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by

Gary S. Fraley

THE INTEGRATED COMPTON CROSS SECTION AND ITS USE IN A MONTE CARLO SCHEME

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ABSTRACT

The differential Compton cross section is integrated over a relativistic Maxwellian electron distribution. The result, the cross section per final energy and angle of scatter, is then used in a Monte Carlo scheme that does not involve the use of large tables.

I. INTRODUCTION

The Compton scattering of a photon off an electron distribution may be handled by integrating the cross section* over the distribution, and then by using the integrated cross section alone without referring again to the elementary cross section. For a Maxwellian distribution, the differential cross section will depend upon the initial photon energy (k_o), the final energy (k), the angle of scatter (θ), and the temperature (T).

$$\frac{\partial\sigma}{\partial k\partial\vec{\Omega}}(k_o \to k,\theta) = \int dn\,(\vec{\beta})\,\frac{\partial\sigma(\vec{\beta})}{\partial k\partial\vec{\Omega}} \quad , \qquad (1)$$

where $n(\vec{\beta})$ is the normalized electron distribution, and

$$\frac{\partial\sigma(\vec{\beta})}{\partial k\partial\vec{\Omega}}$$

is the cross section for an electron with velocity $\vec{\beta}$. Polarization effects are ignored, and the cross section is summed over polarizations. Because the cross section is independent of the azimuthal angle of scatter,

$$\frac{\partial\sigma}{\partial k\partial\cos\theta} = 2\pi\,\frac{\partial\sigma}{\partial k\partial\vec{\Omega}} \quad .$$

*Cross section is the reaction rate per unit electron and photon and includes a factor involving relative velocity.

In a Monte Carlo scheme that picks a new energy and direction after a scattering, the variables f and g are found for which

$$\frac{\partial\sigma}{\partial f\partial g} = \left(\frac{\partial\sigma}{\partial k\partial\cos\theta}\,J\left(\frac{k,\ \cos\theta}{f,\ g}\right)\right)$$

is a constant. For example,

$$f^* = \int_{-1}^{\cos\theta} d\cos\theta\,\frac{\partial\sigma}{\partial k\partial\cos\theta} \quad , \quad \frac{\partial\sigma}{\partial k} = f^*(1) \ ,$$

and

$$g^* = \int_{o}^{k} dk\,\frac{\partial\sigma}{\partial k} \quad , \quad f = f^*/f^*(1),\ g = g^*/g^*(\infty) \ . \qquad (2)$$

The variables f and g are equated to random numbers, and the physical variables are obtained by inverting these functions.

$$k = k(g,k_o,\ T) \quad , \quad \cos\theta = \cos\theta\ (f,g,k_o,T) \ .$$

Because the inversion must be done numerically, k and $\cos\theta$ are found by interpolation in tables. One table is four-dimensional. Because 50,000 is about the largest practical table, the average number of entries per variable is about 15. If the

entries are equi-spaced in the variables, accuracy in some regions may not be good. If the entries are not equi-spaced, searching for entries and using the more complicated interpolation formulae will increase the time spent for interpolation. In any case, interpolation will not be especially fast because it involves 16 entries in a four-dimensional table.

Another method is to pick k and cosθ directly by random numbers, and then compare

$$\frac{\partial\sigma}{\partial k\partial\cos\theta} \Big/ \left(\frac{\partial\sigma}{\partial k\partial\cos\theta}\right)_{\max}$$

to a third random number. If the ratio is greater than the random number, the reaction goes; if not, the procedure is repeated until the ratio is greater. This is not efficient because the ratio is generally small.

A third method is to develop analytical approximations to f and g; f_A and g_A, which should be easily inverted. This method is similar to the second, but the ratio

$$\frac{\partial\sigma}{\partial f_A\partial g_A} \Big/ \left(\frac{\partial\sigma}{\partial f_A\partial g_A}\right)_{\max}$$

is compared to the third random number. To the extent that the approximations are good, the ratio should usually be close to 1, and k and θ will generally come from the first try. This scheme requires an analytical formula for the cross section. The integration in Eq. (1) must be done analytically (it has been done numerically by Stone and Nelson[1]), or at least a sufficiently accurate approximation to the integral must be developed. What is usually the dominant term can be integrated analytically, and the other terms can be approximated fairly easily. The integral is used by the third method in a scheme that may be somewhat faster than interpolation, and which does not require the large storage space.

II. THE INTEGRATED CROSS SECTION

In Eq. (1) we use the (nondegenerate) relativistic Maxwellian distribution

$$dn = \frac{1}{4\pi\, T\, K_2\left(\frac{1}{T}\right)}\, e^{-\frac{\gamma}{T}}\, \gamma^2\beta d\gamma d\cos\theta_e\, d\omega_e \,. \qquad (3)$$

Variables include

T = temperature
γ = relativistic electron energy
θ_e = electron polar angle
ω_e = electron azimuthal angle
k_o = initial photon energy
k = final photon energy
$a = k_o - k$
$k_2 = k_o + k$
θ = angle of scatter (0 for forward scattering)
$C^- = 1-\cos\theta$
$C^+ = 1+\cos\theta$
$k_4 = \sqrt{a^2 + 2kk_oC^-}$.

The electron mass and the speed of light are taken as unity. The polar direction of the coordinate system is in the direction of k_o (Fig. 1). The direction of k is $(\theta, \omega = 0)$. Unprimed quantities refer to the center-of-mass system of the distribution; primed quantities refer to the rest system of the electron.

In Eq. (1), we write

$$\frac{\partial\sigma(\vec{\beta})}{\partial k\partial\vec{\Omega}} = \frac{\partial\sigma'}{\partial k'\partial\Omega'}\,\frac{\partial\sigma}{\partial\sigma'}\,\frac{\partial k'}{\partial k}\,\frac{\partial\Omega'}{\partial\Omega} \,, \qquad (4)$$

where $\partial\sigma'/\partial k'\partial\Omega'$ is the cross section in the rest system of the electron; and $\partial\sigma/\partial\sigma'$, etc., are the appropriate transformation factors to the unprimed system. The cross section in the rest system of the electron is given by the Klein-Nishina formula.[2]

$$\frac{\partial\sigma'}{\partial k'\partial\Omega'} = \frac{r_o^2}{2}\left(\frac{k'}{k_o'}\right)^2\left(\frac{k_o'}{k'} + \frac{k'}{k_o'} - \sin^2\theta 1\right) \times \delta\left(k' - \frac{k_o'}{1+k_o'\,(C^-)'}\right). \qquad (5)$$

The cross-section transformation can be determined by noting that $d\sigma\, n_e n_p$ (where n_e and n_p are electron and photon densities) is an invariant, being the ratio of two invariants, the number of reactions in an element of space-time, and the volume of that element.

$$d\sigma\, n_e n_p = \frac{\partial N}{\partial t\partial x^3} \equiv \frac{\partial N}{\partial x^4} \,. \qquad (6)$$

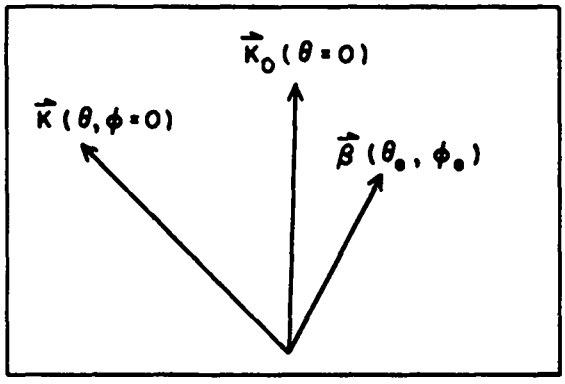

Fig. 1. The electron solid angle.

Then

$$\frac{\partial\sigma}{\partial\sigma'} = \frac{n_e' n_p'}{n_e n_p} \quad .$$

Because n_e and n_p are the time-like components of 4-vectors, $(n,n\vec{v})$, they transform as

$$n = \gamma n' \left(1 + \vec{\beta}\cdot\vec{v}'\right) ,$$

or

$$n' = \gamma n \left(1 - \vec{\beta}\cdot\vec{v}\right) \quad . \tag{7}$$

For the photons $|v| = |v'| = 1$, and for the electrons $\vec{v}' = 0$. Then

$$\frac{\partial\sigma}{\partial\sigma'} = 1 - \beta\cos\theta_e \equiv D_1 \quad . \tag{8}$$

If a coordinate system is temporarily taken in the direction of the electron velocity,

$$\frac{\partial\Omega'}{\partial\Omega} = \frac{\partial\varphi_k'}{\partial\varphi_k}\frac{\partial\cos\theta_k'}{\partial\cos\theta_k} = \frac{1}{\gamma^2 D_2^2} \quad , \tag{9}$$

where

$$D_2 \equiv 1 - \beta\left(\cos\theta_e\cos\theta + \sin\theta\sin\theta_e\cos\varphi_e\right) \tag{10}$$

is determined by using the usual angle-transformation formula and by noting that $\partial\varphi_k'/\partial\varphi_k = 1$, because it only involves coordinates perpendicular to the velocity of transformation.

