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An approximate partial differential matrix equation in the lepton energy for evaluation of Dirac–Coulomb radial integrals

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Abstract. Radial integrals consisting of products of Whittaker functions of the first and second kind arise frequently in expressions for various scattering processes. In particular, the Dirac-Coulomb radial integrals for intermediate energy DWBA lepton pair production and bremsstrahlung consist of products of Whittaker functions that result in slowly converging series expressions. An approximate partial differential matrix equation in the lepton energy is obtained that can be used to numerically propagate Dirac-Coulomb radial integrals along the lepton and photon energy spectrum, resulting in substantial time savings on the computer. Radial integrals for DWBA electron pair production from 10 MeV photons are calculated as an example of the use of the approximate equation that yield three significant digit accuracy.

1. Introduction

Many radial matrix elements that occur in the formulation of a scattering process involve integrals over products of Whittaker functions of the first and second kind. Whittaker functions (Whittaker and Watson 1927) are closely related to numerous other functions of special interest in scattering processes, e.g. Bessel functions, Coulomb functions and Dirac–Coulomb functions. Integrals over products of related functions can therefore be re-expressed into integrals involving products of Whittaker functions. Often, the evaluation of these radial integrals in terms of their infinite series expansions was not possible due to the series being barely convergent or not convergent at all for the momentum variables of the problem.

In recent years, radial integrals over Whittaker functions have been expressed in terms of matrix gamma functions (Onley 1972, Sud *et al* 1976). The matrix gamma function is a generalization of the gamma function consisting of an integral over products of solutions to a first-order differential matrix equation. The matrix gamma function obeys a recurrence relation and a partial differential matrix equation (Wright *et al* 1977) which can be used to reduce the number of direct evaluations of radial matrix elements. This yields a substantial saving on computation time for matrix elements of scattering processes involving large angular momentum components in the incident and outgoing waves.

The difficulties of convergence in the evaluation of radial integrals in the form of the matrix gamma function have been handled for the case of DWBA electron pair production and bremsstrahlung processes at intermediate energies (Kosik 1980, Wright *et al* 1987) by an analytic continuation of the matrix gamma function consisting of direct evaluation in a convergent domain followed by numerical integration of a partial

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differential matrix equation back to the domain of interest. A more general expression for the matrix gamma function in terms of convergent matrix series was given by Wright and Talwar (1986).

Calculation of pair production or bremsstrahlung processes at intermediate energies can now be done without numerical difficulties; however, even with the use of matrix recursion relations, an enormous amount of computer time is still required to calculate matrix elements. For example, the total cross-section for electron pair production has only been calculated in the intermediate energy range (10–50 MeV) at 10 and 20 MeV. In order to save substantial amounts of computation time, approximate partial differential matrix equations have been derived in the photon energy and lepton energy for pair production and bremsstrahlung processes (Sud *et al* 1979, Sud and Sharma 1984). Unfortunately, these approximations are quite restrictive and rather poor when used in a direct manner.

In section 2 I will derive an improved approximate partial differential matrix equation in the lepton energy for the matrix gamma function consisting of Whittaker functions corresponding to Dirac–Coulomb radial integrals. In section 3 I will discuss a technique for avoiding round-off difficulties associated with direct numerical integration of the partial differential matrix equation in the lepton energy. In section 4 I apply these results to the evaluation of Dirac–Coulomb radial integrals that arise in electron pair production of intermediate energy photons in the presence of a point Coulomb field of the atomic nucleus.

2. Approximate partial differential matrix equation in the lepton energy for the matrix gamma function

Whittaker functions arise in the general solution to the differential matrix equation

$$\frac{dU}{dx}=\left(\frac{A}{x}-B\right)U \tag{1}$$

where A, B, and U are 2×2 matrices. For example, a solution to equation (1) involving Whittaker functions of the first kind $M_{k,\mu}$ with a diagonal B matrix has

$$A=\begin{pmatrix}-(k+\frac{1}{2}) & \mu+\kappa+\frac{1}{2}\\ \mu-\kappa-\frac{1}{2} & \kappa+\frac{1}{2}\end{pmatrix}\qquad B=\begin{pmatrix}-\frac{1}{2} & 0\\ 0 & \frac{1}{2}\end{pmatrix} \tag{2}$$

and a solution matrix $U_{\kappa,\mu}$ given as

$$U_{\kappa,\mu}=\frac{1}{x^{1/2}}\begin{pmatrix}M_{\kappa,\mu}(x) & [(\kappa+\mu+\frac{1}{2})/(\kappa-\mu+\frac{1}{2})]M_{\kappa,-\mu}(x)\\ M_{\kappa+1,\mu}(x) & M_{\kappa+1,-\mu}(x)\end{pmatrix}. \tag{3}$$

It is possible and very useful to transform the solution U to equation (1) into a representation where either the matrix A or B is diagonal. The matrices of a given representation are labelled with the appropriate superscript, e.g. $U^{(A)}$.

