0}^{s} b_\mu{}^s (a + \mu c)^{-p-1} \tag{25}$$

is a sum of Laplace transforms.

It is clear that the first integral of Eq. (23) can be evaluated by Gauss–Legendre quadrature. Since $F_s \geqslant 0$, $\mathscr{B}_p^{(2)s} \geqslant 0$, and consequently, one might expect stable recursion relations to exist. These are developed in Appendix I. The integral from 0 to ∞ can be transformed to $-1 \leqslant x \leqslant +1$ by $\xi = (1 + x)/(1 - x)$. This transformation is chosen since $\mathscr{B}^{(2)}$ is of degree $-[3l + 2 + n]$ in ξ for large ξ, and the integrand of Eq. (23) is of degree $-(n + l + 2)$ in ξ. The rapid change of $\mathscr{B}^{(2)}$ for intermediate values of ξ and decay for large values of ξ suggested the above transformation to favor large ξ in a Gauss–Legendre quadrature. In Fig. 1, $a^2\mathscr{B}_0^{(2)2l+1}(a, c)$ is plotted as a function of a. For large ξ, $a \approx h\xi$, and consequently, the transformation $a = (1 + u)/(1 - u)$, $-1 \leqslant u \leqslant 1$, is chosen as a convenience

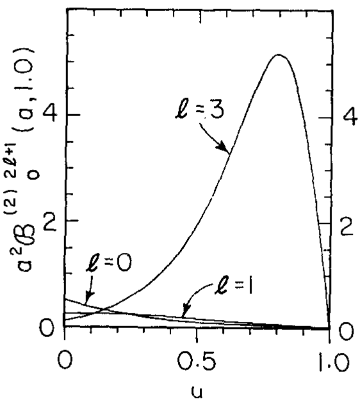


FIG. 1. Demonstration of the near polynomial character of $\mathscr{B}_0^{(2)2l+1}$ over the interval $0 \leqslant u \leqslant 1$ or $1 \leqslant a \leqslant \infty$.

for analysis. Because $a^2\mathscr{B}^{(2)}$ changes slowly for $-1 \leqslant u < 0$, this region is omitted from the figure. The case $n = -l$ is examined because the integrand behaves like a^{-2} for large a.

$a^{2l}\mathscr{B}^{(2)}$ is seen to vary slowly over the range of $0 \leqslant u \leqslant 1$; $\mathscr{B}^{(2)}$ can be well represented by a polynomial in a and hence for $0 < \xi < \infty$. The integrand $(1 + \xi^2)^l \mathscr{B}^{(2)2l+1}_{n+l}(\alpha + h\xi, c)$ will behave like $(a^{2l}/h^{2l})\mathscr{B}^{(2)}$ for large ξ, but for small ξ a slight distortion of the curves will result.

For the above transformations the Gauss–Legendre quadrature becomes

$$B_l^n(\alpha, h, c) = h^l \left\{\sum_{i=1}^{N_1} \omega_i{}^l \mathscr{B}^{(1)2l+1}_{n+l}(\alpha, h\eta_i, c) - \sum_{j=1}^{N_2} \rho_j{}^l \mathscr{B}^{(2)2l+1}_{n+l}(\alpha, h\xi_j, c)\right\}, \quad (26)$$

where

$$\rho_i{}^l = w_i \frac{(1 - x_i)^{-2}(1 + \xi_i{}^2)^l}{2^{l-1} l!} \quad (27)$$

is related to the weights w_i and zeros x_i for Gauss–Legendre quadrature of order N_2. Equation (22) defines $\omega_i{}^l$ for order N_1. Throughout this paper this definition of $\rho_i{}^l$ and the transformation between x_i and ξ_i already mentioned will be retained.

