

JAMES COOK UNIVERSITY OF NORTH QUEENSLAND



POINT COULOMB SOLUTIONS OF THE DIRAC EQUATION:
ANALYTICAL RESULTS REQUIRED FOR THE EVALUATION
OF THE BOUND ELECTRON PROPAGATOR IN QUANTUM
ELECTRODYNAMICS.

by

I. B. WHITTINGHAM

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Physics Department,
James Cook University of North Queensland,
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ABSTRACT

The bound electron propagator in quantum electrodynamics is reviewed and the Brown and Schaefer angular momentum representation of the propagator discussed. Regular and irregular solutions of the radial Dirac equations for both $|E| < mc^2$ and $|E| \geq mc^2$ are required for the computation of the propagator. Analytical expressions for these solutions, and their corresponding Wronskians, are obtained for a point Coulomb potential. Some computational aspects are discussed in an appendix.

1. The bound electron propagator in quantum electrodynamics

In applying Dyson-Feynman covariant perturbation techniques to quantum electrodynamical processes such as Rayleigh scattering, bound Compton scattering and the Lamb shift of atomic energy levels, the Furry or Bound Interaction Picture (Jauch and Rohrlich 1955, p.306; Schweber 1964, p.566) must be used if the external, non-quantized, nuclear field is to be included exactly.

In the Bound Interaction Picture the initial and final electron wave functions $\psi(x)$ obey the external field Dirac equation

$$[\gamma_\mu (\partial_\mu - \frac{ie}{\hbar} A_\mu^{(e)}(x)) + \frac{mc}{\hbar}] \psi(x) = 0 \quad (1.1)$$

and the virtual electron-positron intermediate states are represented by the bound electron propagator $S_F^{(e)}(x, x')$ which satisfies (Schweber 1964, p.570)

$$[\gamma_\mu (\partial_\mu - \frac{ie}{\hbar} A_\mu^{(e)}(x)) + \frac{mc}{\hbar}] S_F^{(e)}(x, x') = 2i\delta^{(4)}(x-x') \quad (1.2)$$

subject to the boundary condition that $S_F^{(e)}(x, x')$ is asymptotic to the free electron propagator $S_F(x-x')$ in the limit of zero external field. In these equations $\gamma_k = -i\beta\alpha_k$ and $\gamma_4 = \beta$ are the Dirac 4×4 matrices,

$$x_\mu = (x, ict), \quad \partial_\mu = \frac{\partial}{\partial x_\mu} = (\nabla, \frac{\partial}{\partial ict}),$$

$A^{(e)} = (A^{(e)}, i\phi^{(e)}/c)$ is the external electromagnetic potential (SI units). Greek subscripts range over 1, 2, 3, 4; Latin subscripts over 1, 2, 3 and the repeated index summation convention is used.

To obtain an expression for the bound electron propagator we rewrite (1.1) as

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}_D \psi \quad (1.3)$$

where

$$\hat{H}_D = c\alpha_k (-i\hbar\partial_k - eA_k^{(e)}(x)) + \beta mc^2 + e\phi^{(e)}(x) \quad (1.4)$$

and observe that for a time independent external field the Dirac wave functions have the form

$$\psi_{E\pm}(x) = \psi_{E\pm}(\underline{x}) e^{\mp iEt/\hbar} \quad (1.5)$$

$\psi_{E\pm}^{(\pm)}(\underline{x})$ are the positive and negative energy eigenfunctions of \hat{H}_D , that is

$$\hat{H}_D \psi_{E\pm}(\underline{x}) = \pm E \psi_{E\pm}(\underline{x}). \quad (1.6)$$

In terms of these positive and negative energy solutions the bound electron propagator is (Akheizer and Berestetskii 1965, p.485; Schweber 1964, p.596)

$$-\frac{1}{2} S_F^{(e)}(x, x') = \begin{cases} \sum_{a, E^+} \psi_{a, E^+}(x) \bar{\psi}_{a, E^+}(x') & t > t' \\ -\sum_{a, E^-} \psi_{a, E^-}(x) \bar{\psi}_{a, E^-}(x') & t < t' \end{cases} \quad (1.7)$$

where $\bar{\psi}(x) \equiv \psi^\dagger(x) \gamma_4$ and the label a represents the other quantum numbers needed to specify the complete set $\{\psi_{a, E^+}(x), \psi_{a, E^-}(x)\}$. With the relation

$$\partial_t \theta(t-t') = \delta(t-t')$$

for the step function

$$\theta(y) = \begin{cases} 1 & y > 0 \\ 0 & y < 0 \end{cases},$$

it is easily shown that (1.7) satisfies (1.2). Also we note that for a time independent external field

$$S_F^{(e)}(x, x') \rightarrow S_F^{(e)}(\underline{x}, \underline{x}', t-t').$$

For quantum electrodynamical processes involving the inner electrons of heavy atoms we have a scalar external potential which can be assumed spherically symmetric. The Dirac Hamiltonian is then

$$\hat{H}_D^{CF} = -i\hbar c \alpha_k \partial_k + \beta m c^2 + V(r) \quad (1.8)$$

where $\underline{x} = (r, \theta, \phi) = (r, \Omega)$ and $V(r) = e\phi^{(e)}(r)$. The wave functions $\psi_{a, E}(\underline{x})$ are then the simultaneous eigenfunctions of \hat{H}_D^{CF} , \hat{j}^2 , \hat{j}_z and $\hat{K} = \beta(\underline{\Sigma} \cdot \hat{j} + \hbar)$ corresponding to the eigenvalues E , $j(j+1)\hbar^2$, $\mu\hbar$ and $-\kappa\hbar$ respectively and have the form (Rose 1961, p.159)

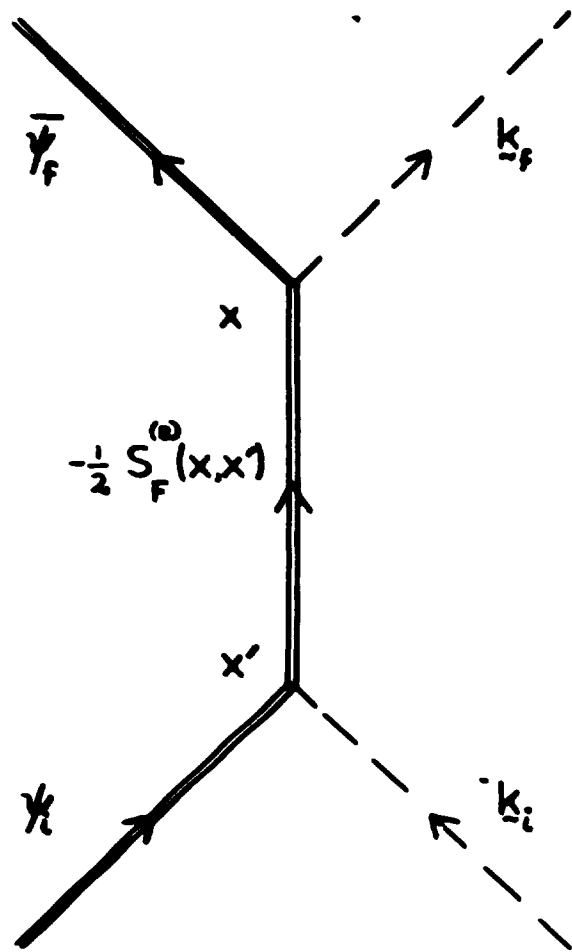
$$\psi_{\kappa, \mu, E}(\underline{x}, t) = \frac{1}{r} \begin{pmatrix} g_{\kappa, E}(r) \chi_{\kappa}^{\mu}(\Omega, \zeta) \\ i f_{\kappa, E}(r) \chi_{-\kappa}^{\mu}(\Omega, \zeta) \end{pmatrix}. \quad (1.9)$$

