Relationship of the relativistic Compton cross section to the momentum distribution of bound electron states. II. Effects of anisotropy and polarization

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An approximate relativistic treatment of the differential cross section for Compton scattering from bound electron states is discussed. A simple relationship between the Compton profile and the differential cross section, valid for anisotropic momentum distributions and arbitrary scattering angles, is found. We also derive a differential-cross-section formula for Compton-scattered polarized photons.

I. INTRODUCTION

During the last years we have seen an increasing interest in the study of inelastically scattered photons.[1,2] The Compton-scattered radiation may give information about the electronic structure of atoms, molecules, and solids. The reason for this is that in the so-called impulse approximation[1,3] the differential cross section is (in the nonrelativistic region) simply proportional to the Compton profile!

$$J(p_z)=\iint dp_x dp_y \rho(\vec{p}) \; . \tag{1}$$

Here, $\rho(\vec{p})$ is the momentum distribution of the electron system before scattering, and p_z is the component of electron momentum along the scattering vector. We have recently shown[4] that the conventional concept of a Compton profile also survives when we use high-energy γ rays, because they force us to take relativistic effects into consideration. We have formulated a simple relationship between the differential cross section and the Compton profile valid for all scattering angles, but restricted to isotropic momentum distributions $\rho(\vec{p})$. Here we will show that a similar relation also can be obtained for *anisotropic* momentum distributions.

As mentioned above, the Compton-scattering technique gives information on the momentum distribution and the electronic structure of the scatterer. As recognized fairly recently, however, the experimental data must be corrected for effects of multiple scattering. Such studies, based on the Monte Carlo technique and the Klein-Nishina formula, have been published by Felsteiner and co-workers.[5] Since the Klein-Nishina formula refers to initial electrons at rest, we will derive here a differential cross section for the general case when both the initial and final photons are polarized. This formula describes the scattering of photons against a nonstationary electron system better than the Klein-Nishina formula. For materials of low atomic number, the multiple scattering contributes about 10% of the total scattering.[5] It is therefore necessary to use an accurate model for the polarization dependence, if one wants to estimate the effect of multiple scattering in a particular Compton experiment.

In Sec. II a relativistic cross section for anisotropic systems is derived. Section III contains a description of a relation between the differential cross section in Sec. II and the Compton profile. The problem of Compton-scattered polarized photons is discussed in Sec. IV. Section V contains a summary. In what follows we use natural units, i.e., $c=1$ and $\hbar=1$.

II. RELATIVISTIC DIFFERENTIAL CROSS SECTION FOR ANISOTROPIC SYSTEMS

Much of the physics and algebra we use in this section has already been described by other authors.[6,7] With the use of the coordinate system in Fig. 1 and a heuristic approach developed in detail elsewhere,[4,6,7] we obtain as a starting point the differential cross section

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{m r_0^2 \omega'}{2\omega[|\vec{k}-\vec{k}'|-(\omega-\omega')p_z'/m]} \times\int dp_x' dp_y' \rho(\vec{p})\overline{X}(K,K') \; , \tag{2}$$

where

$$p_z'=\frac{m(\omega-\omega')-\omega\omega'(1-\cos\theta)}{|\vec{k}-\vec{k}'|} \; , \tag{3}$$

$$\overline{X}(K,K')=K/K'+K'/K+2m^2(1/K-1/K') +m^4(1/K-1/K')^2 \; , \tag{4}$$

$$K=\omega(m-p\cos\alpha) \; , \tag{5}$$

$$K'=K-\omega\omega'(1-\cos\theta) \; . \tag{6}$$

In these equations we have made the assumption that $E\simeq m$. We want to develop Eq. (2) without making approximations for the $\overline{X}$ factor, Eq. (4). We have shown[4] that the second term in the parentheses of Eq. (5) can be written