INTEGRAL III

$$\begin{aligned} D^n_{lm}(\alpha, h, k) &= \int_0^\infty dr\, r^n e^{-\alpha r} j_l(hr)\, j_m(kr) \\ &= a_l(h)\, a_m(k) \\ &\times \int_0^1 d\eta\, (1 - \eta^2)^l \int_0^1 d\bar{\eta}\, (1 - \bar{\eta}^2)^m\, \mathscr{D}_{n+l+m}(\alpha, h\eta, k\bar{\eta}) \end{aligned} \quad (28)$$

with $n \geqslant -l - m$, where

$$\begin{aligned} \mathscr{D}_p(a, h, k) &= \int_0^\infty dr\, r^p e^{-ar} \cos(hr)\cos(kr) \\ &= \tfrac{1}{2}\{C_p(a, h - k) + C_p(a, h + k)\}. \end{aligned} \quad (29)$$

The Fourier transforms are polynomial like in η and $\bar{\eta}$, and therefore, the same transformation and integration techniques may be applied for each dimension of this double integral as described for Integral I. The integrand will be approximately of order $N_1 = l + q$ in η and $N_2 = m + q$ in $\bar{\eta}$ with zeros and weighting factors η_i, $\omega_i{}^l$ and $\bar{\eta}_j$, $\bar{\omega}_j{}^m$ respectively, where $q \approx n + l + m + 1$. Hence

$$D^n_{lm}(\alpha, h, k) = \sum_{i=1}^{N_1} \omega_i{}^l \sum_{j=1}^{N_2} \bar{\omega}_j{}^m \mathscr{D}_{n+l+m}(\alpha, h\eta_i, k\bar{\eta}_j). \quad (30)$$

INTEGRAL IV

$$E_{lm}^{n}(\alpha, h, k, d) = \int_0^\infty dr\, r^n e^{-\alpha r} j_l(hr)\, y_m(kr)\, F_{2m+1}(dr)$$
$$= a_l(h)\, a_m(k)$$
$$\times \left\{ \int_0^1 d\eta\, (1-\eta^2)^l \int_0^\infty d\bar{\eta}\, (1-\bar{\eta}^2)^m\, \mathscr{E}_{n+l+m}^{(1)2m+1}(\alpha, h\eta, k\bar{\eta}, d) \right.$$
$$\left. - \int_0^1 d\eta\, (1-\eta^2)^l \int_0^\infty d\bar{\xi}\, (1+\bar{\xi}^2)^m\, \mathscr{E}_{n+l+m}^{(2)2m+1}(\alpha + k\bar{\xi}, h\eta, d) \right\} \tag{31}$$

with $n \geqslant -l - m$, where

$$\mathscr{E}_p^{(1)t}(a, h, k, d) = \int_0^\infty dr\, r^p e^{-ar} \cos(hr) \sin(kr)\, F_t(dr)$$
$$= \tfrac{1}{2} \sum_{\mu=0}^{t} b_\mu{}^t \{S_p(a + \mu d, h + k) - S_p(a + \mu d, h - k)\}, \tag{32}$$

and

$$\mathscr{E}_p^{(2)t}(a, h, d) = \int_0^\infty dr\, r^p e^{-ar} \cos(hr)\, F_t(dr)$$
$$= \sum_{\mu=0}^{t} b_\mu{}^t C_p(a + \mu d, h). \tag{33}$$

$\mathscr{E}^{(1)}$ is a sum of Fourier sine transforms, and the same argument applied to Integral I applies here. For $\mathscr{E}^{(2)}$ the same transformation used to favor large ξ of Integral II is used here, and the same arguments apply here also. The order of the polynomial fit required is N_1, $N_2 \approx n + l + 3m + 2$ with zeros and weighing factors η_i and $\omega_i{}^l$, $\bar{\eta}_j$ and $\bar{\omega}_j{}^m$, and $\bar{\xi}_j$ and $\bar{\rho}_j{}^m$. Hence Gauss–Legendre quadrature yields

$$E_{lm}^{n}(\alpha, h, k, d) = h^l k^m \left\{ \sum_{i=1}^{N_1} \omega_i{}^l \sum_{j=1}^{N_2} \bar{\omega}_j{}^m \mathscr{E}_{n+l+m}^{(1)2m+1}(\alpha, h\eta_i, k\bar{\eta}_j, d) \right.$$
$$\left. - \sum_{i=1}^{N_1} \omega_i{}^l \sum_{j=1}^{N_2} \bar{\rho}_j{}^m \mathscr{E}_{n+l+m}^{(2)2m+1}(\alpha + k\bar{\xi}_j, h\eta_i, d) \right\}. \tag{34}$$

