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Compton Scattering of Photons from Electrons in Thermal (Maxwellian) Motion: Electron Heating

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EXECUTIVE SUMMARY

The Compton differential scattering of photons from a relativistic Maxwell Distribution of electrons is reviewed and the theory and numerical values verified for application to particle transport codes. We checked the Wienke exact covariant theory, the Wienke-Lathrop isotropic approximation, and the Wienke-Lathrop fitted approximation. Derivation of the approximations from the exact theory are repeated. The Klein-Nishina limiting form of the equations was verified. Numerical calculations, primarily of limiting cases, were made as were comparisons both with Wienke's calculations and among the various theories. An approximate (Cooper and Cummings), simple, accurate, total cross section as a function of photon energy and electron temperature is presented. Azimuthal integration of the exact and isotropic cross sections is performed but rejected for practical use because the results are small differences of large quantities and are algebraically cumbersome.

The isotropic approximation is good for photons below 1 MeV and temperatures below 100 keV. The fitted approximation version discussed here is generally less accurate but does not require integration, replacing the same with a table or with graphs. We recommend that the ordinary Klein-Nishina formula be used up to electron temperatures of 10 keV (errors of $\leq 1.5\%$ in the total cross section and of about 5% or less in the differential cross section.) For greater accuracies, higher temperatures, or better specific detail and no temperature or photon energy limits, the exact theory is recommended. However, the exact theory effectively requires four multiple integrations so that within its accuracy and temperature and energy limits the Wienke-Lathrop isotropic approximation is a simpler solution and is thereby recommended as such.

The mean energy of a photon scattered from a Maxwell distributed electron gas is calculated by four methods: exact; the Wienke-Lathrop isotropic and one-parameter fitted approximations; and the standard (temperature T = 0) Compton energy equation. To about 4% error the simple Compton (T = 0) equation is adequate up to 10-keV temperature. Above that temperature the exact calculation is preferred if it can be efficiently coded for practical use. The isotropic approximation is a suitable compromise between simplicity and accuracy, but at the extreme end of the parameter range (T = 100 keV incident photon energy $\nu' = 1$ keV, scattering angle $\theta = 180^{\circ}$) the error is as high as -28%. For mid-range values like 10 to 25 keV, the errors are generally a percent or so but range up to about 8% (25 keV, 180°). The fitted approximation is generally found to have large errors and is consequently not recommended.

The energy deposited in the electron gas by the Compton scattering of the photon, i.e., the heating, is only adequately given by the exact expression for all parameters in the ranges $1 \le T \le 100$ keV and $1 \le v' \le 1000$ keV. For low depositions the heating is the difference between two large quantities. Thus if one quantity is approximate, orders of magnitude errors can occur. However, for scattered photon energy v >> T the isotropic approximation does well (0.13% error for v' = 1000 keV, $\theta = 180^{\circ}$, T = 10 keV, v = 790.7 keV; and 2.7% error for v' = 1000 keV, $\theta = 90^{\circ}$, v = 583.5 keV, T = 100 keV). The regular T = 0 Compton also does well for $T \le 10$ keV and v >> T (0.7% for v' = 1000 keV, $\theta = 180^{\circ}$, T = 10 keV, v = 790.7 keV; and 2.8%, T = 1000 keV, $\theta = 180^{\circ}$, T = 10 keV, v = 790.7 keV; and 0.08% for v' = 1000 keV, $\theta = 180^{\circ}$, T = 10 keV, v = 790.7 keV; and 0.08% for v' = 1000 keV, $\theta = 180^{\circ}$, T = 1 keV, v = 795.9 keV). The fitted approximation is without merit for heating.

COMPTON SCATTERING OF PHOTONS FROM ELECTRONS IN THERMAL (MAXWELLIAN) MOTION: ELECTRON HEATING

by

Joseph J. Devaney

ABSTRACT

The Compton differential scattering of photons from a relativistic Maxwell distribution of electrons is reviewed. The exact theory and the approximate theories due to Wienke and Lathrop were verified for application to particle transport codes. We find that the ordinary (zero temperature) Klein-Nishina formula can be used up to electron temperatures of 10 keV if errors of less than 1.6% in the total cross section and of about 5% or less in the differential cross section can be tolerated. Otherwise, for photons below 1 MeV and temperatures below 100 keV the Wienke-Lathrop isotropic approximation is recommended. Were it not for the four integrations effectively required to use the exact theory, it would be recommended. An approximate (Cooper and Cummings), simple, accurate, total cross section as a function of photon energy and electron temperature is presented.

I. INTRODUCTION

This report critically reviews the exact Compton differential scattering of a photon from an electron distributed according to a relativistic Maxwell velocity distribution. We base our study on the form derived by Wienke using field theoretic methods.¹⁻⁷ (Particularly Eq. (1) of Ref. 1, whose derivation is presented in Ref. 2.) Wienke was the first known to this writer to point out the simplicity and power of deriving the Compton effect for moving targets by the coordinate covariant (i.e., invariant in form) techniques of modern field theory. His derivation is equivalent to,⁴ but replaced, earlier methods⁸ which involved the tedious and obscure making of a Lorentz transformation to the rest frame of the target electron, applying the Klein-Nishina Formula, and making a Lorentz transformation back to the laboratory frame.

We also critically review the Wienke-Lathrop isotropic approximation⁹ to the exact formula which selectively substitutes electron averages into the exact formula so obviating integration over the electron momenta and colatitude. The electron directions in a Maxwell distribution are, of course, isotropic, hence the name chosen by Wienke and Lathrop.

We verify the theory for the exact expression and the plausibility arguments for the isotropic expression. We verify in detail numerical comparisons between the two theories at selected electron temperatures and initial photon energies. We rewrite the formulas in a form suitable for application, especially for the Los Alamos National Laboratory Monte Carlo neutron-photon code, MCNP.¹⁰

As a further approximation, Wienke and Lathrop have reduced the isotropic approximation to a one- or two-parameter fitted approximation,⁹ which we also review. As always, the choice between the methods is complexity versus accuracy and limitations of parameter ranges.

We include a simple, accurate estimate of the total Compton cross section. We give the mean scattered photon energy and the mean heating of the electron gas by the photon scattering. Both quantities are given as a function of the photon scattering angle, θ ; the electron temperature; and the incident photon energy, v'. We compare these means, v> and H>: as calculated exactly, as calculated with the Wienke-Lathrop isotropic and one-parameter fitted approximations, as well as with the unmodified, regular, T = 0, Compton energy equation results. Recommendations are offered.

Because much of this report is devoted to derivation and verification, we recommend that a user-oriented reader turn first to the recommendations of Section XVI, then for differential cross sections, Sections IX to XI as desired, which give applications together with reference to Figs. 2 through 8, which show the accuracy of the cross-section approximations. For scattered photon energies and heating, refer first to Section XV for comparisons and errors, particularly Fig. 10 and Tables II and III, then as desired Sections XIII to XIV. Refer to the Table of Contents for further guidance.

11. THE EXACT COMPTON SCATTERING OF A PHOTON FROM A RELATIVISTIC MAXWELL ELECTRON DISTRIBUTION

We will follow the notation and largely the method of Wienke^{1,9} and first choose the "natural" system of units in which h = c = 1 and $kT \equiv T$ in keV. Let the incoming photon and electron energies be v' and ε ', and the outgoing be v and ε , with corresponding electron momenta \vec{p} ' and \vec{p} , and photon momenta \vec{q} ' and \vec{q} , respectively. The angle between \vec{q} ' and \vec{q} shall be θ ; q is oriented relative to some fixed laboratory direction by azimuthal angle θ_q . The angle between \vec{q} ' and \vec{p} ' shall be α ' and that between \vec{q} and \vec{p} ' shall be α . The azimuthal angle between the spherical triangle sides $\vec{q}\vec{q}$ ' and $\vec{q}'\vec{p}'$ shall be ϕ . Thus on the surface of a sphere with origin of the vectors \vec{q}, \vec{q}' , and \vec{p}' at the center of the sphere and intersections labelled on the surface thereof, we have the spherical triangle shown in Fig. 1.



Fig. 1. Angular relations.

The law of cosines applied to the triangle of Fig. 1 gives

$$\cos \alpha = \cos \alpha' \cos \theta + \sin \alpha' \sin \theta \cos \phi \quad . \tag{1}$$

In terms of energy, ε , and (vector) momentum, \vec{p} , the four-vector momentum is

$$P \equiv [\varepsilon, \vec{p}] \quad . \tag{2}$$

Its square is

$$P^{2} = \varepsilon^{2} - \dot{P}^{2} \qquad (3)$$

Now all four vectors are required to transform (Lorentz transformation) alike, in particular as the line element

$$ds = [dt, d\vec{x}]$$
(4)

so as to keep $(ds)^2$ invariant. Thus P^2 is invariant.

In the rest frame $\vec{p} \equiv o$, $\epsilon \equiv m$, so that generally for any four-momentum P of mass m,

$$P^2 = m^2 avertee avertee$$

In particular, for photons, $m \equiv 0$, so that their four-momenta, Q, satisfy

$$Q^2 = 0 \qquad (photons) \qquad (6)$$

Consider now the Compton scattering of four-momenta P' + Q' into P + Q. Four-momentum is conserved, so

$$P = P' + Q' - Q$$
 (7)

The square of Eq. (7) yields

$$P'Q' = P'Q + Q'Q , \qquad (8)$$

where we have used Eqs. (6) and (5):

$$p^2 = p'^2 = m^2$$
, $q^2 = q'^2 = 0$.