The photon energies, as the time-like components of 4-vectors, $\underline{k} \equiv (k,\vec{k})$, transform as

$$k_o' = \gamma k_o D_1 \quad \text{and} \quad k' = \gamma k D_2 \quad . \tag{11}$$

The delta function requires that

$$k' = \frac{k_o'}{1 + k_o'(C^-)'} \equiv \frac{k_o'}{1 + k' k_o'(C^-)'/k'} \quad . \tag{12}$$

Because $k'k_o'(C^-)'$ is an invariant ($= \underline{k}'\cdot\underline{k}_o'$), in unprimed quantities we have

$$k = \frac{k_o D_1}{D_2 + \frac{k_o}{\gamma}C^-} \quad . \tag{13}$$

We have $\partial k/\partial\varphi_e$ proportional to $-\sin\varphi_e$, which shows that in the half section of solid angle, $0 \le \varphi_e \le \pi$, there is at most one φ_e (for given θ_e) where the delta function has zero argument. Figure 2 shows lines of constant k over half of the total solid angle.

When the delta function integration over φ_e is done, we have (including a factor of 2 for the two sections of solid angle)

$$\frac{\partial\sigma}{\partial k\partial\vec{\Omega}} = \frac{r_o^2}{4\pi T K_2\left(\frac{1}{T}\right)} \int d\gamma d\cos\theta_e \, e^{-\frac{\gamma}{T}} \gamma^2\beta \left|\frac{\partial\varphi_e}{\partial k}\right| \frac{D_1}{\gamma^2 D_2^2}\left(\left(\frac{k'}{k_o'}\right)^3 + \frac{k'}{k_o'} - \sin^2\theta'\left(\frac{k'}{k_o'}\right)^2\right). \tag{14}$$

From Eq. (13),

$$\frac{\partial k}{\partial\varphi_e} = \frac{-k_o D_1 \beta \sin\theta \sin\theta_e \sin\varphi_e}{\left(D_2 + \frac{k_o}{\gamma}C^-\right)^2}$$

$$= -\beta\sin\theta\sin\theta_e\sin\varphi_e \frac{k^2}{k_o D_1} \quad .$$

From Eq. (12),

$$\sin^2\theta' = 2\left(\frac{1}{k'} - \frac{1}{k_o'}\right) - \left(\frac{1}{k'} - \frac{1}{k_o'}\right)^2 .$$

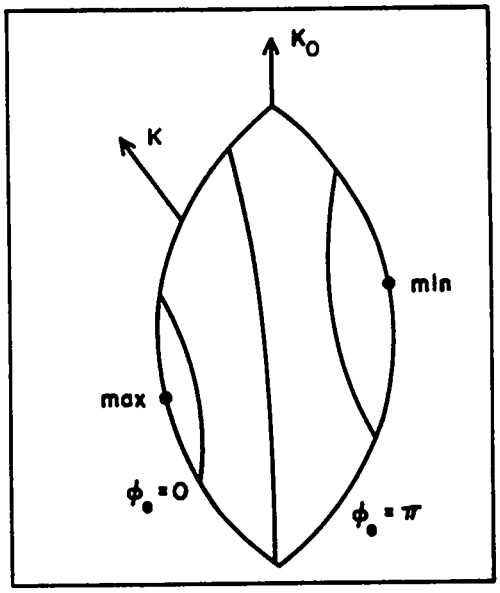

Fig. 2. Lines of constant final energy (k) in the electron solid angle.

In unprimed quantities,

$$\frac{\partial\sigma}{\partial k\partial\vec{\Omega}} = \frac{r_o^2}{4\pi\, T\, K_2\left(\frac{1}{T}\right)}\int dy\, d\cos\theta_e\, e^{-\frac{\gamma}{T}}\, \frac{\beta}{|\beta \sin\theta \sin\theta_e \sin\phi_e|}$$

$$\left(\frac{k}{k_o^2}\,\frac{D_2}{D_1} + \frac{1}{k}\,\frac{D_1}{D_2} - \frac{2}{\gamma D_2 k k_o} + \frac{2}{D_1 k_o^2 \gamma} + \frac{1}{\gamma^2 D_2^2 k^2 k_o} - \frac{2}{\gamma^2 D_1 D_2 k k_o^2} + \frac{1}{D_1^2 k_o^3 \gamma^2}\right) . \qquad (15)$$

We now write

$$\frac{1}{D_1 D_2} = \frac{\gamma}{kC^- D_2} - \frac{\gamma}{k_o C^- D_1} ,$$

$$\frac{D_2}{D_1} = \frac{k_o}{k} - \frac{k_o C^-}{\gamma D_1} \text{ , and } \frac{D_1}{D_2} = \frac{k}{k_o} + \frac{k}{\gamma}\,\frac{C^-}{D_2} .$$

We also have

$$d\cos\theta_e = \frac{d\,D_1}{\beta} = \frac{k}{k_o \beta}\, d\,D_2 .$$

Then Eq. (15) is

$$\frac{\partial\sigma}{\partial k\partial\vec{\Omega}} = \frac{r_o^2}{4\pi\, T\, K_2\left(\frac{1}{T}\right)}\int \frac{d\gamma e^{-\frac{\gamma}{T}}}{|\beta \sin\theta \sin\theta_e \sin\phi_e|}$$

$$\left\{ dD_1\left(\frac{2}{k_o} - \frac{k}{k_o}\,\frac{C^-}{\gamma D_1} + \frac{2}{D_1 k_o^2 \gamma} + \frac{2}{\gamma D_1 k k_o^3 C^-} + \frac{1}{D_1^2 k_o^3 \gamma^2}\right)\right.$$

$$\left. + \frac{k}{k_o}\, dD_2\left(\frac{C^-}{\gamma D_2} - \frac{2}{\gamma D_2 k k_o} + \frac{1}{\gamma^2 D_2^2 k^2 k_o} - \frac{2}{\gamma k^2 k_o^2 C^- D_2}\right)\right\} . \qquad (16)$$

The term $|\beta \sin\theta \sin\theta_e \sin\phi_e|$ may, by Eq. (13), be written as a quadratic in D_1 or D_2.

$$|\beta \sin\theta \sin\theta_e \sin\phi_e| = \sqrt{a_1 D_1^2 + b_1 D_1 + c_1}$$

$$= \sqrt{a_2 D_2^2 + b_2 D_2 + c_2} , \qquad (17)$$

where

$$a_1 = -k_4^2/k^2 ,$$

$$b_1 = 2C^-\left[C^+ + \left(1 + \frac{k_o}{\gamma}\right)\left(\frac{k_o}{k} - \cos\theta\right)\right]$$

$$c_1 = -\frac{C^-}{\gamma^2}\left[C^+ + C^-(\gamma + k_o)^2\right] ,$$

$$a_2 = -\frac{k_4^2}{k_o^2} ,$$

$$b_2 = \frac{2k}{k_o} C^-\left[C^+ + \frac{k_o}{k} - \cos\theta - \frac{k}{\gamma} + \frac{k_o}{\gamma}\cos\theta\right] ,$$

and

$$c_2 = -\frac{C^-}{\gamma^2}\left[C^+ + C^-(\gamma - k)^2\right] .$$

The integrals over $D_1(D_2)$ are then of the type

$$\int \frac{dx}{x^\alpha \sqrt{ax^2 + bx + c}} \qquad a, c < 0,\ b > 0,\ \alpha = 0, 1, 2 .$$

The results usually involve inverse sines. However, when the quadratic is 0, the argument of the

inverse sine is always ± 1. In our case, the quadratic is always 0 at the limits of integration because it has a factor $\sin\theta_e \sin\omega_e$ (Fig. 2). The result is

$$\int_{\sqrt{}=0}^{\sqrt{}=0} \frac{dx}{x^{\alpha}\sqrt{}} = \pi \begin{cases} \frac{1}{\sqrt{-a}} & \alpha = 0 \\ \frac{1}{\sqrt{-c}} & \alpha = 1 \\ \frac{-b}{2c\sqrt{-c}} & \alpha = 2 \end{cases} .$$

Equation (16) reduces to

$$\frac{\partial\sigma}{\partial k \partial\vec{\Omega}} = \frac{r_o^2}{4\,T\,K_2\left(\frac{1}{T}\right)k_o} \int d\gamma e^{-\frac{\gamma}{T}} \left\{ \frac{2k}{k_4} \right.$$

$$+ k\sqrt{C^-}\left(\frac{1}{T_2^{\frac{1}{2}}} - \frac{1}{T_1^{\frac{1}{2}}}\right) + \frac{2}{k_o\sqrt{C^-}}\left(\frac{1}{T_1^{\frac{1}{2}}} - \frac{1}{T_2^{\frac{1}{2}}}\right)\left(1 + \frac{1}{kk_oC^-}\right)$$

$$+ \frac{1}{k_o^2\, k\sqrt{C^-}\, T_1^{\frac{3}{2}}}\left[k_2\,\gamma + k_o\, a + kk_o\, C^-\right]$$

$$\left. + \frac{1}{k_o^2\, k\sqrt{C^-}\, T_2^{\frac{3}{2}}}\left[k_2\,\gamma + ka - kk_o\, C^-\right]\right\} , \qquad (18)$$

where

$$T_1 = C^+ + C^-(\gamma + k_o)^2 ,$$

and

$$T_2 = C^+ + C^-(\gamma - k)^2 .$$

The vertical line in Fig. 3 shows schematically the range of final energies (k) for a given electron energy (γ). The horizontal line shows the range of energies to be integrated over for a given k. The lower limit is that electron energy for which k is the minimum or maximum final photon energy. The extreme values of k occur at $\cos\omega_e = \pm 1$. We replace $\cos\omega_e$ by ± 1 in Eq. (13), differentiate with respect to θ_e, and set the derivative equal to 0. The resulting equation involves k_o, k, C^-, and γ. By solving for γ, we obtain the lower limit of integration

$$\gamma_m = 0.5\left[-a + k_4\left(1 + 2/(kk_oC^-)\right)^{\frac{1}{2}}\right] . \qquad (19)$$

(The $(\pm)$ factor has been squared out.)