INTEGRAL V

$$F_{lm}^{n}(\alpha, h, k, c, d)$$

$$= \int_0^\infty dr\, r^n e^{-\alpha r} y_l(hr)\, F_{2l+1}(cr)\, y_m(kr)\, F_{2m+1}(dr)$$

$$= a_l(h)\, a_m(k)$$

$$\times \Big\{ \int_0^1 d\eta\, (1-\eta^2)^l \int_0^1 d\bar{\eta}\, (1-\bar{\eta}^2)^m\, \mathscr{F}_{n+l+m}^{(1)2l+1\;2m+1}(\alpha, h\eta, k\bar{\eta}, c, d)$$

$$+ \int_0^\infty d\xi\, (1+\xi^2)^l \int_0^\infty d\bar{\xi}\, (1+\bar{\xi}^2)^m\, \mathscr{F}_{n+l+m}^{(2)2l+1\;2m+1}(\alpha + h\xi + k\bar{\xi}, c, d)$$

$$- \int_0^1 d\eta\, (1-\eta^2)^l \int_0^\infty d\bar{\xi}\, (1+\bar{\xi}^2)^m\, \mathscr{F}_{n+l+m}^{(3)2l+1\;2m+1}(\alpha + k\bar{\xi}, h\eta, c, d)$$

$$- \int_0^\infty d\xi\, (1+\xi^2)^l \int_0^1 d\bar{\eta}\, (1-\bar{\eta}^2)^m\, \mathscr{F}_{n+l+m}^{(3)2l+1\;2m+1}(\alpha + h\xi, k\bar{\eta}, c, d)\Big\} \qquad (35)$$

with $n \geqslant -l - m$, where

$$\mathscr{F}_p^{(1)st}(a, h, k, c, d) = \int_0^\infty dr\, r^p e^{-ar} \sin(hr)\, F_s(cr) \sin(kr)\, F_t(dr)$$

$$= \tfrac{1}{2} \sum_{\mu=0}^{s} b_\mu{}^s \sum_{\nu=0}^{t} b_\nu{}^t \{C_p(a + \mu c + \nu d, h - k)$$

$$- C_p(a + \mu c + \nu d, h + k)\}, \qquad (36)$$

$$\mathscr{F}_p^{(2)st}(a, c, d) = \int_0^\infty dr\, r^p e^{-ar} F_s(cr)\, F_t(dr)$$

$$= p! \sum_{\mu=0}^{s} b_\mu{}^s \sum_{\nu=0}^{t} b_\nu{}^t (a + \mu c + \nu d)^{-p-1}, \qquad (37)$$

and

$$\mathscr{F}_p^{(3)st}(a + k, h, c, d) = \int_0^\infty dr\, r^p e^{-(a+k)r} \sin(hr)\, F_s(cr)\, F_t(dr)$$

$$= \sum_{\mu=0}^{s} b_\mu{}^s \sum_{\nu=0}^{t} b_\nu{}^t S_p(a + k + \mu c + \nu d, h). \qquad (38)$$

The integrand of $\mathscr{F}^{(2)}$ is always positive. Stable recursion relations, which are an extension of those developed for $\mathscr{B}^{(2)}$, are presented in Appendix B.

Gauss quadrature yields

$$F^{n}_{lm}(\alpha, h, k, c, d) = h^l k^m \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \{\omega_i{}^l \bar{\omega}_j{}^m \mathscr{F}^{(1)2l+1\ 2m+1}_{n+l+m}(\alpha, h\eta_i, k\bar{\eta}_j, c, d)$$

$$+ \rho_i{}^l \bar{\rho}_j{}^m \mathscr{F}^{(2)2l+1\ 2m+1}_{n+l+m}(\alpha + h\xi_i + k\bar{\xi}_j, c, d)$$

$$- \omega_i{}^l \bar{\rho}_j{}^m \mathscr{F}^{(3)2l+1\ 2m+1}_{n+l+m}(\alpha + k\bar{\xi}_j, h\eta_i, c, d)$$

$$- \rho_i{}^l \bar{\omega}_j{}^m \mathscr{F}^{(3)2l+1\ 2m+1}_{n+l+m}(\alpha + h\xi_i, k\bar{\eta}_j, c, d)\} \tag{39}$$

for polynomial fits of order $n + 3l + 3m + 3$.

