Penetration and Diffusion of Hard X-Rays: Polarization Effects*

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Most calculations of x-ray penetration and diffusion neglect the polarization of the scattered photons. In this paper an investigation is made of the effect of polarization in a typical x-ray penetration problem. The Boltzmann equation for polarizable photons is expanded into suitable angular and spatial polynomial systems; and a calculation based on this Boltzmann equation is compared with a similar calculation which neglects polarization. The polarization effect increases the intensity of the 100–200 kev secondaries by a few percent.

I. INTRODUCTION

In recent years a number of methods have been developed for calculating spectral intensities of scattered x-rays at various penetrations.[1, 1a, 2] Nearly all calculations have neglected the effect of polarization in successive Compton scatterings. It is of interest to know just how far one is justified in this. An attempt to evaluate the effect of polarization was made four years ago by Monte Carlo sampling techniques.[3] The results indicated that the effect is quite small.

It can be argued qualitatively that polarization should increase the x-ray flux slightly at large penetrations since the effect of polarization is to increase the likelihood that the successive directions of scattering of a photon will be coplanar. The effect should be more important at low than at high photon energies.

In this paper we have extended the method of reference 1 to calculate spectral intensities generated by a point isotropic source in an infinite medium, taking into account polarization. The results confirm our expectations of slightly greater flux at great depths than is predicted by the simpler theory. Since the method for performing such a calculation may be of fairly general interest, we present it in some detail in the following sections.

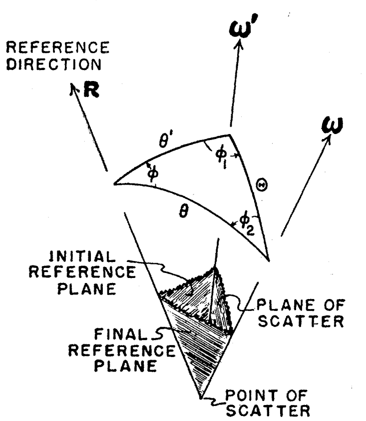

FIG. 1. The geometry of a Compton scattering. A photon traveling initially in the direction $\boldsymbol{\omega}'$ is scattered into a new direction $\boldsymbol{\omega}$. The plane of scatter includes the two photon directions, and the initial and final reference planes relate $\boldsymbol{\omega}'$, $\boldsymbol{\omega}$ to a reference direction **R**.

II. THE DIFFUSION EQUATION

A beam of partially polarized radiation can be completely described by the four parameters of Stokes:[4, 5] I^0, I^1, I^2, and I^3, where I^0 refers to the intensity of the beam, I^1 and I^2 together describe the degree and direction of plane polarization, and I^3 represents the degree of circular polarization. We need not consider circular polarization because it does not affect the penetration of x-rays unless the electrons in the medium are spin polarized.

In order to write down the Boltzmann equation in terms of Stokes parameters we need to know how the Stokes parameters transform if their reference plane is rotated.[6] To determine this we consider a partially polarized beam of photons which passes through a "polarization analyzer." Since the measurement of the analyzer is independent of our description of the beam, the Stokes parameters relating to reference planes inclined to the plane of the analyzer by angles α_1 and α_2 must satisfy the relation[4]

$$I_1^0+I_1^1\cos 2\alpha_1+I_1^2\sin 2\alpha_1 = I_2^0+I_2^1\cos 2\alpha_2+I_2^2\sin 2\alpha_2, \quad (1)$$

where the subscripts on the I's refer to the reference plane. If the angle between the reference planes is Φ, i.e., $\alpha_1+\Phi=\alpha_2$, the I_2's can be obtained from the I_1's by the operation

$$\begin{pmatrix} I_2^0 \\ I_2^1 \\ I_2^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 2\Phi & -\sin 2\Phi \\ 0 & \sin 2\Phi & \cos 2\Phi \end{pmatrix} \cdot \begin{pmatrix} I_1^0 \\ I_1^1 \\ I_1^2 \end{pmatrix}. \quad (2)$$

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[2] G. H. Peebles, Rand Corporation Report RM-653, Part 1, 1951; Part 2, 1952 (unpublished).
[3] L. V. Spencer, National Bureau of Standards Interim Report on Contract with the U. S. Office of Naval Research, 1948 (unpublished).
[4] U. Fano, J. Opt. Soc. Am. **39**, 859 (1949).
[5] S. Chandrasekhar, *Radiative Transfer* (University Press, Oxford, 1950), Chap. I.
[6] The Stokes parameters are defined operationally by means of measurements made with a "polarization analyzer." These measurements are made with the plane of the analyzer inclined several different angles to a so-called arbitrary "reference plane."