The spinor spherical harmonics are

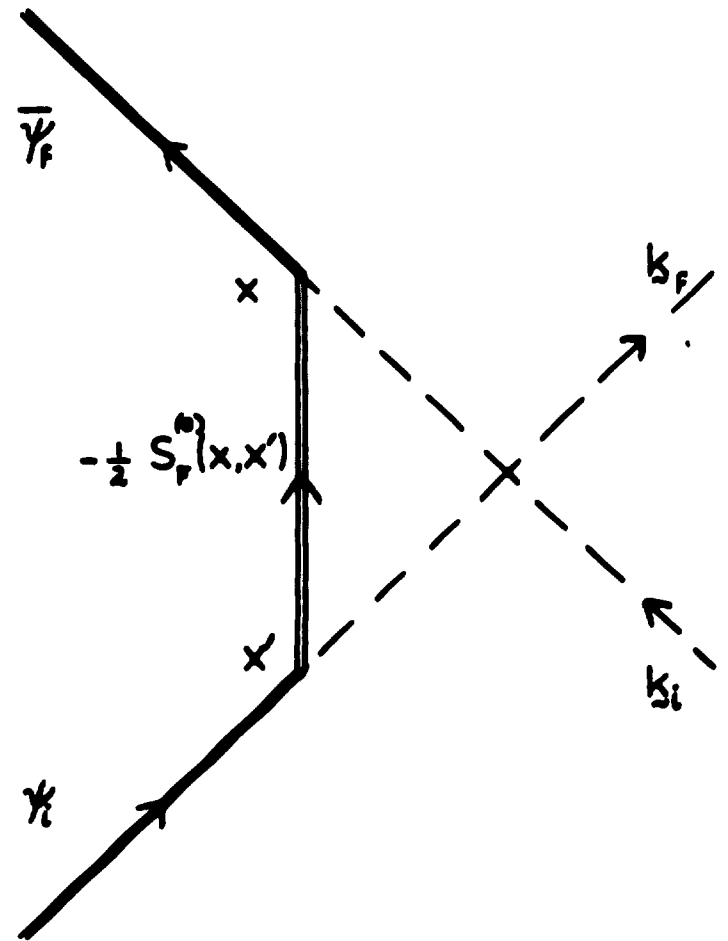
$$\chi_{\kappa}^{\mu}(\Omega, \zeta) = \sum_m C(l, \frac{1}{2}, j; \mu-m, m) Y_l^{\mu-m}(\Omega) \chi_m(\zeta), \quad (1.10)$$

where the notation and phase conventions for the Clebsch-Gordon coefficient $C(j_1, j_2, j; m_1, m_2)$ and spherical harmonic $Y_l^m(\Omega)$ is that of Rose (1957), the $\chi_m(\zeta)$ are the two component Pauli spinors, $\underline{\Sigma} = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$ where the σ are the Pauli 2×2 spin matrices, and the values of the total and orbital angular momentum quantum numbers j and l respectively are obtained from κ via

$$j = |\kappa| - \frac{1}{2}, l = j \pm \frac{1}{2} = \begin{cases} \kappa & \kappa > 0 \\ -\kappa - 1 & \kappa < 0 \end{cases}$$



Absorption First



Emission First

Figure 1. Compton Scattering by a Bound Electron.

The parameter κ takes all non-zero integral values.

The radial functions are solutions of the coupled first order equations

$$\hat{A}_{\kappa, E}(r) \begin{pmatrix} g_{\kappa, E}(r) \\ f_{\kappa, E}(r) \end{pmatrix} = 0 \quad (1.11)$$

where

$$\hat{A}_{\kappa, E}(r) = \begin{pmatrix} \frac{d}{dr} + \frac{\kappa}{r} & -(E + mc^2 - V(r))/\hbar c \\ (E - mc^2 - V(r))/\hbar c & \frac{d}{dr} - \frac{\kappa}{r} \end{pmatrix}. \quad (1.12)$$

In this angular momentum representation the bound electron propagator (1.7) is then (Brown and Schaefer 1956)

$$S_F^{(e)}(\underline{x}, \underline{x}', t-t') = - \int_{\mu, \kappa, E} [c(t-t') + c(E)] \psi_{\kappa, \mu, E}(\underline{x}) \psi_{\kappa, \mu, E}^\dagger(\underline{x}') e^{-iE(t-t')/\hbar} \quad (1.13)$$

where

$$c(y) = \begin{cases} 1 & y > 0 \\ 0 & y = 0 \\ -1 & y < 0 \end{cases},$$

and equation (1.2) becomes for our static central field

$$[\hat{H}_D^{CF}(\underline{x}) - i\hbar \frac{\partial}{\partial t}] S_F^{(e)}(\underline{x}, \underline{x}', t-t') = 2i\hbar\delta(\underline{x}-\underline{x}')\delta(t-t'). \quad (1.14)$$

If we now introduce the mixed representation $S_F^{(e)}(\underline{x}, \underline{x}', E)$ (Brown and Schaefer 1956) of $S_F^{(e)}(\underline{x}, \underline{x}', t-t')$ through the Fourier transform

$$S_F^{(e)}(\underline{x}, \underline{x}', t-t') = \frac{i}{\pi} \int_{-\infty}^{\infty} S_F^{(e)}(\underline{x}, \underline{x}', E) e^{-iE(t-t')/\hbar} dE \quad (1.15)$$

then $S_F^{(e)}(\underline{x}, \underline{x}', E)$ satisfies

$$(\hat{H}_D^{CF} - E) S_F^{(e)}(\underline{x}, \underline{x}', E) = \delta(\underline{x}-\underline{x}'), \quad (1.16)$$

that is $S_F^{(e)}(\underline{x}, \underline{x}', E)$ is a Green function for the Dirac equation.

