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1978 J. Phys. A: Math. Gen. 11 L237

(http://iopscience.iop.org/0305-4470/11/10/001)

J. Phys. A: Math. Gen., Vol. 11, No. 10, 1978. Printed in Great Britain

LETTER TO THE EDITOR

Asymptotic expansions of radial integrals for Dirac–Coulomb functions

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Received 12 July 1978

Abstract. An asymptotic expansion of the Appell's hypergeometric function $F_2(\alpha, a_1, a_2, b_1, b_2; x, y)$ is given for the case when all of its five parameters are large. This result is useful for calculating the radial integrals involving higher angular momentum components in electron wavefunctions.

1. Introduction

The radial matrix elements which arise in the distorted wave Born approximation (DWBA) analysis of an electron scattering in the Coulomb field of the nucleus can be expressed in term of Appell's hypergeometric function F_2 (Überall 1971). Appell's hypergeometric function F_2 is a doubly infinite series:

$$F_2(\alpha, a_1, a_2, b_1, b_2; x, y) = \sum_{m,n} \frac{(\alpha)_{m+n}(a_1)_m(a_2)_n}{(b_1)_m(b_2)_n m!n!} x^m y^n \tag{1}$$

which is convergent for $|x|+|y|<1$ (Erdélyi *et al* 1953). The variables of the F_2 function which occur in calculations of the virtual photon spectrum (inelastic electron scattering) and bremsstrahlung do not satisfy the conditions of convergence. Such F_2 functions require analytic continuation relations which are given in the literature (Gargaro and Onley 1971, Sud and Wright 1976, Sud *et al* 1976). The continuation relations are given in terms of five doubly infinite series (Sud and Wright 1976) and in terms of three series (Gargaro and Onley 1976, Sud and Wright 1976). We shall use the continuation given in terms of three doubly infinite series. The expression for the virtual photon spectrum is given in §2 in terms of an infinite sum over positive definite terms in equation (4), a similar type of expression exists for the bremsstrahlung. The term involving large partial waves corresponds to distant collisions which emit relatively small numbers of photons, yet the series is extremely slowly converging. Consequently, the calculations of the virtual photon spectrum and the bremsstrahlung cross section become very time consuming. In this Letter we give a method to compute the radial matrix elements for terms involving higher angular momentum components in the electron wavefunctions. In § 2 it is shown that Appell's F_2 function for such matrix elements has all its five parameters very large. The F_2 function and the associated series to which it is continued have Barne's integral representations (Slater 1966). In § 3 Barne's integral representations for Q_1, Q_2 and F_3 functions are used to obtain the asymptotic expansion for the F_2 function.

2. Radial integrals for Dirac–Coulomb functions

Here we shall give the expression for the virtual photon spectrum and show that the radial integrals can be evaluated by computing Appell's hypergeometric function F_2. For a relativistic electron in the Coulomb field of a point nucleus, the radial wavefunctions are the solutions of the Dirac equation with $V=-Ze^2/r$:

$$(\alpha \cdot p+\beta m_e+V)\psi=E\psi \tag{2}$$

where

$$\alpha_i=\begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}, \qquad \beta=\begin{bmatrix} I_2 & 0 \\ 0 & -I_2 \end{bmatrix}$$

and σ_i, $i=1, 2, 3$, are the Pauli spin matrics, I_2 is the 2×2 unit matrix. The solutions of the equation (2) (Rose 1961) have the form

$$\psi_\kappa^\mu=\begin{bmatrix} g_\kappa & \chi_\kappa^\mu \\ if_\kappa & \chi_{-\kappa}^\mu \end{bmatrix}$$

The spin-angle functions χ_κ^μ and $\chi_{-\kappa}^\mu$ are eigenfunctions of the operator $\boldsymbol{K}=(\boldsymbol{\sigma}\cdot\boldsymbol{L}+1)$ with eigenvalues $-\kappa$ and κ respectively, and μ is the eigenvalue of the third component of total angular momentum.

