# Relativistic Compton cross section for general central-field Hartree-Fock wave functions

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This paper discusses a rigorous relativistic treatment of the differential cross section for Compton scattering from bound electron states in the impulse approximation. Starting with general relativistic central-field Hartree-Fock wave functions, a simple expression is found which is valid for all completely occupied shells. This expression is then compared with the more approximate expression developed by R. Ribberfors [Phys. Rev. B **12**, 2067 (1975)]. The Compton profile is a well-defined concept in nonrelativistic theory, but it is not categorically applicable in relativistic theory. Therefore this paper also discusses the circumstances in which the concept of a Compton profile is well defined also in a relativistic context.

## I. INTRODUCTION

Methods that give information about the electronic structure of atoms, molecules, and solids are of special interest. A method that offers a sensitive probe of electronic structures is Compton scattering.[1] The reason for this is, so far as nonrelativistic theory is concerned, that the differential cross section is simply proportional to the Compton profile[1,2]

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

Here, $\rho(\mathbf{p})$ is the momentum density of the electron system before scattering and $p_z$ is the component of the electron momentum along the scattering vector. This proportionality can be shown within the so-called impulse approximation.[1-3] The Compton profile $J(p_z)$ is of central importance because $J(p_z)$ is directly related to the momentum density $\rho(\mathbf{p})$, and consequently constitutes a good test of the accuracy of different wave-function models. Furthermore, $J(p_z)$ represents the form in which results of experiments often are presented.

In the impulse approximation it is assumed that the final-state wave function of the excited electron may be approximated by a plane-wave state. This approximation is justifiable when we also assume that the energy transfer to the electron is so large that binding effects are negligible. A very good approximation due to the plane-wave expansion of the initial wave function and the plane-wave approximation of the final state is obtained by letting the potential be canceled out of the energy for an electron in some initial plane-wave state $|\mathbf{p}\rangle$ and final state $|\mathbf{p}'\rangle$. This means that an electron in some of these initial plane-wave states $|\mathbf{p}\rangle$ is assumed to have the same potential as in the final state $|\mathbf{p}'\rangle$. This latter assumption is a central point in the impulse approximation.

A nonrelativistic description of Compton scattering can be applied to x rays below roughly 15 keV. In this energy range relativistic effects are negligible. However, $\gamma$ rays in current use have considerably higher energies than 15 keV. The advantage of using $\gamma$ rays is that the energy transfer to the electron is large enough to allow investigations of both heavy and light elements. Methods using x rays are disadvantageous in that attempts to ensure the validity of the impulse approximation are limited to the investigations of light elements.

A complication stemming from the $\gamma$-ray technique is the possibility of large energy transfers which require a relativistic treatment of the differential cross section. Calculation of the relativistic differential cross section for inelastic photon scattering against a bound-electron system follows general principles which are well known.[4] Even if approximations are made, such calculations would be a heroic undertaking. For this reason, Eisenberger and Reed[5] proposed a "heuristic" approach. Starting from the cross section for scattering of photons by free electrons, i.e., plane waves, available in a closed analytical form,[4,6] they introduced the relativistic momentum density $\rho(\mathbf{p})$ as follows. If the binding effects are ignored, the problem can be seen as that of scattering against a stationary wave packet composed of plane-wave states, and where $\rho(\mathbf{p})d^3p$ can be regarded as the probability for scattering by the plane-wave state $|\mathbf{p}\rangle$. The cross section may then be written as an integral over each plane-wave state times the weight factor $\rho(\mathbf{p})$. The cross section now will be different from the expression given by Jauch and Rohrlich,[6] by an integral over the momentum $\mathbf{p}$ of the momentum density $\rho(\mathbf{p})$ for the initial state times $\rho(\mathbf{p})$. The expressions also differ by a factor that arises from the choice of the flux factor. The choice of the flux factor in the expression of Eisenberger and Reed ($K/E\omega$ has been replaced by 1) is properly revised.[4] The resulting form, however, still is relatively complicated. Eisenberger and Reed therefore have chosen the scattering angle $\theta'$ to be 180°, which simplifies the algebra considerably. In particular, this choice has the effect that certain factors can be moved outside the integration over $\mathbf{p}$ so that the conventional concept of a Compton profile survives also in a relativistic context. However, in order to minimize backscattering from the chamber, experiments often are performed at lesser angles. Thus, the derivation of a more general expression, valid for $\theta'\neq 180°$, seems to be an important problem. This problem has also been solved.

 

The "heuristic" approach of Eisenberger and Reed has been elaborated by Ribberfors.[7] He made a successful choice of coordinate systems that solves many of the difficulties briefly mentioned above. After some algebra, an expression results for the differential cross section that is valid for all scattering angles. Using partial integration, this expression can be approximated to a quite simple form, and within this approximation the Compton profile is a well-defined concept for all scattering angles.[7] The resulting expression for the differential cross section and its approximated form, derived by Ribberfors, is discussed in more detail later.