$S_F^{(e)}(\underline{x}, \underline{x}', E)$ arises naturally in the evaluation of S-matrix elements involving the bound electron propagator. As an illustration we consider bound Compton scattering for which the S-matrix element describing the "absorption first" process (figure 1) is proportional to (Whittingham 1971)

$$S_{fi}^{(a)} = \iint d^4x' d^4x \bar{\psi}_f(x) \gamma_{c(f)} e^{-ik_f \cdot x} S_F^{(e)}(x, x') \gamma_{c(i)} e^{ik_i \cdot x'} \psi_i(x). \quad (1.17)$$

Here $k = (\mathbf{k}, i\omega/c)$ and $\epsilon = (\xi(\mathbf{k}), 0)$ are the photon 4-momentum and 4-polarization respectively. With the aid of (1.15) we can integrate over t, t' and E in (1.17) to obtain

$$S_{fi}^{(a)} = -4\pi i \hbar^2 \delta(E_f + \hbar\omega_f - E_i - \hbar\omega_i) \int d^3x' \int d^3x \\ \times \bar{\psi}_f(\underline{x}) \gamma_\epsilon (f)^\dagger e^{-ik_f \cdot \underline{x}} S_F^{(e)}(\underline{x}, \underline{x}', E_i + \hbar\omega_i) \gamma_\epsilon (i) e^{ik_i \cdot \underline{x}'} \psi_i(\underline{x}'). \quad (1.18)$$

The "emission first" process involves $S_F^{(e)}(\underline{x}, \underline{x}', E_i - \hbar\omega_i)$.

2. The Green function $S_F^{(e)}(\underline{x}, \underline{x}', E)$

In § 1 it was shown that the S-matrix elements for quantum electrodynamical processes involving bound virtual electron-positron states can be expressed in terms of the Green function $S_F^{(e)}(\underline{x}, \underline{x}', E)$. If we introduce the two linearly independent solutions of (1.11), the solution ${}^0y_{\kappa E}(\mathbf{r}) \equiv \begin{pmatrix} {}^0g_{\kappa, E}(\mathbf{r}) \\ {}^0f_{\kappa, E}(\mathbf{r}) \end{pmatrix}$ regular at the origin and the solution ${}^{\infty}y_{\kappa, E}(\mathbf{r})$ regular at infinity, then $S_F^{(e)}(\underline{x}, \underline{x}', E)$ can be expressed as (Brown and Schaefer 1956)

$$S_F^{(e)}(\underline{x}, \underline{x}', E) = \sum_{\mu, \kappa} \left\{ \frac{\theta(r-r')-1}{\Delta_\kappa(E)} {}^0\psi_{\kappa, \mu, E}(\underline{x}) {}^{\infty}\psi_{\kappa, \mu, E}^*(\underline{x}') \right. \\ \left. - \frac{\theta(r-r')}{\Delta_\kappa(E)} {}^{\infty}\psi_{\kappa, \mu, E}(\underline{x}) {}^0\psi_{\kappa, \mu, E}^*(\underline{x}') \right\} \quad (2.1)$$

where, for example

$${}^0\psi_{\kappa, \mu, E}(\underline{x}) = \frac{1}{F} \begin{pmatrix} {}^0g_{\kappa, E}(\mathbf{r}) \chi_\kappa^\mu(\Omega, \zeta) \\ i {}^0f_{\kappa, E}(\mathbf{r}) \chi_{-\kappa}^\mu(\Omega, \zeta) \end{pmatrix} \quad (2.2)$$

and

$${}^{\infty}\psi_{\kappa, \mu, E}^*(\underline{x}) = \frac{1}{F} ({}^0g_{\kappa, E}(\mathbf{r}) \chi_\kappa^{\mu\dagger}(\Omega, \zeta)^\dagger, -i {}^0f_{\kappa, E}(\mathbf{r}) \chi_{-\kappa}^{\mu\dagger}(\Omega, \zeta)). \quad (2.3)$$

$\Delta_\kappa(E)$ is the Wronskian of the two solutions of (1.11), that is

$$\Delta_\kappa(E) = {}^0g_{\kappa, E}(\mathbf{r}) {}^{\infty}f_{\kappa, E}(\mathbf{r}) - {}^{\infty}g_{\kappa, E}(\mathbf{r}) {}^0f_{\kappa, E}(\mathbf{r}). \quad (2.4)$$

As both ${}^0y_{\kappa, E}(\mathbf{r})$ and ${}^{\infty}y_{\kappa, E}(\mathbf{r})$ satisfy (1.11) we have immediately

$$\begin{pmatrix} {}^0f_{\kappa, E}(\mathbf{r}), & {}^0g_{\kappa, E}(\mathbf{r}) \end{pmatrix} \hat{A}_{\kappa, E}(\mathbf{r}) \begin{pmatrix} {}^0g_{\kappa, E}(\mathbf{r}) \\ -{}^0f_{\kappa, E}(\mathbf{r}) \end{pmatrix} + \begin{pmatrix} {}^{\infty}f_{\kappa, E}(\mathbf{r}), & {}^{\infty}g_{\kappa, E}(\mathbf{r}) \end{pmatrix} \hat{A}_{\kappa, E}(\mathbf{r}) \begin{pmatrix} {}^0g_{\kappa, E}(\mathbf{r}) \\ {}^0f_{\kappa, E}(\mathbf{r}) \end{pmatrix} \\ = 0,$$

