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Incoherent scattering of gamma rays in heavy atoms

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Abstract. Exact relativistic differential cross sections for the incoherent scattering of gamma rays by the inner shell electrons of heavy atoms are developed from the second order S matrix element for the electron–photon interaction in the Furry picture. Electron binding is accounted for completely by using the bound electron propagator and Dirac eigenfunctions for the initial and final electron states.

A pure Coulomb potential is used to calculate the energy spectrum and the differential cross section for 662 keV gamma rays scattered by the K electrons of lead. In contrast with the results of Di Lazzaro and Missoni, the energy spectrum maximum is displaced by 10% from the Compton energy towards higher photon energies, and there is no increase in the spectrum at the low-energy end. The relativistic results for the ratio of the bound electron to free electron cross sections are larger than the incoherent scattering function calculations and exceed unity for scattering angles above 52°.

1. Introduction

Theoretical investigations of the incoherent scattering of photons by atomic electrons have until now been essentially non-relativistic in that they are based upon either the atomic form factor approximation, which is valid for low photon energies and low electron binding energies, or the incoherent scattering function approach, whose validity requires the photon energy to be appreciably greater than the electron binding energy. The form factor calculations, which originally used hydrogen wave functions (Wentzel 1929, Bloch 1934, Schnaidt 1934), successfully accounted for the scattering of x-rays by light atoms. Subsequently, Randles (1957), Standing and Jovanovich (1962) and Lambert *et al.* (1966) used relativistic wave functions in evaluating the form factor for the scattering of gamma rays in heavy atoms. The incoherent scattering function approach has been employed predominantly in the investigation of the total x-ray scattering from light atoms (White-Grodstein 1957). Sujkowski and Nagel (1961) and Shimizu *et al.* (1965) have applied the incoherent scattering function to the scattering of gamma rays by individual atomic electrons, and the cross sections obtained using both non-relativistic and relativistic electron states agree qualitatively with the experimental results.

Recently, Di Lazzaro and Missoni (1966) have followed Akhiezer and Berestetskii (1965) in directly evaluating the second-order S matrix element for the Compton process and, although electron binding is neglected in the intermediate and final states, the results explain the general behaviour of the scattering of gamma rays in heavy atoms.

The disagreement between the results of recent measurements of the scattering of medium energy gamma rays by the K electrons of heavy atoms (Brini *et al.* 1960, Sujkowski and Nagel 1961, Motz and Missoni 1961, Varma and Eswaran 1962, Di Lazzaro and Missoni 1963, 1966, Shimizu *et al.* 1965, Ramalinga Reddy *et al.* 1967,

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Pingot 1968, 1969, East and Lewis 1969) confirm the need for a calculation which both accounts fully for the effects of the static nuclear field and is not restricted to low-energy photons.

In this paper the Furry picture (Furry 1951) is used to describe the interaction of an electron and a photon in the presence of a prescribed c number external field. Electron binding is taken into account by using the bound electron propagator and Dirac eigenfunctions for the initial discrete, and final continuum, electron states. Following Brown *et al.* (1954), the completeness properties of the spin spherical harmonics are used in § 2 to separate the angular and radial dependence of the transition amplitude, and the radial dependence of the bound electron propagator is obtained as the solution of an inhomogeneous differential equation.

The summations over electron magnetic quantum numbers and photon polarizations are effected by the Wigner–Eckart theorem and the techniques of Racah algebra in § 3, and the ensuing cross section for the incoherent scattering of unpolarized photons is expressed in terms of a set of radial matrix elements and combinations of angular momentum coupling coefficients.

The structure of the radial matrix elements is examined in § 4 and their numerical computation discussed briefly in § 5.

Finally, in § 6, results are presented for the scattering of 662 keV photons by the K electrons of lead, and a comparison is made with experimental and existing theoretical results.

2. General formalism

The rationalized relativistic unit system $\hbar = m = c = 1$ is used throughout. In these units the fine-structure constant is $\alpha = e^2/4\pi \simeq 1/137$. The scalar product of two 4-vectors is denoted by $A.B = \Sigma_{\mu=0}^{3} A^\mu B_\mu = A_0 B_0 - \boldsymbol{A}.\boldsymbol{B}$ and the conventions for the Dirac matrices are $\gamma^i = \beta\alpha_i$ $(i = 1, 2, 3)$, $\gamma^0 = \beta$. Also, $\bar{\psi} = \psi^\dagger\gamma^0$ where $\psi^\dagger$ is the adjoint of the spinor ψ and c^* denotes the complex conjugate of a scalar c.

The second-order S matrix element, in the Furry picture, for the interaction of a photon and an electron in the presence of the c number electromagnetic field $A_\mu^e(x)$ is

$$S_{fi} = S_{fi}^{(a)} + S_{fi}^{(e)} \tag{1}$$

where

$$S_{fi}^{(a)} = \frac{\alpha}{8\pi^2}(\omega_i\omega_f)^{-1/2}\int\int \mathrm{d}^4x'\,\mathrm{d}^4x\{\bar{\psi}_f(x')\gamma\,.\,\epsilon^{(f)*}\exp(ik_f\,.\,x')S^e(x', x)\gamma\,.\,\epsilon^{(i)} \times \exp(-ik_i\,.\,x)\psi_i(x)\} \tag{2}$$

and

$$S_{fi}^{(e)} = S_{fi}^{(a)}\{k_f \leftrightarrow -k_i,\ \epsilon^{(f)*} \leftrightarrow \epsilon^{(i)}\} \tag{3}$$

are the amplitudes which correspond, respectively, to the absorption of the incident photon before the emission of the final photon and to the emission of the final photon prior to the absorption of the initial photon. The electron states $\psi(x)$ are solutions of

$$\{i\gamma\,.\,\partial - e\gamma\,.\,A^e(x) - 1\}\psi(x) = 0$$

where $\partial = \partial/\partial x^\mu$, and $k = (\omega, \boldsymbol{k})$ and $\epsilon = \epsilon^{(\rho)}(\hat{\boldsymbol{k}}) = (0, \boldsymbol{\epsilon})$ are the 4-momentum and 4-polarization vectors respectively of a photon in a state of circular polarization

denoted by ρ. The bound electron propagator $S^e(x, x')$ is obtained as the solution of (Schweber 1961)

$$\{i\gamma \cdot \partial - e\gamma \cdot A^e(x) - 1\}S^e(x, x') = -2i\delta^{(4)}(x - x')$$

subject to the boundary condition that $S^e(x, x')$ is asymptotic to the free electron propagator $S(x-x')$ for large x.

Introducing the amplitude

$$F^{(a)}(x') = \int d^4x S^e(x', x)\gamma \cdot \epsilon^{(i)} \exp(-ik_i \cdot x)\psi_i(x) \tag{4}$$

and noting that $\psi(x) = \psi_E(x)\exp(-iEx^0)$ and $S^e(x', x) = S^e(\boldsymbol{x}', \boldsymbol{x}, x^{0\prime} - x^0)$ for a time-independent external potential, we obtain, on integrating over $t = x^{0\prime} - x^0$

$$S_{fi}^{(a)} = \delta(E_f + \omega_f - E_i - \omega_i)\mathcal{M}_{fi}^{(a)} \tag{5}$$

where

$$\mathcal{M}_{fi}^{(a)} = -\frac{i\alpha}{2\pi}(\omega_i\omega_f)^{-1/2}\int d^3x' \psi_{E_f}^{\dagger}(\boldsymbol{x}')\boldsymbol{\alpha} \cdot \boldsymbol{\epsilon}^{(f)*}\exp(-i\boldsymbol{k}_f \cdot \boldsymbol{x}')F^{(a)}(\boldsymbol{x}'). \tag{6}$$

