UNION CARBIDE CORPORATION

UCC/DSSD – 206

# THEORETICAL CALCULATIONS OF THE BREMSSTRAHLUNG CROSS SECTION

by Clayton D. Zerby and Henry Brysk

June 24, 1966

Work Performed Under Contract No. NASw-1235
National Aeronautics and Space Administration
Washington, D. C.

Space Science and Engineering Group
Union Carbide Research Institute
Tarrytown, New York

# PREFACE

This report covers work done on the calculation of the Bremsstrahlung cross section (both mathematical analysis and computer programming) under Contracts NASw-906 and NASw-1235.

For the sake of clarity of presentation, the report has been split into two sections. Section A presents the theoretical development incorporated into the current computer program, together with a discussion of the program itself. Section B contains significant work on the problem that is not utilized in the current form of the program, together with a discussion of the reasons for its present exclusion and of the advisability of its consideration for future refinements of the program. A number of lesser results and transitional approaches, which were reported in the quarterly reports, are not reproduced here. Similarly, discussions of test programs and checkout problems have appeared in the quarterly reports but are not given here.

The program is now operational. The continuation of this work will include some further refinements of the program, and an extensive series of production runs for various elements and energies.

TABLE OF CONTENTS

# SECTION A

# THEORETICAL CALCULATIONS AND THE COMPUTER PROGRAM

# I. INTRODUCTION

It is well known that the Bethe-Heitler expression for the electron Bremsstrahlung cross section[1], which was derived using the Born approximation, yields inaccurate results in comparison with experiment.[2] In general at energies below approximately 10 Mev the photon energy spectrum is underestimated over its complete range with the most serious discrepancy occuring at the higher photon energies. As a result, it is estimated that at 1 Mev incident electron energy the average energy release in a radiative collision with Aluminum is underestimated by over 30% while for Gold it is underestimated by as much as 55%.[2]

The reason for the discrepancy can be attributed almost entirely to the use of plane waves for the electron wavefunction in the matrix element as prescribed by the Born approximation. The theoretical estimate can be improved in accuracy by using Coulomb wavefunctions in the matrix element. In this way the influence of the nuclear electrostatic field can be taken into account in the most accurate way. Jaeger and Hulme[3,4,5] were the first to use the more accurate wavefunctions in the closely allied process of electron-positron pair production by photons. Their results were in good agreement with experiment.[3,6] Hence, very accurate results for the theoretical estimate of the Bremsstrahlung cross section can also be expected with the corresponding approach. The difficulty with the improved method, and the reason it has not been used extensively in the past, is that it does not yield a simple analytic formula, but requires extensive numerical procedures to obtain results.

In the present study, the Bremsstrahlung cross section problem is formulated with Dirac wavefunctions for the screened and unscreened nuclear electrostatic field. The screened potential is obtained from

self-consistent-field calculations. This requires that the wavefunctions be expanded in a series of angular momentum states. Hence, the formulation is suitable for calculation only at relatively low incident energies.

The cross section for unpolarized incident electrons is obtained for various polarization states of the photon, differential in the polar angle and energy of the photon. With a simple change in input for the incident particle's charge and/or mass, the program is equally applicable to the calculation of Bremsstrahlung from positrons and positive and negative muons.

The derivation starts in Chapter II with the presentation of the eigenfunctions of the energy and angular momentum operator of the Dirac equation. The eigenfunctions are used in the matrix element for the production of Bremsstrahlung as described in Chapter III. The final derivation of the cross section is given in Chapter IV. In Chapter V, Racah algebra is used to perform the magnetic quantum number sums explicitly, leading to some computational as well as formal simplifications.

For the computation of matrix elements, the procedure, as described in Chapter VI, is to terminate the numerical integration at some moderate radius, and to continue the integration out to infinity analytically by means of an asymptotic evaluation. This involves using asymptotic wavefunctions to perform the integral from the cut-off radius onward, and carrying out the integral itself asymptotically.

Chapter VII clears up an ambiguity in the phase of the Coulomb wavefunctions found in the literature (this was needed to establish the sign of each partial wave in the starting conditions for integration). In Chapter VIII, the analytic limit of the Coulomb wavefunctions as the kinetic energy goes to zero is derived. These are the scattered-electron wavefunctions in the end-point case (electron giving up its entire kinetic energy to the photon).

Initial values and equations for the radial integrals are covered in Chapter IX Phase shift determination by wave-matching at the cut-off radius is described in Chapter X.

Chapter XI explains the procedure used for the computation of normalization factors by matching to the W.K.B. approximation solution.

Chapter XII discusses the self-consistent-field calculations and their application to the computation of the screened potential.

The calculation of the angular distributions at the end of the program is detailed in Chapter XIII.

The structure of the computer program is outlined in Chapter XIV, together with specification of the input and a description of the output.

Chapter XV describes full-scale sample runs of the computer program, used to establish that the results from the program compare with the Born approximation in the expected way.

## II. EIGENFUNCTIONS OF THE ENERGY AND ANGULAR MOMENTUM OPERATORS

The continuum eigenfunctions of the positive energy operator of the Dirac equation for an electron in a central electrostatic field have the form[7]

$$\phi_{\kappa,\mu} = \begin{Bmatrix} -ir^{-1} G_\kappa \Omega_{\kappa,\mu} \\ r^{-1} F_\kappa \Omega_{-\kappa,\mu} \end{Bmatrix} \tag{1}$$

where $\phi_{\kappa,\mu}$ is a bispinor, $\Omega_{\kappa,\mu}$ is a spinor and $G_\kappa$ and $F_\kappa$ are radial functions. The eigenfunctions $\phi_{\kappa,\mu}$ are also eigenfunctions of the operators, $\underline{J}$, $\underline{L}$, $\underline{S}$, and $J_z$ which are the total, orbital and spin angular momentum operators and the z component of the total angular momentum operator, respectively. The eigenvalues belonging to these operators are $j$, $\ell$, $\frac{1}{2}$, and $\mu$, respectively. The non-zero parameter $\kappa$, which can take on all positive and negative integral values, is related to $j$ and $\ell$ by[7]

$$\left.\begin{aligned} \kappa &= -(j+\tfrac{1}{2}) = -(\ell+1), \text{ for } \kappa < 0, \\ \kappa &= j+\tfrac{1}{2} = \ell, \text{ for } \kappa > 0. \end{aligned}\right\} \tag{2}$$

The parameter $\kappa$ is sufficient to designate both $j$ and $\ell$ simultaneously since $j = |\kappa| - \frac{1}{2}$ and $\ell = j+\frac{1}{2}\kappa/|\kappa|$. To indicate the dependence of $j$ and $\ell$ on $\kappa$, the eigenvalue $j$ will be replaced with $j_\kappa$ and $\ell$ will be replaced with $\ell_\kappa$.

The eigenfunctions $\phi_{\kappa,\mu}$ are normalized on the energy scale so that*

---

*The notation $\phi^+$ indicates the complex conjugate transpose of $\phi$ while $\phi^*$ indicates only the complex conjugate of $\phi$.

$$\int \phi^{+}_{\kappa,\mu}(E)\,\phi_{\kappa',\mu'}(E')\,d^3x = \delta_{\kappa,\kappa'}\,\delta_{\mu,\mu'}\,\delta(E-E'). \tag{3}$$

The angular functions $\Omega_{K,\mu}$ that appear in (1) are given by

$$\Omega_{\kappa,\mu} = \sum_n C(\ell_\kappa \tfrac{1}{2} j_\kappa ; \mu-n, n)\, Y_{\ell_\kappa,\mu-n}(\hat{r})\, \eta_{\frac{1}{2},n} \tag{4}$$

where $\eta_{\frac{1}{2},n}$ is the spin-$\frac{1}{2}$ spinor with z-axis projection quantum number n, $Y_{\ell,\mu-n}(\hat{r})$ is a spherical harmonic, and $C(\ell_\kappa \tfrac{1}{2} j_\kappa ; \mu-n,n)$ is a Clebsch-Gordan coefficient.[8] These angular functions are orthonormal on the unit sphere so that

$$\int \Omega^{+}_{\kappa,\mu}\,\Omega_{\kappa',\mu'}\,d\Omega = \delta_{\kappa,\kappa'}\,\delta_{\mu,\mu'} \tag{5}$$

where $d\Omega$ is a differential element of solid angle.

The electron function $\phi_{\kappa,\mu}$ satisfies the equation

$$E\,\phi_{\kappa,\mu} = (-i\underset{\sim}{\alpha}\cdot\underset{\sim}{\nabla}+\beta+V)\,\phi_{\kappa,\mu}. \tag{6}$$

Consequently the radial functions satisfy

$$\left.\begin{aligned} F' - \frac{\kappa}{r}F + (E-V-1)\,G &= 0 \\ G' + \frac{\kappa}{r}G - (E-V+1)\,F &= 0 \end{aligned}\right\} \tag{7}$$

and have the asymptotic forms

$$\left.\begin{aligned} G &\sim \frac{\sqrt{E+1}}{\sqrt{\pi k}}\ \sin\left(kr - \frac{\ell_\kappa \pi}{2} + \delta_\kappa\right) \\ F &\sim \frac{\sqrt{E-1}}{\sqrt{\pi k}}\ \cos\left(kr - \frac{\ell_\kappa \pi}{2} + \delta_\kappa\right) \end{aligned}\right\} \tag{8}$$

where $k = (E^2-1)^{\frac{1}{2}}$ and $\delta_\kappa$ is the phase shift.

In the case of a pure Coulomb field with $V = -\frac{Ze^2}{r}$, the radial functions have the form

$$\left.\begin{aligned} G_\kappa &= \sqrt{E+1}\ \ (H_\kappa + H_\kappa^*) \\ F_\kappa &= i\sqrt{E-1}\ \ (H_\kappa - H_\kappa^*) \end{aligned}\right\} \tag{9}$$

where

$$H_\kappa = A_\kappa e^{-i\frac{1}{2}\pi(\gamma+\frac{1}{2})}\ (2kr)^{-\frac{1}{2}}\ M_{-\frac{1}{2}-i\nu,\gamma}\ (2ikr) \tag{10}$$

with

$$A_K = \frac{|\Gamma(\gamma+i\nu)|\ \ e^{\frac{1}{2}\pi\nu}\ e^{ih(\kappa)}\ (\gamma+i\nu)}{2(\pi k)^{\frac{1}{2}}\ \Gamma(2\gamma+1)} \tag{11}$$

In the above $M_{-\frac{1}{2}-i\nu,\gamma}\ (2ikr)$ is a Whittaker function,[9]

$\gamma = |(\kappa^2 - Z^2e^2)^{\frac{1}{2}}|$ , $\nu = EZe^2/k$, and $\exp[2i\ h(\kappa)] = (-\kappa+i\nu E^{-1})(\gamma+i\nu)^{-1}$.

In the subsequent development it is not advantageous to use the complex conjugate form of $H_\kappa$ shown in (10). Instead, the following relation for the Whittaker function can be used:[9]

$$M_{K,\mu}(z) = e^{i\epsilon\pi(\frac{1}{2}+\mu)}\ M_{-K,\mu}(-z)$$

where $\epsilon=1$ if $Im(z)>0$ and $\epsilon=-1$ if $Im(z)\leq 0$, to obtain the alternative and more useful expression:

$$H_\kappa^* = A_\kappa^*\ e^{-i\frac{1}{2}\pi(\gamma+\frac{1}{2})}\ (2kr)^{-\frac{1}{2}}\ M_{\frac{1}{2}-i\nu,\gamma}\ (2ikr). \tag{12}$$

In the case of the Coulomb field, the asymptotic forms of (8) are replaced with

$$\left.\begin{aligned} G &\sim \frac{\sqrt{E+1}}{\sqrt{\pi k}}\ \sin\left(kr+\nu\ \ell n\ (2kr) - \frac{\ell_\kappa \pi}{2} + \delta_\kappa\right) \\ F &\sim \frac{\sqrt{E-1}}{\sqrt{\pi k}}\ \cos\left(kr+\nu\ \ell n\ (2kr) - \frac{\ell_\kappa \pi}{2} + \delta_\kappa\right) \end{aligned}\right\} \tag{13}$$

where

$$\delta_\kappa = h(\kappa) - \arg\Gamma(\gamma+i\nu) - \frac{\pi}{2}(\gamma-\ell_\kappa-1) \tag{14}$$

## III. THE MATRIX ELEMENT

The matrix element for the production of Bremsstrahlung is[10]

$$M = -e\int \underline{A}_q \cdot (\Psi_f^+(E') \underline{\alpha} \Psi_m(E))\, d^3x \tag{1}$$

where $\underline{\alpha}$ is the Dirac matrix operator. Since we will not be interested in angular or polarization details about the electron leaving the interaction, the final state electron function $\Psi_f(E')$ can be normalized on the energy scale according to the form given in Chapter II, Eq. 1:

$$\Psi_f(E') = \phi_{\kappa',\mu'} = \begin{Bmatrix} -ir^{-1} G_{\kappa'} \Omega_{\kappa',\mu'} \\ r^{-1} F_{\kappa'} \Omega_{-\kappa',\mu'} \end{Bmatrix} . \tag{2}$$

The initial state electron function $\Psi_m(E)$ is normalized on the momentum scale and has the asymptotic form

$$\Psi_m(E) \sim u(m) e^{i\underline{k}\cdot\underline{r}} + Gr^{-1} e^{ikr} \tag{3}$$

where u(m) and G are bispinors. The z component of the spin associated with the plane wave in (3) is designated by m. It can be shown that if the axis of quantization is taken along the direction of propagation of the incident electron, then[7] $\Psi_m(E)$ is given by

$$\Psi_m(E) = \sum_\kappa 2\pi(2Ek)^{-\frac{1}{2}} C_{\kappa,m}\, \phi_{\kappa,m} \tag{4}$$

with

$$C_{\kappa,m} = i^{\ell_\kappa+1} (2\ell_\kappa+1)^{\frac{1}{2}} C(\ell_\kappa \tfrac{1}{2} j_\kappa; om)\, e^{i\delta_\kappa} \tag{5}$$

and $\phi_{\kappa,m}$ as defined in (1) of Chapter II.

The electromagnetic wave in (1) can be represented as a linear combination of waves which are circularly polarized perpendicular to the direction of propagation. If the wave was propagating along the z axis it would have the form

$$\underset{\sim}{A}_q(0) = \sum_{p=\pm 1} a_p \underset{\sim}{A}_p \tag{6}$$

with

$$\underset{\sim}{A}_p = -p\hat{\xi}_p \sqrt{\frac{2\pi}{\epsilon}}\, e^{-iqz} = -p\hat{\xi}_p \sqrt{\frac{2\pi}{\epsilon}} \sum_{\ell} (-i)^{\ell} [4\pi(2\ell+1)]^{\frac{1}{2}} Y_{\ell,0}(\hat{r})\, j_{\ell}(qr) \tag{7}$$

where $\epsilon$ and $q$ are the photon energy and momentum, respectively, $\hat{\xi}_p$ are the spherical basis[8], $j_{\ell}(qr)$ are the spherical Bessel functions, and $a_p$ are constants (to be discussed below). The wave $\underset{\sim}{A}_{+1}$ is l.h. circularly polarized and $\underset{\sim}{A}_{-1}$ is r.h. circularly polarized. Rotation of the coordinate system so that the photon is propagated in an arbitrary direction with respect to the new system yields the required expression

$$\underset{\sim}{A}_p = -p \frac{4\pi}{\sqrt{2\epsilon}} \sum_{\ell} \sum_{\lambda} \sum_{m'=-\lambda}^{+\lambda} (-i)^{\ell} (2\ell+1)^{\frac{1}{2}}\, j_{\ell}(qr) C(\ell\ 1\lambda; 0p)\, D^{\lambda}_{m'p}(\varphi_q, \theta_q, 0) \underset{\sim}{T}_{\lambda \ell m'} \tag{8}$$

where $\varphi_q$ and $\theta_q$ are the azimuthal and polar angle, respectively, of the propagation vector, $D^{\lambda}_{m'p}$ is a rotation matrix[8] and $\underset{\sim}{T}_{\lambda \ell m'}$ is given by[8]

$$\underset{\sim}{T}_{\lambda \ell m'} = \sum_{\nu} C(\ell\ 1\lambda;\ m'-\nu, \nu)\, Y_{\ell, m'-\nu}(\hat{r})\ \hat{\xi}_{\nu} \tag{9}$$

The constants $a_p$ in (6) can be shown to have the forms:

$$\left.\begin{array}{ll} \text{for a l.h. circularly polarized photon,} & a_p = \delta_{p,+1} \\ \text{for a r.h. circularly polarized photon,} & a_p = \delta_{p,-1} \\ \text{for a linearly polarized photon,} & a_p = 2^{-\frac{1}{2}} e^{-ip\varphi_0} \end{array}\right\} . \tag{10}$$

In the case of linear polarization the angles of interest are indicated in Fig. 1.

In the subsequent development it is appropriate to consider the matrix element with $\underset{\sim}{A}_q$ replaced with $\underset{\sim}{A}_p$. The new matrix element M(p) shows p as an argument. Hence

$$M = \sum_{p=\pm 1} a_p \, M(p). \tag{11}$$

The matrix element M(p) is obtained with the use of (1) through (11)

$$M(pm\kappa'\mu') = \frac{4\pi^2 e}{\sqrt{\epsilon E k}} \sum_{\ell} \sum_{\lambda} \; p \, C(\ell 1\lambda; 0p) \sum_{m'=-\lambda}^{+\lambda} D^{\lambda}_{m',p}(\varphi_q, \theta_q, 0) \, F(\lambda \ell \kappa' \mu' m m') \tag{12}$$

where $$F(\lambda\ell\kappa'\mu' mm') = (-i)^{\ell} \, (2\ell+1)^{\frac{1}{2}} \sum_{\nu} \; C(\ell 1\lambda; m'-\nu, \nu) \sum_{\kappa} \; C_{\kappa, m}$$

$$\int j_{\ell}(qr) \, Y_{\ell, m'-\nu}(\hat{r}) \, \phi^{+}_{\kappa', \mu'} \alpha_{\nu} \phi_{\kappa, m} \, d^3x \tag{13}$$

and $$\alpha_{\nu} = \hat{\epsilon}_{\nu} \cdot \underset{\sim}{\alpha}.$$

The integral over the angles in (13) is readily found with the result that (13) becomes

$$F(\lambda\ell\kappa'\mu' mm') = \delta_{\mu'-m, m'} \sqrt{\frac{3}{4\pi}} \qquad A(\lambda\ell\kappa'\mu' m) \tag{14}$$

and, as a result, (12) becomes

$$M(pm\kappa'\mu') = \frac{2\pi\sqrt{3\pi e}}{\sqrt{\epsilon E k}} \sum_{\lambda} \sum_{\ell} \; pC(\ell 1\lambda; 0p) \; D^{\lambda}_{\mu'-m, p}(\varphi_q, \theta_q, 0) A(\lambda\ell\kappa'\mu' m). \tag{15}$$

If we set $\mu' - m = \epsilon$ in (15) and eliminate $\mu'$ we have

$$A(\lambda\ell\kappa'\mu' m) \equiv A(\lambda\ell\kappa' \epsilon m) \tag{16}$$

where

$$A(\lambda\ell\kappa' \epsilon m) = \sum_{\kappa} \left[ H_1(\kappa'\kappa m) \, B_{\ell\lambda}(\kappa', -\kappa\epsilon m) - H_2(\kappa'\kappa m) \, B_{\ell\lambda}(-\kappa'\kappa\epsilon m) \right], \tag{17}$$