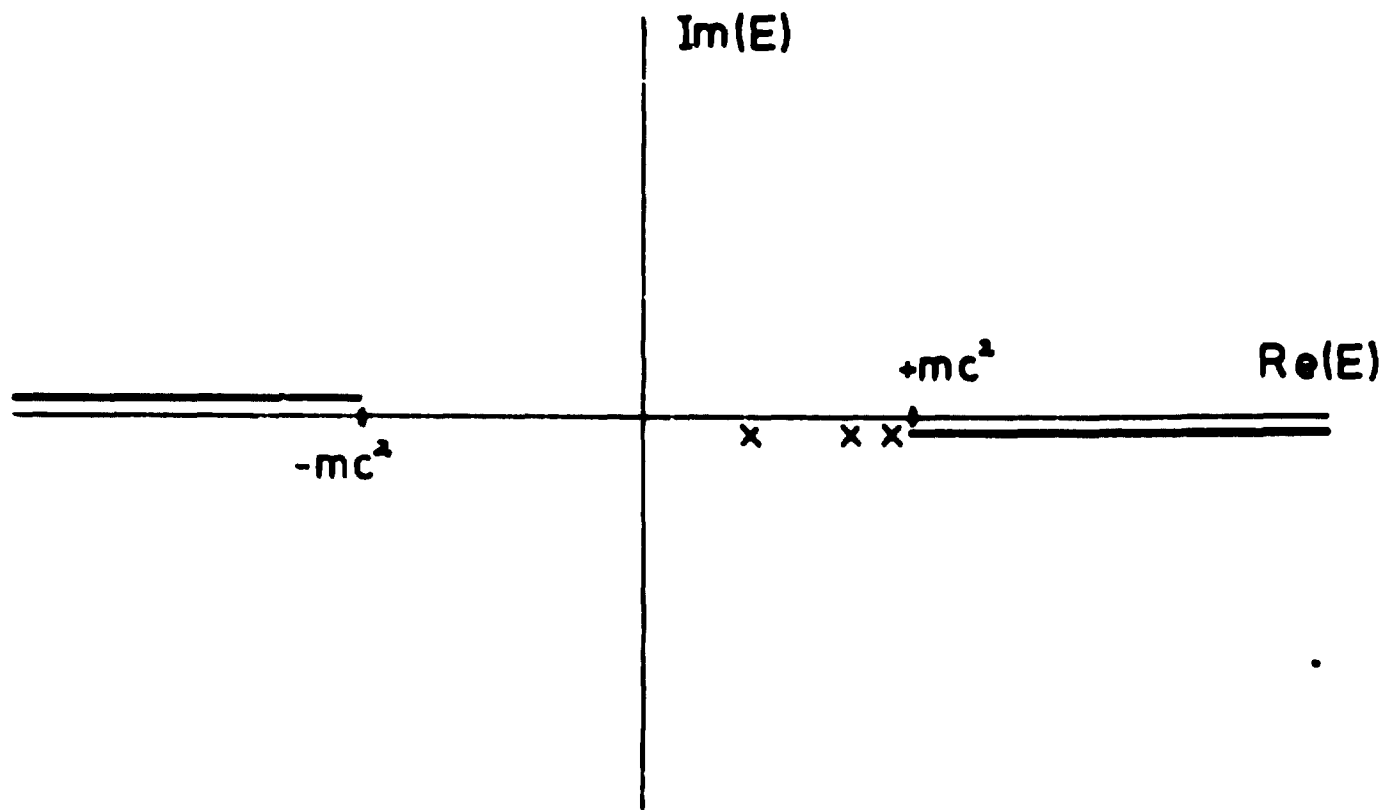


Figure 2. Poles and Branch Lines of $S_F^{(n)}(\underline{x}, \underline{x}', E)$

that is

$$\frac{d}{dr} ({}^0g_{\kappa,E}(r) {}^{\infty}f_{\kappa,E}(r) - {}^{\infty}g_{\kappa,E}(r) {}^0f_{\kappa,E}(r)) = \frac{d}{dr} \Delta_{\kappa}(E) = 0. \quad (2.5)$$

Thus, as indicated by the notation, the Wronskian for solutions of the radial Dirac equations is independent of r .

We shall see later that the solutions ${}^0y_{\kappa,E}(r)$ and ${}^{\infty}y_{\kappa,E}(r)$ become proportional when E is equal to a discrete energy eigenvalue E_n . Thus $\Delta_{\kappa}(E=E_n) = 0$ for all r .

Brown and Schaefer (1956) show that $S_F^{(e)}(x, x', E)$ given by (2.1) is a solution of (1.16) and has all the desired properties of a Green function, that is, considered as a function of E , $S_F^{(e)}(x, x', E)$ has simple poles in the range $0 < E < mc^2$, two branch lines $E \geq mc^2$ and $E \leq -mc^2$, and is regular elsewhere (figure 2). Also, as a function of r (or r') with r' (or r) fixed, $S_F^{(e)}(x, x', E)$ is finite at infinity and at the origin for E not equal to a discrete energy eigenvalue.

To ensure that the Green function satisfies the correct boundary conditions in the limit of large r (or r'), we note that the radial Dirac equations (1.11) have the asymptotic solutions

$$\begin{aligned} g_{\kappa,E}(r) &\xrightarrow{r \rightarrow \infty} (E+mc^2)^{\frac{1}{2}} [a e^{\lambda r} + b e^{-\lambda r}] \\ f_{\kappa,E}(r) &\xrightarrow{r \rightarrow \infty} (mc^2-E)^{\frac{1}{2}} [a e^{\lambda r} - b e^{-\lambda r}] \end{aligned} \quad (2.6)$$

where

$$\lambda = (m^2c^4 - E^2)^{\frac{1}{2}}/hc.$$

For $|E| < mc^2$, λ is real and we must choose

$$\begin{pmatrix} {}^{\infty}g_{\kappa,E}(r) \\ {}^{\infty}f_{\kappa,E}(r) \end{pmatrix} \xrightarrow{r \rightarrow \infty} \pm b (mc^2 \pm E)^{\frac{1}{2}} e^{-\lambda r}. \quad (2.7)$$

For $|E| \geq mc^2$ we have

$$\begin{aligned} \lambda &\rightarrow ip, \quad p = (E^2 - m^2c^4)^{\frac{1}{2}}/hc \\ (mc^2 - E)^{\frac{1}{2}} &\rightarrow i(E - mc^2)^{\frac{1}{2}} \end{aligned} \quad (2.8)$$

and therefore we choose

$$\begin{pmatrix} {}^{\infty}g_{\kappa,E}(r) \\ {}^{\infty}f_{\kappa,E}(r) \end{pmatrix} \xrightarrow{r \rightarrow \infty} a \begin{pmatrix} (E + mc^2)^{\frac{1}{2}} \\ i(E - mc^2)^{\frac{1}{2}} \end{pmatrix} e^{iDr} \quad (2.9)$$

so that, on the half line $E \geq mc^2$, ${}^{\infty}y_{\kappa,E}(r)$ represents outgoing electrons while on the half line $E \leq -mc^2$ it represents outgoing positrons.

If we substitute the angular momentum representation (2.1) for $S_F^{(e)}(\underline{x}, \underline{x}', E)$ into S-matrix elements such as (1.18) and use wave functions of the form (1.9) for the initial and final electron (or positron) states, then all angular integrations can be effected using the orthonormality properties of the spinor spherical harmonics $Y_{\kappa}^{\mu}(\alpha, \kappa)$. Thus the S-matrix elements can be expressed in terms of radial integrals over the various solutions of the radial Dirac equations (1.11) (see, for example, Whittingham 1971, §4). In the remaining sections of this report we will obtain analytical results for the radial functions ${}^{(0, \pm)}g_{\kappa, E}(r)$ and ${}^{(0, \pm)}f_{\kappa, E}(r)$ for $|E| < mc^2$ ($E \neq E_n$) and $|E| \geq mc^2$ for the case of a point Coulomb potential. The corresponding Wronskians will be evaluated.

3. Radial functions for $|E| < mc^2$.

If we introduce the functions $\phi_1(r)$ and $\phi_2(r)$ via

$$\begin{pmatrix} g_{\kappa, E}(r) \\ f_{\kappa, E}(r) \end{pmatrix} = (mc^2 \pm E)^{\frac{1}{2}} e^{-\lambda r} (\phi_1 \pm \phi_2) \quad (3.1)$$

and assume that ϕ_1 and ϕ_2 can be written as power series

$$\begin{pmatrix} \phi_1(\rho) \\ \phi_2(\rho) \end{pmatrix} = \rho^{\gamma} \sum_{n=0}^{\infty} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} \rho^n, \quad (3.2)$$

where $\rho \equiv 2\lambda r$, then for the point-Coulomb potential

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} = -\frac{\alpha \hbar c}{r} \quad (3.3)$$

the recurrence relations for α_n and β_n yield the relation

$$\gamma^2 = \kappa^2 - (\alpha Z)^2.$$

α is the fine structure constant

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} = \frac{1}{137}.$$

For solutions regular at the origin we must choose

$$\gamma = +[\kappa^2 - (\alpha Z)^2]^{\frac{1}{2}} \quad (3.4)$$

and we obtain (Rose 1961, p.175; Akheizer and Berestetskii 1965, p.123)

$$\begin{aligned} \phi_1(\rho) &= \frac{\gamma - \alpha}{\xi - \kappa} \rho^{-\frac{1}{2}} M_{\kappa' - 1, \gamma}(\rho) \\ \phi_2(\rho) &= \rho^{-\frac{1}{2}} M_{\kappa', \gamma}(\rho). \end{aligned} \quad (3.5)$$