The solution to the Dirac equation for a point Coulomb potential can be separated into radial and angular functions (Rose 1961). The radial Dirac–Coulomb functions for a given lepton energy E and mass m are also solutions to an equation of the form of (1) given as

$$\frac{dU_0^{(S)}}{dr}=\left(\frac{A^{(S)}}{r}-B^{(S)}\right)U_0^{(S)} \tag{4}$$

where

$$A^{(S)}=\begin{pmatrix}-\kappa & \alpha Z\\ -\alpha Z & \kappa\end{pmatrix}\qquad B^{(S)}=\begin{pmatrix}0 & -(E+m)\\ (E-m) & 0\end{pmatrix}\tag{5}$$

with a solution matrix given as

$$U_0^{(S)}=\begin{pmatrix}rg_\kappa^R(r) & rg_\kappa^I(r)\\ rf_\kappa^R(r) & rf_\kappa^I(r)\end{pmatrix}.\tag{6}$$

Here the κ is the Dirac quantum number which gives the orbital l and total j angular momentum of the lepton as $l=|\kappa+\frac{1}{2}|-\frac{1}{2}$ and $j=|\kappa|-\frac{1}{2}$, α is the fine-structure constant, Z is the atomic number of the nucleus, and $g_\kappa(r)$ and $f_\kappa(r)$ are the Dirac-Coulomb radial functions (R, regular; I, irregular). The superscript notation (S) is used to indicate that the matrices are in the so-called standard representation of the Dirac-Coulomb radial functions. The subscript 0 is used to indicate that the radial functions are expressed in terms of Whittaker functions of the first kind and therefore can be given as power series expansions.

The normalized solution $U_0^{(S)}$, its transformations to other representations, and the transformation matrices are given by Sud *et al* (1976). In the B-diagonal representation, they obtain the transformed solution

$$U_0^{(B)}=\frac{1}{\sqrt{2ipr}}\begin{pmatrix}M_{-1/2-i\eta,\gamma}(2ipr) & -[(\gamma-i\eta)/(\gamma+i\eta)]M_{-1/2-i\eta,-\gamma}(2ipr)\\ M_{1/2-i\eta,\gamma}(2ipr) & M_{1/2-i\eta,-\gamma}(2ipr)\end{pmatrix}\tag{7}$$

where $\gamma=(\kappa^2-\alpha^2Z^2)^{1/2}$, $\eta=\alpha ZE/p$ and the lepton momentum is $p=(E^2-m^2)^{1/2}$. The matrix function $U_0^{(B)}$ is a solution to equation (4) in the B-diagonal representation with $A^{(B)}$ and $B^{(B)}$ matrices given as

$$A^{(B)}=\begin{pmatrix}i\eta & \gamma-i\eta\\ \gamma+i\eta & -i\eta\end{pmatrix}\qquad B^{(B)}=\begin{pmatrix}-ip & 0\\ 0 & ip\end{pmatrix}.\tag{8}$$

Note that $U_0^{(B)}$ is a solution to equation (1) for Whittaker functions of the first kind and can be written as in equation (3) by identifying the parameters as $\kappa=-\frac{1}{2}-i\eta$ and $\mu=\gamma$ and the variable as $x=2ipr$. Equation (7) can now be seen to be a solution to equation (4) in the B-diagonal representation provided that the momentum p is considered fixed or constant and can be pulled out of the derivative in equation (1).

The radial integrals for point Coulomb scattering processes will contain products of Dirac-Coulomb functions and other functions that are solutions to the type of first-order differential matrix equation given in equation (4) that correspond to different momentum variables so that all radial integrals of interest can be formed by integrating the matrix function

$$W(r)=U_n(2ip_nr)\otimes\ldots\otimes U_2(2ip_2r)\otimes U_1(2ip_1r)\tag{9}$$

where p_i is the momentum variable for each function, U_i are 2×2 matrix functions that satisfy equations of the form of equation (4) and $W(r)$ is an $n\times n$ matrix function. Onley (1972) and Sud *et al* (1976) showed that $W(r)$ is a solution to the first-order matrix differential equation

$$\frac{dW}{dr}=\left(\frac{\mathscr{A}}{r}-\mathscr{B}\right)W\tag{10}$$

where $\mathscr{A}$ and $\mathscr{B}$ are $n\times n$ matrices given as

$$\begin{aligned}\mathscr{A}&=A_n\otimes I_{2n-2}+I_2\otimes A_{n-1}\otimes I_{2n-4}+\ldots+I_{2n-2}\otimes A_1\\ \mathscr{B}&=B_n\otimes I_{2n-2}+\ldots+I_{2n-2}\otimes B_1\end{aligned}\tag{11}$$

and I_n is an $n \times n$ unit matrix. Since the matrices U_i depend upon the Whittaker parameters κ and μ and the momentum variables, $W(r)$ dependence on these variables can be expressed through the matrices in equation (11):

$$W = W(\mathscr{A}, \mathscr{B}; r). \tag{12}$$

An important property of this solution to equation (10) is

$$r^a \, \mathrm{e}^{-br} W(\mathscr{A}, \mathscr{B}; r) = W(\mathscr{A} + a, \mathscr{B} + b; r) \tag{13}$$

where the notation $\mathscr{A} + a$ means $\mathscr{A} + aI_n$. From the same references given above, the matrix gamma function was defined as

$$\Gamma(\mathscr{A} + 1, \mathscr{B}) = \int_{(0)}^{\infty} W(\mathscr{A}, \mathscr{B}; r) \, \mathrm{d}r \tag{14}$$

where the symbol (0) indicates that any simple pole present at the origin has been subtracted out. Contained within the elements of the matrix gamma function are the radial integrals of importance to the scattering problem. The matrix gamma function obeys a recurrence relation that is similar to that for the ordinary gamma function:

$$\mathscr{A}\Gamma(\mathscr{A}, \mathscr{B}) = \mathscr{B}\Gamma(\mathscr{A} + 1, \mathscr{B}). \tag{15}$$

Now consider all momentum variables as fixed except for p_i. Taking the partial derivative of the matrix gamma function in the B-diagonal representation, we obtain

$$\frac{\partial \Gamma^{(B)}}{\partial p_i} = \int_{(0)}^{\infty} U_n^{(B)} \otimes \ldots \otimes \frac{\partial U_i^{(B)}}{\partial p_i} \otimes \ldots \otimes U_1^{(B)} \, \mathrm{d}r. \tag{16}$$