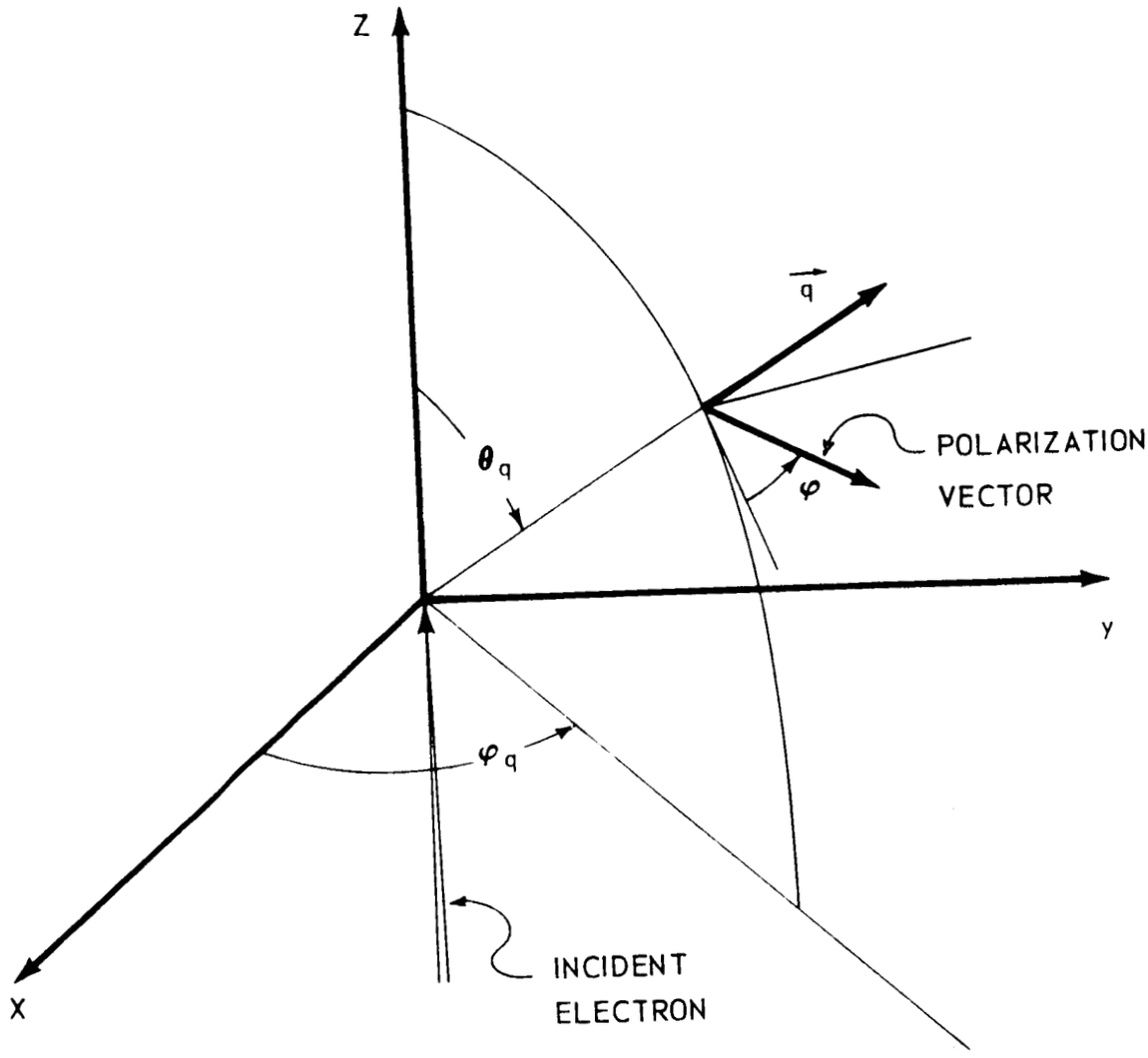


FIGURE 1 GEOMETRY OF BREMSSTRAHLUNG INTERACTION INDICATING THE CASE OF A LINEARLY POLARIZED PHOTON.

with

$$H_1(\nu'\nu m) = i^{\ell+\ell_\nu+1}\,(-1)^{m+1/2}\,(2\ell+1)(2j_\nu+1)^{1/2}\,e^{i\delta_\nu}\,C(j_\nu\,\tfrac{1}{2}\,\ell_\nu;\,-m,m)$$
$$C(\ell\ell_{\nu'}\,\ell_{-\nu};00)\,K_\ell(\nu'\nu) \tag{18}$$

and

$$H_2(\nu'\nu m) = i^{\ell+\ell_\nu+1}\,(-1)^{m+1/2}\,(2\ell+1)(2j_\nu+1)^{1/2}\,e^{i\delta_\nu}\,C(j_\nu\,\tfrac{1}{2}\,\ell_\nu;-m,m)$$
$$C(\ell\ell_{-\nu'},\ell_\nu;00)\,K_\ell\,(\nu\nu') \tag{19}$$

The $B_{\ell\lambda}$ functions in (17) can be determined from

$$B_{\ell\lambda}\,(\nu',-\nu\varepsilon m) = \sum_\delta C(\ell_{\nu'}\tfrac{1}{2}j_{\nu'};\,\varepsilon+m-\delta,\delta)\sum_\beta(-1)^{\delta-\beta}\,C(\tfrac{1}{2}1\tfrac{1}{2};\delta,-\delta+\beta)x$$
$$C(\ell 1\lambda;\varepsilon-\delta+\beta,\delta-\beta)C(\ell_{-\nu}\tfrac{1}{2}j_{-\nu};m-\beta,\beta)C(\ell\ell_{-\nu}\ell_{\nu'};\varepsilon-\delta+\beta,m-\beta). \tag{20}$$

The $K_\ell$ functions in (18) and (19) can be determined from

$$\left.\begin{aligned} K_\ell(\nu'\nu) &= \int_0^\infty j_\ell(qr)\,G_{\nu'}\,(E',r)\,F_\nu\,(E,r)dr \\ \text{and} \\ K_\ell(\nu\nu') &= \int_0^\infty j_\ell(qr)\,G_\nu\,(E,r)\,F_{\nu'}\,(E',r)dr \end{aligned}\right\} \tag{21}$$

## IV. DERIVATION OF THE CROSS SECTION

The cross section for production of Bremsstrahlung by unpolarized incident electrons and without regard for the direction or polarization of the scattered electron or the azimuthal angle of the photon is given by[10]

$$d\sigma = \frac{2\pi}{v} \sum_{m\mu'\mu'} \int_{\varphi_q=0}^{2\pi} \left|M\left(m\mu'\mu'\right)\right|^2 \frac{q^2 dq\, d\mu_q d\varphi_q}{(2\pi)^3} \qquad (1)$$

where the polarization states of the incident electron (designated by m) have been averaged over, v is the incident velocity of the electron and $\mu_q = \cos\theta_q$. Using the matrix elements defined by (11) and (13) of Chapter III,

$$d\sigma = \sum_{p=\pm 1} \left\{ \left|A_p\right|^2 d\sigma_{pp} + A_{-p}^{*} A_p \, d\sigma_{-p,p} \right\} \qquad (2)$$

where $A_p$ is defined in (8) of Chapter III and

$$d\sigma_{p'p} = \frac{\pi}{v} \sum_{m\mu'\mu'} \int_{\varphi_q=0}^{2\pi} M^{+}(p'm\mu'\mu') \, M\left(pm\mu'\mu'\right) \frac{q^2 dq\, d\mu_q d\varphi_q}{(2\pi)^3} \,. \qquad (3)$$

Hence, it follows that

$$\begin{aligned}
d\sigma &= d\sigma_{11} && \text{for l.h. circularly polarized photons} \\
d\sigma &= d\sigma_{-1-1} && \text{for r.h. circularly polarized photons} \qquad (4) \\
d\sigma &= \tfrac{1}{2} \sum_{p=\pm 1} \left(d\sigma_{pp} + e^{-2ip\varphi} \, d\sigma_{-p,p}\right) && \text{for linearly polarized photons}^{*} \\
d\sigma &= \sum_{p=\pm 1} d\sigma_{pp} && \text{for unpolarized photons.}
\end{aligned}$$

The integral over the photon azimuthal angle involves the integral

$$I = \int_0^{2\pi} D^{*\lambda_1}_{\mu'-m,p'}(\varphi_q \theta_q 0) D^{\lambda}_{\mu'-m,p}(\varphi_q \theta_q 0) \, d\varphi_q \qquad (5)$$

Actually the integrand of this integral is independent of $\varphi$ and it is

---

* See Fig. 1.

easily shown that

$$I = 2\pi \sum_j (-1)^{\mu'-m-p'} C(\lambda_1 \lambda j; -\mu+m, \mu'-m) C(\lambda_1 \lambda j; -p', p)$$

$$\left[\frac{(j-|p'-p|)!}{(j+|p'-p|)!}\right]^{1/2} P_{j,|p'-p|}(\theta_q) \qquad (6)$$

In (6), $P_{j,m}$ are the associated Legendre polynomials:

$$P_{j,m}(\theta_q) = \frac{1}{2^j j!} (1-\cos^2\theta_q)^{m/2} \left[\frac{d}{d(\cos\theta)}\right]^{j+m} (\cos^2\theta-1)^j \qquad (7)$$

where m is positive definite. The fact that

$$(-1)^{p'-p} = 1 \qquad (8)$$

in all cases has been used.

With the use of (15) of Chapter III and of (6), the cross section (3) becomes

$$d\sigma_{p'p} = \sum_j d\sigma^j_{p'p} \left[\frac{(j-|p'-p|)!}{(j+|p'-p|)!}\right]^{1/2} P_{j,|p'-p|}(\theta_q) \qquad (9)$$

where, upon setting $v = k/E$ and using $k^2 = E^2-1$,

$$d\sigma^j_{p'p} = 3\pi^2 e^2 \frac{(E-1)}{(E+1)} B_j(p'p)\, y dy d\mu_q \qquad (10)$$

with $y = q(E-1)^{-1}$. Also

$$B_j(p'p) = B^*_j(pp') = B_j(-p',-p) = \sum_{\ell\ell_1} A_j(p'p\ell_1\ell), \qquad (11)$$

where

$$A_j(p'p\ \ell_1\ell) = p\ p' \sum_{\lambda_1\lambda} C(\ell_1\ 1\ \lambda_1;0p')C(\ell 1\lambda;0p)C(\lambda_1\lambda j;-p',p)x$$

$$V_j(\lambda_1\lambda\ell\ell_1). \tag{12}$$

The function $V_j$ in (12) is independent of p and p' and is given by

$$V_j(\lambda_1\lambda\ell_1\ell) = \sum_{\epsilon} (-)^{\epsilon+1}\, C(\lambda_1\lambda j;-\epsilon,\epsilon)\varphi(\lambda_1\lambda\ell_1\ell\epsilon) \tag{13}$$

where, in turn, the $\varphi$ function is

$$\varphi(\lambda_1\lambda\ell_1\ell\epsilon) = \sum_{\kappa'}\sum_{m} A^*(\lambda_1\ell_1\kappa'\epsilon m)\, A(\lambda\ell\kappa'\epsilon m). \tag{14}$$

The A functions in (14) are given in (17) of Chapter III.

Since $B_j(p'p)$ is symmetric with respect to the pairs $(\ell,\lambda)$ and $(\ell_1,\lambda_1)$, both having been summed over in the same way, only the real part of $\varphi$ contributes.

The computer program calculates

$$A_j^{(1)}(\ell_1\ell) = (-1)^j\, 6(2\ell_1+1)^{-1}\,(2\ell+1)^{-1}\, A_j(1\ 1\ \ell_1\ell), \tag{15a}$$

$$A_j^{(2)}(\ell_1\ell) = (-1)^j\, 6(2\ell_1+1)^{-1}\,(2\ell+1)^{-1}\, A_j(1,\ -1\ \ell_1\ell), \tag{15b}$$

and then

$$B_j^{(i)} = \sum_{\ell} (2\ell+1) \sum_{\ell_1\le\ell} (2-\delta_{\ell_1\ell})(2\ell_1+1)A_j^{(i)}(\ell_1\ell). \tag{16}$$

## V. ANGULAR MOMENTUM SUMS

The expressions given for the Bremsstrahlung cross section contain several sums over angular momentum quantum numbers, the summands consisting of products of Clebsch-Gordan coefficients. These sums can be carried out formally, yielding Racah and X coefficients.

Going up the hierarchy of magnetic quantum number sums, there is first

$$B_{\ell\lambda}(\kappa',-\kappa\epsilon m) = \sum_{\delta} C(\ell_\kappa, \tfrac{1}{2}\, j_\kappa,; \epsilon+m-\delta,\delta)\sum_{\beta}(-1)^{\delta-\beta}C(\tfrac{1}{2}\,1\,\tfrac{1}{2};\delta,-\delta+\beta)$$

$$C(\ell 1\lambda;\epsilon-\delta+\beta,\delta-\beta)C(\ell_{-\kappa}\,\tfrac{1}{2}\,j_\kappa;m-\beta,\beta)C(\ell\ell_{-\kappa}\ell_\kappa,;\epsilon-\delta+\beta,m-\beta). \qquad (1)$$

After two recouplings (yielding two Racah coefficients) and an orthogonality relation, the $\beta$ sum reduces to

$$\sum_{\beta} \text{---} = (-1)^{\ell-j_\kappa-\epsilon-m+\frac{1}{2}+\delta}\left[(2\lambda+1)(2\ell_\kappa,+1)(2j_\kappa+1)\right]^{1/2}\sum_{f}(2f+1)^{1/2}$$

$$W(\ell\ell_\kappa,\tfrac{1}{2}\,j_\kappa;\ell_{-\kappa}f)W(1\lambda\tfrac{1}{2}f;\ell\tfrac{1}{2})C(\ell_\kappa,\, j_\kappa f;-\epsilon-m+\delta,m)C(\lambda f\tfrac{1}{2};\epsilon,-\epsilon+\delta). \qquad (2)$$

Similarly, the remaining $\delta$-sum yields

$$\sum_{\delta}(-1)^{\delta+\frac{1}{2}}C(\ell_\kappa j_\kappa f;-\epsilon-m+\delta,m)C(\lambda f\tfrac{1}{2};\epsilon,-\epsilon+\delta)C(\ell_\kappa,\tfrac{1}{2}\,j_\kappa,;\epsilon+m-\delta,\delta)$$

$$=(-1)^{\lambda+f+j_\nu,\ -\frac{1}{2}+\epsilon+m}\,[2(2f+1)]^{1/2}\,W(\ell_\nu,j_\nu\tfrac{1}{2}\lambda;fj_\nu,)C(j_\nu\lambda j_\nu,;m\ \epsilon). \tag{3}$$

On splitting off the magnetic quantum number dependence by

$$B_{\ell\lambda}(\nu',-\nu\epsilon\ m)\equiv\bar{B}_{\ell\lambda}(\nu',-\nu)C(\lambda j_\nu j_\nu,;\epsilon\ m), \tag{4}$$

there remains

$$\bar{B}_{\ell\lambda}(\nu',-\nu)\ =\ (-1)^{\ell}\,[2(2\lambda+1)(2\ell_\nu,+1)(2j_\nu+1)]^{1/2}\sum_{f}(-1)^{f-\frac{1}{2}}\,(2f+1)$$

$$W(\ell\ell_\nu,\tfrac{1}{2}j_\nu;\ell_{-\nu}f)W(1\lambda\tfrac{1}{2}f;\ell\tfrac{1}{2})W(\ell_\nu,j_\nu\ \tfrac{1}{2}\ \lambda;f\ j_\nu,). \tag{5}$$

The f sum is an X-coefficient (after rearrangement), so that

$$\bar{B}_{\ell\lambda}(\nu',-\nu)=-[2(2\lambda+1)(2\ell_\nu,+1)(2j_\nu+1)]^{1/2}\,X(\lambda j_\nu j_\nu,;\ell\ell_{-\nu}\ell_\nu,;1\ \tfrac{1}{2}\ \tfrac{1}{2}). \tag{6}$$

This X-coefficient can be expressed in a more elementary form.

Together with the matching parity Clebsch-Gordan coefficient, the result reduces to[11,12]

$$\bar{\bar{B}}_{\ell\lambda}(\nu',-\nu)\ =\ C(\ell\ell_\nu,\ell_{-\nu};00)\bar{B}_{\ell\lambda}(\nu',-\nu)$$

$$=\ -3^{-1/2}C\,(\lambda j_\nu,j_\nu;0,\ \tfrac{1}{2})\ \ G_{\ell\lambda}(\nu',-\nu), \tag{7}$$

where the dependence on the signs of $\nu$ and $\nu'$ is contained in

$$G_{\ell\lambda}(\nu',\nu)=(\nu'-\nu)[\ell(\ell+1)]^{-1/2}\delta_{\lambda,\ell}+(\nu'+\nu+\ell)[\ell(2\ell+1)]^{-1/2}\delta_{\lambda,\ell-1}$$

$$+\ (\nu'+\nu-\ell-1)[(\ell+1)(2\ell+1)]^{-1/2}\delta_{\lambda,\ell+1} \tag{8}$$

Equation 8 does not hold for $\lambda=0$, but this value is eliminated by the occurrence of a factor $C(\ell 1\lambda;0,\pm1)$ further upstream.

Separating the magnetic quantum number dependence of $A(\lambda\ell\nu'\epsilon m)$,

$$A(\lambda \ell \nu' \epsilon m) \equiv (-1)^{m+1/2} \sum_{\nu} \bar{H}(\lambda \ell \nu' \nu) C(\lambda j_\nu j_{\nu'}; \epsilon m) C(j_\nu \tfrac{1}{2} \ell_\nu ; -m, m) \qquad (9)$$

where, in turn,

$$\bar{H}(\lambda \ell \nu' \nu) = i^{\ell_\nu + \ell + 1} (2\ell+1)(2j_\nu+1)^{1/2} e^{i\delta_\nu} [\bar{\bar{B}}_{\ell\lambda}(\nu', -\nu) K_\ell(\nu' \nu) - \bar{\bar{B}}_{\ell\lambda}(-\nu', \nu) K_\ell(\nu \nu')]. \qquad (10)$$

In the next round of summations now,

$$\varphi(\lambda_1 \lambda \ell_1 \ell \epsilon) = \sum_{\nu'} \sum_{m} A^*(\lambda_1 \ell_1 \nu' \epsilon m) A(\lambda \ell \nu' \epsilon m)$$

$$= \sum_{\nu' \nu \nu_1} \bar{H}^*(\lambda_1 \ell_1 \nu' \nu_1) \bar{H}(\lambda \ell \nu' \nu) \sum_{m} C(\lambda_1 j_{\nu_1} j_{\nu'}; \epsilon m) C(j_{\nu_1} \tfrac{1}{2} \ell_{\nu_1}; -m, m)$$

$$C(\lambda j_\nu j_{\nu'}; \epsilon m) C(j_\nu \tfrac{1}{2} \ell_\nu; -m, m). \qquad (11)$$

Recoupling to separate the $\epsilon$ and m dependence,

$$C(\lambda_1 j_{\nu_1} j_{\nu'}; \epsilon m) C(\lambda j_\nu j_{\nu'}; \epsilon m)$$

$$= (-1)^{\lambda - j_{\nu'} + m} (2j_{\nu'}+1)(2\lambda+1)^{-1/2} \sum_{s} (2s+1)^{1/2} W(\lambda_1 j_{\nu_1} \lambda j_\nu; j_{\nu'} s)$$

$$C(j_{\nu_1} j_\nu s; m, -m) C(\lambda_1 s \lambda; \epsilon 0). \qquad (12)$$

The next step is

$$V_j(\lambda_1 \lambda \ell_1 \ell) = \sum_{\epsilon} (-)^{\epsilon+1} C(\lambda_1 \lambda j; -\epsilon, \epsilon) \varphi(\lambda_1 \lambda \ell_1 \ell \epsilon).$$

The $\epsilon$ sum reduces to

$$\sum_{\epsilon} (-)^{\epsilon+1} C(\lambda_1 \lambda j; -\epsilon, \epsilon) C(\lambda_1 s \lambda; \epsilon 0) = (-1)^{s-\lambda+1} [(2\lambda+1)/(2s+1)]^{1/2} \delta_{sj} \qquad (13)$$

leaving

$$V_j(\lambda_1\lambda\ell_1\ell)=(-1)^{j+1}\sum_{\nu'}(2j_{\nu'}+1)\sum_{\nu\nu_1}\bar{H}^*(\lambda_1\ell_1\nu'\nu_1)\bar{H}(\lambda\ell\nu'\nu)W(\lambda_1 j_{\nu_1}\lambda j_\nu;j_{\nu'},j)$$

$$\sum_m(-1)^{-j_{\nu'}+m}C(j_{\nu_1}j_\nu j;m,-m)C(j_{\nu_1}\tfrac{1}{2}\ell_{\nu_1};-m,m)C(j_\nu\tfrac{1}{2}\ell_\nu;-m,m). \qquad (14)$$

The m sum consists of the two terms $m=\pm\frac{1}{2}$ which differ only in the sign of the magnetic quantum numbers of the Clebsch-Gordan coefficients, hence by a phase factor of $(-1)$ to the power

$$\begin{aligned}&1+(j_{\nu_1}+j_\nu-j)-(j_{\nu_1}+\tfrac{1}{2}-\ell_{\nu_1})-(j_\nu+\tfrac{1}{2}-\ell_\nu)=\ell_\nu+\ell_{\nu_1}-j\\&=(\ell_\nu+\ell_{-\nu'}+\ell)+(\ell_{\nu_1}+\ell_{-\nu'}+\ell_1)-2(\ell_{-\nu'}+\ell+\ell_1)+(\ell+\ell_1-j).\end{aligned} \qquad (15)$$

This yields the selection rule that $V_j(\lambda_1\lambda\ell_1\ell)$ vanishes unless

$$\ell+\ell_1-j = \text{even integer}. \qquad (16)$$

Subject to this condition, the m sum is twice the $m=-\frac{1}{2}$ term. On substituting the explicit value

$$C(j_\nu\tfrac{1}{2}\ell_\nu;\tfrac{1}{2},-\tfrac{1}{2}) = 2^{-1/2}, \qquad (17)$$

$$\begin{aligned}V_j(\lambda_1\lambda\ell_1\ell)=(-1)^j\sum_{\nu'\nu\nu_1}(-1)^{j_{\nu'}-1/2}(2j_{\nu'}+1)\\ \bar{H}^*(\lambda_1\ell_1\nu'\nu_1)\bar{H}(\lambda\ell\nu'\nu)W(\lambda j_\nu\lambda_1 j_{\nu_1};j_{\nu'},j)C(j_\nu j_{\nu_1}j;-\tfrac{1}{2},\tfrac{1}{2}).\end{aligned} \qquad (18)$$

Equation (18) requires the computation of general Racah coefficients. This can be avoided at the cost of performing one magnetic quantum number sum explicitly. Re-expanding,

$$\begin{aligned}&W(\lambda j_\nu\lambda_1 j_{\nu_1};j_{\nu'},j)C(j_\nu j_{\nu_1}j;-\tfrac{1}{2}\,\tfrac{1}{2})\\&=(-1)^{j+j_{\nu'}+1/2+\epsilon}(2j_{\nu'}+1)^{-1}\sum_\epsilon C(\lambda_1 j_{\nu_1}j_{\nu'};\epsilon,-\tfrac{1}{2})C(\lambda j_\nu j_{\nu'};\epsilon,-\tfrac{1}{2})C(\lambda_1\lambda j;-\epsilon,\epsilon),\end{aligned} \qquad (19)$$

so that

$$V_j(\lambda_1\lambda\ell_1\ell) = \sum_{\epsilon} (-1)^{\epsilon+1} C(\lambda_1\lambda j;-\epsilon\ \epsilon)$$

$$\sum_{\nu'\nu\nu_1} \bar{H}^*(\lambda_1\ell_1\nu'\nu_1)\bar{H}(\lambda\ell\nu'\nu)C(\lambda_1 j_{\nu_1} j_{\nu'};\epsilon,-\tfrac{1}{2})C(\lambda j_\nu j_{\nu'};\epsilon,-\tfrac{1}{2}). \tag{20}$$

The second line agrees with (11) upon using (17) and setting the $m=\frac{1}{2}$ term equal to the $m=-\frac{1}{2}$ term.