We have introduced

$$\sigma = \frac{\alpha Z E}{\hbar c \lambda} \quad , \quad k' = \sigma + \frac{1}{2} \quad , \quad \xi = \frac{\alpha Z m c}{\hbar \lambda} \quad . \quad (3.6)$$

The Whittaker function $M_{k', \gamma}$ is related to the confluent hypergeometric function ${}_1F_1(a, b; \rho)$ via (Abramowitz and Stegun 1965), equation 13.1.32)

$$M_{k', \gamma}(\rho) = \rho^{\gamma + \frac{1}{2}} e^{-\rho/2} {}_1F_1\left(\frac{1}{2} + \gamma - k', 2\gamma + 1, \rho\right) . \quad (3.7)$$

Thus the solutions regular at the origin are

$$\begin{pmatrix} \phi_{\kappa, E}^{(o)}(r) \\ \phi_{\kappa, E}^{(c)}(r) \end{pmatrix} = (mc^2 \pm E)^{\frac{1}{2}} (2\lambda r)^{\gamma} e^{-\lambda r} \left\{ \frac{\gamma - \sigma}{\xi - \kappa} {}_1F_1(\gamma - \sigma + 1, 2\gamma + 1, 2\lambda r) \pm {}_1F_1(\gamma - \sigma, 2\gamma + 1, 2\lambda r) \right\} . \quad (3.8)$$

The solutions regular at infinity are (Rose 1961, p.176)

$$\begin{aligned} \phi_1(\rho) &= (\kappa + \xi) \rho^{-\frac{1}{2}} W_{k', -1, \gamma}(\rho) \\ \phi_2(\rho) &= \rho^{-\frac{1}{2}} W_{k', \gamma}(\rho) \end{aligned} \quad (3.9)$$

where the Whittaker function $W_{k', \gamma}$ is (Abramowitz and Stegun 1965, equation 13.1.34)

$$W_{k', \gamma}(\rho) = \frac{\Gamma(-2\gamma)}{\Gamma(\frac{1}{2} - \gamma - k')} M_{k', \gamma}(\rho) + \frac{\Gamma(2\gamma)}{\Gamma(\frac{1}{2} + \gamma - k')} M_{k', \gamma}(\rho) . \quad (3.10)$$

This solution behaves as $\rho^{-\gamma}$ near the origin due to the term $M_{k', -\gamma}$.

For the point-Coulomb potential(3.3) the discrete energy eigenvalues are

$$E_{n, \kappa} = \left[1 + \left(\frac{\alpha Z}{\gamma + n - |\kappa|} \right)^2 \right]^{-\frac{1}{2}} mc^2 \quad n=1, 2, 3, \dots \quad (3.11)$$

and therefore

$$\frac{1}{2} + \gamma - k' = -n . \quad (3.12)$$

Thus $\Gamma(\frac{1}{2} + \gamma - k') = \infty$ and $W_{k', \gamma}$ is proportional to $M_{k', \gamma}$, that is for $E = E_n$ the solution regular at the origin and the solution regular at infinity coalesce and become the (unnormalized) eigenfunction belonging to the eigenvalue E_n .

As the Wronskian is independent of r we can choose to evaluate it at $r = \infty$ where we can use the asymptotic relation (Abramowitz and Stegun 1965, equation 13.5.1)

$$\begin{aligned} {}_1F_1(a, b, z) + \frac{\Gamma(b)}{\Gamma(a)} e^z z^{a-b} \left\{ \sum_{n=0}^{S-1} \frac{(b-a)_n (1-a)_n}{n!} z^{-n} + O(|z|^{-S}) \right\} \\ + \frac{\Gamma(b-a)}{\Gamma(a)} z^{-a} \left\{ \sum_{n=0}^{R-1} \frac{(a)_n (1+a-b)_n}{n!} (\dots)^{-n} + O(|z|^{-R}) \right\} \end{aligned} \quad (3.13)$$

$(a)_n$ is the Pochhammer symbol

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)} = a(a+1)(a+2)\dots(a+n-1)$$

$$(a)_0 = 1.$$

The asymptotic form of the solutions regular at the origin is therefore

$$\begin{aligned} \begin{pmatrix} g_{\kappa, E}(r) \\ f_{\kappa, E}(r) \end{pmatrix} &\xrightarrow{r \rightarrow \infty} (mc^2 \pm E)^{\frac{1}{2}} e^{\lambda r} \frac{(\gamma - \sigma) \Gamma(2\gamma + 1)}{\xi - \kappa \Gamma(\gamma - \sigma + 1)} (2\lambda r)^{-\sigma} \pm \frac{\Gamma(2\gamma + 1)}{\Gamma(\gamma - \sigma)} (2\lambda r)^{-1 - \sigma} \\ &= (mc^2 \pm E)^{\frac{1}{2}} \frac{\gamma - \sigma}{\xi - \kappa} \frac{\Gamma(2\gamma + 1)}{\Gamma(\gamma - \sigma + 1)} e^{\lambda r} (2\lambda r)^{-\sigma}. \end{aligned} \quad (3.14)$$

Noting that

$$W_{k', \gamma}(z) \xrightarrow{z \rightarrow \infty} e^{-z/2} z^{k'} \left(1 + \frac{\gamma^2 - (k' - \frac{1}{2})^2}{z} + O(|z|^{-2}) \right) \quad (3.15)$$

then the asymptotic form of the solutions regular at infinity is

$$\begin{aligned} \begin{pmatrix} g_{\kappa, E}(r) \\ f_{\kappa, E}(r) \end{pmatrix} &\xrightarrow{r \rightarrow \infty} (mc^2 \pm E)^{\frac{1}{2}} (2\lambda r)^{-\frac{1}{2}} \left\{ (\kappa + \xi) e^{-\lambda r} (2\lambda r)^{k' - 1} \right. \\ &\quad \left. \pm e^{-\lambda r} (2\lambda r)^{k'} \left(1 + \frac{(\kappa - \xi)(\kappa + \xi)}{2\lambda r} \right) \right\} \\ &= \pm (mc^2 \pm E)^{\frac{1}{2}} e^{-\lambda r} (2\lambda r)^{k'}. \end{aligned} \quad (3.16)$$

In obtaining this result we have used the relation

$$\gamma^2 - (k' - \frac{1}{2})^2 = (\kappa - \xi)(\kappa + \xi).$$

With the asymptotic forms (3.14) and (3.16) the Wronskian becomes

$$\begin{aligned} \Delta_{\kappa}(E) &= -2 (m^2 c^4 - E^2)^{\frac{1}{2}} \frac{\gamma - \sigma}{\xi - \kappa} \frac{\Gamma(2\gamma + 1)}{\Gamma(\gamma - \sigma + 1)} \\ &= \frac{2\hbar c \lambda}{\kappa - \xi} \frac{\Gamma(2\gamma + 1)}{\Gamma(\gamma - \sigma)} \end{aligned} \quad (3.17)$$

since $\Gamma(z) = (z - 1) \Gamma(z - 1)$.

