Relationship of the relativistic Compton cross section to the momentum distribution of bound electron states

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An approximate relativistic treatment of the differential cross section for Compton scattering against bound electron states is discussed. A simple relationship between the cross section and the Compton profile is found. On contrast to previous work this relationship is valid for all scattering angles.

I. INTRODUCTION

Since its resurgence in the late 1960's, x- and γ-ray Compton scattering has promised to be a delicate probe of the electronic structure of atoms, molecules, and solids.[1,2] 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

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

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. The Compton profile in Eq. (1) is of central importance and represents the form in which experimentalists so far have chosen to present their results. Since $J(p_z)$ is directly related to $\rho(\vec{p})$, the Compton profile constitutes a sensitive test of the accuracy of various model wave functions.

In the impulse approximation it is assumed that the energy transfer is so large that binding effects for the electrons may be neglected and that the final state of the excited electron may be approximated by a plane-wave state. This means that the scattering process can be viewed as a photon being scattered inelastically against a stationary wave packet of superimposed plane-wave states. A scattering event then means that an electron in some initial plane-wave state $|\vec{p}\rangle$ is scattered into the final state $|\vec{p}\,'\rangle$. The probability of such an event is $\rho(\vec{p})$ times the square of the transition matrix element. Such a description applies to x-ray Compton scattering below roughly 15 keV. In this energy range, relativistic effects can be neglected. The use of x rays[1] has some disadvantages, however. The method is limited to only light elements to ensure the validity of the impulse approximation. Besides that, the intensity is low.

Experiments using γ rays[2] have the advantage that the energy transfer is large enough to allow for investigations of a wider class of materials. Typical γ-ray sources in use are ^{241}Am (59.54 keV) and ^{123}Te^m (159.0 keV), but sources with considerably higher energies are currently under consideration. A serious complication of the γ-ray technique is, however, that the energy transfers are so large that relativistic effects must be considered. Although the general principles for the calculation of the relativistic differential cross section for inelastic photon scattering against bound system are well known,[4] an actual evaluation is difficult owing to the complicated matrix elements and the large set of intermediate states to be summed over. This has been clearly demonstrated by Casimir,[5] who evaluated the cross section using plane-wave states for the intermediate states. Even at a scattering angle close to zero, as used by Casimir, such calculations are heroic. Eisenberger and Reed[6] and Manninen *et al.*[7] have therefore proposed an heuristic approach which in brief goes as follows. The cross section for colliding beams of electrons and photons is available in a closed analytical form.[4,8] If we neglect binding effects, as above, we may again consider the case of scattering against a stationary wave packet composed of plane-wave states (or a collection of electron beams), characterized by the probability function $\rho(\vec{p})$. With a properly revised flux factor, the desired relativistic differential cross section may then be written as an integral over each free-particle scattering event times the weight factor $\rho(\vec{p})$. The resulting form is, however, relatively complicated. Eisenberger and Reed[6] and Manninen *et al.*[7] have therefore discussed various simplifying assumptions. In particular, they have chosen the scattering angle θ to be 180°. This choice simplifies the algebra considerably and has the effect that certain factors may be taken outside the integration over $\vec{p}$ so that the conventional concept of a Compton profile survives also in a relativistic context. For $\theta \neq 180°$, however, it is still an open question whether the Compton profile is a well-defined concept or not. This problem seems relatively important since many experiments are performed at lower angles, typically $\simeq 150°$, in order to avoid backscattering from the chamber. By tradition, however, the experimental results are analyzed in the form of a Compton profile with the approximation $\theta = 180°$. Since experimentalists continue to report Compton profiles with increasing accuracy ($\le 1\%$), it seems to be an urgent problem to study the angular dependence of the relativistic differential cross section as well as the definition of the Compton profile itself. The purpose of the present work is to study these problems.

In Sec. II we review the heuristic approach of Eisenberger and Reed[6] and Manninen *et al.*[7] and discuss a convenient choice of coordinate system. In Sec. II an expression for the differential cross section is elaborated, and it is shown that the Compton profile can be defined at all angles θ. Section III also describes an iteration process for $J(p_z)$. In Sec. IV a comparison with previous relativistic treatments is given. Section V contains a summary. Mathematical details are given in Appendixes A and B.