$$p\cos\alpha=D(p_z')+H(p_x') \; , \tag{7}$$

where

$$D\equiv\frac{\omega-\omega'\cos\theta}{|\vec{k}-\vec{k}'|}\,p_z' \tag{8}$$

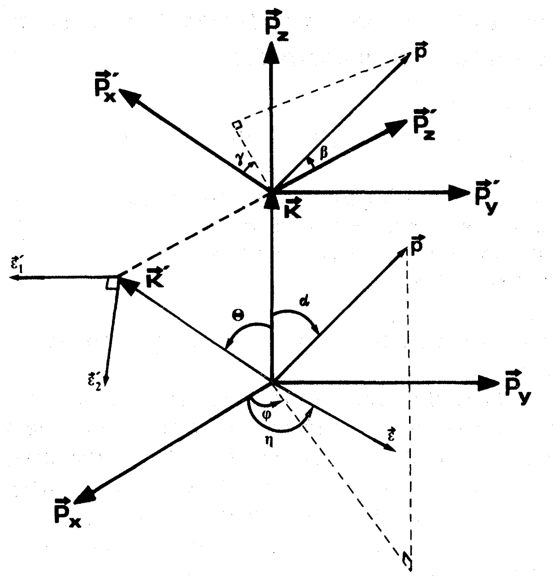

FIG. 1. Coordinate systems (p_x, p_y, p_z) and (p_x', p_y', p_z').

and

$$H \equiv \frac{\omega' \sin\theta}{|\vec{k}-\vec{k}'|} p_x' . \tag{9}$$

Equation (7) is the key to the solution of our problem because this yields for Eq. (4)

$$\bar{X}(K,K') = \bar{X}(p_x', p_z') . \tag{10}$$

It is easy to see that the integral in Eq. (2) can be written

$$\int_{-\infty}^{+\infty} dp_x' \bar{X}(p_x', p_z') R(p_x', p_z') , \tag{11}$$

where

$$R(p_x', p_z') \equiv \int_{-\infty}^{+\infty} \rho(p_x', p_y', p_z') dp_y' , \tag{12}$$

with $\rho(p_x', p_y', p_z')$ as the anisotropic momentum distribution for the electrons in the system considered. If we know the solution to Eq. (12), we can write down the differential cross section, Eq. (2), as a single integral,

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{m r_0^2 \omega'}{2\omega[|\vec{k}-\vec{k}'| - (\omega-\omega')p_z'/m]} \times \int_{-\infty}^{+\infty} dp_x' R(p_x', p_z') \bar{X}(p_x', p_z') . \tag{13}$$

This expression is useful if we want to calculate the differential cross section from a known momentum distribution, $\rho(p_x', p_y', p_z')$.

III. COMPTON PROFILE

The Compton profile in Eq. (1) can be written in the following way using Eq. (12):

$$J(p_z') = \int_{-\infty}^{+\infty} dp_x' R(p_x', p_z') . \tag{14}$$

We separate Eq. (14) into two parts

$$J(p_z') = J_-(p_z') + J_+(p_z') , \tag{15}$$

with

$$J_-(p_z') = \int_{-\infty}^{0} dp_x' R(p_x', p_z') \tag{16}$$

and

$$J_+(p_z') = \int_{0}^{\infty} dp_x' R(p_x', p_z') . \tag{17}$$

We also define the functions

$$J_-(p_x', p_z') = \int_{-\infty}^{p_x'} R(p_x, p_z') dp_x \tag{18}$$

and

$$J_+(p_x', p_z') = \int_{p_x'}^{\infty} R(p_x, p_z') dp_x . \tag{19}$$

A partial integration of Eq. (13) with use of Eqs. (15), (18), and (19) yields the result for the integral

$$\int_{-\infty}^{+\infty} R\bar{X} dp_x' = J(p_z')\bar{X}(0, p_z') + \int_0^{\infty} J_+(p_x', p_z') \frac{d\bar{X}}{dp_x'} dp_x' - \int_{-\infty}^{0} J_-(p_x', p_z') \frac{d\bar{X}}{dp_x'} dp_x' , \tag{20}$$

