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Evaluation of radial integrals in scattering problems

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Abstract. The radial part of many scattering waves can be expressed in terms of Whittaker functions $M_{\kappa,\mu}$ and/or $W_{\kappa,\mu}$, and integrals over products of these waves are required in the analysis of many processes. Integrals over n Whittaker functions of the first kind are generalised hypergeometric series which often have variables outside the range of convergence, or are such that the series are slowly converging. Using matrix series for the Whittaker functions, analytic continuations of the resulting generalised hypergeometric series have been obtained which always result in convergent series apart from a few special cases involving degeneracy. In addition, an asymptotic matrix series for the integral from some radius R to infinity of products of Whittaker functions of the second kind is given. As an example, the Dirac-Coulomb matrix elements arising in bremsstrahlung are evaluated.

1. Introduction

Radial matrix elements that occur in the analysis of many scattering processes in physics consist of integrals over products of two or three oscillatory functions. Many of these matrix elements arise from large angular momentum portions of the incident and outgoing waves and hence can be approximated by regular Whittaker functions $M_{\kappa,\mu}$. Other matrix elements involve penetrating orbits and the integral from the origin to some radius R may have to be done numerically. However, in the portion of the integral outside the range of all non-Coulomb forces, the scattering waves can be expressed in terms of the Whittaker functions of the second kind $W_{\kappa,\mu}$.

Complete integrals over products of Whittaker functions of the first kind result in generalised hypergeometric series. For example, integrals over two Whittaker functions produce one of the Appell functions, F_2, while integrals over three Whittaker functions of the first kind produce a triply infinite series known as the Lauricella function L_A. In many cases of interest, the variables in these series (combinations and ratios of the momenta in the problem) are such that the series are not convergent. A number of analytic continuations of the Appell F_2 functions are known (Erdelyi 1953, Gargaro 1970, Gargaro and Onley 1970, Sud and Wright 1976), and some continuations of the Lauricella function L_A are known (Rozics and Johnson 1964). However, the usefulness of these analytic continuations are limited to special cases.

In this paper we use a first-order matrix differential equation for the Whittaker functions and write integrals over the solutions of this equation as a generalisation of the gamma function (Onley 1972, Sud *et al* 1976) to obtain a new analytic continuation of series of the Appell or Lauricella type. A key ingredient is a partial differential equation obeyed by the generalised gamma function (Wright *et al* 1977).

The matrix series form of the Whittaker functions of the first kind can be integrated from the origin to infinity to obtain a matrix series representation of the integral. In § 2, we give a general technique whereby these matrix series are evaluated in kinematic domains where they are convergent and the results are then transformed by a matrix operator back to the desired kinematic values. This two-step process permits the evaluation of the complete integral over n Whittaker functions of the first kind. At the end of § 2 we give an asymptotic matrix series for integrals over products of Whittaker functions of the second kind from some distance R to infinity. In § 3, we apply our technique for the complete integral to the evaluation of Dirac-Coulomb radial integrals that arise in the calculation of high energy electron bremsstrahlung from the atomic nulceus.

2. Evaluation of radial integrals

Onley (1972) and co-workers (Sud *et al* 1976) have investigated the properties of solutions to the first-order matrix differential equation

$$\mathrm{d}W/\mathrm{d}r = (\mathscr{A}/r - \mathscr{B})W \tag{1}$$

where $\mathscr{A}$ and $\mathscr{B}$ are $n\times n$ constant matrices and $W(\mathscr{A}, \mathscr{B}; r)$ is an $n\times n$ array of functions which can be written as

$$W(\mathscr{A}, \mathscr{B}; r) = U_n(2\mathrm{i}p_n r)\otimes\ldots\otimes U_2(2\mathrm{i}p_2 r)\otimes U_1(2\mathrm{i}p_1 r) \tag{2}$$

where each U_i is a 2×2 matrix of functions which satisfy (1) with the 2×2 matrices A_i and B_i, p_i is the momentum variable for each function and

$$\begin{aligned}\mathscr{A} &= A_n\otimes I_{2n-2} + I_2\otimes A_{n-1}\otimes I_{2n-4} + \ldots + I_{2n-2}\otimes A_1 \\ \mathscr{B} &= B_n\otimes I_{2n-2} + \ldots + I_{2n-2}\otimes B_1.\end{aligned} \tag{3}$$

In general the matrices $\mathscr{A}$ and $\mathscr{B}$ do not commute, so they cannot both be diagonalised simultaneously. It is useful, however, to diagonalise either $\mathscr{A}$ or $\mathscr{B}$. Solutions with diagonal $\mathscr{A}$ or $\mathscr{B}$ will be denoted by superscript (A) or (B). The solution $U^{(A)}$ and $U^{(B)}$ and some of their more useful properties are given in appendix 1. In the A-diagonal representation of (1), a power series solution is easily obtained, while in the B-diagonal representation an inverse power series solution is convenient. Both of these series are given in appendix 2 and are well defined apart from cases with degenerate eigenvalues for A or B, respectively. An important property of solutions to equation (1) is

$$x^a\,\mathrm{e}^{-bx}W(A, B; x) = W(A+a, B+b; x) \tag{4}$$

where $A+a$ means $A+aI_n$, and I_n is the $n\times n$ unit matrix.

