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**K-SHELL COMPTON SCATTERING ON TIN AND GOLD AT
145 keV AND GOLD AT 320 keV**

Leon Arthur Wittwer

August 11, 1972

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**LAWRENCE
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University of California/Livermore

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LAWRENCE LIVERMORE LABORATORY
University of California, Livermore, California, 94550

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Ph. D. Thesis

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K-SHELL COMPTON SCATTERING ON TIN AND GOLD AT 145 keV AND GOLD AT 320 keV

Abstract

A numerical calculation is given for the inelastic K-shell cross sections of tin with an incident energy of 145 keV and of gold at 145 and 320 keV. The calculation is based on second-order perturbation theory. The bound initial state is the relativistic Hartree-Fock-Slater single-particle $1s_{1/2}$ eigenfunction for the particular element concerned. The relativistic scattering solutions are constructed from continuum total spin eigenfunctions of the self-consistent potential field of the parent configuration. The necessity of using both negative and positive energy eigenfunctions is demonstrated when the Dirac relativistic formalism is used. The calculated spectra are the sum of the Compton line and the infrared divergence, with the Compton line being dominant. The Compton line displays the Compton defect and line broadening found at higher incident energies. The Compton line is also almost entirely due to negative-energy, intermediate-state transitions. The infrared divergence, on the other hand, is due entirely to positive-energy, intermediate-state transitions.

I. Introduction

In recent years, several investigators¹⁻⁷ have measured K-shell Compton cross sections in heavy elements such as tin, gold, lead, and tantalum with an incident energy of 662 keV. Additional experiments⁸ are now in progress with tin, gold, iron, and holmium at incident energies of 145, 320 and 662 keV. The existing theoretical calculations^{3,5,8-10} modeling these experiments are of limited value in predicting the differential cross sections and in illuminating the details of the scattering processes. The present calculations are an attempt to remedy the situation by calculating the K-shell Compton cross sections of tin and gold at 145 keV and gold at 320 keV without the approximations and limitations characterizing the work hitherto. This work uses the standard second-order perturbation theory based on wave functions calculated from the relativistic self-consistent Hartree-Fock-Slater potential of the parent configuration.

These experiments and calculations are interesting because the binding effects of the initial electron are now significant in determining the dynamics of the scattering. Previous works are all characterized by having the incident photon energy much larger than the binding energy. For this physical situation, the effects of binding should be small.

The first work was done for the scattering of electrons out of light elements. In the thirties, DuMond and his associates¹¹⁻¹⁴ scattered K x rays from carbon, helium, and hydrogen. The Compton line was broadened as a result of Doppler shifting from the momentum distribution of the initial bound electron. The formula for the half-width so derived was

$$\lambda_{\frac{1}{2}} = 4v\lambda \sin (\theta/2)/c, \quad (1)$$

where

$\lambda_{\frac{1}{2}}$ = wavelength half-width,
 λ = incident photon wavelength,
 v = bound electron velocity, and
 θ = photon scattering angle.

The Compton defect was explained by Ross and Kirkpatrick¹⁶ as due to the scattering of the final electron out of the potential field of the final atomic configuration. Their work resulted in a modified form of the Compton formula,

$$\Delta\lambda = \frac{h}{mc} [1 - \cos (\theta)] - \frac{\lambda^2 kE}{hc}, \quad (2)$$

where

$\Delta\lambda$ = wavelength shift,
 λ = incident photon wavelength,
 E = binding energy,
 θ = photon scattering angle, and
 k = constant of order unity.

Bloch¹⁷ carried out a nonrelativistic screened hydrogenic calculation and theoretically verified these effects for light elements and loosely bound electrons.

More recent work for both light and heavy elements has been based on the impulsive nature of the scattering when the incident photon energy is larger than the initial electron binding energy. It is then assumed the photon-electron interaction occurs in times much smaller than that characteristic of the electron motion. Recently Eisenberger and Platzman¹⁸ demonstrated the usefulness and limits of applicability of the impulse approximation to the study of bound electron momentum distributions in light elements. For heavy elements, the incoherent scattering factor method uses the impulse concept in a very explicit manner. This method assumes the cross section to be the product of two factors. The first, the Klein-Nishina formula,¹⁹ is the probability that the initial electron will acquire some momentum and be scattered through some angle. The second factor, the incoherent scattering factor, is the probability that, having received some momentum, the electron will absorb energy and escape the atom. This method has been used to tabulate atomic Compton cross sections²⁰⁻²¹ and small-angle cross sections in heavy elements at 662 keV.⁵

Two other methods are used for heavy elements of particular note. The first method has been used with some success for large-angle scattering at 662 keV.^{3,5} It consists of assigning to the initial electron a velocity characteristic of its binding energy. The cross section for this velocity, given by Jauch and Rohrlich,²² is then averaged over all velocity directions for the final result. The limitation to large-angle scattering is to insure that the momentum transfer is large compared with the initial electron momentum.

The second method, the form factor method, is derived²³ from the dispersion formula for Compton scattering by assuming that binding can be neglected in the intermediate state. Randles²⁴ used this method to calculate the ratio of coherent to incoherent scattering for large angles at 1 MeV. Schumacher⁹ also used it to calculate cross sections for various electron shells in lead at 662 keV. He achieved reasonable success considering the extra approximations used above and beyond those of the method. He also noted that it was necessary to use relativistic wave functions in calculating the form factor.

Thus far, it has been assumed that the incident photon energy is considerably larger than the binding energy. For the present work, this assumption is no longer true and the just discussed methods are of doubtful applicability. In addition, Schumacher's calculation⁹ does imply the need for a relativistic treatment. The above methods do, to some degree, include relativistic effects, but it is not immediately obvious whether they are adequate in this respect. It is the unknown applicability of the present methods and the execution of the present experiments⁸ that supply the basic motivation for this work.

There are two general approaches that can be used to calculate such second-order processes without the approximations and limitations inherent in previous work. The first, used here, is standard second-order perturbation theory. The second is the Green's function approach as developed by Brown and others.²⁵ To avoid confusion with the present development, which begins with a Green's function equation, the Brown method solves the appropriate inhomogeneous coupled differential equation for the intermediate Green's function. In general, the Green's function is constructed out of unperturbed solutions of the central field of the parent configuration. The present development is begun in this manner to avoid any confusion in the use of both negative and positive energy eigenfunctions and their time propagation in the intermediate state. Brown's method has been used for coherent scattering²⁶⁻²⁸ and for one incoherent calculation.¹⁰ Unfortunately, the work was done with analytic wavefunctions and other approximations that make comparison with the present work rather difficult. Calculations²⁹ using the relativistic Hartree-Fock-Slater model for potentials and Brown's formalism are being contemplated so perhaps useful comparison as to ease of use and computational efficiency can be made in the future.

The present method allows more detailed examination of the intermediate processes such as the relative importance of the Feynman diagrams for Compton scattering. Aside from this comment, the relative merits of the two "rigorous" methods will have

to wait. Of note is a nonrelativistic analytic formalism by Gavrilla³⁰ which may be useful for some physical regimes.

The following sections, starting with the perturbation theory development, will detail the complete formalism used in the calculation. The last three sections discuss the computer codes, calculation details, results, conclusions, and summary.

II. Perturbation Solution for Compton Scattering

A quantum-mechanical wave function propagates as

$$\psi(r', t') = i\epsilon_\omega \int G(r', t'; r, t) \psi(r, t) d^3r, \quad (3)$$

where

$$\begin{aligned} \epsilon_\omega &= 1, \quad W > 0, \\ &= -1, \quad W < 0. \end{aligned}$$

The use of ϵ_ω anticipates the expansion of the Green's function in terms of positive and negative energy eigenfunctions where W is the energy of the particular members of the expansion set. The Green's function satisfies the following equation:

$$\left[i \frac{\partial}{\partial t'} - \frac{1}{\hbar} H(r', t') \right] G(r', t'; r, t) = \sigma^3(r' - r) \sigma(t' - t) \quad (4)$$

where

$$\begin{aligned} H(r', t') &= H_0(r') + V(r', t'), \\ H_0(r') &= \text{unperturbed Dirac Hamiltonian,} \\ V(r', t') &= \text{perturbation potential.} \end{aligned}$$