Expanding the four-momentum products into energy and three-momentum products by, for example,

$$P'Q' = \varepsilon'v' - \vec{p}' \cdot \vec{q}' , \qquad (9)$$

and then using Fig. 1 to determine that, for example,

$$\vec{p}' \cdot \vec{q}' = p'q' \cos \alpha', \qquad (10)$$

where p' and q' are, of course the magnitude of the 3-momenta \vec{p} ' and \vec{q} ', we get finally for Eq. (8)

$$\varepsilon'\nu' - p'\nu'\cos\alpha' = \varepsilon'\nu - p'\nu\cos\alpha + \nu\nu' - \nu\nu'\cos\theta , \qquad (11)$$

where we have used $q'^2 = v'^2$, $q^2 = v^2$ for the zero rest mass photons.

The Compton collision, of course, also conserves 3-momentum so that

$$\vec{p} = \vec{p}' + \vec{q}' - \vec{q} \quad . \tag{12}$$

If now we square Eq. (12) and use the relation

$$\dot{p}^2 + m^2 = \varepsilon^2 \tag{13}$$

plus scalar products determined from Fig. 1 as we did for Eqs. (10) and (11), we get

$$\varepsilon^{2} = \varepsilon'^{2} + \nu'^{2} + \nu'^{2} + 2p'\nu' \cos \alpha' - 2p'\nu \cos \alpha - 2\nu\nu' \cos \theta \quad . \tag{14}$$

The Compton cross section for scattering a photon into a direction solid angle d Ω , and into an energy interval d ν , from a relativistic Maxwell electron distribution, f(\vec{p}'), is given by Wienke¹ to be

$$\frac{d\sigma}{d\Omega d\nu} = \frac{r_o^2}{2} \int d^{32} r' f(p') \cdot \left(\frac{m^2 \nu}{\epsilon' \nu' \epsilon}\right) \cdot \delta (\epsilon' + \nu' - \epsilon - \nu) \cdot K , \quad (15)$$

where

$$K \equiv \left[\left(\frac{m^2}{\epsilon' \nu' - p' \nu' \cos \alpha}, - \frac{m^2}{\epsilon' \nu - p' \nu \cos \alpha} \right)^2 + 2 \left(\frac{m^2}{\epsilon' \nu' - p' \nu' \cos \alpha'} - \frac{m^2}{\epsilon' \nu - p' \nu \cos \alpha} \right) + \frac{\epsilon' \nu' - p' \nu' \cos \alpha'}{\epsilon' \nu - p' \nu \cos \alpha} + \frac{\epsilon' \nu - p' \nu \cos \alpha}{\epsilon' \nu' - p' \nu' \cos \alpha'} \right], \quad (16)$$

m is the electron rest energy (or mass, c = 1), and

 $r_o \equiv e^2/mc^2$ is the classical electron radius.

We integrate over final photon energy in order to remove the δ -function. However, the δ -function is not in the form $\delta(\nu - \nu_0)$, where ν_0 is constant because Eq. (14) shows that $\varepsilon = \varepsilon(\nu)$. We must first use the identity

$$\delta(f(\mathbf{x})) = \left[\frac{\partial f}{\partial \mathbf{x}}\right]^{-1} \Big|_{\mathbf{x}_{o}} \delta(\mathbf{x} - \mathbf{x}_{o}) , \qquad (17)$$

from which, using Eq. (14), then differentiating, then substituting $\epsilon+\nu = \epsilon'+\nu'$, and then Eq. (11),

$$\delta(\varepsilon + \nu - \varepsilon' - \nu') = \frac{\varepsilon(\frac{\nu}{\nu'})}{\varepsilon' - p' \cos \alpha'} \delta(\nu - \nu_0) , \qquad (18)$$

for some constant outgoing photon energy, v_0 .

Substituting in Eq. (15), integrating over ν , and replacing ν_0 by ν (i.e., ν is now the outgoing photon energy), we get

$$\frac{d\sigma}{d\Omega} = \frac{r_o^2}{2} \int d^{3+}p' f(p') \cdot \frac{m^2}{\epsilon'(\epsilon' - p' \cos \alpha')} \left(\frac{\nu}{\nu'}\right)^2 K \quad . \tag{19}$$

Formulas (15) and (16) have been checked by independent calculation by C. Zemach, Theoretical Division, Los Alamos National Laboratory.^{*} In the form of Eqs. (19) and (16) the formulas are the same as those of Pauli⁸ and Ginzburg and Syrovat-Skii¹¹ provided one corrects for the electron motion. The number of events per unit time are equal to the flux times the density of electrons times the cross section times the volume. For an electron of velocity \vec{v} , the number of events per unit time is increased by the factor

$$\left(1 - \frac{\overrightarrow{v} \cdot \overrightarrow{c}}{c^2}\right) = \frac{\varepsilon' - \overrightarrow{p}' \cdot \frac{\overrightarrow{v}'}{v'}}{\varepsilon'} = \frac{\varepsilon' - p' \cos \alpha'}{\varepsilon'} , \qquad (20)$$

where again $c \equiv 1$.

The relativistic Maxwell electron distribution is

$$f(\vec{p}') = (4\pi\gamma)^{-1} e^{-\sqrt{p'^2 + m^2}/T}$$
 (21)

or for

$$\varepsilon' = \mathbf{m} + \mathbf{K}' \quad . \tag{22}$$

K' being the electron kinetic energy, then

$$f = (4\pi\gamma)^{-1} e^{-m/T} \cdot e^{-K'/T}$$
, (23)

where the normalization constant $\boldsymbol{\gamma}$ is given by

$$\gamma = m^{2} T K_{2}(m/T) = m^{2} T \left(\frac{\pi T}{2m}\right)^{1/2} e^{-m/T} \left[1 + \frac{15}{1!} \left(\frac{T}{8m}\right) + \frac{105}{2!} \left(\frac{T}{8m}\right)^{2} - \frac{945}{3!} \left(\frac{T}{8m}\right)^{3} + \frac{31185}{4!} \left(\frac{T}{8m}\right)^{4} + \dots \right], \qquad (24)$$

where ${\rm K}_2$ is the modified Bessel function of the second kind and order. We use

$$f \approx \sqrt{\frac{m}{2\pi T}} \cdot \frac{e^{-K'/T}}{2\pi m^2 T \left[1 + 15\left(\frac{T}{8m}\right) + \frac{105}{2}\left(\frac{T}{8m}\right)^2 - \frac{315}{2}\left(\frac{T}{8m}\right)^3 + \frac{10395}{8}\left(\frac{T}{8m}\right)^4\right]}, \quad (25)$$

which is good for T << 4 MeV, more accurately, for T < 400 keV.

*Information from C. Zemach, November 1982.

We generally prefer to describe electrons by their kinetic energy, K', rather than momentum \vec{p} ', so using $\epsilon'^2 = p'^2 + m^2$ and $\epsilon' = m + K'$ we have

$$p'^{2} dp' = (K' + m) \cdot \sqrt{K'^{2} + 2mK'} dK'$$
, (26)

also

$$d^{3}_{p'} = p'^{2} dp' d\cos \alpha' d\phi \qquad (27)$$

We put

 $\mu \equiv \cos \theta , \qquad (28)$

thus

$$d\mu = -\sin \theta \, d\theta$$
.

For convenience, define

$$\kappa \equiv \varepsilon'/m = 1 + (K'/m) , \qquad (29)$$

$$\kappa_1 \equiv m^{-1} (\epsilon' - p' \cos \alpha') = \kappa - \sqrt{\kappa^2 - 1} \cos \alpha' , \qquad (30)$$

and

$$\kappa_2 \equiv m^{-1} (\varepsilon' - p' \cos \alpha) = \kappa - \sqrt{\kappa^2 - 1} \cos \alpha \quad . \tag{31}$$

Substituting into the energy equation ((11)) we get simply

$$\kappa_{1}^{m\nu'} = \nu\nu'(1 - \mu) + \kappa_{2}^{m\nu} .$$
 (32)

Substituting into Eq. (16) and with a little rearranging,

$$K = \left[\frac{(1-\mu)^2}{\kappa_1^2 \kappa_2^2} - \frac{2(1-\mu)}{\kappa_1 \kappa_2} + \frac{\nu' \kappa_1}{\nu \kappa_2} + \frac{\nu \kappa_2}{\nu' \kappa_1} \right], \qquad (33)$$

and the cross section, Eq. (19), becomes

$$\frac{d\sigma}{d\Omega} = \frac{r_o^2}{2} \int dK' (K' + m) \sqrt{K'^2 + 2mK'} \cdot f(K') \cdot \frac{1}{\kappa \kappa_1} \cdot \left(\frac{\nu}{\nu'}\right)^2$$
(34)

 \times K • d • d cos α ' .