where

$$\bar{X}(0, p_z') \equiv \tilde{X} = R/R' + R'/R + 2m^2(1/R - 1/R') + m^4(1/R - 1/R')^2 , \tag{21}$$

$$R \equiv \omega[m - (\omega - \omega' \cos\theta) p_z' / |\vec{k}-\vec{k}'|] , \tag{22a}$$

$$R' \equiv R - \omega\omega'(1-\cos\theta) . \tag{22b}$$

This is exactly the same $\bar{X}$ factor as for an isotropic system.[4]

The last two terms in Eq. (20) are very small and we will estimate them. To do this we replace the anisotropic quantities, Eqs. (18) and (19), by their averaged functions

$$J_+'(p_x', p_z') = \langle J_+(p_x', p_z') \rangle = \int_{p_x'}^{\infty} R'(p_x, p_z') dp_x , \tag{23}$$

$$J_-'(p_x', p_z') = \langle J_-(p_x', p_z') \rangle = \int_{-\infty}^{p_x'} R'(p_x, p_z') dp_x , \tag{24}$$

$$R'(p_x, p_z) = \int_{-\infty}^{+\infty} \langle \rho(\vec{p}) \rangle dp_y . \tag{25}$$

The averaged anisotropic momentum distribution is written $\langle \rho(\vec{p}) \rangle$. Of course we can write

$$\langle\rho(\vec{p})\rangle=\rho'(|\vec{p}|)=\rho'(|p_x'|,\ |p_y'|,\ |p_z'|)\ . \qquad (26)$$

This symmetry relation gives us a connection between Eqs. (23) and (24)

$$J_-'(-p_x',p_z')=J_+'(p_x',p_z')\ , \qquad (27)$$

which is easily shown from the definitions. With the substitution $p_x'\to -p_x'$ in the last term of Eq. (20), the result of Eq. (13) is

$$\frac{d^2\sigma}{d\omega'\,d\Omega'}=\frac{mr_0^2\omega'}{2\omega[|\vec{k}-\vec{k}'|-(\omega-\omega')p_z'/m]}\left[\bar{X}J(p_z')+\int_0^\infty J_+'(p_x',p_z')\left(\frac{d\bar{X}(p_x')}{dp_x'}+\frac{d\bar{X}(-p_x')}{dp_x'}\right)dp_x'\right]\ . \qquad (28)$$

An explicit calculation of the derivatives of the $\bar{X}$ factor, Eq. (10), yields

$$\frac{d\bar{X}(p_x')}{dp_x'}+\frac{d\bar{X}(-p_x')}{dp_x'}=4p_x'\left(\frac{\omega'\sin\theta}{|\vec{k}-\vec{k}'|}\right)^2\left[F\left(\frac{m-D-W}{T^2}-\frac{m-D}{S^2}\right)+\frac{3m^4}{\omega^2}\left(\frac{(m-D)^2+2H^2}{S^3}+\frac{(m-D-W)^2+2H^2}{T^3}\right)\right], \qquad (29)$$

where

$$W\equiv\omega'(1-\cos\theta)\ , \qquad (30)$$

$$F\equiv W-2m^2/\omega-2m^4/(\omega^2W)\ , \qquad (31)$$

$$S\equiv(m-D)^2-H^2\ , \qquad (32)$$

$$T\equiv(m-D-W)^2-H^2\ . \qquad (33)$$

D and H are defined by Eqs. (8) and (9). Because normally $(m-D)^2\gg H^2$ and $(m-D-W)^2\gg H^2$, we have good reasons to write

$$S\simeq(m-D)^2 \quad\text{and}\quad T\simeq(m-D-W)^2\ . \qquad (34)$$

This gives, for Eq. (29),

$$\frac{d\bar{X}(p_x')}{dp_x'}+\frac{d\bar{X}(-p_x')}{dp_x'}\simeq 4p_x'C\ , \qquad (35)$$