On splitting the $\epsilon$ sum into positive and negative values,

$$V_j(\lambda_1\lambda\ell_1\ell)=\frac{1}{2}\sum_{\epsilon\geq 0} (-1)^{\epsilon+1}(2-\delta_{\epsilon 0})\ [C(\lambda_1\lambda j;-\epsilon\epsilon)\varphi(\lambda_1\lambda\ell_1\ell\epsilon)$$

$$+C(\lambda_1\lambda j;\epsilon,-\epsilon)\varphi(\lambda_1\lambda\ell_1\ell,-\epsilon)]. \tag{21}$$

Going back to (11), a change of size of $\epsilon$ (when accompanied by a change in the name of the dummy variable from m to -m), simply introduces a phase factor of (-1) to the power

$$(\lambda_1+j_{\nu_1}-j_{\nu'})-(j_{\nu_1}+\tfrac{1}{2}-\ell_{\nu_1})-(\lambda+j_\nu-j_{\nu'})+(j_\nu+\tfrac{1}{2}-\ell_\nu)=\lambda_1-\lambda+\ell_{\nu_1}-\ell_\nu \tag{22}$$

for $\varphi$ and of $\lambda+\lambda_1-j$ for the Clebsch-Gordan coefficient. In view of (15) and (16), the two terms in the bracket of (21) are equal and

$$V_j(\lambda_1\lambda\ell_1\ell)= \sum_{\epsilon\geq 0} (-1)^{\epsilon+1}(2-\delta_{\epsilon 0})C(\lambda_1\lambda j;-\epsilon\epsilon)\varphi(\lambda_1\lambda\ell_1\ell\epsilon). \tag{23}$$

On defining

$$H(\lambda\ell\nu'\nu)=C(\lambda j_{\nu'} j_\nu;0\tfrac{1}{2})\ [G_{\ell\lambda}(\nu',-\nu)K_\ell(\nu'\nu)-G_{\ell\lambda}(-\nu',\nu)K_\ell(\nu\nu')], \tag{24}$$

there results

$$\mathrm{Re}[\varphi(\lambda_1\lambda\ell_1\ell\epsilon)]=(-1)^{\lambda+\lambda_1}(1/3)(2\ell+1)(2\ell_1+1)\bar{\varphi}(\lambda_1\lambda\ell_1\ell\epsilon) \tag{25}$$

where

$$\bar{\varphi}(\lambda_1\lambda\ell_1\ell\epsilon) =\sum_{\nu'\nu\nu_1} (2j_{\nu'}+1)H(\lambda_1\ell_1\nu'\nu_1)H(\lambda\ell\nu'\nu)i^{\ell_\nu-\ell_{\nu_1}+\ell-\ell_1}\cos(\delta_\nu-\delta_{\nu_1})$$

$$C(\lambda_1 j_{\nu'} j_{\nu_1};\epsilon,-\epsilon+\tfrac{1}{2})C(\lambda j_\nu j_{\nu'};\epsilon,-\epsilon+\tfrac{1}{2}) \tag{26}$$

making use of the fact that

$$\ell_\kappa - \ell_{\kappa_1} + \ell - \ell_1 = (\ell_\kappa + \ell + \ell_{-\kappa}) - (\ell_{\kappa_1} + \ell_1 + \ell_{-\kappa'}) = \text{even integer} \qquad (27)$$

whence i to this power is real.

## VI. ASYMPTOTIC EVALUATION OF MATRIX ELEMENT TAILS

If the potential can be neglected beyond r = a (i.e. if the error in the phase shift from truncating the potential at r = a is small), the wavefunctions for r > a are given analytically by

$$F_\kappa = S(\kappa)\left[(E-1)/k\right]^{1/2} kr\left[\cos\delta_\kappa\, j_{\ell(-\kappa)}(kr) - \sin\delta_\kappa\, y_{\ell(-\kappa)}(kr)\right], \qquad (1)$$

$$G_\kappa = \left[(E+1)/k\right]^{1/2}\left[\cos\delta_\kappa\, j_{\ell(\kappa)}(kr) - \sin\delta_\kappa\, y_{\ell(\kappa)}(kr)\right]. \qquad (2)$$

The tail of the matrix element (the integral from r = a to infinity) then reduces to an integral over a product of spherical Bessel and Neumann functions which, in principle, can be carried out analytically.

The spherical Bessel or Neumann functions can be written as sines and cosines times polynomials in inverse powers of r (the order of the Bessel function determining the order of the polynomial). The resultant integrals can be reduced to sums of sine and cosine integrals of various orders. Formally, this leads to a closed solution. In practical terms, however, it is unsatisfactory because a large number of terms occur which are of comparable magnitude and varying sign, casting doubt on the ultimate precision.

It is simpler and safer to invoke from the start the fact that the matrix element tail calculation is intended for large r and use asymptotic values for the wavefunctions and asymptotic evaluation of the integrals. Explicitly, keeping the two leading terms in the asymptotic expansion,[13]

$$j_\ell(z) = z^{-1}\sin(z-\ell\pi/2) + \ell(\ell+1)(2z^2)^{-1}\cos(z-\ell\pi/2), \qquad (3)$$

$$y_\ell(z) = -z^{-1}\cos(z-\ell\pi/2) + \ell(\ell+1)(2z^2)^{-1}\sin(z-\ell\pi/2). \qquad (4)$$

The wavefunctions take the form (apart from a numerical factor)

$$kr[\cos\delta_\ell\, j_\ell(kr) - \sin\delta_\ell\, y_\ell(kr)] \sim$$

$$\sin(kr+\delta_\ell - \ell\pi/2) + \ell(\ell+1)(2kr)^{-1}\cos(kr+\delta_\ell - \ell\pi/2). \qquad (5)$$

Consistently, when the integrand is formed by a product of such expressions the terms of order higher than the second in $1/r$ are discarded. Elementary trigonometric manipulation then allows the integrand to be expressed as a sum of single sines or cosines times $r^{-1}$ or $r^{-2}$. The integrals are then carried out by integration-by-parts in the direction of increasing inverse powers of r, again stopping after two terms. The basic integral is

$$\int_a^\infty \frac{\sin(kr+\phi)}{r^n}\, dr = \frac{\cos(ka+\phi)}{k\, a^n} + \frac{n\,\sin(ka+\phi)}{k^2 a^{n+1}}, \qquad (6)$$

with neglect of terms of order $a^{-n-2}$, where n = 1 or 2.

## VII. PHASE OF COULOMB WAVEFUNCTIONS

The continuum solution of the Dirac equation for a Coulomb field contains an ambiguity of $\pi$ in the phase shift. In computing matrix elements for electromagnetic interactions, it is necessary to adhere to a consistent convention for the phase. Since there is an established sign convention for the free particle solution, it provides a suitable calibration.

The relative phase of the two radial functions is well-defined, so it is sufficient to examine only the "large" component. The Coulomb function, normalized on the energy scale, is

$$G_\kappa = \frac{|\Gamma(\gamma+i\nu)|e^{\nu\pi/2}(E+1)^{1/2}(2kr)^\gamma}{2\Gamma(2\gamma+1)(\pi k)^{1/2}} \left[e^{-ikr+i\eta}(\gamma+i\nu)_1F_1(\gamma+1+i\nu, 2\gamma+1;2ikr) + c.c.\right] \quad (1)$$

$$\text{with } \exp(2i\eta) = -(\kappa-i\nu/E)/(\gamma+i\nu) \quad (2)$$

$$\text{and} \quad \nu = (E/k)(\alpha Z),\ \gamma = (\kappa^2-\alpha^2Z^2)^{1/2}. \quad (3)$$

The corresponding free particle function is

$$G^o_\kappa = (E+1)^{1/2}(\pi k)^{-1/2} kr\, j_{\ell(\kappa)}(kr). \quad (4)$$

It is desired to fix the choice of the square root of Eq. 2 to be used for $\exp(i\eta)$ by requiring that Eq. 1 reduce to Eq. 4 in the limit as Z goes to zero (causing the potential to vanish).

As $Z \longrightarrow 0$, $\nu \longrightarrow 0$, and $\gamma \longrightarrow |\kappa|$. With these, Eq. 2 reduces to $-\kappa/|\kappa|$. By Kummer's transformation,[9]

$$_1F_1(|\kappa|+1,2|\kappa|+1;-2ikr) = \exp(-2ikr)\ _1F_1(|\kappa|,2|\kappa|+1;2ikr). \quad (5)$$

Factoring $\exp(-i\eta)$ out of Eq. 1 and letting $\exp(2i\eta) = -\kappa/|\kappa|$ :

$$G_\kappa \longrightarrow \frac{\Gamma(|\kappa|)}{4\Gamma(2|\kappa|)} \left(\frac{E+1}{\pi k}\right)^{1/2} (2kr)^{|\kappa|} e^{-i\eta - ikr} \left[-\frac{\kappa}{|\kappa|} {}_1F_1(|\kappa|+1, 2|\kappa|+1; 2ikr)\right.$$

$$\left. + {}_1F_1(|\kappa|, 2|\kappa|+1; 2ikr)\right]. \qquad (6)$$

For $\kappa < 0$, the expression in brackets is[9]

$${}_1F_1(|\kappa|+1, 2|\kappa|+1; 2ikr) + {}_1F_1(|\kappa|, 2|\kappa|+1; 2ikr) = 2\,{}_1F_1(|\kappa|, 2|\kappa|; 2ikr) \qquad (7)$$

while $\ell(\kappa) = |\kappa| - 1$ and

$$kr\, j_{|\kappa|-1}(kr) = \frac{\pi^{1/2}}{\Gamma(|\kappa|+1/2)} \left(\frac{kr}{2}\right)^{|\kappa|} e^{-ikr}\, {}_1F_1(|\kappa|, 2|\kappa|; 2ikr). \qquad (8)$$

Using the doubling formula[9]

$$\Gamma(2|\kappa|) = 2^{2|\kappa|-1} \pi^{-1/2} \Gamma(|\kappa|)\Gamma(|\kappa| + 1/2), \qquad (9)$$

the limit reduces to

$$G_{-|\kappa|} \longrightarrow \exp(-i\eta)\, (E+1)^{1/2}\, (\pi k)^{-1/2}\, kr\, j_{|\kappa|-1}(kr). \qquad (10)$$

Comparing with Eq. 4, the correct limit is $\exp(i\eta) \longrightarrow 1$.

For $\kappa > 0$, the expression in brackets is[9]

$${}_1F_1(\kappa+1, 2\kappa+1; 2ikr) - {}_1F_1(\kappa, 2\kappa+1; 2ikr) = 2ikr\, {}_1F_1(\kappa+1, 2\kappa+2; 2ikr)/(2\gamma+1) \qquad (11)$$

while $\ell(\kappa) = \kappa$. The limit then reduces to

$$G_{|\kappa|} \longrightarrow -i \exp(-i\eta)(E+1)^{1/2} (\pi k)^{-1/2}\, kr\, j_{|\kappa|}(kr). \qquad (12)$$

The equivalence now yields $\exp(i\eta) \longrightarrow -i$.

Splitting $\exp(2i\eta)$ into real and imaginary parts,

$$\cos 2\eta = (-\kappa\gamma + \nu^2/E)/(\gamma^2+\nu^2) = 2\cos^2\eta - 1, \qquad (13)$$

$$\sin 2\eta = \nu(\kappa + \gamma/E)/(\gamma^2+\nu^2) = 2 \sin\eta \cos\eta. \qquad (14)$$

Thus, with $\epsilon = +1$ or $-1$,

$$\cos\eta = \epsilon[(1+\cos 2\eta)/2]^{1/2}, \qquad (15)$$

$$\sin\eta = \sin 2\eta/(2\cos\eta). \qquad (16)$$

If Eqs. 15 and 16 are used to compute $\exp(i\eta)$, the phase convention is given by specifying $\epsilon$. This choice is determined by the $Z \longrightarrow 0$ limits obtained above.

For $\kappa < 0$, the limit is $\cos \eta \longrightarrow 1$, so $\epsilon = 1$. For $\kappa > 0$, the limit yields $\cos \eta \longrightarrow 0$ (which leaves the sign undetermined) and $\sin \eta \longrightarrow -1$. Since $|\kappa| > |\kappa|\ /E > \gamma/E$, the sign of $\sin 2\eta$ is unaffected by E; for electrons, it is the same as that of $\kappa$. For $\kappa > 0$, then, $\sin 2\eta > 0$ while $\sin \eta < 0$, so $\cos \eta < 0$, and $\epsilon = -1$. Positron wave functions are obtained by taking Z negative, hence $\nu$ negative. The sign of $\sin 2\eta$ then reverses, and $\epsilon = 1$ for $\kappa > 0$. Combining the results, the prescription for using Eqs. 15 and 16 is:

electrons: $\epsilon = -\kappa/|\kappa|$,

positrons: $\epsilon = 1$.

The relation between positron and electron phases is

$$(e^{i\eta})_{pos} = - \frac{\kappa}{|\kappa|} (e^{-i\eta})_{el}. \qquad (17)$$

In the limit of small kinetic energy ($k \longrightarrow 0$), $\nu$ becomes infinite and $\exp(2i\eta) \longrightarrow 1$. For an electron, then, $\exp(i\eta) = -\kappa/|\kappa|$. The limit is meaningless for a positron, as its wavefunction then tends to a delta function at infinity.

## VIII. ZERO KINETIC ENERGY LIMIT OF COULOMB WAVEFUNCTION

The "small" component Coulomb wavefunction is

$$F_\kappa = \frac{i\,|\Gamma(\gamma+i\nu)|\,e^{\nu\pi/2}(E-1)^{1/2}(2kr)^\gamma}{2\Gamma(2\gamma+1)(\pi k)^{1/2}}\,[e^{-ikr+i\eta}(\gamma+i\nu)_1F_1(\gamma+1+i\nu;2\gamma+1;2ikr)-c.c.]. \quad (1)$$

In the limit of vanishing kinetic energy ($k \longrightarrow 0$), $\nu = E\alpha Z/k$ goes to infinity (through positive values for an electron, negative for a positron). Going to the limit on the various factors:[13]

$$\lim_{|\nu|\longrightarrow\infty} (2\pi)^{-1/2}\,|\Gamma(\gamma+i\nu)|\,e^{|\nu|\pi/2}\,|\nu|^{1/2-\gamma} = 1. \quad (2)$$

$$\lim_{a\longrightarrow\infty} {}_1F_1(a,b;-z/a)/\Gamma(b) = z^{(1/2)(1-b)}J_{b-1}(2\,z^{1/2}) \quad (3)$$

yields, with

$$a = \gamma+1+i\nu, \qquad b = 2\gamma+1,$$

$$z = -2ikr\,(\gamma+1+i\nu) \approx 2\,\alpha\,Zr,$$

$$\lim_{\nu\longrightarrow\infty} {}_1F_1(\gamma+1+i\nu,2\gamma+1;2ikr) = \Gamma(2\gamma+1)(2\,\alpha\,Zr)^{-\gamma}\,J_{2\gamma}\,[2(2\,\alpha\,Zr)^{1/2}]. \quad (4)$$

Inasmuch as the source reference did not establish the validity of this result when a increases through imaginary rather than real values, it was verified by writing out the confluent hypergeometric series and going to the limit term by term.

$$[E-1]^{1/2} = [(k^2+1)^{1/2}-1]^{1/2} \approx [(1+k^2/2)-1]^{1/2} = 2^{-1/2}k \quad (5)$$

$$(\gamma+i\nu) - c.c. = 2i\nu \approx 2i(\alpha\,Z/k) \quad (6)$$

$$\exp(-ikr+i\eta) \approx -\kappa/|\kappa| \text{ for an electron.} \quad (7)$$

Combining these results, the electron wavefunction ($\nu > 0$) is

$$F_\kappa = (\kappa/|\kappa|)\,(\alpha\,Z)^{1/2}\,J_{2\gamma}\,[2(2\,\alpha\,Zr)^{1/2}]. \quad (8)$$

For $G_\kappa$, the analogous procedure becomes more complicated because there occurs

$$(\gamma+i\nu) + \text{c.c.} = 2\gamma, \tag{9}$$

so that a term involving $\nu$ times the second term in the limiting expression for the confluent hypergeometric function must be included. It is simpler to resort to the differential equation:

$$F_\kappa' - (\kappa/r)F_\kappa = -(E-V-1)G_\kappa \approx -(\alpha Z/r)G_\kappa . \tag{10}$$

$$F_\kappa' = (\kappa/|\kappa|)(\alpha Z)^{1/2}\,(d/dr)\,J_{2\gamma}\,[2(2\alpha Zr)^{1/2}] \tag{11}$$

$$= (\kappa/|\kappa|)(\alpha Z)^{1/2}(2\alpha Z/r)^{1/2}\left\{ J_{2\gamma-1}[2(2\alpha Zr)^{1/2}] - \gamma(2\alpha Zr)^{-1/2}J_{2\gamma}[2(2\alpha Zr)^{1/2}] \right\}.$$

$$G_\kappa = -(\kappa/|\kappa|)(\alpha Z)^{-1/2}\left\{(2\alpha Zr)^{1/2}J_{2\gamma-1}[2(2\alpha Zr)^{1/2}] - (\gamma+\kappa)J_{2\gamma}[2(2\alpha Zr)^{1/2}]\right\}. \tag{12}$$

In the positron case ($\nu < 0$), the exponentials no longer cancel, but lead instead to a factor $\exp(-|\nu|\pi)$ which tends to zero. Thus, the positron wavefunction vanishes. Actually, the limits were attained while holding r fixed and finite, and the wave function behaves as a delta function at infinity. The physical explanation is that the positron is repelled by the (positive charge) Coulomb center of force, and can only approach it to the extent that its momentum can overcome the repulsion; as the kinetic energy goes to zero, so does the probability of the positron being within a finite distance of the center of force.

The matrix elements for Bremsstrahlung involve in the integrand a product of initial and final Coulomb wave functions. For a positron, the overlap vanishes as the kinetic energy of the positron after interaction goes to zero. Thus, while an electron can give up essentially all its kinetic energy to the photon in Bremsstrahlung, a positron cannot. On the other hand, the positron can lose all of its energy (including rest energy) through annihilation to photons.

## IX. STARTING CONDITIONS FOR INTEGRATION

Near the origin the screened nuclear potential has the form $V \approx C + Ze^2/r$, where C is a constant contributed by the potential of the electrons. If this relation is substituted into (Chapter II, Eq. 7) the coupled equations become

$$\left.\begin{aligned} F' - \frac{\kappa}{r} F + \frac{Ze^2}{r} G + (E_o - 1) G = 0 \\ G' + \frac{\kappa}{r} G - \frac{Ze^2}{r} F + (E_o + 1) F = 0 \end{aligned}\right\}, \tag{1}$$

where $E_o = E + C$. These equations, which are essentially radial equations with a pure Coulomb potential, provide a means of obtaining the form of the wavefunction and its derivative near the origin.