The expressions (32), (33), (34), (25) (or (23) and (24)), and (1) constitute the exact Compton scattering cross section of a photon of energy ν' from a relativistic Maxwell distribution of electrons, f(K'), into the solid angle $d\Omega = \sin \theta \ d\theta \ d\phi_q$. The ϕ -integration can be carried out analytically, see Appendix A, but we found the result both too cumbersome and too inaccurate for practical use. The latter was caused by small differences of very large, but exact, quantities that our calculator could not handle.

In the limit $T \rightarrow 0$, Eq. (34) or Eq. (19) should reduce to the Klein-Nishina Formula (i.e., Compton for zero velocity electrons). So it does, as we now show. Observe that the relativistic Maxwellian is normalized such that

$$\int f d^{3} \dot{p}' = 1$$
(35)

and from Eq. (25) for $T \rightarrow 0$ that for $K' \neq 0, f = 0$ and for $K' = 0, f = \infty$, so that we may write

$$\begin{array}{ccc} f & d^{3} \dot{p}' & \rightarrow & \delta(p') & dp' \\ & T & 0 \end{array}$$
 (36)

because the δ -function, $\delta(x)$, is defined as

$$\delta(\mathbf{x} \neq \mathbf{o}) = \mathbf{o}$$

$$\delta(\mathbf{o}) = \infty$$

$$\int \delta(\mathbf{x}) \, d\mathbf{x} = 1 \quad . \tag{37}$$

Substituting Eq. (36) in Eq. (19), using Eq. (33) and Eqs. (29), (30), and (31), (i.e., $\kappa = 1 = \kappa_1 = \kappa_2$), we get the usual Compton energy equation from Eq. (32).

$$m\nu' = \nu\nu'(1 - \mu) + \nu m$$
 (initially stationary electron) (38)

and the Klein-Nishina Formula^{10,12} for unpolarized light,

$$\frac{d\sigma}{d\Omega} = \frac{r_o^2}{2} \left(\frac{\nu}{\nu'}\right)^2 \left[\frac{\nu'}{\nu} + \frac{\nu}{\nu}\right] + \mu^2 - 1, \qquad (39)$$

as we should.

III. NUMERICAL VERIFICATION OF THE EXACT COMPTON SCATTERING FROM A MAXWELL DISTRIBUTION

Integration over ϕ in Eq. (34) is possible analytically but is both complicated and leads to small differences in large quantities (see Appendix A). Accordingly, we have used Simpson's rule to integrate over ϕ , α ', and K' to provide $d\sigma/d\theta$ vs θ . By symmetry the cross section is independent of ϕ_q . We used angular intervals of 22.50° and variable electron kinetic energy intervals appropriate to yielding an error of about 1% or less. Our numerical calculations agree with Wienke and Lathrop⁹ to about 1% or better except at T = 1 keV, ν' = 1000 keV, and θ = 30°, where the agreement was only 3.5% because of our using a coarse K' interval. We found and checked with Wienke that his latest communication (Ref. 9, February 15, 1983) has an erroneous exact curve in Fig. 6. (T = 100 keV, ν' = 1 keV); however, we agree with earlier Wienke-Lathrop exact calculations for these parameters. The parameter sets for which we have numerically checked the Wienke-Lathrop exact angular distributions are given in Table I.

TABLE I

TEMPERATURE T (keV)	INCIDENT PHOTON ENERGY v'(keV)	PHOTON SCATTERING ANGLES, O
100	1	45°, 90°, 100° 135°
100	1000	45°, 90°, 135°
1	1	60°, 140°
1	1000	30°

PARAMETER SETS AT WHICH THE EXACT WIENKE-LATHROP FORMULAS FOR do/d0 WERE VERIFIED

(As noted, agreement is within the error of our Simpson's rule approximation error, i.e., $\simeq 1\%$ except, 1, 1000, 30°: $\simeq 3.5\%$.)

IV. THE WIENKE-LATHROP ISOTROPIC APPROXIMATION FOR THE COMPTON SCATTERING OF A PHOTON FROM A RELATIVISTIC MAXWELL ELECTRON DISTRIBUTION

The exact Compton formula (34) requires three integrations to provide the differential scattering cross section $d\sigma/d\Omega$. It requires four integrations to provide the total scattering cross section (the fifth integration over ϕ_q is trivial, yielding 2π because of symmetry). Accordingly, an approximate form of Eq. (34) without such integrations could be quite useful when the errors of the approximation can be tolerated. We derive the Wienke-Lathrop isotropic approximation by a plausibility argument. This approximation removes the integration over p' and α' . In place of averaging the covariant Compton expression over a Maxwell spectrum, key parameters are averaged in that expression, an inexact but reasonable approach leading to a simpler expression.

Because the relativistic Maxwell distribution is isotropic, it is clear that

$$\langle \cos \alpha' \rangle = 0$$
, (40)

where the average, $\langle \rangle$, is the Maxwell average over K' and α' . The first approximation then is to replace $\cos \alpha'$ by its average

$$\cos \alpha' \to \langle \cos \alpha' \rangle = o \tag{41}$$

so that

$$\sin \alpha' = \sqrt{1 - \cos^2 \alpha'} = 1 \tag{42}$$

and Eq. (1) becomes

 $\cos \alpha = \sin \theta \cos \phi \quad . \tag{43}$

Consequently, by Eq. (30)

 $\kappa_1 = \kappa \quad . \tag{44}$

Since (Eq. (24)) $\kappa \equiv \epsilon'/m$, one might, for example, choose $\kappa = \langle \epsilon' \rangle/m$, but Wienke chooses rather to set

$$\varepsilon' = \sqrt{\langle p'^2 \rangle + m^2} , \qquad (45)$$

which he shows and we verify and expand to be

$$\kappa = \epsilon'/m = \sqrt{1 + \frac{3T}{m} \cdot \frac{K_3(m/T)}{K_2(m/T)}}$$
$$= \sqrt{1 + \frac{3T}{m}} \left[1 + 20(\frac{T}{8m}) + 120(\frac{T}{8m})^2 - 960(\frac{T}{8m})^3 + 4320(\frac{T}{8m})^4 + \cdots \right] .(46)$$

Substituting Eq. (42) into Eq. (31) yields

$$\kappa_2 = \kappa - \sqrt{\kappa^2 - 1} \cdot (\sin \theta \cos \phi) \quad . \tag{47}$$

Eq. (32) reduces by Eq. (44) to

$$\frac{\nu}{\nu'} = \frac{\kappa}{\frac{\nu'}{m} (1-\mu) + \kappa_2}$$
(48)

Remembering that the Maxwell averaging operator,

$$\int \frac{d^3 \dot{p'}}{d\phi} f (p')$$

(i.e., except for ϕ) now applies solely to cos α ', where it gives zero, and to $\langle p' \rangle^2$, where it yields Eqs. (45) and (46), we perform that averaging in Eq. (19) with K taken to be Eq. (33) to obtain the isotropic approximation for the differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{r_o^2}{4\pi} \cdot \frac{1}{\kappa^2} \int_0^{2\pi} \left[\left(\frac{\nu}{\nu'} \right)^2 \frac{\left(1-\mu\right)^2}{\left(\kappa\kappa_2\right)^2} - \frac{2\left(1-\mu\right)}{\kappa\kappa_2} + \frac{\nu'\kappa}{\nu\kappa_2} + \frac{\nu\kappa_2}{\nu'\kappa} \right] d\phi \quad , \quad (49)$$

where $r_0 \equiv e^2/mc^2$ is the classical electron radius, κ_2 is given by Eq. (47), κ by Eq. (46), $\mu = \cos \theta$, and ν/ν' is given by Eq. (48).

$$\frac{d\sigma}{d\Omega} \equiv \frac{d\sigma}{\sin\theta d\theta d\phi_{\rm q}} = \frac{d\sigma}{2\pi \sin\theta d\theta}$$
(50)

because of φ_q symmetry of the problem. Thus

$$\frac{d\sigma}{d\theta} = r_0^2 \cdot \frac{\sin \theta}{\kappa^2} \int_0^{\pi} d\phi \left(\frac{\nu}{\nu'}\right)^2 \left[\frac{(1-\mu)^2}{(\kappa\kappa_2)^2} - \frac{2(1-\mu)}{\kappa\kappa_2} + \frac{\nu'}{\nu} \frac{\kappa}{\kappa_2} + \frac{\nu\kappa_2}{\nu'\kappa}\right] \cdot (51)$$

The ϕ -integration of Eqs. (49) or (51) can be performed analytically, but we found the result to be small differences of very large quantities leading to inaccuracies in small computers as well as to be algebraically cumbersome. Accordingly, we found it simpler to use direct numerical integration by Simpson's rule. For angles, only 8 intervals gave sufficient accuracy for our purposes.