II. RELATIVISTIC CROSS SECTION FOR ISOTROPIC SYSTEMS

A. General

In this section we will assume natural units, i.e., $c=1$ and $\hbar = 1$. We will start from an expression for the total relativistic cross section for scattering of a photon, which is in an initial state characterized by the four-vector $\kappa = (\vec{k}, i\omega)$. Here $\vec{k}$ stands for the wave vector and ω is the frequency of the photon. The target is a free electron characterized by $\pi = (\vec{p}, iE)$, where $\vec{p}$ is the momentum and E the total relativistic energy of the electron. After scattering, the electron is in the state $\pi' = (\vec{p}', iE')$ and the photon in $\kappa' = (\vec{k}', i\omega')$. Jauch and Rohrlich[8] give the following expression for the total relativistic cross section for the photon:

$$\sigma = m^2 r_0^2 \int d^3k'\, d^3p' \frac{1}{2KE'\omega'} \times X(K, K')\delta(\pi + \kappa - \pi' - \kappa') , \qquad (2)$$

where

$$K = E\omega - \vec{p}\cdot\vec{k} , \qquad (3)$$

$$K' = E\omega' - \vec{p}\cdot\vec{k}' = K + \kappa\kappa' = K - \omega\omega'(1-\cos\theta) , \qquad (4)$$

$$X(K, K') = \frac{K}{K'} + \frac{K'}{K} + 2m^2\left(\frac{1}{K} - \frac{1}{K'}\right) + m^4\left(\frac{1}{K} - \frac{1}{K'}\right)^2 , \qquad (5)$$

and

$$\delta(\pi + \kappa - \pi' - \kappa') \equiv \delta(\vec{p} + \vec{k} - \vec{p}' - \vec{k}')\delta(E + \omega - E' - \omega') . \qquad (6)$$

This formula thus refers to an experiment with colliding beams. The polarization of the photon is not observed in the initial or in the final state.

In the present case we are interested in the differential cross section for the scattering of photons against electrons in bound states, characterized by the momentum distribution $\rho(\vec{p})$. The target is at rest, i.e., $\langle \vec{p} \rangle = 0$. In the spirit of the impulse approximation, we may then from Eq. (2) write the differential cross section as

$$\frac{d^2\sigma}{d\omega'\, d\Omega'} = \frac{m^2 r_0^2}{2\omega} \int d^3p\, d^3p'\, \rho(\vec{p}) \frac{\omega'}{EE'} \overline{X}(K, K') \times \delta(\pi + \kappa - \pi' - \kappa') . \qquad (7)$$

To obtain Eq. (7) we have used $d^3k' = \omega'^2 d\omega'\, d\Omega'$, where $d\Omega'$ is the solid-angle element in the direction of $\vec{k}'$. We have also taken the derivative of σ with respect to ω' and Ω'. The flux factor $K/E\omega$ in Eq. (2) refers to colliding beams, and has therefore to be replaced here by one ($c=1$).[4] Integration over $\vec{p}'$ gives

$$\frac{d^2\sigma}{d\omega'\, d\Omega'} = \frac{m^2 r_0^2 \omega'}{2\omega} \int d^3p\, \rho(\vec{p}) \frac{\overline{X}(K, K')}{EE'} \times \delta(E + \omega - E' - \omega') . \qquad (8)$$

B. Choice of coordinate systems

It is convenient to introduce two coordinate systems (see Fig. 1). In the first system (x, y, z), the z axis has been chosen in the direction of $\vec{k}$. The angle between $\vec{p}$ and $\vec{k}$ is α and the azimuthal angle for $\vec{p}$ in the xy plane is ϕ. System (x', y', z') is obtained by rotating the system (x, y, z) around the y axis in such a way that z' coincides with $\vec{k} - \vec{k}'$. The vectors $\vec{k}'$ and $\vec{k}$ are in the xz plane, and the angle between them is θ. The vector $\vec{p}$ has components in the system (x', y', z') determined by the spherical angles β and γ. In the system (x', y', z'), the volume element for $\vec{p}$ can be written

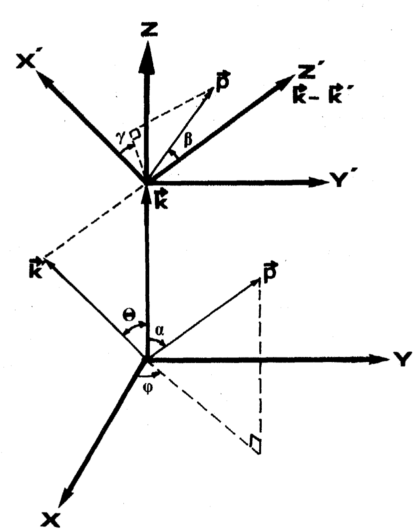

FIG. 1. Definition of the coordinate systems (x, y, z) and (x', y', z').

$$p \equiv |\vec{p}| , \tag{9}$$

$$d^3p = d\gamma \, d\beta \, dp \sin\beta \, p^2 . \tag{10}$$

We now evaluate the integral

$$\int \delta(E + \omega - E' - \omega') \sin\beta \, d\beta , \tag{11}$$

in which ω and ω' are to be held constant, and E is independent of $\cos\beta$ for constant p. We can therefore write

$$\int \delta(E + \omega - E' - \omega') \sin\beta \, d\beta$$

$$= -\int \delta(E + \omega - E' - \omega') \, d(\cos\beta)$$

$$= |\delta E'/\delta(\cos\beta)|^{-1} . \tag{12}$$

Since

$$E' = (|\vec{p}'|^2 + m^2)^{1/2} = (|\vec{p} + \vec{k} - \vec{k}'|^2 + m^2)^{1/2}$$
$$= (E^2 + |\vec{k} - \vec{k}'|^2 + 2|\vec{p}|\,|\vec{k} - \vec{k}'| \cos\beta)^{1/2} , \tag{13}$$

the result is

$$\int \delta(E + \omega - E' - \omega') \sin\beta \, d\beta$$

$$= \left(\frac{E'}{p|\vec{k} - \vec{k}'|} \right)_{E' + \omega' = E + \omega} . \tag{14}$$