Onley and co-workers defined integrals over the solutions of equation (1) by writing

$$\Gamma(\mathscr{A}+1, \mathscr{B}) \equiv \int_{(0)}^{\infty} W(\mathscr{A}, \mathscr{B}; r)\,\mathrm{d}r \tag{5}$$

where the symbol (0) indicates that finite order poles have been subtracted out at the origin. The formal definition of the matrix gamma function is given in Onley (1972) and Sud *et al* (1976). The matrix gamma function defined in equation (5) has the very useful property:

$$\mathscr{A}\Gamma(\mathscr{A}, \mathscr{B}) = \mathscr{B}\Gamma(\mathscr{A}+1, \mathscr{B}). \tag{6}$$

In the analysis of scattering processes we require both integrals over all space defined by (5) and integrals from some distance R to infinity defined by

$$\Gamma(\mathscr{A}+1, \mathscr{B}; R) = \int_R^\infty W(\mathscr{A}, \mathscr{B}; r)\,\mathrm{d}r. \tag{7}$$

We refer to this latter integral as the incomplete matrix gamma function, and it will prove to be useful when using asymptotic series for the integrand.

For non-penetrating orbits we require integrals over n regular Whittaker functions of the first kind which can be represented by the first column of $W(\mathscr{A}, \mathscr{B}; r)$. Thus, we consider the vector gamma function defined by

$$\boldsymbol{\Gamma}_0(\mathscr{A}^{(A)}+1, \mathscr{B}^{(A)}+\Delta) = \int_0^\infty \mathrm{e}^{-\Delta r}\boldsymbol{W}(\mathscr{A}, \mathscr{B}; r)\,\mathrm{d}r \tag{8}$$

where we have included $\exp(-\Delta r)$ for convenience. The n-element vector of the functions $\boldsymbol{W}$ is given by

$$\boldsymbol{W}(\mathscr{A}, \mathscr{B}; r) = \boldsymbol{U}_n^{(A)}\otimes\ldots\otimes \boldsymbol{U}_1^{(A)} \tag{9}$$

where $\boldsymbol{U}_i^{(A)}$ represents the first column of the Whittaker functions given in equation (A1.11). Using the power series of equation (A2.2) we can write

$$\boldsymbol{W}(\mathscr{A}, \mathscr{B}; r) = N\sum_{m=0}^{\infty} r^{m+\mathscr{A}_{11}}\boldsymbol{V}_m \tag{10}$$

where the normalisation $N=(2\mathrm{i}p_n)^{\mu_n}\ldots(2\mathrm{i}p_2)^{\mu_2}(2\mathrm{i}p_1)^{\mu_1}$ and $\boldsymbol{V}_m$ can be obtained from the recursion relation

$$(\boldsymbol{V}_m)_i = \frac{-\mathscr{B}_{ij}(\boldsymbol{V}_{m-1})_j}{\mathscr{A}_{11}-\mathscr{A}_{ii}+m} \tag{11}$$

where $(\boldsymbol{V}_0)_i = \delta_{i,1}$. Substituting (10) into (8) and integrating term by term we obtain the singly infinite matrix series

$$\boldsymbol{\Gamma}_0(\mathscr{A}^{(A)}+1, \mathscr{B}^{(A)}+\Delta) = N\sum_{m=1}^{\infty}\frac{\Gamma(\mathscr{A}_{11}+m+1)\boldsymbol{V}_m}{\Delta^{\mathscr{A}_{11}+m+1}}. \tag{12}$$

The convergence of this series is not easily investigated directly and the results look puzzling in the limit $\Delta\to 0$. However, this apparent difficulty can easily be remedied by extracting a scalar factor from B by writing $\mathscr{B}' = \mathscr{B} - \mathrm{i}(p_1+p_2+\ldots+p_n)I_n$. Now using $\mathscr{B}'$ in (11), the series in (12) becomes

$$\boldsymbol{\Gamma}_0(\mathscr{A}^{(A)}+1, \mathscr{B}^{(A)}+\Delta) = N\sum_{m=0}^{\infty}\frac{\Gamma(\mathscr{A}_{11}+m+1)\boldsymbol{V}'_m}{[\Delta+\mathrm{i}(p_1+p_2+\ldots+p_n)]^{\mathscr{A}_{11}+m+1}} \tag{13}$$

where letting $\Delta\to 0$ causes no apparent problems, and the prime on V indicates that $\mathscr{B}'$ is to be used in (11). In order to integrate a power series term by term to infinity, we require an exponential factor which can always be extracted from $\mathscr{B}$.