The approximation (49) also reduces in the limit $T \rightarrow o$ to the Klein-Nishina formula¹²,¹⁰ for unpolarized light, as it should. In Eq. (46) setting T = 0 gives $\kappa = 1$, which in Eq. (47) then gives $\kappa_2 = 1$, i.e., κ_2 is now no longer a function of ϕ , and thus yields from Eq. (48)

$$\frac{\nu}{\nu'} = \frac{1}{\frac{\nu'}{m} (1 - \mu) + 1}, \qquad (T \neq 0)$$
(52)

which is identical to Eq. (38), and from Eq. (49) (with $\int d\phi = 2\pi$) yields the unpolarized Klein-Nishina Formula (39)

$$\frac{d\sigma}{d\Omega} = \frac{r_o^2}{2} \cdot \left(\frac{\nu}{\nu^*}\right)^2 \cdot \left[\frac{\nu^*}{\nu} + \frac{\nu}{\nu^*} + \mu^2 - 1\right] \quad . \qquad (T \neq 0)$$
(53)

V. NUMERICAL VERIFICATION OF THE WIENKE-LATHROP ISOTROPIC APPROXIMATION OF COMPTON SCATTERING

We have numerically verified Eq. (51) against the independent calculations of Wienke and Lathrop.⁹ We find all points in agreement to within our error in reading the curves of Wienke and Lathrop and possibly also including the difference in our use of more terms for κ , Eq. (46). We verified the formula (51) for $\theta = 30^{\circ}$, 60° , 90° , 120° , and 150° for all parameter sets. In addition, for T = 100 keV, $\nu' = 1$ keV, the differential cross section was verified at $\theta = 80^{\circ}$, 100° , 110° , and 115° because of the peaked behavior of the approximation near 100° (see Fig. 5).

VI. COMPARISON OF THE WIENKE-LATHROP APPROXIMATION TO THE EXACT COMPTON SCATTERING OF PHOTONS FROM A MAXWELLIAN ELECTRON GAS

In Figs. 2 through 6 we compare the isotropic approximation versus the exact differential Compton scattering cross sections, $d\sigma/d\theta$. T refers to the electron temperature, and the photon energy is the initial photon energy v'. The isotropic approximation curves are dashed and are taken from Eq. (51) (integrated over ϕ). The solid curves are the exact curves from Eqs. (34) and (50) after numerical integration over K', ϕ , and α '. The Wienke-Lathrop approximation is a good one except for T large and T \gg v'. However, the total Compton cross section, σ , is very well represented by the Wienke-Lathrop approximation. Figs. 7 and 8 show the Compton cross sections integrated over the photon scattering angle, θ . Again, dashed is the isotropic approximation, solid the exact. It is evident that the two total cross sections, isotropic and exact, are nearly indistinguishable up to 100-keV temperature. Figures 2, 3, 6, 7, and 8 are reproduced, by permission, from Ref. 9 (February 15, 1983). Figures 4 and 5 also contain the Wienke-Lathrop fitted approximation curves (dot-dash), which we discuss next.

VII. WIENKE-LATHROP FITTED APPROXIMATION TO COMPTON SCATTERING

In the event that a poorer approximation (the present version - it could be made better) than the isotropic is satisfactory, Wienke and Lathrop⁹ offer a "fitted approximation" that avoids even the ϕ -integration of their isotropic approximation. However, an adjunct plot or plots or tables of the parameters $\langle \kappa_1 \rangle$ and $\langle \kappa_2 \rangle$ versus T and ν ' are required. Moreover the isotropic approximation can be integrated analytically, but perhaps uselessly (see Appendix B). In Eq. (34) the functions κ_1 and κ_2 are replaced by the fitting parameters $\langle \kappa_1 \rangle$ and $\langle \kappa_2 \rangle$ and κ is taken to be the average (46) independent of K' so that integration over the Maxwell distribution is trivially performed:

$$\int dK' \cdot (K' + m) \cdot \sqrt{K^2 + 2mK'} \cdot f(K') \cdot d\cos \alpha' d\phi = 1$$
(54)

and we are left with

$$\frac{d\sigma}{d\mu} = \frac{d\sigma}{\sin\theta \ d\theta} = \pi \ r_{o}^{2} \cdot \frac{1}{\kappa \langle \kappa_{1} \rangle} \left(\frac{\nu}{\nu'}\right)^{2} K_{f}$$
(55)

with now,

$$K_{f} = \left[\frac{(1-\mu)^{2}}{\langle\kappa_{1}\rangle^{2}\langle\kappa_{2}\rangle^{2}} - \frac{2(1-\mu)}{\langle\kappa_{1}\rangle\langle\kappa_{2}\rangle} + \frac{\nu'}{\nu} \cdot \frac{\langle\kappa_{1}\rangle}{\langle\kappa_{2}\rangle} + \frac{\nu}{\nu'} \cdot \frac{\langle\kappa_{2}\rangle}{\langle\kappa_{1}\rangle}\right], \quad (56)$$

and from Eq. (32),

$$\left(\frac{\nu}{\nu'}\right) = \frac{\langle \kappa_1 \rangle^m}{\nu'(1-\mu) + \langle \kappa_2 \rangle^m} \quad .$$
 (57)

Equations (55), (56), and (57) can now be fitted to exact curves to determine the parameters $\langle \kappa_1 \rangle$ and $\langle \kappa_2 \rangle$, and the resulting values tabulated or graphed for computational use. Wienke and Lathrop⁹ have carried out such a fitting to the total cross section. It is not the most general, however, because one parameter, $\langle \kappa_2 \rangle$, is fixed, $\langle \kappa_2 \rangle = \kappa$, thus reducing the problem to a one-parameter fit. They also simplify Eq. (56) by omitting the κ -factors from the last two terms. Their one parameter fit is then of the form

$$\left(\frac{\nu}{\nu'}\right) = \frac{\langle \kappa_1 \rangle m}{\nu'(1-\mu) + \kappa m}$$
(58)

and

$$K_{f1} = \left[\frac{(1-\mu)^2}{\langle \kappa_1 \rangle^2 \kappa^2} - \frac{2(1-\mu)}{\langle \kappa_1 \rangle \kappa} + \frac{\nu'}{\nu} + \frac{\nu}{\nu'}\right]$$
(59)

with $\langle \kappa_1 \rangle$ given by them⁹ in Fig. 9 (reproduced by permission) so as to match the total cross section (checked by us at T = 100 keV and 1 kev, and $\nu' = 1$ keV). κ is given by Eq. (46). Equations (58) and (59) are substituted in Eq. (55) to get the differential scattering cross section $d\sigma/d\theta$. As alleged, this procedure does eliminate integrations, but requires use of a table or graph, Fig. 9. We have calculated the differential cross section by this one-parameter fitted cross section for T = 1 keV, $\nu' = 1$ keV and found it indistinguishable from the isotropic for these parameters. However, for T = 25 keV = ν' , Fig. 3, and T = 100 keV, $\nu' = 1$ keV, Fig. 4, the differences are appreciable. We label the one-parameter approximation in Figs. 4 and 5 as "approximate (fitted)." Especially from Fig. 4 do we conclude that the isotropic approximation is superior at least to the one-parameter fitted approximation of Eqs. (58), (59), and (55). Of course, one may be able to improve the fits by the use of additional parameters such as $\langle \kappa_2 \rangle$. But again such use means additional complication, additional tables.

VIII. THE TOTAL COMPTON SCATTERING CROSS SECTION AT TEMPERATURE T

Following Cooper and Cummings,¹³ we give a fit to the total Compton scattering cross section in the range T = 0 to 150 keV and v' in the range 1 to 1000 keV. The accuracy is better than 1%, except at v = 300 keV, T = 150 keV, where an error of 1.9% appears. At higher temperatures up to 200 keV the error is 3.7% or less. We numerically verified for T = 10 and 100 keV and for v' = 1to 1000 keV that the difference between this fit and both the Devaney and Wienke-Lathrop exact total cross sections was less than could be discerned on the graphs, Figs. 7 and 8 (i.e., < 1%).

For unpolarized light the total Compton cross section for electrons at rest is given by:12,14

1

$$\sigma_{c} = 2\pi r_{o}^{2} \left\{ \frac{1+\gamma}{\gamma^{3}} \left[\frac{2\gamma(1+\gamma)}{1+2\gamma} - \ln(1+2\gamma) \right] + \frac{1}{2\gamma} \ln(1+2\gamma) - \frac{1+3\gamma}{(1+2\gamma)^{2}} \right\},$$
(60)

where

$$\gamma \equiv \nu'/m$$
 (m the rest mass energy of the electron)

and

$$r_o = e^2/m_e c^2$$

is the classical electron radius. For low photon energies, $\gamma <<< 1$, small computers fail to calculate logarithms accurately enough, so that below 10 keV to an accuracy of six significant figures or better Eq. (60) can be replaced by12

$$\sigma_{\rm c} = \frac{8\pi}{3} r_{\rm o}^2 \left(1 - 2\gamma + \frac{26}{5} \gamma^2 \right) .$$
 (61)

The terms outside the bracket constitute the Thomson scattering cross section, which is, of course, the limit of the Compton cross section at low energy. The Thomson cross section gives the elastic scattering of a photon by an effectively free electron.

For electrons in thermal Maxwellian motion we correct Eqs. (60) or (61) by the factor (in brackets)¹³

$$\sigma_{c}(\nu' = m\gamma, T) = \sigma_{c} \cdot \left[1 - \frac{\nu'T}{47703 \cdot + 637 \cdot 69\nu'}\right]$$
(62)

with accuracies noted above. Refer to Figs. 7 and 8 for a plot of Eq. (62) at T = 10 and 100 keV. Eq. (62) is indistinguishable from the exact curve there, error $\Delta < 1\%$.