The normalised wavefunctions f_κ and g_κ are given as

$$\begin{Bmatrix} f_\kappa \\ g_\kappa \end{Bmatrix}=\begin{Bmatrix} -(E-m_e)/p \\ 1 \end{Bmatrix}\frac{(pr)^{\gamma-1}2^\gamma e^{\pi/2}|\Gamma(\gamma+i\eta)|}{\Gamma(2\gamma+1)}$$
$$\times\begin{Bmatrix} \mathrm{Im} \\ \mathrm{Re} \end{Bmatrix}[(\gamma+i\eta)e^{-i(pr-\phi)}{}_1F_1(\gamma+1+i\eta, 2\gamma+1; 2ipr)] \tag{3}$$

where

$$p=(E^2-m_e^2)^{1/2}, \qquad \gamma=(\kappa^2-\alpha^2Z^2)^{1/2}, \qquad \eta=\alpha ZE/p$$
$$e^{2i\phi}=e^{-i\pi}\frac{\kappa-i\alpha Zm_e/p}{\gamma+i\eta}, \qquad -\pi<\phi<0.$$

The phase shift of this solution is

$$-\arg|\Gamma(\gamma+i\eta)+\phi-\tfrac{1}{2}\pi+\tfrac{1}{2}|\kappa|\pi|.$$

The subscript 1 (or 2) will be used to denote the incident (final) state of the electron. The expression for the virtual photon spectrum (for details see Gargaro and Onley 1971), is given as

$$N^{(\lambda L)}(E_1, W)=\frac{\alpha}{\pi}\frac{p_2}{p_1}\frac{(E_1+m_e)(E_2+m_e)W^4}{2L+1}$$
$$\times\sum_{\kappa_1\kappa_2} S(\lambda)(2j_1+1)(2j_2+1)|C(j_1, j_2, L; -\tfrac{1}{2}, \tfrac{1}{2})R^\lambda(\kappa_1, L, \kappa_2)|^2 \tag{4}$$

where $E_2=E_1-W$; and the operator $S(\lambda)$ enforces the selection rule; l_1+l_2+L is even for electric transitions and odd for magnetic transitions. We also have

$$j=|k|-\tfrac{1}{2}; \qquad l=\begin{cases} \kappa & \text{for } \kappa>0 \\ \kappa-1 & \text{for } \kappa<0. \end{cases}$$

The radial integrals involve products of incoming and outgoing electron wavefunctions and the radial part of the electromagnetic Green function. The explicit expressions are given as

$$R^{(EL)}(\kappa_1,\kappa_2,W)$$

$$=\left(\frac{L}{L+1}\right)^{1/2}\int_0^\infty r^2\,\mathrm{d}r\Big[h^1_{L-1}(Wr)(f_{\kappa_1}(p_1r)g_{\kappa_2}(p_2r)-g_{\kappa_1}(p_1r)f_{\kappa_2}(p_2r))$$

$$+\left(\frac{\kappa_1-\kappa_2}{L}\right)h^1_{L-1}(Wr)(f_{\kappa_1}(p_1r)g_{\kappa_2}(p_2r)+g_{\kappa_1}(p_1r)f_{\kappa_2}(p_2r))$$

$$-h^1_L(Wr)(f_{\kappa_1}(p_1r)f_{\kappa_2}(p_2r)+g_{\kappa_1}(p_1r)g_{\kappa_2}(p_2r))\Big] \tag{5}$$

and

$$\mathrm{R}^{(ML)}(\kappa_1,\kappa_2,W)$$

$$=\frac{\kappa_1+\kappa_2}{[L(L+1)]^{1/2}}\int_0^\infty r^2\,\mathrm{d}r\,h^1_L(Wr)(f_{\kappa_1}(p_1r)g_{\kappa_2}(p_2r)+g_{\kappa_1}(p_1r)f_{\kappa_2}(p_2r)). \tag{6}$$

By using finite expansion for the spherical Hankel function,

$$h^{(1)}_L(Wr)=-\mathrm{e}^{\mathrm{i}Wr}\sum_{n=1}^{L+1}\frac{\Gamma(L+n)}{\Gamma(n)\Gamma(L+2-n)}2^{1-n}\mathrm{i}^{n-2}\rho^{n-2} \tag{7}$$

and g_κ and f_κ as given in equation (3), we can express the integrals in equations (5) and (6) as a sum of the following integrals:

$$I(l,m,n)=\int_0^\infty \mathrm{d}r\,r^{\gamma_1+\gamma_2-n}\exp[\mathrm{i}(p_2-p_1+W)r]$$

$$\times\,{}_1F_1(\gamma_1+l-1+\mathrm{i}\eta_1,2\gamma_1+1;2\mathrm{i}p_1r)\,{}_1F_1(\gamma_2+2-m-\mathrm{i}\eta_2,2\gamma_2+1;2\mathrm{i}p_2r) \tag{8}$$

where $l, m=1,2$. The above integral can be written in general notation as follows:

$$I=\int_0^\infty \mathrm{d}r\,\mathrm{e}^{-\Delta r}r^{\alpha-1}\,{}_1F_1(a_1,b_1;k_1r)\,{}_1F_1(a_2,b_2;k_2r)$$

$$=\Gamma(\alpha)\Delta^{-\alpha}F_2(\alpha,a_1,a_2,b_1,b_2;k_1/\Delta,k_2/\Delta). \tag{9}$$

For large values of Dirac angular momentum quantum numbers $\kappa_1(\gamma_1)$ and $\kappa_2(\gamma_2)$, all the five parameters of the F_2 function become large. In the next section we give the asymptotic expansion of such a function.