To examine the convergence of the series in equation (13) we first consider a particular case, namely the integral over only two Whittaker functions of the first kind, i.e. let $\boldsymbol{W} = \boldsymbol{U}_2^{(A)}\otimes \boldsymbol{U}_1^{(A)}$. Clearly the resulting $\boldsymbol{\Gamma}$ vector has four elements which can be written as

$$\Gamma_0(\mathscr{A}+1, \mathscr{B}+\Delta) = \int_0^\infty \mathrm{d}r\, \mathrm{e}^{-\Delta r}$$

$$\times \begin{pmatrix} M_{\kappa_2+\frac{1}{2},\mu_2-\frac{1}{2}}(2\mathrm{i}p_2 r) M_{\kappa_1+\frac{1}{2},\mu_1-\frac{1}{2}}(2\mathrm{i}p_1 r) \\ \dfrac{-(\mu_1-\kappa_1-\frac{1}{2})}{2\mu_1(2\mu_1+1)} M_{\kappa_2+\frac{1}{2},\mu_2-\frac{1}{2}}(2\mathrm{i}p_2 r) M_{\kappa_1+\frac{1}{2},\mu_1+\frac{1}{2}}(2\mathrm{i}p_1 r) \\ \dfrac{-(\mu_2-\kappa_2-\frac{1}{2})}{2\mu_2(2\mu_2+1)} M_{\kappa_2+\frac{1}{2},\mu_2+\frac{1}{2}}(2\mathrm{i}p_2 r) M_{\kappa_1+\frac{1}{2},\mu_1-\frac{1}{2}}(2\mathrm{i}p_1 r) \\ \dfrac{(\mu_2-\kappa_2-\frac{1}{2})(\mu_1-\kappa_1-\frac{1}{2})}{2\mu_2 2\mu_1(2\mu_2+1)(2\mu_1+1)} M_{\kappa_2+\frac{1}{2},\mu_2+\frac{1}{2}}(2\mathrm{i}p_2 r) M_{\kappa_1+\frac{1}{2},\mu_1+\frac{1}{2}}(2\mathrm{i}p_1 r) \end{pmatrix} \qquad (14)$$

Expressing the M in terms of ${}_1F_1$ by means of equation (A1.1), each of these elements can be integrated term by term and is proportional to an Appell function F_2 given by the doubly infinite series

$$F_2(\alpha, a_2, a_1, b_2, b_1; x, y) = \sum_{m,n} \frac{(\alpha)_{m+n}(a_2)_m(a_1)_n}{(b_2)_m(b_1)_n m!\, n!} x^m y^n \qquad (15)$$

where the parameter values for the first element are

$$\alpha = \mu_1+\mu_2+1 \qquad b_2 = 2\mu_2 \qquad b_1 = 2\mu_1$$

$$a_2 = \mu_2-\kappa_2-\tfrac{1}{2} \qquad a_1 = \mu_1-\kappa_1-\tfrac{1}{2}$$

and the variables for all four elements are

$$x = 2\mathrm{i}p_2/[\Delta+\mathrm{i}(p_1+p_2)] \qquad y = 2\mathrm{i}p_1/[\Delta+\mathrm{i}(p_1+p_2)]. \qquad (16)$$

This series is absolutely convergent for $|x|+|y|<1$.

It is straightforward, but tedious, to confirm that the singly infinite matrix series given in (13) generates the four Appell series coming from (14). Therefore, we can examine the convergence properties of the matrix series by using the known convergence properties of the Appell F_2-type series. In our 2×2 example, $|x|+|y| = (|2p_1|+|2p_2|)/|\Delta+\mathrm{i}(p_1+p_2)|$ and is not convergent for $\Delta=0$. In the $n\times n$ case, each element of the gamma vector will be an n-dimensional series of the Appell F_2 structure. For example, for $n=3$ each element is a Lauricella series given by

$$L_A(\alpha, a_3, a_2, a_1, b_3, b_2, b_1; x, y, z) = \sum_{l,m,n} \frac{(\alpha)_{l+m+n}(a_3)_l(a_2)_m(a_1)_n}{(b_3)_l(b_2)_m(b_1)_n l!\, m!\, n!} x^l y^m z^n \qquad (17)$$