Note that the use of the Sampson equations,¹⁵ also suggested earlier,¹⁶ is limited to T and $\nu' << 100$ keV and they are less accurate (< 4%).

IX. APPLICATION TO MONTE CARLO (OR OTHER) CODES: THE EXACT EQUATIONS

The exact differential cross section for the Compton scattering of a photon of energy ν ' from a Maxwell gas of electrons at a temperature T is given by Eqs. (1), (34), (33), (32), and (25) (or (23) and (24)). The scattering is to photon energy, ν , and is in a direction solid angle $d\Omega = \sin \theta \ d\theta \ d\phi_q$ and

is symmetric in ϕ_q . The total scattering cross section (i.e., integrated over all five variables) is given by Eqs. (60) or (61) and (62). All quantities possible are in energy units.

The equations give the cross section, or with the total cross section the relative probability, of a particular event. For example, to determine a particular scattering $(\nu' \rightarrow \nu, \theta, \phi_q)$ by a particular electron (K', α', ϕ) no integration of Eq. (34) is required. However, usually a user is interested (because of ϕ_q symmetry) only in $d\sigma/d\theta$, the differential scattering cross section of the photon into an angle, θ , and to energy, ν . Thus the other four variables must be integrated over. The succeeding sections give approximate methods for such integrations.

"The simplest application of Monte Carlo is the evaluation of integrals."¹⁷ In fact, highly multi-dimensional integrals are likely to be efficiently solved by Monte Carlo methods.¹⁰ "Every Monte Carlo computation that leads to quantitative results may be regarded as estimating the value of a multiple integral."¹⁸ Thus, the above equations are amenable to formal solution by Monte Carlo methods. The equivalent Monte Carlo particle transport methods¹⁰ may also be employed. At first inspection one might imagine sampling for electron kinetic energy, K', from the Maxwell distribution, Eq. (25) (or (23) plus (24)), and for the isotropic spherical directions α ' and ϕ , then applying these to Eq. (33) and (34) as well as to (32) to determine probabilities. The actual detailed applications of Monte Carlo to the exact equations are beyond the scope of this work.

X. APPLICATION TO MONTE CARLO (OR OTHER) CODES: THE WIENKE-LATHROP ISO-TROPIC APPROXIMATION

If the accuracy of Wienke-Lathrop isotropic approximation is satisfactory, see for example, Figs. 1 to 7 for a comparison of it with the exact scattering cross section, then considerable simplification in the formulas can be achieved. Note from the figures that for temperatures well below 100 keV, say 25 keV or lower, the isotropic cross section does very well. Note further that the total cross section is extremely well represented by the approximation, as Figs. 7 and 8 show. Thus, if a problem is insensitive to angular distributions, indeed if fore and aft symmetry only is required, then the isotropic approximation is good even up to 100-keV temperature. Also note that Figs. 2, 3, 5, and 6 show extreme behavior so that Fig. 5, the worst, describes a rare



Fig. 2. Isotropic differential photon-Maxwellian electron cross sections.



Fig. 3. Isotropic differential photon-Maxwellian electron cross sections.







Fig. 5. Compton cross-section electron temperature, T = 100 keV; initial photon energy, v' = 1 keV.



Fig. 6. Isotropic differential photon-Maxwellian electron cross sections.



Fig. 7. Isotropic photon-Maxwellian electron cross sections (Total).



Fig. 8. Isotropic photon-Maxwellian electron cross sections (Total).

event out of a large totality for most problems. Thus, the isotropic approximation may well be the practical means of choice for most Monte Carlo calculations. It involves only one integration over ϕ , and in fact not even that for the integrals can be integrated analytically (done in Appendix B). Unfortunately, the result involves small differences of very large quantities for some of our parameters and considerable complexity so this author recommends rather numerical or other (e.g., Monte Carlo) quadrature. The accuracy even with intervals as large as 22.5° appears good so that numerical methods can give good accuracy and reasonable calculational efficiency. The total Compton cross section is given by Eqs. (60) or (61) and (62). The differential isotropic cross section is given by Eqs. (51), (48), (47), and (46).

XI. APPLICATION TO MONTE CARLO (OR OTHER) CODES: THE WIENKE-LATHROP FITTED APPROXIMATION

If a somewhat poorer approximation than the isotropic is tolerable, the Wienke-Lathrop fitted approximation is perhaps the simplest to use. See Figs. 4 and 5 for comparisons of the three cross sections: exact, isotropic, and fitted. In place of integration over ϕ , a graph or table is required. The particular one-parameter fit to the total cross section suggested by Wienke and Lathrop⁹ yields the differential cross section (55) with K_f given in Eq. (59) and (ν/ν') given in Eq. (58). The parameter $\langle \kappa_1 \rangle$ is obtained in Fig. 8. The total Compton cross section is given by Eqs. (60) or (61) and (62).

XII. THE MEAN SCATTERED PHOTON ENERGY, HEATING: THE EXACT THEORY

From Eq. (32) the exact scattered photon energy is

$$\nu = \nu' \kappa_1 / \left[\frac{\nu'(1-\mu)}{m} + \kappa_2 \right] , \qquad (63)$$

with κ_1 and κ_2 given by Eqs. (30), (31), and (1). The energy deposition in, or heating H of, the electron gas by the photon is, of course,

$$H \equiv v' - v \quad . \tag{64}$$

We will calculate the mean heating of a relativistic Maxwell electron gas by the Compton scattering of a photon, ν ', through the angle, θ . Using the same notation as in Appendix A, we define

$$a \equiv \kappa - \sqrt{\kappa^2 - 1} \cos \alpha' \cos \theta$$
 (65)

$$b \equiv -\sqrt{\kappa^2} -1 \sin \alpha' \sin \theta$$
 (66)

$$c \equiv (v'/m)(1 - \mu)$$
, (67)

where

 $\mu \equiv \cos \theta$.

By Eq. (30) and (1)

 $\kappa_2 = a + b \cos \phi , \qquad (68)$

and by Eq. (31)

$$\kappa_1 = \kappa - \sqrt{\kappa^2 - 1} \cos \alpha' \quad . \tag{69}$$

Eq. (29) gives

$$\kappa = 1 + \left(\frac{K'}{m}\right) \quad . \tag{70}$$

We average Eq. (64) over the relativistic Maxwell distribution (25). We first integrate over the azimuthal angle ϕ ; our equation is, using Eq. (A10),

$$\langle H \rangle_{\phi} = \nu' \left[1 - \frac{\kappa_1}{\pi} \int_{0}^{\pi} \frac{d\phi}{c + a + b \cos \phi} \right]$$
(71)

with solution

$$\langle H \rangle_{\phi} = \nu' \left[1 - \frac{\kappa_1}{\sqrt{(c+a)^2 - b^2}} \right]$$
 (72)

Let

$$\cos \alpha' \equiv x$$
, (73)

and define

$$A \equiv \kappa^2 - 1$$
 (Note A>0, see Eq. (70)) (74)

$$B \equiv -2\mu\nu\kappa^2 - 1 (c + \kappa)$$
(75)

$$C \equiv c^{2} + 2c\kappa + \kappa^{2}\mu^{2} + 1 - \mu^{2}$$
 (76)

Then our average over the angle of elevation, $\boldsymbol{\alpha}^{\boldsymbol{\cdot}},$ is given by

$$\langle H \rangle_{\phi, \mathbf{x}} = \nu' \left[1 - \frac{1}{2} \int_{-1}^{1} \frac{(\kappa - \sqrt{\kappa^2 - 1} \mathbf{x}) d\mathbf{x}}{\sqrt{Ax^2 + Bx + C}} \right]$$
(77)

with solution

$$\langle H \rangle_{\phi, \kappa} = \nu' \left[1 - \mu - \frac{1}{2\sqrt{\kappa^2 - 1}} \left(\kappa - \mu(c + \kappa) \right) \right]$$

$$\times \ln \left| \frac{c + \kappa + \sqrt{\kappa^2 - 1}}{c + \kappa - \sqrt{\kappa^2 - 1}} \right| .$$

$$(78)$$

Finally, we integrate over electron kinetic energy, K', or in terms of κ from Eq. (70),

$$\langle H \rangle_{\phi, \mathbf{x}, \kappa} \equiv H \rangle = \frac{m^{3} \nu'}{\gamma} \int_{1}^{\infty} \kappa d\kappa \cdot \sqrt{\kappa^{2} - 1} \cdot e^{-(\mathbf{m}\kappa/\mathbf{T})} \\ \times \left\{ (1 - \mu) - \frac{1}{2\sqrt{\kappa^{2} - 1}} \left[(\mathbf{c} + \kappa)(1 - \mu) - \mathbf{c} \right] \right. \\ \left. \times \ln \left| \frac{\mathbf{c} + \kappa + \sqrt{\kappa^{2} - 1}}{\mathbf{c} + \kappa - \sqrt{\kappa^{2} - 1}} \right| \right\},$$
(79)

where we simply write H> for the full Maxwellian average. We evaluate the integral (79) numerically. By Eq. (64) and the distributive law of integration over addition,

$$v \rangle = v' - H \rangle \quad . \tag{80}$$

Eqs. (79) and (80) give the exact mean electron heating and scattered photon energy, v', scattered through an angle θ , after impacting on a relativistic Maxwell electron gas.