3. Asymptotic expansion for the F_2 function

We shall use following analytic continuations (see Sud *et al* 1976) of the F_2 function:

$$F_2(\alpha,a_1,a_2,b_1,b_2;x,y)=Q'_1+Q'_2+Q'_3. \tag{10}$$

The Q'_1, Q'_2 and Q'_3 series are given explicitly as

$$Q'_1=\frac{\Gamma(b_2)\Gamma(a_2-\alpha)}{\Gamma(a_2)\Gamma(b_2-\alpha)}(-y)^{-\alpha}Q_1 \tag{11}$$

$$Q_2' = \frac{\Gamma(b_2)\Gamma(\alpha-a_2)\Gamma(b_1)\Gamma(a_1+a_2-\alpha)}{\Gamma(\alpha)\Gamma(b_2-a_2)\Gamma(a_1)\Gamma(b_1+a_2-\alpha)}\left(\frac{x}{y}\right)^{a_2}(-x)^{-\alpha}Q_2 \tag{12}$$

$$Q_3' = \frac{\Gamma(b_2)\Gamma(b_1)\Gamma(\alpha-a_1-a_2)}{\Gamma(\alpha)\Gamma(b_2-a_2)\Gamma(b_1-a_1)}(-y)^{-a_2}(-x)^{-a_1}$$
$$\times F_3(a_1, a_2, 1-b_1+a_1, 1-b_2-a_2 : 1+a_1-a_2-\alpha : 1/x, 1/x) \tag{13}$$

where

$$Q_1 = \sum_{m,n} \frac{(\alpha)_{m+n}(1-b_2+\alpha)_{m+n}(a_1)_m}{(1-a_2+\alpha)_{m+n}(b_1)_n\, m!n!}\left(\frac{1}{y}\right)^m\left(-\frac{x}{y}\right)^n$$

and

$$Q_2 = \sum_{m,n} \frac{(a_2)_n(1-b_2+a_2)_n(a_1+a_2-\alpha)_{n-m}}{(b_1+a_2-\alpha)_{n-m}(1+a_2-\alpha)_{n-m}m!n!}\left(-\frac{1}{x}\right)^m\left(-\frac{x}{y}\right)^n.$$

For large values of κ_1 and κ_2 all the parameters of the F_2 function are large but a few parameters of the Q_1, Q_2 and F_3 series become small. For the Q_1 series the parameter $(1-b_2+\alpha)$, for the Q_2 series the parameter $(a_1+a_2-\alpha)$ and for the F_3 function the parameter $(1+a_1+a_2-\alpha)$ are small. We will obtain the asymptotic expansions for Q_1, Q_2 and F_3 series when one parameter in each series is small.

We describe here in detail the method used to obtain the asymptotic expansion for the Q_1 series. The Barnes integral representation for the Q_1 series is given as

$$Q_1(a, b, c : d, e : x, y)$$
$$= \frac{\Gamma(d)\Gamma(e)}{\Gamma(a)\Gamma(b)\Gamma(c)}\frac{1}{(2\pi i)^2}\int\int_{-i\infty}^{+i\infty} ds\, dt \frac{\Gamma(a+s+t)\Gamma(b+s+t)}{\Gamma(d+s+t)\Gamma(e+t)}$$
$$\times\Gamma(c+s)\Gamma(-s)\Gamma(-t)(-x)^s(-y)^t. \tag{14}$$

The integrand has the following sequences of poles: an increasing sequences of poles at

$$s=n, t=n \qquad \text{where } n = 0, 1, 2, \ldots$$

and the decreasing sequence of poles at

$$s=-c-n \qquad \text{where } n = 0, 1, 2, \ldots.$$

The Q_1 series is obtained by closing the contours in the s and t planes on the right-hand side of the imaginary axis, and integrating by making use of the residue theorem. The asymptotic expression for the $\Gamma(c+s)$ for large values of c (Erdélyi *et al* 1953) is given as

