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Legendre Polynomial Expansion for the Klein–Nishina Formula for Nonstationary Electrons*

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This paper presents energy integrated coefficients for a Legendre expansion of the angular dependence of the differential cross section which describes Compton scattering from nonstationary electrons. The electrons are assumed to have a Maxwellian velocity distribution and an analytic fit is presented for the dependence of these coefficients on photon energy and electron distribution temperature. If one wishes to use a Legendre expansion of the scattering kernel in a gray transport calculation, these coefficients may be used to aid in determining the degree of expansion required for the particular situations to be encountered in the problem. The fits presented will yield integrated coefficients whose accuracy are good to approximately one percent for photon energies between 0 and 1000 keV, and for electron distribution temperatures between 0 and 20 KeV. These well-behaved, smoothly varying energy integrated coefficients also serve as a check on the accuracy of arbitrarily constructed multigroup coefficients.

1. INTRODUCTION

The Klein–Nishina formula [1] for the differential cross section which describes the scatter of unpolarized photons from stationary electrons may be used to describe scattering from nonstationary electrons by the use of a Lorentz transformation [2]. If one considers an ensemble of free electrons which may be characterized by a relativistic Maxwellian distribution function, the expression for the

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averaged differential scattering cross section over all possible electron velocities has been shown to be [2]

$$\sigma_S(\epsilon \to \epsilon', \hat{\Omega} \to \hat{\Omega}'; T_e) = \int_{\mathbf{v}} \sigma_S^{KN}(\epsilon_0 \to \epsilon_0'; \mu_0)\, F(\mathbf{v}; T_e)\, \frac{D}{\lambda D'}\, d^3v. \tag{1}$$

Here σ_S is the differential cross section for the scatter of a photon of energy ϵ with incident direction $\hat{\Omega}$ scattered to direction $\hat{\Omega}'$ with final energy ϵ', from electrons whose distribution temperature is T_e. The term σ_S^{KN} is the Klein–Nishina cross section for scattering in the rest frame of a given electron. The energies ϵ_0 and ϵ_0' are the photon energies whose values in the laboratory frame are ϵ and ϵ'. Similarly, the cosine of the scattering angle in the rest frame of the electron, μ_0, has an angular cosine in the laboratory frame which is given by the inner product $\hat{\Omega} \cdot \hat{\Omega}'$. The quantity $\mathbf{v}$ is the electron velocity, and the F function is the relativistic Maxwellian velocity distribution function given by [2]

$$F(\mathbf{v}; T_e) = \frac{m\lambda^5}{4\pi c k T_e} \frac{\exp(-mc^2\lambda/kT_e)}{K_2(mc^2/kT_e)} \tag{2}$$

where,

$K_2(x)$ is the modified Bessel function of order 2, where for $x \gg 1$, [3]

$$K_2(x) = [\pi/2x]^{1/2}\, e^{-x} \left[1 + \frac{15}{8x} + \frac{1}{2}\frac{15 \cdot 7}{(8x)^2} - \frac{1}{6}\frac{15 \cdot 7 \cdot 9}{(8x)^3} + \cdots\right].$$

Also,

$$\begin{aligned} \lambda &= [1 - v^2/c^2]^{-1/2} \\ D &= 1 - \hat{\Omega} \cdot \mathbf{v}/c; \\ D' &= 1 - \hat{\Omega}' \cdot \mathbf{v}'/c; \qquad \text{and} \\ k &= \text{Boltzmann's constant} = 8.6164 \times 10^{-2}(\text{KeV}^{0}K^{-1}). \end{aligned} \tag{3}$$

Stone and Nelson [4] presented a method for calculating the differential scattering cross section as a function of the initial and final photon energies, the cosine of the scatter angle, and the electron distribution temperature. The computer routines which they developed are available through the Computer Information Center of the Lawrence Livermore Laboratory [5]. These routines were the tool used by the authors and by others referenced, to generate all differential scattering cross sections for the case of nonstationary electrons.