The heuristic approach, proposed by Eisenberger and Reed, and elaborated by Ribberfors, gives results that agree very well with empirical results.[8] The purpose of the work presented in this paper is to verify this heuristic approach. Furthermore, to obtain the Compton profile, an approximation must be carried out. Therefore the concept of a Compton profile in a relativistic context is also discussed here. Since researchers now analyze empirical findings expressed as Compton profiles and continue to report Compton profiles with increasing accuracy, it seems important to study the following question: When is the Compton profile an applicable concept?

In Sec. II we review the differential cross section as defined by Ribberfors. In Sec. III we start with general relativistic central-field Hartree-Fock bound states to derive an expression for the differential cross section that is more general than those previously used. In Sec. IV our expression is compared to the Ribberfors expression for some scattering angles and energies of the incoming photon. In Sec. V we investigate at what point the definition of a Compton profile is significant in a relativistic context. Section VI contains a summary.

## II. RELATIVISTIC CROSS SECTION FOR ISOTROPIC SYSTEMS IN THE MOMENTUM-DENSITY APPROACH

Throughout this paper we use natural units, i.e., $c=1$ and $\hbar=1$. Compton scattering involves an incoming photon and an electron in the initial state, which we characterize by the four-vectors $\kappa=(\mathbf{k},i\omega)$ and $\pi=(\mathbf{p},iE)$, respectively. Here $\mathbf{k}$ stands for the wave vector or the momentum, and $\omega$ for the frequency or the energy of the photon. Furthermore, $\mathbf{p}$ is the momentum and $E$ the relativistic energy of a free electron. After scattering, we characterize these by $\kappa'=(\mathbf{k}',i\omega')$ and $\pi'=(\mathbf{p}',iE')$, respectively. These designations are used in the following descriptions. In Ref. 6 (Jauch and Rohrlich[6]) the following expression for the total relativistic cross section for scattering of photons against free electrons can be found:

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

where

$$K=-\pi\cdot\kappa=E\omega-\mathbf{p}\cdot\mathbf{k} , \quad (3)$$

$$K'=-\pi\cdot\kappa'=E\omega'-\mathbf{p}\cdot\mathbf{k}'=K-\omega\omega'(1-\cos\theta') , \quad (4)$$

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

$$E=(m^2+p^2)^{1/2} , \quad (6)$$

$$E'=(m^2+p'^2)^{1/2} , \quad (7)$$

and $\theta'$ stands for the scattering angle. This formula describes an experiment with colliding beams, where the polarization of the photons is not observed in either the initial or the final state.

The present paper's interest will focus on the differential cross section for the scattering of photons against bound electrons, characterized by the momentum density $\rho(\mathbf{p})$. Applying the heuristic approach of Eisenberger and Reed[5] to Eq. (2) the cross section can be written as

$$\sigma=m^2r_0^2\int d^3k'd^3p'd^3p\frac{\bar{X}(K,K')}{2EE'\omega\omega'}\rho(\mathbf{p})\delta(\mathbf{p}+\mathbf{k}-\mathbf{p}'-\mathbf{k}')\times\delta(E+\omega-E'-\omega') . \quad (8)$$

The flux factor $K/E\omega$ in Eq. (2) refers to colliding beams, and has therefore been replaced by 1.[4] Knowing that $d^3k'=\omega'^2d\omega'd\Omega'$, after an integration over $\mathbf{p}'$ we can write the differential cross section as

$$\frac{d^2\sigma}{d\omega'd\Omega'}=\frac{m^2r_0^2\omega'}{2\omega}\int d^3p\frac{\bar{X}(K,K')}{EE'}\times\rho(\mathbf{p})\delta(E+\omega-E'-\omega') . \quad (9)$$

Inside the integral in Eq. (9), the angle dependence in $\bar{X}(K,K')$ will cause some trouble. However, if the momentum density is isotropic, the integral in Eq. (9) can be transformed into a form that solves the problem. A convenient choice of coordinate systems can be performed in such a way that one overcomes the problem of angle dependence. This has been done by Ribberfors,[7] and after some algebra the result can be written as

$$\frac{d^2\sigma}{d\omega'd\Omega'}=\frac{m^2r_0^2\omega'}{2\omega q}\int_{|p_z|}^{\infty}\frac{\bar{X}_{\rm int}(p)}{E(p)}2\pi\rho(p)p\,dp , \quad (10)$$

where

$$E=E(p)=(m^2+p^2)^{1/2} , \quad (11)$$

$$q=|\mathbf{k}-\mathbf{k}'|=(\omega^2+\omega'^2-2\omega\omega'\cos\theta')^{1/2} , \quad (12)$$

$$\bar{X}_{\rm int}(p)=2+F\{[(E-D-W)^2-H^2]^{-1/2}-[(E-D)^2-H^2]^{-1/2}\}+\frac{m^4}{\omega^2}(E-D-W)[(E-D-W)^2-H^2]^{-3/2}+\frac{m^4}{\omega^2}(E-D)[(E-D)^2-H^2]^{-3/2} , \quad (13)$$