Two-Electron Integrals

Integral VI

$$W^{pq}_{lm}(\alpha, h; \beta, k) = \int_0^\infty dr\, r^p e^{-\alpha r} j_l(hr) \int_r^\infty dv\, v^q e^{-\beta v} j_m(kv)$$

$$= a_l(h)\, a_m(k)$$

$$\times \int_0^1 d\eta\, (1 - \eta^2)^l \int_0^1 d\bar{\eta}\, (1 - \bar{\eta}^2)^m\, Q^{00}_{p+l\ q+m}(\alpha, h\eta; \beta, k\bar{\eta})$$

$$= h^l k^m \sum_i \sum_j \omega_i{}^l \bar{\omega}_j{}^m Q^{00}_{p+l\ q+m}(\alpha, h\eta_i; \beta, k\bar{\eta}_j) \tag{40}$$

where $p \geqslant -l$ and $q \geqslant -m$.

The functions $Q^{\sigma\epsilon}_{pq}$ are discussed in Appendix C.

Integral VII

$$\mathrm{X}^{pq}_{lm}(\alpha, h; \beta, k, d)$$

$$= \int_0^\infty dr\, r^p e^{-\alpha r} j_l(hr) \int_r^\infty dv\, v^q e^{-\beta v} y_m(kv)\, F_{2m+1}(dv)$$

$$= a_l(h)\, a_m(k) \left\{ \int_0^1 d\eta\, (1 - \eta^2)^l \int_0^1 d\bar{\eta}\, (1 - \bar{\eta}^2)^m\, \mathscr{X}^{(1)2m+1}_{p+l\ q+m}(\alpha, h\eta; k\bar{\eta}, \beta, d) \right.$$

$$\left. - \int_0^1 d\eta\, (1 - \eta^2)^l \int_0^\infty d\bar{\xi}\, (1 + \bar{\xi}^2)^m\, \mathscr{X}^{(2)2m+1}_{p+l\ q+m}(\alpha, h\eta; \beta + k\bar{\xi}, d) \right\}, \tag{41}$$

with $p \geqslant -l$ and $q \geqslant -m$, where

$$\mathscr{X}^{(1)t}_{pq}(\alpha, h; k, \beta, d) = \int_0^\infty dr\, r^p e^{-\alpha r} \cos(hr) \int_r^\infty dv\, v^q e^{-\beta v} \sin(kv)\, F_t(dv)$$

$$= \sum_{\mu=0}^{t} b_\mu{}^t Q^{0\,\pi/2}_{pq}(\alpha, h; \beta + \mu d, k), \tag{42}$$

and

$$\mathscr{X}^{(2)t}_{pq}(\alpha, h; \beta, d) = \int_0^\infty dr\, r^p e^{-\alpha r} \cos(hr) \int_r^\infty dv\, v^q e^{-\beta v} F_t(dv)$$

$$= \sum_{\mu=0}^{t} b_\mu{}^t Q^{00}_{pq}(\alpha, h; \beta + \mu d, 0). \tag{43}$$

Hence

$$X^{pq}_{lm}(\alpha, h; \beta, k, d) = h^l k^m \sum_i \sum_j \{\omega_i{}^l \bar{\omega}_j{}^m \mathscr{X}^{(1)2m+1}_{p+l\; q+m}(\alpha, h\eta_i\, ; k\bar{\eta}_j\, , \beta, d)$$

$$- \omega_i{}^l \bar{\rho}_j{}^m \mathscr{X}^{(2)2m+1}_{p+l\; q+m}(\alpha, h\eta_i\, ; \beta + k\bar{\xi}_j\, , d)\}. \tag{44}$$

INTEGRAL VIII

$$Y^{qp}_{lm}(\alpha, h, c; \beta, k) = \int_0^\infty dr\, r^p e^{-\alpha r} y_l(hr)\, F_{2l+1}(cr) \int_r^\infty dv\, v^q e^{-\beta v} j_m(kv)$$

$$= A_m{}^q(\beta, k)\, B_l{}^p(\alpha, h, c) - X^{qp}_{ml}(\beta, k; \alpha, h, c). \tag{45}$$