The derivative acting on $U_i^{(B)}$ within the integral can be expressed as

$$\frac{\partial U_i^{(B)}}{\partial p_i} = \frac{\partial U_i^{(B)}(x)}{\partial x} \frac{\partial x}{\partial p_i} + \frac{\partial U_i^{(B)}}{\partial y_i} \frac{\partial y_i}{\partial p_i} \tag{17}$$

where $x = 2ip_i r$ and $y_i = -\mathrm{i}\eta_i$. The second term occurs when parameters in $U_i^{(B)}$ depend upon η_i which in turn depends upon the momentum p_i. When this occurs, $U_i^{(B)}$ is considered to be a function of x and the parameter y_i. This is the case for the Dirac-Coulomb functions. Substituting equation (1) into the first term of equation (17) yields

$$\frac{\partial U_i^{(B)}(x)}{\partial x} \frac{\partial x}{\partial p_i} = \left(\frac{A_i}{2ip_i r} - B \right) (2ir) U_i^{(B)} = (A_i^{(B)} - B_i^{(B)} r) \left(\frac{U_i^{(B)}}{p_i} \right). \tag{18}$$

The second term in equation (17) can be evaluated for the Dirac-Coulomb radial functions by first considering the derivative of one of the Whittaker functions that make up the matrix $U_i^{(B)}$. The Whittaker function $M_{\kappa,\mu}(x)$ can be expressed in terms of the confluent hypergeometric series ${}_1F_1$ as (Slater 1960)

$$M_{\kappa,\mu} = \mathrm{e}^{-x/2} x^{\mu+1/2} \, {}_1F_1(\mu - \kappa + \tfrac{1}{2}, 2\mu + 1; x) \tag{19}$$

where the confluent hypergeometric function has an integral representation given as

$${}_1F_1(a, c; x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 \mathrm{e}^{xt} t^{a-1} (1-t)^{c-a-1} \, \mathrm{d}t \tag{20}$$

provided that

$$\ldots \Re(c) > \Re(a) > 0.$$

Taking the derivative of equation (19) with respect to the parameter κ gives

$$\frac{\partial M_{\kappa,\mu}}{\partial \kappa} = e^{-x/2}\, x^{\mu+1/2} \frac{\partial\, {}_1F_1(\mu-\kappa+\frac{1}{2}, 2\mu+1; x)}{\partial \kappa} \tag{21}$$

The derivative of the confluent hypergeometric function becomes

$$\frac{\partial\, {}_1F_1}{\partial \kappa} = \frac{\partial}{\partial \kappa}\left(\frac{\Gamma(2\mu+1)}{\Gamma(\mu-\kappa+\frac{1}{2})\Gamma(\mu+\kappa+\frac{1}{2})}\int_0^1 e^{xt}\, t^{\mu-\kappa-1/2}(1-t)^{\mu+\kappa-1/2}\, dt\right). \tag{22}$$

From the definition of the digamma function $\psi(z)$ (Erdelyi *et al* 1953) the derivative of the gamma function is given as

$$\frac{d\Gamma(z)}{dz} = \Gamma(z)\psi(z). \tag{23}$$

Using this in equation (22) gives

$$\frac{\partial\, {}_1F_1}{\partial \kappa} = [\psi(\mu-\kappa+\tfrac{1}{2}) - \psi(\mu+\kappa+\tfrac{1}{2})]\, {}_1F_1 + \frac{\Gamma(2\mu+1)}{\Gamma(\mu-\kappa+\frac{1}{2})\Gamma(\mu+\kappa+\frac{1}{2})}\frac{\partial I(\kappa, \mu; x)}{\partial \kappa} \tag{24}$$

where

$$I(\kappa, \mu; x) = \int_0^1 e^{xt}\, t^{\mu-\kappa-1/2}(1-t)^{\mu+\kappa-1/2}\, dt. \tag{25}$$

The derivative of the integral I in equation (24) can be evaluated by expanding the exponential in the integral in a power series and taking the derivative of the result term by term, giving

$$\frac{\partial I}{\partial \kappa} = \frac{\partial}{\partial \kappa}\left(\sum_{n=0}^{\infty}\frac{x^n}{n!}\int_0^1 t^{\mu+n-k-1/2}(1-t)^{\mu+\kappa-1/2}\, dt\right) = \sum_{n=0}^{\infty}\frac{x^n}{n!}\frac{\partial B(\mu+n-\kappa+\frac{1}{2}, \mu+\kappa+\frac{1}{2})}{\partial \kappa} \tag{26}$$

where $B(x, y)$ is a beta function. Since the beta function can be expressed as

$$B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \tag{27}$$

then using this and equation (23) in equation (26) yields the result

$$\frac{\partial I}{\partial \kappa} = [\psi(\mu+\kappa+\tfrac{1}{2}) - \psi(\mu-\kappa+\tfrac{1}{2})]I(\kappa, \mu; x) - \left[\sum_{n=1}^{\infty}\frac{x^n}{n!}\left(\sum_{m=0}^{n-1}\frac{1}{(\mu+m-\kappa+\frac{1}{2})}\right)\frac{\Gamma(\mu+n-\kappa+\frac{1}{2})\Gamma(\mu+\kappa+\frac{1}{2})}{\Gamma(2\mu+1+n)}\right]. \tag{28}$$