In (1) use will be made of the operator notation

$$r^n \frac{d^n}{dr^n} = \delta(\delta-1) \cdots\cdot (\delta-n+1). \tag{2}$$

This is done for convenience since it can be shown that

$$f(\delta) r^n = f(n) r^n. \tag{3}$$

Thus, when (1) is multiplied through by r and the operator notation is used, the coupled equations become

$$\left.\begin{aligned} \delta F - \kappa F + Ze^2 G + (E_o - 1) rG = 0 \\ \delta G + \kappa G - Ze^2 F - (E+1) rF = 0 \end{aligned}\right\}. \tag{4}$$

Now substitute

$$\left.\begin{aligned} G = \sum_{\ell=0}^{\infty} a_\ell r^{\ell+\gamma} \\ F = \sum_{\ell=0}^{\infty} b_\ell r^{\ell+\gamma} \end{aligned}\right\} \tag{5}$$

into (4) and use (3) to get

$$[(\gamma+\kappa)a_o - Ze^2 b_o]r^\gamma + \sum_{\ell=1}^{\infty} [(\ell+\gamma)a_\ell + \kappa a_\ell - Ze^2 b_\ell - (E_o+1)b_{\ell-1}]r^{\ell+\gamma} = 0$$

$$[(\gamma-\kappa)b_o + Ze^2 a_o]r^\gamma + \sum_{\ell=1}^{\infty} [(\ell+\gamma)b_\ell - nb_\ell + Ze^2 a_\ell + (E_o-1)a_{\ell-1}]r^{\ell+\gamma} = 0. \quad (6)$$

When the coefficient of each power of r is set equal to zero in (6), then the relationship between the coefficients of (5) is established. The relationship between the first few coefficients is given by the following equations:

$$a_o = \frac{Ze^2}{\gamma+\kappa} b_o, \quad (7)$$

$$b_o = \frac{Ze^2}{\kappa-\gamma} a_o, \quad (8)$$

with

$$\gamma = \left|(\kappa^2 - Z^2e^4)^{1/2}\right| \quad (9)$$

and

$$a_1 = -b_o \left[\frac{(\kappa-\gamma-1)(E_o-1) + (\kappa-\gamma)(E_o+1)}{1+2\gamma}\right], \quad (10)$$

$$b_1 = -a_o \left[\frac{(\kappa+\gamma+1)(E_o-1) + (\kappa+\gamma)(E_o+1)}{1+2\gamma}\right]. \quad (11)$$

The positive square root in (9) is taken so the wavefunctions will be finite at the origin.

For Z close to zero, the denominator in (7) is small for $\kappa<0$ while the denominator of (8) is small for $\kappa>0$. Thus, in general, to make the program applicable for all Z, the procedure adopted for selecting the coefficients was to choose $b_o$ and use (7) to obtain $a_o$ when $\kappa>0$, and to choose $a_o$ and use (8) to obtain $b_o$ when $\kappa<0$.

Since the wavefunction and its first derivative are both zero at the origin, as can be seen from (5) through (11), there is difficulty with starting the numerical integration. This trouble can be circumvented by making a transformation to the functions

$$\left.\begin{aligned} G_o &= r^{-\gamma} G \\ F_o &= r^{-\gamma} F \end{aligned}\right\} \tag{12}$$

which satisfy the equations

$$\left.\begin{aligned} F_o' + \frac{(\gamma-\kappa)}{r} F_o + (E-V-1)G_o &= 0 \\ G_o' + \frac{(\gamma+\kappa)}{r} G_o - (E-V+1)F_o &= 0 \end{aligned}\right\} . \tag{13}$$

Thus, at the origin,

$$\left.\begin{aligned} G_o &= a_o \quad , \quad F_o = b_o, \\ G_o' &= a_1 \quad , \quad F_o' = b_1 . \end{aligned}\right\} \quad r = 0 \tag{14}$$

The procedure is to integrate (13) out to some convenient radius (e.g. $r = 1$) and then transform to (Chapter II, Eq. 7).

## X. PHASE SHIFTS (NON-COULOMB)

The free particle solution to (Chapter II, Eq. 7) is required to determine the normalization and phase shift for the numerical solution of the radial equation. These are obtained from (Chapter II, Eq. 7) with V=0 as

$$G_f = \sqrt{\frac{E+1}{\pi k}}\ kr\ j_{\ell_\kappa}(kr) \sim \sqrt{\frac{E+1}{\pi k}}\ \sin\left(kr - \frac{\ell_\kappa \pi}{2}\right)$$

$$F_f = \sqrt{\frac{E-1}{\pi k}}\ \frac{\kappa}{|\kappa|}\ kr\ j_{\ell_{-\kappa}}(kr) \sim \sqrt{\frac{E-1}{\pi k}}\ \cos\left(kr - \frac{\ell_\kappa \pi}{2}\right), \tag{1}$$

where $j_\ell$ is a spherical Bessel function. Also required are the two new functions S(r) and C(r) which are defined by the equations

$$G = \sqrt{\frac{E+1}{E-1}}\ S\,F_f + C G_f \sim \sqrt{\frac{E+1}{\pi k}}\left[\sin\delta_\kappa \cos\left(kr - \frac{\ell_\kappa \pi}{2}\right) + \cos\delta_\kappa \sin\left(kr - \frac{\ell_\kappa \pi}{2}\right)\right]$$

$$F = C\,F_f - \sqrt{\frac{E-1}{E+1}}\ S G_f \sim \sqrt{\frac{E-1}{\pi k}}\left[\cos\delta_\kappa \cos\left(kr - \frac{\ell_\kappa \pi}{2}\right) - \sin\delta_\kappa \sin\left(kr - \frac{\ell_\kappa \pi}{2}\right)\right]. \tag{2}$$

From the asymptotic forms given in Chapter III, Eqs. 13 and 14 one can deduce

$$\left.\begin{aligned} C(r) &\sim \cos\delta_\kappa \\ S(r) &\sim \sin\delta_\kappa \end{aligned}\right\}, \tag{3}$$

$$C^2(r) + S^2(r) \sim 1. \tag{4}$$

If $G_N$ and $F_N$ are the numerical solutions to the radial wave equations, they will not be properly normalized because of the arbitrary selection of one constant in the starting conditions. (The procedure is to start with the normalization appropriate to a pure Coulomb potential.) Thus they will differ from the correct solution by a normalization constant N such that $F=NF_N$ and $G=NG_N$. Substitution of these equations into (2) yields

$$S(r) = N \frac{\left( \frac{G_N}{\sqrt{E+1}} \frac{F_f}{\sqrt{E-1}} - \frac{F_N}{\sqrt{E-1}} \frac{G_f}{\sqrt{E+1}} \right)}{\left( \frac{F_f^2}{E-1} + \frac{G_f^2}{E+1} \right)} \tag{5}$$

$$C(r) = N \frac{\left( \frac{G_N G_f}{E+1} + \frac{F_N F_f}{E-1} \right)}{\left( \frac{F_f^2}{E-1} + \frac{G_f^2}{E+1} \right)}$$

Upon completion of the numerical integration, Eqs. 4 and 5 are used to determine the phase shifts.

## XI. W.K.B. APPROXIMATION AND NORMALIZATION

The radial equations can be combined into the second order equation

$$G_\kappa'' + (E-V+1)^{-1}V'G_\kappa' + \left\{ (E-V)^2-1-[\kappa(\kappa+1)/r^2]+(\kappa/r)(E-V+1)^{-1}V' \right\} G_\kappa=0. \quad (1)$$

To get a form appropriate for a W.K.B. treatment, the first derivative term must be eliminated. This is achieved by the change of dependent variable

$$R_\kappa(r) = (E-V+1)^{-1/2}\, G_\kappa(r) \quad (2)$$

which results in

$$R_\kappa'' + \left[ -\frac{V''}{2(E-V+1)} - \frac{3}{4}\frac{V'^2}{(E-V+1)^2} + \frac{\kappa}{r}\frac{V'}{E-V+1} + (E-V)^2-1-\frac{\kappa(\kappa+1)}{r^2}\right] R_\kappa=0. \quad (3)$$

This can now be assumed of the form

$$R_\kappa'' + p^2(r)\, R_\kappa = 0 \quad (4)$$

for r sufficiently large that the quantity in brackets is positive. The formal analogy with the non-relativistic solution can be extended by writing

$$p^2(r) = k^2-U(r)-\ell_\kappa(\ell_\kappa+1)/r^2, \quad (5)$$

so that the known W.K.B. approximation of the more familiar case can be taken over. using the "equivalent potential" U(r). For this purpose, note that

$$\kappa(\kappa+1) = \ell_\kappa(\ell_\kappa+1), \quad (6)$$

$$(E-V)^2-1 = k^2-2EV+V^2, \quad (7)$$

so that

$$U(r) = (1/2)V''(E-V+1)^{-1}+(3/4)V'^2(E-V+1)^{-2}-(\kappa/r)V'(E-V+1)^{-1}+2EV-V^2. \quad (8)$$

The W.K.B. solution is

$$R_\kappa = (\pi p)^{-1/2} \sin\left(\int p\, dr + \delta_\kappa\right), \quad (9)$$

with the normalization set by comparison with the asymptotic value of the exact solution for $G_\kappa$.

The numerical solution of the exact radial equations yields unnormalized wavefunctions. The normalization is obtained by proceeding out to an r sufficiently large that the asymptotic form of the wavefunction is attained, and setting the normalization by comparison with the known normalized asymptotic wavefunction. This usually means that, for the sake of ascertaining the normalization, the numerical integration has to be carried well past the values of r necessary for the evaluation of the matrix element integrals.

For a well-behaved potential, the W.K.B. solution will satisfactorily approximate the exact wavefunction long before the asymptotic region is reached. This suggests the alternative approach of obtaining the normalization by comparing the numerical unnormalized wavefunction with the W.K.B. solution. The procedure then becomes that of carrying out the numerical solution as far as it is needed for the evaluation of the matrix elements. At the cut-off radius, the wave matching is then carried out as described below. Note that the normalization must precede correction of the matrix elements for the tail contribution (Chapter VI).

Denoting by $\bar{R}_\nu$ the unnormalized numerical solution of the exact equations for $R_\nu$ and by A the associated normalization constant, matching $\bar{R}_\nu$ to the W.K.B. solution yields

$$\bar{R}_\nu = A(\pi p)^{-1/2} \sin \left( \int p \, dr + \delta_\nu \right). \tag{10}$$

If the W.K.B. solution is a reasonable approximation at the value of r being considered, the derivatives can also be matched:

$$\bar{R}'_\nu = -(p'/2p)\, \bar{R}_\nu + A(\pi p)^{-1/2} \, p \cos \left( \int p \, dr + \delta_\nu \right), \tag{11}$$

or more conveniently,

$$A(\pi p)^{-1/2} \cos\left(\int p\,dr + \delta_\kappa\right) = p^{-1}\,\bar{R}_\kappa' + (p'/2p^2)\,\bar{R}_\kappa . \qquad (12)$$

Squaring and summing Eqs. 10 and 12,

$$A^2 = \pi p \left\{ \bar{R}_\kappa^2 + \left[p^{-1}\bar{R}_\kappa' + (p'/2p^2)\,\bar{R}_\kappa\right]^2 \right\} . \qquad (13)$$

For an r below the validity limit for the W.K.B. approximation, the above expression for $\bar{R}_\kappa$ can still be used provided that A and $\delta_\kappa$ are considered functions of r instead of constants. When both are allowed to vary, the description is underdetermined. The resultant freedom permits an arbitrary choice of a supplementary relation. A legitimate choice is to require that $\bar{R}_\kappa'$ retain the form given above, i.e. that the additional terms obtained on differentiating the expression for $\bar{R}_\kappa$ cancel:

$$A' \sin\left(\int p\,dr + \delta_\kappa\right) + A\,\delta_\kappa' \cos\left(\int p\,dr + \delta_\kappa\right) = 0. \qquad (14)$$

The expression given for $A^2$ is then still valid, but the value obtained may vary with r. The normalization constant has been attained, then, if $|dA/d(kr)| \ll |A|$ for all r above the value in question. To obtain A', differentiate Eq. 12:

$$A' \cos\left(\int p\,dr + \delta_\kappa\right) - A\,p \sin\left(\int p\,dr + \delta_\kappa\right) - A\,\delta_\kappa' \sin\left(\int p\,dr + \delta_\kappa\right)$$

$$= \pi^{1/2} p^{-1/2} \bar{R}_\kappa'' + (\pi^{1/2}/2)\,\bar{R}_\kappa \left[p'' p^{-3/2} - (3/2) p'^2 p^{-5/2}\right]. \qquad (15)$$

Substituting Eqs. 4 and 10,

$$\pi^{1/2} p^{-1/2} \bar{R}_\kappa'' = -\pi^{1/2} p^{3/2} \bar{R}_\kappa = -Ap \sin\left(\int p\,dr + \delta_\kappa\right). \qquad (16)$$

Using also Eq. 14,

$$A' \cos\left(\int p\,dr + \delta_\kappa\right) - A\,\delta_\kappa' \sin\left(\int p\,dr + \delta_\kappa\right) = A'/\cos\left(\int p\,dr + \delta_\kappa\right)$$

$$= A \sin\left(\int p\,dr + \delta_\kappa\right)\left[(1/2)\,p'' p^{-2} - (3/4) p'^2 p^{-3}\right]. \qquad (17)$$

To eliminate the masking effect of oscillations of the sinusoidal factor, note that

$$\left|\sin\left(\int p\,dr + \delta_\mu\right)\cos\left(\int p\,dr + \delta_\mu\right)\right| \leq 1/2. \qquad (18)$$

The relation $k^{-1}|A'| \ll A$ then reduces to

$$(8kp^3)^{-1}\left|2p''p-3p'^2\right| \ll 1. \qquad (19)$$

It should be noted that the procedure outlined results in the evaluation of the normalization factor while leaving the phase shift undetermined. In principle, the W.K.B. approximation can also be used to compute the phase shift. This requires, however, the evaluation of $\int p\,dr$ out to infinity (or at least to the asymptotic region) and this has to be done numerically because of the complicated expression for p.

The W.K.B. approximation as applied to the normalization of the wavefunctions requires an expression involving the potential and its first three derivatives. For a screened potential, which is known only numerically, computation of these derivatives by differencing would be unreliable. Instead, use is made of the fact that the screening factor (ratio of screened to unscreened potential) is nearly exponential. The exponent appropriate to the radius at which the numerical integration stops is obtained by taking the logarithm of the ratio of the screening factor at that radius to the screening factor at a slightly larger radius. The analytical form of the screening factor thus arrived at is then used to calculate the derivatives. This procedure has been used to obtain the normalization of the wavefunctions in the screened case.

## XII. ELECTROSTATIC POTENTIAL AND SELF-CONSISTENT FIELD CALCULATIONS

The electrostatic potential of a spherically symmetric charge distribution of an atom is given by:

$$V(r) = \frac{4\pi}{r} \int_0^r \rho(r')\, r'^2\, dr' + 4\pi \int_0^\infty \frac{\rho(r')}{r'}\, r'^2\, dr' \qquad (1)$$

where $\rho(r)$ is the volume charge density, r is the distance from the center of the charge distribution and $V(r)$ is the electrostatic potential. The units used here are those for which $\hbar=e=m=1$. Note that these atomic units differ from the natural units used in the cross section calculation. Different units have been chosen in this context to be consistent with the results of self-consistent field (SCF) calculations which will be used to obtain $\rho(r)$.

In terms of single electron orbitals, $\Psi_{n\ell}$, $\rho(r)$ is given by:

$$\rho(r) = \sum_{n\ell} 2(2\ell+1)\, \Psi^2_{n\ell} \qquad (2)$$

where n is the principal quantum number and $\ell$ is the orbital angular momentum quantum number. The cross terms in (2) have been eliminated by the angular intergrations in (1) which have already been made and are not shown. The "occupation" function $2(2\ell+1)$ shown in equation (2) is correct only for filled electron shells. For partially filled shells this must be reduced appropriately.

In performing SCF calculations, it is most convenient to solve for $P_{n\ell} = r\,\Psi_{n\ell}$ rather than $\Psi_{n\ell}$. In terms of $P_{n\ell}$, the expression for V becomes:

$$V(r) = \frac{4\pi}{r}\int_0^r \sum_{n\ell} \omega P^2_{n\ell}(r')dr' + 4\pi\int_r^\infty \sum_{n\ell} \omega \frac{P^2_{n\ell}(r')}{r'}\,dr' \quad (3)$$

where the symbol $\omega$ has been introduced to represent the occupation function.

The $P_{n\ell}$ functions are obtained from Hartree-Fock type of calculations[14]. These are essentially iterative solutions of the multi-electron wave equation obtained by first assuming a net potential, solving for the wavefunctions and then recalculating the potential. The process is repeated until self-consistency is achieved. The usual measure of self-consistency is the energy of the atomic state under consideration. This energy must be minimized.

The solutions are obtained either by numerical integration[15] or by expansion in suitable orthogonalized functions[16]. A computer code[16] which performs these calculations has been obtained and is now in production operation. This code calculates exponents and coefficients appropriate to finite expansions of the $P_{n\ell}$ functions in terms of "Slater orbitals":

$$P_{n\ell} = \sum_p \left[(2m_{\ell p})!\right]^{-\frac{1}{2}} C_{n\ell p}\,(2\xi_{\ell p})^{m_{\ell p}+\frac{1}{2}}\, r^{m_{\ell p}}\, e^{-\xi_{\ell p} r}\,. \quad (4)$$

Here $C_{n\ell p}$ and $\xi_{\ell p}$ are the constants obtained from the code and $m_{\ell p}$ are suitable integers. Methods for choosing $m_{\ell p}$ and making initial estimates of $C_{n\ell p}$ and $\xi_{\ell p}$ are given by Roothaan[16].

The integrals required in (3) are

$$I_1 = \frac{1}{r} \int_0^r \sum_{n\ell} \omega \, P_{n\ell}^2 \, (r') \, dr' \tag{5}$$

$$I_2 = \int_r^\infty \sum_{n\ell} \frac{\omega \, P_{n\ell}^2 \, (r')}{r'} \, dr'. \tag{6}$$

From (4),

$$P_{n\ell}^2 = \sum_{p,q} \left[(2m_{\ell p})!\right]^{-\frac{1}{2}} \left[(2m_{\ell q})!\right]^{-\frac{1}{2}} C_{n\ell p} \, C_{n\ell q} (2\xi_{\ell p})^{m_{\ell p}+\frac{1}{2}} (2\xi_{\ell q})^{m_{\ell q}+\frac{1}{2}} \, r^{(m_{\ell p}+m_{\ell q})}$$

$$\cdot \, e^{-(\xi_{\ell p}+\xi_{\ell q})\, r}. \tag{7}$$

Now (5) and (6) become:

$$I_1 = \sum_{n\ell} \omega_{n\ell} \sum_{p,q} \left[(2m_{\ell p})!(2m_{\ell q})!\right]^{-\frac{1}{2}} C_{n\ell p} \, C_{n\ell q} (2\xi_{\ell p})^{m_{\ell p}+\frac{1}{2}} (2\xi_{\ell q})^{m_{\ell q}+\frac{1}{2}}$$

$$\cdot \, \frac{1}{r} \int_0^r r'^{(m_{\ell p}+m_{\ell q})} \, e^{-(\xi_{\ell p}+\xi_{\ell q})r'} \, dr' \tag{8}$$

$$I_2 = \sum_{n\ell} \omega_{n\ell} \sum_{p,q} \left[(2m_{\ell p})!(2m_{\ell q})!\right]^{-\frac{1}{2}} C_{n\ell p} \, C_{n\ell q} \, (2\xi_{\ell p})^{m_{\ell p}+\frac{1}{2}} \, (2\xi_{\ell q})^{m_{\ell q}+\frac{1}{2}}$$

$$\int_r^\infty r'^{(m_{\ell p}+m_{\ell q}-1)} \, e^{-(\xi_{\ell p}+\xi_{\ell q})r'} \, dr'. \tag{9}$$

Two types of integrals appear in (8) and (9):

$$I_A(m,a) = \int_0^r x^m \, e^{-ax} \, dx \tag{10}$$

$$I_B(m,a) = \int_r^\infty x^m \, e^{-ax} \, dx \tag{11}$$

where m is always an integer and always ≥ 1. These integrals can be found in standard tables[17] and obey the recurrence relations:

$$I_A(m,a) = \frac{-r^m e^{-ar}}{a} + \frac{m}{a} I_A(m-1,a), \tag{12}$$

$$I_B(m,a) = \frac{r^m e^{-ar}}{a} + \frac{m}{a} I_B(m-1,a). \tag{13}$$

For m = 1:

$$I_A(1,a) = \frac{1}{a^2} \left[ 1 - (1 + ar)\, e^{-ar} \right], \tag{14}$$

$$I_B(1,a) = \frac{1}{a^2} \left[ (1 + ar)\, e^{-ar} \right]. \tag{15}$$

Starting with (14) and (15), values of $I_A$ and $I_B$ are obtained for any m using (12) and (13). This completes the analytic evaluation of the integrals.

As input, the code which has been written requires specification of all of the constants associated with (4) and specification of a radial grid on which the potential is to be calculated for use in the main cross section code. Suitable transformations are made so that both input and output of the potential code are in "natural units" although the actual calculation is done in "atomic units". The output consists of values of the screening factor (ratio of screened to Coulomb potential) as a function of r for the particular element. These are written in binary form on a library tape.

In the Bremsstrahlung program, the library tape is searched for the appropriate element, and a table of screening factors and radii is read in. The program interpolates on this table to obtain the potential at the current point. The tabulation is done in terms

of the screening factor because of its smooth behavior as a function of r. In this procedure, the SCF calculation is done once for each element, and can then serve for many Bremsstrahlung runs at different energies.

## XIII. ANGULAR DISTRIBUTIONS

The full description of the cross sections requires reconstituting the angular distributions from the Legendre coefficients, for unpolarized and linearly polarized photons. In addition, values of $\mu_q$ and $\mu_q^2$ averaged over the angular distributions give a compact characterization of these distributions (of value in some applications).