In the problem treated in this paper, $H_0(r')$ is the central field Dirac Hamiltonian and $V(r', t')$ is the photon interaction operator. The Green's function above, in general, cannot be found, but it can be approximated by a series in $G_0(r', t'; r, t)$, the unperturbed Green's function, where

$$\left[i \frac{\partial}{\partial t'} - \frac{1}{\hbar} H_0(r') \right] G_0(r', t'; r, t) = \sigma^3(r' - r) \sigma(t' - t), \quad (5)$$

$$\begin{aligned} G(r', t'; r, t) &= G_0(r', t'; r, t) + \frac{1}{\hbar} \int G_0(r', t'; r_i, t_i) \\ &\quad \times V(r_i, t_i) G_0(r_i, t_i; r, t) d^3r_i dt_i \\ &\quad + \frac{1}{\hbar^2} \int G_0(r', t'; r_j, t_j) V(r_j, t_j) G_0(r_j, t_j; r_i, t_i) \\ &\quad \times V(r_i, t_i) G_0(r_i, t_i; r, t) d^3r_i d^3r_j dt_i dt_j + \dots \quad (6) \end{aligned}$$

The last term is appropriate for Compton scattering and will be referred to as the Compton term. The unperturbed Green's function can be expressed as a time function times any complete set of solutions of the unperturbed Hamiltonian. The time function determines the direction of propagation in time. If the time direction is forward, the Green's function is called retarded. If it is backward, the function is called advanced Green's function. In terms of the spherical basic set, the unperturbed Green's function can be written as

$$\begin{aligned}
 G_0(r', t'; r, t) = & \lim_{\epsilon \rightarrow 0^+} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\omega(t' - t)}}{\omega + i\epsilon} d\omega \\
 & \left[\sum_{\kappa\nu} \int_{mc^2}^{\infty} \psi_{\kappa\nu}(qr') \psi_{\kappa\nu}^*(qr) e^{-\frac{1}{\hbar}(t' - t)W} dW \right. \\
 & \left. + \sum_{n\kappa\nu} \psi_{n\kappa\nu}(r') \psi_{n\kappa\nu}^*(r) e^{-\frac{1}{\hbar}(t' - t)W} \right]_{n\kappa} \\
 & + \lim_{\epsilon \rightarrow 0^+} \frac{-1}{2\pi} \int_{\infty}^{\infty} \frac{e^{-i\omega(t' - t)}}{\omega - i\epsilon} d\omega \\
 & \left[\sum_{\kappa\nu} \int_{\infty}^{-mc^2} \psi_{\kappa\nu}(qr') \psi_{\kappa\nu}^*(qr) e^{-\frac{1}{\hbar}(t' - t)W} dW \right]. \quad (7)
 \end{aligned}$$

The unperturbed Green's function above is the sum of a retarded and an advanced function. This is because the positive energy eigenfunction propagates forward and the negative energy eigenfunction propagates backward in time. The backward propagating negative energy electrons are dynamically equivalent to positrons going forward in time.

The unperturbed Green's function can also be expanded in scattering solutions. In the present work, only the positive energy portion of the expansion is needed.

$$G_0(r', t'; r, t) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\omega(t' - t)}}{\omega + i\epsilon} d\omega$$

$$\sum_{\eta} \int \psi_{\eta}(\vec{q} \cdot \vec{r}) \psi_{\eta}^{\ast}(\vec{q} \cdot \vec{r}') e^{-\frac{i}{\hbar}(t' - t)\omega} \frac{\omega}{\hbar^2 c^2} d\omega d\Omega_{\vec{q}}. \quad (8)$$

The first unperturbed Green's function on the right in the Compton term merely serves to propagate the initial electron state. The retarded portion of the unperturbed Green's function constructed from the spherical basic set is appropriate as the initial state is a positive energy bound state. The intermediate unperturbed Green's function is taken to be the entire spherical basis set expansion as the intermediate state can be either a negative or positive energy eigenfunction. The last unperturbed Green's function must give a result composed of scattering solutions so Eq. (8) is used.

The two interaction operators in the Compton term represent a photon absorption and emission event. Their roll in the Compton process can best be understood by use of the four Feynman diagrams needed to describe the alternative ways the scattering can occur.

As seen in the diagrams, either absorption or emission can occur first. The first two diagrams are from the positive energy portion of the intermediate state and the last two are from the negative energy portion. These diagrams are summed coherently as there is no way in principle to determine through which diagram a particular event occurred.

The final propagated state can now be found. This is done by substituting the appropriate forms of the unperturbed Green's functions in the Compton term of Eq. (6), summing over the two time orderings of emission and absorption, and using the

resulting expression for $G(r', t'; r, t)$ in Eq. (1). By taking the matrix element between the final propagated state and any particular final scattering solution, one then gets the amplitude to transition from the initial state to that final scattering solution. The resulting amplitude is

$$\begin{aligned} \langle \gamma' \alpha'; q' \eta' | H' | \gamma \alpha; n_i \kappa_i \nu_i \rangle &= \sum_{\kappa' \nu'} \frac{\hbar c}{\langle q' W \rangle^{\frac{1}{2}}} (-i)^{\lambda' + 1} e^{i \sigma_{\kappa'}} \\ &\times C(\lambda' \frac{1}{2} j', \nu' - \eta', \eta', \nu') \left(Y_{\lambda'}^{\nu' - \eta'}(\hat{q}') \right) \\ &\left\{ \lim_{\epsilon \rightarrow 0^+} \sum_{\kappa \nu} \int_W \left[\frac{\langle q' \kappa' \nu' | V'(\alpha') | q \kappa \nu \rangle \langle q \kappa \nu | V(\alpha) | n_i \kappa_i \nu_i \rangle}{W - W_{n_i \kappa_i} - \hbar c \gamma - i \epsilon_{\omega} \epsilon} \right. \right. \\ &+ \frac{\langle q' \kappa' \nu' | V(\alpha) | q \kappa \nu \rangle \langle q \kappa \nu | V'(\alpha') | n_i \kappa_i \nu_i \rangle}{W - W_{n_i \kappa_i} + \hbar c \gamma' - i \epsilon_{\omega} \epsilon} \Big] dW \\ &+ \sum_{n \kappa \nu} \left[\frac{\langle q' \kappa' \nu' | V'(\alpha') | n \kappa \nu \rangle \langle n \kappa \nu | V(\alpha) | n_i \kappa_i \nu_i \rangle}{W_n - W_{n_i \kappa_i} - \hbar c \gamma} \right. \\ &\left. \left. + \frac{\langle q' \kappa' \nu' | V(\alpha) | n \kappa \nu \rangle \langle n \kappa \nu | V'(\alpha') | n_i \kappa_i \nu_i \rangle}{W_{n \kappa} - W_{n_i \kappa_i} + \hbar c \gamma'} \right] \right\}, \quad (9) \end{aligned}$$

where

$$\begin{aligned} V(\alpha) e^{-i c \gamma t} &= \text{photon absorption operator,} \\ V'(\alpha') e^{i c \gamma' t} &= \text{photon emission operator,} \\ \alpha &= \text{initial photon quantum numbers, and} \\ \alpha' &= \text{final photon quantum numbers.} \end{aligned}$$

The intermediate energy integration is over all continuum intermediate energies. The time dependence in the amplitude above has been omitted. It can be expressed as $f(\tau)$ where

$$f(\tau)^2 \approx \frac{2\pi}{\hbar} \tau \sigma(W' + \hbar c \gamma' - W_{n_i \kappa_i} - \hbar c \gamma),$$

where τ = duration of scattering process.

The initial photon field is normalized to unit flux and the final field to a volume V . The transition rate for the scattering is found by complex-squaring the amplitude and $f(\tau)$, dividing by τ , and integrating over all available phase space. The cross

section is then found by noting that the incident flux times the total cross section equals the transition rate.

The differential cross section is

$$\frac{d^2\sigma(\theta', \gamma')}{d\Omega_{\gamma'} d(\hbar c \gamma')} = \frac{1}{N} \int \sum_1 \left| \sum_2 \langle \gamma' \alpha'; q' \eta' | H' | \gamma \alpha; n_1 \kappa_1 \nu_1 \rangle \right|^2 \\ \times \frac{W' q'}{\hbar^2 c^2} \sigma(W' + \hbar c \gamma' - W_{n_1 \kappa_1} - \hbar c \gamma) dW' d\Omega_{q'} \frac{2\pi}{\hbar} \frac{V}{(2\pi)^3} \frac{\gamma'^2}{\hbar c}. \quad (10)$$

The average over initial states and sum over final states is represented by $\sum_1/N$, and $\sum_2$ represents any internal sums necessary to the matrix element. The units of the differential cross sections are $\text{cm}^2 \text{erg}^{-1} \text{s}^{-1}$. The following sections will develop the detailed formalism necessary to evaluate the differential cross section.