(See the appendix for the details leading to the result in equation (28).) Substituting this into equation (24) gives

$$\frac{\partial\, {}_1F_1}{\partial \kappa} = -\sum_{n=1}^{\infty}\frac{(\mu-\kappa+\frac{1}{2})_n x^n}{(2\mu+1)_n n!}\left(\sum_{m=0}^{n-1}\frac{1}{(\mu+m-\kappa+\frac{1}{2})}\right) \tag{29}$$

where $(z)_n = \Gamma(z+n)/\Gamma(z)$ is a Pochhammer symbol. The result given in equation (29) could now be used to find an expression for the second term in equation (17) that is open ended but would require an enormous amount of numerical effort to evaluate directly. What is needed is an approximate expression that will lead to a simple first-order differential matrix equation for the matrix gamma function that can be rapidly evaluated on the computer. To this end, consider making the approximation of replacing the sum in parenthesis in equation (29) by the overestimate given as

$$\left(\sum_{m=0}^{n-1} \frac{1}{(\mu+m-\kappa+\frac{1}{2})}\right) \approx \frac{n}{(\mu-\kappa+\frac{1}{2})}. \tag{30}$$

Substituting this approximation into equation (29) yields

$$\begin{aligned}\frac{\partial\, {}_1F_1}{\partial\kappa} &\approx -\sum_{n=1}^{\infty} \frac{(\mu-\kappa+\frac{1}{2})(\mu-\kappa+\frac{1}{2}+1)_{(n-1)}x^n}{(2\mu+1)(2\mu+1+1)_{(n-1)}(n-1)!(\mu-\kappa+\frac{1}{2})} \\ &\approx \left(\frac{-x}{2\mu+1}\right) \sum_{n=1}^{\infty} \frac{(\mu-\kappa+\frac{1}{2})_{(n-1)}x^{n-1}}{(2\mu+1)_{(n-1)}(n-1)!}\end{aligned} \tag{31}$$

or

$$\frac{\partial\, {}_1F_1}{\partial\kappa} \approx \left(\frac{-x}{2\mu+1}\right) {}_1F_1 \tag{32}$$

where a further approximation was made in neglecting the 1's in the Pochhammer symbols. Since the Whittaker functions that occur in the B-diagonal representation have parameters given as

$$\kappa = -\tfrac{1}{2}+y \qquad \mu = \gamma \tag{33}$$

κ will not change much in the interior region of the energy spectrum where $E \gg m$ so that to a good approximation in this region $\kappa \approx -\frac{1}{2} - i\alpha Z(1+m^2/2p^2)$. Therefore, most γ values will exceed κ values in magnitude with a resulting improvement in the approximations made in equation (32) as γ becomes large.

Although the approximation in equation (30) is rather harsh for large n, it is workable because the dominant contributions to the radial integrals will require a small number n of terms in equation (29) to reach a point where the onset of convergence occurs. This can be seen to be true by examining the ratio $\mathcal{R}$ of a term at $n+1$ over a term at n in equation (29):

$$\begin{aligned}\mathcal{R} &= \frac{(\mu+n-\kappa+\frac{1}{2})x}{(2\mu+1+n)(n+1)} \frac{(\Sigma_{m=0}^{n} 1/(\mu+m-\kappa+\frac{1}{2}))}{(\Sigma_{m=0}^{n-1} 1/(\mu+m-\kappa+\frac{1}{2}))} \\ &\approx \frac{(\mu+n-\kappa+\frac{1}{2})x}{(2\mu+1+n)(n+1)}.\end{aligned} \tag{34}$$

Desiring for convergence, $|\mathcal{R}| < 1$, and noting that dominant contributions occur when $|x| \sim |2pr| \sim |2l| \sim |2\kappa|$, then $n < |2\kappa|$.

Substituting equation (32) into equation (21) gives

$$\frac{\partial M_{\kappa,\mu}}{\partial\kappa} \approx \left(\frac{-x}{2\mu+1}\right) M_{\kappa,\mu} \tag{35}$$

Using equations (7), (33) and (35), the second term of equation (17) becomes

$$\frac{\partial U_i^{(B)}}{\partial y_i}\frac{\partial y_i}{\partial p_i} \approx \left(\frac{i\alpha Z m^2}{E_i p_i^2}\right)\left(\frac{-2ip_i r U_i^{(B)}}{2\gamma_i+1} + D_i V_i^{(B)}\right) \tag{36}$$

where

$$D=\begin{pmatrix}2\gamma/(\gamma^2-y^2) & 0\\ 0 & 0\end{pmatrix} \tag{37}$$

and $V_i^{(B)}$ is the same as $U_i^{(B)}$ with the first column of functions set to zero.

Now consider the case where the parameters of $U_i^{(B)}$ are independent of the momentum variable p_i. The second term in equation (17) will then be zero. Substituting equations (18) and (17) into equation (16) yields the differential matrix equation

$$\frac{\partial\Gamma^{(B)}}{\partial p_i}=\int_{(0)}^{\infty} U_n^{(B)}\otimes\ldots\otimes\left(\frac{A_i^{(B)}-B_i^{(B)}r}{p_i}\right)U_i^{(B)}\otimes\ldots\otimes U_1^{(B)}\,\mathrm{d}r. \tag{38}$$

Using equations (13) and (15), equation (38) becomes

$$\begin{aligned}\frac{\partial\Gamma^{(B)}}{\partial p_i}&=\left(\frac{I_{2n-2i}\otimes A_i^{(B)}\otimes I_{2i-2}}{p_i}\right)\Gamma^{(B)}(\mathscr{A}+1,\mathscr{B})-\left(\frac{I_{2n-2i}\otimes B_i^{(B)}\otimes I_{2i-2}}{p_i}\right)\Gamma^{(B)}(\mathscr{A}+2,\mathscr{B})\\&=\left[\left(\frac{1}{p_i}\right)[(I_{2n-2i}\otimes A_i^{(B)}\otimes I_{2i-2})-(I_{2n-2i}\otimes B_i^{(B)}\otimes I_{2i-2})\mathscr{B}^{-1}(\mathscr{A}+1)]\right]\Gamma^{(B)}\end{aligned} \tag{39}$$

or

$$\frac{\partial\Gamma^{(B)}}{\partial p_i}=T_i\Gamma^{(B)}\qquad\text{(independent parameter)} \tag{40}$$

where T_i is the matrix given in the square brackets of equation (40). This is the result obtained by Wright *et al* (1977) and is essentially the same type of approximate partial differential matrix equation used by Sud and Sharma (1984) in their calculation of electron pair production in the tip region of the energy spectrum where the parameter y that arises in the radial Dirac–Coulomb functions is approximately constant.