and the convergence condition is $|x|+|y|+|z|<1$. For our case, this would be $|x|+|y|+|z| = (|2p_1|+|2p_2|+|2p_3|)/|\Delta+\mathrm{i}(p_1+p_2+p_3)|$ and again would not be convergent for $\Delta=0$. This pattern clearly continues for the $n\times n$ case. However, if we choose the parameter Δ in (13) sufficiently large, then clearly $|\Delta+\mathrm{i}(p_1+\ldots+p_n)| \gg |2p_n|+|2p_{n-1}|+\ldots+|2p_1|$ and the matrix series in (12) is rapidly convergent. For this step, the parameter Δ can be complex, but in order to obtain the result with $\Delta=0$, we will need to choose a Δ which is real as will be shown below.

Our procedure is to first choose a sufficiently large real Δ to easily evaluate the vector gamma function $\Gamma_0(\mathscr{A}+1, \mathscr{B}+\Delta)$ of (13). In order to obtain the gamma vector at $\Delta=0$, we make use of the fact that the gamma vector obeys a first-order matrix differential equation in Δ. For our case we require only a simple version of the general result (Wright *et al* 1977) for which we give a brief derivation.

Differentiating equation (8) with respect to Δ we obtain

$$\frac{\mathrm{d}\boldsymbol{\Gamma}(\mathscr{A}+1, \mathscr{B}+\Delta)}{\mathrm{d}\Delta} = \int_0^\infty -r\,\mathrm{e}^{-\Delta r}\boldsymbol{W}(\mathscr{A}, \mathscr{B}; r)\,\mathrm{d}r. \tag{18}$$

Using the fundamental property of the matrix gamma function given in equation (6), we can rewrite the right-hand side as follows:

$$\frac{\mathrm{d}\boldsymbol{\Gamma}(\mathscr{A}+1, \mathscr{B}+\Delta)}{\mathrm{d}\Delta} = -(\mathscr{B}+\Delta)^{-1}(\mathscr{A}+1)\boldsymbol{\Gamma}(\mathscr{A}+1, \mathscr{B}+\Delta). \tag{19}$$

Unlike the more general case discussed by Wright *et al* (1977), this first-order matrix differential equation can be directly integrated to obtain

$$\boldsymbol{\Gamma}(\mathscr{A}^{(B)}+1, \mathscr{B}^{(B)}+\Delta_0-x) = S(x)\boldsymbol{\Gamma}(\mathscr{A}^{(B)}+1, \mathscr{B}^{(B)}+\Delta_0) \tag{20}$$

where we have written $\Delta = \Delta_0 - x$ and the $n\times n$ matrix operator $S(x)$ is given by

$$S(x) = \sum_{l=0}^{\infty} T_l x^l \tag{21}$$

where

$$T_0 = I_n$$

$$T_l = (\mathscr{B}^{(B)}+\Delta_0)^{-1}\left(\frac{\mathscr{A}^{(B)}+l}{l}\right)T_{l-1}. \tag{22}$$

For large l, the recurrence relation for T_l becomes diagonal, and one sees that the convergence of the series in equation (21) reduces to that of a geometrical series. The conditions for the matrix series S to converge in all of its elements can be written as

$$\frac{|x|}{|\mathscr{B}_{ii}+\Delta_0|} < 1 \qquad \text{for } i = 1, 2, \ldots, n. \tag{23}$$

Since in the B-diagonal form, the $\mathscr{B}_{ii}$ are $\pm$ combinations of the $\{2\mathrm{i}p_i\}$, we see that if Δ_0 is real then the series in equation (21) is absolutely convergent for all x such that $|x| \leqslant |\Delta_0|$. In particular, choosing $x = \Delta_0$ allows the evaluation of the integral given in equation(8) for $\Delta = 0$ if none of the $\mathscr{B}_{ii}$ vanish, i.e.

$$\boldsymbol{\Gamma}(\mathscr{A}^{(A)}+1, \mathscr{B}^{(A)}) = \mathscr{C}^{AB}S(\Delta_0)(\mathscr{C}^{AB})^{-1}\boldsymbol{\Gamma}(\mathscr{A}^{(A)}+1, \mathscr{B}^{(A)}+\Delta_0) \tag{24}$$

where the $\mathscr{C}^{AB}$ transforms the n-element vector of Whittaker functions from a B-diagonal to A-diagonal basis and is obtained from the 2×2 matrix following (A1.11) by the procedure given in (3). The gamma vector on the right-hand side can be evaluated with the series given in (13), while the $n\times n$ matrix operator S can be evaluated by the series given in (21).