4. Radial functions for $|E| > mc^2$

4.1 Solutions regular at the origin

The solutions regular at the origin can be obtained by the analytical continuation (2.8) of the solutions (3.8) for $|E| < mc^2$, that is

$$\begin{pmatrix} g_{\kappa, E}(r) \\ f_{\kappa, E}(r) \end{pmatrix} = \begin{pmatrix} (E+mc^2)^{\frac{1}{2}} \\ i(E-mc^2)^{\frac{1}{2}} \end{pmatrix} (2pr)^{\gamma} e^{-ipr} \left\{ -\frac{\gamma+iv}{\kappa+i\xi} {}_1F_1(\gamma+iv+1, 2\gamma+1, 2ipr) \right. \\ \left. \pm {}_1F_1(\gamma+iv, 2\gamma+1, 2ipr) \right\} \quad (4.1)$$

where $v = i\sigma = \frac{\alpha ZE}{\hbar cp}$. (4.2)

Since $|\gamma+iv|^2 = \gamma^2 + \left(\frac{\alpha ZE}{\hbar cp}\right)^2 = \kappa^2 + \left(\frac{\alpha Zmc}{\hbar p}\right)^2$ (4.3)

$$= |\kappa + i\xi|^2$$

we can rewrite (4.1) as

$$\begin{pmatrix} g_{\kappa, E}(r) \\ f_{\kappa, E}(r) \end{pmatrix} = \begin{pmatrix} (E+mc^2)^{\frac{1}{2}} \\ i(E-mc^2)^{\frac{1}{2}} \end{pmatrix} \frac{\gamma+iv}{|\kappa+i\xi|} (2pr)^{\gamma} e^{-ipr} \\ \times \left\{ (\gamma+iv) \left[-\frac{\gamma-iv}{\kappa+i\xi} \right] {}_1F_1(\gamma+iv+1, 2\gamma+1, 2ipr) \right. \\ \left. \pm (\gamma-iv) {}_1F_1(\gamma+iv, 2\gamma+1, 2ipr) \right\} . \quad (4.4)$$

Thus with the definition

$$e^{2i\eta(\gamma)} = -\frac{\kappa-i\xi}{\gamma+iv} = -\frac{\kappa-imc^2 v/E}{\gamma+iv} \quad (4.5)$$

and use of the Kummer transformation (Abramowitz and Stegun 1965, equation 13.1.27)

$$\begin{aligned} {}_1F_1(\gamma+iv, 2\gamma+1, 2ipr) &= e^{2ipr} {}_1F_1(\gamma-iv+1, 2\gamma+1, -2ipr) \\ &= e^{2ipr} {}_1F_1^*(\gamma+iv+1, 2\gamma+1, 2ipr) \end{aligned} \quad (4.6)$$

we finally obtain for the solution regular at the origin

$$\begin{pmatrix} g_{\kappa, E}(r) \\ f_{\kappa, E}(r) \end{pmatrix} = N \begin{pmatrix} (E+mc^2)^{\frac{1}{2}} \\ i(E-mc^2)^{\frac{1}{2}} \end{pmatrix} (2pr)^{\gamma} (\gamma+iv) e^{-ipr+i\eta(\gamma)} {}_1F_1(\gamma+iv+1, 2\gamma+1, 2ipr) \\ \pm \text{ complex conjugate} \} . \quad (4.7)$$

The constant N is unimportant in constructing $S_F^{(e)}(\underline{x}, \underline{x}', E)$ since the Wronskian will also contain N as a factor. However for convenience later we will normalize the solutions (4.7) according to

$$\int d^3x \psi_{\kappa, \mu, E}^{\dagger}(\underline{x}) \psi_{\kappa', \mu', E'}(\underline{x}) = \delta_{\mu\mu'} \delta_{\kappa\kappa'} \delta(E-E'), \quad (4.8)$$

that is

$$\int_0^{\infty} \{g_{\kappa,E}(r) g_{\kappa,E}(r) + f_{\kappa,E}(r) f_{\kappa,E}(r)\} dr = \delta(E-E') \quad (4.9)$$

The normalization constant is (Rose 1961,p.193)

$$N(\gamma) = \frac{e^{\pi\nu/2} |\Gamma(\gamma+i\nu)|}{2(\pi p \hbar c)^{1/2} \Gamma(2\gamma+1)} \quad (4.10)$$

The asymptotic form of (4.7) is then (Rose 1961,p.194)

$$\begin{pmatrix} g_{\kappa,E}(r) \\ f_{\kappa,E}(r) \end{pmatrix} \xrightarrow{r \rightarrow \infty} \pm \left(\frac{E \pm mc^2}{\pi p \hbar c} \right)^{1/2} \begin{pmatrix} \cos \\ \sin \end{pmatrix} [pr + \delta_{\kappa}(\gamma)] \quad (4.11)$$

where the phase is

$$\delta_{\kappa}(\gamma) = \nu \ln 2pr - \arg \Gamma(\gamma+i\nu) + \eta(\gamma) - \pi\gamma/2. \quad (4.12)$$

From (4.5) the phase contribution $\eta(\gamma)$ is given by

$$\eta(\gamma) = \frac{1}{2} [\arg(-\kappa+i\xi) - \arg(\gamma+i\nu)].$$

Since $-\kappa+i\xi$ is in the second or first quadrant depending on κ being positive or negative respectively, and $\gamma+i\nu$ is the first quadrant, we have

$$\eta(\gamma) = \begin{cases} \frac{1}{2} [\pm\pi - \tan^{-1} \left| \frac{mc^2 \nu}{\kappa E} \right| - \tan^{-1} \left| \frac{\nu}{\gamma} \right|] & \kappa > 0 \\ \frac{1}{2} [\tan^{-1} \left| \frac{mc^2 \nu}{\kappa E} \right| - \tan^{-1} \left| \frac{\nu}{\gamma} \right|] & \kappa < 0 \end{cases} \quad (4.13)$$

To remove this ambiguity in $\eta(\gamma)$ for $\kappa > 0$ we insist that, in the limit $Z \rightarrow 0$ (4.11) must reduce to the free field solutions for which (Rose 1961,p.206)

$$\delta_{\kappa}(Z=0) = -\frac{\kappa+1}{2} \pi = \begin{cases} -\frac{\kappa+1}{2} \pi & \kappa > 0 \\ +\frac{\kappa}{2} \pi & \kappa < 0 \end{cases} \quad (4.14)$$