When considering scattering in a solution to the equation for the radiative transfer of energy, it has often been found useful to expand the angular dependence of the differential scattering cross section in a series of Legendre polynomials. The first four coefficients of such an expansion were calculated by Matteson, Pomraning, and Wilson for ten electron temperatures and over a fairly large range of initial and final photon energies [6]. These coefficients may be used in any method which considers scattering from one discrete energy to another.

If one wishes to apply a multienergy group solution to a problem, then one must obtain integrals of these coefficients over appropriate energy limits. Stephan and Bridgman have obtained such a set of group-to-group scattering coefficients which are defined by the following relationship [7]

$$\sigma_{s_l}^{K\to K'}(\theta_e) = \frac{\int_{\epsilon_K}^{\epsilon_{K+1}} d\epsilon\, W(\epsilon;\, \theta_e) \int_{\epsilon_{K'}}^{\epsilon_{K'+1}} d\epsilon'\, \sigma_{s_l}(\epsilon \to \epsilon';\, \theta_e)}{\int_{\epsilon_K}^{\epsilon_{K+1}} d\epsilon\, W(\epsilon;\, \theta_e)}, \tag{4}$$

where W is the equilibrium Wien weighting function, written in terms of photon number density.[1] The coefficients were obtained for 134 energy groups for photon energies from 0.05 to 400 KeV.

In another paper, Stephan and Bridgman [9] report a systematic investigation of a thermal X-ray, discrete ordinates, benchmark problem in which the order of the angular quadrature, the number of energy groups, and the degree of anisotropy of the scattering kernel, as well as the photon and target electron temperatures were all systematically varied. Their results were relative, showing the variation in transmission as these parameters were changed. They found that a two or three term Legendre expansion of the scattering kernel was sufficient for thin slab geometries. In general, a more absolute measure of the number of Legendre terms necessary in the expansion of the scattering kernel is needed. Such a measure is developed here by calculating a set of Legendre coefficients, integrated over scattered energies, similar to those presented by Renken for the case of stationary electrons [10]. Renken obtained coefficients for the following expansion.

$$\mathscr{A}_l(\epsilon) = \frac{1}{\sigma_{\text{th}}} \int_{4\pi} d\Omega\, \sigma_{KN}(\epsilon, \mu)\, P_l(\mu). \tag{5}$$

The parameter σ_{th} is the classical Thompson cross section, which was taken to be 665.1606 millibarns per free electron. The integral over all solid angles is, in reality, an integral over all final scattered photon energies as well. This is due to the constraint between the ratio of the initial and scattered photon energies and the cosine of the angle of scatter off a stationary electron [11]

$$\epsilon/\epsilon' = 1 + \alpha(1 - \mu), \tag{6}$$

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[1] The Wien function was chosen because the cross sections were developed for a calculation which did not consider the nonlinear induced terms in the scattering integrals. The inclusion of induced terms leads to an equilibrium distribution which would be described by a Planckian function.

where α is the energy of the incident photon expressed in units of the electron rest energy. This constraint is often written in the form of a Dirac delta function, and included in the Klein–Nishina formula. The result of electron motion is a Doppler broadening of this constraint, making a range of scattered energies possible for a given initial energy and cosine of scatter angle. Graphical representation of this effect was displayed by Stone and Nelson [4]. To obtain a set of coefficients like those defined in Eq. (5) for the case of nonstationary electrons, one would have to perform an integration over the final scattered photon energies as well. The resultant one-group coefficients might not be of significance for use in "grey" calculations as such calculations would only be approximate, but other uses for the coefficients are worth noting. If one were using a multigroup transport technique to describe a situation which required angular resolution of the scattering process, these energy integrated coefficients would be useful in two respects. First, they would be a quantitative check for determining the relative importance of the various scattering coefficients to determine the degree of expansion required on the scattering kernel. Second, they would serve as physical checks upon the group-to-group scattering coefficients which one would construct for the calculation. For the zeroth order case, this would be an application of the principle of conservation of total cross section. For higher order coefficients a generalization of this principle could be used to assure accuracy of the group-to-group coefficients.