where

$$C\equiv\left(\frac{\omega'\sin\theta}{|\vec{k}-\vec{k}'|}\right)^2\left[F\left(\frac{1}{(m-D-W)^3}-\frac{1}{(m-D)^3}\right)+\frac{3m^4}{\omega^2}\left(\frac{1}{(m-D-W)^4}+\frac{1}{(m-D)^4}\right)\right]\ , \qquad (36)$$

with C independent of p_x'. The last term in the bracket of Eq. (28) is, with Eq. (35),

$$4C\int_0^\infty dp_x'\,p_x'J_+'(p_x',p_z')\ , \qquad (37)$$

or, with Eq. (23),

$$4C\int_0^\infty dp_x'\,p_x'\int_{p_x'}^\infty dp_x R'(p_x,p_z')\ , \qquad (38)$$

where the domain of integration is the shaded area in Fig. 2. We can easily see, from the figure, that we can write Eq. (38) in a second way,

$$4C\int_0^\infty R'(p_x,p_z')dp_x\int_0^{p_x}p_x'dp_x'$$

$$=2C\int_0^\infty p_x^2R'(p_x,p_z')dp_x\ . \qquad (39)$$

We now introduce spherical coordinates

$$p_x=p\sin\alpha\cos\phi\ ,$$

$$p_y=p\sin\alpha\sin\phi\ , \qquad (40)$$

$$p_z'=p\cos\alpha=\text{const}\ ,$$

and obtain after integration and the substitution $p_z'/\cos\alpha\to p$ for Eq. (39)

$$C\pi\int_{|p_z'|}^\infty p\rho'(p)(p^2-p_z'^2)dp\ . \qquad (41)$$

A simple partial integration yields for Eq. (41)

$$C\int_{|p_z'|}^\infty pJ'(p)dp\ , \qquad (42)$$

with

$$J'(p)\equiv\int_p^\infty 2\pi p'\langle\rho(\vec{p}')\rangle dp'=\langle J(p)\rangle\ , \qquad (43)$$

which is the definition of the isotropic Compton profile. The final result will be important for the anisotropic Compton profile [Eq. (28)]:

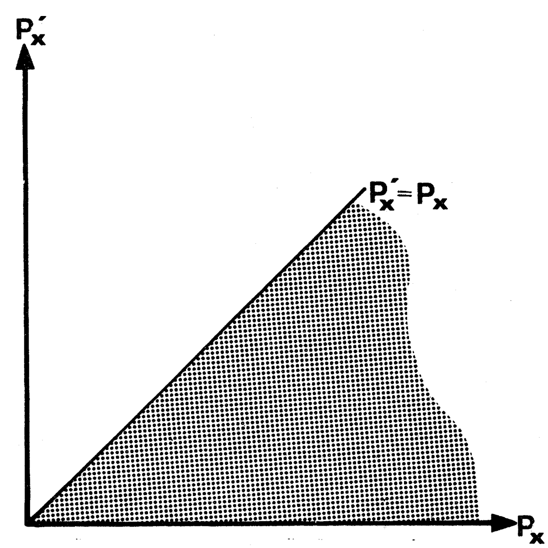

FIG. 2. Domain of integration in Eqs. (38) and (39).

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{m r_0^2 \omega'}{2\omega[|\vec{k}-\vec{k}'| - (\omega-\omega')p_z'/m]} \times \left(\tilde{X} J(p_z') + C \int_{|p_z'|}^{\infty} p \langle J(p) \rangle dp \right), \quad (44)$$

where the second term is very small compared to the first.[4] Equation (44) is powerful if we want to calculate the anisotropic Compton profile from experimental differential-cross-section data. We may observe that the second term in Eq. (44) can be used in an iterative way to get a better value of $J(p_z')$.[4] In most cases, however, we can neglect C in Eq. (44) in relation to the other term. One may mention the striking similarity between Eq. (44) and the cross-section formula developed for the isotropic case.[4] The functional forms and the constants are the same in the two expressions. Furthermore, it is interesting to note that Eq. (44) reduces to the formula used by Eisenberger and Reed[6] and Manninen *et al.*[7] if we put $\theta = 180°$.