If the Stokes parameters of incident and scattered radiation are referred to the plane of scatter,[7] the Klein-Nishina cross section can be expressed as a matrix which relates the parameters of the scattered radiation to the parameters of the incident radiation:[4]

$$\frac{3}{8}\frac{\lambda'}{\lambda}\mu_{\mathrm{Th}}\begin{pmatrix} 1+\cos^2\Xi+\left(\frac{1}{\lambda'}-\frac{1}{\lambda}\right)(1-\cos\Xi) & -\sin^2\Xi & 0 \\ -\sin^2\Xi & 1+\cos^2\Xi & 0 \\ 0 & 0 & 2\cos\Xi \end{pmatrix} = \frac{3}{8}\frac{\lambda'}{\lambda}\mu_{\mathrm{Th}}\begin{pmatrix} k_{00}(\lambda',\lambda) & k_{01}(\lambda',\lambda) & 0 \\ k_{10}(\lambda',\lambda) & k_{11}(\lambda',\lambda) & 0 \\ 0 & 0 & k_{22}(\lambda',\lambda) \end{pmatrix}, \quad (3)$$

where λ', λ are the wavelengths in Compton units of the incident and scattered radiation respectively, $\cos\Xi$ is $(1-\lambda+\lambda')$ and must, according to the Compton condition, equal $\cos\Theta$ where Θ is the angle between incident and scattered directions, and μ_{Th} is the Thomson scattering cross section.

We now want to consider a beam of photons which is traveling in a direction $\boldsymbol{\omega}'$ and which is described by Stokes parameters relating to a plane defined by the direction $\boldsymbol{\omega}'$ and a reference direction $\mathbf{R}$. If these photons are scattered into a direction $\boldsymbol{\omega}$, we shall want the Stokes parameters of the scattered radiation related to the plane $(\boldsymbol{\omega}, \mathbf{R})$. To this end we rotate the reference plane of the original parameters through an angle ϕ_1 into coincidence with the plane of scatter (see Fig. 1), apply the Klein-Nishina scattering matrix (3), and finally rotate the plane of the scattered photons back to the new reference plane through an angle $(\phi_2+\pi)$. This sequence of operations is expressed in the following manner:

$$\begin{pmatrix} I_2^0 \\ I_2' \\ I_2^2 \end{pmatrix} = \frac{3}{8}\frac{\lambda'}{\lambda}\mu_{\mathrm{Th}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 2(\phi_2+\pi) & -\sin 2(\phi_2+\pi) \\ 0 & \sin 2(\phi_2+\pi) & \cos 2(\phi_2+\pi) \end{pmatrix}\cdot\begin{pmatrix} k_{00}(\lambda',\lambda) & k_{01}(\lambda',\lambda) & 0 \\ k_{10}(\lambda',\lambda) & k_{11}(\lambda',\lambda) & 0 \\ 0 & 0 & k_{22}(\lambda',\lambda) \end{pmatrix}$$
$$\cdot\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 2\phi_1 & -\sin 2\phi_1 \\ 0 & \sin 2\phi_1 & \cos 2\phi_1 \end{pmatrix}\cdot\begin{pmatrix} I_1^0 \\ I_1^1 \\ I_1^2 \end{pmatrix}. \quad (4)$$