For the case where the matrix solution $U_i^{(B)}$ contain Whittaker functions of the first kind corresponding to radial Dirac–Coulomb functions, the parameters of $U_i^{(B)}$ will be dependent upon the momentum variable p_i. Simple first-order partial differential matrix equations can be obtained for each column of the gamma matrix function. These equations are of two types depending upon whether the derivative with respect to the parameters acts on the first or second column of $U_i^{(B)}$. For the first column of $U_i^{(B)}$, substitution of equations (36), (18) and (17) into equation (16) will yield the same right-hand side as in equation (40) for the first term and using equations (13) and (15) for the second term gives

$$\frac{\partial\Gamma_1^{(B)}}{\partial p_i}\approx(T_i+R_i)\Gamma_1^{(B)}\qquad\text{(dependent parameter)} \tag{41}$$

where the matrix R_i is given by

$$R_i=\left(\frac{2\alpha Zm^2}{E_ip_i(2\gamma_i+1)}\right)\mathscr{B}^{-1}(\mathscr{A}+1). \tag{42}$$

The matrix gamma function $\Gamma_1^{(B)}$ is an n-element column vector of $\Gamma^{(B)}$ formed from the first column of $U_i^{(B)}$. Likewise to the above, the second column of $U_i^{(B)}$ yields the

result

$$\frac{\partial \Gamma_2^{(B)}}{\partial p_i} \approx (T_i + S_i)\Gamma_2^{(B)} \qquad \text{(dependent parameter)} \tag{43}$$

where the matrix S_i is given by

$$S_i = R_i + \left(\frac{i\alpha Z m^2}{E_i p_i^2}\right)(I_{2n-2i} \otimes D_i \otimes I_{2i-2}). \tag{44}$$

An improved approximate first-order partial differential matrix equation in the lepton energy is obtained by taking the derivative of $\Gamma_j^{(B)}$ with respect to the lepton energy E_i as

$$\frac{\partial \Gamma_j^{(B)}}{\partial E_i} = \sum_{k=1}^{n} \frac{\partial \Gamma_j^{(B)}}{\partial p_k} \frac{\partial p_k}{\partial E_i} \tag{45}$$

where $j = 1, 2$ and $i = 1, \ldots, n$ with the additional partial derivatives in the above equation present to allow for the possible dependence of momentum variables on the energy E_i, as for instance would be required by conservation of energy in a scattering process. Use of equation (45) along with equations (40), (41) and (43) enable rapid numerical integration of the vector gamma function from some initial lepton energy to a range of other adjacent lepton energies for the radial Dirac–Coulomb functions.

3. Numerical integration of the vector gamma function

The $n \times n$ $\mathscr{B}$ matrix in *B-diagonal representation* consists of elements that span all combinations of signs between the individual elements of each $B_i^{(B)}$. Since the radial integrals for the scattering problem will contain products of matrix functions corresponding to different momentum $U_i^{(B)}(2ip_i r)$ that are solutions to equations of the form of equation (4), then we will find $B_i^{(B)}$ of the form of equation (8). Hence, $\mathscr{B}$ will contain elements like $(\pm ip_n \pm \ldots \pm ip_i \pm \ldots \pm ip_1)$. The numerical evaluation of equation (45) requires the formation of $\mathscr{B}^{-1}$ and therefore the inversion of the elements in $\mathscr{B}$. At intermediate and higher lepton energies $E \approx p$ and because of energy conservation in the scattering process, one of the elements of $\mathscr{B}^{-1}$ will be *nearly* singular. This causes significant loss of precision in the numerical integration of the vector gamma function in equation (45).

To alleviate this numerical difficulty, consider as a first step numerically integrating equation (45) for a momentum variable p that has independent parameters and where all other momentum variables are fixed. Equation (45) along with equation (40) give for this case the exact expression

$$\frac{\partial \Gamma_j^{(B)}}{\partial E} = \left(\frac{\partial p}{\partial E}\right) T \Gamma_j^{(B)} \qquad \text{(independent } p\text{)}. \tag{46}$$

Having obtained the vector gamma function at a non-physical value of the energy E', the near singularity in the inverse matrix $\mathscr{B}^{-1}$ is removed. The second step is to now numerically integrate equation (45) for the energy variable of interest, maintaining conservation of energy and the energy difference $\delta E = E' - E$. After the desired vector gamma function at $E'' = \delta E + E'''$ is calculated, the third step is to use equation (46)

in reverse to numerically integrate the vector gamma function back to the physical E''' required by energy conservation. The diagram below illustrates this three-step procedure for numerical precision:

$$\begin{array}{ccc} \Gamma(E, E_{(i)}) & \rightarrow & \Gamma(E', E_{(i)}) \\ \Downarrow & & \downarrow \\ \Gamma(E''', E_{(j)}) & \leftarrow & \Gamma(E'', E_{(j)}) \end{array}$$

where $E_{(i)}$ represents the set of all energy variables that Γ depends upon except E. Although the near singularity occurs in the first and last steps of the above procedure, it only exists over a few of the numerical integration steps and therefore does not cause a significant loss in precision.