The result given in (24) works for all non-penetrating integrals, but as noted in the introduction some waves do penetrate, so we now turn to evaluating the integrals from some radius R to infinity. That is, we evaluate the incomplete gamma function defined in (7). In the B-diagonal representation we can write

$$\Gamma_\infty(\mathscr{A}^{(B)}+1, \mathscr{B}^{(B)}; R) = \int_R^\infty W_\infty(\mathscr{A}^{(B)}, \mathscr{B}^{(B)}; r)\,\mathrm{d}r \tag{25}$$

where $W_\infty = U_n \otimes U_{n-1} \otimes \ldots \otimes U_1$ and the U are given in (A1.9). Writing the asymptotic matrix series for W given in (A2.4) of appendix 2 for our case we find

$$W(\mathscr{A}^{(B)}, \mathscr{B}^{(B)}; r) = \sum_{m=0} D_m r^{\mathscr{A}-m}\,\mathrm{e}^{-\mathscr{B}r}\mathscr{N} \tag{26}$$

where $\mathscr{A}$ and $\mathscr{B}$ are given in terms of the 2×2 A and B matrices in (A1.7) by (3), and the normalisation matrix $\mathscr{N} = N_n \otimes N_{n-1} \otimes \ldots \otimes N_1$ where

$$N_i = (2\mathrm{i}p_i)^{\bar{\mathscr{A}}_i}. \tag{27}$$

The notation $\bar{\mathscr{A}}$ means the diagonal part of the $\mathscr{A}$ matrix. Inserting (26) into (25), and integrating term by term we obtain

$$\Gamma_\infty(\mathscr{A}^{(B)}+1, \mathscr{B}^{(B)}; R) = \sum_{m=0} D_m \Gamma(\bar{\mathscr{A}}+1-m; \mathscr{B}R)\mathscr{B}^{-(\bar{\mathscr{A}}+1-m)}\mathscr{N}. \tag{28}$$

Each element in (28) is diagonal apart from the D_m matrix which is defined by $D_0 = I_n$, and the recursion scheme given in (A2.5) and (A2.6).

The behaviour of the matrix series in (21) can be investigated by standard techniques. It is not surprising, perhaps, to find that the criterion for using this matrix asymptotic series to represent the integral from R to ∞ is that $|2\mathrm{i}p_iR| \gg 1$, for $i = 1, n$. This is just the union of the criteria that each function in the integrand be well represented by an asymptotic series at the point $2\mathrm{i}p_iR$.

3. The evaluation of Dirac–Coulomb radial integrals

To illustrate the power of this technique consider the radial integrals arising in the analysis of bremsstrahlung accompanying high energy electron scattering from the nucleus (Sud *et al* 1976). Using matrix notation, the integrand required for the bremsstrahlung integrals is

$$W(\mathscr{A}, \mathscr{B}; r) = U_3(2\mathrm{i}\omega r) \otimes U_2(2\mathrm{i}p_2 r) \otimes U_1(2\mathrm{i}p_1 r) \tag{29}$$

where the regular functions are given by

$$U_3(2\mathrm{i}\omega r) = \begin{pmatrix} \mathrm{i}j_{L-1}(\omega r) \\ j_L(\omega r) \end{pmatrix} \qquad A_3 = \begin{pmatrix} L-1 & 0 \\ 0 & -L-1 \end{pmatrix} \qquad B_3 = \begin{pmatrix} 0 & \mathrm{i}\omega \\ \mathrm{i}\omega & 0 \end{pmatrix} \tag{30}$$

and

$$U_j^{(A)}(2\mathrm{i}p_j r) = N(\gamma_j) \begin{pmatrix} M_{-\mathrm{i}\eta_j, \gamma_j - \frac{1}{2}}(2\mathrm{i}p_j r) \\ \dfrac{-(\gamma_j + \mathrm{i}\eta_j)}{2\gamma_j(2\gamma_j+1)} M_{-\mathrm{i}\eta_j, \gamma_j + \frac{1}{2}}(2\mathrm{i}p_j r) \end{pmatrix} \tag{31}$$

where

$$A_j = \begin{pmatrix} \gamma_j & 0 \\ 0 & -\gamma_j \end{pmatrix} \qquad B_j = \frac{\mathrm{i}p_j}{\gamma_j} \begin{pmatrix} -\mathrm{i}\eta_j & \gamma_j - \mathrm{i}\eta_j \\ \gamma_j + \mathrm{i}\eta_j & \mathrm{i}\eta_j \end{pmatrix} \qquad j = 1, 2$$

and $\gamma_j = (\kappa_j^2 - \alpha^2 Z^2)^{1/2}$, $\eta_j = \alpha Z E_j / p_j$ and the Dirac quantum number κ_j is a non-zero integer. The fine structure constant is denoted by α, $E_j(p_j)$ are the incident and final electron energy (momentum) and $\omega = E_1 - E_2$ is the energy of the emitted photon.