2. ENERGY INTEGRATED COEFFICIENTS

The Zero Order Coefficient

For the case of scattering from nonstationary electrons, we shall call the quantity which corresponds to Renken's energy integrated cross section $\sigma(\epsilon, \mu; \theta_e)$, where

$$\sigma(\epsilon, \mu; \theta_e) = \int_0^\infty d\epsilon' \sigma_S(\epsilon \to \epsilon', \mu; \theta_e). \tag{7}$$

When the angular dependence of this quantity is represented in a Legendre polynomial expansion, it is of the same form as that which was presented by Renken, namely

$$\sigma(\epsilon, \mu; \theta_e) = \sigma_{th} \sum_l [(2_l + 1)/4\pi] \mathscr{A}_l(\epsilon; \theta_e) P_l(\mu). \tag{8}$$

The coefficients $\mathscr{A}_l$ are obtained by

$$\mathscr{A}_l(\epsilon; \theta_e) = \frac{1}{\sigma_{th}} \int_{4\pi} d\Omega\, P_l(\mu) \int_0^\infty d\epsilon'\, \sigma_S(\epsilon \to \epsilon', \mu; \theta_e). \tag{9}$$

The zeroth order coefficient is, by definition, the normalized total Compton scattering cross section. This cross section was available directly from the Stone and Nelson routines, and the values obtained were fit over the following energy and temperature ranges:

$$0 \leqslant \theta_e \leqslant 20 \text{ KeV},$$
$$0 \leqslant \epsilon \leqslant 1000 \text{ KeV}.$$

The accuracy of the Stone and Nelson data was represented to be within 0.1 % for the quadrature option chosen, and the precision of the fit obtained was within 1.0 % agreement with the data. The zero order coefficient was observed to be a monotonically decreasing function of initial photon energy for a given electron temperature. For this reason and the fact that in the limit of zero photon energy and stationary electrons the value of $\mathscr{A}_0$ is unity, the following form was chosen for the dependence of $\mathscr{A}_0$. For photons of energy (keV) scattering off of a Maxwellian distribution of electrons whose temperature is T(keV).

$$\mathscr{A}_0(\epsilon; T_e) = 1 - \epsilon/[B_{00}(T_e) + B_{01}(T_e) \cdot \epsilon + B_{02}(T_e) \cdot \epsilon^2]. \qquad (10)$$

The coefficients B were nearly linearly dependent upon the electron temperature, and a second degree polynomial was used to describe this dependence. Thus, the two parameter fit for $\mathscr{A}_0$ was

$$\mathscr{A}_0(\epsilon; T_e) = 1 - \epsilon\Big/\left[\sum_{M=0}^{2} \epsilon^M \sum_{N=0}^{2} C_{0,M,N} \cdot T_e{}^N\right] \qquad (11)$$

The fits of Eq. (11) were obtained using a least-squares fitting routine [12], and the coefficients C_{0MN} are presented in Table I.

Energy Integrated Higher Order Coefficients

The values of the energy integrated higher order expansion coefficients were not available from the Stone and Nelson routines. Therefore, a numerical integration was performed to obtain the coefficients defined in Eq. (9). A point is worth noting here. In the limit of forward scatter, the differential cross section becomes a delta function. The Stone and Nelson routines return a value for the energy integrated value of the differential cross section in the limit of forward scattering through the use of a limit function which they derived [4].

For this reason, it was expedient first to perform the energy integration in Eq. (9) for a set of scattering cosines chosen to cover the range of possible scatter directions. An examination of the differential scattering cross section resulted in the following observations.