4. Evaluation of Dirac–Coulomb radial integrals for electron pair production

As an example application of the approximate partial differential matrix equation in the lepton energy for the matrix gamma function, consider the vector gamma function that contains as elements the radial integrals needed for calculation of DWBA matrix elements in electron pair production (Wright *et al* 1987). This vector gamma function consists of the integrand

$$W(\mathscr{A}^{(S)}, \mathscr{B}^{(S)}; r) = U_3^{(S)}(ip_3 r) \otimes U_2^{(S)}(ip_2 r) \otimes U_1^{(S)}(ip_1 r) \tag{47}$$

where $U_1^{(S)}$ and $U_2^{(S)}$ are column vectors of regular Dirac–Coulomb functions given as

$$U_j^{(S)} = \begin{pmatrix} rg_j^R(p_j r) \\ rf_j^R(p_j r) \end{pmatrix} \tag{48}$$

with $(j = 1, 2)$ and $U_3^{(S)}$ is a column vector of spherical Bessel functions given as

$$U_3^{(S)} = \begin{pmatrix} j_L(\omega r) \\ j_{L-1}(\omega r) \end{pmatrix} \tag{49}$$

with L the angular momentum quantum number of the incoming photon. The radial functions in $U_2^{(S)}$ are from the radial part of the outgoing electron wavefunction with energy E_2 and momentum p_2. The outgoing positron radial functions in $U_1^{(S)}$ are obtained from $U_2^{(S)}$ by replacing the energy variables for the electron wavefunctions with $E_2 \rightarrow -E_1$ and the momentum variables with $p_2 \rightarrow -p_1$. The energy of the incoming photon is $E_3 = \omega$ with a momentum $p_3 = \omega \hat{p}_3$. In the standard representation, the matrices $A^{(S)}$ and $B^{(S)}$ of equation (4) for the electrons are as given in equation (5) with the appropriate replacements for the energy and momentum variables mentioned above. For the spherical Bessel functions of $U_3^{(S)}$, the matrices are given as

$$A_3^{(S)} = \begin{pmatrix} -L-1 & 0 \\ 0 & L-1 \end{pmatrix} \qquad B_3^{(S)} = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}. \tag{50}$$

Using the transformation equations $U_i^{(S)} = C_i^{SB} U_i^{(B)}$, equation (47) can be expressed as

$$W(\mathscr{A}^{(S)}, \mathscr{B}^{(S)}; r) = (C_3^{SB} \otimes C_2^{SB} \otimes C_1^{SB}) W(\mathscr{A}^{(B)}, \mathscr{B}^{(B)}; r). \tag{51}$$

The transformation matrices C_i^{SB} are given as (Sud *et al* 1976)

$$C_2^{SB} = \frac{ip_2(\gamma_2 - y_2)^2}{2(\gamma_2 + y_2)(\kappa_2 - i\beta_2)} \begin{pmatrix} \dfrac{\kappa_2 - i\beta_2}{\sqrt{E_2 - m}} & \dfrac{-(\gamma_2 + y_2)}{\sqrt{E_2 - m}} \\ \dfrac{i(\kappa_2 - i\beta_2)}{\sqrt{E_2 + m}} & \dfrac{i(\gamma_2 + y_2)}{\sqrt{E_2 + m}} \end{pmatrix}$$

$$C_3^{SB} = \frac{1}{2}\begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix} \tag{52}$$

where $\beta = \alpha Zm/p$ and C_1^{SB} is obtained from C_2^{SB} by replacing the electron variables with positron variables as discussed above for $U_j^{(S)}$. From equation (14), equation (51) gives for the vector gamma function of pair production

$$\Gamma_1^{(S)} = (C_3^{SB} \otimes C_2^{SB} \otimes C_1^{SB})\Gamma_1^{(B)}. \tag{53}$$

The normalized transformed matrices which make up the integrand of $\Gamma_1^{(B)}$ are given as

$$U_j^{(B)} = N(\gamma_j, y_j)\begin{pmatrix} M_{-1/2+y_j,\gamma_j}(2ip_jr) \\ M_{1/2+y_j,\gamma_j}(2ip_jr) \end{pmatrix} \tag{54}$$

with

$$A_j^{(B)} = \begin{pmatrix} -y_j & \gamma_j + y_j \\ \gamma_j - y_j & y_j \end{pmatrix} \qquad B_j^{(B)} = \begin{pmatrix} -ip_j & 0 \\ 0 & ip_j \end{pmatrix} \tag{55}$$

and $N(\gamma_j, y_j)$ is the normalization factor given as

$$N(\gamma_j, y_j) = -\begin{pmatrix} \dfrac{e^{i\eta_{\kappa_j}} i^{1-\gamma_j} e^{\pi\eta_j/2}(\gamma_j + y_j)}{p_j\sqrt{E_j + m}\,(\gamma_j - y_j)} & \dfrac{|\Gamma(\gamma_j - y_j)|}{\Gamma(2\gamma_j + 1)} \end{pmatrix} \tag{56}$$

where

$$\eta_{\kappa_j} = -\frac{\pi}{2}\left(\frac{\kappa_j + |\kappa_j|}{2|\kappa_j|}\right) - \tfrac{1}{2}\tan^{-1}\left(\frac{\eta_j(\kappa_j + \gamma_j m/E_j)}{\kappa_j\gamma_j - \eta_j^2 m/E_j}\right) \qquad j = 1, 2$$

and for the $U_3^{(B)}$ matrix

$$U_3^{(B)} = \begin{pmatrix} ij_L(\omega r) + j_{L-1}(\omega r) \\ -ij_L(\omega r) + j_{L-1}(\omega r) \end{pmatrix} \tag{57}$$

with

$$A_3^{(B)} = \begin{pmatrix} -1 & L \\ L & -1 \end{pmatrix} \qquad B_3^{(B)} = \begin{pmatrix} -i\omega & 0 \\ 0 & i\omega \end{pmatrix}. \tag{58}$$