From Eqs. (8) and (14), we then have

$$\frac{d^2\sigma}{d\omega' \, d\Omega'} = \frac{m^2 r_0^2 \omega'}{2|\vec{k} - \vec{k}'|\omega} \int dp \, d\gamma \, p\rho(\vec{p}) \frac{\overline{X}}{E(p)} . \tag{15}$$

The value of p in this expression follows from conservation of momentum and energy,

$$p = \frac{E(\omega - \omega') - \omega\omega'(1 - \cos\theta)}{|\vec{k} - \vec{k}'| \cos\beta} . \tag{16}$$

The expression for the differential cross section in Eq. (15) is valid for any type of momentum distribution $\rho(\vec{p})$. Here we shall restrict ourselves, however, to isotropic distributions. This restriction will allow the integration over γ to be done analytically.

The $\overline{X}$ factor in Eq. (15) is a function of $p \cos\alpha$ because

$$K = \omega(E - p\cos\alpha) \quad \text{and} \quad K' = K - \omega\omega'(1 - \cos\theta) . \tag{17}$$

Since $\rho(\vec{p})$ is independent of γ, we are now able to perform the integration over γ if only the transformation of $p\cos\alpha$ from (x, y, z) to (x', y', z') is known.

We write $\vec{p}$ in the two systems as

$$\vec{p} = |\vec{p}| (\sin\alpha \cos\phi \, \hat{x} + \sin\alpha \sin\phi \, \hat{y} + \cos\alpha \, \hat{z}) , \tag{18}$$

$$\vec{p} = |\vec{p}| (\sin\beta \cos\gamma \, \hat{x}' + \sin\beta \sin\gamma \, \hat{y}' + \cos\beta \, \hat{z}') , \tag{19}$$

where $(\hat{x}, \hat{y}, \hat{z})$ and $(\hat{x}', \hat{y}', \hat{z}')$ are unit vectors. From Fig. 1 it follows that

$$\hat{z}' = (\vec{k} - \vec{k}')/|\vec{k} - \vec{k}'| , \tag{20}$$

$$\hat{y}' = \hat{y} , \tag{21}$$

$$\vec{k} = \omega\hat{z} , \tag{21a}$$

$$\vec{k}' = \omega' \cos\theta \, \hat{z} + \omega' \sin\theta \, \hat{x} . \tag{21b}$$

Insertion of Eqs. (21a) and (21b) into Eq. (20) gives

$$\hat{z}' = [(\omega - \omega' \cos\theta)\hat{z} - \omega' \sin\theta \, \hat{x}]/|\vec{k} - \vec{k}'| . \tag{22}$$

Equations (21) and (22) combine to yield

$$\hat{x}' = \hat{y}' \times \hat{z}' = [(\omega - \omega' \cos\theta)\hat{x} + \omega' \sin\theta \, \hat{z}]/|\vec{k} - \vec{k}'| . \tag{23}$$

If Eqs. (21), (22), and (23) are inserted into Eq. (19) and the z components in Eqs. (18) and (19) are compared, one finds

$$p\cos\alpha = p\sin\beta \cos\gamma \frac{\omega' \sin\theta}{|\vec{k} - \vec{k}'|} + \frac{p\cos\beta(\omega - \omega' \cos\theta)}{|\vec{k} - \vec{k}'|} . \tag{24}$$

Define the quantities

$$D \equiv (\omega - \omega' \cos\theta)(p\cos\beta)/|\vec{k} - \vec{k}'| \tag{25}$$

and

$$H \equiv (\omega' \sin\theta \, p\sin\beta)/|\vec{k} - \vec{k}'| . \tag{26}$$

With these notations, Eq. (24) reads

$$p\cos\alpha = D(p) + H(p)\cos\gamma . \tag{27}$$

This is a useful result, and we will return to it in the following sections. Of course, $\sin\beta$ and $\cos\beta$ are functions of p [cf. Eq. (16)].