The amplitude $F^{(a)}(\boldsymbol{x}')$ satisfies

$$\{H_D(\boldsymbol{x}') - (E_i + \omega_i)\}F^{(a)}(\boldsymbol{x}') = \mathcal{Q}^{(a)}(\boldsymbol{x}') \tag{7}$$

where

$$\mathcal{Q}^{(a)}(\boldsymbol{x}) = -\boldsymbol{\alpha} \cdot \boldsymbol{\epsilon}^{(i)}\exp(i\boldsymbol{k}_i \cdot \boldsymbol{x})\psi_{E_i}(\boldsymbol{x}) \tag{8}$$

and, for a scalar external field, the Dirac Hamiltonian $H_D(\boldsymbol{x})$ is

$$H_D(\boldsymbol{x}) = -i\boldsymbol{\alpha} \cdot \partial + eA_0^e(\boldsymbol{x}) + \beta. \tag{9}$$

The inner electrons of heavy atoms can be accurately assumed to move in a spherically symmetric potential $V(r) = eA_0^e(r)$ and therefore the eigenfunctions $\psi_{E_i}(\boldsymbol{x})$ have the form (Rose 1961)

$$\psi_E(r, \theta, \phi) = \frac{1}{r}\begin{pmatrix} g_{\kappa,E}(r)\chi_\kappa^\mu(\Omega) \\ if_{\kappa,E}(r)\chi_{-\kappa}^\mu(\Omega) \end{pmatrix}. \tag{10}$$

Here, $(r, \theta, \phi) = (r, \Omega)$ are spherical polar coordinates and the $\chi_\kappa^\mu(\Omega)$ are the spinor spherical harmonics

$$\chi_\kappa^\mu(\Omega) = \sum_m C(l\tfrac{1}{2}j; \mu - m, m)Y_l^{\mu-m}(\Omega)\chi^m.$$

The notation and phase convention for the Clebsch–Gordan coefficient

$$C(j_1 j_2 j; m_1, m - m_1)$$

and the spherical harmonic $Y_l^m(\Omega)$ is that of Rose (1957), the χ^m are the two component Pauli spinors, and j, l_κ and $l_{-\kappa}$ are obtained from κ by

$$j = |\kappa| - \tfrac{1}{2},\ l = l_\kappa = \begin{cases} \kappa & \kappa > 0 \\ -\kappa - 1 & \kappa < 0 \end{cases} \qquad l' = l_{-\kappa} = l_\kappa - \frac{\kappa}{|\kappa|}.$$

The parameter κ takes all non-zero integral values. The radial functions are solutions

of the Dirac equations

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

where

$$A(r, E) = \begin{pmatrix} \mathrm{d}/\mathrm{d}r + \kappa/r & -\{E+1-V(r)\} \\ E-1-V(r) & \mathrm{d}/\mathrm{d}r - \kappa/r \end{pmatrix}.$$

Using the standard representation

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$$

for the Dirac matrices, the σ_i being the 2×2 Pauli matrices, and introducing the components

$$\sigma_{\pm 1} = \mp \frac{1}{\sqrt{2}}(\sigma_x \pm \mathrm{i}\sigma_y),\ \sigma_0 = \sigma_z$$

and

$$\epsilon^{(\rho)}_{\pm 1} = \mp \frac{1}{\sqrt{2}}(\epsilon^{(\rho)}_x \pm \mathrm{i}\epsilon^{(\rho)}_y),\ \epsilon^{(\rho)}_0 = \epsilon^{(\rho)}_z$$

of $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ respectively in a spherical basis, $\mathcal{Q}^{(a)}(\boldsymbol{x})$ becomes

$$\begin{pmatrix} {}^{u}\mathcal{Q}^{(a)}(\boldsymbol{x}) \\ {}^{l}\mathcal{Q}^{(a)}(\boldsymbol{x}) \end{pmatrix} = -\frac{1}{r}\sum_{\lambda=-1}^{1} \exp(\mathrm{i}\boldsymbol{k}_i \cdot \boldsymbol{x})\sigma_\lambda \epsilon^{(i)*}_\lambda \begin{pmatrix} \mathrm{i}f_{\kappa_i E_i}(r)\chi^{\mu_i}_{-\kappa_i}(\Omega) \\ g_{\kappa_i E_i}(r)\chi^{\mu_i}_{\kappa_i}(\Omega) \end{pmatrix}. \tag{11}$$

The completeness properties of the spinor spherical harmonics allow the expansion

$$\begin{pmatrix} {}^{u}\mathcal{Q}^{(a)}(\boldsymbol{x}) \\ {}^{l}\mathcal{Q}^{(a)}(\boldsymbol{x}) \end{pmatrix} = \frac{1}{r}\sum_{\mu\kappa} \begin{pmatrix} Q^{(a)\mu}_{\kappa}(r)\chi^{\mu}_{\kappa}(\Omega) \\ \mathrm{i}P^{(a)\mu}_{\kappa}(r)\chi^{\mu}_{-\kappa}(\Omega) \end{pmatrix} \tag{12}$$

with the expansion coefficients

$$r^{-1}Q^{(a)\mu}_{\kappa}(r) = \langle \chi^{\mu}_{\kappa}(\Omega) | {}^{u}\mathcal{Q}^{(a)}(\boldsymbol{x}) \rangle \tag{13}$$

and

$$\mathrm{i}r^{-1}P^{(a)\mu}_{\kappa}(r) = \langle \chi^{\mu}_{-\kappa}(\Omega) | {}^{l}\mathcal{Q}^{(a)}(\boldsymbol{x}) \rangle. \tag{14}$$

A similar expansion

$$F^{(a)}(\boldsymbol{x}) = \frac{1}{r}\sum_{\mu\kappa} \begin{pmatrix} S^{(a)\mu}_{\kappa}(r)\chi^{\mu}_{\kappa}(\Omega) \\ \mathrm{i}R^{(a)\mu}_{\kappa}(r)\chi^{\mu}_{-\kappa}(\Omega) \end{pmatrix} \tag{15}$$

and the use of the orthogonality properties of the χ^{μ}_{κ} reduces equation (7) to the inhomogeneous Dirac equations (cf. Johnson and Feiock 1968)

$$A(r, E = E_i + \omega_i)\begin{pmatrix} S^{(a)\mu}_{\kappa}(r) \\ R^{(a)\mu}_{\kappa}(r) \end{pmatrix} = \begin{pmatrix} P^{(a)\mu}_{\kappa}(r) \\ -Q^{(a)\mu}_{\kappa}(r) \end{pmatrix}. \tag{16}$$

For heavy atoms it is necessary to consider only electron transitions to continuous states and, as no observation is made upon the atomic electron after collision, the

asymptotic form of these states is unimportant. With the choice (10) for ψ_{E_f}, the function

$$\Pi^{(a)}(\boldsymbol{x}) = -\boldsymbol{\alpha}^{\dagger} \cdot \boldsymbol{\epsilon}^{(f)} \exp(\mathrm{i}\boldsymbol{k}_f \cdot \boldsymbol{x})\psi_{E_f} \tag{17}$$

can be expanded in the same manner as $\mathcal{Q}^{(a)}(\boldsymbol{x})$ above, the expansion coefficients in this case being denoted $L^{(a)\mu}_{\kappa}(r)$ and $M^{(a)\mu}_{\kappa}(r)$. Consequently, with the orthogonality of the χ^{μ}_{κ}, the transition amplitude

$$\mathscr{M}^{(a)}_{fi} = \frac{\mathrm{i}\alpha}{2\pi}(\omega_i\omega_f)^{-1/2}\int \mathrm{d}^3x\, \Pi^{(a)\dagger}(\boldsymbol{x})F^{(a)}(\boldsymbol{x}) \tag{18}$$

becomes

$$\mathscr{M}^{(a)}_{fi} = \frac{\mathrm{i}\alpha}{2\pi}(\omega_i\omega_f)^{-1/2}\sum_{\mu\kappa}\int_0^{\infty} \mathrm{d}r\{L^{(a)\mu}_{\kappa}{}^*(r)S^{(a)\mu}_{\kappa}(r) + M^{(a)\mu}_{\kappa}{}^*(r)R^{(a)\mu}_{\kappa}(r)\}. \tag{19}$$