In order to numerically propagate the vector gamma function for pair production across the physical electron energy spectrum, the photon energy is considered fixed and the electron and positron energy is allowed to vary such that the total energy of the process is conserved, $\omega = E_1 + E_2$. Equation (45) yields for this situation the result

$$\frac{\partial\Gamma_1^{(B)}}{\partial E_2} = \frac{\partial\Gamma_1^{(B)}}{\partial p_2}\frac{\partial p_2}{\partial E_2} + \frac{\partial\Gamma_1^{(B)}}{\partial p_1}\frac{\partial p_1}{\partial E_2} = \left(\frac{E_2}{p_2}\right)\frac{\partial\Gamma_1^{(B)}}{\partial p_2} - \left(\frac{E_1}{p_1}\right)\frac{\partial\Gamma_1^{(B)}}{\partial p_1} \tag{59}$$

and a similiar equation for the derivative with respect to E_1. The derivatives of $\Gamma_1^{(B)}$ contain dependent parameters requiring the use of the approximate equation (41).

However, the vector gamma function for pair production contains the additional normalization factors with momentum dependence. The simplest procedure to follow is to remove the normalization factors before applying equation (59) and then restore them upon completion of the numerical propagation. In addition to removing and restoring the normalization factors, the procedure outlined in section 3 is followed to improve the numerical precision of the result.

The inverse transformation from the standard to the B-diagonal representation of equation (53) is used on $\Gamma_1^{(S)}$ calculated exactly at the energies ω, E_1 and E_2. For the first step, E_1 and E_2 are considered fixed and equation (46) is used to propagate $\Gamma_1^{(B)}$ to the non-physical value of the photon energy ω'. In the second step, ω' is fixed and E_1 and E_2 are allowed to vary with $\omega = E_1 + E_2$. Equation (59) is used to propagate $\Gamma_1'^{(B)}$ to its value at the desired final energies E_1' and E_2'. Finally, in the third step, E_1' and E_2' are fixed and equation (46) is used in reverse to propagate $\Gamma_1''^{(B)}$ to the physical value $\Gamma_1'''^{(B)}$ at energies ω, E_1', and E_2' and is then transformed back to $\Gamma_1'''^{(S)}$.

The tables show a comparison of the results of this procedure (*approximate*) to the results obtained exactly (*exact*), with $R_i = 0$ (*fixed parameter*), and with $\omega = \omega'$ and $R_i = 0$ (*nearly singular*) for the first element of $\Gamma_1^{(S)}$ which is the radial integral

$$R_1 = \int_0^\infty j_L(\omega r) g_2^R(p_2 r) g_1^R(p_1 r) r^2 \, dr. \tag{60}$$

Table 1 shows the results of propagation away from the middle of the electron energy spectrum. About three significant digit or better agreement can be seen between the *exact* and *approximate* results. The good agreement that occurs when $\kappa_1 \sim \kappa_2$ is a result of the parameter terms in equation (59) giving nearly equal but opposite contributions tending to cancel out of the calculation. The poorer agreement that occurs when κ_1 or κ_2 is small and the other κ is large is due to the approximation becoming worse with small $\gamma(\kappa)$ and an asymmetry in the two parameter terms of equation (59). In all cases the *approximate* calculation leads to a notable improvement in the results.

Table 1. Comparison of values of the radial integral R_1 calculated by exact, approximate, fixed parameter and nearly singular means for electron pair production in the presence of a uranium nucleus ($Z = 92$). The initial energies are $\omega = 10$ MeV, $\omega' = 13$ MeV, $E_2 = 5$ MeV and $E_1 = 5$ MeV. The final electron energies are $E_2' = 5.5$ MeV and $E_1' = 4.5$ MeV. All numbers in the table are to be multiplied by the factor 1×10^{-4}.

κ_1	1	1	5	10
κ_2	1	10	6	1
L	1	10	6	10
Exact	−23.509 3	−3.281 95	−7.930 82	3.952 43
Approximate	−23.514 5	−3.277 86	−7.929 57	3.969 30
Fixed parameter	−23.492 0	−3.302 91	−7.928 52	3.973 77
Nearly singular	−23.411 0	−3.319 14	−7.926 41	3.976 49

In table 2 the propagation is from the edge of the electron energy spectrum. Again, about three significant digit agreement can be seen. Note the dramatic agreement for the case where $\kappa_1 \sim \kappa_2$. Because of the asymmetry in the electron energies, cancellation of the parameter terms in equation (59) is not the cause of the dramatic agreement, but instead must be a result of the larger values of $\gamma(\kappa)$. The non-physical photon energy ω' is smaller here in order to reduce the round-off error associated with the

Table 2. *Comparison of values of the radial integral R_1 calculated by exact, approximate,* fixed parameter and nearly singular means for electron pair production in the presence of a uranium nucleus ($Z = 92$). The initial energies are $\omega = 10$ MeV, $\omega' = 11$ MeV $E_2 = 1$ MeV and $E_1 = 9$ MeV. The final electron energies are $E_2' = 1.5$ MeV and $E_1' = 8.5$ MeV. All numbers in the table are to be multiplied by the factor 1×10^{-5}.