First, for electron temperatures which are low in comparison with the initial

TABLE I

Coefficients which Define the Dependence of the Normalized Legendre Coefficients which Describe the Angular Dependence of the Energy Integrated Differential Cross Section for Compton Scatters

L	N	M: 0	1	2	3	4	5	6
0	0	2.255 + 2[a]	1.311	−1.018 − 4				
	1	−1.245	1.817 − 3	−1.788 − 6				
	2	4.015 − 3	−5.487 − 7	4.251 − 9				
1	0	0	1.410 − 3	−7.011 − 6	1.873 − 8	−2.729 − 11	2.020 − 14	−5.919 − 18
	1	−5.341 − 4	6.256 − 6	−4.787 − 8	1.609 − 10	−2.652 − 13	2.110 − 16	−6.479 − 20
	2	−1.045 − 5	4.929 − 9	−2.812 − 11	1.258 − 13	−2.648 − 16	2.486 − 15	−8.598 − 23
2	0	0.1	−3.264 − 4	1.888 − 6	−5.650 − 9	8.757 − 12	−6.714 − 15	2.012 − 18
	1	−1.241 − 3	2.407 − 6	9.023 − 10	−2.024 − 11	4.518 − 14	−4.084 − 17	1.343 − 20
	2	1.24 − 5	−2.572 − 8	5.460 − 11	−8.572 − 14	9.475 − 17	−6.725 − 20	2.117 − 23
3	0	0	1.511 − 4	−4.954 − 7	1.210 − 9	−1.773 − 12	1.343 − 15	−4.024 − 19
	1	3.682 − 4	−3.163 − 6	1.095 − 8	−2.304 − 11	2.882 − 14	−1.923 − 17	5.238 − 21
	2	−6.299 − 6	2.878 − 8	−8.975 − 11	1.633 − 13	−1.913 − 16	1.258 − 19	−3.498 − 23

[a] 2.255 + 2–2.255 × 10^2.

photon energy, the cross section is very nearly a spike which is centered about the final scattered energy which one would compute for cold Compton scatter.

Second, for relatively high electron temperatures, the function becomes much broader, and the peak is shifted slightly to higher final scattered energies. The reason for this upward shift of the peak may be attributed to the fact that for higher electron temperatures, upscattering may occur for any angle of scatter. This leads to a larger set of possible energies above the stationary Compton value. The probable energies below this value are bounded from below by zero. An example of this observed behavior is shown in Fig. 1 for photons which are backscattered from an initial energy of 1 KeV.

The numerical integrations over final energies were carried out using Simpson's Rule. Fifty equidistant energy intervals were set up on either side of the cold Compton scattered energy for a given cosine of the scatter angle. Twelve equally spaced cosine intervals were considered requiring twelve discrete values besides that for the forward scattering returned by the Stone and Nelson routines. Thirty-five initial photon energies were considered. They range from 0.1 KeV to 1000 KeV, for ten electron temperatures which range from 0.5 to 20 KeV. Renken's data

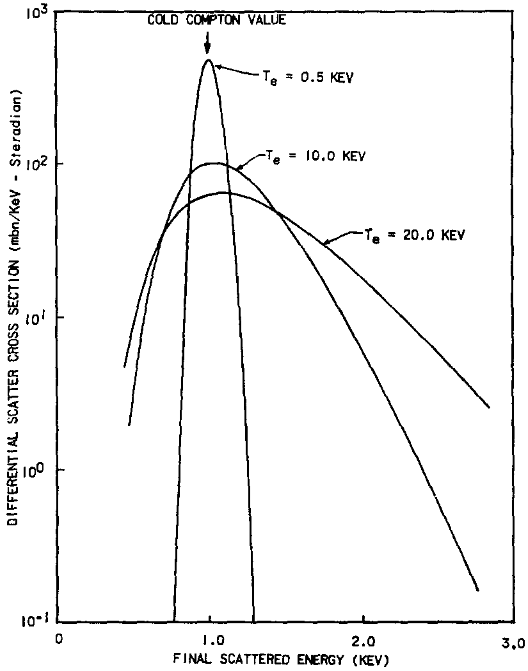

FIG. 1. Differential scattering cross section for backscatter from an initial photon energy of 1.0 KeV.

supplied a check on the values of the coefficients for the stationary electron case. These stationary values were calculated with a separate integration scheme to provide the coefficients at the thirty-five photon energies chosen. The agreement with Renken's data was within 0.05 percent for the points which he published [10].