$$\Gamma(c+s) \sim (2\pi)^{1/2}\, e^{-c}\, e^{s+c-\frac{1}{2}}, \tag{15}$$

when $c \to \infty$; if $|\arg(s+c)| \leq \pi-\delta$, $|\arg c| \leq \pi-\delta$, where δ is any positive parameter. On substituting in equation (14), the asymptotic values of the gamma functions $\Gamma(a+s+t)$, $\Gamma(c+s)$, $\Gamma(d+s+t)$ and $\Gamma(e+t)$, for large values of their parameters a, c, d and e, we obtain

$$Q_1(a, b, c : d, e : x, y)$$
$$= \frac{1}{\Gamma(b)}\frac{1}{(\pi i)^2}\int\int_{-i\infty}^{+i\infty} ds\, dt\Gamma(b+s+t)\Gamma(-s)\Gamma(-t)\left(-\frac{ac}{d}x\right)^s\left(-\frac{a}{de}y\right)^t. \tag{16}$$

Integrating equation (16) by enclosing the contours in s and t planes on the right-hand side of the imaginary axis by using the residue theorem:

$$Q_1(a, b, c:d, e:x, y) = \sum_{m,n} \frac{(b)_{m+n}}{m!n!}\left(\frac{ac}{d}x\right)^m\left(\frac{a}{de}y\right)^n. \tag{17}$$

Similarly, we can obtain the asymptotic expansions for Q_2 and F_3 series:

$$Q_2(a, b, c:d, e:x, y) = \sum_{m,n} \frac{(c)_{n-m}}{m!n!}(dex)^n\left(\frac{ab}{de}y\right)^n \tag{18}$$

and

$$F_3(a_1, a_2, b_1, b_2:c:x, y) = \sum_{m,n} \frac{1}{(c)_{m+n}m!n!}(a_1b_1x)^m(a_2b_2y)^n. \tag{19}$$

On substituting the asymptotic expansions for Q_1, Q_2 and F_3 functions (as given by equations (17), (18) and (19)) in equation (10), we obtain the asymptotic expansion of the F_2 function when all of its five parameters have large values:

$$F_2(\alpha, a_1, a_2, b_1, b_2: x, y)$$
$$= \left(\frac{\Gamma(b_2)\Gamma(a_2-\alpha)}{\Gamma(a_2)\Gamma(b_2-\alpha)}(-y)^{-\alpha}\right) \sum_{m,n} \frac{(1-b_2+\alpha)_{m+n}}{m!n!}\left(\frac{\alpha a_1}{(1-a_2+\alpha)y}\right)^m$$
$$\times\left(-\frac{\alpha}{(1-a_2+\alpha)b_1}\frac{x}{y}\right)^n + \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(a_1+a_2-\alpha)\Gamma(\alpha-a_2)}{\Gamma(\alpha)\Gamma(b_2-a_2)\Gamma(a_1)\Gamma(b_1+a_2-\alpha)}\left(\frac{x}{y}\right)^{a_2}(-x)^{-\alpha}$$
$$\times\sum_{m,n} \frac{(a_1+a_2-\alpha)_{n-m}}{m!n!}[(b_1+a_2-\alpha)(1+a_2-\alpha)x]^n$$
$$\times\left(\frac{a_2(1-b_2+a_2)y}{(b_1+a_2-\alpha)(1+a_2-\alpha)}\right)^m + \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(\alpha-a_1-a_2)}{\Gamma(\alpha)\Gamma(b_2-a_2)\Gamma(b_1-a_1)}(-y)^{-a_2}(-x)^{-a_1}$$
$$\times\sum_{m,n} \frac{1}{(1+a_1+a_2-\alpha)_{m+n}}\frac{1}{m!n!}\left(\frac{a_1(1+a_1-b_1)}{x}\right)^m\left(\frac{a_2(1+a_2-b_2)}{y}\right)^n. \tag{20}$$

The expression given in equation (20) may be used to compute the radial integrals involving higher angular momentum components in the electron wavefunctions.

References

Erdélyi A, Magnus W, Oberhettinger F, and Tricomi F C 1953 *Higher Transcendental Functions* vol. 1 (New York: McGraw-Hill)

Gargaro W W and Onley D S 1971 *Phys. Rev.* C 4 1032

Rose M E 1961 *Relativistic Electron Theory* (New York: Wiley)

Slater L J 1966 *Generalized Hypergeometric Functions* ((Cambridge: Cambridge University Press)

Sud K K and Wright L E 1976 *J. Math. Phys.* **17** 1719

Sud K K, Wright L E and Onley D S 1976 *J. Math. Phys.* **17** 2175

Überall H 1971 *Electron Scattering from Complex Nuclei* (New York, London: Academic)