By means of Eq. (17), we can write Eqs. (3) and (4) as

$$K = \omega(E - D - H\cos\gamma) , \tag{28}$$

$$K' = \omega[E - D - H\cos\gamma - \omega'(1 - \cos\theta)] . \tag{29}$$

With the abbreviations

$$W \equiv \omega'(1 - \cos\theta) \tag{30}$$

and

$$f(\gamma) = D(p) + H(p)\cos\gamma , \tag{31}$$

one obtains

$$\overline{X} = 2 + F\left(\frac{1}{E - W - f} - \frac{1}{E - f} \right) + \frac{m^4}{\omega^2} \left(\frac{1}{(E - f)^2} + \frac{1}{(E - W - f)^2} \right) , \tag{32}$$

where

$$F \equiv W - 2m^2/\omega - 2m^4/\omega^2 W . \tag{33}$$

K and K' can be expressed as

$$C(E - p\cos\epsilon) = Cp(E/p - \cos\epsilon) , \tag{34}$$

where $E/p = (1 + m^2/p^2)^{1/2} > 1$, and C is a constant. Because of this, K and K' have no real roots. Hence, the integration of $\overline{X}$ over γ can be performed without restrictions as

$$\int_0^{2\pi} \overline{X}(D+H\cos\gamma)\,d\gamma = \int_0^{\pi} [\overline{X}(D+H\cos\gamma)+\overline{X}(D-H\cos\gamma)]\,d\gamma \,. \quad (35)$$

These integrals are elementary, and the result is

$$\int_0^{2\pi} \overline{X}\,d\gamma = 2\pi \overline{X}_{\rm int} \,, \quad (36)$$

with

$$\overline{X}_{\rm int} \equiv 2 + F\left(\frac{1}{[(E-W-D)^2-H^2]^{1/2}} - \frac{1}{[(E-D)^2-H^2]^{1/2}}\right) + \frac{m^4}{\omega^2}\left(\frac{E-D}{[(E-D)^2-H^2]^{3/2}} + \frac{E-D-W}{[(E-D-W)^2-H^2]^{3/2}}\right), \quad (37)$$

and D, H, and F as defined in Eqs. (25), (26), and (33). The expression for the differential cross section is then

$$\frac{d^2\sigma}{d\omega'\,d\Omega'} = \frac{m^2 r_0^2 \omega' 2\pi}{2\omega|\vec{k}-\vec{k}'|}\int_{p_{\rm min}}^{\infty} \frac{p\rho(p)\overline{X}_{\rm int}}{E(p)}\,dp \,, \quad (38)$$

$$p_{\rm min} = \frac{|E(\omega-\omega')-\omega\omega'(1-\cos\theta)|}{|\vec{k}-\vec{k}'|}\,, \quad E=(p_{\rm min}^2+m^2)^{1/2} \,. \quad (39)$$

Expression (38) is of central importance in the present work. It allows us to calculate, within the framework of the impulse approximation, differential cross sections for arbitrary scattering angles θ for any given isotropic momentum distribution $\rho(p)$.

A good first approximation to $p_{\rm min}$ in Eqs. (38) and (39) is

$$p_{\rm min} = \frac{|m(\omega-\omega')-\omega\omega'(1-\cos\theta)|}{|\vec{k}-\vec{k}'|} = p_z \,. \quad (40)$$

An improved approximation may be obtained by combining Eqs. (39) and (40):

$$p_{\rm min} = p_z\left(1 \pm \frac{(\omega-\omega')p_z}{2m|\vec{k}-\vec{k}'|}\right) . \quad (41)$$

The minus sign refers to the high-energy side of the spectrum, or $m(\omega-\omega')-\omega\omega'(1-\cos\theta)<0$. The correction term in Eq. (41), however, is small in most cases.

For later use, we define

$$A(p) \equiv E(p)(\omega-\omega') - \omega\omega'(1-\cos\theta) \,, \quad (42)$$

and rewrite Eqs. (25), (26), and (39) as

$$p_{\rm min} = |A(p)|/|\vec{k}-\vec{k}'| \,, \quad (43)$$

$$D = (\omega - \omega'\cos\theta)A(p)/|\vec{k}-\vec{k}'|^2 \,, \quad (44)$$

$$H = (\omega'\sin\theta/|\vec{k}-\vec{k}'|)(p^2-p_{\rm min}^2)^{1/2} \,. \quad (45)$$

III. COMPTON PROFILE

As mentioned in the Introduction, the choice of a scattering angle θ of 180° has the effect that the Compton profile in Eq. (1) may be defined also when relativistic effects come into play.[6,7] We will here discuss whether this is also true for other values of θ. For reasons given in the Introduction, this question is important.