The energy integrated differential cross sections were found to be smoothly varying functions of the cosine of the scattering angle. For low electron temperatures and low photon energies, they had essentially a parabolic form. As the photon energy increased, this cross section became strongly biased in the forward direction. The effect of elevated electron temperature was to spread the scattering probability out more evenly over all scatter cosines as is illustrated in Figs. 2 and 3.

The numerical integrals required over all solid angles in Eq. (9) may be written as the product of 2π and the integral over all scattering cosines. The integration was carried out over the twelve intervals using Weddel's rule, a sixth-order accurate integration scheme. This method requires a number of equispaced intervals which is some multiple of six [13]. A convenient means for checking the accuracy of the overall integration procedure was to compare the zeroth-order coefficients calculated against the value of the total cross section which was returned by the

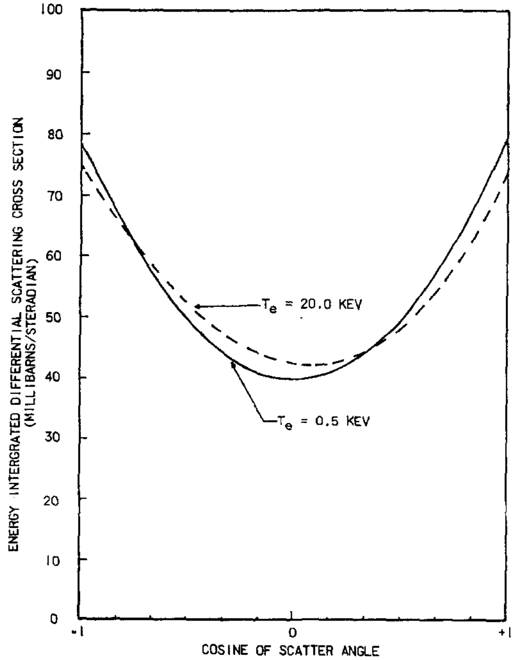

FIG. 2. Energy integrated differential scattering cross section for an initial photon energy of 0.1 KeV.

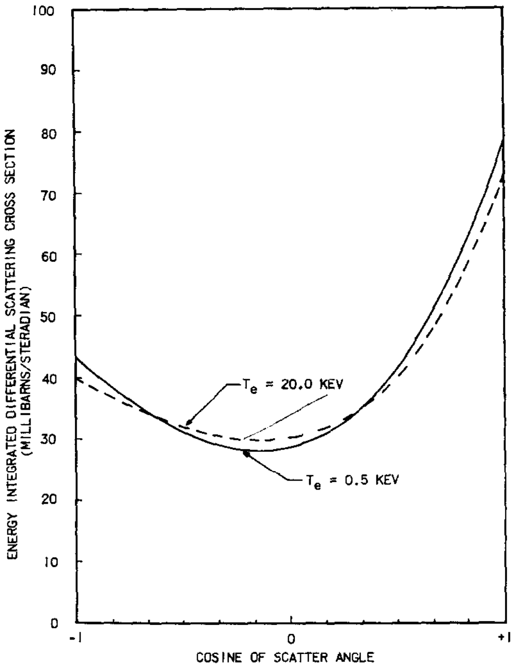

FIG. 3. Energy integrated differential scattering cross section for an initial photon energy of 100 KeV.

Stone and Nelson routines. The precision of the integration scheme was within 1 % of the Stone and Nelson data for all cases. Because of the order of accuracy of the integration scheme, it is reasonable to expect the values calculated for the first- through third-order coefficients to be of similar accuracy [14].