By writing the spherical Bessel function in terms of the Hankel function, the integral over each element of W in (29) can be expressed as a sum of L Appell F_2 series, and the use of more conventional analytic continuations permit their evaluation (Sud *et al* 1976). Each Appell series is expressed as a sum of three doubly infinite series designated by Q_1, Q_2 and Q_3. These series converge well for typical kinematics of importance to electron scattering from the nucleus, but when the Q are added together and the spherical Bessel function is extracted from the spherical Hankel function there can be substantial numerical cancellation.

To illustrate this point consider the integral

$$I_L = \int_0^\infty j_L(\omega r) f_{\kappa_1}(p_1 r) f_{\kappa_2}(p_2 r) r^2 \, \mathrm{d}r$$

where f_κ, the large Dirac-Coulomb radial function, is real and is defined explicitly in terms of the Whittaker functions by Sud *et al* (1976). Integrals of this form enter all inelastic electron scattering processes from the nucleus. The use of the Appell series to evaluate this integral suffers extensive numerical cancellations for large L as shown in table 1 where we compare the Appell series value to the value calculated with (24) which has no numerical difficulties. The precision can be confirmed by checking recurrence relations over the label L which follow from equation (A1.12), and the values calculated with (24) are good to more than 11 digits.

Table 1. Values of the radial integral I_L calculated with the Appell series (a) and with the matrix series (b) for different L values. The other parameters are: $E_1 = 100.511$ MeV, $\omega = 20$ MeV, $Z = 92$, $\kappa_1 = 10$ and $\kappa_2 = 10$. The length units are MeV^{-1} and all the integrals are multiplied by a factor of 10^5. The underlined digits are wrong and demonstrate loss of precision when using the Appell series.

L	1	7	14	17
a	−0.130 771 81	0.994 803 0$\underline{1}$	0.121 $\underline{289}$ $\underline{01}$	−0.$\underline{481}$ $\underline{680}$ $\underline{04}$
b	−0.130 771 81	0.994 803 00	0.121 263 61	−0.747 278 40

In calculating the Coulomb correction to the radiation tail accompanying elastic scattering from the nucleus, we have evaluated the electric and magnetic multipoles radial integrals for L values up to 30, and for κ values from 1 to 50 and have found no numerical difficulties with the use of (24), although we did have to return to $\Delta = 0$ in a number of steps. When one or more elements of $\mathscr{B}_{ii}$ is small the operator S in (21) needs to be calculated at $\Delta_0/2$ to obtain Γ at $\Delta_0/2$, then the process is repeated at $\Delta_0/4$, etc. Once $\Delta_0/2n$ becomes comparable to the small elements of $\mathscr{B}_{ii}$ the remaining distance can be covered in one step. We find that about 15 to 20 Zeno-like steps give a final integral good to about 11 significant figures.

In conclusion, we have found a general method of evaluating radial integrals for scattering problems. For non-penetrating orbits the complete integral can be evaluated by means of (24), while for penetrating orbits the integral from some radius R to infinity can be evaluated by (26). We have demonstrated that this technique works for the notoriously difficult Dirac-Coulomb radial integrals and believe that it will work equally well for other radial integrals arising in scattering problems, particularly in cases where the long-range character of the Coulomb field causes difficulties.

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Appendix 1

The Whittaker function $M_{\kappa,\mu}(x)$ is given in terms of the hypergeometric series ${}_1F_1$ by (Slater 1960)

$$M_{\kappa,\mu}(x) = \mathrm{e}^{-x/2}x^{\mu+\frac{1}{2}}{}_1F_1(\mu-\kappa+\tfrac{1}{2}, 2\mu+1; x) \tag{A1.1}$$

where

$${}_1F_1(a, c; x) = \sum_{l=0}^{\infty} \frac{(a)_l x^l}{(c)_l l!}. \tag{A1.2}$$

The second Whittaker function $W_{\kappa,\mu}(x)$ can be defined in terms of $M_{\kappa,\mu}(x)$ by the relation (Slater 1960)

$$W_{\kappa,\mu}(x) = \frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2}-\mu-\kappa)} M_{\kappa,\mu}(x) + \frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2}+\mu-\kappa)} M_{\kappa,-\mu}(x). \tag{A1.3}$$