For an isotropic system, Eq. (1) may be written[1]

$$J(p_z) = \int_{p_z}^{\infty} 2\pi p\rho(p)\,dp \,. \quad (46)$$

$J(p_z)$ is a positive, monotonically decreasing function. Hence we can formally write the primitive function to $2\pi p\rho(p)$ as $-J(p)$, with $J(\infty)=0$. A simple partial integration of Eq. (38) yields

$$\frac{d^2\sigma}{d\omega'\,d\Omega'} = \frac{m^2 r_0^2\omega'}{2\omega|\vec{k}-\vec{k}'|}\left(-J(p)\frac{\overline{X}_{\rm int}}{E}\Bigg|_{p_{\rm min}}^{\infty} + \int_{p_{\rm min}}^{\infty}\frac{J(p)}{E}\frac{d\overline{X}_{\rm int}}{dp}\,dp - \int_{p_{\rm min}}^{\infty} J(p)\overline{X}_{\rm int}\frac{p}{E^3}\,dp\right). \quad (47)$$

The first term inside the large parentheses gives

$$J(p_{\rm min})\overline{X}_{\rm int}(p_{\rm min})/E(p_{\rm min}) \,, \quad (48)$$

because $J(\infty)=0$ and $\overline{X}_{\rm int}$ is limited. The second term has the character of a correction, and is small compared to the first term (see Appendix A). The third term can be neglected right off because it is of the order $1/m^3$. $\overline{X}_{\rm int}(p_{\rm min})$ can be simplified and rewritten

$$\tilde{X} \equiv X_{\rm int}(p_{\rm min}) = \frac{R}{R'} + \frac{R'}{R} + 2m^2\left(\frac{1}{R}-\frac{1}{R'}\right) + m^4\left(\frac{1}{R}-\frac{1}{R'}\right)^2 , \quad (49)$$

where

$$R \equiv \omega[E(p_{\rm min}) - D(p_{\rm min})] \,, \quad (50)$$

$$R' \equiv R - \omega\omega'(1-\cos\theta) \,. \quad (51)$$

With

$$S \equiv [(m-D)^2-H^2]^{1/2} \text{ and } T \equiv [(m-D-W)^2-H^2]^{1/2} \,,$$

we get

$$\frac{d\overline{X}_{\rm int}}{dp} = p\left(\frac{\omega'\sin\theta}{|\vec{k}-\vec{k}'|}\right)^2 \times\left[F\left(\frac{1}{T^3}-\frac{1}{S^3}\right) + \frac{3m^4}{\omega^2}\left(\frac{m-D}{S^5}+\frac{m-D-W}{T^5}\right)\right]. \quad (52)$$

Here we have $D \simeq$ const and $E \simeq m$. As a final result, we obtain

$$\frac{d^2\sigma}{d\omega'\,d\Omega'} = \frac{m^2 r_0^2\omega'}{2\omega|\vec{k}-\vec{k}'|}\left(J(p_{\rm min})\frac{\tilde{X}}{E(p_{\rm min})} + \int_{p_{\rm min}}^{\infty}\frac{J(p)}{E(p)}\frac{d\overline{X}_{\rm int}}{dp}\,dp\right) . \quad (53)$$

It is pleasing to note that Eq. (49) reduces exactly to the constant X factor used by Eisenberger and Reed[6] and Manninen *et al.*[7] if we put $\theta = 180°$. At the same time the second term in Eq. (53) vanishes,

TABLE I. Convergence of the Compton profile as described in text. The component p_z is given in natural units ($c=1$, $\hbar=1$); atomic units are obtained by multiplication with 137.04/510.98. The Compton profiles are given in units of keV^{-1}.

$J_0(P_z)$	$J_1(p_z)$	$J(p_z)$	ω' (keV)	p_z
(a)				
$\omega=160$ keV, $\theta=90°$, $Z=10$, $\omega'_{max}=157.8$ keV				
0.228 236-1	0.227 643-1	0.227 635-1	121.80	0.1563
0.168 135-1	0.167 650-1	0.167 648-1	125.55	12.2173
0.789 572-2	0.786 629-2	0.786 608-2	129.30	24.3100
0.314 100-2	0.312 507-2	0.312 468-2	133.05	36.1239
0.125 495-2	0.124 642-2	0.124 583-2	136.80	47.6618
(b)				
$\omega=160$ keV, $\theta=150°$, $Z=10$, $\omega'_{max}=149.0$ keV				
0.227 899-1	0.227 648-1	0.227 647-1	101.0	0.0283
0.208 948-1	0.208 711-1	0.208 708-1	103.0	6.3908
0.164 313-1	0.164 112-1	0.164 109-1	105.0	12.6590
0.115 286-1	0.115 127-1	0.115 124-1	107.0	18.8348
0.753 104-2	0.751 905-2	0.751 876-2	109.0	24.9203

and Eq. (53) reduces to the conventional expression.

Equation (53) is useful if we want to calculate the Compton profile from experimental cross-section data, because the second term is small (of the order p_z/m, as shown in Appendix A). We therefore have good reason to neglect it. Solving for $J(p_{min})$ gives

$$J_0(p_{min}) = \frac{2\omega|\vec{k}-\vec{k}'|E(p_{min})}{m^2 r_0^2 \omega' \bar{X}} \frac{d^2\sigma}{d\omega' d\Omega'} . \quad (54)$$

We observe that in this formula there are no restrictions on the scattering angle. If we want to calculate $J(p_{min})$ with greater accuracy than in Eq. (54), we can write Eq. (53) as

$$J(p_{min}) = J_0(p_{min}) - \frac{E(p_{min})}{\bar{X}} \int_{p_{min}}^{p_{max}} \frac{J_0(p)}{E(p)} \frac{d\bar{X}_{int}}{dp} dp , \quad (55)$$

with $J_0(p)$ as a first approximation [from, e.g., Eq. (54)]. Equation (55) is a diagonal-dominant system of equations, which rapidly converge to the correct values, $J(p_{min})$. In the next section we show how this iteration method works for a hydrogenlike system.