III. Bound Relativistic Wave Functions

The formalism used for these wave functions is due to Schiff.³¹ The form of the functions is as follows:

$$\psi_{n\kappa\nu}(r) \equiv \langle r | n\kappa\nu \rangle = \begin{pmatrix} -i F_{n\kappa}(r)/r \phi_{L,S}(\kappa\nu) \\ G_{n\kappa}(r)/r \phi_{S,L}(\kappa\nu) \end{pmatrix}, \quad (11)$$

where

$$\kappa = \pm(j + \frac{1}{2}),$$

$$j = \text{total spin,}$$

$$n = \text{principal quantum number,}$$

$$\nu = z \text{ projection of total spin, and}$$

$\phi_{L,S}$ is a j-j coupled spinor wave function constructed with spherical harmonics and spin functions.

$$\phi_{L,S}(\kappa\nu) = \begin{pmatrix} C(\ell_{L,S}^{\frac{1}{2}} j; \nu - \frac{1}{2}, \frac{1}{2}, \nu) Y_{\ell_{L,S}}^{\nu - \frac{1}{2}}(\hat{r}) \\ C(\ell_{L,S}^{\frac{1}{2}} j; \nu + \frac{1}{2}, -\frac{1}{2}, \nu) Y_{\ell_{L,S}}^{\nu + \frac{1}{2}}(\hat{r}) \end{pmatrix} \equiv \langle \hat{r} | \kappa\nu \ell_{L,S} \rangle. \quad (12)$$

where

$$\begin{aligned} \ell_{L,S} &= \kappa - 1, \quad \kappa > 0 \\ &= -\kappa, \quad -\kappa - 1, \quad \kappa < 0. \end{aligned}$$

The wave functions are thus seen to be bispinors. $F(r)$ is the large component and $G(r)$ is the small component of the wave functions. These functions satisfy the following simultaneous equations:

$$\begin{aligned} [W - mc^2 - V(r)] F_{n\kappa}(r) + \hbar c \frac{dG_{n\kappa}(r)}{dr} + \frac{\hbar c \kappa}{r} G_{n\kappa}(r) &= 0 \\ [W + mc^2 - V(r)] G_{n\kappa}(r) - \hbar c \frac{dF_{n\kappa}(r)}{dr} + \frac{\hbar c \kappa}{r} F_{n\kappa}(r) &= 0, \end{aligned} \quad (13)$$

where

W = total relativistic energy,

m = electron rest mass,

c = speed of light,

$\hbar$ = Planck's constant, and

$V(r)$ = spherically symmetric spin-independent potential.

The dependence on κ is explicit. The dependence on n is manifested by requiring the components to have a certain number of radial nodes.

The wave functions are normalized to unity:

$$\int \psi_{n'\kappa'\nu'}^* (r) \psi_{n\kappa\nu}(r) dV = \delta_{nn'} \delta_{\kappa\kappa'} \delta_{\nu\nu'}. \quad (14)$$

The above orthogonality is assured as long as all eigenfunctions are numerically generated from a common potential.

IV. Continuum Relativistic Wave Functions

The form of the solutions for the continuum wave functions is similar to that of the bound wave functions, with a few important exceptions. The total energy, W , is greater than mc^2 or less than $-mc^2$ and, as a result, the radial functions do not vanish at large r but become sinusoidal. Then " n ", the principle quantum number, is dropped as the solutions have an infinite number of nodes.

The asymptotic form of the wave function, where the potential is pure Coulomb, is

$$r \langle r | q\kappa\nu \rangle \sim \begin{pmatrix} -i f_{\kappa, W} \sqrt{\frac{W + mc^2}{2q\hbar^2 c}} \sin \left(qr - \frac{\ell\pi}{2} + \sigma_{\kappa} \right) \phi_L(\kappa\nu) \\ g_{\kappa, W} \sqrt{\frac{W - mc^2}{2q\hbar^2 c}} \cos \left(qr - \frac{\lambda\pi}{2} + \sigma_{\kappa} \right) \phi_S(\kappa\nu) \end{pmatrix}. \quad (15)$$

where

$$\begin{aligned}\sigma_{\kappa} &= \frac{Ze^2}{\hbar v} \log(2qr) + \sigma'_{\kappa}, \\ Ze &= \text{asymptotic Coulomb charge,} \\ v &= \text{relative electron velocity,} \\ \sigma'_{\kappa} &= \text{constant phase shift, and} \\ \lambda &= \ell_L = \kappa - 1, \quad \kappa > 0; \quad = -\kappa, \quad \kappa < 0.\end{aligned}$$

If $W > mc^2$, then $f_{\kappa, W} = g_{\kappa, W} = 1$. If $W < -mc^2$, then $f_{\kappa, W} = -g_{\kappa, W} = 1$ for $\kappa > 0$ and -1 for $\kappa < 0$. If the potential decreases faster than $1/r$ in the asymptotic region there is no logarithmic phase shift, only a constant shift. In the limit of no potential, $Z \rightarrow 0$ and $\sigma_{\kappa} \rightarrow 0$. The radial wave functions then become half-integer Bessel functions.

The normalization can be written as

$$\int \psi_{\kappa' \nu'}^* (q' r) \psi_{\kappa \nu} (qr) dV = \epsilon_{\omega} \delta_{\kappa' \kappa} \delta_{\nu' \nu} \delta(W' - W) \quad (16)$$

where

$$\begin{aligned}\epsilon_{\omega} &= 1, \quad W > mc^2 \\ &= -1, \quad W < -mc^2.\end{aligned}$$

The delta function is defined as follows:

$$\begin{aligned}W > mc^2, \quad \int_{mc^2}^{\infty} \delta(W - W') dW &= 1 \\ W < -mc^2, \quad \int_{-\infty}^{-mc^2} \delta(W - W') dW &= 1.\end{aligned}$$

The above solutions are known as the spherical basis set of solutions for the particular potential. Another useful set is the scattering set. Only the positive energy set will be considered here.

$$\begin{aligned}\psi_{\eta}^{\pm}(\vec{q} \cdot \vec{r}) \equiv \langle \vec{r} | \vec{q} \eta \rangle^{\pm} &= \mu_{\eta}^{\pm} e^{i \left[\vec{q} \cdot \vec{r} \pm \frac{Z' Ze^2}{\hbar v} \log(qr \mp \vec{q} \cdot \vec{r}) \right]} \\ &\quad + F_{\eta}^{\pm} \frac{e}{r} \left[qr - \frac{Z' Ze^2}{\hbar v} \log(2qr) \right], \quad (17)\end{aligned}$$

where $\mu_{\eta}^{\pm}$ and $F_{\eta}^{\pm}$ are bispinors.

The proper expansions of these functions are (see Appendix):

$$\psi_{\eta}^{\pm}(\vec{q} \cdot \vec{r}) = \sum_{\kappa \nu} \frac{\hbar c}{(qW)^{\frac{1}{2}}} i^{\lambda+1} e^{\pm i \sigma_{\kappa}} C(\lambda \frac{1}{2} j; \nu - \eta, \eta, \nu) Y_{\lambda}^{\nu - \eta*}(\hat{q}) \psi_{\kappa \nu}(qr). \quad (18)$$

The normalization is in momentum space;

$$\int \psi_{\eta'}^{\pm}(\vec{q} \cdot \vec{r}) \psi_{\eta}^{\pm}(\vec{q} \cdot \vec{r}) dV = \delta_{\eta' \eta} \delta(\vec{q}' - \vec{q}). \quad (19)$$

V. Interaction Hamiltonian

The interaction Hamiltonian for a point charge in an electromagnetic field is

$$H^i(\vec{r}, t) = -e\vec{\alpha} \cdot \vec{A}, \quad (20)$$

where

$$\vec{\alpha} = \begin{vmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix},$$

$\vec{\sigma}$ = vector spin operator, and

$\vec{A}$ = vector potential.

The vector potential of polarization $\hat{\epsilon}_M$ and momentum $\vec{\gamma}$ is represented as

$$\vec{A}_M(\vec{\gamma} \cdot \vec{r}) = \frac{\hat{\epsilon}_M}{V^{1/2}} \left[a_{\vec{\gamma}M} e^{i(\vec{\gamma} \cdot \vec{r} - \gamma ct)} + a_{\vec{\gamma}M}^{\dagger} e^{-i(\vec{\gamma} \cdot \vec{r} - \gamma ct)} \right], \quad (21)$$

where

$$\hat{\epsilon}_1 = -\frac{1}{\sqrt{2}} (\hat{e}_x + i\hat{e}_y),$$

$$\hat{\epsilon}_0 = \hat{e}_z,$$

$$\hat{\epsilon}_{-1} = \frac{1}{\sqrt{2}} (\hat{e}_x - i\hat{e}_y),$$

$$\hat{\epsilon}_M \cdot \vec{\gamma} = 0,$$

V = normalization volume,

$a_{\vec{\gamma}M}$ = photon destruction operator, and

$a_{\vec{\gamma}M}^{\dagger}$ = photon creation operator.