IV. RELATIVISTIC DIFFERENTIAL CROSS SECTION FOR COMPTON–SCATTERED POLARIZED PHOTONS

A. Derivation

We use the vectors and designations given in Fig. 1. The X factor for polarized photons is given by Jauch and Rohrlich.[8]

$$X = \tfrac{1}{2}(K/K' + K'/K) - 1 + 2\left(\vec{\epsilon}\cdot\vec{\epsilon}' + \frac{\vec{\epsilon}\cdot\vec{p}\,\vec{\epsilon}'\cdot\vec{p}'}{K} - \frac{\vec{\epsilon}'\cdot\vec{p}\,\vec{\epsilon}\cdot\vec{p}'}{K'}\right)^2 \quad (45)$$

(K and K' are defined as before).

With the help of Fig. 1 we see that it is possible to express the different quantities in the (p_x, p_y, p_z) system.

$$\vec{\epsilon} = (\cos\eta, \sin\eta, 0)\,, \quad (46)$$

$$\vec{\epsilon}_1' = (0, -1, 0)\,, \quad (47)$$

$$\vec{\epsilon}_2' = (\cos\theta, 0, -\sin\theta)\,, \quad (48)$$

$$\vec{p} = p(\sin\alpha\cos\phi, \sin\alpha\sin\phi, \cos\alpha) = (Lp_x' - Np_z', p_y', Np_x' + Lp_z')\,, \quad (49)$$

$$N \equiv \omega' \sin\theta / |\vec{k} - \vec{k}'|\,, \quad (50)$$

$$L \equiv (\omega - \omega'\cos\theta)/|\vec{k} - \vec{k}'|\,, \quad (51)$$

$$\vec{k} = (0, 0, \omega)\,, \quad (52)$$

$$\vec{k}' = (\omega'\sin\theta, 0, \omega'\cos\theta)\,. \quad (53)$$

It is straightforward to express Eq. (45) with Eqs. (46)–(53). Because $X = X(p_x', p_y', p_z')$, we have to restrict ourselves to isotropic momentum distribution and write for the differential cross section[4] in the spherical system (p, β, γ):

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{m r_0^2 \omega'}{2\omega|\vec{k}-\vec{k}'|} \int dp\, d\gamma\, p\rho(p) X(p, \beta, \gamma)\,, \quad (54)$$

$$p\cos\beta = \frac{m(\omega - \omega') - \omega\omega'(1-\cos\theta)}{|\vec{k}-\vec{k}'|} = p_z'\,. \quad (55)$$

Because $p\cos\beta$ is constant, it is suitable to write

$$X(p_x', p_y', p_z') = X((p^2 - p_z'^2)^{1/2}\cos\gamma,\ (p^2 - p_z'^2)^{1/2}\sin\gamma,\ p_z')\,, \quad (56)$$

that is, we are able to write the integral in Eq. (54)

$$\int dp\, d\gamma\, p\,\rho(p) X(p, \beta, \gamma) = \int_{|p_z'|}^{\infty} dp\, p\,\rho(p) \int_0^{2\pi} d\gamma\, X(p, p_z', \gamma)\,. \quad (57)$$

It is possible to perform the angular integration, and we get integrals of the form

$$\int_0^{2\pi} \frac{\sin^k\gamma \cos^n\gamma}{(b - H\cos\gamma)^l} d\gamma\,, \qquad k = 0, 1\,, \quad n = 0, 1, 2, 3, 4\,, \quad l = 1, 2\,. \quad (58)$$