A. Iteration of the Compton profile

In order to test the convergency properties of Eq. (55), we consider the case of a hydrogenlike system. In this case the differential cross section in Eq. (38) can be worked out analytically (see Appendix B). We may say that this particular cross section simulates a set of experimental data, and defines a first estimate of the Compton profile, $J_0(p_z)$, in accordance with Eq. (54). Iteration by means of Eq. (55) should then yield the conventional profile for a $1s$ system,

$$J(p_z) = 8\epsilon^5/3\pi(\epsilon^2 + p_z^3)^3 \quad (56)$$

(ϵ is defined in Appendix B).

We have considered two cases: (a) $\omega=160$ keV, $\theta=90°$, and $Z=10$; (b) $\omega=160$ keV, $\theta=150°$, and $Z=10$. Table I shows the results for J_0, J_1 (after one iteration), and the correct J according to Eq. (56). Table I also shows that the convergence is rapid and that one iteration is sufficient; in treating experimental data, J_0 is probably accurate enough.

IV. COMPARISON BETWEEN THE CORRECT X FACTOR AND THE X FACTOR IN THE "180° APPROXIMATION"

As mentioned, the approximate methods of Eisenberger and Reed[6] and Manninen *et al.*[7] for calculating the Compton profile rely on a constant X factor calculated for $\theta=180°$. For the high-energy side we get $[X_{180°} \equiv X(\theta=180°)]$:

$$J_{180°}(p_z) = \frac{2\omega[|\vec{k}-\vec{k}'| + p_z(\omega-\omega')/m]E}{m^2 r_0^2 \omega' X_{180°}} \frac{d^2\sigma}{d\omega' d\Omega'} . \quad (57)$$

Until now, experimental profiles have been derived by means of Eq. (57) or slight variations thereof.

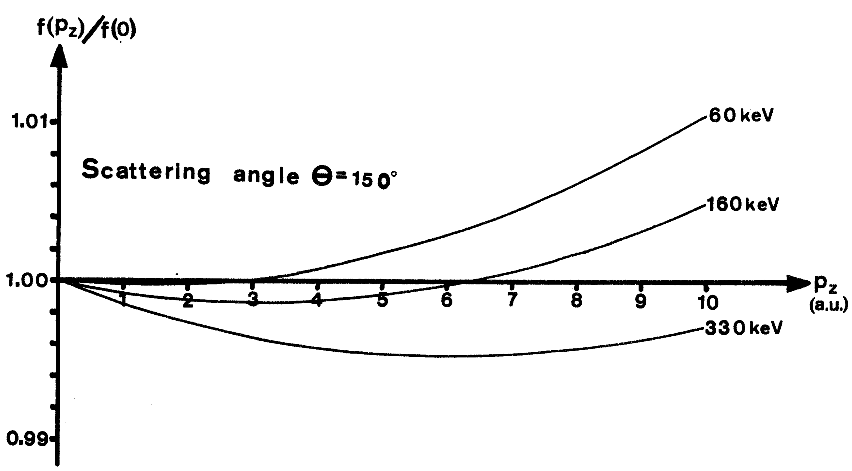

FIG. 2. Corrections to the Compton profile according to Eq. (58) and $\theta=150°$.

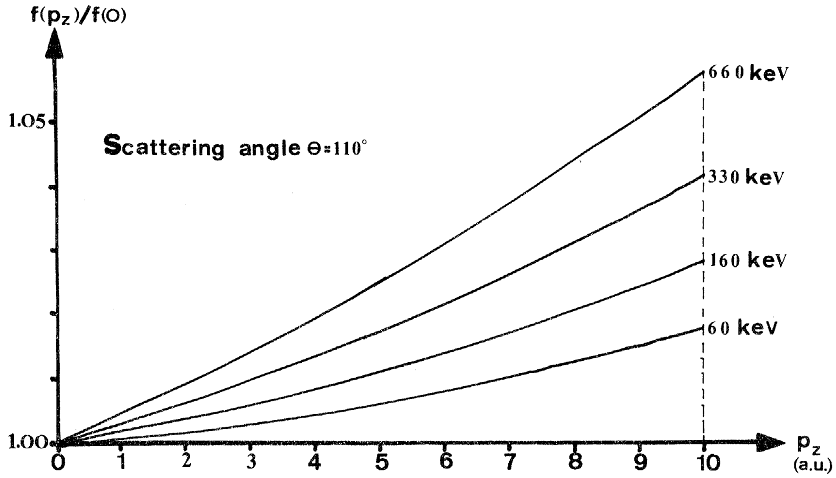

FIG. 3. Corrections to the Compton profile according to Eq. (58) and $\theta=110°$.