If we define

$$\mathbf{I} \equiv \begin{pmatrix} I^0 \\ I^1 \\ I^2 \end{pmatrix},$$

and if we perform the multiplications, we may write this relation in the form $\mathbf{I}_2 = \mathbf{S}\cdot\mathbf{I}_1$, where

$$\mathbf{S} = \frac{3}{8}\frac{\lambda'}{\lambda}\mu_{\mathrm{Th}}\begin{pmatrix} k_{00} & k_{01}\cos 2\phi_1 & -k_{01}\sin 2\phi_1 \\ k_{10}\cos 2\phi_2 & k_{11}\cos 2\phi_2\cos 2\phi_1 - k_{22}\sin 2\phi_2\sin 2\phi_1 & -k_{11}\cos 2\phi_2\sin 2\phi_1 - k_{22}\sin 2\phi_2\cos 2\phi_1 \\ k_{10}\sin 2\phi_2 & k_{11}\sin 2\phi_2\cos 2\phi_1 + k_{22}\cos 2\phi_2\sin 2\phi_1 & -k_{11}\sin 2\phi_2\sin 2\phi_1 + k_{22}\cos 2\phi_2\cos 2\phi_1 \end{pmatrix}. \quad (5)$$

With these definitions, the equation governing the propagation of radiation is the following:

$$\boldsymbol{\omega}\cdot\operatorname{grad}\mathbf{I}(\mathbf{r},\boldsymbol{\omega},\lambda) = -\mu(\lambda)\mathbf{I}(\mathbf{r},\boldsymbol{\omega},\lambda) + \int_0^\lambda d\lambda' \int_{4\pi} d\boldsymbol{\omega}'(1/2\pi)\delta(\boldsymbol{\omega}\cdot\boldsymbol{\omega}'-\cos\Xi)\mathbf{S}\cdot\mathbf{I}(\mathbf{r},\boldsymbol{\omega}',\lambda') + \text{source}, \quad (6)$$

where

$$\mathbf{I}(\mathbf{r},\boldsymbol{\omega},\lambda) = \begin{pmatrix} I^0(\mathbf{r},\boldsymbol{\omega},\lambda) \\ I^1(\mathbf{r},\boldsymbol{\omega},\lambda) \\ I^2(\mathbf{r},\boldsymbol{\omega},\lambda) \end{pmatrix}. \quad (7)$$

In these relations, $I^0(\mathbf{r},\boldsymbol{\omega},\lambda)$ is the spectral energy density of the x-rays,[1a] $\mathbf{r}$ is the position vector, $\mu(\lambda)$ is the total narrow beam attenuation coefficient, $\boldsymbol{\omega}, \boldsymbol{\omega}'$ are unit direction vectors, δ is the Dirac delta-function, and $\cos\Xi = (1-\lambda+\lambda')$.

[7] The plane of scatter is the plane which includes the photon directions before and after the scattering.

If we restrict ourselves to a point isotropic source, the only position parameter necessary is the distance of the photon from the source. If, further, we specify a monoenergetic source and choose as a reference direction $\mathbf{R}$ the line from the source to the position of the photon, Eq. (7) becomes[1]

$$\omega_r\frac{\partial\mathbf{I}(r,\omega_r,\lambda)}{\partial r}+\frac{(1-\omega_r^2)}{r}\frac{\partial\mathbf{I}(r,\omega_r,\lambda)}{\partial\omega_r}=-\mu(\lambda)\mathbf{I}(r,\omega_r,\lambda)+\int_{\lambda_0}^{\lambda}d\lambda'\int_{4\pi}d\omega'(1/2\pi)\delta(\cos\Theta-\cos\Xi)\mathbf{S}\cdot\mathbf{I}(r,\omega_r',\lambda')+\lambda_0\delta(\lambda-\lambda_0)\frac{\delta(r)}{4\pi r^2}\mathbf{1} \quad (8)$$

where

$$\mathbf{1}=\begin{pmatrix}1\\0\\0\end{pmatrix},$$

$r=|\mathbf{r}|$, $\omega_r=\boldsymbol{\omega}\cdot\mathbf{R}=\cos\vartheta$, $\omega_r'=\boldsymbol{\omega}'\cdot\mathbf{R}=\cos\vartheta'$, $\cos\Theta=\boldsymbol{\omega}\cdot\boldsymbol{\omega}'$, and λ_0 is the wavelength of the source radiation.