The first term in Eq. (18) involves γ only in the exponential and can be done explicitly. The other terms probably cannot be done explicitly. They are of the type

$$I = \frac{1}{T}\int_{\gamma_m}^{\infty} d\gamma e^{-\frac{\gamma}{T}} f(\gamma) . \qquad (20)$$

For temperatures small compared to 500 keV, I can be approximated by pulling $f(\gamma)$ from the integral. A better approximation is to change to the variable $s = e^{-(\gamma - \gamma_m)/T}$ and then do Gaussian quadratures.

Second-order quadratures give

$$I \approx 0.5\, e^{-\frac{\gamma_m}{T}}\left[f(\gamma_m + 0.237\,T) + f(\gamma_m + 1.554\,T)\right] . \qquad (21)$$

This gives an accuracy of 1% or better to temperatures up to 200 keV and 3% to temperatures up to 500 keV.

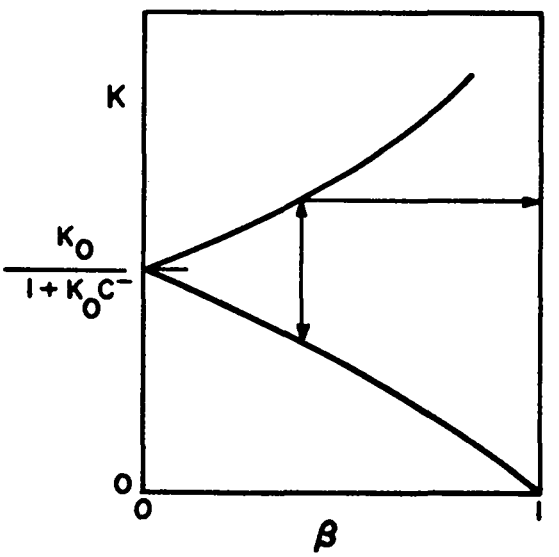

Fig. 3. Range of final energies as function of electron velocity.

The Klein-Nishina formula has a factor

$$\left(\frac{k_o'}{k'} + \frac{k'}{k_o'} - \sin^2\theta'\right)$$

$$= \left(2 + \left(\frac{k'}{k_o'} + \frac{k_o'}{k'} - 2\right) - \sin^2\theta'\right) .$$

The exact term (that integrated explicitly) comes from the 2.

Because

$$\frac{k_o'}{k'} = 1 + k_o' (C^-)', \quad \frac{k'}{k_o'} = 1 - k' (C^-)' ,$$

and

$$\frac{1}{k'} - \frac{1}{k_o'} = (C^-)' ,$$

then

$$\frac{k'}{k_o'} + \frac{k_o'}{k'} - 2 = (C^-') (k_o' - k')$$

$$= k'k_o' (C^-)' \left(\frac{1}{k'} - \frac{1}{k_o'}\right) = kk_o C^- (C^-)' . \quad (22)$$

($kk_o C^-$ is invariant.)

The cross section is then

$$\frac{\partial\sigma}{\partial k \partial\Omega} = \frac{r_o^2}{k_o^4 K_2\left(\frac{1}{T}\right)} \frac{2k}{k_4} e^{-\frac{\gamma_m}{T}}$$

$$\left[1 + 0.5\, kk_o\, C^- \langle (C^-)' \rangle - 0.5 \langle \sin^2\theta' \rangle\right] , \quad (23)$$

where $\langle\ \rangle$ indicates the appropriate average over the electron distribution. For fairly small T and γ_m, $\langle (C^-)' \rangle \approx C^-$, and

$$\frac{\partial\sigma}{\partial k \partial\Omega} \approx \frac{r_o^2}{4k_o K_2\left(\frac{1}{T}\right)} \frac{2k}{k_4} e^{-\frac{\gamma_m}{T}}$$

$$\left[1 + 0.5 \left(kk_o (C^-)^2 - \sin^2\theta\right)\right] . \quad (24)$$

This gives better than 10% accuracy for $T < 25$ keV and $\gamma_m < 1.3$.

An approximation intermediate in accuracy to the two cases above is to approximate

$$\frac{1}{T} \int_{\gamma_m}^{\infty} e^{-\frac{\gamma}{T}} f(\gamma) \text{ by } f(\gamma_m) .$$

It is exact in the limit of low temperature. Figure 2 shows that the integration over solid angle degnerates to integration over a point at $\gamma = \gamma_m$. This approximation then amounts to replacing

$\langle (C^-)' \rangle$ by the $(C^-)'$ of that point (denoted by C_m).

$\langle (C^-)' \rangle$ comes from the terms

$$k\sqrt{C^-} \left(\frac{1}{T_2^{\frac{1}{2}}} - \frac{1}{T_1^{\frac{1}{2}}}\right) \text{ in Eq. (18).}$$

We have

$$C_m = \frac{k_4\sqrt{C^-}}{C^- kk_o} \left(\frac{1}{T_2^{\frac{1}{2}}} - \frac{1}{T_1^{\frac{1}{2}}}\right) ,$$

where

$$T_1^{\frac{1}{2}} = \left[2 + C^- \left((\gamma_m + k_o)^2 - 1\right)\right]^{\frac{1}{2}} ,$$

and

$$T_2^{\frac{1}{2}} = \left[2 + C^- \left((\gamma_m - k)^2 - 1\right)\right]^{\frac{1}{2}} .$$

The formula is complicated by square roots inside of square roots, due to γ_m. These may be eliminated by the algebraic identity

$$\sqrt{a \pm \sqrt{b}} \equiv \frac{1}{\sqrt{2}}$$

$$\left(\sqrt{a + \sqrt{(a^2 - b)}} \pm \sqrt{a - \sqrt{a^2 - b}}\right) \quad (25)$$

if $(a^2 - b)$ is a perfect square. It is nearly always a perfect square for the functions associated with Compton scattering. We obtain

$$T_1^{\frac{1}{2}} = 0.5\sqrt{C^-}\left(k_2\sqrt{1 + 2/kk_oC^-} + k_4\right) ,$$

and

$$T_2^{\frac{1}{2}} = 0.5\sqrt{C^-}\left(k_2\sqrt{1 + 2/kk_oC^-} - k_4\right) .$$

$$C_m = 2\,\frac{\left(a^2 + 2kk_o\,C^-\right)}{k_2^{\,2} + k^2k_o^{\,2}\,C^-C^+} \quad . \tag{26}$$

Two things are noted: $C_m(C^- = 2)$ is 2 for all cases; if terms of $O(kk_o)$ are ignored, C_m is linear in C^-. The cross-section approximation is

$$\frac{\partial\sigma}{\partial k\partial\vec{\Omega}} \approx \frac{r_o^{\,2}}{4k_o\,K_2\left(\frac{1}{T}\right)}\,\frac{2k}{k_4}\,e^{-\frac{\gamma_m}{T}}$$

$$\left[1 - C_m(1 - 0.5\,kk_oC^-) + 0.5\,C_m^{\,2}\right] . \tag{27}$$

The dominant factor in the cross section is usually γ_m. Figure 4 shows γ_m, for fixed k, as a function of cosθ. Unless $k = k_o$, γ_m goes to infinity for forward scattering. For all $k \neq k_o$, the cross section for forward scattering is 0, but it is infinite for $k = k_o$. γ_m has a minimum at

$$C^- = \left|\frac{1}{k_o} - \frac{1}{k}\right| \quad .$$

For $k > k_o/(1 - 2k_o)$ or $k < k_o/(1 + 2k_o)$, this minimum is at an unphysical angle, and the real minimum is at $C^- = 2$. Figure 5 shows the cross sections

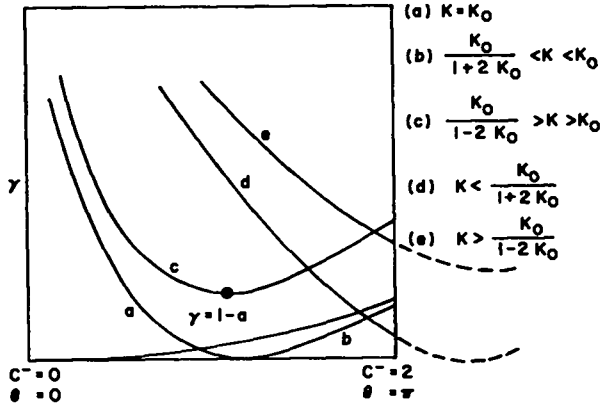

Fig. 4. Minimum electron energy as function of scattering angle (for constant k).