Since in the limit $Z \rightarrow 0$

$$\nu \rightarrow 0, \gamma \rightarrow |\kappa|, \arg \Gamma(\gamma+i\nu) \rightarrow \arg \Gamma(|\kappa|) = 0$$

we have

$$\delta_{\kappa}(\gamma) \rightarrow \eta(Z=0) - \frac{\pi|\kappa|}{2},$$

that is

$$\eta(Z=0) = \begin{cases} -\frac{\pi}{2} & \kappa > 0 \\ 0 & \kappa < 0 \end{cases} \quad (4.15)$$

Thus we have finally

$$\eta(\gamma) = \begin{cases} -\frac{1}{2} [\pi + \tan^{-1} \left| \frac{mc^2 \nu}{\kappa E} \right| + \tan^{-1} \left| \frac{\nu}{\gamma} \right|] & \kappa > 0 \\ \frac{1}{2} [\tan^{-1} \left| \frac{mc^2 \nu}{\kappa E} \right| - \tan^{-1} \left| \frac{\nu}{\gamma} \right|] & \kappa < 0 \end{cases} \quad (4.16)$$

4.2 Solution irregular at the origin

In order to construct a second linearly independent solution of the Dirac equation for $|E| > mc^2$ it is convenient to introduce the solutions obtained from (4.7) by changing the sign of γ (Yennie et al 1954, Rawitscher 1958), that is

$$\begin{pmatrix} \bar{G}_{\kappa, E}(r) \\ \bar{F}_{\kappa, E}(r) \end{pmatrix} = N(-\gamma) \begin{pmatrix} (E+mc^2)^{\frac{1}{2}} \\ i(E-mc^2)^{\frac{1}{2}} \end{pmatrix} (2pr)^{-\gamma} \{ (-\gamma+iv)e^{-ipr} + i\eta(-\gamma) \\ \times {}_1F_1(-\gamma+iv+1, -2\gamma+1, 2ipr) \pm \text{compl. conj.} \} \quad (4.17)$$

where

$$e^{2i\eta(-\gamma)} = \frac{-\kappa+i mc^2 v/E}{-\gamma+iv} \quad (4.18)$$

As indicated in §3 these solutions will behave as $r^{-\gamma}$ at the origin. Their behaviour for large r is

$$\begin{pmatrix} \bar{G}_{\kappa, E}(r) \\ \bar{F}_{\kappa, E}(r) \end{pmatrix} \rightarrow \pm \begin{pmatrix} E+mc^2 \\ \mp p\hbar c \end{pmatrix}^{\frac{1}{2}} \begin{matrix} \cos \\ \sin \end{matrix} [pr + \delta_{\kappa}(-\gamma)] \quad (4.19)$$

where

$$\delta_{\kappa}(-\gamma) = v \ln 2pr - \arg \Gamma(-\gamma+iv) + \eta(-\gamma) + \pi\gamma/2. \quad (4.20)$$

From (4.18) we have

$$\eta(-\gamma) = \begin{cases} \frac{1}{2} [\tan^{-1} \frac{v}{\gamma} - \tan^{-1} \frac{mc^2 v}{\kappa E}] & \kappa > 0 \\ \frac{1}{2} [\pm\pi + \tan^{-1} \frac{v}{\gamma} + \tan^{-1} \frac{mc^2 v}{\kappa E}] & \kappa < 0 \end{cases} \quad (4.21)$$

so that, if we choose the positive sign in (4.21),

$$\eta(-\gamma) = \eta(\gamma) + \tan^{-1} \frac{v}{\gamma} + \frac{\pi}{2} \quad (4.22)$$

and

$$\delta_{\kappa}(-\gamma) = \delta_{\kappa}(\gamma) + \pi\gamma + \tan^{-1} \frac{v}{\gamma} + \frac{\pi}{2} + \arg \Gamma(\gamma+iv) - \arg \Gamma(-\gamma+iv). \quad (4.23)$$

Recalling the identity (Abramowitz and Stegun 1965, equation 6.1.17)

$$\Gamma(-z) = \frac{-\pi}{z \sin \pi z \Gamma(z)}, \quad (4.24)$$

that is

$$\arg \Gamma(-z) = -\arg z - \arg \sin \pi z - \arg \Gamma(z) \pm \pi,$$

then

$$\begin{aligned} \arg \Gamma(-\gamma+iv) &= -\arg \Gamma(-\gamma-iv) \\ &= \arg(\gamma+iv) + \arg[\sin \pi(\gamma+iv)] - \arg \Gamma(\gamma+iv) \pm \pi. \end{aligned} \quad (4.25)$$

From (4.23) we therefore obtain

$$\delta_{\kappa}(-\gamma) = \delta_{\kappa}(\gamma) + \delta \quad (4.26)$$

where

$$\delta = \pi\gamma_0 + \frac{\pi}{2} - \arg [\sin \pi(\gamma + i\nu)] \pm \pi \quad (4.27)$$

Unlike the non-relativistic result, the phases of the regular and irregular point-Coulomb solutions do not differ by $\pi/2$.

4.3 Solutions asymptotic to outgoing waves

For the bound electron propagator to be asymptotic to the free electron propagator in the limit of large r (or r') - where the external field is assumed to be zero - we require solutions of the radial Dirac equation which, for $|E| > mc^2$, have the form of outgoing waves at large r (see equation (2.9)). We can construct these outgoing wave solutions from a linear combination of the regular and irregular solutions discussed in §4.1 and §4.2 respectively. We require

$$a \begin{pmatrix} g_{\kappa, E}(r) \\ f_{\kappa, E}(r) \end{pmatrix} + b \begin{pmatrix} \bar{g}_{\kappa, E}(r) \\ \bar{f}_{\kappa, E}(r) \end{pmatrix} \xrightarrow{r \rightarrow \infty} \pm \left[\frac{E + mc^2}{\pi \hbar c} \right]^{\frac{1}{2}} e^{i[pr + \delta_{\kappa}(\gamma)]} \quad (4.28)$$

Using the asymptotic forms (4.11) and (4.19) together with the relation (4.26) between $\delta_{\kappa}(\gamma)$ and $\delta_{\kappa}(-\gamma)$, (4.28) yields the requirements

$$a + b e^{i\delta} = 2, \quad a + b e^{-i\delta} = 0. \quad (4.29)$$

The solutions of these equations are

$$a = 1 + i \cot \delta, \quad b = -i \operatorname{cosec} \delta \quad (4.30)$$

or, defining δ' via

$$\delta = \delta' + \frac{\pi}{2} \pm \pi, \quad (4.31)$$

that is

$$\delta' = \pi\gamma - \arg [\sin \pi(\gamma + i\nu)], \quad (4.32)$$

then

$$a = 1 - i \tan \delta', \quad b = i \sec \delta'. \quad (4.33)$$

The phase difference δ' may be written in the form

$$\begin{aligned} \delta' &= \pi\gamma - \tan^{-1} \left\{ \frac{\cos \pi\gamma \sinh \pi\nu}{\sin \pi\gamma \cosh \pi\nu} \right\} \\ &= \pi\gamma - \tan^{-1} (\cot \pi\gamma \tanh \pi\nu). \end{aligned} \quad (4.34)$$

In the ultrarelativistic limit $E \gg mc^2$, $v \rightarrow \alpha Z$ and (4.34) agrees with the result of Yennie et al (1954).