It has been decided to calculate the cross sections in units of

$$\bar{\sigma} = \alpha\, r_e^2\, Z(Z+1) \tag{1}$$

where Z is the nuclear charge, $r_e$ is the classical electron radius and $\alpha$ is the fine structure constant. These units have been chosen to make the results directly comparable with data generated with the Bethe-Heitler equation, in the form favored by Heitler[10], with the change $Z^2 \longrightarrow Z(Z+1)$ to correct it approximately for electron-electron Bremsstrahlung[2].

In terms of the unit $\bar{\sigma}$ for the cross section, Eq. 10 of Chapter IV becomes

$$\frac{d\sigma^j_{p'p}}{dy\, d\mu_q} = \frac{3\pi}{\alpha^2 Z(Z+1)} \frac{(E-1)}{(E+1)}\, y\, B_j(p'p). \tag{2}$$

In (2) energy variables have units of $mc^2$, momentum variables have units of mc, length variables have units of $\hbar/mc$, and $y=z(E-1)^{-1}$. For convenience, let

$$\sigma_A \equiv \sigma_{1,1} \tag{3a}$$

and

$$\sigma_B \equiv \sigma_{1,-1} \quad , \tag{3b}$$

then

$$\frac{d\sigma_A}{dy\, d\mu_q} = \sum_j \frac{d\sigma^j_A}{dy\, d\mu_q} P_j(\mu_q) \tag{4a}$$

and

$$\frac{d\sigma_B}{dy\, d\mu_q} = \sum_{j\geq 2} \frac{d\sigma^j_B}{dy\, d\mu_q} \left[(j+2)(j+1)j(j-1)\right]^{-\frac{1}{2}} P_{j,2}(\mu_q). \tag{4b}$$

To find the average values of $\mu_q$ and $\mu_q^2$ it will be necessary to derive an expression for

$$I = \int_{-1}^{+1} x^n \, P_{j,2}(x)dx. \tag{5}$$

This can be done using Rodrigues' expression

$$P_{j,2}(x) = (1-x^2) \, \frac{d^2P_j(x)}{dx^2} \, . \tag{6}$$

Inserting (6) into (5) and integrating by parts twice yields

$$I = (x^n - x^{n+2}) \, \frac{dP_j(x)}{dx} \Bigg|_{-1}^{+1} - \left[n\, x^{n-1} - (n+2)x^{n+1}\right] \, P_j(x) \Bigg|_{-1}^{+1} +$$

$$+ n(n-1) \int_{-1}^{+1} x^{n-2} \, P_j(x)dx - (n+2)(n+1) \int_{-1}^{+1} x^n \, P_j(x)dx. \tag{7}$$

The first term on the r.h. side of (7) is zero and the second term can be evaluated using

$$\left.\begin{aligned} P_j(1) &= 1 \\ P_j(-1) &= (-1)^j \end{aligned}\right\}. \tag{8}$$

The remaining integrals in (9) can be found using the relation[18]

$$B(n,j) \equiv \int_{-1}^{+1} x^n \, P_j(x)dx = \frac{n! \, \Gamma(\frac{n-j+1}{2})}{2^j (n-j)! \, \Gamma(\frac{n+j+3}{2})}, \quad \text{for } n \geq j \text{ and } n-j \text{ even or zero,}$$

$$= 0 \, , \quad \text{otherwise.} \tag{9}$$

Thus (7) reduces to

$$I = 4+n(n-1)B(n-2,j) - (n+2)(n+1)B(n,j), \text{for } n-j \text{ even or zero,}$$

$$= 0 \quad , \quad \text{otherwise.} \tag{10}$$

From (9) and (10) we have

$$\int_{-1}^{+1} P_{j,2}(x)dx = \begin{cases} 4 & j \text{ even and } \geq 2 \\ 0 & j \text{ odd} \end{cases} \tag{11a}$$

$$\int_{-1}^{+1} xP_{j,2}(x)dx = \begin{cases} 4 & j \text{ odd and } \geq 3 \\ 0 & j \text{ even} \end{cases} \tag{11b}$$

$$\int_{-1}^{+1} x^2P_{j,2}(x)dx = \begin{cases} 4/5 & j = 2 \\ 4 & j \text{ even and } \geq 4 \\ 0 & j \text{ odd} \end{cases} \tag{11c}$$

$$\int_{-1}^{+1} P_j(x)dx = 2\,\delta_{j,0} \tag{11d}$$

$$\int_{-1}^{+1} xP_j(x)dx = 2/3\,\delta_{j,1} \tag{11e}$$

and

$$\int_{-1}^{+1} x^2P_j(x)dx = 4/5\,\delta_{j,2} + 2/3\,\delta_{j,0} \tag{11f}$$

Since the cross section for circular polarization is one half that for unpolarized photons it will only be necessary to obtain expressions for one of these. In the following, the expression for unpolarized photons is given along with expression for linearly polarization states. With the use of (3), (4) and (11a) through (11f), the cross section which is differential with respect to y becomes

$$U = \frac{d\sigma}{dy} = 4\left(\frac{d\sigma_A^0}{dy\ d\mu_q}\right), \tag{12}$$

for unpolarized photons, and

$$P \equiv \frac{d\sigma}{dy} = 2\left(\frac{d\sigma_A^0}{dy\ d\mu_q}\right) + \cos 2\varphi \sum_{\substack{j\geq 2 \\ j \text{ even}}} 4\left(\frac{d\sigma_B^j}{dy\ d\mu_q}\right)\left[(j+2)(j+1)j(j-1)\right]^{-\frac{1}{2}}, \quad (13)$$

for polarized photons. The average $\mu_q$ is given by

$$\overline{\mu}_q = U^{-1}\frac{4}{3}\left(\frac{d\sigma_A^1}{dy\ d\mu_q}\right), \quad (14)$$

for unpolarized photons, and

$$\overline{\mu}_q = P^{-1}\left\{\frac{2}{3}\left(\frac{d\sigma_A^1}{dy\ d\mu_q}\right) + \cos 2\varphi \sum_{\substack{j\geq 3 \\ j \text{ odd}}} 4\left(\frac{d\sigma_B^j}{dy\ d\mu_q}\right)\left[(j+2)(j+1)j(j-1)\right]^{-\frac{1}{2}}\right\}, \quad (15)$$

for polarized photons. The average value of $\overline{\mu_q^2}$ is given by

$$\overline{\mu_q^2} = U^{-1}\frac{4}{3}\left(\frac{d\sigma_A^0}{dy\ d\mu_q}\right) + \frac{8}{5}\left(\frac{d\sigma_A^2}{dy\ d\mu_q}\right), \quad (16)$$

for unpolarized photons, and

$$\overline{\mu_q^2} = P^{-1}\left[\frac{2}{5}\left(\frac{d\sigma_A^0}{dy\ d\mu_q}\right) + \frac{4}{5}\left(\frac{d\sigma_A^2}{dy\ d\mu_q}\right) + \cos 2\varphi\left\{\frac{2}{5\sqrt{6}}\left(\frac{d\sigma_B^2}{dy\ d\mu_q}\right) + \sum_{\substack{j\geq 4 \\ j \text{ even}}} 4\left(\frac{d\sigma_B^j}{dy\ d\mu_q}\right)\left[(j+2)(j+1)j(j-1)\right]^{-\frac{1}{2}}\right\}\right] \quad (17)$$

for polarized photons.

The computer output presents values of the differential cross section at two-degree intervals of the polar angle. For the case of linear polarization, the polar angular distribution is also given at thirty degree intervals of $\varphi$. The output also includes an evaluation of (12) through (17).

## XIV. THE COMPUTER PROGRAM

The main routine (BREMS) sets up some numerical constants, reads the input parameters and checks them, then calls subroutines to do the bulk of the calculations, and finally computes the Legendre functions and puts together the cross sections and writes them out. All ordinary input/output is done in BREMS. Supplementary diagnostic and checkout output is now generated by some subroutines, but would not occur in production operation.

The structure of subroutine calls is schematized in Fig. 2.

The first subroutine called is SELECT. It starts from the input specification of the maximum orbital angular momenta to be considered, runs through the selection rules to determine what matrix elements will occur, and indexes these matrix elements and the corresponding quantum numbers.

If screening is to be considered, SETAPE scans the tape bearing the screening factors and finds the section of it containing the data for the required element.

FINTEG is the control subroutine for the radial matrix elements. It sets up the required arrays for the wavefunctions and matrix elements and their derivatives, computes their initial values and the coefficients of the differential equations, calls other subroutines to do the actual integrating, computes the phase shifts, then calls subroutines to normalize the matrix elements, asymptotically evaluate their tail, and form reduced matrix elements including an X-coefficient.

From the origin to r=1, the indicial behavior, $r^{\gamma}$, is factored out of the wavefunctions. The Runge-Kutta integration is performed by RKUTTA, which calls DIRAC to supply the derivatives from the differential equations. For larger r, the wavefunctions are used directly; the

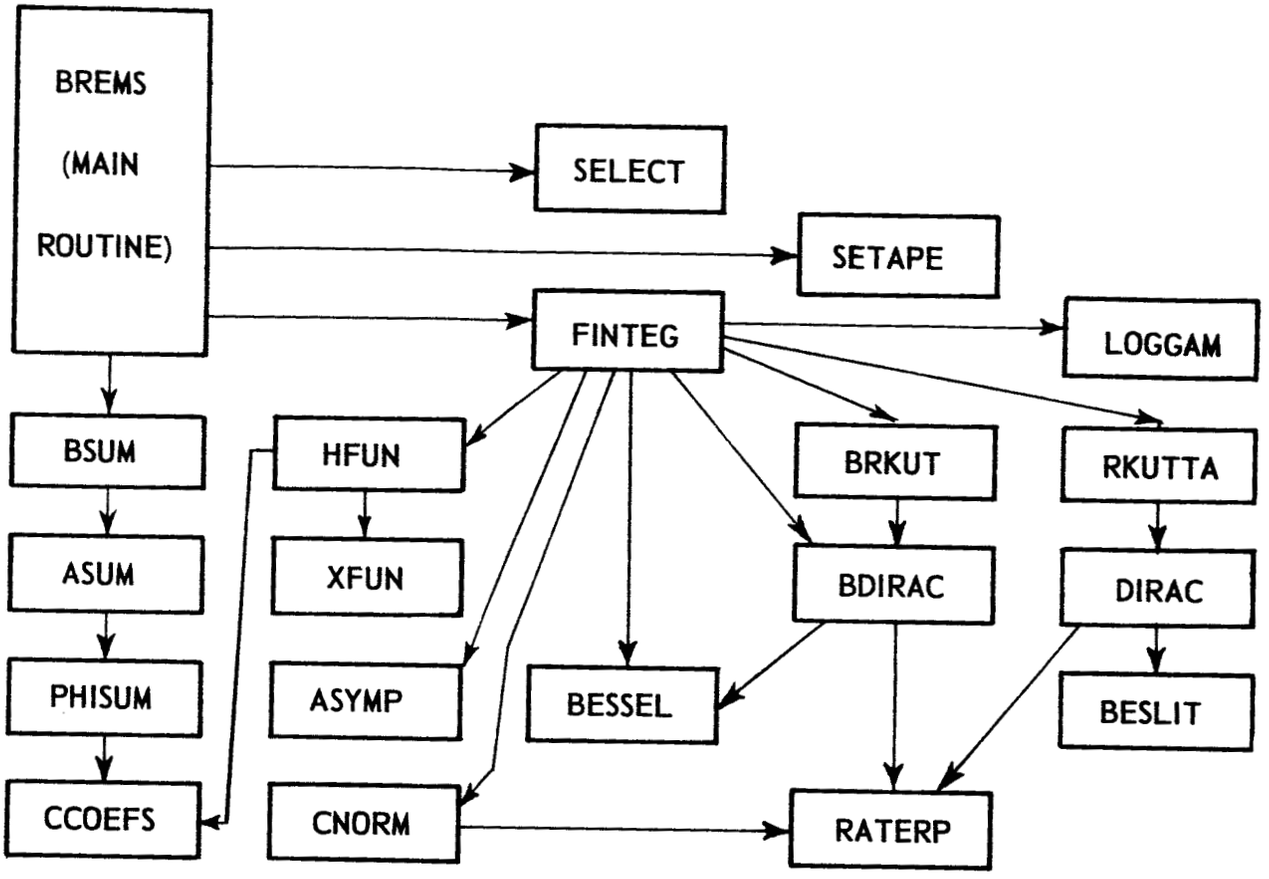


**FIGURE 2 CALLING SEQUENCES**

This flow-chart shows the communication among subroutines of the Bremsstrahlung program through calls. The arrow goes from the subroutine in which the call occurs to the subroutine being called (a return is implied). In addition, there is transfer of information through Common (labelled and unlabelled).

corresponding subroutines are BRKUT and BDIRAC. If screening is taken into account, the screening factor (ratio of screened potential to Coulomb potential) is supplied by RATERP, which reads values from tape and interpolates.

Upon completion of the integration, normalization factors are computed in CNORM by matching the wavefunctions to their W.K.B. approximation (see Chapter XI) and the matrix elements are then normalized.

The asymptotic evaluation of the tail of the matrix elements (see Chapter VI) is performed in ASYMP, and the correction is added on.

In HFUN, the calculation is carried forward to the reduced matrix elements $H(\lambda\ \ell\kappa'\kappa)$, incorporating an implicit sum over a couple of magnetic quantum numbers (see Chapter V, Eq. 24).

The remaining angular momentum sums are performed through the chain BSUM-ASUM-PHISUM. The sums over all $\kappa$'s are performed in PHISUM, with appropriate phase shifts and Clebsch-Gordan coefficients, to yield $\bar{\varphi}(\lambda_1 \lambda \ell_1 \ell \epsilon)$ (see Chapter V, Eq. 26). Further sums over $\epsilon$ and the $\lambda$'s are carried out in ASUM, again with Clebsch-Gordan coefficients, to yield $A_j^{(i)}(\ell_1 \ell)$ (see Chapter IV, Eq. 15). BSUM sums over the $\ell$'s to yield $B_j^{(i)}$ (see Chapter IV, Eq. 16).

The remaining subroutines compute special functions. LOGGAM is an NYU program[19] to compute the logarithm of the gamma function for complex argument (converted to FORTRAN IV at UCC), used for the Coulomb wavefunctions and phase shifts. BESSEL computes spherical Bessel functions, using the explicit expressions in terms of trigonometric functions for $\ell$=0 and 1, and recursion relations for larger $\ell$. BESLIT is the same as BESSEL except that if the argument is less than 1 the power series are used for $\ell > 0$. CCOEFS computes Clebsch-Gordan coefficients, using

explicit formulas if the smallest j is 2 or less, the general formula otherwise[20]. XFUN yields the factor denoted by $G_{\ell\lambda}(\kappa',\kappa)$ in the explicit expression for the special X-coefficient arising from the magnetic quantum number sums (see Chapter V, Eq. 8).

## Input

The input consists of two data cards per problem. The program recycles, picking up the next pair of data cards on completion of each problem.

Card I, in FORMAT (6I5), contains KEY, JM, LM, LM1, LM2, NTAPE. KEY = 0 indicates a pure Coulomb problem. KEY = 1 indicates that screening is to be included. KEY = -1 triggers CALL EXIT (thus, the last card in the input should be a Card I starting with -1; a matching Card II is not required). The next four entries are cut-off maxima for angular momenta, constrained by the dimensions in the program to lie between 0 and 10, inclusive. JM refers to the Legendre coefficients in the angular distribution, LM, LM1, and LM2 to the orbital angular momentum of the photon, the incident particle, and the scattered particle, respectively. The program dimensions limit the number of wavefunctions and matrix elements to 2000; this imposes a combined constraint on the LM's somewhat more restrictive than the 10 limit on each LM, and satisfaction of this constraint is checked at the start. NTAPE is the FORTRAN number of the tape unit on which is mounted the tape containing the screening data.

Card II, in FORMAT (6F10.0), contains RATIO, Z, E0, X0, ZEL, RCUT. RATIO is the ratio of the particle mass to the mass of an electron. Z is the atomic number. E0 is the kinetic energy of the incident particle in Mev; X0 is the fraction of this energy going to the photon (between 0 and 1.0). ZEL is the ratio of the particle charge to the charge of an

electron (1.0 for an electron, -1.0 for a positron, etc.). RCUT is the cut-off radius for numerical integration (in the natural units $\hbar/mc$), beyond which the tail of the matrix elements is evaluated asymptotically.

## Output

The output consists of a restatement of the input data, followed by cross section tabulations. Cross sections are expressed in units of $\alpha\, r_e^2\, Z(Z+1)$ per unit interval of the ratio of the photon energy to the kinetic energy of the incident particle, following Heitler[10] ($\alpha$ is the fine-structure constant, $r_e$ the classical electron radius). The differential cross section is tabulated per unit interval of $\cos\theta$, where $\theta$ is the angle between the photon and the incident particle, for $\theta$ values between 0 degrees and 180 degrees in steps of 2 degrees. The cross section integrated over all angles, and values of $\cos\theta$ and $\cos^2\theta$ averaged over the differential cross section are also listed. All these are given for unpolarized photons, and also for linearly polarized photons at six values of the polarization angle ($\phi$ = 0,30,60,90,120, and 150 degrees).

## XV. SAMPLE RUNS: COMPARISON WITH BORN APPROXIMATION

In the course of the development of the program, a large number of piecemeal numerical checks were carried out - comparisons of special functions with tabulated values, artificial cases with analytic answers, spot checks by hand computation, etc... Ultimately, however, the only completely convincing check is to relate the output from a full-scale run of the program with previously known results.

The only theoretical results available in the relevant energy range are those obtained from the Born approximation: the Bethe-Heitler integral cross section[1] and the Sauter differential cross section[21]. To facilitate comparisons, a computer program was written to compute these cross sections.

The Born approximation is a perturbation calculation in which the potential energy is treated as small compared with the kinetic energy. The approach to this limit is, unfortunately, forbidding in the present case. On the one hand, the kinetic energy cannot be raised indefinitely because the number of partial waves required increases (pushing storage capacity, running time, and numerical precision). On the other hand, the potential cannot strictly be made small everywhere for a Coulomb field (which is singular at the origin). The artifice of letting Z tend to zero is not satisfactory: The matrix elements all vanish in that limit, and the computed results are then dominated by the numerical integration errors. The best that can be done is to settle for moderate values of the parameters, and verify that the deviations from the Born approximation are in the expected direction.

Fig. 3 presents the differential cross section for a 0.5 Mev electron radiating a 0.25 Mev photon (unpolarized). The dotted curve is

the Born approximation result. The solid curve comes from a computer run with the present program for hydrogen (with the pure Coulomb option). The dashed curve comes from a similar computer run with Z set equal to 0.5. The theoretical expectation is that the Born approximation should give reasonable results in the forward direction and provide an underestimate for large angles. There is, indeed, good agreement at small angles (better for Z = 0.5 than Z = 1). The discrepancy at large angles is in the right direction, though larger than expected.

Table I lists the cross sections integrated over angle corresponding to Fig. 3. The agreement is fair.

The comparison thus indicates that the computer program yields reasonable results. An appreciably more extensive series of runs is obviously desirable to reinforce this conclusion.

The ultimate test of a theoretical calculation is, of course, comparison with experiment. In the next phase of this project, a considerable number of production runs of the computer program are planned, and these will be correlated with the available experimental data. The experiments usually yield the cross section integrated over angle and, frequently, further integrated over the photon spectrum for a given incident electron energy. Hence, an appreciable accumulation of computer runs is required before undertaking a significant comparison with experiment.