Obviously, this is permitted for θ not too far from 180° (e.g., in the experiments of Eisenberger and Reed, $\theta=173°$). For other cases, previously published profiles may be corrected approximately by multiplication with

$$f(p_z)=\frac{X_{180°}}{\tilde{X}[1+p_z(\omega-\omega')/m\,|\vec{k}-\vec{k}'|]}, \tag{58}$$

and then renormalized. Figures 2 and 3 show $f(p_z)/f(0)$ for two different scattering angles and different energies. The value of $f(0)$ varies strongly with θ and ω and thus with the value of the differential cross section itself. However, after renormalization of $f(p_z)$, deviations from the correct profile may not be large. For example, $\theta=150°$, $f(p_z)$ is almost constant, which results in a very small error in the normalized profile. For smaller angles corrections become increasingly important, as shown by Fig. 3.

V. SUMMARY

We have considered the differential cross section for Compton scattering against an isotropic momentum distribution. The heuristic approach of Eisenberger and Reed[6] and Manninen *et al.*[7] has been elaborated, and it has been found that the Compton profile is a well-defined concept at all scattering angles. To obtain a high accuracy in $J(p_z)$, a rapidly convergent iteration process is proposed. For most purposes, however, the zeroth-order estimate is accurate enough. Our new form for the differential cross section is as simple as those previously used, and should replace them. The present results can be extended to anisotropic Compton scattering, as well as to the polarization dependence of the differential cross section. This will be presented in a separate publication.

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APPENDIX A: CONTRIBUTION FROM THE SECOND TERM IN EQUATION (53)

The normalization of the Compton profile is usually chosen to be

$$\int_0^\infty dp_z\,J(p_z)=\frac{n}{2}, \tag{A1}$$

where n stands for the number of electrons in the atomic system. We define

$$N(p)=\int_p^\infty J(p_z)\,dp_z\,. \tag{A2}$$

With $E(p_{\min})\simeq m$, and $p_{\min}=p_z$, we get for Eq. (53)

$$\frac{d^2\sigma}{d\omega'\,d\Omega'}=\frac{mr_0^2\omega'}{2\omega\,|\vec{k}-\vec{k}'|}\left(\tilde{X}J(p_z)+\int_{p_z}^\infty J(p)\frac{d\overline{X}_{\rm int}}{dp}\,dp\right). \tag{A3}$$

Define

$$\mathrm{Rem}\equiv\int_{p_z}^\infty J(p)\frac{d\overline{X}_{\rm int}}{dp}\,dp\,, \tag{A4}$$

$$|\mathrm{Rem}|=\left|-N(p)\frac{d\overline{X}_{\rm int}}{dp}\right|_{p_z}^\infty+\int_{p_z}^\infty N(p)\frac{d^2\overline{X}_{\rm int}}{dp^2}\,dp\right|$$

$$=\left|N(p_z)\left(\frac{d\overline{X}_{\rm int}}{dp}\right)_{p_z}+N(\xi)\int_{p_z}^\infty\frac{d^2\overline{X}_{\rm int}}{dp^2}\,dp\right|,$$

$$p_z<\xi<\infty,\quad N(p_z)>N(\xi)>0\,; \tag{A5}$$

$$|\mathrm{Rem}|<N(p_z)\left|\frac{d\overline{X}_{\rm int}}{dp}\right|_{p=p_z}. \tag{A6}$$

From Eq. (52), we obtain

$$\left|\frac{d\overline{X}_{\rm int}}{dp}\right|_{p=p_z}=p_z\left(\frac{\omega'\sin\theta}{|\vec{k}-\vec{k}'|}\right)^2\left[F\left(\frac{1}{(m-W-D)^3}-\frac{1}{(m-D)^3}\right)\right.$$

$$+\frac{3m^4}{\omega^2}\left(\frac{1}{(m-D)^4}+\frac{1}{(m-D-W)^4}\right)\Bigg] . \quad \text{(A7)}$$

If this expression is expanded in powers of $1/(m-D)$, the dominating term in $|\text{Rem}|$ is

$$|\text{Rem}| \simeq 12N(p_z)\frac{p_z}{m}\left(\frac{\omega' \sin\theta}{|\vec{k}-\vec{k}'|}\right)^2 \frac{\omega'(1-\cos\theta)}{\omega^2} . \quad \text{(A8)}$$

We solve for $J(p_z)$ in Eq. (53):

$$J(p_z)=\frac{d^2\sigma}{d\omega'\,d\Omega'}\Bigg/\left(\frac{m r_0^2 \omega'}{2\omega|\vec{k}-\vec{k}'|}\tilde{X}\right) \pm \frac{|\text{Rem}|}{\tilde{X}} . \quad \text{(A9)}$$