3. Derivation and reduction of differential cross section

With the expansion

$$\exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}) = 4\pi \sum_n \sum_m \mathrm{i}^n \mathrm{j}_n(\omega r)\, Y^{m*}_n(\hat{\boldsymbol{k}})\, Y^m_n(\Omega)$$

where the $\mathrm{j}_n(\omega r)$ are the spherical Bessel functions of order n, the expansion coefficients (13) and (14) are

$$\begin{pmatrix} Q^{(a)\mu}_{\kappa}(r) \\ P^{(a)\mu}_{\kappa}(r) \end{pmatrix} = \mp 4\pi\mathrm{i} \sum_{mn\lambda} \mathrm{i}^n \mathrm{j}_n(\omega_i r)\, Y^{m*}_n(\hat{\boldsymbol{k}}_i)\epsilon^{(i)*}_{\lambda} \begin{pmatrix} f_{\kappa_i E_i}(r) I^m_{n\lambda}(\kappa, -\kappa_i) \\ g_{\kappa_i E_i}(r) I^m_{n\lambda}(-\kappa, \kappa_i) \end{pmatrix}. \tag{20}$$

The matrix element

$$I^m_{n\lambda}(\kappa, -\kappa_i) = \langle \chi^{\mu}_{\kappa}(\Omega) | \sigma_{\lambda} Y^m_n(\Omega) | \chi^{\mu_i}_{-\kappa_i}(\Omega) \rangle \tag{21}$$

has been evaluated with the aid of the Wigner–Eckart theorem by Alling and Johnson (1965). They obtain

$$I^m_{n\lambda}(\kappa, -\kappa_i) = \left(\frac{3}{4\pi}\right)^{1/2} \frac{[l_i'][n]}{[l]}\, [C](l_i' n l; 00)\delta_{m,\mu-\mu_i-\lambda} J_{n\lambda}(\kappa, -\kappa_i) \tag{22}$$

where

$$J_{n\lambda}(\kappa, -\kappa_i) = \sqrt{2}[l][j_i] \sum_f [f] W(nl_i' j\tfrac{1}{2} lf) W(1\tfrac{1}{2} f l_i' \tfrac{1}{2} j_i) C(nfj; \mu-\mu_i-\lambda, \mu_i+\lambda)$$
$$\times C(j_i 1 f; \mu_i, \lambda). \tag{23}$$

$W(abcdef)$ is the Racah coefficient and $[a] = (2a+1)^{1/2}$.

The corresponding results for the coefficients $L^{(a)\mu}_{\kappa}$ and $M^{(a)\mu}_{\kappa}$ are obtained by the replacements $(\omega_i, \boldsymbol{k}_i) \to (\omega_f, \boldsymbol{k}_f)$, $\epsilon^{(i)*} \to \epsilon^{(f)}$ and $(\kappa_i E_i) \to (\kappa_f E_f)$ in the above results.

The following calculations are greatly simplified by choosing the coordinate system such that $\hat{\boldsymbol{k}}_i$ is along the z axis and $\hat{\boldsymbol{k}}_f$ lies in the x–z plane and makes an angle $\Theta = \cos^{-1}(\hat{\boldsymbol{k}}_i \cdot \hat{\boldsymbol{k}}_f)$ with the z axis. Thus

$$Y^m_n(\hat{\boldsymbol{k}}_i) = \frac{[n]}{(4\pi)^{1/2}}\delta_{m,0}$$

and

$$Y_n^{m*}(\hat{\boldsymbol{k}}_f) = \frac{[n]}{(4\pi)^{1/2}} D_{m,0}^{n}(0, \Theta, 0)$$

where $D_{mm'}^{j}(\alpha\beta\gamma)$ is the Wigner rotation matrix for a rotation through the Euler angles α, β and γ. (The phase convention is that of Rose 1957.)

The expansion coefficients can now be written

$$\begin{pmatrix} Q^{(a)\mu}_{\kappa}(r) \\ P^{(a)\mu}_{\kappa}(r) \end{pmatrix} = \sum_{nf} a^{(a)\mu}_{nf\kappa} \begin{pmatrix} Q^{(a)}_{nf\kappa}(r) \\ P^{(a)}_{nf\kappa}(r) \end{pmatrix} \tag{24}$$

and

$$\begin{pmatrix} L^{(a)\mu}_{\kappa}(r) \\ M^{(a)\mu}_{\kappa}(r) \end{pmatrix} = \sum_{nf} b^{(a)\mu}_{nf\kappa} \begin{pmatrix} L^{(a)}_{nf\kappa}(r) \\ M^{(a)}_{nf\kappa}(r) \end{pmatrix} \tag{25}$$

where all dependence on projection quantum numbers and photon polarizations is carried in the coefficients

$$a^{(a)\mu}_{nf\kappa} = \mathrm{i}^{n-1}\sqrt{6}[n][f][j_i]C(nfj; 0\mu)C(j_i 1f; \mu_i, \mu-\mu_i)\epsilon^{(i)*}_{\mu-\mu_i} \tag{26}$$

$$b^{(a)\mu}_{nf\kappa} = \mathrm{i}^{n-1}\sqrt{6}[n][f][j_f] \sum_{\lambda} C(nfj; \mu-\mu_f-\lambda, \mu_f+\lambda)C(j_f 1f; \mu_f, \lambda) \times D^{n}_{\mu-\mu_f-\lambda,0}(0, \Theta, 0)\epsilon^{(f)*}_{\lambda} \tag{27}$$

and the radial dependence is restricted to the factors

$$Q^{(a)}_{nf\kappa}(r) = (-1)^{l_i} f_{\kappa_i E_i}(r)\mathrm{j}_n(\omega_i r)[l][l_i']C(l_i' l n; 00)W(nl_i' j\tfrac{1}{2} lf)W(1\tfrac{1}{2} fl_i'\tfrac{1}{2} j_i) \tag{28}$$

$$P^{(a)}_{nf\kappa}(r) = -(-1)^{l_i} g_{\kappa_i E_i}(r)\mathrm{j}_n(\omega_i r)[l'][l_i]C(l_i l' n; 00)W(nl_i j\tfrac{1}{2} l' f)W(1\tfrac{1}{2} fl_i\tfrac{1}{2} j_i). \tag{29}$$

The factors $L^{(a)}_{nf\kappa}(r)$ and $M^{(a)}_{nf\kappa}(r)$ are obtained from $Q^{(a)}_{nf\kappa}(r)$ and $P^{(a)}_{nf\kappa}(r)$ respectively by the replacements $(\kappa_i E_i \omega_i) \to (\kappa_f E_f \omega_f)$.

Defining the functions

$$\begin{pmatrix} S^{(a)\mu}_{\kappa}(r) \\ R^{(a)\mu}_{\kappa}(r) \end{pmatrix} = \sum_{nf} a^{(a)\mu}_{nf\kappa} \begin{pmatrix} S^{(a)}_{nf\kappa}(r) \\ R^{(a)}_{nf\kappa}(r) \end{pmatrix} \tag{30}$$

which are obtained as solutions of

$$A(r, E = E_i + \omega_i)\begin{pmatrix} S^{(a)}_{nf\kappa}(r) \\ R^{(a)}_{nf\kappa}(r) \end{pmatrix} = \begin{pmatrix} P^{(a)}_{nf\kappa}(r) \\ -Q^{(a)}_{nf\kappa}(r) \end{pmatrix} \tag{31}$$

the transition amplitude $\mathscr{M}^{(a)}_{fi}$ becomes

$$\mathscr{M}^{(a)}_{fi} = \frac{\mathrm{i}\alpha}{2\pi}(\omega_i\omega_f)^{-1/2} \sum_{\mu\kappa} \sum_{nf} \sum_{n'f'} \alpha^{(a)}{}_{\kappa}{}^{\mu}(n'f'nf)X^{(a)}_{\kappa}(n'f'nf) \tag{32}$$

where

$$\alpha^{(a)\mu}_{\kappa}(n'f'nf) = b^{(a)}_{n'f'\kappa}{}^{\mu *}\, a^{(a)\mu}_{nf\kappa} \tag{33}$$

and

$$X^{(a)}_{\kappa}(n'f'nf) = \int_0^{\infty} \mathrm{d}r\{L^{(a)*}_{n'f'\kappa}(r)S^{(a)}_{nf\kappa}(r) + M^{(a)*}_{n'f'\kappa}(r)R^{(a)}_{nf\kappa}(r)\}. \tag{34}$$