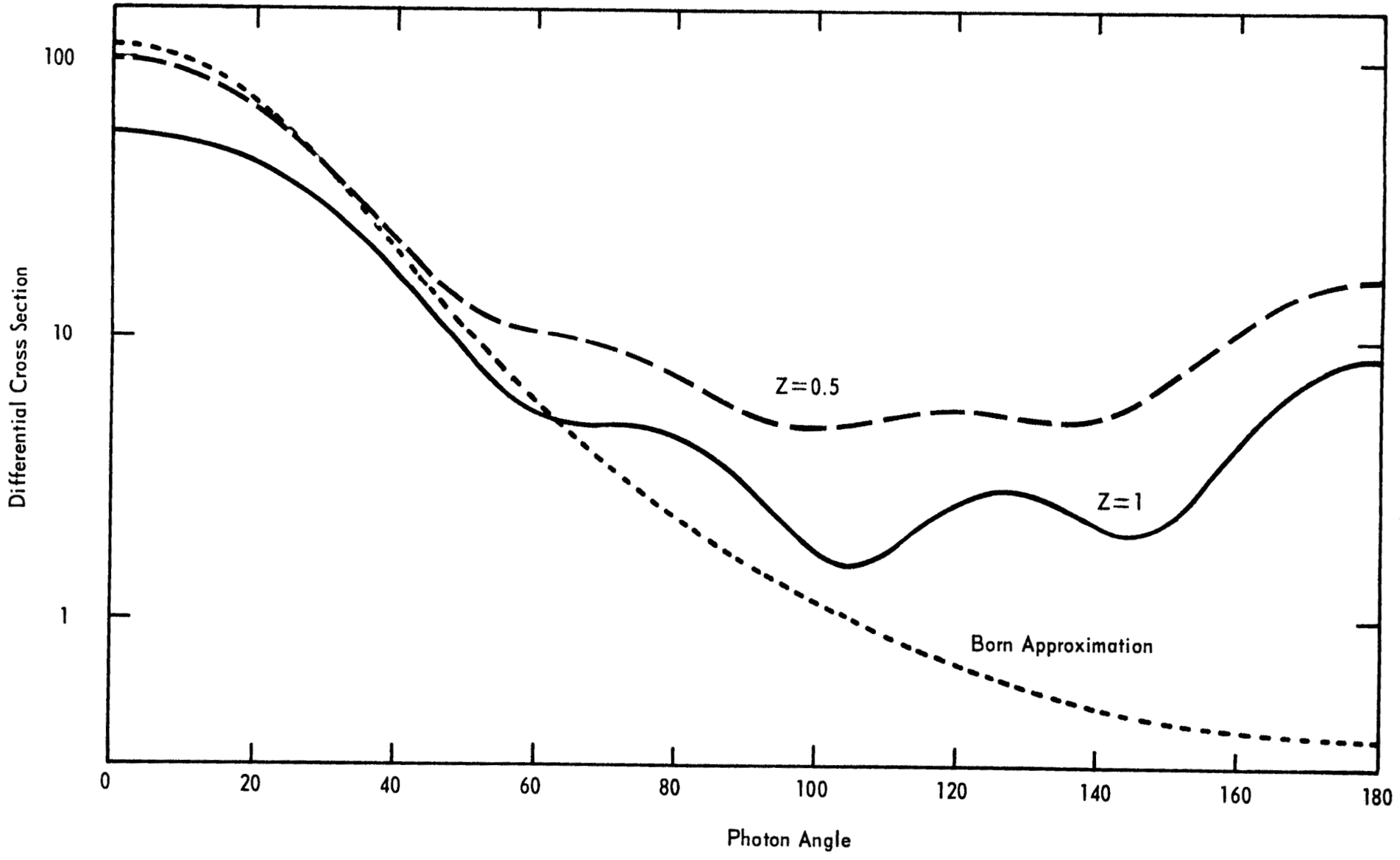


FIGURE 3 DIFFERENTIAL CROSS SECTION FOR A 0.5 Mev ELECTRON RADIATING A 0.25 Mev PHOTON (UNPOLARIZED).

| Case | Cross Section |
|---|---|
| Born approximation | 17.2 |
| Z = 0.5 | 25.8 |
| Z = 1 | 15.2 |

Table I. Cross section integrated over angle for a 0.5 MeV electron radiating a 0.25 Mev photon (unpolarized).

# SECTION B

# SUPPLEMENTARY RESULTS

# I. INTRODUCTION

This section reports results which are not directly utilized in the current version of the Bremsstrahlung calculation, but which are nonetheless considered of interest, and many of which have the potential for implementation in future extensions of the work. Brief mention will be made here of the considerations in the present absence of the particular feature from the program and in its possible value in refinements of the program or supplementary calculations.

Chapter II derives an integral representation for the phase shifts, which was used to good effect in the test program. This method of obtaining the phase shifts is inherently more accurate than wave matching. Its use requires, however, the performance of additional integrals as well as some program changes and rearrangements. Chapter III presents a reformulation of the problem using a Green's function approach and the Fredholm theory of integral equations. In this formulation, the phase shifts occur in integral representation without additional integrals, and the oscillations in the wavefunctions are reproduced with greater precision in principle, at the cost of a somewhat more complicated integral. Implementation of this approach should be investigated as part of an effort to achieve an optimum program; it was not done because it required appreciable programming changes and the existing version worked satisfactorily.

Chapter IV describes a convergence factor technique for evaluating the matrix elements. The technique worked reasonably well, but it

required the choice of a pair of adjustable parameters whose optimum values varied (albeit slowly) with the electron and photon energies. A better alternative was subsequently found, namely the truncation of the integrals followed by the asymptotic evaluation of the tail of the matrix elements. The technique is presented here nevertheless because of its generality and its possible usefulness in other contexts.

A great deal of effort has gone into the analysis of the end point of the photon spectrum (i.e. the case in which the entire kinetic energy of the incident electron goes to the photon). In this limiting case, the Born approximation yields zero for the cross section but the exact cross section is not expected to vanish. Apart from thus showing a maximum discrepancy between the exact and approximate results, this case is of great practical interest because it corresponds to the deepest radiation penetration. The formally correct way to get to this limit is to first compute the matrix elements for a small but finite kinetic energy of the scattered electron and then to go to the limit of vanishing kinetic energy. The original plan was to carry out this case as a separate program. The main program would then be checked against the Born approximation in one limit and against the end-point result in another. There was a hope (unfulfilled, as it turned out) that some analytic simplifications would occur in the limit. Chapter V presents the analysis for the end point case. In Chapter VI the treatment of an anomalous case not covered in Chapter V is sketched out. The computer programming to implement this analysis has not been done because of time limitations. Instead, the more limited plan was followed of interchanging the order of limits –

i.e. going to the zero kinetic energy limit for the scattered electron wavefunction first and then carrying out the matrix element integrals in the usual way. This interchange is valid only if the matrix elements and their derivatives with respect to the kinetic energy of the scattered electron are continuous at the end point; preliminary results are consistent with this being so. There is still theoretical interest in the original plan for the end point calculation. Its implementation at a later date is feasible if there is a willingness to expend the sizable effort required.

## II. INTEGRALS FOR PHASE SHIFTS

The free particle solutions to the Dirac radial equations are

$$G_f = \sqrt{\frac{E+1}{\pi k}}\ kr\ j_{\ell_\kappa}(kr) \sim \sqrt{\frac{E+1}{\pi k}}\ \sin\left(kr - \frac{\ell_\kappa \pi}{2}\right) \tag{1}$$

$$F_f = \sqrt{\frac{E-1}{\pi k}}\ \frac{\kappa}{|\kappa|}\ kr\ j_{\ell_{-\kappa}}(kr) \sim \sqrt{\frac{E-1}{\pi k}}\ \cos\left(kr - \frac{\ell_\kappa \pi}{2}\right), \tag{2}$$

where $j_\ell$ is a spherical Bessel function. Introducing the functions $S(r)$ and $C(r)$ which are defined by the equations

$$G = \sqrt{\frac{E+1}{E-1}}\ S\ F_f + C G_f \sim \sqrt{\frac{E+1}{\pi k}}\ \left[\sin\delta_\kappa \cos\left(kr - \frac{\ell_\kappa \pi}{2}\right) + \cos\delta_\kappa \sin\left(kr - \frac{\ell_\kappa \pi}{2}\right)\right]$$

$$F = C F_f - \sqrt{\frac{E-1}{E+1}}\ S G \sim \sqrt{\frac{E-1}{\pi k}}\ \left[\cos\delta_\kappa \cos\left(kr - \frac{\ell_\kappa \pi}{2}\right) - \sin\delta_\kappa \sin\left(kr - \frac{\ell_\kappa \pi}{2}\right)\right]. \tag{3}$$

From the asymptotic forms, by comparison,

$$C(r) \sim \cos\delta_\kappa,$$

$$S(r) \sim \sin\delta_\kappa. \tag{4}$$

Solving for $S(r)$ and $C(r)$ in general,

$$S(r) = \frac{\left(\frac{G}{\sqrt{E+1}}\ \frac{F_f}{\sqrt{E-1}} - \frac{F}{\sqrt{E-1}}\ \frac{G_f}{E+1}\right)}{\left(\frac{F_f^2}{E-1} + \frac{G_f^2}{E+1}\right)}, \tag{5}$$

$$C(r) = \frac{\left(\frac{GG_f}{E+1} + \frac{FF_f}{E-1}\right)}{\left(\frac{F_f^2}{E-1} + \frac{G_f^2}{E+1}\right)} \tag{6}$$

Noting that asymptotically

$$\pi k \left(\frac{F_f^2}{E-1} + \frac{G_f^2}{E+1}\right) \sim 1, \tag{7}$$

new functions $\bar{S}(r)$ and $\bar{C}(r)$ can be defined as

$$\bar{S}(r) = \pi(G\,F_f - F\,G_f), \tag{8}$$

$$C(r) = \pi k\left(\frac{G\,G_f}{E+1} + \frac{F\,F_f}{E-1}\right). \tag{9}$$

Asymptotically, $\bar{S}$ and $\bar{C}$ also tend to the sine and cosine of the phase shift; but they differ from S and C for smaller r. Differentiating and then substituting from the Dirac radial equations,

$$\begin{aligned} d\bar{S}/dr &= \pi(G'F_f + GF_f' - F'G_f - FG_f') \\ &= \pi F_f\left[-\frac{\kappa}{r}G + (E+1)F - VF\right] + \pi G\left[\frac{\kappa}{r}F_f - (E-1)G_f\right] \\ &= -\pi G_f\left[\frac{\kappa}{r}F - (E-1)G + VG\right] - \pi F\left[-\frac{\kappa}{r}G_f + (E+1)F_f\right] \\ &= -\pi\,V(FF_f + GG_f). \end{aligned} \tag{10}$$

At the origin, $\bar{S}$ vanishes (in fact, $d\bar{S}/dr$ also) because the F's and G's (r times the wave functions) all vanish. Integrating the last equation,

$$\bar{S}(r) = -\pi\int_0^r dr\; V(FF_f + GG_f). \tag{11}$$

The corresponding procedure with $\bar{C}(r)$ yields

$$\bar{C}(r) = \pi k\int_0^r dr\left[\frac{2\kappa}{r}\left(\frac{FF_f}{E-1} - \frac{GG_f}{E+1}\right) - V\left(\frac{FG_f}{E+1} - \frac{GF_f}{E-1}\right)\right]. \tag{12}$$

The integral representation of $\bar{S}(r)$ suggests its interpretation as the value that would be obtained for the sine of the phase shift upon neglecting the tail of the potential beyond r. This is only strictly true if F and G are the normalized wave functions obtained without truncation (wave functions for the truncated potential will differ in the value of the normalization constant). Thus the integral representation can be useful in estimating theerror made in evaluating the phase shift if the potential is truncated, and even in analytically approximating the contribution of the tail.

There is no simple interpretation of $\bar{C}(r)$ short of its asymptotic value. Note that $\bar{S}^2(r) + \bar{C}^2(r) \neq 1$ except asymptotically. Similarly, there is no simple interpretation of either $S(r)$ or $C(r)$ short of their asymptotic value. For smaller r, it should not be overlooked that the barred and unbarred quantities vary with r in different ways.

## III. DRUKAREV TRANSFORMATION OF DIRAC EQUATION

Drukarev has transformed the Fredholm equation that is the Green's function formulation of the solution of the Schrodinger equation into a Volterra equation[22]. The theoretical and computational advantages of this approach have been discussed previously[23]. The present chapter exhibits the corresponding result for the Dirac equation.

The Green's function formulation of the Dirac equation for a central potential was given by Rose[24]. Denoting as usual by F and G the radial functions multiplied by r, by $F_o$ and $G_o$ the free-space functions (regular solution), and by $\bar{F}_o$ and $\bar{G}_o$ the corresponding irregular solution,

$$F = F_o \left[1+\int_r^\infty (F\bar{F}_o + G\bar{G}_o)Vdr'\right] + \bar{F}_o \int_o^r (FF_o+GG_o)Vdr', \qquad (1a)$$

$$G = F_o \left[1+\int_r^\infty (F\bar{F}_o + G\bar{G}_o)Vdr'\right] + \bar{G}_o \int_o^r (FF_o+GG_o)Vdr', \qquad (1b)$$

where, explicitly,

$$F_o = S(\kappa)\,[(E-1)/k]^{1/2}\, kr\, j_{\ell(-\kappa)}(kr), \qquad (2a)$$

$$G_o = [(E+1)/k]^{1/2}\, kr\, j_{\ell(\kappa)}(kr), \qquad (2b)$$

and the irregular solutions are obtained by replacing the Bessel functions by Neumann functions (i.e. $j_\ell \longrightarrow y_\ell$). More generally (as Rose points out), $F_o$ and $G_o$ could be wave functions of a potential $V_o$ (typically, a Coulomb potential), in which case V in Eqs. 1 would be replaced by $V-V_o$.

Following Drukarev's approach, Eqs. 1 are rewritten as

$$F = F_o\left[1+\int_o^\infty (F\bar{F}_o+G\bar{G}_o)Vdr'\right]-F_o\int_o^r (F\bar{F}_o+G\bar{G}_o)Vdr'+\bar{F}_o\int_o^r (FF_o+GG_o)Vdr', \qquad (3a)$$

$$G = F_o\left[1+\int_o^\infty (F\bar{F}_o+G\bar{G}_o)Vdr'\right]-G_o\int_o^r (F\bar{F}_o+G\bar{G}_o)Vdr'+\bar{G}_o\int_o^r (FF_o+GG_o)Vdr'. \qquad (3b)$$

The change of variable

$$\varphi = CF \quad , \quad \Gamma = CG \tag{4}$$

is then introduced, where

$$C = [1+\int_0^\infty (F\bar{F}_0+G\bar{G}_0)Vdr']^{-1} = [1+C^{-1}\int_0^\infty (\varphi\bar{F}_0+\Gamma\bar{G}_0)Vdr']^{-1} \tag{5}$$

or, on inverting,

$$C = 1 - \int_0^\infty (\varphi\bar{F}_0+\Gamma\bar{G}_0)Vdr'. \tag{6}$$

Eqs. 3 then reduce to a coupled pair of Volterra equations. With the convenient notation,

$$C(r) = 1 - \int_0^r (\varphi\bar{F}_0+\Gamma\bar{G}_0)V\ dr', \tag{7a}$$

$$S(r) = - \int_0^r (\varphi F_0+\Gamma G_0)V\ dr', \tag{7b}$$

the Volterra equations are

$$\varphi(r) = C(r)\ F_0(r) - S(r)\ \bar{F}_0(r), \tag{8a}$$

$$\Gamma(r) = C(r)\ G_0(r) - S(r)\ \bar{G}_0(r). \tag{8b}$$

Asymptotically,

$$\Gamma \sim [(E+1)/k]^{1/2}\ [C\ \sin(kr-\ell(\nu)\pi/2)-S\ \cos(kr-\ell(\nu)\pi/2)], \tag{9}$$

$$G = C^{-1}\ \Gamma \sim [(E+1)/k]^{1/2}\ [\sin(kr-\ell(\nu)\pi/2)-(S/C)\ \cos(kr-\ell(\nu)\pi/2)], \tag{10}$$

leading to the identification

$$\tan\ \delta_\nu = \frac{S(\infty)}{C(\infty)} = - \frac{\int_0^\infty (\varphi F_0+\Gamma G_0)\ V\ dr'}{1-\int_0^\infty(\varphi\bar{F}_0+\Gamma\bar{G}_0)\ V\ dr'}\ . \tag{11}$$

For the alternative normalization convention

$$\begin{aligned} G &\sim [(E+1)/k]^{1/2}\ \sin\ [kr-\ell(\nu)(\pi/2)+\delta_\nu] \\ &= [(E+1)/k]^{1/2}\ [\cos\ \delta_\nu\ \sin(kr-\ell(\nu)\pi/2)+\sin\ \delta_\nu\ \cos(kr-\ell(\nu)\pi/2)], \end{aligned} \tag{12}$$

there results

$$\cos \delta_\kappa = C(\infty)/[C^2(\infty)+S^2(\infty)]^{1/2}, \quad \sin \delta_\kappa = S(\infty)/[C^2(\infty)+S^2(\infty)]^{1/2}. \qquad (13)$$

The formal properties of this approach have been fully discussed previously[23].

Some remarks pertinent to numerical solution are presented here:

(1) There is no normalization problem, as the solutions start out with the free-space functions.

(2) The direct numerical solution of the radial equations requires numerical integration for the wavefunctions which (away from the origin) are oscillatory - a delicate procedure. Here, the numerical integration is for the slowly varying functions C(r) and S(r), the oscillatory behavior appearing in terms of analytic functions (the spherical Bessel and Neumann functions, expressible as sines and cosines times polynomials in 1/r).

(3) The integration procedure directly yields S(r) and C(r), integrals whose limits are sin δ and cos δ. This integral representation of the phase shift converges faster and more dependably than does the determination of the phase shift by matching the wave to its asymptotic form.

(4) If the potential cuts off at r=a, then for r > a Eqs. 8 become

$$\varphi(r) = C(a)\, F_o(r) - S(a)\, \bar{F}_o(r), \qquad (14a)$$

$$\Gamma(r) = C(a)\, G_o(r) - S(a)\, \bar{G}_o(r), \qquad (14b)$$

yielding directly the appropriate analytical form for the wave functions, not only their numerical value at the cut-off.

(5) The last observation leads into a simple iterative device for improving on a foreshortened solution: From Eqs. 7,

$$C(\infty) = C(a) - \int_a^\infty (\varphi\bar{F}_o + \Gamma\bar{G}_o)\, V dr', \tag{15a}$$

$$S(\infty) = S(a) - \int_a^\infty (\varphi F_o + \Gamma G_o)\, V dr'. \tag{15b}$$

Suppose now that the numerical integration has been stopped at r=a, but the potential extends beyond. The contribution from the tail to the phase shift can be evaluated approximately by carrying out the integral in Eq. 15 with $\varphi$ and $\Gamma$ represented by Eqs. 14. If the potential is given analytically (or is fitted to an analytic expression for $r > a$), the integral may be carried out analytically. If the error in the phase shift upon truncation at r=a is of order $\epsilon$, after this approximate evaluation of the tail contribution there will be an error of order $\epsilon^2$ only.

## IV. CONVERGENCE FACTOR TECHNIQUE

For purposes of this discussion a function F(x) will be defined as

$$F(x) = \int_0^x f(r)dr. \tag{1}$$

In the limit $x \longrightarrow \infty$ this function will be assumed to be equal to one of the required radial matrix elements. Hence f(r) represents the product of the three radial wave functions. The function F(x) starts at zero at x = o and increases monotonically as x increases until it starts fluctuating about its asymptotic value with a gradually decreasing amplitude. The problem is how to deduce the asymptotic value from the integral at intermediate values of x.

This problem has been partially solved previously[25] and will be reviewed here along with current developments. In analytic work it is customary to introduce an exponential convergence factor in the integrand and take the limit as the exponent goes to zero. Thus

$$F(x) = \lim_{b \to o} F(x,b) \equiv \lim_{b \to o} \int_0^x e^{-br} f(r)dr. \tag{2}$$

In numerical work the same procedure can be used, only F(x,b) would have to be calculated for various values of b and extrapolated to b = o.

Note that this numerical procedure effectively changes the problem of approximating the asymptotic value of F(x), which is an oscillating function, to one of estimating the zero point value of a well behaved function. As an example consider the integral where

$$f(r) = r^{-1} \sin r.$$

Then

$$F(x) = \int_0^x \frac{\sin r}{r}\, dr$$

which oscillates about the asymptotic value $F = \pi/2$. However, for x large

$$F(x,b) \cong F(\infty,b) = \int_0^\infty e^{-br}\ \frac{\sin r}{r}\ dr = \tan^{-1}\ \frac{1}{b}\ .$$

This is a monotonic function of b which is relatively easy to extrapolate to b = o. A convenient method of performing the required extrapolation is with Lagrange's interpolation formula:

$$F(x,b) \simeq \sum_{s=1}^{n} F(x,a_s) \prod_{\substack{r=1 \\ r\neq s}}^{n} \left(\frac{b-a_r}{a_s-a_r}\right) \tag{3}$$

where the values of $a_s$ are selected values of b. For $a_t = ta$, where a is some convenient interval or spacing, and b = o, Lagrange's formula becomes

$$F(x,o) \cong \sum_{s=1}^{n} F(x,sa) \prod_{\substack{r=1 \\ r\neq s}}^{n} \left(\frac{-r}{s-r}\right)$$

$$= \sum_{s=1}^{n} F(x,sa)\ (-1)^{s+1}\ \frac{n!}{s!(n-s)!} \tag{4}$$

Thus

$$F(x) \cong \int_0^x (-1) \sum_{s=1}^{n} \frac{n!}{s!(n-s)!}\ (-e^{-ar})^s\ f(r)dr$$

$$= \int_0^x \left\{1 - \sum_{s=0}^{n} \frac{n!}{s!(n-s)!}\ (-e^{-ar})^s\right\} f(r)dr =$$

$$\int_0^x \left[1-(1-e^{-ar})^n\right] f(r)dr \tag{5}$$

Equation (5) is similar to (2) except that a different convergence factor appears which should give a better approximation to the function

$$F = \lim_{x \longrightarrow \infty} F(x). \tag{6}$$

The reason for this is that the parameters a and n can be chosen so the integrand becomes negligible for $r \geq x$. Since there are two parameters, this allows for the possibility of an optimum convergence factor.