If $|\text{Rem}|$ is neglected, there will be an error of the order

$$\Delta J(p_z) = \pm\,|\text{Rem}|/\tilde{X} . \quad \text{(A10)}$$

We now estimate $N(p_z)$ in Eq. (A8). A straight-line approximation of $J(p_z)$ is

$$J(p_z) \simeq n/p_{\max}(1-p_z/p_{\max}) , \quad \text{(A11)}$$

with $p_{\max}$ as the largest experimental value of p_z. Equation (A11) is normalized as

$$\int_0^{p_{\max}} J(p_z)\,dp_z = \frac{n}{2} . \quad \text{(A12)}$$

We get from Eqs. (A2) and (A11)

$$N(p_z)=\int_{p_z}^{p_{\max}} \frac{n}{p_{\max}}\left(1-\frac{p_z}{p_{\max}}\right)dp_z = \frac{n}{2}\left(1-\frac{p_z}{p_{\max}}\right)^2 . \quad \text{(A13)}$$

With $\tilde{X} \simeq 2$ the final estimate is

$$\Delta J(p_z) = \pm\, 6n\left(1-\frac{p_z}{p_{\max}}\right)^2 \frac{p_z}{m}\frac{\omega'^3}{\omega^2|\vec{k}-\vec{k}'|^2}\sin^2\theta\,\sin^2\frac{\theta}{2} . \quad \text{(A14)}$$

APPENDIX B: DIFFERENTIAL CROSS SECTION FOR A HYDROGENLIKE SYSTEM

The nonrelativistic wave function for a hydrogenlike system is

$$\psi_{1s} = (Z^3/\pi a^3)^{1/2} e^{-zr/a} , \quad \text{(B1)}$$

where Z is the atomic number and a the Bohr radius. [There is no restriction in choosing a nonrelativistic ground-state distribution in Eq. (7). In fact, the relativistic effects are, in the present context, mainly associated with the final states.]

We transform Eq. (B1) to $\vec{p}$ space as

$$\chi(\vec{p}) = \frac{1}{(2\pi)^{3/2}}\int d^3r\, e^{-i\vec{p}\cdot\vec{r}}\,\Psi(\vec{r}) . \quad \text{(B2)}$$

Then

$$\rho(p) = \frac{8\epsilon^5}{\pi^2}\frac{1}{(\epsilon^2+p^2)^4} , \quad \text{(B3)}$$

where $\epsilon = \alpha m Z$; α is the fine-structure constant. The distribution is isotropic, and we get from Eq. (38)

$$\frac{d^2\sigma}{d\omega'\,d\Omega'} = \frac{m r_0^2 \omega' 2\pi 8\epsilon^5}{2\omega|\vec{k}-\vec{k}'|\pi^2}\int_{p_z}^{\infty}\frac{\overline{X}_{\text{int}}\,p}{(\epsilon^2+p^2)^4}\,dp , \quad \text{(B4)}$$

where we have put $E(p)=m$ in the denominator. It is convenient, however, to keep the $E(p)$ dependence in $\overline{X}_{\text{int}}$ to avoid nonphysical singularities. Equation (B4) can be integrated by elementary methods.

With

$$T \equiv |\vec{k}-\vec{k}'|^2/(\omega'\sin\theta)^2 , \quad \text{(B5)}$$

$$U \equiv (\epsilon^2+p_z^2)/T , \quad \text{(B6)}$$

and F given by Eq. (33), we define the function

$$R_\pm(N) = \pm\frac{8\epsilon^5 F}{\pi T^3}\left(\frac{N}{6(U+N^2)U^3}+\frac{5}{24}\frac{N}{(U+N^2)^2U^2}+\frac{5N}{16(U+N^2)^3U}+\frac{5}{32(U+N^2)^{7/2}}\ln\left|\frac{(U+N^2)^{1/2}+N}{(U+N^2)^{1/2}-N}\right|\right)$$
$$+\frac{8\epsilon^5 m^4}{\pi T^3\omega^2}\left(\frac{11N^2}{24(U+N^2)^3U^2}+\frac{19N^2}{16(U+N^2)^4U}+\frac{N^2}{6(U+N^2)^2U^3}\right.$$
$$\left.-\frac{1}{(U+N^2)^4}+\frac{35N}{32(U+N^2)^{9/2}}\ln\left|\frac{(U+N^2)^{1/2}+N}{(U+N^2)^{1/2}-N}\right|\right) . \quad \text{(B7)}$$

The analytic expression for the differential cross section is then

$$\frac{d^2\sigma}{d\omega'\,d\Omega'} = \frac{m r_0^2\omega'}{|\vec{k}-\vec{k}'|\,\omega}\left[J(p_z)+R_+(m-D)+R_-(m-D-W)\right] . \quad \text{(B8)}$$

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