In this way we obtain

$$\int_0^{2\pi} d\gamma\, X(p, p_z', \gamma) \equiv 2\pi X_{\rm int}((p^2 - p_z'^2)^{1/2}, p_z')\,. \quad (59)$$

We are now able to integrate Eq. (54) partially and neglect the second small term[4]:

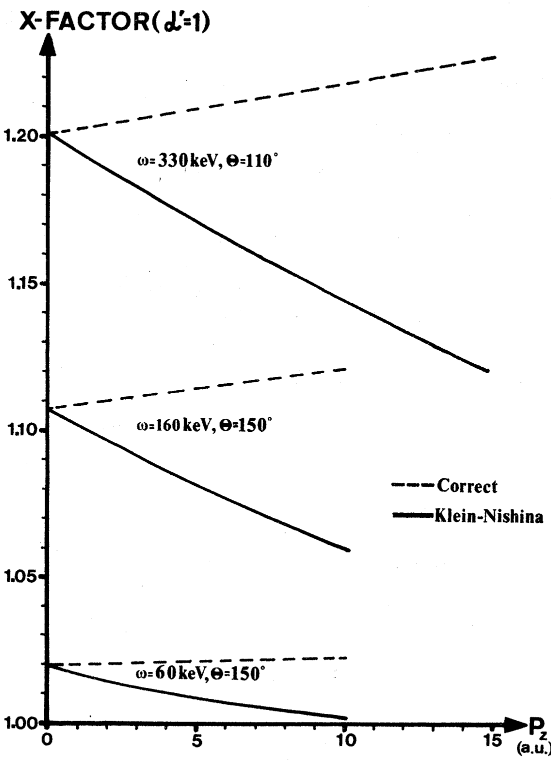

FIG. 3. Comparisons between X factors for $\vec{\epsilon}_1'$ given by Eqs. (65) and (66). Incoming radiation is unpolarized.

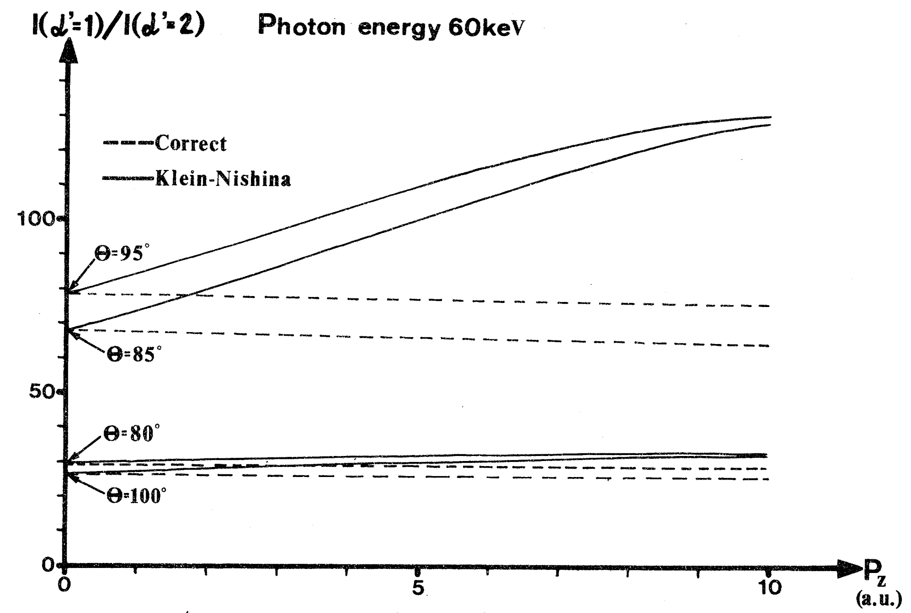

FIG. 4. Ratio X_1/X_2 given by Eqs. (65) and (66) for incoming unpolarized 60-keV radiation.