## V. SPECTRUM END-POINT (PURE COULOMB CASE)

In the case of the pure Coulomb field, the radial matrix elements can be found under restricted conditions. To find the integral write the spherical Bessel function[9] as

$$j_\ell(qr) = \sum_{n=o}^{\ell} \frac{(-i)^{\ell+1-n}}{n!} \frac{(\ell+n)!}{(\ell-n)!} \frac{e^{iqr}}{(2qr)^{n+1}} + c.c. \qquad (1)$$

where c.c. stands for complex conjugate of the first term. Inserting this expression and the Coulomb wavefunctions into the radial integrals yields

$$K_\ell(\nu'\nu) = \sqrt{(E'+1)(E-1)} \sum_{n=o}^{\ell} \frac{(-i)^{\ell+1}}{n!} \frac{(\ell+n)!}{(\ell-n)!} e^{-i\frac{1}{2}\pi(\gamma'-\gamma)} [R_n(\nu',\nu) + S_n(\nu',\nu)] + c.c. \qquad (2a)$$

$$K_\ell(\nu\nu') = \sqrt{(E+1)(E'-1)} \sum_{n=o}^{\ell} \frac{(-i)^{\ell+1}}{n!} \frac{(\ell+n)!}{(\ell-n)!} e^{-i\frac{1}{2}\pi(\gamma'-\gamma)} [R_n(\nu',\nu) - S_n(\nu',\nu)] + c.c. \qquad (2b)$$

where

$$R_n(\nu',\nu) = A_{\nu'}A_\nu I_n(-\tfrac{1}{2}-i\nu', \tfrac{1}{2}+i\nu) - A^*_{\nu'} A^*_\nu I_n(\tfrac{1}{2}-i\nu', -\tfrac{1}{2}+i\nu) \qquad (3a)$$

$$S_n(\nu',\nu) = -A_{\nu'} A^*_\nu I_n(-\tfrac{1}{2}-i\nu', -\tfrac{1}{2}+i\nu) + A^*_{\nu'}A_\nu I_n(\tfrac{1}{2}-i\nu', \tfrac{1}{2}+i\nu) \qquad (3b)$$

and

$$I_n(K',K) = \frac{(-i)^n i}{(2q)^{n+1} 2(k'k)^{\frac{1}{2}}} \int_o^\infty e^{iqr} r^{-n-2} M_{K',\gamma'}(2ik'r) M_{K,\gamma}(-2ikr)\, dr \qquad (4)$$

In (4) a convergence factor $e^{-sr}$ can be inserted in the integrand to make the integral properly convergent and the limit taken as $s \longrightarrow 0$. Integrals of this type have been found by Erdelyi[26] in the form

$$\int e^{-(s-iq)r}\, r^{-n-2}\, M_{K',\gamma'}(2ik'r)\, M_{K,\gamma}(-2ikr)\, dr =$$

$$(2ik')^{\gamma'+\frac{1}{2}}(-2ik)^{\gamma+\frac{1}{2}}\,(S-iq+ik'-ik)^{-\gamma'-\gamma+n}\,\Gamma(\gamma'+\gamma-n)\;X$$

$$F_2\left(\gamma'+\gamma-n,\gamma'+\tfrac{1}{2}-K',\gamma+\tfrac{1}{2}-K;2\gamma'+1,2\gamma+1;\ \frac{-2k'}{is+q-k'+k'},\ \frac{2k}{is+q-k'+k}\right) \qquad (5)$$

which holds for Re $(\gamma'+\gamma-n) >$ and Re $(s-iq \pm ik' \pm ik) > o$. The function $F_2$ in (5) is an Appell function, or hypergeometric function of two variables[9]. A convergent series representation for $F_2$ will be discussed below.

In the limit as $s \longrightarrow o$ the function given in (4) is

$$I_n(K',K) = (-1)^{n+\gamma'+1}\,(2q)^{-1}\,(-x)^{\gamma'}\,y^{\gamma}\,z^{-n}\,\Gamma(\gamma'+\gamma-n)\;\mathbf{X}$$

$$F_2(\gamma'+\gamma-n,\ \gamma'+\tfrac{1}{2}-K',\ \gamma+\tfrac{1}{2}-K;\ 2\gamma'+1,\ 2\gamma+1;\ x,y) \qquad (6)$$

where

$$\left.\begin{aligned} x &= -2k'\,(q-k'+k)^{-1} \\ y &= 2k\,(q-k'+k)^{-1} \\ z &= 2q\,(q-k'+k)^{-1} \end{aligned}\right\} \qquad (7)$$

The four Appell functions required in (3a) and (3b) can be represented by

$$\left.\begin{aligned} K_1(\alpha) &= F_2(\alpha;\beta' \ ;\ \beta \ ;\ \delta',\delta;\ x,y) \\ K_2(\alpha) &= F_2(\alpha;\beta'+1;\ \beta \ ;\ \delta',\delta;\ x,y) \\ K_3(\alpha) &= F_2(\alpha;\beta' \ ;\ \beta+1;\ \delta',\delta;\ x,y) \\ K_4(\alpha) &= F_2(\alpha;\alpha'+1;\ \beta+1;\ \delta',\delta;\ x,y) \end{aligned}\right\} \qquad (8)$$

where $\beta' = \gamma' + i\nu'$, $\beta = \gamma - i\nu$, $\delta' = 2\gamma'+1$, $\delta = 2\gamma+1$, and $\gamma'+\gamma-\ell \leq \alpha \leq \gamma'+\gamma$. The parameter $\alpha$ indexes by unity in the sum over n in (2a) and (2b) and it is useful to use the recursion relations derived by Jaeger and Hulme to minimize the work required:[27]

$$\alpha K_1(\alpha+1) = (\alpha-\beta-\beta')\, K_1(\alpha) + \beta' K_2(\alpha) + \beta\, K_3(\alpha)$$

$$(1-x)\alpha K_2(\alpha+1) = (\delta'-1-\beta')\, K_1(\alpha) + (\beta'+1-\delta'+\alpha-\beta)\, K_2(\alpha) + \beta\, K_4(\alpha)$$

$$(1-y)\alpha K_3(\alpha+1) = (\delta-1-\beta)\, K_1(\alpha) + (\beta+1-\delta+\alpha-\beta')\, K_3(\alpha) + f' K_4(\alpha) \qquad (9)$$

$$(1-x-y)\alpha\, K_4(\alpha+1) = (\delta-1-\beta)\, K_2(\alpha) + (\delta'-1-\beta')\, K_3(\alpha) + (\alpha+\beta+\beta'-\delta-\delta'+2)\, K_4(\alpha)$$

Returning now to the representation of the Appell function, it should be noted that the usual series representation

$$F_2(\alpha;\beta',\beta;\delta',\delta;x,y) = \sum_{n,m=0}^{\infty} \frac{(\alpha)_{n+m}\,(\beta')_n\,(\beta)_m\, x^n y^m}{n!\; m!\; (\delta')_n\,(\delta)_m} \qquad (10)$$

is convergent only for $|x| + |y| < 1$. This inequality does not obtain in the case of Bremsstrahlung since $k > k'+q$, because of momentum transfer to the nucleus, and hence $2k > k'+k+q > -k'+k+q > 0$ which implies $|y| = |2k\,(q-k'+k)^{-1}| > 1$ The Appell function can be analytically continued to find a series representation that can be used in the case of Bremsstrahlung. Erdelyi[28] showed that the hypergeometric function of two variables $H_2$, which appears in Horn's list,[9] can be continued according to

$$H_2(\alpha,\beta,\gamma,\delta,\epsilon;x,y) = \frac{\Gamma(1-\alpha)\Gamma(\delta-\gamma)}{\Gamma(\delta)\Gamma(1-\alpha-\gamma)}\; y^{-\gamma}\, F_2(\alpha+\gamma;\beta,\gamma;\epsilon,1+\gamma-\delta;x,-\frac{1}{y}) + \frac{\Gamma(1-\alpha)\Gamma(\gamma-\delta)}{\Gamma(\gamma)\Gamma(1-\alpha-\delta)}$$

$$y^{-\delta}\, F_2\,(\alpha+\delta;\beta,\delta;\epsilon,1+\delta-\gamma,x,-\frac{1}{y}).$$

He also indicated that $F_2$ could not be made a linear combination of the $H_2$ functions, but in fact

$$F_2(x,-\frac{1}{y}) = CH_2(x,y) + DE(x,y)$$

where $E(x,y)$ is a hypergeometric function of two variables which does not appear in Horn's list.* By analytic continuation it is possible to prove that

$$F_2(\alpha;\beta',\beta;\delta',\delta;x,y) = \frac{\Gamma(\delta-\alpha-\beta)\Gamma(\delta)}{\Gamma(\delta-\alpha)\Gamma(\delta-\beta)}\ y^{-\alpha}\ E(\alpha;\beta',\alpha+1-\delta;\delta',\ \alpha+\beta+1-\delta;\ \frac{x}{y},\ \frac{y-1}{y})$$

$$+ \frac{\Gamma(\alpha+\beta-\delta)\Gamma(\delta)}{\Gamma(\beta)\Gamma(\alpha)}\left(\frac{1}{1-y}\right)^{\alpha}\left(\frac{y}{1-y}\right)^{\beta-\delta} H_2(\alpha+\beta-\delta;\ \beta',\delta-\beta,1-\beta;\ \delta';\ \frac{x}{1-y}\ \frac{1-y}{y}) \qquad (11)$$

where

$$E(\alpha;\ \beta,\gamma;\ \delta,\epsilon;\ x,y) = \sum_{n,m} \frac{(\alpha)_{n+m}\ (\beta)_n\ (\gamma)_{n+m}\ x^n\ y^m}{n!\ m!\ (\delta)_n\ (\epsilon)_{n+m}} \quad \text{for } |x| + |y| < 1 \qquad (12)$$

and

$$H_2(\alpha;\ \beta,\gamma,\delta;\epsilon;\ x,y) = \sum_{n,m} \frac{(\alpha)_{n-m}\ (\beta)_n\ (\gamma)_m\ (\delta)_m\ x^n\ y^m}{n!\ m!\ (\epsilon)_n} \quad \text{for } |x| < 1$$

$$\text{and } |y| < \frac{1}{1+|x|} \qquad (13)$$

The function E of (12) corresponds to Erdelyi's function E.

The representation (11) for $F_2$ yields convergent series provided $\left|\frac{x}{y}\right| + \left|\frac{y-1}{y}\right| < 1$, $\left|\frac{x}{1-y}\right| < 1$ and $\left|\frac{1-y}{y}\right| < \left(1+\left|\frac{x}{1-y}\right|\right)^{-1}$. If we restrict the calculation to the case $k' \leq q$, then all the inequalities are satisfied.

---

* Erdelyi does not give a representation for his function.

Of interest in the Bremsstrahlung calculation is the end point value when $k' \longrightarrow 0$ (all incident kinetic energy is given to the photon). To find the cross section at this point we should reduce (2a) and (2b). A relation that is helpful in the reduction is:

$$(\beta')_n = (\tau+i\nu')_n = (\tau+n-1+i\nu')(\tau+n-2+i\nu').... (\tau+i\nu')\cdot 1$$

$$= (i\nu')^n + A_{n-1}(i\nu')^{n-1} +.... + A_1(i\nu') + A_0 \qquad (14)$$

where $$A_{n-1} = \sum_{j=0}^{n-1} (\tau+j) = n\,\tau + \frac{(n-1)n}{2} \qquad (15)$$

Thus in the limit as $k' \longrightarrow 0$ (and remembering that $\nu' = \frac{E'Ze^2}{k'}$) we have

$$\lim_{k \longrightarrow 0} (\beta')_n\, x^n = \left(\frac{-2iZe^2}{q+k}\right)^n \equiv (-ig)^n \qquad (16a)$$

$$\lim_{k \longrightarrow 0} (\beta')_n \left(\frac{x}{y}\right)^n = \left(\frac{-iZe^2}{k}\right)^n \equiv (-ir)^n \qquad (16b)$$

and

$$\lim_{k \longrightarrow 0} (\beta')_n \left(\frac{x}{1-y}\right)^n = \left(\frac{2iZe^2}{k-q}\right)^n \equiv (is)^n . \qquad (16c)$$

With the use of (16a), (16b) and (16c), (11) reduces to

$$\lim_{k' \longrightarrow 0} F_2(\alpha;\beta',\beta;\delta',\delta;x,y) = \Psi_1(\alpha;\beta;\gamma',\gamma;-ig,y_o)$$

$$= \frac{\Gamma(\delta-\alpha-\beta)\Gamma(\delta)}{\Gamma(\delta-\alpha)\Gamma(\delta-\beta)}\, y_o^{-\alpha}\, \Gamma\left(\alpha+\beta-\delta,\delta-\beta;1-\beta,\delta';-ir,\frac{1-y_o}{y_o}\right)$$

$$+ \frac{\Gamma(\alpha+\beta-\delta)\Gamma(\delta)}{\Gamma(\beta)\Gamma(\alpha)} \left(\frac{1}{1-y_o}\right)^{\alpha} \left(\frac{y_o}{1-y_o}\right)^{\beta-\delta} H_{11}\left(\alpha+\beta-\delta;\delta-\beta,1-\beta;\delta';is,\frac{1-y_o}{y_o}\right) \qquad (17)$$

where

$$y_o = \frac{2k}{k+q} \tag{18a}$$

$$\Gamma(\alpha,\beta;\gamma,\delta;x,y) = \sum_{n,m} \frac{(\alpha)_{n+m}\,(\beta)_{n+m}}{n!m!\,(\gamma)_n(\delta)_{n+m}}\, x^n y^m \quad \text{for } |y| < 1 \tag{18b}$$

$$H_{11}(\alpha;\beta,\gamma;\delta;x,y) = \sum_{n,m} \frac{(\alpha)_{n-m}\,(\beta)_m\,(\gamma)_m}{n!m!\,(\delta)_n}\, x^n y^m \quad \text{for } |y| < 1 \tag{18c}$$

As a result of the limiting process we have that

$$\left.\begin{aligned} K_1(\alpha) &= K_2(\alpha) = \Psi_1(\alpha;\beta;\delta',\delta;-ig,y_o) \\ \text{and} \\ K_3(\alpha) &= K_4(\alpha) = \Psi_1(\alpha;\beta+1;\delta',\delta;-ig,y_o) \end{aligned}\right\} \text{for } k' \longrightarrow 0 \tag{19}$$

Also, the recursion relations (9) reduce to

$$\left.\begin{aligned} \alpha K_1(\alpha+1) &= (\gamma-\beta)K_1(\alpha)+\beta K_3(\alpha) \\ (1-y_o)\alpha K_3(\alpha+1) &= (\delta-1-\beta)K_1(\alpha)+(\beta+1-\delta+\alpha)K_3(\alpha) \end{aligned}\right\} \text{for } k' \longrightarrow 0 \tag{20}$$

To proceed with the reduction of (2a) and (2b) we will require the following

$$\lim_{k' \longrightarrow 0} |\Gamma(\gamma'+i\nu')| = \lim_{k' \longrightarrow 0} \nu'^{\gamma'-\frac{1}{2}}\, e^{\frac{\pi}{2}\nu'}\, (2\pi)^{\frac{1}{2}}, \tag{21a}$$

$$\lim_{k' \longrightarrow 0} (\gamma'+i\nu')\, e^{i\eta(\varkappa')} = \lim_{k' \longrightarrow 0} \frac{(\gamma'-\varkappa')}{2} + i\nu', \tag{21b}$$

$$\lim_{k' \longrightarrow 0} A_{k'} = \lim_{k' \longrightarrow 0} \frac{|\Gamma(\gamma'+i\nu')|\; e^{\frac{1}{2}\pi\nu'}\; e^{i\eta(\varkappa')}(\gamma'+i\nu')}{2(\pi k')^{\frac{1}{2}}\,\Gamma(2\gamma'+1)}$$

$$= \lim_{k' \longrightarrow 0} \nu'^{\gamma'}\left[i\nu' + \frac{(\gamma'-\varkappa')}{2}\right](2Ze^2)^{-\frac{1}{2}}, \tag{21c}$$

$$\lim_{k' \to 0} \sqrt{E'-1} = \lim_{k' \to 0} \frac{Ze^2}{\sqrt{2}\,\nu'}, \tag{21d}$$

$$\lim_{k' \to 0} \sqrt{E'+1} = \sqrt{2}, \tag{21e}$$

$$\lim_{k' \to 0} A_{\nu'} (-x)^{\gamma'} = \lim_{k' \to 0} g^{\gamma'} (2Ze^2)^{\frac{1}{2}} \left[ i\nu' + \frac{(\gamma'-\nu)}{2} \right] \tag{21f}$$

$$\lim_{k' \to 0} A^*_{\nu'} (-x)^{\gamma'} = \lim_{k' \to 0} g^{\gamma'} (2Ze^2)^{\frac{1}{2}} \left[ -i\nu' + \frac{(\gamma'-\nu)}{2} \right] \tag{21g}$$

Now, if we let

$$H_n^j = g^{\gamma} (2Ze^2)^{\frac{1}{2}} (-1)^{n+\gamma'+1} (2q)^{-1} y_o^{\gamma} z_o^{-n} \Gamma(\gamma'+\gamma-n) K_j(\alpha), \tag{22}$$

where $y_o = 2k\,(k+q)^{-1}$ and $z_o = 2q\,(k+q)^{-1}$, then (3a) and (3b) reduce to

$$\lim_{k' \to 0} R_n(\nu',\nu) = \lim_{k' \to 0} \left\{ A_\nu H_n^1 \left[ i\nu' + \frac{(\gamma'-\nu)}{2} \right] - A^*_\nu H_n^3 \left[ -i\nu' + \frac{(\gamma'-\nu)}{2} \right] \right\} \tag{23a}$$

and

$$\lim_{k' \to 0} S_n(\nu',\nu) = \lim_{k' \to 0} \left\{ -A^*_\nu H_n^3 \left[ i\nu' + \frac{(\gamma'-\nu)}{2} \right] + A_\nu H_n^1 \left[ -i\nu' + \frac{(\gamma'-\nu)}{2} \right] \right\} \tag{23b}$$

Hence the desired result is

$$\lim_{k' \to 0} K_\ell(\nu'\nu) = (E-1)^{\frac{1}{2}} \sum_{n=0}^{\ell} \frac{(-i)^{\ell+1}\,(\ell+n)!}{n!\,(\ell-n)!}\, e^{-i\frac{\pi}{2}(\gamma'-\gamma)}\, T_n + \text{c.c.}, \tag{24a}$$

and

$$\lim_{k' \to 0} K_\ell(\nu\nu') = (E+1)^{\frac{1}{2}} \sum_{n=0}^{\ell} \frac{(-i)^{\ell+1}\,(\ell+n)!}{n!\,(\ell-n)!}\, e^{-i\frac{\pi}{2}(\gamma'-\gamma)}\, V_n + \text{c.c.}, \tag{24b}$$

where

$$T_n = \lim_{k' \to 0} \sqrt{E'+1} \left[ R_n(\nu',\nu) + S_n(\nu',\nu) \right] =$$

$$= \sqrt{2}\,(\gamma'-\nu) \left[ A_\nu H_n^1 - A^*_K H_n^3 \right], \tag{25a}$$

and

$$V_n = \lim_{k' \longrightarrow 0} \sqrt{E'-1}\ \left[R_n(\varkappa',\varkappa) - S_n(\varkappa',\varkappa)\right] =$$

$$= i\sqrt{2}\ Ze^2 \left[A_\varkappa\ H_n^1 + A_\varkappa^*\ H_n^3\right]. \qquad (25b)$$

## VI. SPECTRUM END-POINT (PURE COULOMB CASE) - SUPPLEMENT

The Appell function result is subject to the condition $\gamma+\gamma'-\ell > 0$, in order for the radial integral in question to have an integrand less singular than $1/r$ at the origin. On the other hand, the selection rules allow terms for which $\gamma+\gamma'-\ell < 0 < \gamma+\gamma'-\ell+1$. To verify this, note that the selection rules impose the restriction $\ell \geq \ell_{-\kappa}+\ell_{\kappa}$, for one set of terms and $\ell \geq \ell_{\kappa}+\ell_{-\kappa}$, for the other (with the additional constraint that the sum of the three $\ell$'s be even). In turn, $\ell_{\pm\kappa} \leq |\kappa|$ (equal if the subscript is positive, one less if negative). Since $\gamma = (\kappa^2-\alpha^2Z^2)^{1/2} < |\kappa|$ , the most singular case, $\ell = |\kappa| + |\kappa'|$, has $\gamma+\gamma'-\ell < |\kappa| + |\kappa'| -\ell = 0$. On the other hand, $\gamma > |\kappa| - 1/2; (\kappa^2-\alpha^2Z^2 > \kappa^2-|\kappa|+1/4$ or $\alpha^2Z^2 < |\kappa| - 1/4$ is always satisfied; at worst, for $|\kappa| = 1$, it implies $Z < 118$. Hence, $\gamma+\gamma'-\ell > |\kappa| + |\kappa'| -\ell-1 = -1$. When the singular integral occurs for $n = \ell$, this does not imply an intrinsic divergence in the problem. The difficulty arises from the split in terms of imaginary exponentials. The integral with exp(iqr) diverges, and so does its complex conjugate, but, if the two terms are combined in the integrand to yield sin qr, the combination (sin qr)/qr goes to unity at the origin and the integrand (effectively one power of r less at the origin) is well behaved.

Considering the scattered electron wavefunction as a function of k' and expanding it about its k'=0 value, the most critical r-behavior is exhibited by the leading term and so the solution is here demonstrated for it. The calculation is carried out for the matrix element $K_\ell(\kappa\,\kappa')$ in which $F_\kappa$, is the zero-energy wavefunction; the treatment of $K_\ell(\kappa'\,\kappa)$ differs in very minor respects.