INTEGRAL IX

$$Z^{pq}_{lm}(\alpha, h, c; \beta, k, d)$$

$$= \int_0^\infty dr\, r^p e^{-\alpha r} y_l(hr)\, F_s(cr) \int_r^\infty dv\, v^q e^{-\beta v} y_m(kv)\, F_t(dv)$$

$$= a_l(h)\, a_m(k) \left\{ \int_0^1 d\eta\, (1 - \eta^2)^l \int_0^1 d\bar{\eta}\, (1 - \bar{\eta}^2)^m\, \mathscr{Z}^{(1)st}_{p+l,q+m}(\alpha, h\eta, c; \beta, k\bar{\eta}, d) \right.$$

$$+ \int_0^\infty d\xi\, (1 + \xi^2)^l \int_0^\infty d\bar{\xi}\, (1 + \bar{\xi}^2)^m\, \mathscr{Z}^{(2)st}_{p+l,q+m}(\alpha + h\xi, c; \beta + k\bar{\xi}, d)$$

$$- \int_0^1 d\eta\, (1 - \eta^2)^l \int_0^\infty d\bar{\xi}\, (1 + \bar{\xi}^2)^m\, \mathscr{Z}^{(3)st}_{p+l,q+m}(\alpha, h\eta, c; \beta + k\bar{\xi}, d)$$

$$\left. - \int_0^\infty d\xi\, (1 + \xi^2)^l \int_0^1 d\bar{\eta}\, (1 - \bar{\eta}^2)^m\, \mathscr{Z}^{(4)st}_{p+l,q+m}(\alpha + h\xi, c; \beta, k\bar{\eta}, d) \right\}, \tag{46}$$

with $p \geqslant -l$, $q \geqslant -m$, $s = 2l + 1$, and $t = 2m + 1$, where

$$\mathscr{X}_{pq}^{(1)st}(\alpha, h, c; \beta, k, d) = \int_0^\infty dr\, r^p e^{-\alpha r} \sin(hr)\, F_s(cr) \int_r^\infty dv\, v^q e^{-\beta v} \sin(kv)\, F_t(dv)$$

$$= \sum_{\mu=0}^{s} b_\mu{}^s \sum_{\nu=0}^{t} b_\nu{}^t Q_{pq}^{\pi/2\ \pi/2}(\alpha + \mu c, h; \beta + \nu d, k), \tag{47}$$

$$\mathscr{X}_{pq}^{(2)st}(\alpha, c; \beta, d) = \int_0^\infty dr\, r^p e^{-\alpha r} F_s(cr) \int_r^\infty dv\, v^q e^{-\beta v} F_t(dv)$$

$$= \sum_{\mu=0}^{s} b_\mu{}^s \sum_{\nu=0}^{t} b_\nu{}^t Q_{pq}^{00}(\alpha + \mu c, 0; \beta + \nu d, 0), \tag{48}$$

$$\mathscr{X}_{pq}^{(3)st}(\alpha, h, c; \beta, d) = \int_0^\infty dr\, r^p e^{-\alpha r} \sin(hr)\, F_s(cr) \int_r^\infty dv\, v^q e^{-\beta v} F_t(dv)$$

$$= \sum_{\mu=0}^{s} b_\mu{}^s \sum_{\nu=0}^{t} b_\nu{}^t Q_{pq}^{\pi/2\ 0}(\alpha + \mu c, h; \beta + \nu d, 0), \tag{49}$$

and

$$\mathscr{X}_{pq}^{(4)st}(\alpha, c; \beta, k, d) = \int_0^\infty dr\, r^p e^{-\alpha r} F_s(cr) \int_r^\infty dv\, v^q e^{-\beta v} \sin(kv)\, F_t(dv)$$

$$= \sum_{\mu=0}^{s} b_\mu{}^s \sum_{\nu=0}^{t} b_\nu{}^t Q_{pq}^{0\ \pi/2}(\alpha + \mu c, 0; \beta + \nu d, k). \tag{50}$$

The final formula for Gauss-quadrature follows, but it will be omitted here.