The corresponding results for $\mathcal{M}_{fi}^{(e)}$ follow from the above results for $\mathcal{M}_{fi}^{(a)}$ by noting that $\alpha^{(e)} = \alpha^{(a)}(\kappa_i\mu_i \leftrightarrow \kappa_f\mu_f)$, by interchanging ω_i and ω_f in the radial functions (28) and (29) and by solving

$$A(r, E = E_i - \omega_f)\begin{pmatrix} S_{nf\kappa}^{(e)}(r) \\ R_{nf\kappa}^{(e)}(r) \end{pmatrix} = \begin{pmatrix} P_{nf\kappa}^{(e)}(r) \\ -Q_{nf\kappa}^{(e)}(r) \end{pmatrix}.$$

As we are interested in the differential cross section for the scattering of unpolarized photons by all of the electrons in a specified atomic shell or subshell, no reference being made to the final state of the atomic electron, the transition probability per unit time

$$\mathrm{d}P_{fi} = \frac{1}{2\pi}\delta(E_f + \omega_f - E_i - \omega_i)|\mathcal{M}_{fi}|^2 \mathrm{d}^3k_f$$

where $\mathcal{M}_{fi}\,(= \mathcal{M}_{fi}^{(a)} + \mathcal{M}_{fi}^{(e)})$ must be averaged over incident, and summed over final, photon polarizations; summed over all possible initial and final electron states and divided by the incident photon flux $(2\pi)^{-3}$. Thus the differential cross section for the scattering of unpolarized photons through an angle Θ into the solid angle $\mathrm{d}\Omega$ and energy interval $\mathrm{d}\omega_f$ is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega\,\mathrm{d}\omega_f} = \frac{(2\pi)^2}{2}\sum_{\rho_i\rho_f}\sum_{\kappa_f\mu_f}\sum_{\mu_i}\omega_f^2|\mathcal{M}_{fi}|^2. \tag{35}$$

With the expansion (32) for $\mathcal{M}_{fi}$, the differential cross section for all photons scattered into $\mathrm{d}\Omega$ is

$$\begin{aligned}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\alpha^2}{2}\sum_{\kappa_f\bar{\kappa}\kappa}\sum_{\bar{\beta}\beta}\int \mathrm{d}\omega_f \frac{\omega_f}{\omega_i}\,[&B_1(\bar{\kappa}\bar{\beta}\,\kappa\beta)X_{\bar{\kappa}\bar{\beta}}^{(a)*}X_{\kappa\beta}^{(a)} + B_3(\bar{\kappa}\bar{\beta}\,\kappa\beta)X_{\bar{\kappa}\bar{\beta}}^{(e)*}X_{\kappa\beta}^{(e)} \\ &+ 2\mathrm{Re}\{B_2(\bar{\kappa}\bar{\beta}\,\kappa\beta)X_{\bar{\kappa}\bar{\beta}}^{(a)*}X_{\kappa\beta}^{(e)}\}]\end{aligned} \tag{36}$$

where the integration over final photon energies is taken between the limits zero and $E_i + \omega_i - 1$, the B coefficients are

$$\begin{aligned} B_1(\bar{\kappa}\bar{\beta}\kappa\beta) &= \sum_{\eta}\alpha_{\bar{\kappa}\bar{\beta}}^{(a)\bar{\mu}*}\alpha_{\kappa\beta}^{(a)\mu} \\ B_2(\bar{\kappa}\bar{\beta}\kappa\beta) &= \sum_{\eta}\alpha_{\bar{\kappa}\bar{\beta}}^{(a)\bar{\mu}*}\alpha_{\kappa\beta}^{(e)\mu} \\ B_3(\bar{\kappa}\bar{\beta}\kappa\beta) &= \sum_{\eta}\alpha_{\bar{\kappa}\bar{\beta}}^{(e)\bar{\mu}*}\alpha_{\kappa\beta}^{(e)\mu} \end{aligned} \tag{37}$$

and the parameters β and η denote the sets of indices $(n'f'nf)$ and $(\mu\bar{\mu}\rho_i\rho_f\mu_i\mu_f)$ respectively.

The completeness relation

$$\sum_{\rho=\pm 1}\epsilon_m^{(\rho)*}(\hat{\boldsymbol{k}})\epsilon_n^{(\rho)}(\hat{\boldsymbol{k}}) = \delta_{m,n} - \frac{4\pi}{3}Y_1^{m*}(\hat{\boldsymbol{k}})\,Y_1^n(\hat{\boldsymbol{k}})$$

for the vectors $\boldsymbol{\epsilon}^{(1)}$, $\boldsymbol{\epsilon}^{(-1)}$ and $\hat{\boldsymbol{k}}$ in a spherical basis, is used to perform the summations over the photon polarizations. With the chosen orientation of the coordinate system, the polarization sums are

$$\sum_{\rho_i}\epsilon_m^{(\rho_i)*}\epsilon_n^{(\rho_i)} = \delta_{m,n} - \delta_{m,0}\delta_{n,0} \tag{38}$$

and

$$\sum_{\rho_f}\epsilon_m^{(\rho_f)*}\epsilon_n^{(\rho_f)} = \delta_{m,n} - D_{m,0}^1(0, \Theta, 0)D_{n,0}^1(0, \Theta, 0). \tag{39}$$

In order to sum over the magnetic quantum numbers, the Clebsch–Gordan series (Rose 1957—§ 14) is used to reduce the products of rotation matrices to a single matrix of the form $D^t_{\rho,0}\ (0, \Theta, 0)$ and the resulting products of Clebsch–Gordan coefficients are then summed over using the relations of Rose (1957—§ 23). Details of these calculations are too lengthy to be included here but are given in Whittingham (1970—PhD thesis unpublished). We obtain

(i)
$$B_1(\bar\kappa\bar\beta\kappa\beta) = \mathrm{i}^{\bar n'+n-\bar n-n'}\sum_{i=1}^{4}\mathrm{B}^i_1(\bar\kappa\bar\beta\kappa\beta) \tag{40}$$

with

$$B^1_1(\bar\kappa\bar\beta\kappa\beta) = -(-1)^{f+f'}\delta_{f,\bar f}\delta_{f',\bar f'}36([j_i][j_f][f][f'])^2\sum_t Z(\bar n\bar jnjft)Z(\bar n'\bar jn'jf't)\mathrm{P}_t(\cos\Theta) \tag{41}$$

$$B^2_1(\bar\kappa\bar\beta\kappa\beta) = -(-1)^{f+f'+\bar f'+j_f}\delta_{f,\bar f}12\frac{([j_i][f'][f][\bar f'])^2}{[j][\bar j]}\sum_{uvt}Z(\bar n'\bar j1j_f\bar f'u)Z(n'j1j_ff'v)$$
$$\times Z(u\bar jvjj_ft)Z(\bar n\bar jnjft)\mathrm{P}_t(\cos\Theta) \tag{42}$$

$$B^3_1(\bar\kappa\bar\beta\kappa\beta) = B^2_1(\bar\kappa\bar\beta\kappa\beta)\{(j_i\bar nnf\bar f)\leftrightarrow(j_f\bar n'n'\bar f'f')\} \tag{43}$$

$$B^4_1(\bar\kappa\bar\beta\kappa\beta) = -(-1)^{f+f'+\bar f+\bar f'+j_i+j_f}b([j][\bar j])^{-2}\sum_{uvswt}Z(\bar n'\bar j1j_f\bar f'u)Z(n'j1j_{\bar j}f'v)$$
$$\times Z(\bar nj1j_i\bar fs)Z(nj1j_ifw)Z(u\bar jvjj_ft)Z(s\bar jwjj_it)\mathrm{P}_t(\cos\Theta) \tag{44}$$