When $\gamma+\gamma'-\ell > 0$, $j_\ell(qr)$ is expanded in terms of imaginary exponentials as above, while

$$F_{\kappa'} = (\kappa/|\kappa|)(\alpha Z)^{1/2} J_{2\gamma'}[2(2\alpha Zr)^{1/2}] = (\kappa/|\kappa|)(\alpha Z)^{1/2} \frac{(2\alpha Zr)^{\gamma'}}{\Gamma(2\gamma'+1)} \; {}_0F_1(2\gamma'+1;-2\alpha Zr)$$

$$= (\kappa/|\kappa|)(\alpha Z)^{1/2} (2\alpha Zr)^{\gamma'} \sum_{s=0}^{\infty} (-2\alpha Zr)^s/s!\, \Gamma(2\gamma'+1+s), \qquad (1)$$

$$G_\kappa = \frac{|\Gamma(\gamma+i\nu)|\, e^{\nu\pi/2}(E+1)^{1/2}}{2\Gamma(2\gamma+1)(\pi k)^{1/2}} (\gamma+i\nu) i^{-\gamma-1/2} e^{i\eta} (2kr)^{-1/2} M_{-1/2-i\nu,\gamma}(2ikr) + c.c. \qquad (2)$$

After insertion of an integration factor $\exp(-\varepsilon r)$ (where $\varepsilon$ will subsequently be set equal to zero), the basic integral that is required is[29]

$$(2k)^{-1/2}\, i^{-\gamma-1/2} \int_0^\infty dr\, r^{s-n+\gamma'-3/2}\, e^{-(\varepsilon-iq)r}\, M_{-1/2-i\nu,\gamma}(2ikr) \qquad (3)$$

$$= (2k)^\gamma\, \Gamma(\gamma+\gamma'+s-n)(\varepsilon-iq+ik)^{-(\gamma+\gamma'+s-n)}\; {}_2F_1\left(\gamma+\gamma'+s-n, \gamma+1+i\nu; 2\gamma+1; \frac{2ik}{\varepsilon-iq+ik}\right).$$

Comparing this procedure with the Appell function approach, there is the same finite sum over n from the expansion of the spherical Bessel function in both cases, and the same ultimate necessity for analytic continuation at the end. Previously, the Appell function constituted a double infinite sum in two variables. Now, there is an infinite sum (over s) containing as a factor a hypergeometric function which represents another infinite sum. The computational effort can be reduced by expressing all the hypergeometric functions as derivatives of one basic one: Let $m = \ell+s-n$ (so that m is positive definite for all s and n). Let

$$z = 2ik\,(\varepsilon-iq+ik)^{-1} \qquad (4)$$

Then (9)

$$\Gamma(\gamma+\gamma'-\ell+m)\; z^{\gamma+\gamma'-\ell-1}\; {}_2F_1(\gamma+\gamma'-\ell+m,\gamma+1+i\nu;2\gamma+1;z)$$

$$= \Gamma(\gamma+\gamma'-\ell)\; \frac{d^m}{dz^m}\; [z^{\gamma+\gamma'-\ell-1+m}\; {}_2F_1(\gamma+\gamma'-\ell,\gamma+1+i\nu;2\gamma+1;z)]. \tag{5}$$

For $\gamma+\gamma'-\ell < 0$, the $n=\ell$ terms must be kept together:

$$\text{term} = \frac{(2\ell)!}{\ell!}\; (2qr)^{-\ell}\; \frac{\sin qr}{r}\; . \tag{6}$$

An expansion for $\sin qr/qr$ is (9)

$$\sin qr/qr = \exp(-iqr)\; {}_1F_1(1,2;2iqr). \tag{7}$$

Combining the two series,

$${}_0F_1\; (2\gamma'+1;-2\;\alpha\; Zr)\; {}_1F_1(1,2;2iqr)$$

$$= \sum_{s=0}^{\infty} \frac{\Gamma(2\gamma'+1)}{\Gamma(2\gamma'+1+s)}\; \frac{(-2\;\alpha\; Zr)^s}{s!}\; \sum_{t=0}^{\infty} \frac{\Gamma(t+1)\Gamma(2)}{\Gamma(1)\Gamma(t+2)}\; \frac{(2iqr)^t}{t!}$$

$$= \sum_{s=0}^{\infty} \frac{\Gamma(2\gamma'+1)}{\Gamma(2\gamma'+1+s)}\; \frac{(-2\;\alpha\; Zr)^s}{s!}\; \sum_{t=0}^{\infty}\; \frac{(2iqr)^t}{(t+1)!}\; . \tag{8}$$

Let $n = s+t$. Then

$$\frac{1}{(t+1)!} = \frac{1}{(n-s+1)!} = \frac{1}{\Gamma(n-s+2)} = (-1)^s\; \frac{\Gamma(-n-1+s)}{\Gamma(-n-1)\Gamma(n+2)} = \frac{1}{(n+1)!}\; (-1)^s\; \frac{\Gamma(-n-1+s)}{\Gamma(-n-1)} \tag{9}$$

$${}_0F_1\; (2\gamma'+1;-2\;\alpha\; Zr)\; {}_1F_1(1,2;2iqr)$$

$$= \sum_{s=0}^{\infty}\; \frac{\left(\frac{\alpha\; Z}{i\; q}\right)^s}{s!}\; \frac{1}{(2\gamma'+1)_s}\; \sum_{n=s}^{\infty}\; \frac{(2iqr)^n}{(n+1)!}\; (-n-1)_s$$

$$= \sum_{n=0}^{\infty}\; \frac{(2iqr)^n}{(n+1)!}\; \sum_{s=0}^{n}\; \frac{(-n-1)_s}{(2\gamma'+1)_s}\; \frac{\left(\frac{\alpha\; Z}{i\; q}\right)^s}{s!}\; . \tag{10}$$

The s sum does not depend on r. The integration is now the same as above.

ACKNOWLEDGEMENT

The authors take this opportunity to acknowledge the help received on this project from colleagues at Union Carbide: Dr. J. Agresta contributed the screened potential computations and the angular distribution routine. Programming assistance was provided by Mr. R. A. Fronapfel in the first year and Mr. A. Glick in the second, and on a smaller scale by Miss C. Currie and Mr. J. W. Nostrand, Jr.

## REFERENCES


1. H. A. Bethe and W. Heitler, Proc. Royal Soc. (London) A146, 83 (1934).

2. H. W. Koch and J. W. Motz, Rev. of Mod. Phys. 31, 920 (1959).

3. J. C. Jaeger and H. R. Hulme, Proc. Royal Soc. (London) A153, 443 (1936).

4. J. C. Jaeger, Nature 137, 781 (1936).

5. J. C. Jaeger, Nature 148, 86 (1941).

6. Rosenblum, Shroder, and Warner, Phys. Rev. 88, 612 (1952); I. E. Dayton, Phys. Rev. 89, 544 (1953); H. I. West, Jr., Phys. Rev. 101, 915 (1956); C. D. Zerby and H. S. Moran, "A Semi-Empirical Equation for Pair Production Below 5 Mev", ORNL-CF-56-12-4 (1956).

7. A. I. Akhiezer and V. B. Berestetsky, Quantum Electrodynamics (State Technico-Theoretical Literature Press, Moscow, 1953) translated version: Technical Information Service Extension, Oak Ridge, Tenn., AEC-tr-2876.

8. M. E. Rose, Elementary Theory of Angular Momentum, (John Wiley and Sons, New York, 1957).

9. A. Erdelyi, et al., Higher Transcendental Functions (McGraw-Hill Book Company, New York, 1953) Vol. I and II.

10. W. Heitler, The Quantum Theory of Radiation, (Oxford University Press, London, 1954).

11. M. E. Rose and L. C. Biedenharn, "Theory of the Photoelectric Effect. I. Formal Aspects," Oak Ridge National Laboratory Report ORNL 1779 (1954).

12. M. E. Rose, "On the Relation Between Certain 9-j and 6-j Symbols," (unpublished).

13. M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, National Bureau of Standards (Washington, D. C., 1964).

14. D. R. Hartree, The Calculation of Atomic Structures (John Wiley and Sons, Inc., New York, 1957).

15. F. Herman and S. Skillman, Atomic Structure Calculations (Prentice-Hall, Inc., Englewood Cliffs, N.J., 1963).

16. C. C. J. Roothaan and P. S. Bagus, "Atomic Self-Consistent Field Calculations by the Expansion Method," Methods in Computational Physics, Volume II, 47, (Academic Press, New York, 1963).

17. B. O. Peirce, A Short Table of Integrals, No. 403, (Ginn and Company, Boston, 1929).

18. J. Irving and N. Mullineux, Mathematics in Physics and Engineering, (Academic Press, New York, 1959), p. 180.

19. Miriam S. Shapiro and Max Goldstein, "A Collection of Mathematical Computer Routines," NYO-1480-14 (1965).

20. E. U. Condon and G. H. Shortley, Theory of Atomic Spectra, (Cambridge University Press, 1935).

21. F. Sauter, Ann. Physik (5), 20, 404 (1934).

22. G. F. Drukarev, Zh. Eksperim. i Teor. Fiz. 25, 139 (1953).

23. H. Brysk, Phys. Rev. 133, B-1625 (1964). The reader is referred to this article for extensive references.

24. M. E. Rose, Phys. Rev. 82, 389 (1961).

25. C. D. Zerby, "Electromagnetic Production of Pion Pairs," ORNL 3033 (1961), and Phys. Rev. 124, 2029 (1961).

26. A. Erdelyi, Math. Z. 40, 693 (1936).

27. J. C. Jaeger and H. R. Hulme, Proc. Royal Soc. A148, 708 (1935).

28. A. Erdelyi, Proc. Royal Soc. of Edinburgh A62, 378 (1948).

29. A. Erdelyi et al., Tables of Integral Transforms, Vol. I (McGraw Hill Book Company, New York, 1954).

Jet Propulsion Laboratory
Pasadena, California, 91103
Attention: Mr. Dwain F. Spencer (Mail Stop 354-4219)
Dr. Robert V. Meghreblian (Mail Stop 354-4040)
Dr. Robert J. Mackin (Mail Stop 354-4110)
Mr. Bruce E. Anspaugh (Mail Stop T-141)
Mr. Ed Divita (Mail Stop T-141)

National Bureau of Standards
Washington, D.C., 20234
Attention: Dr. Martin J. Berger, Radiation Theory Branch
Dr. Joseph W. Motz, Radiation Physics Division

U.S. Naval Radiological Defense Laboratory
San Francisco, California, 94135
Attention: Dr. William Kreger

Air Force Cambridge Research Center
L. G. Hanscom Field, Massachusetts
Attention: Dr. Ludwig Katz

U.S. Naval School of Aviation Medicine
Pensacola, Florida 32512
Attention: Dr. H. J. Schaefer

Office of Naval Research
Washington, D. C.
Attention: Dr. Sol Krasner

Air Force Weapons Laboratory
WLRB-1
Kirtland Air Force Base, New Mexico

Air Force Space Systems Division
SSTA
Air Force Unit Post Office
Los Angeles 45, California

Air Force Institute of Technology (NETF)
Wright-Patterson AFB, Ohio
Attention: L/C James R. Bohannon

Space Systems Division (SSTDS)
Los Angeles 45, California
Attention: Lt. V. H. Bouquet

Defense Atomic Support Agency
Pentagon
Washington, D. C.
Attention: L/C Charles D. Daniel, Jr.

Commanding General
U.S. Army Electronics Command
Fort Monmouth, New Jersey 07703
Attn: AMSEL-KL-I

DISTRIBUTION LIST

NASA/Headquarters
Washington, D.C., 20546
Attention: Mr. Arthur Reetz, Jr. (Code RV-1)
Mr. J. Warren Keller (Code RV-1)
Dr. Jacob Trombka (Code SM)
Mr. Leo Fox (Code RBH)
Dr. Harry Harrison (Code RRE)
Office of Technology Utilization (Code AT)

NASA/Marshall Space Flight Center
Huntsville, Alabama, 35812
Attention: Dr. Russell D. Shelton (Code R-RP-N)
Dr. Nat Edmonson (Code R-RP-N)
Mr. Henry E. Stern (Code R-RP-N)
Mr. Martin O. Burrell (Code R-RP-N)
Mr. Eugene W. Urban (Code R-RP-N)

NASA/Goddard Space Flight Center
Greenbelt, Maryland 20771
Attention: Dr. Wilmot N. Hess (Code 640)
Dr. George F. Pieper (Code 600)
Mr. Robert J. Janda (Code 636)

NASA/Langley Research Center
Langley Field, Va., 23365
Attention: Dr. Trutz Foelsche (Mail Stop 304)
Mr. Herbert D. Hendricks (Mail Stop 499)
Dr. John E. Duberg (Mail Stop 116)
Mr. Raymond M. Hansen (Mail Stop 235)
Mr. Edwin T. Kruszewski (Mail Stop 188B)
Mr. William C. Hulten (Mail Stop 900)
Dr. Albert Lieber (Mail Stop 400)

NASA/Manned Spacecraft Center
Houston, Texas 77001
Attention: Mr. Jerry Modisette (Code ET32)
Mr. Peter Higgins (Code ET32)
Mr. Donald E. Robbins (Code ET32)
Mr. Clarence E. Humphries (Code EP2)

NASA/Ames Research Center
Moffett Field, California 94035
Attention: Mr. J. Michael Coogan (Mail Stop 207-1)
Dr. Fred Casal (Mail Stop 207-1)

NASA/Lewis Research Center
Cleveland, Ohio 44135
Attention: Mr. Irving M. Karp (Mail Stop 54-1)
Mr. Robert I. Hildebrand (Mail Stop 54-1)
Mr. Gerald V. Brown (Mail Stop 301-1)
Dr. James W. Blue (Mail Stop 49-2)

Air Force Weapons Lab.(WLDN-2)
Kirtland AFB, New Mexico
Attention: Lt. Nelson S. DeMuth, Jr.

U.S. Army Nuclear Defense Lab (AMXND-C)
Edgewood Arsenal, Maryland
Attention: Dr. Herman J. Donnert

Air Force Weapons Lab (SLRPH)
Kirtland AFB, New Mexico
Attention: Capt. Roy E. Herman

Air Force Systems Command (SCTR)
Andrews AFB, Maryland
Attention: Major Russell E. Linkous

Systems Engineering Group (SESSV)
Wright-Patterson AFB, Ohio
Attention: Mr. Thomas J. McGuire

Air Force Systems Command (SCLDS)
Andrews AFB, Maryland
Attention: Major Robert F. Mitchell

6570th Aerospace Medical Research Lab.
Wright-Patterson AFB, Ohio
Attention: Mr. Loren H. Pittman

Aerospace Medical Division (AMRL)
Brooks AFB, Texas
Attention: L/C A. G. Swan

Air Force Flight Dynamics Lab.(FDFE)
Wright-Patterson AFB, Ohio
Attention: Mr. Ronald White

Aerospace Corporation
2400 El Segundo Blvd.
El Segundo, California
Attention: Dr. Stan Freden
Dr. Robert Pruett

North American Aviation, Inc.
12214 S. Lakewood Blvd.
Downey, California
Attention: Mr. Fred Raymes (Dept. 695, Group 224)
Mr. E. R. Beever
Mr. J. D. Fletcher

General Atomic
P.O. Box 608
San Diego, California 92112
Attention: Mr. Clyde Jupiter
Mr. George Joanou
Dr. Richard Scalettar

Boeing Company
Aero-Space Division
P.O. Box 3707
Seattle, Washington
Attention: Dr. Glenn Keister
Mr. Maynard Pearson
Mr. Brian Mar

General Dynamics/Fort Worth
P.O. Box 748
Fort Worth, Texas
Attention: Mr. E. C. Kidd (Zone Y71, Dept. 641)
Mr. R. A. Miller (Zone Y71, Dept. 641)
Mr. C. F. Johnson (Zone Y71, Dept. 641)

United Nuclear Corporation
Grasslands Road
Elmsford, New York
Attention: Dr. Richard Ross

Union Carbide Research Institute
P.O. Box 278
Tarrytown, New York 10591
Attention: Dr. Clay Zerby
Dr. F. L. Keller

Ling-Temco-Vought Research Center
P.O. Box 5907
Dallas, Texas 75222
Attention: Dr. Jim Johnson
Dr. David Rester
Dr. William Dance

Oak Ridge National Laboratory
P.O. Box X
Oak Ridge, Tennessee 37831
Attention: Dr. F. C. Maienschein
Dr. R. G. Alsmiller
Mr. S. K. Penny

Lockheed-Georgia Company
Marietta, Georgia
Attention: Mr. Charles W. Hill (Dept 73-69, Zone 64)

Republic Aviation Corporation
Power Conversion Systems Division
Farmingdale, L.I., New York
Attention: Mr. Ed Kuhn

Bendix Systems Division
3300 Plymouth Road
Ann Arbor, Michigan
Attention: Mr. Keith More

College of William & Mary
Department of Physics
Williamsburg, Virginia
Attention: Dr. Robert Siegel

Rice University
Houston, Texas
Attention: Dr. John W. Freeman

Lockheed Missiles and Space Company
Bldg. 204, Dept. 52-10
3251 Hanover Street
San Jose, California
Attention: Dr. Richard A. Glass
Mr. Thomas Powers

Advanced Research Corporation
715 Miami Circle N.E.
Atlanta, Georgia 30324
Attention: Dr. Ed Rollor, Jr.

Radiation Research Associates
1314 Hurley Avenue
Fort Worth, Texas
Attention: Mr. Robert L. French
Dr. Norman Schaeffer

Ion Physics Corporation
Burlington, Massachusetts
Attention: Dr. Sam V. Nablo

General Electric Company
P.O. Box 8555
Philadelphia 1, Pennsylvania
Attention: Dr. R. C. Good, Jr.

Northrop Space Laboratories
Hawthorne, California
Attention: Mr. R. E. Fortney
Mr. M. C. Chapman

The Martin Company
Baltimore 3, Maryland
Attention: Dr. Sidney Russak (Mail No. 325)

University of California
Lawrence Radiation Laboratory
Berkeley, California 94720
Attention: Dr. Cornelius Tobias
Dr. Roger Wallace

Bellcomm, Inc.
1100 17th Street, N.W.
Washington, D.C., 20036
Attention: Dr. Tim Orrok
Dr. Robert Hilberg

Grumman Aircraft Engineering Corporation
Bethpage, Long Island, New York
Attention: Mr. E. M. Finkelman

McDonnell Aircraft Corporation
P.O. Box 516
St. Louis, Missouri 63166
Attention: Mr. Robert L. Kloster (Dept. 401, Bldg. 106)
Mr. R. V. Glowszwski (Dept. 401, Bldg. 106)

General Dynamics/Convair
P.O. Box 166
San Diego, California 92112
Attention: Mr. D. H. Robey (Mail Zone 503-00)
Dr. A. W. McReynolds (Mail Zone 596-00)
Mr. Edward L. Noon (Mail Zone 528-40)
Mr. David Sowle (Mail Zone 596-00)

Westinghouse Electric Company
Research and Development Center
Pittsburgh 35, Pennsylvania
Attention: Dr. D. W. Drawbaugh
Dr. S. H. Autler

University of Arizona
Tuscon, Arizona
Attention: Dr. Robert L. Seale

Douglas Aircraft Company
Missile and Space Division
3000 Ocean Park Blvd.
Santa Monica, California
Attention: Robert W. Langley

University of Uppsala
The Gustaf Werner Institute
Uppsala, Sweden
Attention: Dr. Borje Larsson

Massachusetts Institute of Technology
Cambridge, Massachusetts
Attention: Dr. Robley D. Evans
Professor of Physics

Guggenheim Aerospace Laboratories
New York University
University Heights, New York 53, N. Y.
Attention: Professor B. S. P. Shen

Scientific & Technical Information Facility
P.O. Box 33
College Park, Maryland 20740
Attention: NASA Representative

Battelle Memorial Institute
505 King Avenue
Columbus, Ohio
Attention: Mr. Lee H. Bettenhausen

Clarkson College of Technology
Potsdam, New York
Attention: Dr. Richard Madey, Chairman
Physics Department

Texas Christian University
Fort Worth, Texas
Attention: Dr. Leo Baggerly
Physics Department

AVCO/Everett Research Laboratory
2385 Revere Beach Parkway
Everett, Massachusetts 02149
Attention: Dr. Richard Levy

Exotech Incorporated
525 School Street, S.W.
Washington, D.C. 20024
Attention: Mr. Mathew Barrett

Chattanooga State Technical Institute
400 Chestnut Street
Chattanooga, Tennessee
Attention: Mr. W. Wayne Scott

Physics International Company
2700 Merced Street
San Leamdro, California 94577
Attention: Mr. Larry Behrmann

Georgia Institute of Technology
Atlanta, Georgia 30332
Attention: Dr. R. M. Ahrens
Physics Department

Ottawa University
Ottawa, Kansas 66067
Attention: Dr. L. V. Spencer
Physics Department

Mathematical Applications Group Incorporated
221 East Hartsdale Avenue
Hartsdale, New York
Attention: Dr. Phillip S. Mittelman, President