Conclusion

To check some of the integral calculations, the following limiting forms were used to relate some of the more complex integrals to the simpler ones.

$$A_l^{n+m}(\alpha, h) = \lim_{k\to 0} d_m(k)\, D_{lm}^n(\alpha, h, k),$$

$$B_m^{n+l}(\alpha, k, c) = \lim_{h\to 0} d_l(h)\, E_{lm}^n(\alpha, h, k, c)$$

$$A_l{}^p(\alpha + \beta, h) = \beta \lim_{k\to 0} W_{l0}^{p0}(\alpha, h; \beta, k)$$

$$B_l{}^p(\alpha + \beta, h, c) = \beta \lim_{k\to 0} Y_{l0}^{p0}(\alpha, h, c; \beta, k)$$

In all cases the basic limiting form for j_l was used, i.e.,

$$\lim_{k\to 0} j_l(kr) = \frac{2^l k^l l!}{(2l+1)!} = [d_l(k)]^{-1}.$$

Although the computation time for numerical quadrature is greater than the evaluation by analytical techniques, this route is taken as a first step in the calculation of scattering integrals. Analytic techniques are currently being developed to evaluate these integrals.

Use of proper asymptotic forms, viz. Bessel functions of the first and second kinds, should result in more compact expansions of the scattering wavefunction. The increased computation time required to compute integrals involving both j_l and y_l over that required when y_l is replaced by ϕ_l of Eq. (6) may be somewhat offset because fewer bound-like terms should be required in the scattering function.

Appendix A

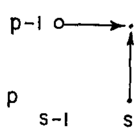
Evaluation of

$$\mathscr{B}_p^{(2)s}(a, c) = \int_0^\infty dr\, r^p e^{-ar} F_s(cr) \qquad \text{(A.1)}$$

proceeds from the following recursion relation obtained after integration by parts:

$$\mathscr{B}_{p+1}^{(2)s}(a, c) = \frac{p+1}{a}\, \mathscr{B}_p^{(2)s}(a, c) + \frac{cs}{a}\, \mathscr{B}_{p+1}^{(2)s-1}(a+c, c). \qquad \text{(A.2)}$$

This formula is stable for recursion outward as indicated in the diagram below.



The dots represent the "a" plane and circles the "$a + c$" plane.

To obtain the $\mathscr{B}_p^{(2)s}(a, c)$ one must first construct $\mathscr{B}_0^{(2)j}(a + [s-j]c, c)$ for $j = 1, 2,..., s$, and $\mathscr{B}_k^{(2)0}(a + sc, c)$ for $k = 1, 2,..., p$ with the recursion formulae

$$\mathscr{B}_0^{(2)j+1}(a, c) = \frac{c(j+1)}{a}\, \mathscr{B}_0^{(2)j}(a + c, c), \qquad (j \geqslant 0), \qquad \text{(A.3)}$$

and

$$\mathscr{B}_{k+1}^{(2)0}(a, c) = \frac{k+1}{a} \mathscr{B}_k^{(2)0}(a, c), \qquad (k \geqslant 0). \tag{A.4}$$

The recursion scheme begins with the first element

$$\mathscr{B}_0^{(2)0}(a + sc, c) = \frac{1}{a + sc} \tag{A.5}$$

denoted by 1 in Fig. 2. Then Eqs. (A.3) and (A.4) are used to generate respectively the elements labelled 2 and 3. With Eq. (A.2) element 4 and all others in the plane to the coordinate (a, s, p) are calculated. Examination of the recursion relations shows the a^{-p-s-1} dependence of Integral (A.1).

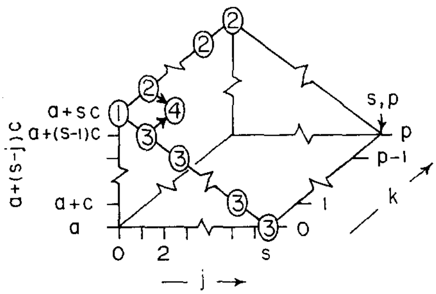


FIG. 2. Recursion scheme for $\mathscr{B}_p^{(2)s}$. The elements are generated in the order denoted.

APPENDIX B

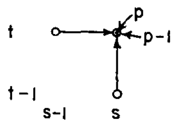
Evaluation of

$$\mathscr{F}_p^{(2)st}(a, c, d) = \int_0^\infty dr\, r^p e^{-ar} F_s(cr)\, F_t(dr) \tag{B.1}$$

proceeds from the following recursion relation obtained after integration by parts (the superscript (2) will be omitted):

$$\mathscr{F}_{p+1}^{st}(a, c, d)$$
$$= \frac{p+1}{a} \mathscr{F}_p^{st}(a, c, d) + \frac{sc}{a} \mathscr{F}_{p+1}^{s-1\,t}(a + c, c, d) + \frac{td}{a} \mathscr{F}_{p+1}^{s\,t-1}(a + d, c, d). \tag{B.2}$$

This relation is stable for recursion outward as indicated in the diagram below.