In addition, $W_{\kappa,\mu}(x)$ has an asymptotic series expansion given by

$$W_{\kappa,\mu}(x) = \mathrm{e}^{-x/2}x^{\kappa}{}_2F_0(\tfrac{1}{2}+\mu-\kappa, \tfrac{1}{2}-\mu-\kappa; -1/x) \tag{A1.4}$$

where

$${}_2F_0(a, b; x) = \sum_{l=0} \frac{(a)_l(b)_l}{l!} x^l. \tag{A1.5}$$

The Whittaker functions are solutions to an equation of the form of (1),

$$\frac{\mathrm{d}U^{(B)}}{\mathrm{d}r} = \left(\frac{A^{(B)}}{r} - B^{(B)}\right) U^{(B)} \tag{A1.6}$$

where

$$A^{(B)} = \begin{pmatrix} -(\kappa+\frac{1}{2}) & \mu+\kappa+\frac{1}{2} \\ \mu-\kappa-\frac{1}{2} & \kappa+\frac{1}{2} \end{pmatrix} \qquad B^{(B)} = \begin{pmatrix} -\mathrm{i}p & 0 \\ 0 & \mathrm{i}p \end{pmatrix}. \tag{A1.7}$$

For scattering waves the argument of the Whittaker function is $x = 2\mathrm{i}pr$. The matrix of Whittaker functions $U^{(B)}$ satisfying (A1.6) is

$$U_0^{(B)} = \frac{1}{x^{1/2}} \begin{pmatrix} M_{\kappa,\mu}(x) & [\kappa+\mu+\frac{1}{2}/(\kappa-\mu+\frac{1}{2})]M_{\kappa,-\mu}(x) \\ M_{\kappa+1,\mu}(x) & M_{\kappa+1,-\mu}(x) \end{pmatrix} \tag{A1.8}$$

or

$$U_\infty^{(B)} = \frac{1}{x^{1/2}} \begin{pmatrix} W_{-\kappa,\mu}(-x)\exp(-\mathrm{i}\pi\varepsilon\kappa) & -(\mu+\kappa+\frac{1}{2})W_{\kappa,\mu}(x) \\ (\mu-\kappa-\frac{1}{2})W_{-\kappa-1,\mu}(-x)\exp[-\mathrm{i}\pi\varepsilon(\kappa+1)] & W_{\kappa+1,\mu}(x) \end{pmatrix} \tag{A1.9}$$

where $\varepsilon = \mathrm{sgn}(\mathrm{Im}(x))$ and the subscripts 0 and ∞ denote power series and asymptotic series solutions respectively. Using (A1.3) we can write $U_0^{(B)} = U_\infty^{(B)}T$, where the matrix T is given by

$$T = \begin{pmatrix} \dfrac{\Gamma(2\mu+1)}{\Gamma(\mu-\kappa+\frac{1}{2})} & \dfrac{(-\mu-\kappa-\frac{1}{2})\Gamma(-2\mu+1)}{(\mu-\kappa-\frac{1}{2})\Gamma(-\mu-\kappa+\frac{1}{2})} \\ \dfrac{\Gamma(2\mu+1)\exp[\mathrm{i}\pi(\mu-\kappa-\frac{1}{2})]}{\Gamma(\mu+\kappa+\frac{3}{2})} & \dfrac{\Gamma(-2\mu+1)\exp[-\mathrm{i}\pi(\mu+\kappa+\frac{1}{2})]}{\Gamma(-\mu+\kappa+\frac{3}{2})} \end{pmatrix}. \tag{A1.10}$$

The array of Whittaker functions of the second kind given in (A1.9) is generated by the matrix asymptotic series in (A2.4).

In order to make use of the matrix power series solution, we transform (A1.6) to the A-diagonal representation by writing $U^{(A)} = C^{AB}U^{(B)}$ where

$$U_0^{(A)} = \begin{pmatrix} M_{\kappa+\frac{1}{2},\mu-\frac{1}{2}}(x) & \dfrac{\mu+\kappa+\frac{1}{2}}{2\mu(2\mu-1)} M_{\kappa+\frac{1}{2},-\mu+\frac{1}{2}}(x) \\ \dfrac{-(\mu-\kappa-\frac{1}{2})}{2\mu(2\mu+1)} M_{\kappa+\frac{1}{2},\mu+\frac{1}{2}}(x) & M_{\kappa+\frac{1}{2},-\mu-\frac{1}{2}}(x) \end{pmatrix} \tag{A1.11}$$

and

$$C^{AB} = \frac{1}{2\mu}\begin{pmatrix} \mu-\kappa-\frac{1}{2} & \mu+\kappa+\frac{1}{2} \\ -(\mu-\kappa-\frac{1}{2}) & \mu-\kappa-\frac{1}{2} \end{pmatrix}.$$

The A and B matrices in A-diagonal form are

$$A^{(A)} = \begin{pmatrix} \mu & 0 \\ 0 & -\mu \end{pmatrix} \qquad B^{(A)} = \frac{\mathrm{i}p}{\mu}\begin{pmatrix} \kappa+\frac{1}{2} & \mu+\kappa+\frac{1}{2} \\ \mu-\kappa-\frac{1}{2} & -(\kappa+\frac{1}{2}) \end{pmatrix}.$$

The array of solutions in equation (A1.11) are generated by the matrix power series given in (A2.2) of appendix 2.