Thus we have for our outgoing waves solution

$$\begin{pmatrix} \bar{g}_{\kappa,E}(r) \\ \bar{f}_{\kappa,E}(r) \end{pmatrix} = (1 - i \tan \delta') \begin{pmatrix} {}^o g_{\kappa,E}(r) \\ {}^o f_{\kappa,E}(r) \end{pmatrix} + i \sec \delta' \begin{pmatrix} \bar{g}_{\kappa,E}(r) \\ \bar{f}_{\kappa,E}(r) \end{pmatrix}. \quad (4.35)$$

Having obtained our desired two sets of linearly independent solutions (4.7) and (4.35), we can now use their asymptotic forms for large r to evaluate their Wronskian. We have

$$\begin{aligned} \Delta_{\kappa}(E) &= {}^o g_{\kappa,E}(r) \bar{f}_{\kappa,E}(r) - \bar{g}_{\kappa,E}(r) {}^o f_{\kappa,E}(r) \\ &= i \sec \delta' \{ {}^c g_{\kappa,E}(r) \bar{f}_{\kappa,E}(r) - \bar{g}_{\kappa,E}(r) {}^o f_{\kappa,E}(r) \} \end{aligned} \quad (4.36)$$

or, using (4.11) and (4.19)

$$\begin{aligned} \Delta_{\kappa}(E) &= - \sec \delta' \left(\frac{E+mc^2}{\pi p \hbar c} \right)^{\frac{1}{2}} \left(\frac{E-mc^2}{\pi p \hbar c} \right)^{\frac{1}{2}} \\ &\quad \times \{ \cos [pr + \delta_{\kappa}(\gamma)] \sin [pr + \delta_{\kappa}(-\gamma)] \\ &\quad \quad - \sin [pr + \delta_{\kappa}(\gamma)] \cos [pr + \delta_{\kappa}(-\gamma)] \} \\ &= -i \frac{\sec \delta'}{\pi} \sin [\delta_{\kappa}(-\gamma) - \delta_{\kappa}(\gamma)] \\ &= 1/\pi. \end{aligned} \quad (4.37)$$

5. Remarks

The expressions developed in this report for the various point-Coulomb solutions of the Dirac equation have been essential in assessing the accuracy and stability of the numerical methods used by the author in a series of calculations of the spectral distribution of γ rays incoherently scattered by the K electrons of medium to heavy elements (Whittingham, 1978 a,b). For this purpose computer routines were written to generate the Whittaker functions $M_{k',\gamma}$ and $W_{k',\gamma}$ for real and complex arguments. Aspects of the computation of these functions are discussed in the appendix of this report.

APPENDIX: COMPUTATION OF WHITTAKER FUNCTIONS

The Whittaker functions $M_{k', \gamma}$ and $W_{k', \gamma}$ are related to the regular and irregular Kummer functions $M(a, b, z)$ and $U(a, b, z)$ respectively via (Abramowitz and Stegun 1965, equations 13.1.32, 13.1.33)

$$M_{k', \gamma}(z) = e^{-z/2} z^{\gamma+1/2} M\left(\frac{1}{2} + \gamma - k', 2\gamma+1, z\right) \quad (A.1)$$

$$W_{k', \gamma}(z) = e^{-z/2} z^{\gamma+1/2} U\left(\frac{1}{2} + \gamma - k', 2\gamma+1, z\right). \quad (A.2)$$

The regular Kummer function $M(a, b, z)$ is just the confluent hypergeometric function ${}_1F_1(a, b, z)$, whereas the irregular Kummer function is given by (Abramowitz and Stegun 1965, equation 13.1.3)

$$U(a, b, z) = \frac{\pi}{\sin \pi b} \left\{ \frac{M(a, b, z)}{\Gamma(1+a-b)\Gamma(b)} - z^{1-b} \frac{M(1+a-b, 2-b, z)}{\Gamma(a)\Gamma(2-b)} \right\}. \quad (A.3)$$

For $|z| \leq 20$ the expansion (Abramowitz and Stegun 1965, equation 13.1.2)

$$M(a, b, z) = 1 + \frac{az}{c} + \frac{az}{c} \frac{(a+1)z}{2(c+1)} + \frac{az}{c} \frac{(a+1)z}{2(c+1)} \frac{(a+2)z}{3(c+2)} + \dots \quad (A.4)$$

was used. $U(a, b, z)$ was then computed directly from (A.3).

For $|z| > 20$ the following expansions were used (Abramowitz and Stegun 1965, equations 13.5.1, 13.5.2):

$$M(a, b, z) = \Gamma(b) \left\{ \frac{z^{-a}}{\Gamma(b-a)} \left[1 + \frac{a(1+a-b)}{z} + \frac{a(1+a-b)}{z} \frac{(a+1)(1+a-b+1)}{2z} \right. \right. \\ \left. \left. + \frac{a(1+a-b)}{z} \frac{(a+1)(1+a-b+1)}{2z} \frac{(a+2)(1+a-b+2)}{3z} + \dots \right] \right. \\ \left. + \frac{z^{a-b}}{\Gamma(a)} \left[1 + \frac{(b-a)(1-a)}{z} + \frac{(b-a)(1-a)}{z} \frac{(b-a+1)(1-a+1)}{2z} \right. \right. \\ \left. \left. + \frac{(b-a)(1-a)}{z} \frac{(b-a+1)(1-a+1)}{2z} \frac{(b-a+2)(1-a+2)}{3z} + \dots \right] \right\}, \quad (A.5)$$

$$U(a, b, z) = z^{-a} \left[1 + \frac{a(1+a-b)}{z} + \frac{a(1+a-b)}{z} \frac{(a+1)(1+a-b+1)}{2z} \right. \\ \left. + \frac{a(1+a-b)}{z} \frac{(a+1)(1+a-b+1)}{2z} \frac{(a+2)(1+a-b+2)}{3z} + \dots \right]. \quad (A.6)$$

The Γ function of complex argument was computed by firstly using the relationship $\Gamma(z+1) = z\Gamma(z)$ to ensure that $|z| \geq 10$ and then using the expansion (Abramowitz and Stegun 1965, equation 6.1.41)

(ii)

$$\begin{aligned} \ln \Gamma(z) - (z - \frac{1}{2}) \ln z - z + \frac{1}{2} \ln(2\pi) + \frac{1}{12z} - \frac{1}{360z^3} \\ + \frac{1}{1260z^5} - \frac{1}{1680z^7} + \frac{1}{1188z^9} - \dots \end{aligned} \quad (\text{A.7})$$

The routines for $M(a,b,c)$, $U(a,b,z)$ and $\ln\Gamma(z)$ were written in double precision arithmetic. The series (A.4),(A.5),(A.6) were terminated when the ratio of the last computed term to the sum of computed terms was less than 10^{-9} .

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JAMES COOK UNIVERSITY OF NORTH QUEENSLAND

POST OFFICE, JAMES COOK UNIVERSITY, QLD 4811 TELEPHONES: Douglas 792711; Pindico 792193; TELEX: AA77669

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