(ii)
$$B_2(\bar\kappa\bar\beta\kappa\beta) = \mathrm{i}^{\bar n'+n'-\bar n-n}\sum_{i=1}^{3}B^i_2(\bar\kappa\bar\beta\kappa\beta) \tag{45}$$

with

$$B^1_2(\bar\kappa\bar\beta\kappa\beta) = (-1)^{\sigma-f-\bar f}9b\frac{[j_i]^2[j_f]^2[j][\bar j][n][\bar n']}{[f][\bar f']}\sum_{tuvw}\sum_\rho(-1)^v[u][v]$$
$$\times C(\bar n'nt;00)W(wf1j_i\bar f1)W(wf'1j_f\bar f'1)X(\bar n'nt;\bar f'jv;\bar jfu)$$
$$\times Z(\bar n\bar jwf\bar fu;0\rho)Z(n'jw\bar f'f'v;0\rho)C(uvt;\rho\rho)\left\{\frac{(t-2\rho)!}{(t+2\rho)!}\right\}^{1/2}\mathrm{P}^{2\rho}_t(\cos\Theta) \tag{46}$$

$$B^2_2(\bar\kappa\bar\beta\kappa\beta) = -(-1)^\sigma 2b\sum_{tuvws}(-1)^w[u][v][w][s]C(uvt;00)Z(\bar n'\bar j1j_f\bar f'u)$$
$$\times Z(nj1j_ifv)X(uvt;j_fjw;\bar jj_is)Z(\bar nj\bar j1j_i\bar fs;01)$$
$$\times Z(n'j1j_ff'w;01)C(swt;1,1)\left\{\frac{(t-2)!}{(t+2)!}\right\}^{1/2}\mathrm{P}^2_t(\cos\Theta) \tag{47}$$

$$B^3_2(\bar\kappa\bar\beta\kappa\beta) = (-1)^\sigma b[n][n']\sum_{tuvws}\sum_\rho(-1)^v[u][v]C(\bar n'nt;00)Z(n'j1j_ff'w)$$
$$\times Z(\bar nj\bar j1j_i\bar fs)X(\bar n'nt;\bar f'jv;\bar jfu)Z(u\bar j1j_ifs;\rho,-\rho)Z(vj1j_f\bar f'w;\rho,-\rho)$$
$$\times C(uvt;\rho\rho)\left\{\frac{(t-2\rho)!}{(t+2\rho)!}\right\}^{1/2}\mathrm{P}^{2\rho}_t(\cos\Theta) \tag{48}$$

and

(iii)
$$B_3(\bar\kappa\bar\beta\kappa\beta) = B_1(\bar\kappa\bar\beta\kappa\beta). \tag{49}$$

In these expressions, the constants b and σ are given by $b = 4([f][f'][\bar{f}][\bar{f}'])^2$ and $\sigma = \bar{n}'+j+\bar{j}+f+f'+\bar{f}+\bar{f}'$, $P_n^m(x)$ is the normalized associated Legendre polynomial of order n and degree m related to the rotation matrices via

$$D^n_{m,0}(0, \Theta, 0) = \left\{\frac{(n-m)!}{(n+m)!}\right\}^{1/2} P_n^m(\cos\Theta)$$

the coefficient

$$Z(abcdef; \alpha\beta) = [a][b][c][d]C(acf; \alpha\beta)W(abcdef)$$

is a generalization of the Z coefficient of Biedenharn *et al.* (1952), and $X(abe; cdf; ghi)$ is the X coefficient of Rose (1957—§ 35). The notation $P_t(\cos\Theta) = P_t^0(\cos\Theta)$ and $Z(abcdef) = Z(abcdef; 00)$ is employed. The limits on the summation parameters are determined from the triangle conditions for the vanishing of the angular momentum coefficients.

The B coefficients are real since $\bar{n}'+n-\bar{n}-n'$ and $\bar{n}'+n'-\bar{n}-n$ are even integers. In addition, since a rotation of the coordinate system so that the new z axis is along $\hat{\boldsymbol{k}}_f$ merely interchanges $\alpha^{(a)}$ and $\alpha^{(e)}$ while leaving the physical system unaltered, it is clear that the B coefficients are invariant under the interchanges $(j_i\bar{n}nff) \leftrightarrow (j_f\bar{n}'n'\bar{f}'f')$ and the identity (49) follows immediately.

4. The radial matrix elements

The radial matrix elements $X_{\kappa\beta}$, defined by equation (34), involve the solutions $S_{nf\kappa}(r)$ and $R_{nf\kappa}(r)$ of the inhomogeneous Dirac equations (31). The boundary conditions upon the solution of these equations are determined from the asymptotic form of the amplitude $F(x')$ introduced in § 2. This amplitude is the wave function of the electron after the first photon interaction and must, for large x', either vanish or represent a free electron, depending upon whether the electron is in a discrete or continuum state as a result of the interaction. The radial equations (31) have the asymptotic solutions

$$S(r) \simeq a\{\exp(\sigma r) + b\exp(-\sigma r)\}$$

$$R(r) \simeq \frac{\sigma}{E+1}\{a\exp(\sigma r) - b\exp(-\sigma r)\}$$

where $\sigma = (1-E^2)^{1/2}$. For the case in which the photon is emitted first, $E = E_i - \omega_f$ and σ is real for $\omega_i < 2$. Consequently, the radial functions must vanish at infinity. For the absorption first case, $E = E_i + \omega_i$ and σ is pure imaginary for all incident photon energies greater than the binding energy $B_i = 1 - E_i$ of the atomic electron. In this case we must therefore require $S_{nf\kappa}(r)$ and $R_{nf\kappa}(r)$ to be asymptotic to outgoing waves.

The method of Laplace integrals has been used (Johansson 1942, Forssner 1968) to obtain analytical solutions of (31) for the case where $V(r)$ is Coulombic and the initial state is that of a K electron. However, these solutions are unsuitable as they involve an expansion in αZ, and immediate recourse will be made here to numerical methods of solution.

As indicated by Brown and Schaefer (1956), the problem of numerical solution of inhomogeneous differential equations subject to two-point boundary conditions

can be avoided by using the variation of parameters method to solve the imhomogeneous Dirac equations in the form

$$\begin{pmatrix} S_{nf\kappa}(r) \\ R_{nf\kappa}(r) \end{pmatrix} = -\frac{1}{\Delta_\kappa(E)}\left\{\begin{pmatrix} {}^0S_\kappa(r) \\ {}^0R_\kappa(r) \end{pmatrix}\int_r^\infty \mathrm{d}x\{{}^\infty S_\kappa(x)Q_{nf\kappa}(x)+{}^\infty R_\kappa(x)P_{nf\kappa}(x)\}\right.$$
$$\left.+\begin{pmatrix} {}^\infty S_\kappa(r) \\ {}^\infty R_\kappa(r) \end{pmatrix}\int_0^r \mathrm{d}x\{{}^0S_\kappa(x)Q_{nf\kappa}(x)+{}^0R_\kappa(x)P_{nf\kappa}(x)\}\right\}. \tag{50}$$

The functions

$$\begin{pmatrix} {}^0S_\kappa(r) \\ {}^0R_\kappa(r) \end{pmatrix} \text{ and } \begin{pmatrix} {}^\infty S_\kappa(r) \\ {}^\infty R_\kappa(r) \end{pmatrix}$$

hereafter denoted by ${}^0y_\kappa(r)$ and ${}^\infty y_\kappa(r)$, are the linearly independent sets of solutions regular at the origin and infinity respectively of the homogeneous Dirac equations. The Wronskian of these solutions is denoted by $\Delta_\kappa(E)$ and is independent of r. For the absorption first case, the solutions regular at infinity must be chosen to be asymptotic to outgoing waves.