The A-diagonal solution also has a useful recursive property on the label μ. If we designate the first column of (A1.11) by $U_\mu^{(1)}$, then by manipulating the recursion relations of the Gauss ${}_1F_1$ functions, one can show that

$$U_{\mu+1}^{(1)} = \left(C_\mu^{(1)}/x - D_\mu^{(1)}\right) U_\mu^{(1)} \tag{A1.12}$$

where

$$C_\mu^{(1)} = \frac{2\mu(2\mu+1)^2(2\mu+2)}{(\kappa+\mu+\frac{3}{2})(\kappa-\mu+\frac{1}{2})}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

and

$$D_\mu^{(1)} = \frac{2\mu+1}{(\kappa+\mu+\frac{3}{2})(\kappa-\mu+\frac{1}{2})}\begin{pmatrix} 0 & -2\mu(\kappa+\mu+\frac{3}{2}) \\ (2\mu+2)(\kappa-\mu+\frac{1}{2}) & 2\kappa(2\mu+1) \end{pmatrix}.$$

The second column $U_\mu^{(2)}$ of (A1.11) is obtained from the first by the operation $U_\mu^{(2)} = KU_{-\mu}^{(1)}$ where $K = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ interchanges elements. Therefore

$$U_{\mu+1}^{(2)} = (C_\mu^{(2)}/x - D_\mu^{(2)})\, U_\mu^{(2)} \tag{A1.13}$$

where

$$C_\mu^{(2)} = KC_{-\mu}^{(1)}K \qquad \text{and} \qquad D_\mu^{(2)} = KD_{-\mu}^{(1)}K.$$

Appendix 2

Consider the first-order matrix differential equation

$$\frac{\mathrm{d}W(A, B; x)}{\mathrm{d}x} = \left(\frac{A}{x} - B\right) W(A, B; x) \tag{A2.1}$$

where A, B and W are $n \times n$ matrices. In a representation where the A matrix is diagonal, denoted by a superscript (A), a power series to (A2.1) is easily obtained (Sud *et al* 1976, Onley 1972):

$$W_0^{(A)}(A, B; x) = \sum_{m=0}^{\infty} V_m x^{m+A} \tag{A2.2}$$

where

$$V_0 = I_n$$

and

$$\{V_m\}_{ij} = \{-B^{(A)} V_{m-1}\}_{ij} / (A_{jj} - A_{ii} + m). \tag{A2.3}$$

A scalar to a diagonal matrix power is to be interpreted as a diagonal matrix with elements $\{x^{A_{ii}}\}_{ii}$.

An asymptotic series solution to equation (A2.1) can be given in a B-diagonal representation. It is (Sud *et al* 1976, Onley 1972)

$$W_\infty^{(B)}(A, B; x) = \sum_{m=0} D_m x^{\bar{A}-m} \, \mathrm{e}^{-Bx} \tag{A2.4}$$

where $D_0 = I_n$, and the diagonal matrix $\bar{A}$ consists of the diagonal elements of the A matrix. Defining the matrix $\bar{\bar{A}} = A - \bar{A}$, which only has non-diagonal elements, the recursion relation for the matrices D_m can be written for $i \neq j$ as

$$\{D_m\}_{ij} = \frac{\{(\bar{\bar{A}} + m - 1)D_{m-1}\}_{ij} + (A_{ii} - A_{jj})\{D_{m-1}\}_{ij}}{B_{ii} - B_{jj}} \tag{A2.5}$$

and for $i = j$

$$\{D_m\}_{ii} = -\frac{1}{m} \sum_{k \neq i} A_{ik} \{D_m\}_{ki}. \tag{A2.6}$$

Note that these two equations in Sud *et al* (1976) contain sign errors.

Both the power series solutions and the asymptotic series solutions can be transformed to either the B-diagonal or A-diagonal representation as need arises. Furthermore, since W_0 and W_∞ represent the general solution to the differential equation, then $W_0 = W_\infty T$ where T is an $n \times n$ constant matrix which depends on the particular problem under consideration.

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