κ_1	1	1	5	10
κ_2	1	10	6	1
L	1	10	6	10
Exact	−382.712	4.938 14	−12.738 7	−128.112
Approximate	−383.125	4.564 90	−12.687 9	−133.351
Fixed parameter	−388.464	4.438 15	−13.666 2	−119.208
Nearly singular	−396.637	4.557 41	−15.081 0	−108.885

number of steps in the numerical integration. As before, small values of κ give poorer results and in every case the *approximate* result gives a notable improvement.

For numerical propagation along the photon spectrum, one of the electron's energy is considered fixed (say in this case E_1) and the other electron's energy (E_2) and photon energy are allowed to vary such that the total energy of the process is conserved $E_1 = \omega - E_2$. Equation (45) yields in this case

$$\frac{\partial \Gamma_1^{(B)}}{\partial \omega} = \left(\frac{E_2}{p_2}\right) \frac{\partial \Gamma_1^{(B)}}{\partial p_2}\bigg|_{\substack{E_1, E_2 \\ \text{const}}} + \frac{\partial \Gamma_1^{(B)}}{\partial \omega}\bigg|_{\substack{E_1, \omega \\ \text{const}}} . \tag{61}$$

The numerical procedure is the same as before except that step two is a modified to have E_1 fixed and E_2 and ω' as the varying variables with $E_1 = \omega - E_2$ and $\omega' - \omega$ kept constant with equation (61) used in the numerical propagation.

Table 3 shows the result of propagation away from the middle of the electron energy spectrum. There is almost five significant digit agreement for the case where $\kappa_1 \sim \kappa_2$, even though the propagation has been carried out over a much larger range than in the previous examples. This improved agreement can be attributed to the decreasing contribution of the parameter term in equation (61) as the photon energy ω and therefore the electron energy E_2 increases. As before, the *approximate* results give the best overall agreement to the *exact* results.

In conclusion, use of the approximate partial differential matrix equation derived in this paper can greatly reduce the time required to calculate radial integrals containing

Table 3. Comparison of values of the radial integral R_1 calculated by exact, approximate, fixed parameter and nearly singular means for electron pair production in the presence of a uranium nucleus ($Z = 92$). The initial energies are $\omega = 10$ MeV, $\omega' = 11$ MeV, $E_2 = 5$ MeV and $E_1 = 5$ MeV. The final energies are $E_2' = 8$ MeV and $\omega''' = 13$ MeV. All numbers in the table are to be multiplied by the factor 1×10^{-4}.

κ_1	1	1	5	10
κ_2	1	10	6	1
L	1	10	6	10
Exact	−10.201 3	−3.483 87	−4.927 71	2.732 95
Approximate	−10.182 2	−3.481 86	−4.927 83	2.743 48
Fixed parameter	−10.176 1	−3.495 17	−4.923 63	2.749 63
Nearly singular	−10.116 5	−3.511 12	−4.918 68	2.758 42

Dirac-Coulomb functions and still yield a sufficiently useful number of significant digits in the result. For the examples given above, the time savings was a factor of approximately $\frac{1}{5}$–$\frac{1}{10}$ of the time required for an exact calculation. With further adjustment of the parameters involved in the numerical integrations, some improvement in these results should be possible.

Appendix

The evaluation of the derivative of $I(\kappa, \mu; x)$ leading to equation (28) begins with substituting equation (27) into equation (26), yielding

$$\frac{\partial I}{\partial \kappa} = \sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{\partial}{\partial \kappa} \left(\frac{\Gamma(\mu+n-\kappa+\frac{1}{2})\Gamma(\mu+\kappa+\frac{1}{2})}{\Gamma(2\mu+1+n)} \right)$$

$$= \psi(\mu+\kappa+\tfrac{1}{2}) I - \left(\sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{\psi(\mu+n-\kappa+\frac{1}{2})\Gamma(\mu+n-\kappa+\frac{1}{2})\Gamma(\mu+\kappa+\frac{1}{2})}{\Gamma(2\mu+1+n)} \right). \tag{A1}$$

Now using the recursion relation obeyed by the digamma function (Erdelyi *et al* 1953) given as

$$\psi(z+n) = \frac{1}{z} + \frac{1}{z+1} + \ldots + \frac{1}{z+n-1} + \psi(z) \qquad \text{for } n = 1, 2, 3, \ldots \tag{A2}$$

equation (A1) becomes

$$\frac{\partial I}{\partial \kappa} = \psi(\mu+\kappa+\tfrac{1}{2}) I - \left[\sum_{n=0}^{\infty} \frac{x^n}{n!} \left(\sum_{m=0}^{n-1} \frac{1}{(\mu+m-\kappa+\frac{1}{2})} + \psi(\mu-\kappa+\tfrac{1}{2}) \right) \times \frac{\Gamma(\mu+n-\kappa+\frac{1}{2})\Gamma(\mu+\kappa+\frac{1}{2})}{\Gamma(2\mu+1+n)} \right] \tag{A3}$$

where the upper limit $(n-1)$ is understood to mean that no terms exist when it is negative. Factoring out the ψ term yields

$$\frac{\partial I}{\partial \kappa} = [\psi(\mu+\kappa+\tfrac{1}{2}) - \psi(\mu-\kappa+\tfrac{1}{2})] I - \left[\sum_{n=1}^{\infty} \left(\sum_{m=0}^{n-1} \frac{1}{(\mu+m-\kappa+\frac{1}{2})} \right) \frac{\Gamma(\mu+n-\kappa+\frac{1}{2})\Gamma(\mu+\kappa+\frac{1}{2})}{\Gamma(2\mu+1+n)} \right] \tag{A4}$$

which is the result given in equation (28).

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