The connection between the indices and the parameter a is related as follows: for $s = 2l + 1$, $t = 2m + 1$ the argument is a, but for some $\bar{s}$ and $\bar{t}$ the value of the argument in the recursion relation will be $a + (2l + 1 - \bar{s})c + (2m + 1 - \bar{t})d$. In order to generate this array one needs

$$\mathscr{F}_0^{\bar{s}\bar{t}}(a + [2l + 1 - \bar{s}]\, c + [2m + 1 - \bar{t}]\, d, c, d), \tag{B.3}$$

$$\mathscr{F}_{\bar{p}}^{\bar{s}0}(a + [2l + 1 - \bar{s}]\, c + [2m + 1]\, d, c, d), \tag{B.4}$$

and

$$\mathscr{F}_{\bar{p}}^{0\bar{t}}(a + [2m + 1 - \bar{t}]\, c + [2l + 1]\, d, c, d), \tag{B.5}$$

for $0 \leqslant \bar{s} \leqslant s$, $0 \leqslant \bar{t} \leqslant t$, and $0 \leqslant \bar{p} \leqslant p$.

Functions (B.4) and (B.5) are $\mathscr{B}_p^{(2)\bar{s}}$ and $\mathscr{B}_p^{(2)\bar{t}}$ which were developed in Appendix I.

Function (B.3) is obtained with the recursion relation

$$\mathscr{F}_0^{st}(a, c, d) = \frac{\delta_{s0}\delta_{t0}}{a} + \frac{sc}{a}\, \mathscr{F}_0^{s-1\,t}(a + c, c, d) + \frac{td}{a}\, \mathscr{F}_0^{st-1}(a + d, c, d).$$

The recursion scheme begins with calculation of the arrays of the functions (B.3), (B.4), and (B.5). Then the recursion relationship (B.2) is used to generate all elements in the three dimensional array of $\bar{s}$, $\bar{t}$, and $\bar{p}$ until $\mathscr{F}_p^{st}$ is obtained. The implicit dependence of the argument a on $\bar{s}$ and $\bar{t}$ permits use of a three dimensional recursion scheme.

Appendix C

Recursion Relations for $Q_{pq}^{\sigma\epsilon}$

The four exchange integrals are in a form in which the integrands contain sine and cosine functions. By defining

$$Q_{pq}^{\sigma\epsilon}(\alpha, h; \beta, k) = \int_0^\infty dr\, r^p e^{-\alpha r} \cos(hx - \sigma)\, \mathscr{C}_q^{\epsilon}(\beta, k, r), \tag{C.1}$$

where

$$\mathscr{C}_q^{\epsilon}(\beta, k, r) = \int_r^{\infty} dv\, v^q e^{-\beta v} \cos(kv - \epsilon) \tag{C.2}$$

is an incomplete Fourier transform, all possible integrands for the exchange integrals are obtained by setting σ and ϵ equal to 0 and/or $\pi/2$. Integrating Eq. (C.2) twice by parts yields

$$\begin{aligned}
&\mathscr{C}_q^{\epsilon}(\beta, k, r) \\
&\quad = \{-k \sin(kr - \epsilon)\, r^q e^{-\beta r} - q \cos(kr - \epsilon)\, r^{q-1} e^{-\beta r} + \beta \cos(kr - \epsilon)\, r^q e^{-\beta r} \\
&\qquad - q(q-1)\, \mathscr{C}_{q-2}^{\epsilon}(\beta, k, r) + 2q\beta \mathscr{C}_{q-1}^{\epsilon}(\beta, k, r)\}/(k^2 + \beta^2),
\end{aligned} \tag{C.3}$$