In terms of the coefficients

$$\begin{aligned}
\lambda_1'(n'f'\kappa) &= (-1)^{l'}[l][l_f']C(l_f'ln';00)W(n'l_f'j\tfrac{1}{2}lf')W(1\tfrac{1}{2}f'l_f'\tfrac{1}{2}j_f) \\
\lambda_2'(n'f'\kappa) &= -\lambda_1'(n'f'\kappa)\{l\to l',\ l_f'\to l_f\} \\
\lambda_1(nf\kappa) &= \lambda_1'(nf\kappa)\{l_f'\to l_i',\ j_f\to j_i\} \\
\lambda_2(nf\kappa) &= -\lambda_1(nf\kappa)\{l_i'\to l_i,\ l\to l'\}
\end{aligned} \tag{51}$$

and the integrals

$$\begin{aligned}
{}^0I_{n\kappa}(r) &= \int_0^r f_{\kappa_i E_i}(x)\mathrm{j}_n(\omega x){}^0S_\kappa(x)\,\mathrm{d}x \\
{}^\infty I_{n\kappa}(r) &= \int_r^\infty f_{\kappa_i E_i}(x)\mathrm{j}_n(\omega x){}^\infty S_\kappa(x)\,\mathrm{d}x \\
\begin{pmatrix} {}^0J_{n\kappa}(r) \\ {}^\infty J_{n\kappa}(r) \end{pmatrix} &= \begin{pmatrix} {}^0I_{n\kappa}(r) \\ {}^\infty I_{n\kappa}(r) \end{pmatrix}\{f_{\kappa_i E_i}\to g_{\kappa_i E_i},\ S_\kappa\to R_\kappa\}
\end{aligned} \tag{52}$$

the radial matrix elements have the factorized form

$$X_{\kappa\beta} = \alpha_1(\kappa\beta)I_{n'n\kappa}+\alpha_2(\kappa\beta)J_{n'n\kappa}+\alpha_3(\kappa\beta)U_{n'n\kappa}+\alpha_4(\kappa\beta)V_{n'n\kappa}. \tag{53}$$

The dependance of $X_{\kappa\beta}$ upon f and f' is restricted to the coefficients

$$\alpha_{2(i-1)+j}(\kappa\beta) = \lambda_i'(n'f'\kappa)\lambda_j(nf\kappa) \qquad (i,j=1,2) \tag{54}$$

while the f-independent integrals are

$$\begin{pmatrix} I_{n'n\kappa} \\ J_{n'n\kappa} \end{pmatrix} = -\frac{1}{\Delta_\kappa(E)}\int_0^\infty \mathrm{d}r f^*_{\kappa_f E_f}(r)\mathrm{j}_{n'}(\omega' r)\left\{{}^0S_\kappa(r)\begin{pmatrix} {}^\infty I_{n\kappa}(r) \\ {}^\infty J_{n\kappa}(r) \end{pmatrix}+{}^\infty S_\kappa(r)\begin{pmatrix} {}^0I_{n\kappa}(r) \\ {}^0J_{n\kappa}(r) \end{pmatrix}\right\} \tag{55}$$

$$\begin{pmatrix} U_{n'n\kappa} \\ V_{n'n\kappa} \end{pmatrix} = \begin{pmatrix} I_{n'n\kappa} \\ J_{n'n\kappa} \end{pmatrix}\{f_{\kappa_f E_f}\to g_{\kappa_f E_f},\ S_\kappa\to R_\kappa\}. \tag{56}$$

In these, and the following expressions, $\omega=\omega_i$, $\omega'=\omega_f$, $E=E_i+\omega_i$ for the absorption first case; $\omega=\omega_f$, $\omega'=\omega_i$, $E=E_i-\omega_f$ for the emission first case.

Insertion of (53) for $X_{\kappa\beta}$ into (36) finally yields the differential cross section as a combination of the radial integrals I_γ, J_γ, U_γ and V_γ, $(\gamma = (\kappa n' n))$, and the 32 coefficients

$$h^k_m(\bar\gamma\gamma) = \sum_{\bar f \bar f'} \sum_{f f'} \alpha_i(\bar\kappa\bar\beta)\alpha_j(\kappa\beta)B_k(\bar\kappa\bar\beta\kappa\beta) \tag{57}$$

where $k = 1, 2$; $i, j = 1, ..., 4$ and $m = 4(i-1)+j = 1, ..., 16$. That is

$$\frac{\mathrm{d}\sigma(E_i\omega_i\Theta)}{\mathrm{d}\Omega} = \frac{\alpha^2}{2}\sum_{\kappa_f}\sum_{\bar\gamma\gamma}\int \mathrm{d}\omega_f \frac{\omega_f}{\omega_i}(A^{(a)}+B+A^{(e)}) \tag{58}$$

where, for example

$$A^{(a)} = h^1_1(\bar\gamma\gamma)I^{(a)*}_{\bar\gamma}I^{(a)}_\gamma + h^1_2(\bar\gamma\gamma)I^{(a)*}_{\bar\gamma}J^{(a)}_\gamma + \ \dots\ + h^1_{16}(\bar\gamma\gamma)V^{(a)*}_{\bar\gamma}V^{(a)}_\gamma \tag{59}$$

and

$$B = 2\,\mathrm{Re}\{h^2_1(\bar\gamma\gamma)I^{(a)*}_{\bar\gamma}I^{(e)}_\gamma + h^2_2(\bar\gamma\gamma)I^{(a)*}_{\bar\gamma}J^{(e)}_\gamma + \ \dots\ + h^2_{16}(\bar\gamma\gamma)V^{(a)*}_{\bar\gamma}V^{(e)}_\gamma\}. \tag{60}$$

The radial integrals (55) and (56) involve several sets of continuum and discrete state solutions of the homogeneous Dirac equations. Before discussing these solutions some comments are required about the form of the potential function $V(r)$. The major contribution to the radial integrals is expected from the region $r \lesssim 1/\Delta k$ (Randles 1957), where $\Delta k = |\boldsymbol{k}_i - \boldsymbol{k}_f|$ is the momentum transfer to the atom. For medium to large angle scattering, where incoherent scattering is the dominant process, and for $\omega_i \simeq 1$, the momentum transfer is approximately unity and the interaction occurs mainly in the immediate neighbourhood of the nucleus. In this region the atomic wave functions differ from the pure Coulombic form only in normalization (Brysk and Rose 1958, Pratt 1960) and consequently the major effects of electron screening upon the differential cross section are restricted to a change in the initial bound state normalization factor. For Z greater than 75, this change is of the order of 0·01% and 0·1% for K and L electrons respectively and there is no significant loss of accuracy by choosing $V(r)$ to be Coulombic.

For $V(r) = -\alpha Z/r$, the required radial functions can be expressed in terms of the confluent hypergeometric function ${}_1F_1(a, c, x)$. However, for the continuum states, the parameters a and x are complex and the computation of ${}_1F_1(a, c, x)$ involves the summation of a slowly convergent complex series. Consequently we choose to integrate the Dirac equation directly for each required function, a procedure which has the added advantage that only minor alterations are required for the consideration of non-Coulombic potentials.