The photon wave functions are normalized in a box of volume V . The creation and destruction operators are now replaced by their eigenvalues;

$$a_{\vec{\gamma}M} | \dots, n_{\vec{\gamma}M}, \dots \rangle = \left(\frac{2\pi\hbar c}{V} \frac{n_{\vec{\gamma}M}}{\gamma} \right)^{1/2} | \dots, n_{\vec{\gamma}M}-1, \dots \rangle$$

$$a_{\vec{\gamma}M}^{\dagger} | \dots, n_{\vec{\gamma}M}, \dots \rangle = \left[\frac{2\pi\hbar c (n_{\vec{\gamma}M} + 1)}{V} \right]^{1/2} | \dots, n_{\vec{\gamma}M}+1, \dots \rangle \quad (22)$$

where $| \dots, n_{\vec{\gamma}M}, \dots \rangle$ is the ket describing the photon field, and $n_{\vec{\gamma}M}$ is the number of photons in the normalization volume of momentum $\vec{\gamma}$ and polarization M ,

Now

$$\vec{A}_M(\vec{\gamma} \cdot \vec{r}) = \hat{\epsilon}_M \left\{ \left[\frac{2\pi\hbar c}{\gamma} \left(\frac{n_{\vec{\gamma}} M}{V} \right) \right]^{\frac{1}{2}} e^{i(\vec{\gamma} \cdot \vec{r} - \gamma ct)} + \left[\frac{2\pi\hbar c}{\gamma} \left(\frac{n_{\vec{\gamma}} M + 1}{V} \right) \right]^{\frac{1}{2}} e^{-i(\vec{\gamma} \cdot \vec{r} - \gamma ct)} \right\}. \quad (23)$$

After expanding,

$$\hat{\epsilon}_M e^{i\vec{\gamma} \cdot \vec{r}} = 4\pi \hat{\epsilon}_M \sum_{\ell} i^{\ell} j_{\ell}(\gamma r) \sum_{\bar{m}} Y_{\ell}^{m*}(\hat{\gamma}) Y_{\ell}^{\bar{m}}(\hat{r}). \quad (24)$$

Now

$$Y_{\ell}^m(\hat{r}) \hat{\epsilon}_M = \sum_L C(\ell 1 L; m, M, m+M) T_{L\ell}^{m+M}(\hat{r}),$$

where

$C(\)$ = Clebsch-Gordan coefficient, and
 $T_{L\ell}^{m+M}$ = vector spherical harmonics.

The electric and magnetic multipole contributions to the interaction are

$L = \ell$, magnetic multipoles, and

$L = \ell \pm 1$, electric multipoles.

Next,

$$\hat{\epsilon}_M e^{i\vec{\gamma} \cdot \vec{r}} = 4\pi \sum_{\ell} i^{\ell} j_{\ell}(\gamma r) \sum_L Y_{\ell}^{m*}(\hat{\gamma}) \sum C(\ell 1 L; m, M, m+M) T_{L\ell}^{m+M} \quad (25)$$

Also,

$$\hat{\epsilon}_M e^{-i\vec{\gamma} \cdot \vec{r}} = 4\pi \sum_{\ell} (-1)^{\ell} i^{\ell} j_{\ell}(\gamma r) \sum_{m'} Y_{\ell}^{m'*}(\hat{\gamma}) \sum_L C(\ell 1 L; m', M, m'+M) T_{L\ell}^{m'+M}(\hat{r}). \quad (26)$$

Finally,

$$\begin{aligned} \vec{A}_M(\vec{\gamma} \cdot \vec{r}) &= 4\pi \sum_{\ell} \sum_L i^{\ell} j_{\ell}(\gamma r) \left\{ \left[\frac{2\pi\hbar c}{\gamma} \left(\frac{n_{\vec{\gamma}} M}{V} \right) \right]^{\frac{1}{2}} e^{-i\gamma ct} \right. \\ &\times \sum_m Y_{\ell}^{m*}(\hat{\gamma}) C(\ell 1 L; m, M, m+M) T_{L\ell}^{m+M}(\hat{r}) + \left[\frac{2\pi\hbar c}{\gamma} \left(\frac{n_{\vec{\gamma}} M + 1}{V} \right) \right]^{\frac{1}{2}} \\ &\times e^{i\gamma ct} (-1)^{\ell} \sum_{m'} Y_{\ell}^{m'*}(\hat{\gamma}) C(\ell 1 L; m', M, m'+M) T_{L\ell}^{m'+M}(\hat{r}) \left. \right\}. \quad (27) \end{aligned}$$

The $\vec{\alpha}$ operator operates on the $T_{L\ell}^{m+M}(\hat{r})$. First

$$\vec{\alpha} \cdot T_{L\ell}^{m+M}(\hat{r}) = \vec{\sigma} \cdot T_{L\ell}^{m+M} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}. \quad (28)$$

Now

$$\vec{\sigma} \cdot T_{L\ell}^{m+M} = \sum_{\mu} C(\ell 1 L; m+M-\mu, \mu, M+m) Y_{\ell}^{m+M-\mu}(\hat{r}) (\vec{\sigma} \cdot \hat{\epsilon}_{\mu}), \quad \vec{\sigma} \cdot \hat{\epsilon}_{\mu} = \sigma_{\mu} \quad (29)$$

$$\vec{\sigma} \cdot T_{L\ell}^{m+M} = \sum_{\mu} C(\ell 1 L; m+M-\mu, \mu, M+m) Y_{\ell}^{m+M-\mu}(\hat{r}) \sigma_{\mu} = [Y_{\ell} \otimes \sigma_1]_L^{m+M}, \quad (30)$$

where the bracket term is the tensor product of Y_{ℓ} and σ_1 .

The interaction operator can now be written, parameterized by ℓ, m, L, M , and $\vec{\gamma}$. The operator is also divided into absorption and emission portions and the convention is adopted of describing the emission field by primed variables. In addition, both operators must be appropriately normalized. For absorption, the normalization is for a unit photon flux on the scattering center. The final state is normalized in a box of volume V with $n_{\vec{\gamma}, M'} = 0$ and $\vec{\gamma} \cdot \hat{e}_n = 0$ where $\hat{e}_n$ is the polarization vector of the final state. The polarization vector is defined to be perpendicular to the propagation vector. If the polar and azimuthal angles of the final photon state are θ' and ϕ' , then

$$\hat{e}_1 = \sum_M A_M^1(\theta')^* \hat{\epsilon}_M e^{-iM\phi'}, \quad (31)$$

where

$$A_1^1(\theta') = -\frac{1}{\sqrt{2}},$$

$$A_0^1(\theta') = 0, \text{ and}$$

$$A_{-1}^1(\theta') = \frac{1}{\sqrt{2}}.$$

$$\hat{e}_2 = \sum_M A_M^2(\theta')^* \hat{\epsilon}_M e^{-iM\phi'}, \quad (32)$$

where

$$A_1^2(\theta') = -\frac{\cos \theta'}{\sqrt{2}},$$

$$A_0^2(\theta') = -\sin \theta', \text{ and}$$

$$A_{-1}^2(\theta') = \frac{\cos \theta'}{\sqrt{2}}.$$

The absorption Hamiltonian is

$$H'(\vec{r}; t; \ell m L M) = -4\pi e i^{\ell} j_{\ell}(\gamma r) \left(\frac{2\pi \hbar c}{\gamma} \right)^{\frac{1}{2}} e^{-i\gamma c t} \rho^{\frac{1}{2}} \\ \times Y_{\ell}^{m*}(\hat{\gamma}) C(\ell 1 L; m, M, m+M) \left[Y_{\ell} \otimes \sigma_1 \right]_{L}^{m+M} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \quad (33)$$

where $\rho = 3.33 \times 10^{-11} / \text{cm}^3$.