Examination of the behavior of the higher order coefficients revealed that their dependence upon initial photon energy for a given order coefficient was qualitatively similar over the range of electron temperatures considered. For this reason, the higher order coefficients were first fit as a function of photon energy for a given electron temperature as

$$\mathscr{A}_L(\epsilon; T_e) = \sum_{M=0}^{6} B_{L,M}(T_e) \cdot \epsilon^M \tag{12}$$

The variation of the coefficients $B_{L,M}$ was then seen to be a nearly linear function of electron temperature. This variation was fit with a set of second-degree polynomials, so that the expression for the higher order coefficients was

$$\mathscr{A}_L(\epsilon; T_e) = \sum_{M=0}^{6} \epsilon^M \sum_{N=0}^{2} C_{L,M,N} T_e^N \tag{13}$$

In performing the fits, the coefficients $C_{1,0,0}$ and $C_{3,0,0}$ were constrained to be zero and $C_{2,0,0}$ was constrained to be 0.1. These values represent the values of the coefficients $\mathscr{A}_1$, $\mathscr{A}_2$, and $\mathscr{A}_3$ in the classical limit of Thompson scatter. The least-squares fits were performed by setting the values of $C_{1,0,01}$, $C_{2,0,0}$, and $C_{3,0,0}$ and then letting the routine choose the values of the other $C_{L,M,N}$. The values of the higher order coefficients are given in Table I. By using these fits over the ranges specified for the electron temperatures and photon energies, the maximum deviations from the calculated values of $\mathscr{A}_1$, $\mathscr{A}_2$, $\mathscr{A}_3$ were within ± 0.0008 in all cases. Since the true value for $\mathscr{A}_1$ and $\mathscr{A}_3$ is zero for the limiting case of Thompson scatter, percentage deviations were not relevant for these coefficients. The maximum deviation from the value of $\mathscr{A}_2$ was found to be less than 1 %.

Figure 4 shows the dependence upon photon energy of the $\mathscr{A}$'s for various electron temperatures. As was shown by Renken, the order of the expansion

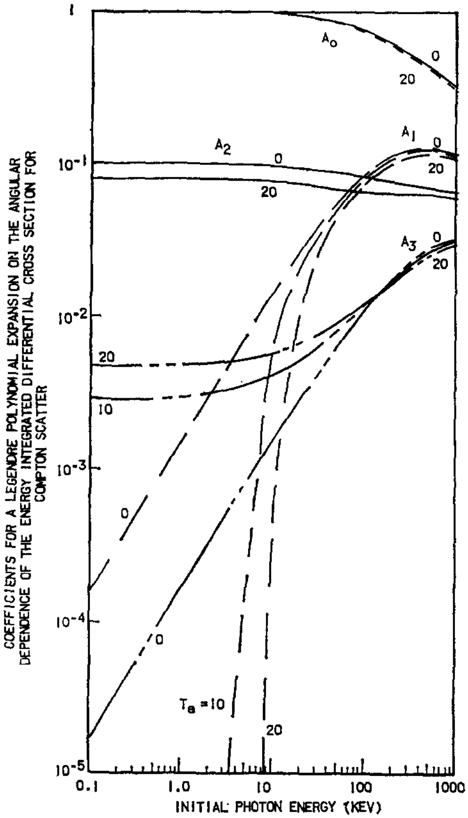

FIG. 4. Electron temperature and photon energy dependence of first four Legendre expansion coefficients.

required for an adequate description of scattering increases with increasing photon energy for cold Compton scatter. While it might appear that the influence of the coefficients $\mathscr{A}_1$ is decreasing with increasing electron temperature for low photon energies, it should be pointed out that it may have negative values in this range. For example, with a 20 keV electron temperature, the value of $\mathscr{A}_1$ approaches approximately -0.0156 as the photon energy approaches zero. As the photon energy becomes very large in comparison with the electron temperature, the values of all four coefficients appear to converge to the values for the cold case.

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