III. REDUCTION OF THE DIFFUSION EQUATION

We want to expand Eqs. (8) into spherical harmonics. In making this expansion, we find that each of the elements of $\mathbf{S}$ leads to integrals which are special cases of the quantity

$$D(m_1,m_2)=(1/2\pi)\int_0^{2\pi}d\phi e^{i(m_1\phi_1+m_2\phi_2)}\delta(\cos\Theta-\cos\Xi). \quad (9)$$

The evaluation of $D(m_1, m_2)$ can be accomplished by means of the symmetrical top wave functions $\psi(l, m_1, m_2)$.[8] These functions are especially adapted to this problem because they relate to the most general possible rotation of axes, involving all three Euler angles.

If we make use of the orthogonality property of these wave functions we may write

$$D(m_1,m_2)=(1/2\pi)\int_0^{2\pi}d\phi e^{i(m_1\phi_1+m_2\phi_2)}4\pi^2\sum_l\psi(l,m_1,m_2;0,\Xi,0)\psi(l,m_1,m_2;0,\Theta,0)$$
$$=e^{-im_2\pi}(1/2\pi)\int_0^{2\pi}d\phi 4\pi^2\sum_l\psi(l,m_1,m_2;0,\Xi,0)\psi(l,m_1,m_2;\phi_1,\Theta,\pi+\phi_2). \quad (10)$$

We now want to make use of an addition formula for the ψ's which relates to the fact (see Fig. 1) that a general rotation of axes involving:

(a) A rotation around one axis by an angle ϕ_1,
(b) A tipping of this axis by an angle Θ,
(c) Another rotation around the tipped axis by an angle $\pi+\phi_2$, which is the transformation to which $\psi(l, m_1, m_2; \phi_1, \Theta, \pi+\phi_2)$ corresponds, is identical to the following transformation:

(a) A tipping of the axis by an angle ϑ',
(b) A rotation around the tipped axis by an angle $(\pi-\phi)$,
(c) A further tipping of the axis by an angle ϑ.
(d) A rotation about this final axis by the angle π.

The addition formula relating to this identity is the following:

$$\psi(l,m_1,m_2;\phi_1,\Theta,\pi+\phi_2)=\sum_i\left(\frac{8\pi^2}{2l+1}\right)^{\frac{1}{2}}\psi(l,m_1,i;0,\vartheta',\pi-\phi)\psi(l,i,m_2;0,\vartheta,\pi). \quad (11)$$

[8] These (normalized) functions are given by the following formula (l, m_1, m_2 integers):

$$\psi(l,m_1,m_2;\phi_1,\Theta,\phi_2)=Ae^{i(m_1\phi_1+m_2\phi_2)}[\tfrac{1}{2}(1-\cos\Theta)]^{d/2}[\tfrac{1}{2}(1+\cos\Theta)]^{s/2}F[-p,(1+d+s+p);(1+d);\tfrac{1}{2}(1-\cos\Theta)],$$

where

$$A=\left\{\frac{2l+1}{8\pi^2}\frac{(d+s+p)!(d+p)!}{p!(d!)^2(s+p)!}\right\}^{\frac{1}{2}},$$
$$d=|m_1-m_2|,\quad s=|m_1+m_2|,\quad p=l-\tfrac{1}{2}(s+d).$$

We obtained this formula for the normalized functions from Ruark and Urey, *Atoms, Molecules, and Quanta*, p. 671 (McGraw-Hill Book Company, Inc., New York, 1930). The ψ's are also called the representations $\mathfrak{D}^{(l)}$ of the group of space rotations. We are very grateful to U. Fano for this method of evaluating $D(m_1, m_2)$.

If we substitute this into (10) and carry out the integration, we have the result:

$$D(m_1, m_2)=4\pi^2\sum_l\left(\frac{8\pi^2}{2l+1}\right)^{\frac{1}{2}}\psi(l, m_1, m_2; 0, \Xi, 0)\psi(l, m_1, 0; 0, \vartheta', 0)\psi(l, 0, m_2; 0, \vartheta, 0)$$

$$=4\pi^2\sum_l\left\{\frac{2l+1}{8\pi^2}\frac{(l-m_1)!(l-m_2)!}{(l+m_1)!(l+m_2)!}\right\}^{\frac{1}{2}}\psi(l, m_1, m_2; 0, \Xi, 0)P_l^{m_1}(\omega_r')P_l^{m_2}(\omega_r). \tag{12}$$