and substitution into Eq. (C.1) yields the recursion relation

$$\begin{aligned}
&(k^2 + \beta^2)\, Q_{pq}^{\sigma\epsilon}(\alpha, h; \beta, k) \\
&\quad = -k \mathscr{G}_{p+q}^{\sigma\,\epsilon+\pi/2}(\alpha + \beta, h, k) - q \mathscr{G}_{p+q-1}^{\sigma\epsilon}(\alpha + \beta, h, k) + \beta \mathscr{G}_{p+q}^{\sigma\epsilon}(\alpha + \beta, h, k) \\
&\qquad - q(q-1)\, Q_{pq-2}^{\sigma\epsilon}(\alpha, h; \beta, k) + 2q\beta Q_{pq-1}^{\sigma\epsilon}(\alpha, h; \beta, k),
\end{aligned} \tag{C.4}$$

where the Fourier-like transform

$$\mathscr{G}_p^{\sigma\epsilon}(\alpha, h, k) = \int_0^{\infty} dr\, r^p e^{-\alpha r} \cos(hr - \sigma) \cos(kr - \epsilon) \tag{C.5}$$

must be added into the recursion relation when one proceeds along q as indicated below.

$$p \quad \underset{q-2}{\bullet} \longrightarrow \underset{q-1}{\bullet} \longrightarrow \underset{q}{\bullet}$$

Integration of the outer integral of Expression (C.1) by parts twice yields

$$\begin{aligned}
&(h^2 + \alpha^2)\, Q_{pq}^{\sigma\epsilon}(\alpha, h; \beta, k) \\
&\quad = \delta_{0p} h \sin \sigma \mathscr{C}_q^{\epsilon}(\beta, k, 0) - \delta_{1p} \cos \sigma \mathscr{C}_q^{\epsilon}(\beta, k, 0) + \delta_{0p} \alpha \cos \sigma \mathscr{C}_q^{\epsilon}(\beta, k, 0) \\
&\qquad + p \mathscr{G}_{p+q-1}^{\sigma\epsilon}(\alpha + \beta, h, k) - \alpha \mathscr{G}_{p+q}^{\sigma\epsilon}(\alpha + \beta, h, k) + h \mathscr{G}_{p+q}^{\sigma+\pi/2\,\epsilon}(\alpha + \beta, h, k) \\
&\qquad - p(p-1)\, Q_{p-2\,q}^{\sigma\epsilon}(\alpha, h; \beta, k) + 2p\alpha Q_{p-1\,q}^{\sigma\epsilon}(\alpha, h; \beta, k),
\end{aligned} \tag{C.6}$$

where $\mathscr{C}_q^{\epsilon}(\beta, k, 0)$ is a Fourier sine or cosine transform respectively when $\epsilon = \pi/2$

and 0. Recursion with addition of $\mathscr{G}$ and $\mathscr{C}$ proceeds along p as indicated below.

$$q \quad \cdot\longrightarrow\cdot\longrightarrow\cdot$$
$$p-2 \qquad p-1 \qquad p$$

Recursion Relation (C.4) is used to move along q for fixed p whereas Eq. (C.6) is used to move along p for fixed q. $\mathscr{G}_p^{\sigma\epsilon}$ is related to Fourier transforms, and it is calculated as needed. To start the procedure $Q_{00}^{\sigma\epsilon}(\alpha, h; \beta, k)$ must be calculated and a simple integration yields

$$Q_{00}^{00} = \left[-\frac{k}{2}[A+B] + \frac{\beta}{2}[C+D]\right] \Big/ (k^2+\beta^2), \tag{C.7}$$

$$Q_{00}^{0\ \pi/2} = \left[\frac{k}{2}[C+D] + \frac{\beta}{2}[A+B]\right] \Big/ (k^2+\beta^2), \tag{C.8}$$

$$Q_{00}^{\pi/2\ 0} = \left[\frac{k}{2}[C-D] + \frac{\beta}{2}[A-B]\right] \Big/ (k^2+\beta^2), \tag{C.9}$$

and

$$Q_{00}^{\pi/2\ \pi/2} = \left[\frac{k}{2}[A-B] + \frac{\beta}{2}[D-C]\right] \Big/ (k^2+\beta^2), \tag{C.10}$$

where

$$A = (h+k)[(h+k)^2 + (\alpha+\beta)^2]^{-1},$$
$$B = (k-h)[(k-h)^2 + (\alpha+\beta)^2]^{-1},$$
$$C = (\alpha+\beta)[(h+k)^2 + (\alpha+\beta)^2]^{-1},$$

and

$$D = (\alpha+\beta)[(h-k)^2 + (\alpha+\beta)^2]^{-1},$$

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