Results of the exact heating calculations using Eq. (79) are found in Table III. Selected results of the exact scattered photon energy (Eq. (80)) are found in Figs. 10a, b, and c. The exact results are compared with the isotropic and fitted approximations of Wienke and Lathrop,⁹ and with the unmodified T = 0 Compton energy equation.

XIII. THE MEAN SCATTERED PHOTON ENERGY, HEATING: THE WIENKE-LATHROP ISOTROPIC APPROXIMATION

For the isotropic approximation, Eq. (48) gives the scattered photon energy

$$\nu = \nu' \kappa / \left[\frac{\nu'}{m} (1 - \mu) + \kappa_2 \right] , \qquad (81)$$

where κ is given now by Eq. (46):

$$\kappa = \sqrt{1 + \frac{3T}{m} \left[1 + 20\left(\frac{T}{8m}\right) + 120\left(\frac{T}{8m}\right)^2 - 960\left(\frac{T}{8m}\right)^3 + 4320\left(\frac{T}{8m}\right)^4 + \dots \right]}$$
(82)

and κ_2 by Eq. (47):

$$\kappa_2 = \kappa - \sqrt{\kappa^2 - 1} \cdot (\sin \theta \cos \phi) \quad . \tag{83}$$

The isotropic approximation heating, H_{I} , is

$$H_{I} = \nu' - \nu = \nu' \left[1 - \frac{\kappa}{c + \kappa + e \cos \phi} \right]$$
(84)

using Eq. (67) and defining

$$e \equiv -\sqrt{\kappa^2 - 1} \sin \theta \quad . \tag{85}$$

The mean heating is given by the average over the azimuthal angle ϕ :

$$H_{I} > = \langle H_{I} \rangle_{\phi} = \frac{\nu'}{\pi} \int_{0}^{\pi} d\phi \left[1 - \frac{\kappa}{c + \kappa + e \cos \phi} \right]$$
(86)

using again Eq. (A10), with solution

$$H_{I} > = \nu' \left[1 - \frac{\kappa}{\sqrt{(c + \kappa)^{2} - (\kappa^{2} - 1)(1 - \mu)^{2}}} \right], \qquad (87)$$

where $\mu = \cos \theta$.

Eqs. (87), (70), (67), and (82) give the mean heating in the isotropic approximation of a photon of energy ν ' Compton scattered through an angle θ , ($\mu = \cos \theta$), by a Maxwellian electron gas at a temperature T. The corresponding mean scattered photon energy, ν >, is from Eq. (80):

$$v_{I} = v' - H_{I} > .$$
(88)

XIV. THE MEAN SCATTERED PHOTON ENERGY, HEATING: THE WIENKE-LATHROP ONE-PARAMETER FITTED APPROXIMATION

Equation (58) gives the one-parameter, i.e., $\langle \kappa_1 \rangle$, fitted approximation of Wienke and Lathrop.⁹ $\langle \kappa_1 \rangle$ is found in Fig. 9 and κ is given by Eq. (82) or (46).

$$\nu = \nu' \frac{\langle \kappa_1 \rangle}{c + \kappa} , \qquad (89)$$

where as before (Eq. (67)),

$$c \equiv (\nu'/m) \cdot (1 - \mu)$$
 (90)

The fitted heating is then

$$H_{F} \equiv \nu' - \nu \equiv \nu' \left[1 - \frac{\langle \kappa_{1} \rangle}{c + \kappa} \right] .$$
(91)

Equations (89), (91), (90), and (82) together with Fig. 9 give the one-parameter fitted approximation to the heating and scattered photon energy of a photon of energy ν ' incident on a Maxwell gas of electrons at temperature T.

XV. COMPARISONS OF THE MEAN SCATTERED PHOTON ENERGY AND THE MEAN HEATING AS GIVEN BY THE EXACT, THE ISOTROPIC APPROXIMATION, AND THE FITTED APPROXI-MATION THEORIES

A. Scattered Photon Energy

The ability of the Wienke-Lathrop isotropic approximation to give accurately the mean Compton scattered photon energy corresponds to its ability to give accurately the differential cross section: both are accurate for T small and then for v' large compared to T. Figure 10 shows a comparison of the mean scattered photon energies at the higher temperatures of 100 and 25 keV. For the lower temperatures of 10 keV, the isotropic is in error at most only 3.8%, and for 1-keV temperature in error only at most 0.39% (both at $\theta = 180^{\circ}$, v' = 1). The same plots of these temperatures would fail to show significant differences with the two theories and so were omitted. Because of the displaced 0 in Figs. 9a, b, and c, the differences between exact and approximate



Fig. 9. Wienke-Lathrop fitting parameter, $\langle k \rangle$, versus initial photon energy, ν ', and electron temperature, T.



Fig. 10. Comparisons of exact versus isotropic approximation mean scattered photon energy, v, as a function of angle θ .

are emphasized. The worst scattered photon energy error, as noted, is in Fig. 9c for T large, namely 100 keV, and for $\nu' << T$, namely $\nu' = 1$ keV, at $\theta = 180^{\circ}$ where the error of the isotropic is -28%. Again, as noted in Section X, incident photon energy near $\nu' = 1$ keV when $T_{electron} = 100$ keV is not likely in the totality of problems to be a large fraction of incident photons, so that examination of usual problems reveals that the somewhat large errors of $\nu' = 1$ keV and T = 100 keV usually play but a small role. Thus, the isotropic approximation is certainly a useful approximation in the ranges 0 < T < 100 keV, $1 < \nu' < 1000$ keV.

Up to 10 keV, however, the ordinary, T = 0, Compton equation (Ref. 1, Eq. (38)) is adequate. Its error is less than 4% at 10 keV (-3.8% or less absolutely) and less than 0.4% at 1 keV (-0.39% or less absolutely).

On the other hand the fitted approximation values for the scattered photon energy are simply poor (except at low temperature, but T = 0 Compton is better) and for the most part exceed the ranges of Figs. 10a, b, and c. The fitted approximation errors relative to the exact results are given in Table II. The ordinary T = 0 Compton energy equation (Eq. (38)) is superior to fitted energy equation (Eq. (58)) at all incident photon energies up to T = 100 keV. In fact at T = 100 keV the T = 0 errors are 2 to 29%.

TABLE II

THE ONE-PARAMETER FITTED APPROXIMATION ERRORS IN THE SCATTERED PHOTON ENERGY IN (PERCENT)

 $(\text{Error} \equiv 100 \cdot \frac{-v(\text{exact}) + v(\text{fitted})}{v(\text{exact})})$. T is electron temperature (keV), v' is incident photon energy in keV.

Photon Scattering Angle, θ :	0°	<u>45°</u>	<u>90°</u>	<u>135°</u>	<u>180°</u>
$T = 1, v^* = 1$	1.6%	1.5	1.3	1.3	1.2
$T = 1, v^* = 1000$	-2.2	-2.2	-2.2	-2.3	-2.3
T = 10, v' = 1	11.2%	10.5	9.0	7.5	7.0
$T = 10, v^* = 10$	10.5	9.9	8.5	7.1	6.5
$T = 10, v^* = 20$	10.2	9.6	8.2	7.0	6.5
T = 10, v' = 100	8.4	7.9	6.8	6.1	5.8
$T = 10, v^* = 1000$	4.6	4.7	4.3	4.1	4.1
T = 25, v' = 25	19.5%	17.9	14.3	11.2	10.0
T = 100, v' = 1	52.9%	44.3	27.2	13.7	9.2
$T = 100, v^* = 10$	51.1	42.8	26.5	13.6	9.6
$T = 100, v^* = 100$	41.8	35.6	24.9	17.7	15.4
$T = 100, v^* = 1000$	39.4	41.1	38.5	36.3	35.6

The fitted approximation for the cross section is, however, the simplest algebraically, although one must append Fig. 9 or a table thereof. We recommend use of the standard Compton energy equation (Eq. (38)) if the fitted approximation is used. Note that a two (or more) parameter fitted approximation could be constructed with the expectation of greater accuracy. Again one would require yet another additional graph or table.

B. Heating

Because the energy deposited in the electron gas by the scattering of the photon is often the small difference of relatively large numbers, approximate results are bound to give very poor heating numbers (see Table III). In short, for accurate mean heating of an electron gas by Compton scattering at all parameter values, the exact theory must be used. Note that the greatest error in the isotropic heating occurs for the least heating, so that for many problems the worst discrepancies of Table III overstate the total heating error by a considerable amount. It is clear from Table III that the best heating numbers (although very poor for incident photon energies near the electron temperature), are given by the isotropic approximation, next best T = 0Compton, and the fitted heating numbers are essentially useless.

XVI. RECOMMENDATIONS

In the spirit of the founding fathers of Monte Carlo particle transport, E. D. Cashwell and C. J. Everett, one should always use the best and most precise physics that is practicable. There is also a very real, very pragmatic further reason to do so. Sooner or later every code and every theory will be used beyond the domain originally intended by the creators. Here, use of the exact theory is suitable for any parameter range provided only that one remembers that the Compton effect is not the only photon process (photo-electric, pair production, etc., exist and can be dominant) and that the electron distribution specifically considered is the Maxwellian. (The reader may substitute his own normalized distribution, f(p') in Eq. (19) or f(K') in Eq. (34) if desired.) In contrast, the isotropic approximation is appropriate for a limited range: $0 < T \le 100$ keV and $1 \le v' \le 1000$ keV. Indeed, as Fig. 4 shows, significant departure from the exact angular distribution begins for T = 100 keV and v' = 1 keV, although in most calculations the total effect will be small (see the discussion in Section X).