Notice that according to (12), $D(m_1, m_2)$ is real. The part of $D(m_1, m_2)$ which changes sign if the signs of both ϕ_1 and ϕ_2 are reversed vanishes with the integration over ϕ. Now, the elements of **S** are either even or odd with respect to a reversal of the sign of both ϕ_1 and ϕ_2. Since all elements lead to the integrals $D(m_1, m_2)$ (plus or minus the complex conjugate), those elements which are odd vanish when the integral over ϕ is performed. We may as well omit these odd elements and write

$$\mathbf{S}=\frac{3}{8}\frac{\lambda'}{\lambda}\mu_{\mathrm{Th}}\begin{pmatrix} k_{00} & k_{01}\cos 2\phi_1 & 0 \\ k_{10}\cos 2\phi_2 & k_{11}\cos 2\phi_2\cos 2\phi_1-k_{22}\sin 2\phi_2\sin 2\phi_1 & 0 \\ 0 & 0 & -k_{11}\sin 2\phi_2\sin 2\phi_1+k_{22}\cos 2\phi_2\cos 2\phi_1\end{pmatrix}. \tag{13}$$

It is apparent from (13) that the lower right corner element of **S** is isolated. This has the consequence that, if the source radiation is unpolarized, $I^2(r, \omega_r, \lambda)$ remains identically zero, since there is no means by which it can be generated. (This result can be readily obtained directly from symmetry considerations.)

If we define quantities I_{ln}^0, I_{ln}^1 by the relations

$$\begin{aligned} I_{ln}^0(\lambda)&=(n!)^{-1}\int_0^\infty dr(4\pi r^2)r^n\int_{4\pi}d\boldsymbol{\omega}(2\pi)^{-1}P_l(\omega_r)I^0(r, \omega_r, \lambda),\\ I_{ln}^1(\lambda)&=(n!)^{-1}\int_0^\infty dr(4\pi r^2)r^n\int_{4\pi}d\boldsymbol{\omega}(2\pi)^{-1}P_l^2(\omega_r)I'(r, \omega_r, \lambda),\end{aligned} \tag{14}$$

and if we expand (8) after the manner of reference 1, Eq. (23), we obtain the following interlinked system of equations:

$$\begin{aligned} -\frac{1}{n(2l+1)}&[(l+1)(n-l)I_{l+1,n-1}^0(\lambda)+l(l+n+1)I_{l-1,n-1}^0(\lambda)]=-\mu(\lambda)I_{ln}^0(\lambda)\\ &+\int_{\lambda_0}^{\lambda}d\lambda'\left\{k_{00}P_l(\cos\Xi)I_{ln}^0(\lambda')+k_{01}\frac{(l-2)!}{(l+2)!}P_l^2(\cos\Xi)I_{ln}^1(\lambda')\right\}+\delta(\lambda-\lambda_0)\delta_{n0}\delta_{l0},\\ -\frac{1}{n(2l+1)}&[(l-1)(n-l)I_{l+1,n-1}^1(\lambda)+(l+2)(l+n+1)I_{l-1,n-1}^1(\lambda)]=-\mu(\lambda)I_{ln}^1(\lambda)\\ &+\int_{\lambda_0}^{\lambda}d\lambda'\{k_{10}P_l^2(\cos\Xi)I_{ln}^0(\lambda')+\tfrac{1}{2}[k_{11}\{\psi(l,2,2)-\psi(l,2,-2)\}+k_{22}\{\psi(l,2,2)+\psi(l,2,-2)\}]I_{ln}^1(\lambda')\},\end{aligned} \tag{15}$$

where $k_{ij}=k_{ij}(\lambda', \lambda)$ and $\psi(l, 2, \pm 2)=\psi(l, 2, \pm 2; 0, \Xi, 0)$.