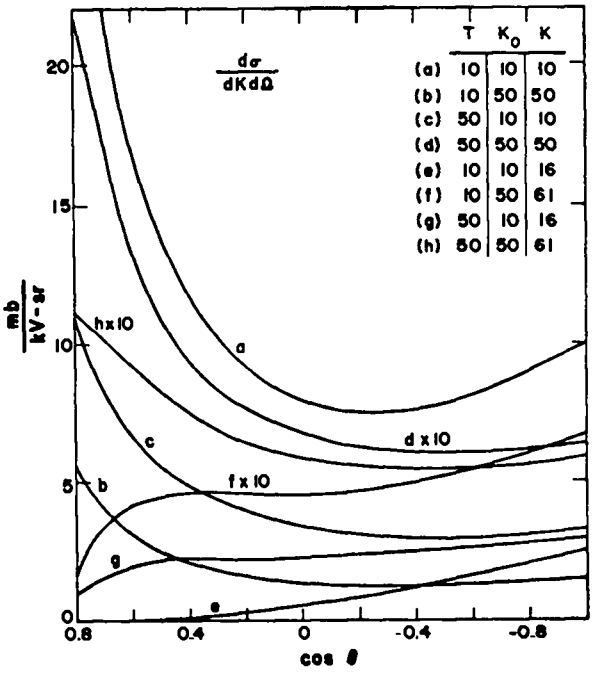

Fig. 5. Differential cross sections.

for some typical cases in units of millibarns per keV per steradian.

III. THE MONTE CARLO SCATTERING SCHEME

The approximations to the indefinite integrals (discussed in Sec. I) should be chosen to minimize the amount of calculation. This will depend upon the complexity of the formulae and the number of times the process must be repeated to get a scattering. The integration of the exact term found in Sec. II fits these conditions fairly well. The third random number is compared to

$$\frac{\left[1 - 0.5\,\langle\sin^2\theta'\rangle + 0.5\,kk_o\,C^-\,\langle(C^-)'\rangle\right]}{\left[1 - 0.5\,\langle\sin^2\theta'\rangle + 0.5\,kk_o\,C^-\,\langle(C^-)'\rangle\right]_{max}} \tag{28}$$

For energies small compared to 500 keV, this is about

$$1 - 0.5\,\langle\sin^2\theta'\rangle \quad .$$

Because the average value of $\langle\sin^2\theta'\rangle \approx \frac{2}{3}$, the number of times the process must be repeated is

$$1 + \frac{1}{3} + \frac{1}{9} + \ldots = 1.5 \quad .$$

The maximum is unbounded because k may be arbitrarily large. However, the maximum may be replaced by

$$\left[1 + 2\, k_a k_o\right] , \quad k_a = k_o + \alpha T . \tag{29}$$

Then

$$\gamma_m \,(k > k_a) > 1 + \alpha T .$$

The replacement underestimates the cross section for $k > k_a$ for backward scattering, but because the cross section is small by some exponential factor, it is not important.

Where the exact term is denoted by σ_1,

$$\frac{\partial \sigma_1}{\partial k \partial \cos\theta} = \frac{k k_o}{k_4}\; e^{-\frac{\gamma}{T}} . \tag{30}$$

A constant factor in front, as well as the subscript on γ_m has been dropped. The inversion of Eq. (19) gives

$$C^- = \left(\gamma^2 + \gamma a - 1 \pm \alpha_1 \alpha_2\right) / k k_o , \tag{31}$$

where

$$\alpha_2 = \sqrt{\gamma^2 - 1} ,$$

and

$$\alpha_1 = \sqrt{(\gamma + a)^2 - 1} .$$

The $\pm$ refers to two different branches. The range of the branches over k and γ is shown in Fig. 6. The minus branch exists above the curve (1) in the figure. The curve is defined by putting $C^- = 2$ into Eq. (19). Both branches exist between the curve and the straight line $\gamma = 1$ and $\gamma = 1 - k_o + k$.

The plus branch exists only for

$$1 \le \gamma \le \gamma_1 = \begin{cases} 1 + 2k_o^2 \big/ (1 - 2k_o) , & k_o < \frac{1}{2} \\ \infty , & k_o \ge \frac{1}{2} \end{cases} .$$

The values of k on curve (1) in Fig. 6 are

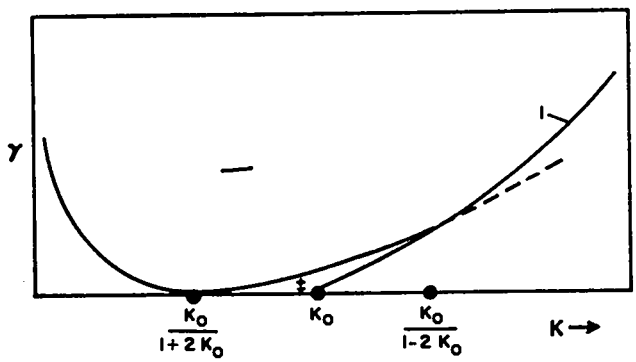

Fig. 6. Range of the independent variables γ and k.

$$k_m = \frac{k_o \left(2\gamma^2 + 2\gamma k_o - 1 - 2\,(\gamma + k_o)\,\alpha_2\right)}{1 + 4\gamma k_o + 4 k_o^2}$$

and

$$k_p = \frac{k_o \left(2\gamma^2 + 2\gamma k_o - 1 + 2\,(\gamma + k_o)\,\alpha_2\right)}{1 + 4\gamma k_o + 4 k_o^2} . \tag{32}$$

With the use of identity (25)

$$\frac{1}{k_4} = \frac{\alpha_1 \mp \gamma_2}{a(2\gamma + a)}$$

and

$$\frac{\partial C^-}{\partial \gamma} = \frac{(2\gamma + a)}{k k_o} \left(1 \pm \frac{(\gamma^2 + \gamma\alpha - 1)}{\alpha_1 \alpha_2}\right) . \tag{33}$$

Then, when the independent variable is changed from C^- to γ,

$$\frac{\partial \sigma_1}{\partial k \partial \gamma} = \left| \frac{\gamma + \alpha}{\alpha_1} \pm \frac{\gamma}{\alpha_2} \right| e^{-\frac{\gamma}{T}} . \tag{34}$$

A value of γ is found by picking a random number P_1, and solving

$$\int_1^{\gamma} \frac{\partial \sigma_1}{\partial \gamma}\, d\gamma = P_1 \int_1^{\infty} \frac{\partial \sigma_1}{\partial \gamma}\, d\gamma , \tag{35}$$

where $\partial \sigma_1 / \partial \gamma$ is the integral of Eq. (34) over all relevant k. The branches are summed over (Table 1).

TABLE I

PROPERTIES OF THE INTEGRAL OVER K

Group	Branch	k limits	a_1	a_2	Integral over Group
I	-	$k_m \le k \le k_o$	1	1	$e^{-\frac{\gamma}{T}} 2 k_m k_o/\alpha_2$
II	-	$k_o \le k \le \gamma - 1 + k_o$ $[k_o \le k \le k_p]$	-1	-1	$e^{-\frac{\gamma}{T}} (\gamma - 1)/\alpha_2$ $\left[e^{-\frac{\gamma}{T}} 2 k_p k_o/\alpha_2\right]$
III	+	$k_p \le k \le \gamma - 1 + k_o$	1	-1	$e^{-\frac{\gamma}{T}} \frac{(2k_p k_o - \gamma + 1)}{\alpha_2}$ [0]

Quantities in brackets are for $\gamma > \gamma_1$.

When γ is known, k is picked by equating a random number P_2 to the indefinite integral over k of $\partial\sigma_1/\partial k \partial\gamma$. This is

$$\int \frac{\partial\sigma_1}{\partial k \partial\gamma}\, dk = \left(a_1 \frac{k\gamma}{\alpha_2} + a_2 \alpha_1\right) e^{-\frac{\gamma}{T}} \quad ,$$

$$|a_1| = |a_2| = 1 \, . \tag{36}$$

The range of k may be divided into three groups. For each group, Table I gives a_1, a_2, and other properties.