5. Numerical integration

The discrete state solutions ${}^0y^{(e)}_\kappa(r)$ and ${}^\infty y^{(e)}_\kappa(r)$ behave as $r^{\pm\gamma}$, $\gamma = \{\kappa^2-(\alpha Z)^2\}^{1/2}$, and $\exp(\pm\lambda r)$, $\lambda = (1-E^2)^{1/2}$, for small and large r respectively. For large γ and λ it is essential to introduce the smoothed functions (Brown and Mayers 1959)

$${}^{(0,\infty)}\mathscr{Y}^{(e)}_\kappa(r) = r^{\pm\gamma}\exp(\pm\lambda r)^{(0,\infty)}y^{(e)}_\kappa(r) \tag{61}$$

which satisfy the modified differential equations

$$\mathscr{Y}'_\kappa = a(r, \gamma, \lambda)\mathscr{Y}_\kappa(r) \tag{62}$$

where

$$a(r,\gamma,\lambda)=\begin{pmatrix} -\dfrac{\kappa\pm\gamma}{r}\mp\lambda & E\div 1+\dfrac{\alpha Z}{r} \\ 1-E-\dfrac{\alpha Z}{r} & \dfrac{\kappa\mp\gamma}{r}\mp\lambda \end{pmatrix}. \tag{63}$$

Here the upper and lower signs refer to the functions regular at $r=0$ and $r=\infty$ respectively, and $y'(r)$ denotes differentiation with respect to r. The functions regular at the origin are obtained by outward integration of (62) from the origin, the starting values being generated by series approximations for $\mathscr{Y}^{(e)}(r)$ near the origin. The functions regular at infinity are obtained by inward integration from a point $r_{\inf}$ where the asymptotic form of the Coulombic solutions can be used as starting values. The determination of $r_{\inf}$ will be discussed later.

For the case where the photon is first absorbed, the solutions ${}^0y^{(a)}(r)$ are chosen to be the set of (real) continuum states which are regular at the origin and asymptotic to standing waves. These solutions increase as r^γ until the point $r_s \simeq |\kappa|/p$, $p=(E^2-1)^{1/2}$, where they become oscillatory with approximately constant amplitude. Following Pratt *et al.* (1964) and Schmickley and Pratt (1967), the smoothed functions

$${}^0\mathscr{Y}^{(a)}_\kappa(r)=r^{-\gamma}\,{}^0y^{(a)}_\kappa(r) \tag{64}$$

are integrated outwards from $r=0$ until the first maximum or minimum of ${}^0y^{(a)}$ is reached, where a switch is made to the computation of ${}^0y^{(a)}(r)$. The starting values are again obtained from series approximations about the origin.

The solutions which are asymptotic to outgoing waves at infinity are evaluated from the combination

$${}^\infty y^{(a)}_\kappa(r)={}^0y^{(a)}_\kappa-\mathrm{i}[{}^0y^{(a)}_\kappa(r)]_{\mathrm{irreg}} \tag{65}$$

of the normalized regular standing wave solutions ${}^0y^{(a)}_\kappa$ and the irregular standing wave solutions $[{}^0y^{(a)}_\kappa]_{\mathrm{irreg}}$. The irregular solutions are computed by inward integration of the differential equations from the point $r=120$ where the potential can be neglected and the asymptotic (free field) solutions are valid. This integration is pursued to $r=r_s$ where a switch is made to the computation of the smoothed functions

$$[{}^0\mathscr{Y}^{(a)}_\kappa]_{\mathrm{irreg}}=r^\gamma[{}^0y^{(a)}_\kappa]_{\mathrm{irreg}}. \tag{66}$$

The differential equations are integrated with the fifth-order Adams–Bashforth–Moulton predictor-corrector system (cf. Smith and Johnson 1967), a modifier being used to replace the iteration of the corrector. The rapid propagation of initial errors that arises from the r^{-1} term in $a(r,\gamma,\lambda)$ during the outward integrations is controlled by the use of the series expansions for the first $2|\kappa|$ points of the integration mesh. The expected constancy of the Wronskian of the two sets of solutions provides a useful check on the accuracy of the integration procedures.

Integrals of the type ${}^0I_{n\kappa}(r)$ and ${}^\infty I_{n\kappa}(r)$ are smoothed and computed as solutions of their associated first-order differential equations (cf. Brown and Mayers 1959), while Bodes integration formula is used for the quadrature of the final state integrals I_γ, J_γ, U_γ and V_γ. The practical upper limit $r_{\inf}$ and the integration interval h are determined from the asymptotic form of a typical integrand

$$u_{n'n\kappa}(r)=f_{\kappa_f E_f}(r)\mathrm{j}_{n'}(\omega' r)\{{}^0S_\kappa(r)\,{}^\infty I_{n\kappa}(r)+{}^\infty S_\kappa(r)\,{}^0I_{n\kappa}(r)\} \tag{67}$$

of these final state integrals. For the emission first case, the choice $r_{\text{inf}} = 20/\lambda_i$ ensures that $f_{\kappa_f E_f}(r)$ and $j_{n'}(\omega' r)$ have attained their oscillatory regions and that the integrand $u(r)$ is exponentially decreasing. However, for the absorption first case, $u(r)$ has the asymptotic behaviour of $\sin(br)/r$ for $r = 20/\lambda_i$ and a convergence factor $\exp(-\nu r)$ must be inserted. Computation of the integrals for several values of ν and extrapolation to $\nu = 0$ is avoided by the use of the result of Zerby and Brysk (1966)

$$I = \int_0^{\infty} u(r)\,\mathrm{d}r = \int_0^{r_{\text{inf}}} [1-\{1-\exp(-ar)\}^n]u(r)\,\mathrm{d}r$$

which is based upon a nth-order Lagrangian interpolation formula. The parameters $a = \nu_{i+1} - \nu_i$ and n can be chosen for optimum convergence.

The most rapidly varying factor in the integrand (67) has a period of $2\pi/|\omega_i + p_f|$ and $2\pi/|\omega_f + p_f + p|$, where $p = \{(E_i+\omega_i)^2 - 1\}^{1/2}$ and $p_f = (E_f^2 - 1)^{1/2}$, for the emission first and absorption first cases respectively. For K shell scattering the choice $h = 0{\cdot}1$ therefore ensures that the integrations use at least 12 ordinates per period of the rapidly varying functions.

Finally, a composite Simpson's rule is used to integrate over the scattered photon energy ω_f in terms of the momentum p_f of the continuum electron.

6. Results and discussion

The present calculations of the differential cross section and the energy spectrum of the scattered photons are restricted to the important case of the scattering of 662 keV gamma rays by the K electrons of lead and are presented in table 1.

Table 1. Energy spectrum† and differential cross sections‡ for scattering of 662 keV photons by K electrons of Pb

	Energy spectrum							Differential cross section
θ(deg) \ $p_f(mc)$ / $\omega_f(mc^2)$	0·230 / 1·071	0·461 / 0·996	0·691 / 0·881	0·921 / 0·737	1·152 / 0·571	1·382 / 0·391	1·613 / 0·199	
0	5·49	4·07	2·42	1·30	0·97	0·85	0·80	1·75
20	10·5	7·75	4·50	2·04	1·00	0·88	0·88	2·79
40	11·9	10·3	7·05	3·84	1·93	1·14	0·93	3·94
60	4·47	5·62	6·10	4·87	2·79	1·38	1·01	3·33
80	1·60	2·37	3·78	4·79	3·72	1·78	1·07	2·75
100	0·74	1·22	2·26	3·81	4·20	2·21	1·14	2·48
120	0·51	0·77	1·38	2·50	3·72	2·87	1·49	2·21
140	0·24	0·53	0·96	1·70	2·84	3·30	2·34	2·09
160	0·05	0·21	0·69	1·46	2·28	2·84	2·76	1·89
180	0·03	0·19	0·56	1·22	2·37	2·92	2·87	1·90

†Relativistic units $\times 10^{-5}(2{\cdot}92 \times 10^{-29}$ cm^2 keV^{-1} sr^{-1}).
‡Relativistic units $\times 10^{-5}(1{\cdot}49 \times 10^{-26}$ cm^2 sr^{-1}).

In § 4 the differential cross section was expressed as an infinite series in κ, $\bar{\kappa}$ ($\leqslant \kappa$) and κ_f. These series were truncated when the radial integrals had decreased sufficiently to ensure that the truncation error incurred was consistent with other sources of error within the calculation. The largest errors are of the order of 0·1% and arise from (i) the matching of the continuum irregular functions with the asymptotic

solutions and (ii) the convergence of the final state integrals for the absorption first case. With $|\kappa_{max}| = 8$ and $|(\kappa_f)_{max}| = 4$ most radial integrals had decreased by at least two orders of magnitude and the resulting error in the differential cross section is accordingly estimated to be approximately 1%.