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{mr_0^2\omega'}{2\omega|\vec{k}-\vec{k}'|}\int_{|p_z'|}^{\infty} dp\, p\, \rho(p)\, 2\pi X_{\text{int}}$$

$$\simeq\frac{mr_0^2\omega'}{2\omega|\vec{k}-\vec{k}'|}\, J(|p_z'|)X_{\text{int}}(0,p_z') \; . \qquad (60)$$

We easily get expressions for $X_{\text{int}}(0, p_z')$, namely,

$$X_1=\tfrac{1}{2}(R/R+R'/R)-1+2\sin^2\eta \qquad \text{for } \vec{\epsilon}'=\vec{\epsilon}_1' \; , \qquad (61)$$

and

$$X_2=\tfrac{1}{2}(R/R'+R'/R)-1+2[\cos\theta + C(1/R-1/R')]^2\cos^2\eta \qquad \text{for } \vec{\epsilon}'=\vec{\epsilon}_2' \; , \qquad (62)$$

where

$$C\equiv\frac{\omega\omega' p_z'\sin^2\theta}{|\vec{k}-\vec{k}'|}\left(1+\frac{p_z'}{|\vec{k}-\vec{k}'|}\right) \; , \qquad (63)$$

R and R' are defined by Eqs. (22a) and (22b). One can show that

$$C\left(\frac{1}{R}-\frac{1}{R'}\right)\sim-\frac{\omega\omega' p_z'}{m^2|\vec{k}-\vec{k}'|} \times\left(1+\frac{p_z'}{|\vec{k}-\vec{k}'|}\right)\sin^2\theta(1-\cos\theta) \; , \qquad (64)$$

which is a very small quantity. We therefore have good reasons to neglect it and write, as a final result for Eqs. (61) and (62),

$$X=\frac{1}{2}\left(\frac{R}{R'}+\frac{R'}{R}\right)-1+2(\vec{\epsilon}\cdot\vec{\epsilon}')^2 \; . \qquad (65)$$

This is an important result because we can see how the polarization of the photon affects the differential cross section when we consider a bound-state system. Equation (65) reduces to the correct Klein-Nishina X factor when $p_z'\to 0$ (electron at rest):

$$X_{\text{Klein-Nishina}}=\frac{1}{2}\left(\frac{\omega}{\omega'}+\frac{\omega'}{\omega}\right)-1+2(\vec{\epsilon}\cdot\vec{\epsilon}')^2 \; . \qquad (66)$$

It is interesting to note that we obtain Eq. (65), even for an *anisotropic* system, if we neglect the very small $1/K$ and $1/K'$ terms in Eq. (45) and use the same arguments as in Sec. III.

If we average over the polarization of the incoming photon and sum over the two polarization states of the scattered photon, we obtain for Eq. (65)

$$\overline{X}=\frac{R}{R'}+\frac{R'}{R}-\sin^2\theta \; , \qquad (67)$$

which is very close to the correct $\overline{X}$ factor for unpolarized radiation given by Eq. (21).

B. Comparisons with Klein-Nishina

Because the Klein-Nishina X factor, Eq. (66), is used in many applications, for instance in multiple-scattering calculations, even when the target electron is nonstationary, it is interesting and necessary to study differences in the two expressions, Eqs. (65) and (66). Figure 3 shows the value of the X_1 factors if we consider $\vec{\epsilon}_1'$ and the incoming photon is unpolarized. The difference between the curves increases with increasing momentum of the electron and cannot be neglected. Figures 4–6 show the ratio X_1/X_2, which is also the ratio between the intensities of scattered radiation with polarization vectors $\vec{\epsilon}_1'$ and $\vec{\epsilon}_2'$, respectively. The deviations are especially significant for scattering angles close to 90°. The incoming unpolar-