For emission,

$$H'(\vec{r}; t; \ell' m' L' M') = -4\pi e i^{\ell'} j_{\ell'}(\gamma' r) \left(\frac{2\pi \hbar c}{\gamma' V} \right)^{\frac{1}{2}} e^{i\gamma' c t} (-1)^{\ell'} \\ \times Y_{\ell'}^{m'*}(\hat{\gamma}') \sum_n A_n^{M'}(\theta')^* e^{-in\phi'} C(\ell' 1 L'; m', n, m'+n) \left[Y_{\ell'} \otimes \sigma_1 \right]_{L'}^{n+m'} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}. \quad (34)$$

VI. Matrix Elements Between κ Eigenstates

In the last section, the interaction operators were developed. In this section, the details of the matrix elements between κ eigenstates are developed. In the matrix integral, the final state appears as a row vector:

$$r \langle n' \kappa' \nu' | r \rangle = (iF_{n' \kappa'}(r) \phi_{L'}(\kappa' \nu') \quad G_{n' \kappa'}(r) \phi_{S'}(\kappa' \nu')). \quad (35)$$

The initial state is a column vector and is first operated on by

$$\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}$$

which inverts it. It then appears as

$$r \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \langle r | n \kappa \nu \rangle = \begin{pmatrix} G_{n \kappa}(r) \phi_S(\kappa \nu) \\ -iF_{n \kappa}(r) \phi_L(\kappa \nu) \end{pmatrix}. \quad (36)$$

The above is the form if both κ eigenfunctions are bound. If one or both are continuum functions, then n, n' or both are dropped and q, q' , or both are added to specify the total electron state.

In the following, nothing depends explicitly on n, q, n' , or q' so all reference is dropped. The matrix element for absorption can now be written

$$\begin{aligned}
\langle \kappa' \nu' | H'(\vec{r} \vec{\gamma} t; \ell m L M) | \kappa \nu \rangle &= -4\pi e i^{\ell+1} \left(\frac{2\pi \hbar c}{\gamma} \right)^{\frac{1}{2}} e^{-i\gamma c t} Y_{\ell}^{m*}(\hat{\gamma}) \rho^{\frac{1}{2}} \\
&\times C(\ell 1 L; m, M, m+M) \left\{ \int_0^{\infty} F_{\kappa'}(r) j_{\ell}(\gamma r) G_{\kappa}(r) dr \right. \\
&\times \langle \kappa' \nu' \ell_L | [Y_{\ell} \otimes \sigma_1]_L^{m+M} | \kappa \nu \ell_S \rangle - \int_0^{\infty} G_{\kappa'}(r) j_{\ell}(\gamma r) F_{\kappa}(r) dr \\
&\left. \times \langle \kappa' \nu' \ell_S | [Y_{\ell} \otimes \sigma_1]_L^{m+M} | \kappa \nu \ell_L \rangle \right\}. \quad (37)
\end{aligned}$$

The L associated with $|\kappa \nu \ell_L\rangle$ should not be confused with the L in the tensor operator. The former just means that value of ℓ associated with the large component of the initial wave function.

The matrix elements between the spinors can be evaluated by using the Wigner-Eckart theorem and associated relations:

$$\langle \kappa' \nu' \ell_L | [Y_{\ell} \otimes \sigma_1]_L^{m+M} | \kappa \nu \ell_S \rangle = (-1)^{j'-\nu'} \begin{pmatrix} j' & L & j \\ -\nu' & m+M & \nu \end{pmatrix} \langle j' \ell_L | [Y_{\ell} \otimes \sigma_1] j \ell_S \rangle$$

where

$$\begin{aligned}
j' &= |\kappa'| - \frac{1}{2} \\
j &= |\kappa| - \frac{1}{2} \\
\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= 3-j \text{ coefficient}
\end{aligned}$$

$$\begin{aligned}
\langle j' \ell_L | [Y_{\ell} \otimes \sigma_1] j \ell_S \rangle &= \sqrt{(2j'+1)(2L+1)(2j+1)} \\
&\times \begin{pmatrix} \ell_L & \frac{1}{2} & j' \\ \ell_S & \frac{1}{2} & j \\ \ell & 1 & L \end{pmatrix} \langle \ell_L | Y_{\ell} | \ell_S \rangle \langle \frac{1}{2} | \sigma_1 | \frac{1}{2} \rangle, \quad (38)
\end{aligned}$$

and

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{pmatrix} = 9-j \text{ coefficient.}$$

and

$$\langle \ell_{L'} | Y_{\ell} | \ell_S \rangle = (-1)^{\ell_{L'}} \sqrt{\frac{(2\ell_{L'} + 1)(2\ell + 1)(2\ell_S + 1)}{4\pi}} \begin{pmatrix} \ell_{L'} & \ell & \ell_S \\ 0 & 0 & 0 \end{pmatrix} \times \langle \frac{1}{2} | \sigma_1 | \frac{1}{2} \rangle = \sqrt{6}. \quad (39)$$

The Clebsch-Gordan coefficient is now converted to a 3-j coefficient. The final result is

$$\begin{aligned} \langle \kappa' \nu' | H'(\vec{r} \vec{\gamma} t; \ell m L M) | \kappa \nu \rangle &= 4\pi \sqrt{6} \, i^{\ell+1} Y_{\ell}^{m*}(\hat{\gamma}) \\ &\times (-1)^{-\ell-m-M-j'-\nu'} \left(\frac{2\pi \hbar c}{\gamma} \right)^{\frac{1}{2}} e^{-i\gamma c t} (2L+1) \begin{pmatrix} \ell & 1 & L \\ m & M & -m-M \end{pmatrix} \rho^{\frac{1}{2}} \\ &\times \begin{pmatrix} j' & L & j \\ -\nu' & m+M & \nu \end{pmatrix} \sqrt{\frac{(2j'+1)(2j+1)(2\ell+1)}{4\pi}} \left[(-1)^{\ell_{L'}} \right. \\ &\times \sqrt{(2\ell_{L'}+1)(2\ell_S+1)} \\ &\times \begin{pmatrix} \ell_{L'} & \ell & \ell_S \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_{L'} & \frac{1}{2} & j' \\ \ell_S & \frac{1}{2} & j \\ \ell & 1 & L \end{pmatrix} \int_0^{\infty} F_{\kappa'}(r) j_{\ell}(\gamma r) G_{\kappa}(r) dr \\ &- (-1)^{\ell_{S'}} \sqrt{(2\ell_{S'}+1)(2\ell_L+1)} \begin{pmatrix} \ell_{S'} & \ell & \ell_L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_{S'} & \frac{1}{2} & j' \\ \ell_L & \frac{1}{2} & j \\ \ell & 1 & L \end{pmatrix} \\ &\left. \times \int_0^{\infty} G_{\kappa'}(r) j_{\ell}(\gamma r) F_{\kappa}(r) dr \right]. \quad (40) \end{aligned}$$

For convenience in the sections that follow, a new coefficient will be defined. For the absorption element,

$$\langle \kappa' \nu' | H'(\vec{r} \vec{\gamma} t; \ell m L M) | \kappa \nu \rangle$$

$$= e^{-i\gamma t} \frac{i^{\ell+1}}{(\gamma)^{\frac{1}{2}}} D(W' W_{\gamma}; \kappa' \nu' \kappa \nu; \ell m L M) Y_{\ell}^{m'}(\hat{\gamma}) \rho^{\frac{1}{2}}. \quad (41)$$

For emission,

$$\begin{aligned} \langle \kappa' \nu' | H'(\vec{r} \vec{\gamma} t; \ell' m' L' M') | \kappa \nu \rangle &= e^{i\gamma' t} (-1)^{\ell'} \frac{i^{\ell'+1}}{(V\gamma')^{\frac{1}{2}}} \\ &\times Y_{\ell'}^{m'}(\hat{\gamma}') \sum_n A_n^{M'}(\theta')^* e^{-in\phi'} D(W' W_{\gamma'}; \kappa' \nu' \kappa \nu; \ell' m' L' n). \end{aligned} \quad (42)$$

A useful property of the D coefficient,

$$D(W' W_{\gamma}; \kappa' \nu' \kappa \nu; \ell m L M),$$

is that it is nonzero only if

$$\nu' = m + M + \nu.$$

VII. K-Shell Compton Cross-Section Development

From Eq. (10), the differential cross section can be written

$$\begin{aligned} \frac{d^2\sigma(\theta', \phi', \gamma')}{d\Omega_{\gamma'} d(\hbar c \gamma')} &= \frac{1}{N} \int \sum \left| \sum \langle \gamma' \alpha'; q' \eta' | H' | \gamma \alpha; 11 \nu_1 \rangle \right|^2 \\ &\frac{W' q'}{\hbar^2 c^2} \sigma(W' + \hbar c \gamma' - W_{11} - \hbar c \gamma) dW' d\Omega_{q'} \frac{2\pi}{\hbar} \frac{V}{(2\pi)^3} \frac{\gamma'^2}{\hbar c}. \end{aligned} \quad (43)$$