The angular dependence of the ratio $d\sigma_K/d\sigma_F$ of the bound electron cross section $d\sigma_K$ and the free electron (Klein–Nishina) cross section $d\sigma_F$ is given in figure 1. The full relativistic results are significantly larger than the incoherent scattering

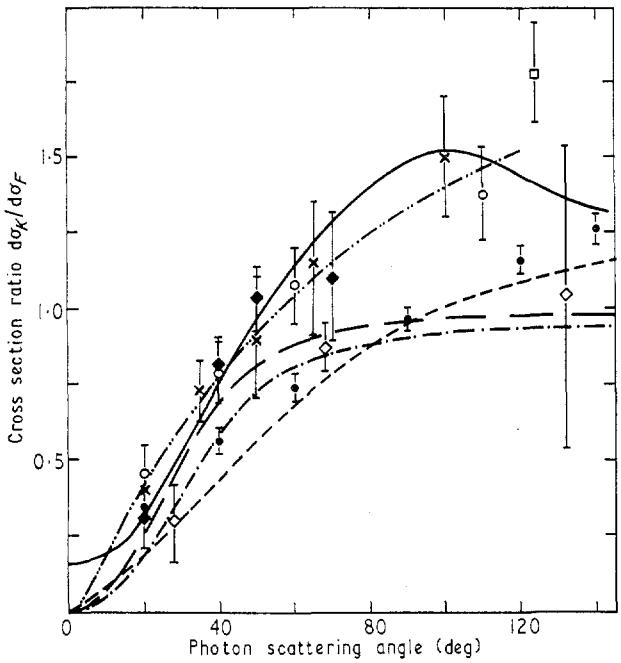

Figure 1. Angular dependence of cross section ratio $d\sigma_K/d\sigma_F$ for scattering of 662 keV photons. *Theoretical results*: ——— present work Pb; – · · – approximate relativistic theory of Di Lazzaro and Missoni (1966) Au; – – – – incoherent scattering function of Shimizu *et al.* (1965) Pb; — — non-relativistic scattering function of Sujkowski and Nagel (1961) Pb; – · – relativistic scattering function of Sujkowski and Nagel (1961) Pb. *Experimental results*: ◇ Sujkowski and Nagel (1961) Pb; ◇ Motz and Missoni (1961) Au; ◇ Varma and Eswaran (1962) Pb; ◇ Shimizu *et al.* (1965) Pb; ◆ Pingot (1968) Au; ◆ East and Lewis (1969) Au.

function calculations and agree well with the experimental results for scattering angles below 100°. The decrease in the cross section ratio for larger angles is probably spurious since the major contributions to $d\sigma_K$ correspond to high values of the continuum electron momentum (see table 1) for which the convergence of the κ_f summation is poorer. Available computing facilities do not allow any present improvement in the calculation of these high-angle cross sections.

The large difference between the present relativistic calculations and the predictions of the three incoherent scattering functions clearly indicates that for heavy atoms it is not valid to factorize the transition probability into a term representing the interaction of the photon with a free electron, and a term describing the transition

made by the electron as a consequence of the momentum transferred to it from the photon.

The non-zero cross section for zero-angle incoherent scattering of photons by bound electrons is in contrast with that for a free electron where the energy and momentum conservation relations allow only coherent scattering. However, momentum is not conserved in the interaction of a photon with a bound electron and the energy conservation relation allows incoherent scattering at all angles provided the electron undergoes a transition.

The differential cross sections per electron for incoherent and coherent scattering from K electrons, and for Compton scattering by a free electron, are shown in figure 2. For zero-angle scattering the incoherent process is significant while small in comparison with the coherent process, but for scattering angles above 33° the incoherent process becomes dominant with a maximum at 40°.

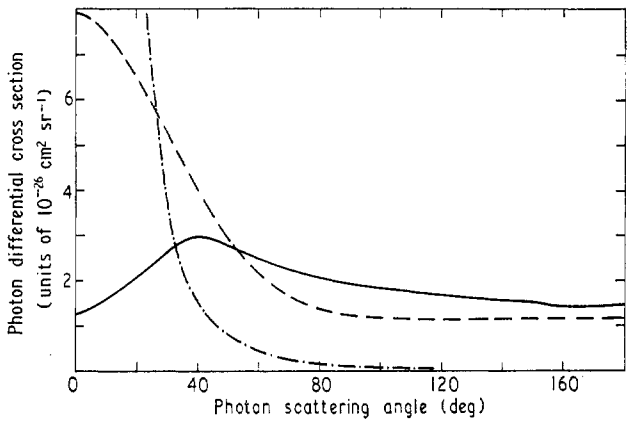

Figure 2. Differential cross sections for scattering of 662 keV photons: —— K electron incoherent scattering in Pb (present work); – – – free electron scattering (Klein–Nishina); – · – K electron coherent scattering in Hg (Brown and Mayers 1957).

The energy spectrum of gamma rays incoherently scattered by K electrons of heavy atoms has been measured by Varma and Eswaran (1962), Di Lazzaro and Missoni (1966) and East and Lewis (1969). Varma and Eswaran, and East and Lewis, found that the spectrum was broadened in relation to that of a free electron and that there was no significant shift of the peak of the spectrum from the free-electron Compton energy. However, Di Lazzaro and Missoni observed a peak shift of 10% towards lower photon energies and a marked increase in the spectrum at low scattered photon energies. These features were supported by their calculated energy spectrum.

The energy spectrum of 1·296 mc^2 photons scattered through 60° by the K shell of lead is presented in figure 3 and compared with the approximate non-relativistic spectrum of Schnaidt (1934). The shape of the spectrum is in accordance with that measured by Varma and Eswaran, and East and Lewis, and does not exhibit any increase at low energies. Although this region corresponds to high momentum of the continuum electron, and consequently the region of least accuracy in the computed results, any significant change in the shape of the photon spectrum with improved accuracy seems unlikely.

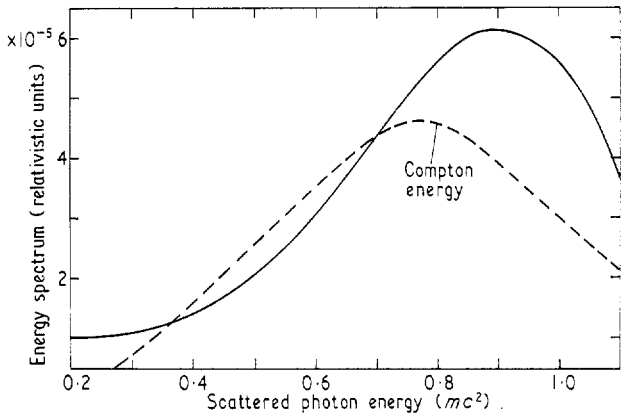

Figure 3. Energy spectrum of 1·296 mc^2 (662 keV) photons scattered through 60° by K electrons of Pb: —— relativistic (present work); – – non-relativistic (Schnaidt 1934).

The relativistic energy spectrum is shifted by 10% from the Compton energy but in the opposite direction to that obtained by Di Lazzaro and Missoni. The shift towards higher photon energies is in agreement with the early non-relativistic calculations of Wentzel (1929) and Bloch (1934) which predicted an energy shift

$$(\omega_f^{-1})_{\text{bound}} - (\omega_f^{-1})_{\text{free}} = -bB/\omega_i^2$$

where B is the binding energy of the atomic electron and b is a numerical constant of the order of unity. A peak shift of 10% for lead would require $b = 1{\cdot}3$. The disagreement between existing measurements of the scattered photon spectrum is due to the difficulty of correctly selecting only those scattering processes which are accompanied by the emission of a K x-ray, and any possible confirmation of a peak shift towards higher photon energies must await additional and improved experimental results.

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