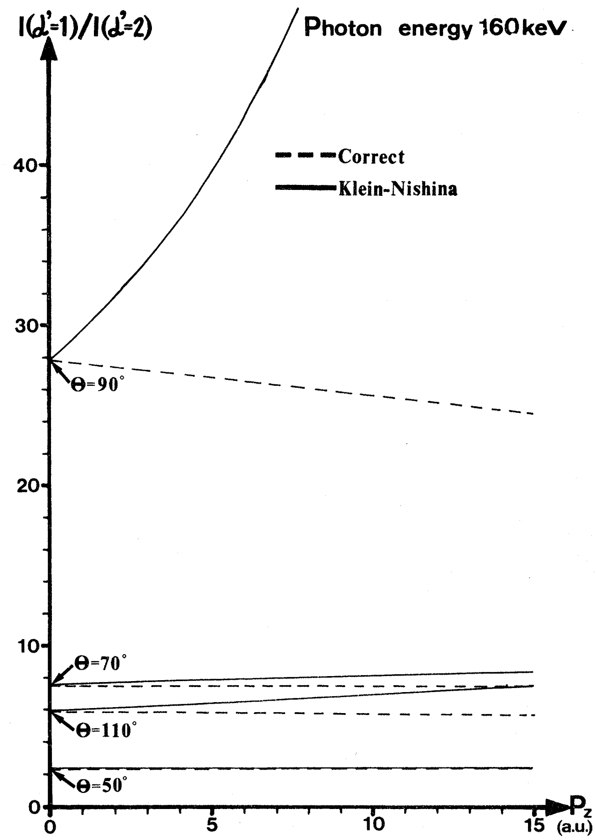

FIG. 5. Ratio X_1/X_2 given by Eqs. (65) and (66) for incoming unpolarized 160-keV radiation.

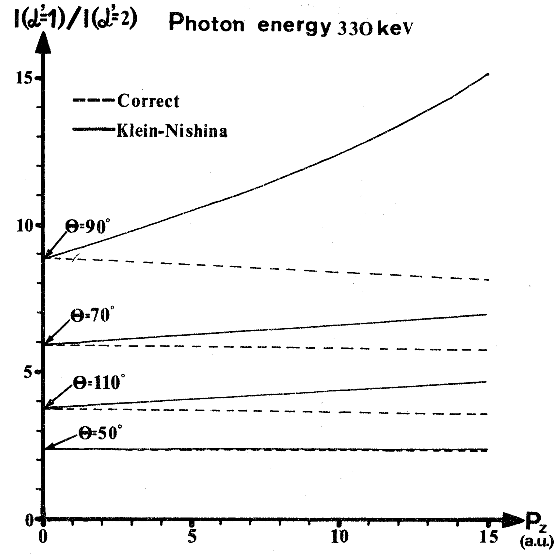

FIG. 6. Ratio X_1/X_2 given by Eqs. (65) and (66) for incoming unpolarized 330-keV radiation.

ized radiation will not be so strongly polarized as predicted by the Klein-Nishina formula if the target electron is in movement. The conclusion must be that Eq. (65) shall replace Eq. (66) when we handle systems with moving electrons.

V. SUMMARY

We have developed a useful method for calculating the anisotropic Compton profile from experimental differential-cross-section data. This method is not limited to scattering angles close to 180°. As a result, this allows us to analyze in a simple way Compton experiments with lower scattering angles also. This is advantageous because lower scattering angles result in decreasing backscattering effects from the chamber.

In our opinion there are good reasons to use the present theory, especially since it is not more difficult to handle than earlier ones. We have also shown that it is possible to replace the Klein-Nishina X factor, Eq. (66), by formulas, Eqs. (60) and (65), which describe the polarization dependence better, and therefore are useful for multiple scattering calculations.[5]

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[8]J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Addison-Wesley, Cambridge, Mass., 1955), pp. 163–169 and 228–235. A tedious calculation shows that the correct polarization-dependent X factor is given by Eq. (45) and not by Eq. (11-13) in p. 231. We are indebted to Professor F. Rohrlich for verifying the correctness of Eq. (45) (private communication).