From Section VI and Eq. (9), the following identifications are made:

$$\alpha' = \ell' m' L' M'$$

$$\alpha = \ell m L M$$

$$V(r) = \sum_{\ell' m' L'} \sum_{\ell m L} H'(\vec{r} \vec{\gamma} t; \ell' m' L' M') e^{-i\gamma' t}$$

$$V(r) = \sum_{\ell} \sum_m \sum_L H'(\vec{r} \vec{\gamma} t; \ell m L M) e^{i\gamma t}$$

$$\begin{aligned}
\sum \langle \gamma' \alpha'; q' \eta' | H | \gamma \alpha; 11 \nu_i \rangle &= \sum_{\ell \ell'} \sum_{mm'} \sum_{LL'} \sum_{\kappa'} \sum_n (-1)^{\lambda' + \ell'} \\
&\times i^{\lambda' + \ell + \ell' + 1} \frac{e^{i\sigma_{\kappa'}}}{(\gamma' \gamma V)^{\frac{1}{2}}} \frac{\hbar c \rho^{\frac{1}{2}}}{(W' Q')^{\frac{1}{2}}} A_n^{M'}(\theta') e^{-in\phi'} C(\lambda' \frac{1}{2} j'; \nu' - \eta', \eta', \nu') \\
&\times Y_{\lambda'}^{\nu' - \eta'}(\hat{q}') Y_{\ell}^{m'}(\hat{\gamma}) Y_{\ell'}^{m'}(\hat{\gamma}') B'_{\kappa', \nu', m', m, n, M, \nu_i, \ell, \ell', L, L'} \quad (44)
\end{aligned}$$

where $\rho = 3.33 \times 10^{-11} / \text{cm}^3$.

$$\begin{aligned}
B(\kappa', \nu', m', m, n, M, \nu_i, \ell, \ell', L, L') &= \sum_{\kappa} \left\{ \lim_{\epsilon \rightarrow 0^+} \right. \\
&\times \int \left(\frac{D(W' W \gamma'; \kappa' \nu' \kappa \nu; \ell' m' L' n) D(W W_{11} \gamma; \kappa \nu 1 \nu_i; \ell m L M)}{W - W_{11} - \hbar c \gamma - i \epsilon \epsilon_{\omega}} \right. \\
&+ \frac{D(W' W \gamma; \kappa' \nu' \kappa \nu''; \ell m L M) D(W W_{11} \gamma'; \kappa \nu'' 1 \nu_i; \ell' m' L' n)}{W - W_{11} + \hbar c \gamma'} dW \\
&+ \sum_{n'} \frac{D(W' W_{n' \kappa} \gamma'; \kappa' \nu' \kappa \nu; \ell' m' L' n) D(W_{n' \kappa} W_{11} \gamma; \kappa \nu 1 \nu_i; \ell m L M)}{W_{n' \kappa} - W_{11} - \hbar c \gamma} \\
&\left. + \frac{D(W' W_{n' \kappa} \gamma; \kappa' \nu' \kappa \nu''; \ell m L M) D(W_{n' \kappa} W_{11} \gamma'; \kappa \nu'' 1 \nu_i; \ell' m' L' n)}{W_{n' \kappa} - W_{11} + \hbar c \gamma'} \right) \quad (45)
\end{aligned}$$

and

$$\nu' = m' + m + M + n + \nu_i.$$

$$\nu = m + M + \nu_i.$$

$$\nu'' = m' + n + \nu_i.$$

The summations over ν' and ν in Eq. (7) have been eliminated by D-coefficient selection rule ϵ .

The next step is to take the complex square. The variables associated with the complex conjugate term will be subscripted with a 2 while the second term in the product will remain unchanged.

$$\begin{aligned}
& \left| \sum \langle \gamma' \ell' m' L' M'; q' \eta' | H | \gamma \ell m L m; 11 \nu_1 \rangle \right|^2 \\
&= \sum_{\ell \ell' \ell_2 \ell_2'} \sum_{m m' m_2 m_2'} \sum_{L L' L_2 L_2'} \sum_{\kappa' \kappa_2'} \sum_{n n_2} \frac{\hbar^2 c^2}{W' q'} \frac{e^{i(\sigma_{\kappa'} - \sigma_{\kappa_2'})}}{V \gamma' \gamma} \rho \\
&\quad \times e^{-i(n - n_2)\phi'} A_n^{M'^*}(\theta') A_{n_2}^{M'}(\theta') (-1)^{\lambda' + \ell_2' + \ell'} \\
&\quad \times \lambda_2'^1 + \lambda + \ell_2 + \ell_2' + \ell + \ell' \\
&\quad \times Y_{\ell}^{m*}(\hat{\gamma}) Y_{\ell_2}^{m_2}(\hat{\gamma}) Y_{\ell'}^{m'^*}(\hat{\gamma}') Y_{\ell_2'}^{m_2'}(\hat{\gamma}') C(\lambda_2' \frac{1}{2} j_2'; \nu_2' - \eta', \eta', \nu_2') \\
&\quad \times C(\lambda' \frac{1}{2} j'; \nu' - \eta', \eta', \nu') Y_{\lambda_2'}^{\nu_2' - \eta'}(\hat{Q}') Y_{\lambda'}^{\nu' - \eta'}(\hat{Q}') B(\kappa_2', m_2', m_2, \\
&\quad \times n_2, M, \nu_1, \ell_2, \ell_2', L_2, L_2')^* B(\kappa', m', m, n, M, \nu_1, \ell, \ell', L, L') \quad (46)
\end{aligned}$$

where

$$\begin{aligned}
\nu_2' &= m_2' + m_2 + M + n_2 + \nu_1, \\
\nu' &= m' + m + M + n + \nu_1.
\end{aligned}$$

The second argument in the B coefficients has been omitted as it is uniquely determined by the remaining arguments. All final electron propagation directions can now be integrated out as the recoiling atom conserves total momentum without significantly affecting the final electron energy via the conservation of energy requirement. The integration over $d\Omega q'$ results in

$$\lambda_2' = \lambda_2, m_2' + m_2 + n_2 = m' + m + n.$$

Since the incident photon flux is in the positive z direction, $m_2 = m = 0$. The sum over η' is now taken with the result

$$j' = j_2, \quad \kappa' = \kappa_2.$$

The differential cross section is written as

$$\begin{aligned}
\frac{d^2\sigma(\theta', \phi', \gamma')}{d\Omega_{\gamma'}^2 d(hc\gamma')} &= \frac{1}{4} \sum_{\nu_1} \sum_M \sum_{M'} \sum_{\ell \ell' \ell_2 \ell_2'} \sum_{m' m_2'} \sum_{LL'} \sum_{L_2 L_2'} \sum_{\kappa'} \\
&\times \sum_{nn_2} \frac{\gamma'}{\gamma} \frac{e^{-i(n-n_2)\phi'}}{(2\pi)^2 \hbar^2 c} A_n^{M'+*}(\theta') A_{n_2}^{M'}(\theta') (-1)^{\ell_2+\ell'} \rho \\
&\times i^{\ell_2+\ell_2'+\ell'+\ell} Y_{\ell}^{0*}(0) Y_{\ell_2}^0(0) Y_{\ell'}^{m'+*}(\hat{\gamma}') Y_{\ell_2'}^{m_2'}(\hat{\gamma}') \\
&\times B(\kappa', m_2', 0, n_2, M, \nu_1, \ell_2, \ell_2', L_2, L_2') B(\kappa', m', 0, n, M, \nu_1, \ell, \ell', L, L'), \quad (47)
\end{aligned}$$

where $n_2 + m_2' = n + m'$.

The factor of 1/4 is for averaging over all initial states. These states are specified by $\nu_1 = \pm 1/2$ and $M = \pm 1$. It is now noted that

$$\begin{aligned}
Y_{\ell}^{0*}(0) Y_{\ell_2}^0(0) &= \left[\frac{(2\ell+1)(2\ell_2+1)}{(4\pi)^2} \right]^{\frac{1}{2}} \\
\times Y_{\ell'}^{m'+*}(\hat{\gamma}') Y_{\ell_2'}^{m_2'}(\hat{\gamma}') &= \left[\frac{(2\ell'+1)(2\ell_2'+1)(\ell'-m')!(\ell_2'-m_2')!}{(4\pi)^2(\ell'+m')!(\ell_2'+m_2')!} \right]^{\frac{1}{2}} \\
&\times P_{\ell'}^{m'}(\cos \theta') P_{\ell_2'}^{m_2'}(\cos \theta') e^{-i(m'-m_2')\phi'}.
\end{aligned}$$

The differential cross section is now recast:

$$\begin{aligned}
\frac{d^2\sigma(\theta', \phi', \gamma')}{d\Omega_{\gamma'}^2 d(hc\gamma')} &= \frac{\gamma'}{\gamma} \frac{1}{256\pi^4 \hbar^2 c} \sum_{\nu_1} \sum_M \sum_{M'} \sum_{\ell \ell' \ell_2 \ell_2'} \sum_{m' m_2'} \\
&\times \sum_{LL'} \sum_{L_2 L_2'} \sum_{\kappa'} \sum_{nn_2} A_n^{M'+*}(\theta') A_{n_2}^{M'}(\theta') (-1)^{\ell_2+\ell'} i^{\ell_2+\ell_2'+\ell'+\ell} \rho \\
&\times \left[\frac{(2\ell+1)(2\ell_2+1)(2\ell'+1)(2\ell_2'+1)(\ell'-m')!(\ell_2'-m_2')!}{(\ell'+m')!(\ell_2'+m_2')!} \right]^{\frac{1}{2}} P_{\ell'}^{m'}(\cos \theta')
\end{aligned}$$

$$\times P_{\ell_2'}^{m_2'} (\cos \theta') B(\kappa', m_2', 0, n_2, M, \nu_1, \ell_2, \ell_2', L_2, L_2')^* \\ \times B(\kappa', m', 0, n, M, \nu_1, \ell, \ell', L, L'), \quad (48)$$

where $n_2 + m_2' = n + m'$.