The value of $\partial\sigma_1/\partial\gamma$ is

$$\frac{\partial\sigma_1}{\partial\gamma} = \frac{4k_o^2}{\alpha_2} \frac{(2\gamma^2 + 2\gamma k_o - 1)}{1 + 4\gamma k_o + 4k_o^2} e^{-\frac{\gamma}{T}} \, . \tag{37}$$

This cannot be integrated explicitly, but if some of the factors are expanded about $\gamma = 1$, the approximation can be integrated in terms of the error function.

$$\frac{\partial\sigma_1}{\partial\gamma} \approx \frac{\partial\sigma_2}{\partial\gamma} =$$

$$e^{-\frac{\gamma}{T}} \frac{4k_o^2}{(1 + 2k_o)\sqrt{2}} \frac{\left[1 + F_1 (\gamma-1) + F_2(\gamma-1)^2\right]}{\sqrt{\gamma - 1}} \, , \tag{38}$$

where

$$F_1 = \left(3.75 + 5k_o + 3k_o^2\right) \Big/ \left(1 + 2k_o\right)^2 \quad ,$$

and

$$F_2 = \frac{1}{32} - \frac{2}{(1 + 2k_o)^3} \left[1 - \frac{2}{(1 + 2k_o)}\right] - \frac{F_1}{4} \, .$$

The equation now to be solved is

$$P_1 \frac{\sqrt{\pi}}{2} F_3 = F_3 \int_o^x e^{-w^2} dw - F_4 e^{-x^2} \quad , \tag{39}$$

where

$$x^2 = (\gamma-1)/T \, ,$$

$$F_3 = 1 + F_1 \frac{T}{2} + \frac{3}{4} F_2 T^2 \, ,$$

and

$$F_4 = F_2 T^2 \frac{x^3}{2} + \frac{3}{4} F_2 T^2 x + F_1 T \frac{x}{2} \, .$$

The integral is the error function, which may be tabulated. The following gives x better than one part in 10^3 for temperatures less than about 100 keV. Where

$$G_1 = F_1 T/2,$$

$$x_2 = x_1 \left[1 + G_1 \Big/ \left(1 + G_1 (1 + G_1) x_1^2\right)\right],$$

where

$$P_1 \frac{\sqrt{\pi}}{2} = \int_o^{x_1} e^{-w^2} dw \, .$$

The value of x_1 may be obtained from a tabulation of the inverse of the error function. Then x is obtained from x_2 by one application of Newton's method.

A distribution of γ corresponding to $\partial\sigma_1/\partial\gamma$ may be obtained by comparing a random number P_4 to

$$\frac{(2\gamma^2 + 2\gamma k_o - 1)}{1 + 4\gamma k_o + 4k_o^2} \frac{\sqrt{2}}{\sqrt{\gamma + 1}} \frac{(1 + 2k_o)}{\left(1 + F_1 (\gamma-1) + F_2 (\gamma - 1)^2\right)} \, . \tag{40}$$

If P_4 is greater than the ratio, a new value of P_1 is picked. The ratio must always be less than 1. This will be true if $k_o < 0.111$. For $k_o > 0.111$, it is true if F_2 is replaced by 0. For $\gamma < 2$, the ratio is always greater than

$$\begin{cases} 1/\left[1 + 0.035\ (\gamma-1)\right] & , \quad k_o < 0.111 \\ 1/\left[1 + 0.13\ (\gamma-1)\right] & , \quad k_o > 0.111 \ . \end{cases}$$

If P_4 is less than this simpler expression (and it almost always is), the calculation of the more complicated term may be avoided.

When γ is known, one picks a random number P_2 and calculates

$$A = 2k_o \left(P_2\ (k_m + k_p) - k_m\right), \qquad (41)$$

which is essentially equivalent to

$$\int_{k_o}^{k} \frac{\partial \sigma_1}{\partial k \partial \gamma}\, dk \ .$$

There are three possibilities for A. After some algebra, which is not included here, one has

(1) $A > \gamma - 1$. Then k is on the positive branch.

Let

$$A_1 = -A + 2k_o k_p \ ,$$

and

$$A_2 = A_1 + \gamma \ .$$

Then $k = \gamma + k_o - \gamma A_2 + \alpha_2 \sqrt{A_2^{\,2} - 1}$,

and

$$C^- = (\gamma - 1 + A_1)/kk_o \ .$$

A will not be greater than $(\gamma - 1)$ if the positive branch does not exist at that value of γ.

(2) $0 \le A \le \gamma - 1$.

$$k = k_o - A\gamma + \alpha_2 \sqrt{A\ (A + 2)} \ ,$$

and

$$C^- = A/kk_o \ .$$

(3) $A < 0$,

$$k = k_o + A\gamma - \alpha_2 \sqrt{A^2 - 2A} \ ,$$

$$C^- = -A/kk_o \ .$$

Then a random number P_3 is compared to

$$\left[1 - 0.5\ \langle \sin^2 \theta' \rangle + 0.5kk_oC^-\ \langle (C^-)' \rangle\right] \Big/ \left[1 + 2k_ak_o\right] \ . \qquad (42)$$

The calculation of the ratio in Eq. (42) may be rather lengthy, therefore it is avoided if possible. If P_3 is less than $0.5/[1 + 2k_ak_o]$, it is less than the ratio in Eq. (42), and no further calculation is required. Otherwise, we calculate

$$A = \left[1 - 0.5\ \sin^2 \theta + 0.5kk_o(C^-)^2\right] \Big/ \left[1 + 2k_ak_o\right] .$$

It was empirically found that expression (42) is greater than

$$A \times \text{Minimum}\left[\frac{(1 + 4.02\ T)}{(1 + 8.14\ T)}\ ,\ \ 1.35 - 0.39\gamma\right], \qquad (43)$$

and less than

$$A \times \text{Maximum}\left[\frac{1 + 8.\ T}{1 + 5.5\ T}\ ,\ \ 0.51 + 0.53\gamma\right] . \qquad (44)$$

If P_3 is less than Eq. (43), the reaction goes. If it is greater than Eq. (44), the entire procedure must be started over. If P_3 is between Eqs. (43) and (44), it must be compared to an acceptably accurate approximation to Eq. (42), for example, from Eq. (21).

If care is taken to predefine all factors occurring more than once, somewhat more than 100 operations (additions, division, etc.) are required each time through the procedure. An exponential and two square roots are also required. Also, one usually must go through the procedure about 1-1/2 times to get a scattering.

IV THE TOTAL CROSS SECTION AND EXPECTATION ENERGY LOSS

The total cross section is needed to determine the position where the photon scatters. At the point of scattering one may deposit in the material energy proportional to $(k_o - k)$. Depending upon the temperature and initial energy, this method may require a large number of scatterings for the energy deposition to settle down to its expectation value. One scheme, which has been used to reduce the fluctuation in energy deposition, is to deposit the expectation energy loss, $\langle k_o - k \rangle$, at each scattering. Energy is then conserved only statistically.

The total cross section is

$$\sigma_T = \frac{1}{2TK_2\left(\frac{1}{T}\right)} \int_1^\infty d\gamma\, e^{-\gamma} \beta \gamma^2 \int_{-1}^{1} dx\, (1-\beta x)\, \sigma_T'(k_o') \quad . \tag{45}$$

The cross section should include a factor $(1 + n_k)$, where $n_k(k,\Omega)$ is the number of photons per final state, but this is neglected.

The expectation energy loss is

$$\langle k_o - k \rangle = k_o - \frac{1}{\sigma_T\, 2T\, K_2\left(\frac{1}{T}\right)} \int_1^\gamma d r\, e^{-\gamma} \beta \gamma^2 \int_{-1}^{1} dx\, (1-\beta x) \int d\Omega' \frac{\partial \sigma'}{\partial \Omega'}(k_o', \Omega')k \quad . \tag{46}$$

The cross section in the rest system of the electron depends upon the photon energy in that system,

$$k_o' = k_o \gamma (1-\beta x) \quad .$$

It is obtained by integrating Eq. (5) over the solid angle.

$$\sigma_T'(k_o') = \pi r_o^2 \left\{ \log(1 + 2k_o') \left(\frac{1}{k_o'} - \frac{2}{k_o'^3} - \frac{2}{k_o'^2} \right) + \frac{4}{k_o'^2} + \frac{1}{(1 + 2k_o')} + \frac{1}{(1 + 2k_o')^2} \right\} \quad . \tag{47}$$

For any $\sigma_T'(k_o')$, Eq. (45) may be reduced to a one-dimensional integral by changing the variable of integration from x to k_o' and then by inverting the order of integration.*

$$\frac{\partial k_o'}{\partial x} = -\beta \gamma k_o \quad .$$

Then Eq. (45) is

$$\sigma_T = \frac{1}{2TK_2\left(\frac{1}{T}\right)k_o^2} \int_1^\infty d\gamma e^{-\frac{\gamma}{T}} \int_{\gamma k_o(1-\beta)}^{\gamma k_o(1+\beta)} dk_o' k_o' \sigma_T'(k_o') \quad . \tag{48}$$