This double system of equations can best be interpreted with the aid of Fig. 2. If l is zero or one, I_{ln}^1 is identically zero. This is a consequence of (14) rather than (15). If l is equal to n, the interlinkage terms $I_{l+1,n-1}^0$, $I_{l+1,n-1}^1$ in (15) are destroyed by the factor $(n-l)$. This means that the elements in Fig. 2 which are left of the diagonal are not linked to the elements which are to the right of the diagonal. The integral equations for I_{ln}^0, I_{ln}^1 must in general be solved simultaneously, since both quantities appear in both integral terms of (15). As in reference 1, by proceeding from small to large n it is possible to unravel the system (15) and solve for as many I_{ln}^0, I_{ln}^1 as desired, since the inhomogeneous terms in the equations for $I_{l,n+1}^0$, $I_{l,n+1}^1$ involve only quantities which have already been determined at an earlier stage of calculation.

IV. CALCULATIONS

For purposes of comparison, two calculations were performed by identical methods. In the first (polariza-

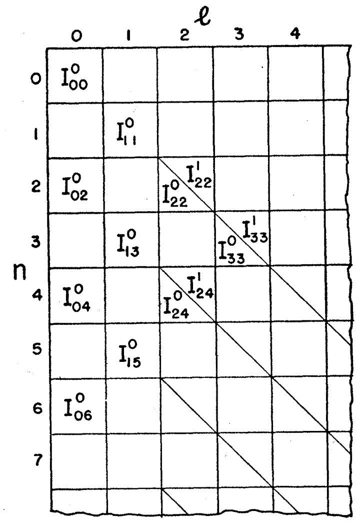

FIG. 2. A diagram showing the quantities determined in the polarization calculation. Two quantities within the same square must be solved for simultaneously. The solution starts in the upper left corner and proceeds down and to the right.

tion included) calculation, a number of Eqs. (15) were solved numerically. In the second (polarization neglected), the corresponding equations of reference 1 were used. (These are the equations obtained by arbitrarily setting all I_{ln}^1 equal to zero.)

The position variable was taken to be the dimensionless quantity $(\mu_0 r)$, μ_0 being the total attenuation coefficient of the source radiation. The source energy was chosen to be 1.277 Mev and the scattering medium was water. The solution was not carried out directly for the space moments $I_{ln}^{0,1}$, but rather for the coefficients of the $U_n^l(\mu_0 r)$ polynomials,[1,9] which are small differences between the $I_{ln}^{0,1}$ moments.

The integration was performed in accordance with Stirling's formula, with an adjustment for situations involving an odd number of integration steps. No integrations were performed for photon energies below 116 kev. The quantities determined correspond with those listed explicitly in Fig. 2, i.e., the coefficients of the first four $U_n^0(\mu_0 r)$ polynomials in the polynomial expansion of the spectral energy density. A considerable simplification in the integration results from the fact that $k_{01}(\lambda,\lambda)=k_{10}(\lambda,\lambda)=0$. Because of this the simultaneous solution of the equations for I_{ln}^0, I_{ln}^1 does not involve awkward algebraic difficulties.

V. RESULTS

The results of these calculations are summarized in Fig. 3, in which is plotted the percentage increase in

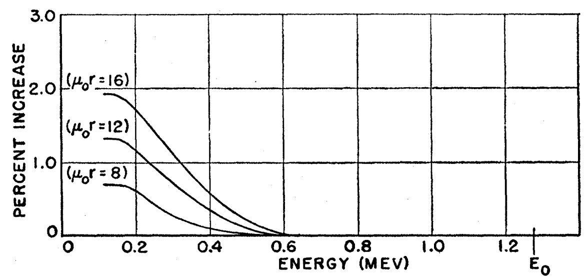

FIG. 3. The percentage increase in the spectral energy density due to polarization. The source energy is $E_0=1.277$ Mev. The leveling off at low energies relates to the fact that photon directional distributions become isotropic at low energies.

the spectral energy density at a given depth resulting from polarization. The effect is small (~1 percent) and positive, as expected. It disappears at high energies. At low energies it is constant because the angular distributions are isotropic. One characteristic which does not appear in Fig. 3 is an approach to an equilibrium (maximum) effect as r increases. It is difficult to predict the penetration at which this maximum effect will be reached, and it is perhaps not surprising that Fig. 3 does not show it.

[9] L. V. Spencer and F. Stinson, Phys. Rev. 85, 662 (1952).