The cross-section expression has some useful properties. First due to parity conservation, the sum of the ℓ values must always be even. Second, the interchange of the pairs (ℓ, ℓ') and (ℓ_2, ℓ_2') is equivalent to the complex conjugate operation on the term, assuming all other sums are carried to completion. These features greatly simplify the numerical evaluation of the cross section by reducing the actual amount of calculation.

A third feature is the $1/\gamma'$ divergence as γ' goes to zero. This is known as the infrared divergence effect. As a result of this effect, the total cross section diverges at the lower limit. This failure is a result of neglecting the e^4 radiative correction to the photoelectric effect. This term diverges similarly at the lower limit, but with opposite sign. Thus when the radiative correction is combined incoherently with the total Compton cross section, the divergence disappears and is replaced by a term which is dependent on $\gamma'_{\min}$ which is the smallest detectable photon energy for a given experiment. This procedure in removing the divergence is physically justified by the indistinguishability of a photoelectric event and a Compton event with the emission of a photon with $\gamma' < \gamma'_{\min}$. One does not know whether a photon was emitted and not detected or no photon was emitted. The first correct explanation and method of removal of the infrared divergence in modern field theory was by Brown and Feynman³² in 1952.

VIII. Program Description and Calculation

GENERAL PROGRAM DESCRIPTION

Two codes are used to calculate the Compton cross sections. The first is a Hartree-Fock-Slater, self-consistent relativistic program normally used to generate single-particle eigenfunctions and eigenvalues. For present purposes, this program provides the central potential of the parent configuration for the scattering process.

The second computer program, using the potential data from the first program, has two phases. The first is the calculation of the wave functions from the central potential, followed by integration for the radial matrix elements. The second phase is the combining of the radial matrix elements with the necessary angular spin factors to form the resultant cross section.

These programs were run on a CDC 7600 computer. This machine has a 65,000 decimal word small (fast) core memory and a 512,000 decimal-word, large-core

memory. The large amount of available storage and the extremely rapid transmission rate between memories was the most important factor in making this calculation feasible. Even then, the problem required approximately 4 hr of CPU time per element.

APPROXIMATIONS

Two approximations are used in this calculation aside from the initial perturbation theory and finite difference approximations.

The first and most important approximation is the truncation of the multipole expansion of the initial and final electromagnetic fields. This calculation truncates both expansions with $\ell = 2$ where ℓ is the angular momentum of the multipole operator. The truncation error was estimated by calculating the cross-section contribution of the most important terms from the $\ell = 3$ operators. These terms change the final differential cross section by about 3% in gold and 5% in tin at 145 keV. For gold at 320 keV, the change is about 10%. The rapid convergence indicates the total truncation error is of this magnitude.

The second approximation is the neglect of the intermediate bound states. These states were included in one of the calculations executed and their contribution was negligible.

Aside from the multipole truncation, the only other source of major error is from the finite difference methods. The finite difference error in the dominant matrix elements are small, being $\leq 0.1\%$. The only other source of finite difference error is the integration over the intermediate energy continuum. The resulting error in the cross section from this integration is $\pm 5\%$. The greatest drawback of the calculational method is the difficulty in achieving reasonable accuracy with the smallest number of intermediate energies. The total estimated errors are: gold at 145 keV — $\pm 7\%$, tin at 145 keV — $\pm 8\%$, and gold at 320 keV — $\pm 12\%$.

IX. Results and Conclusions

The results of the calculation are found in Figs. 1-18. Figures 1-6 contain the angular distributions, and Figs. 7-12 show the final photon energy spectra. The remaining figures are the angular differential cross sections and the incoherent scattering factors for the three calculations. The total cross section in barns per electron are: tin at 145 keV = 0.27, gold at 145 keV = 0.29, and gold at 320 keV = 0.24. These numbers were calculated by a histogram integration over the entire allowed energy range. The energy cutoff for the three cases respectively are 116, 64, and 239 keV.

There are several features of particular note in these results. The first, and most unexpected, is the size of the infrared divergence effect. This effect is manifested by a $1/\gamma'$ behavior in the energy spectrum at all angles, with some emphasis on the forward angles. The effect is dominant in gold at 145 keV and of lesser importance,

Fig. 1. Angular distributions for tin ($\gamma = 145$ keV).

Fig. 2. Angular distributions for tin ($\gamma = 145$ keV).

Fig. 3. Angular distributions for gold ($\gamma = 145$ keV).

Fig. 4. Angular distributions for gold ($\gamma = 145$ keV).

Fig. 5. Angular distributions for gold ($\gamma = 320$ keV).

Fig. 6. Angular distributions for gold ($\gamma = 320$ keV).

Fig. 7. Energy spectra for tin ($\gamma = 145$ keV).

Fig. 8. Energy spectra for tin ($\gamma = 145$ keV).

Fig. 9. Energy spectra for gold ($\gamma = 145$ keV).

Fig. 10. Energy spectra for gold ($\gamma = 145$ keV).

Fig. 11. Energy spectra for gold ($\gamma = 320$ keV).

Fig. 12. Energy spectra for gold ($\gamma = 320$ keV).

Fig. 13. Angular distribution for tin ($\gamma = 145$ keV).

Fig. 14. Angular distribution for gold ($\gamma = 145$ keV).

Fig. 15. Angular distribution for gold ($\gamma = 320$ keV).

Fig. 16. Incoherent scattering factor for tin ($\gamma = 145$ keV).

Fig. 17. Incoherent scattering factor for gold ($\gamma = 145$ keV).

Fig. 18. Incoherent scattering factor for gold ($\gamma = 320$ keV).

but still apparent in the other two cases. The 320-keV calculation was done with the expectation that the infrared divergence, as calculated, would be visible in regions accessible to present experiments.⁸ The present experimental limit is about 30 keV. Since, in the 320-keV calculation, the divergence behavior is present to about 90 keV, the future comparison with experimental data should confirm one way or the other the correctness of the calculation.

A second feature of the calculation is the dominance of negative energy transitions in forming the Compton line. This same result, for free Compton scattering, was noted by Fermi in 1932.³³ In fact, Fermi found in the low-energy limit that negative energy transitions accounted for the entire Compton line. The present work implies the same result for low energies in bound scattering except for the presence of the infrared divergence which results from positive energy transitions.

This calculation sheds some light on the usefulness of some of the approximate methods discussed earlier for heavy elements, particularly the incoherent scattering factor method. This factor when evaluated using either relativistic or nonrelativistic wave functions is never greater than 1. Also, it predicts no zero-angle scattering. Both of these predictions appear to be incorrect. For gold at 320 keV, the incoherent scattering factor becomes as large as 1.1 although this result is not conclusive because of the possible calculation error in this work. This result, however, is not surprising as experiments¹⁻⁷ at 662 keV indicate the incoherent scattering factor to be as large as 1.7. The nonzero formal scattering result apparently has not been examined experimentally, but there is no physical reason to expect a zero result.

The presence of the infrared divergence is indicative of a partial failure of all the approximate methods. In most cases, however, this failure does not appear to be serious as the Compton line, when present, predominates over the divergence. Thus the divergence is important only at low energies when the Compton line is not at least partially present.

The necessity of using a relativistic formalism is not clear, although Schumacher's form factor calculation would seem to indicate this. The difference between relativistic and nonrelativistic results will probably be in the magnitude of the total cross section and not so much on the detailed structure. This structure is determined primarily by momentum transfer considerations which might well be independent of any particular formalism.

The present work demonstrates the need for more research, both experimental and theoretical. There is a need for more experimental measurements of K-shell cross sections at low energies such as 145 and 320 keV. These measurements should measure the energy spectrum to as low an energy as possible. This would allow useful comparison with the theoretically calculated infrared divergence.