After the order of integration is inverted,

$$\sigma_T = \frac{1}{2\, K_2\left(\frac{1}{T}\right)k_o^2} \int_0^\infty dk_o' k_o' \sigma_T'(k_o') \, e^{-\frac{1}{2}\left(\frac{k_o'}{k_o} + \frac{k_o'}{k_o}\right)} \Big/ T$$

$$= \frac{1}{2\, K_2\left(\frac{1}{T}\right)} \sum_{\pm} \int_1^\infty \frac{d\gamma\, e^{-\frac{\gamma}{T}}}{\sqrt{\gamma^2 - 1}} \left(\gamma \pm \sqrt{\gamma^2 - 1}\right)^2 \sigma_T\left[k_o\left(\gamma \pm \sqrt{\gamma^2 - 1}\right)\right] . \tag{49}$$

Let

$$A = 1/(1 + 4k_o\gamma + 4k_o^2) \quad ,$$

$$A_1 = \log\left[1 + 2k_o\left(\gamma + \sqrt{\gamma^2 - 1}\right)\right] \quad ,$$

and

$$A_2 = \log\left[1 + 2k_o\left(\gamma - \sqrt{\gamma^2 - 1}\right)\right] .$$

* The idea for the change of variable and inversion came from a memorandum by the Mathematical Applications Group, Inc., White Plains, N.Y. However, the formula in the memorandum is incorrect due to an error in the Doppler shift and the cross-section transformation.

Then

$$\sigma_T = \frac{\pi r_o^2}{K_2\left(\frac{1}{T}\right)} \int_1^\infty \frac{d\gamma\, e^{-\frac{\gamma}{T}}}{\sqrt{\gamma^2 - 1}} \left[\frac{1}{2}(A_1 + A_2)\right.$$

$$\left(\frac{\gamma}{k_o} - \frac{2\gamma}{k_o^3} - \frac{2}{k_o^2}\right) + \frac{1}{2}\sqrt{\gamma^2 - 1}\,(A_1 - A_2)$$

$$\left.\left(\frac{1}{k_o} + \frac{2}{k_o^3}\right) + \frac{4}{k_o^2} + A^2 2(\gamma^2 - 1) + 2A\gamma(\gamma + k_o)\right] . \tag{50}$$

The integral in Eq. (46) (denoted by I) can be treated in the same way in a slightly more complicated manner. The differential cross section depends upon both k_o' and the angle of scatter. Also,

$$k = \gamma k' \left[1 + \beta(\cos\theta' \cos\theta_e' + \sin\theta_e' \sin\theta' \cos(\omega' - \omega_e')\right] , \tag{51}$$

where

$$\cos\theta_e' = \frac{x - \beta}{1 - \beta x}$$

by the usual angle transformation formula.

Integration over $d\varphi'$ multiplies the first two terms of k by 2π and cancels the last one.

$$I = 2\pi \int_1^\infty d\gamma e^{-\gamma} \beta\gamma^3 \int_{-1}^{1} dx \left\{(1 - \beta x) f(k_o') + \beta(x - \beta) g(k_o')\right\} , \tag{52}$$

where

$$f(k_o') = \int d\cos\theta'\, k' \frac{\partial\sigma'}{\partial\cos\theta'}$$

and

$$g(k_o') = \int d\cos\theta'\, k' \cos\theta' \frac{\partial\sigma'}{\partial\cos\theta'} .$$

After the change of variable from x to k_o' and the inversion of order of integration,

$$I = \frac{2\pi}{k_o} \int_\gamma^\infty d k_o'\, e^{-\frac{1}{2}\left(\frac{k_o'}{k_o} + \frac{k_o}{k_o'}\right)} \Big/ T$$

$$\left\{\left[f(k_o') - g(k_o')\right] \frac{k_o'}{k_o}(\gamma + T) + g(k_o')\right\}$$

$$= 2\pi \sum_{\pm} \int_1^\infty \frac{e^{-\frac{\gamma}{T}} d\gamma}{\sqrt{\gamma^2 - 1}} \left(\gamma \pm \sqrt{\gamma^2 - 1}\right)$$

$$\left\{\left(f\left[k_o\left(\gamma \pm \sqrt{\gamma^2 - 1}\right)\right]\right.\right.$$

$$\left.\left. - g\left[k_o\left(\gamma \pm \sqrt{\gamma^2 - 1}\right)\right]\right)(\gamma + T)\left(\gamma \pm \sqrt{\gamma^2 - 1}\right)\right.$$

$$\left. + g\left[k_o\left(\gamma \pm \sqrt{\gamma^2 - 1}\right)\right]\right\} . \tag{53}$$

For Compton scattering,

$$f(k_o') = \frac{r_o^2}{2}\left[\frac{4}{3} + \frac{1}{1 + 2k_o'} - \frac{2}{k_o'} - \frac{1}{3(1 + 2k_o')^3} + \frac{\log\left[1 + 2k_o'\right]}{k_o'^2}\right] \tag{54}$$

and

$$g(k_o') = \frac{r_o^2}{2}\left[-\frac{6}{k_o'^2} + \frac{4}{3} - \frac{4}{3(1+2k_o')}\right.$$

$$- \frac{1}{3(1+2k_o')^2} + \frac{1}{3(1+2k_o')^3}$$

$$\left. + \log(1+2k_o')\left[\frac{3}{k_o'^3} + \frac{3}{k_o'^2} - \frac{1}{k_o'}\right]\right] .$$

Then

$$I = \frac{\pi r_o^2}{K_2\left(\frac{1}{T}\right)} \int_1^\infty \frac{d\gamma\, e^{-\frac{\gamma}{T}}}{\sqrt{\gamma^2-1}} \left[-\frac{6\gamma}{k_o^2} + \frac{4\gamma}{3}\right.$$

$$- \frac{4}{3}A(\gamma + 2k_o) - \frac{1}{3}A^2(\gamma + 4k_o + 4k_o^2\gamma)$$

$$+ \frac{A^3}{3}\left[\gamma + 6k_o + 12k_o^2\gamma + 8k_o^3(2\gamma^2-1)\right]$$

$$+ \frac{1}{2}(A_1 + A_2)\left[\frac{3}{k_o^3}(2\gamma^2-1) + \frac{3\gamma}{k_o^2} - \frac{1}{k_o}\right]$$

$$+ \frac{1}{2}(A_2 - A_1)\sqrt{\gamma^2-1}\left[\frac{6\gamma}{k_o^3} + \frac{3}{k_o^2}\right]$$

$$+ (\gamma + T)\left\{-\frac{2\gamma}{k_o} + \frac{6}{k_o^2} + \frac{7}{3}A(2\gamma^2 - 1 + 2k_o\gamma)\right.$$

$$+ \frac{A^2}{3}(2\gamma^2 - 1 + 4k_o\gamma + 4k_o^2) - \frac{2}{3}A^3(2\gamma^2 - 1$$

$$+ 6k_o\gamma + 12k_o^2 + 8k_o^3\gamma) + \frac{1}{2}(A_1 + A_2)$$

$$\left(\frac{\gamma}{k_o} - \frac{2}{k_o^2} - \frac{3\gamma}{k_o^3}\right) + \frac{1}{2}(A_1 - A_2)\sqrt{\gamma^2-1}$$

$$\left.\left.\left(\frac{3}{k_o^3} + \frac{1}{k_o}\right)\right\}\right] . \qquad (55)$$

These have been integrated numerically. Table II gives results up to about 200 keV. The upper entry is σ_T in terms of the Thomson cross section, $\frac{8}{3}\pi r_o^2$, and the lower entry is $\langle k_o - k\rangle/k_o$.

For small values of k_o, σ_T', $f(k_o')$, and $g(k_o')$ can be expanded in a power series. The first few terms are

$$\sigma_T' \approx \frac{8}{3}\pi r_o^2 (1 - 2k_o') ,$$

$$g(k_o') \approx \frac{r_o^2}{2}\frac{16}{5}k_o'^2 ,$$

$$f(k_o') \approx \frac{r_o^2}{2}\left(\frac{8}{3}k_o' - 8k_o'^2\right) . \qquad (56)$$

With these approximations,

$$I = \left(\frac{8\pi}{3}r_o^2\right) 2TK_2\left(\frac{1}{T}\right)k_o \left\{1 + 16T^2 + 4Tx\right.$$

$$\left. - k_o\left(36T + 504T^3 + x(3 + 129T^2)\right)\right\} ,$$

and

$$\sigma_T = \left(\frac{8}{3}\pi r_o^2\right)\left\{1 - 2k_o(x + 4T)\right\} , \qquad (57$$

where

$$x = K_1\left(\frac{1}{T}\right)\Big/K_2\left(\frac{1}{T}\right) .$$

Higher-order terms have much larger coefficients, so the series is of little use except for low energies. Better approximations may be obtained by expanding the integrand (with respect to γ) about $\gamma = 1$. For low energies and temperature,

$$\langle k_o - k\rangle/k_o \approx -4T + k_o . \qquad (58)$$

Deposition of the expectation energy loss at the point of scattering may be expanded to deposition of the expectation loss along the path of the particle (up to a certain optical depth). Each Monte Carlo particle which represents a large number of physical particles, does two things; (1) it produces a secondary distribution of particles, and (2) it deposits energy along the line of flight. Although these are physically connected, they may be formally dissociated. Because each additional photon necessitates extra work, the secondary distribution is represented by (usually) one photon chosen in an entirely stochastic manner. For each