TABLE III

MEAN ENERGY DEPOSITION OR HEATING, HD, OF A MAXWELL ELECTRON GAS AT A TEMPERATURE, T, BY A PHOTON OF INITIAL ENERGY, v', COMPTON SCATTERED THROUGH AN ANGLE 0

		<u> </u>					θ				
T (keV)	v' (keV)	H> Theory	0	22.5*	45°	67.5*	90°	112.5°	135•	157.5°	180°
1	1	Exact Isotropic Fitted T = 0 Compton	0 0 -1.6(-2) 0	-2.68(-7) -2.81(-4) -1.58(-2) +1.49(-4)	-7.89(-7) -8.96(-4) -1.54(-2) 5.73(-4)	-8.94(-7) -1.30(-3) -1.47(-2) 1.21(-3)	1.58(-8) -9.81(-4) -1.40(-2) -1.95(-3)	2.03(-6) 1.98(-4) -1.32(-2) 2.70(-3)	4.61(-6) 1.87(-3) -1.26(-2) 3.33(-3)	6.78(-6) 3.32(-3) -1.22(-2) 3.75(-3)	7.62(-6) 3.89(-3) -1.20(-2) 3.90(-3)
1	1000	Exact	0	129.4	363.7	546.4	661.1	729.5	769.0	789.6	795.9
		Isotropic Fitted T = 0 Compton	0 22.1 0	129.0 148.6 129.6	363.3 377.7 364.3	546.1 556.4 547.1	661.0 668.7 661.8	729.5 735.6 730.2	769.1 774.2 769.6	789.6 794.3 790.2	796.0 800.5 796.5
10	1	Exact Isotropic	0 0	-1.36(-2) -4.13(-3)	-5.21(-3) -1.43(-2)	-1,10(-2) -2.45(-2)	-1.77(-2) -2.83(-2)	-2.45(-2) -2.29(-2)	-3.02(-2) -1.15(-2)	-3.40(-2) -5.90(-4)	-3.53(-2) +3.78(-3)
		Fitted T = 0 Compton	112 0	111 +1.49(-4)	111 5.73(-4)	110 1.21(-3)	109 1.95(-3)	109 2.70(-3)	108 3.33(-3)	108 3.75(-3)	107 3.90(-3)
10	10	Exact Isotropic Fitted T = 0 Compton	0 0 -1.05 0	-2.57(-4) -2.82(-2) -1.04 1.49(-2)	-7.43(-4) -9.05(-2) 993 5.70(-2)	-7.96(-4) 132 926 0.119	+1.37(-4) 100 848 0.192	2.10(-3) +1.82(-2) -0.771 0.264	4.54(-3) .179 707 .323	6.56(-3) .314 664 .363	7.34(-3) .366 649 .377
10	20	Exact Isotropic Fitted T = 0 Compton	0 0 -2.04 0	+2.89(-2) -2.72(-2) -1.98 +5.94(-2)	.111 -6.68(-2) -1.80 .227	.235 -2.10(-2) -1.54 .472	.380 +.191 -1.23 .753	.525 .558 940 1.03	.648 .973 698 1.25	.730 1.29 539 1.40	.758 1.41 484 1.45
10	100	Exact Isotropic	0 0	1.31 1.02	4.85 4.01	9.69 8.66	14.81 14.18	19.37 19.54	22.87 23.85	25.05 26.59	25.78 27.53

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TABLE III(cont)

MEAN ENERGY DEPOSITION OF HEATING, H>, OF A MAXWELL ELECTRON GAS At a temperature, T, by a photon of initial knergy, v'. Compton scattered through an angle 0

							ее				
T (ke¥)	v' (keV)	H> Theory	0	22.5°	45°	67.5*	90•	112.5°	135•	157.5*	180•
	• • • •	Fitted T = 0 Compton	-8.35 ·	-6.81 1.47	-2.64 5.42	+3.02 10.8	8.94 16.4	14.18 21.3	18.18 25.0	20.65 27.4	21.48 28.1
10	1000	Exact Isotropic Fitted T = 0 Compton	0 0 -45.5 0	127.1 123.5 +86.6 129.6	358.1 353.6 328.2 364.3	539.5 537.3 518.7 547.1	654.4 653.9 639.4 661.8	723.3 723.7 711.7 730.2	763.3 764.1 753.6 769.6	784.2 785.1 775.4 790.2	790.7 791.7 782.1 796.5
25	25	Exact Isotropic Fitted	0 0 -4.86	-3.77(-3) 175 -4.76	-1.05(-2) 572 -4.47	-1.02(-2) 846 -4.05	+4.68(-3) 639 -3.57	3.36(-2) +.101 -3.10	6.81(-2) 1.05 -2.72	9,57(-2) 1,80 -2,47	.106 2.08 -2.38
100	1	Exact Isotropic Fitted	0 0 529	-1.54(-2) -3.67(-2) 529	-5.90(-2) 145 528	124 296 528	201 378 527	277 294 526	342 142 525	385 -3.38(-2) 525	-,400 +2.83(-3) 525
100	10	Exact	0		-,537		-1.78		-2.94		-3.40
		Isotropic Fitted	0 -5.11	356 -5.10	-1.39 -5.05	-2.79 -4.98	-3.46 -4.90	-2.57 -4.82	-1.11 -4.76	-7.32(-2) -4.71	+.276 -4.70
100	100	Exact Isotropic Fitted	0 0 -41.8	-2.49 -40.3	413 -8.68 -36.1	-13.52 -30.4	+.604 -9.96 -24.17	+1.16 -18.55	3.03 12.43 -14.16	19.66 -11.41	4.23 22.07 -10.47
100	1000	Exact Isotropic Fitted	0 0 -394,2	104.4 70.5 -258.5	301.6 247.0 14.6	468.9 432.6 256.2	583.5 568.2 423.0	656.6 653.8 528.7	700.7 704.4 592.1	724.3 730.9 625.7	731.7 739.1 636.2

I feel the ultimate reliability of a theory used in ranges unexpected by the author is a very strong argument for physical and mathematical rigour as I've indicated above. Not fully in contrast is the fact that much data, many theories, and the significance of the results alike do not warrant great accuracy. In short, many calculations err in using needless precision.

In view of the foregoing considerations, I recommend the ordinary Klein-Nishina Formula and the T = 0 Compton energy equation for most problems up to an electron temperature of 10 keV. The formula and equation are already in MCNP and other Los Alamos Monte Carlo codes. One may then expect accuracies of better than 1.5% in the total Compton cross section [from Eq. (62), maximum v' = 1000 keV and about 5% or better in the differential cross section. The error in the scattered photon energy is 4% or better. For higher accuracies or for special results, such as photon energy upscatter or heating, one should use the full temperature dependent theories. Even as high as T = 25 keV, the error of the total Compton (Klein-Nishina) cross section is 3.6% or less (maximum v' = 1000 keV) and of the differential cross section is of the order of or less than 10%. (Specifically, at T = 25 keV, v' = 25 keV, the differential crosssection errors are +5.8% at θ = 45°, +8% at 90°, and -0.9% at 135°.) For scattered photon energy the error is 0.4% (22.5°) to 8.5% (180°). At 1-keV temperature the error of the total Klein-Nishina cross section drops to 0.15% (v' = 1000 keV) or less, and the error of the Klein-Nishina differential cross section is 0.5% or less. The error in the scattered photon energy ranges from 0.015 to 0.39%.

For higher temperatures (than say 10 keV or so), greater accuracies, or better specific detail, we recommend the exact equations as summarized in Sections IX and XII. This recommendation is only made with the proviso that an efficient cross-section computational algorithm can be found. Otherwise we recommend the Wienke-Lathrop isotropic approximation summarized in Sections X and XIII with numerical integration over ϕ for the cross section. Such approximation should be limited to $0 < T \leq 100$ keV and $1 \leq \nu' \leq 1000$ keV, (but use Klein-Nishina below about 10-keV temperature). Formally, as we've shown, both the exact and the isotropic reduce to the Klein-Nishina for T $\neq 0$.

The fitted approximation is not recommended. Its complexity is not sufficiently less than the isotropic to justify the larger errors it introduces. For heating, only the exact theory will do. Except only for $\nu' \gg T$ will the isotropic approximation yield a good or even fair approximation. The regular T = 0 Compton equation requires both T \leq 10 keV and $\nu \gg$ T in order to yield fair to good heating numbers.