The present theoretical work should be extended in several directions. Investigation is needed of the value of the Brown-Pierls formalism with regard to efficiency and ease of use. The size and complexity of these calculations make it imperative that the best methodology be found. More work is needed in extending the calculation

to other elements. The possibility of using higher incident energies and other than K-shell electrons should also be investigated. Hopefully, this paper will provide the incentive to others in carrying on more work in this and related areas.

X. Summary

The K-shell Compton collision cross sections for tin and gold at 145 keV and gold at 320 keV have been calculated using second-order perturbation theory based on the relativistic Hartree-Fock-Slater model. The necessity of both negative and positive energy eigenfunctions in the intermediate state is demonstrated.

The energy spectra are a combination of the Compton line and the infrared divergence. The Compton line displays the Compton defect and line broadening found at higher energies. Also, the line is almost totally a result of negative energy transition and is dominant over the infrared divergence when present.

The infrared divergence indicates a general failure of the three approximate methods discussed for heavy atoms. This failure, however, is only important when the Compton line is not present. The present results also indicate a failure in the incoherent scattering factor method as the incoherent scattering factor for gold at 320 keV becomes greater than 1.

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Appendix

Distorted Coulomb Scattering Solutions

In scattering problems, there are two solutions of interest—the ingoing (-) and outgoing (+) forms:

$$\psi_{\eta}^{\pm}(\vec{q} \cdot \vec{r}) = \mu_{\eta}^{\pm} e^{i\left[\vec{q} \cdot \vec{r} \pm \frac{z'ze^2}{\hbar v} \log(qr - \vec{q} \cdot \vec{r})\right]} + F_{\eta}^{\pm} e^{\pm i\left[qr - \frac{z'ze^2}{\hbar v} \log(2qr)\right]}, \quad (A-1)$$

where $\mu_{\eta}^{\pm}$ and $F_{\eta}^{\pm}$ are bispinors,

$z'e$ = charge of scattered particle,

ze = charge of scattering center, and

v = scattered particle velocity relative to scatterer.

In what follows, only the large component need be considered. Once the large component is known, the small component can be uniquely determined. Any solution can be represented as

$$\psi_{\eta}^{\pm}(\vec{q} \cdot \vec{r}) = \begin{vmatrix} \theta \\ \chi \end{vmatrix}, \quad (A-2)$$

where

θ is the large component, and

χ is the small component.

Then

$$\chi = \left(\frac{c\vec{\sigma} \cdot \vec{p}}{W + mc^2 - V(r)} \right) \theta, \quad (A-3)$$

where

$\vec{\sigma}$ = Pauli spin vector,

$\vec{p}$ = momentum operator, and

$V(r)$ = scattering potential.

The large component of μ_{η} is

$$\theta_{\eta} = \begin{vmatrix} 1 \\ 0 \end{vmatrix}, \quad \eta = \frac{1}{2}$$

$$\theta_{\eta} = \begin{vmatrix} 0 \\ 1 \end{vmatrix}, \quad \eta = -\frac{1}{2}.$$

Also,

$$\begin{aligned}
& \lim_{\substack{\hat{q} \cdot \hat{r} \rightarrow \mp 1 \\ qr \rightarrow \infty}} e^{i[\vec{q} \cdot \vec{r} \pm \frac{zz'e^2}{\hbar v} \log(qr \mp \vec{q} \cdot \vec{r})]} \\
&= 4\pi \sum_{\lambda} i^{\lambda} \frac{\sin[qr - \frac{zz'e^2}{\hbar v} \log(2qr) - \lambda\pi/2]}{qr} \sum_m Y_{\lambda}^{m*}(\hat{q}) Y_{\lambda}^m(\hat{r}). \quad (A-4)
\end{aligned}$$

At first glance, the above seems incorrect until it is noted that q and r are antiparallel and parallel respectively in the two versions. Now

$$\begin{aligned}
& \lim_{\substack{\hat{q} \cdot \hat{r} \rightarrow \mp 1 \\ qr \rightarrow \infty}} e^{i[\vec{q} \cdot \vec{r} \pm \frac{zz'e^2}{\hbar v} \log(qr \mp \vec{q} \cdot \vec{r})]} \\
&= 4\pi \sum_{\kappa\nu} i^{\lambda} C(\lambda \frac{1}{2} j; \nu - \eta, \eta, \nu) Y_{\lambda}^{\nu - \eta*}(\hat{q}) \phi_L(\kappa\nu) \\
&\quad \times \sin[qr - \frac{\lambda\pi}{2} - \frac{z'ze^2}{\hbar v} \log(2qr)]/qr, \quad (A-5)
\end{aligned}$$

where

$$\begin{aligned}
j &= |\kappa| - \frac{1}{2}, \\
\lambda &= \ell_L = \kappa - 1, \quad \kappa > 0, \\
&= -\kappa, \quad \kappa < 0, \text{ and} \\
\phi_L(\kappa, \nu) &= (j - j) \text{ coupled spinor.}
\end{aligned}$$

The sum has been converted into more conventional relativistic notation, and the spin-angular momentum coupled spinors have been introduced. The above expression, combined with the ingoing or outgoing wave, can be expanded in terms of either negative or positive energy solution of the spherical basic set. The negative energy expansion would be useful for calculations where either the initial or final electron state was a positron. For the present work, only the positive energy expansion is necessary.

$$\psi_{\eta}^{\pm}(\vec{q} \cdot \vec{r}) = \sum_{\kappa\nu} C_{\kappa\nu}^{\pm} \psi_{\kappa\nu}(qr). \quad (A-6)$$

In terms of the large components, neglecting the normalization of the spherical basic set,

$$\begin{aligned}
& \sum_{\kappa\nu} C_{\kappa\nu}^{\pm} (-1) \sin \left[qr - \frac{zz'e^2}{\hbar\nu} \log(2qr) - \frac{\lambda\pi}{2} + \sigma_{\kappa}^{\pm} \right] \phi_L(\kappa\nu)/qr \\
&= 4\pi \sum_{\kappa\nu} i^{\lambda} C(\lambda_{\frac{1}{2}j}; \nu - \eta, \eta, \nu) Y_{\lambda}^{\nu - \eta*}(\hat{\zeta}) \phi_L(\kappa\nu) \sin \left[qr - \frac{zz'e^2}{\hbar\nu} \right. \\
&\quad \times \left. \log(2qr) - \frac{\lambda\pi}{2} \right] / qr + \frac{f^{\pm}}{r} e^{\pm i \left[qr - \frac{zz'e^2}{\hbar\nu} \log(2qr) \right]}. \quad (A-7)
\end{aligned}$$

$C_{\kappa\nu}^{\pm}$ and $f^{\pm}$ can be found by eliminating either e^{-iqr} or e^{iqr} , depending on which solution is desired. The coefficients are:

$$C_{\kappa\nu}^{\pm} = 4\pi i^{\lambda+1} e^{\pm i\sigma_{\kappa}^{\pm}} C(\lambda_{\frac{1}{2}j}; \nu - \eta, \eta, \nu) Y_{\lambda}^{\nu - \eta*}(\hat{q}), \quad (A-8)$$

$$f^{\pm} = \pm \sum_{\kappa\nu} \frac{2\pi}{iq} i^{\lambda} C(\lambda_{\frac{1}{2}j}; \nu - \eta, \eta, \nu) Y_{\lambda}^{\nu - \eta*}(\hat{q}) e^{\mp i\lambda\pi/2} (e^{\pm 2i\sigma_{\kappa}^{\pm}} - 1) \phi_L(\kappa\nu). \quad (A-9)$$

The final form of the two scattering solutions is

$$\psi_{\eta}^{\pm}(\vec{q} \cdot \vec{r}) = \sum_{\kappa\nu} \frac{\hbar c}{(qW)^{\frac{1}{2}}} i^{\lambda+1} e^{\pm i\sigma_{\kappa}^{\pm}} C(\lambda_{\frac{1}{2}j}; \nu - \eta, \eta, \nu) Y_{\lambda}^{\nu - \eta*}(\hat{q}) \psi_{\kappa\nu}(qr), \quad (A-10)$$

where

$$\int \psi_{\eta'}^{\pm*}(\vec{q}' \cdot \vec{r}) \psi_{\eta}^{\pm}(\vec{q} \cdot \vec{r}) dV = \delta_{\eta\eta'} \sigma(\vec{q}' - \vec{q}),$$

$$\int \sigma(\vec{q}' \cdot \vec{q}) q^2 dq d\Omega_q = 1, \text{ and}$$

$$q^2 dq d\Omega_q = \frac{qW}{\hbar^2 c^2} dW d\Omega_q. \quad (A-11)$$