TABLE II

COMPTON CROSS SECTION AND AVERAGE ENERGY LOSS

k_o \ T	0.0	0.04	0.08	0.2	0.16	0.20	0.24	0.28	0.32	0.36	0.40
0	1.000 0	1.000 -0.1765	1.000 -0.3875	1.000 -0.6355	1.000 -0.9223	1.000 -1.249	1.000 -1.618	1.000 -2.030	1.000 -2.485	1.000 -2.985	1.000 -3.530
0.04	0.9275 $0.3678\bar{1}$	0.9211 -0.1132	0.9146 -0.2867	0.9080 -0.4836	0.9013 -0.7037	0.8947 -0.9466	0.8881 -1.212	0.8812 -1.498	0.8745 -1.806	0.8677 -2.134	0.8608 -2.481
0.08	0.8676 $0.6813\bar{1}$	0.8574 $-0.6235\bar{1}$	0.8471 -0.2099	0.8370 -0.3741	0.8270 -0.5542	0.8171 -0.7495	0.8076 -0.9594	0.7979 -1.183	0.7885 -1.420	0.7793 -1.670	0.7702 -1.932
0.12	0.8171 $0.9527\bar{1}$	0.8046 $-0.2024\bar{1}$	0.7923 -0.1490	0.7802 -0.2903	0.7684 -0.4435	0.7570 -0.6080	0.7458 -0.7832	0.7351 -0.9686	0.7244 -1.163	0.7141 -1.367	0.7041 -1.580
0.16	0.7741 0.1191	0.7602 $0.1537\bar{1}$	0.7466 $-0.9897\bar{1}$	0.7335 -0.2234	0.7208 -0.3572	0.7085 -0.5000	0.6966 -0.6512	0.6853 -0.8102	0.6742 -0.9767	0.6634 -1.150	0.6530 -1.330
0.20	0.7369 0.1402	0.7221 $0.4604\bar{1}$	0.7079 $-0.5696\bar{1}$	0.6942 -0.1683	0.6810 -0.2874	0.6683 -0.4139	0.6562 -0.5473	0.6445 -0.6871	0.6330 -0.8327	0.6223 -0.9852	0.6118 -1.142
0.24	0.7044 0.1591	0.6892 $0.7284\bar{1}$	0.6746 $-0.2095\bar{1}$	0.6606 -0.1219	0.6471 -0.2294	0.6343 -0.3432	0.6221 -0.4627	0.6103 -0.5878	0.5991 -0.7179	0.5882 -0.8528	0.5777 -0.9928
0.28	0.6758 0.1761	0.6603 $0.9657\bar{1}$	0.6455 $-0.1040\bar{1}$	0.6314 -0.81951	0.6179 -0.1801	0.6051 -0.2836	0.5928 -0.3921	0.5811 -0.5053	0.5699 -0.6229	0.5592 -0.7446	0.5487 -0.8702
0.32	0.6503 0.1917	0.6347 0.1178	0.6199 $0.3807\bar{1}$	0.6057 $-0.4713\bar{1}$	0.5923 -0.1374	0.5795 -0.2324	0.5673 -0.3319	0.5557 -0.4354	0.5446 -0.5428	0.5340 -0.6535	0.5237 -0.7681
0.36	0.6274 0.2059	0.6118 0.1370	0.5970 $0.6275\bar{1}$	0.5830 $-0.1637\bar{1}$	0.5696 -0.1000	0.5569 -0.1879	0.5449 -0.2797	0.5334 -0.3752	0.5224 -0.4741	0.5119 -0.5761	0.5018 -0.6811
0.40	0.6067 0.2191	0.5912 0.1544	0.5765 $0.8498\bar{1}$	0.5626 $0.1111\bar{1}$	0.5493 $-0.6687\bar{1}$	0.5368 -0.1486	0.5249 -0.2339	0.5134 -0.3225	0.5026 -0.4142	0.4923 -0.5086	0.4824 -0.6058

($0.3678\bar{1} \equiv 0.3678 \times 10^{-1}$)

existing photon, the extra work of calculating the energy loss in each zone is small.

Up to an optical depth, s_1, the expectation loss is deposited in each zone; beyond s_1 the expectation loss for a particle of reduced weight e^{-s_1} is deposited at a point chosen stochastically. We calculate the variance in energy deposition, find the minimum variance, and compare this to the more conventional case, $s_1 = 0$.

Consider a zone of optical depth Δs ($\Delta s \ll 1$) centered at the origin in homogeneous material. The number of particles originating at s in the direction of the zone is

$$dn = n_o\, ds \quad . \tag{59}$$

For $0 \leq s \leq s_1$, the number of particles depositing energy is

$$dn_e = dn \quad , \tag{60}$$

and the deposition per particle is $E\, e^{-s} \Delta s$, where E is the expectation loss (for a full weight particle).

For

$$s_1 \leq s \leq \infty \, ,$$

$$dn_e = dn\, e^{-(s - s_1)}\, \Delta s \quad , \tag{61}$$

and the energy deposited is $E\, e^{-s_1}$.

Let the variance per particle ΔE_p, be the energy deposited times a factor α. The total variance is taken as

$$(\Delta E)^2 = \sum_{\text{particles}} (\Delta Ep)^2$$

$$\longrightarrow \int_0^{s_1} n_o ds\, \alpha^2 E^2\, e^{-2s}\, (\Delta s)^2$$

$$+ \int_{s_1}^{\infty} n_o ds\, e^{-(s - s_1)}\, \Delta s\, \alpha^2 E^2\, e^{-2s_1}$$

$$= \alpha^2 E^2\, n_o\, \Delta s \left[\frac{\Delta s}{2}\,(1 - e^{-2s_1}) + e^{-2s_1}\right] . \qquad (62)$$

E is proportional to the weight of the particle: $E = A/n_o$. The stochastic deposition is usually one optical depth beyond s_1. The work required (computer time) is $W = Bn_o\,(1 + s_1)$.

Then

$$(\Delta E)^2 = \alpha^2 A^2\, \frac{B(1 + s_1)}{W}\, \Delta s \left[\frac{\Delta s}{2}\,(1 - e^{-2s_1}) + e^{-2s_1}\right] . \qquad (63)$$

The minimum value depends upon Δs. For a fairly thin zone, $\Delta s = 0.01$, the minimum value occurs at $s_1 = 3.7$, where

$$(1 + s_1)\left[\frac{\Delta s}{2}\,(1 - e^{-2s_1}) + e^{-2s_1}\right] = 0.026$$

as compared to 1 for $s_1 = 0$. For the seme variance about 1/40 as much work is required.

V. THE CROSS SECTION INTEGRATED OVER SOLID ANGLE

Other cross sections of interest are

$$\frac{\partial \sigma^n}{\partial k} = \int d\cos\theta\, P_n(\cos\theta)\, \frac{\partial \sigma}{\partial k \partial \cos\theta} . \qquad (64)$$

These can be reduced to one-dimensional integrals by inverting the order of integration in Eq. (18). The integration over $\cos\theta$ is elementary. Here it is done for $n = 0$.

The upper limit for $\cos\theta$ is given by

$$C^- = (\gamma^2 + \gamma a - 1 - \alpha_1 \alpha_2)/kk_o . \qquad (65)$$

The integral over γ can then be divided into two regions, A and B, depending upon the lower limit of $\cos\theta$ (Fig. 4). In A the lower limit is given by

$$C^- = (\gamma^2 + \gamma a - 1 + \alpha_1 \alpha_2)/kk_o . \qquad (66)$$

The range of A is

$$\gamma_1 = [1 - \min(o,a)] \leq \gamma \leq \gamma_2 ,$$

where

$$\gamma_2 = 0.5\,(-a + k_2 \sqrt{1 + 1/kk_o}) . \qquad (67)$$

A exists only for cases (a), (b), and (c) of Fig. 4. B covers $\gamma_2 \leq \gamma < \infty$, and the lower limit of $\cos\theta$ is -1.