ACKNOWLEDGMENTS

It is a pleasure to thank John Hendricks, Group X-6, for his interest, encouragement, and patience; Charles Zemach, T-DO, for help in field theory and for verifying the basic exact covariant theory; Bruce Wienke, C-3, for developing the basic theory and then generalizing his isotropic approximation (with B. Lathrop) for developing a fitted approximation and for countless calculations, graphs, and conversations having the objective of benefiting Monte Carlo applications; Art Forster, X-6, for suggesting alternative integration methods; Judi Briesmeister, X-6, and Marge Devaney, C-8, for brief reviews of integration as done in the Los Alamos Central Computing Facility (CCF); Tom Booth for suggesting how to include the master library integration subroutine of TI-59 calculator; Peter Herczeg, T-5, for a lucid explanation of certain δ -function properties; Peter Noerdlinger, X-7, for criticism and suggestions; and Tyce McLarty for an HP15C coding suggestion.

APPENDIX A

$\phi-$ INTEGRATION OF THE EXACT COMPTON DIFFERENTIAL CROSS SECTION

We rewrite Eq. (34) in the form

$$\frac{d\sigma}{d\Omega} = \frac{r_o^2}{2} \int dK' \cdot (K' + m) \cdot \sqrt{K'^2 + 2mK'} \cdot f(K') \cdot \frac{\sin\alpha'}{\kappa\kappa_1} d\alpha' \cdot I, (A1)$$

where I is the $\boldsymbol{\varphi}\text{-integral}$ which we shall analytically evaluate,

$$I \equiv \int_{0}^{\pi} d\phi \cdot \left(\frac{\nu}{\nu^{*}}\right)^{2} K \quad . \tag{A2}$$

Substituting Eq. (1) into Eq. (32) we get

$$\kappa_2 = \kappa - \sqrt{\kappa^2 - 1} \cos \alpha' \cos \theta - \sqrt{\kappa^2 - 1} \sin \alpha' \sin \theta \cos \phi \quad (A3)$$

For convenience define

$$a \equiv \kappa - \sqrt{\kappa^2 - 1} \cos \alpha' \cos \theta \tag{A4}$$

$$b \equiv -\sqrt{\kappa^2 - 1} \sin \alpha' \sin \theta \tag{A5}$$

$$c \equiv (\nu'/m)(1 - \mu) \tag{A6}$$

as before $\mu \equiv \cos \theta$. Then

$$\kappa_2 = a + b \cos \phi , \qquad (A7)$$

and by Eq. (32)

$$\frac{\nu}{\nu'} = \frac{\kappa_1}{\frac{\nu'}{m}(1-\mu)+\kappa_2} = \frac{\kappa_1}{c+a+b\cos\phi} \equiv \frac{\kappa_1}{a'+b\cos\phi} , \quad (A8)$$

where we have defined

a' = c + a =
$$(\nu'/m)(1 - \mu) + \kappa - \sqrt{\kappa^2 - 1} \cos \alpha' \cos \theta$$
 (A9)

Observe that

$$\int_{0}^{2\pi} (\text{function of } \cos \theta) \, d\theta = 2 \int_{0}^{\pi} (\text{function of } \cos \theta) \, d\theta \quad . \tag{A10}$$

Substituting Eqs. (A10), (A8), (A6), and (33) into Eq. (A2), we have

$$I = 2 \int_{0}^{\pi} d\phi \cdot \left(\frac{\kappa_{1}}{c + \kappa_{2}}\right) \left[\frac{(1 - \mu)^{2}}{\kappa_{1}^{2} \kappa_{2}^{2}} - \frac{2(1 - \mu)^{2}}{\kappa_{1}^{2} \kappa_{2}} + \frac{c + \kappa_{2}}{\kappa_{2}} + \frac{\kappa_{2}}{c + \kappa_{2}}\right] \cdot (A11)$$

Expanding in partial fractions and collecting terms of the same $\boldsymbol{\varphi}$ dependence gives

$$I = 2 \int_{0}^{\pi} d\phi \left[\frac{A_{1}}{c + \kappa_{2}} + \frac{A_{2}}{(c + \kappa_{2})^{2}} + \frac{A_{3}}{(c + \kappa_{2})^{3}} - \frac{A_{1}}{\kappa_{2}} + \frac{B_{2}}{\kappa_{2}^{2}} \right] , \quad (A12)$$

where

$$A_{1} \equiv \left[\frac{2(1-\mu)^{2}}{c^{3}} - \frac{\kappa_{1}^{2}}{c} + \frac{2\kappa_{1}(1-\mu)}{c^{2}}\right]$$
(A13)

$$A_{2} \equiv \left[\frac{(1-\mu)^{2}}{c^{2}} + \frac{2\kappa_{1}(1-\mu)}{c} + \kappa_{1}^{2}\right]$$
(A14)

$$A_3 \equiv -c\kappa_1^2/(c + \kappa_2)^3$$
 (A15)

$$B_2 = (1 - \mu)^2 / c^2 \quad . \tag{A16}$$

Defining

$$I(n,a,b) \equiv \int_{0}^{\pi} \frac{d\phi}{(a+b \cos \phi)^{n}} , \qquad (A17)$$

we have in Eq. (A12) the five integrals

I(1,a',b), I(2,a',b), I(3,a',b), I(1,a,b), and I(2,a,b).

Evaluating these integrals with the help of tables, 18

$$I(1,a',b) = \frac{\pi}{\sqrt{a'^2 - b^2}}, \quad I(1,a,b) = \frac{\pi}{\sqrt{a^2 - b^2}}.$$
 (A18)

$$I(2,a',b) = \frac{\pi a'}{(a'^2 - b^2)}, \quad I(2,a,b) = \frac{\pi a}{(a^2 - b^2)^{3/2}}$$
(A19)

$$I(3,a',b) = \frac{\pi(2a'^2 + b^2)}{2(a'^2 - b^2)^{5/2}}$$
(A20)

so that

-

$$I = 2\pi \left[\frac{A_1}{\sqrt{a'^2 - b^2}} + \frac{a'A_2}{(a'^2 - b^2)^{3/2}} + \frac{(2a'^2 + b^2)A_3}{2(a'^2 - b^2)^{5/2}} - \frac{A_1}{\sqrt{a^2 - b^2}} \right] + \frac{aB_2}{(a^2 - b^2)^{3/2}} + \frac{aB_2}{(a^2 - b^2)^{3/2}$$

Eq. (A21) together with Eq. (A1) is our desired solution.

Using Eqs. (A4) to (A6) to evaluate Eqs. (A13) to (A16), we get

$$A_{1} = \frac{m^{3}}{\nu'^{3}(1-\mu)} \left[2 - \frac{\nu_{1}^{2}\kappa_{1}^{2}}{m^{3}} + \frac{2\nu_{1}\kappa_{1}}{m} \right]$$
(A22)

$$A_2 = \left(\frac{m}{v} + \kappa_1\right)^2 \tag{A23}$$

$$A_{3} = -\frac{\nu'\kappa_{1}^{2}}{m}(1-\mu)$$
(A24)

$$B_2 = (m/v')^2$$
 (A25)

$$a^{2} - b^{2} = 1 + (\kappa^{2} - 1)(\mu^{2} + \cos^{2}\alpha') - 2\kappa\mu \cos \alpha' \sqrt{\kappa^{2} - 1}$$
 (A26)

$$a'^2 - b^2 = 1 - (\kappa^2 - 1)(\mu^2 + \cos^2 \alpha') - 2\kappa\mu \cos \alpha' \sqrt{\kappa^2 - 1}$$

$$+ \frac{\nu'}{m} (1 - \mu) \left[2\kappa - 2\sqrt{\kappa^2 - 1} \mu \cos \alpha' + \frac{\nu'}{m} (1 - \mu) \right] . \quad (A27)$$

Of course, by Eq. (30)

$$\kappa_1 = \kappa - \sqrt{\kappa^2 - 1} \cos \alpha' \quad . \tag{A28}$$

The complexity of the above algebra is such that we found it easier to evaluate the ϕ -integral numerically by Simpson's rule. We found the interval number n = 8 to be adequate to reproduce the Wienke-Lathrop results of Figs. 2, 3, 4, and 5 to roughly the accuracy of reading the graphs.

APPENDIX B

\phi-INTEGRATION OF THE ISOTROPIC APPROXIMATION COMPTON DIFFERENTIAL CROSS SECTION

Using Eqs. (A10), (A6), and (48) into Eq. (49), we must evaluate

$$d\sigma/d\Omega = \frac{r_o^2}{2\pi} \cdot \int_o^{\pi} d\phi \cdot \frac{1}{(c + \kappa_2)} \cdot \left[\frac{(1 - \mu)^2}{\kappa_2^2} \frac{2(1 - \mu)}{\kappa_2} + \frac{(c + \kappa_2)}{\kappa_2} + \frac{\kappa_2}{c + \kappa_2} \right].$$
(B1)

Comparing Eq. (B1) with Eq. (All), we see that

$$d\sigma/dQ = \frac{r_o^2}{4\pi\kappa^2} I \text{ (with } \kappa_1 \rightarrow \kappa) \equiv \frac{r_o^2}{4\pi\kappa^2} J ,$$
 (B2)

defining J:

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 $J \equiv I(with \kappa_1 \rightarrow \kappa) \quad . \tag{B3}$

Eq. (B2) is our result where J is then given literally by Eq. (A21) but the constants in Eq. (A21) are those of Eqs. (A22) through (A24) with κ_1 replaced by κ and those of Eqs. (A25) through (A27) additionally.

Again, we found the above algebra complicated so we carried out our ϕ -integration numerically by Simpson's rule.

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