The indefinite integral of the brackets, $\{\}$, in Eq. (18) with respect to $d\cos\theta$ is

$$\frac{1}{k_o}\left\{- 2k_4 + \frac{T_1^{1/2}}{\sqrt{C^-}}\left[\frac{kk_oC^-}{g_1} + \frac{2}{kk_o}\right]\right.$$

$$-\sqrt{\frac{T_2}{C^-}}\left[\frac{kk_oC^-}{g_2} + \frac{2}{kk_o}\right] - \sqrt{\frac{C^-}{T_1}}\left[\frac{k_2\gamma + k_oa}{kk_o} - \frac{2}{g_1}\right]$$

$$-\sqrt{\frac{C^-}{T_2}}\left[\frac{k_2\gamma + k_a}{kk_o} + \frac{2}{g_2}\right]$$

$$-\left[\frac{kk_o + 1}{g_1} + 2\right]\frac{2}{\sqrt{g_1}}\log\left(\sqrt{T_1} + \sqrt{g_1C^-}\right)$$

$$\left.+\left[\frac{kk_o + 1}{g_2} + 2\right]\frac{2}{\sqrt{g_2}}\log\left(\sqrt{T_2} + \sqrt{g_2C^-}\right)\right\}, \qquad (68)$$

where

$$g_1 = (\gamma + k_o)^2 - 1$$

and

$$g_2 = (\gamma - k)^2 - 1 \ .$$

If $g_2 < 0$, $\frac{2}{g_2}$ [. . .] is replaced by

$$-\frac{1}{\sqrt{-g_2}} \sin^{-1} [1 + g_2 C^-] \ .$$

Where

$$C^- = (\gamma^2 + \gamma a - 1 \pm \alpha_1 \alpha_2)/kk_o \ ,$$

the identity of Eq. (25) may be used to give

$$k_4 = \alpha_1 \pm \alpha_2 \ ,$$

$$\sqrt{\frac{T_1}{C^=}} = (k_o \alpha_1 \mp k\alpha_2)/a, \qquad (69)$$

and

$$\sqrt{\frac{T_2}{C^=}} = (k \alpha_1 \mp k_o \alpha_2)/a \ .$$

For the lower sign, the right-hand side of Eq. (69) is multiplied by -1 for negative a.

Let

$$\alpha_< = \min (\alpha_1, \alpha_2) \ ,$$

$$k_< = \min (k, k_o) \ ,$$

$$\alpha_> = \max (\alpha_1, \alpha_2) \ ,$$

$$k_> = \max (k, k_o) \ ,$$

and

$$\textcircled{\pm} = \begin{cases} + & k_o > k \\ - & k_o < k \end{cases} \ . \qquad (70)$$

Then

$$\frac{\partial \sigma}{\partial k} = \frac{\pi r_o^2}{2 k_o^2 TK_2\left(\frac{1}{T}\right)} \int d\gamma \, e^{-\frac{\gamma}{T}} f \ ,$$

where

$$f_A = 2\alpha_< \left\{ -\frac{2}{kk_o} + \left(1 + \frac{1}{kk_o}\right) \left[k < \frac{(\gamma + k_o)}{g_1} \right. \right.$$

$$\left. \left. - k > \frac{(\gamma - k)}{g_2} \right] \right\}$$

$$+ \left[2 + \frac{1 + kk_o}{g_1}\right] \frac{2}{\sqrt{g_1}} \left[\log \left(\frac{\gamma^2 + \gamma a - 1 + \alpha_1 \alpha_2}{|a|} \right) \right.$$

$$\left. + \log \left(\frac{\sqrt{g_1}\, a + k_o \alpha_1 - k\alpha_2}{\sqrt{g_1}\, a \textcircled{\pm} (k_o \alpha_1 + k\alpha_2)} \right) \right]$$

$$- \left[2 + \frac{1 + kk_o}{g_2}\right] \frac{2}{\sqrt{g_2}} \left[\log \left(\frac{\gamma^2 + \gamma a - 1 + \alpha_1 \alpha_2}{|a|} \right) \right.$$

$$\left. + \log \left(\frac{\sqrt{g_2}\, a + k\alpha_1 - k_o \alpha_2}{\sqrt{g_2}\, a \textcircled{\pm} (k\alpha_1 + k_o \alpha_2)} \right) \right] ,$$

and

$$f_B = \frac{2}{kk_o} (\alpha_> - \alpha_<)$$

$$+ \left(1 + \frac{1}{kk_o}\right) \left\{ \frac{\gamma - k}{g_2} \ (k < \alpha_> - k > \alpha_<) \right.$$

$$\left. - \frac{\gamma + k_o}{g_1} \ (k > \alpha_> - k < \alpha_<) \right\}$$

$$+ 2k_2 + 2 (1 + kk_o) \left\{ \frac{\gamma - k}{g_2} - \frac{\gamma + k_o}{g_1} \right\}$$

$$+ \left[2 + \frac{1 + kk_o}{g_1}\right] \frac{1}{\sqrt{g_1}} \left[\log \left(\frac{2kk_o}{\gamma^2 + \gamma a - 1 - \alpha_1 \alpha_2} \right) \right.$$

$$\left. + 2 \log \left(\frac{\sqrt{g_1}\, a + a (\gamma + k_o)}{\sqrt{g_1}\, a \textcircled{\pm} (k_o \alpha_1 + k\alpha_2)} \right) \right]$$

$$- \left[2 + \frac{1 + kk_o}{g_2}\right] \frac{1}{\sqrt{g_2}} \left[\log \left(\frac{2kk_o}{\gamma^2 + \gamma a - 1 - \alpha_1 \alpha_2} \right) \right.$$

$$+ 2 \log\left(\frac{a\sqrt{g_2} + a(\gamma - k')}{a\sqrt{g_2} \pm (k\alpha_1 + k_o\alpha_2)}\right)\Bigg] . \qquad (71)$$

When $g_2 < 0$, in f_A the quantity $\frac{2}{\sqrt{g_2}}$ [. . .] is replaced by

$$\frac{-1}{\sqrt{-g_2}} \sin^{-1}\left[\frac{2\sqrt{-g_2}\,\alpha_2}{k^2}(\gamma^2 - 1 - \gamma k)\right], \quad k < k_o ,$$

or by

$$\frac{-1}{\sqrt{-g_2}} \sin^{-1}\left[\frac{2\sqrt{-g_2}\,\alpha_1}{k_o^2}\left[\alpha_1^2 - k_o(\gamma + a)\right]\right], \quad k > k_o .$$

In f_B, $\frac{1}{\sqrt{g_2}}$ [. . .] goes to

$$\frac{1}{\sqrt{-g_2}}\left\{\sin^{-1}\left[1 + \frac{g_2}{kk_o}(\gamma^2 - 1 + \gamma a - \alpha_1\alpha_2\right]\right.$$

$$\left. - \sin^{-1}(1 + 2g_2)\right\} .$$

For an idea of the approximate size of $\frac{\partial\sigma}{\partial k}$, the first term in the brackets of Eq. (18) may be integrated alone. This is

$$\frac{\partial\sigma_1}{\partial k} = \frac{\pi r_o^2}{k_o^2 TK_2\left(\frac{1}{T}\right)}\left\{\int_{\gamma_1}^{\gamma_2} 2\alpha_< e^{-\frac{\gamma}{T}} d\gamma\right.$$

$$\left. + \int_{\gamma_2}^{\infty} d\gamma e^{-\frac{\gamma}{T}} [k_2 - \alpha_> + \alpha_<]\right\} . \qquad (72)$$

Then

$$\frac{\partial\sigma}{\partial k} = \frac{\partial\sigma_1}{\partial k}\left[1 + 0.5kk_o\langle C^-(C^-)'\rangle - 0.5\langle\sin^2\theta'\rangle\right] , \qquad (73)$$

where the averaging is now over both the electron distribution and the angle of scatter.

For $k = k_o$,

$$\frac{\partial\sigma_1}{\partial k} = \frac{\pi r_o^2}{k_o^2 TK_2\left(\frac{1}{T}\right)}\left\{\int_1^{\gamma_2} 2\alpha_2 e^{-\frac{\gamma}{T}} d\gamma\right.$$

$$\left. + \int_{\gamma_2}^{\infty} k_2 e^{-\frac{\gamma}{T}} d\gamma\right\} . \qquad (74)$$

For $T \ll \gamma_2 - 1$, and k_o small (so $\gamma_2 - 1 \approx k_o^2/2$),

$$\frac{\partial\sigma_1}{\partial k} \approx \frac{\pi r_o^2 2}{k_o^2} . \qquad (75)$$

This is just that part of the Klein-Nishina formula from which this term is taken.

For $T \gg k_o^2/2$, the first integral is negligible and

$$\frac{\partial\sigma_1}{\partial k} \approx \frac{\pi r_o^2 e^{-\frac{\gamma_2}{T}} 2k_o}{k_o^2 K_2\left(\frac{1}{T}\right)} \approx \frac{2r_o^2\sqrt{2\pi}}{k_o T^{1/2}} . \qquad (76)$$

The temperature $T \approx k_o^2/2$ is a transition point between what may be called a zero-temperature region and a finite-temperature region. In the first region, the Klein-Nishina formula is a good approximation and there is a strong correlation between final energy and scattering angle. The quantity $\langle|k - k_o|\rangle \approx k_o^2$. In the finite-temperature region there is little correlation between final energy and scattering angle, and $\langle|k - k_o|\rangle \approx k_o T^{1/2}$. For $k_o = 1$ keV, the transition temperature, $k_o^2/2$ is, for example, about 1 eV.

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