$$A = A(p) = \frac{1}{q}[(\omega-\omega')E(p)-\omega\omega'(1-\cos\theta')] , \tag{14}$$

$$D = D(p) = \frac{1}{q}(\omega-\omega'\cos\theta')A(p) , \tag{15}$$

$$H = H(p) = \frac{\omega'}{q}\sin\theta'[p^2 - A^2(p)]^{1/2} , \tag{16}$$

$$W = \omega'(1-\cos\theta') , \tag{17}$$

$$F = W - \frac{2m^2}{\omega} - \frac{2m^4}{\omega^2 W} , \tag{18}$$

and

$$|p_z| = |A(p_z)| = \left|\frac{1}{q}[(\omega-\omega')(m^2+p_z^2)^{1/2} - \omega\omega'(1-\cos\theta')]\right| . \tag{19}$$

The expression in Eq. (10) is valid for any given isotropic momentum density $\rho(p)$ of the nonperturbed system.

The last equation, i.e., Eq. (19), follows from the conservation of momentum and energy. The condition in Eq. (19) allows one to choose a relationship between $p_z$ and $\omega'$. The relation usually chosen is

$$p_z = \frac{q}{2} - (\omega-\omega')\left[\frac{1}{4} + \frac{m^2}{2\omega\omega'(1-\cos\theta')}\right]^{1/2} , \tag{20}$$

which also can be written as

$$\omega' = \begin{cases} \xi/\zeta + (\xi^2/\zeta^2 - m^2\omega^2/\zeta)^{1/2} & \text{when } p_z > 0 \\ m\omega/[\omega(1-\cos\theta')+m] & \text{when } p_z = 0 \\ \xi/\zeta - (\xi^2/\zeta^2 - m^2\omega^2/\zeta)^{1/2} & \text{when } p_z < 0 . \end{cases} \tag{21}$$

The quantities $\xi$ and $\zeta$ are derived from the following equations:

$$\xi = \omega^2 E(p_z)(1-\cos\theta') + \omega E^2(p_z) - \omega p_z^2\cos\theta' \tag{22}$$

and

$$\zeta = [\omega(1-\cos\theta') + E(p_z)]^2 - p_z^2 . \tag{23}$$

The above choice causes $p_z$ to increase when $\omega'$ increases.

As mentioned in Sec. I, a relativistic expression containing the Compton profile would be of interest. Such an expression can also be developed from Eq. (10). After a partial integration, we are able to find the following approximation of the expression in Eq. (10):[7]

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{m^2 r_0^2 \omega'}{2\omega q}\frac{\bar{X}_{\rm int}(|p_z|)}{E(p_z)}J(p_z) , \tag{24}$$

where

$$J(p_z) = \int_{|p_z|}^{\infty} 2\pi\rho(p)p\,dp , \tag{25}$$

i.e., the Compton profile for the isotropic momentum density. The factor $\bar{X}_{\rm int}(|p_z|)$ can be rewritten more simply as follows:

$$\bar{X}_{\rm int}(|p_z|) = \frac{R}{R'} + \frac{R'}{R} + 2m^2\left[\frac{1}{R} - \frac{1}{R'}\right] + m^4\left[\frac{1}{R} - \frac{1}{R'}\right]^2 , \tag{26}$$

where

$$R = \omega[E(p_z) - D(|p_z|)] \tag{27}$$

and

$$R' = R - \omega\omega'(1-\cos\theta') . \tag{28}$$

We will return to expressions (10) and (24) when we are able to compare them with the one that we derive in this paper. [Note that when we write "the Ribberfors expression" or "the Ribberfors method" we are referring to Eq. (10) and not Eq. (24).]

## III. RELATIVISTIC CROSS SECTION FOR GENERAL RELATIVISTIC CENTRAL-FIELD HARTREE-FOCK BOUND STATES

In this section we derive an expression for the differential cross section in a more rigorous way than has been done in previous works within this field. We use the impulse approximation and a general relativistic wave function in the central-field approximation that can be written in the following form:[9]

$$\psi_{nljm_j}(\mathbf{r}) = \begin{bmatrix} g_{nlj}(r) & 0 \\ 0 & if_{nlj}(r) \end{bmatrix}\begin{bmatrix} y_{jl}^{m_j}(\theta,\phi) \\ y_{jl'}^{m_j}(\theta,\phi) \end{bmatrix} , \tag{29}$$

where $n$, $l$, $j$, and $m_j$ are quantum numbers. The number $l'$ can be expressed in terms of the other numbers as follows:

$$l' = \begin{cases} l+1 & \text{when } j = l+1/2 \quad (l \geq 0) \\ l-1 & \text{when } j = l-1/2 \quad (l > 0) . \end{cases} \tag{30}$$

The function $y_{jl}^{m_j}$ can be written as[9]

$$y_{jl}^{m_j}(\theta,\phi) = (2l+1)^{-1/2} \times \begin{bmatrix} (l+m_j+1/2)^{1/2}Y_{l,m_j-1/2}(\theta,\phi) \\ (l-m_j+1/2)^{1/2}Y_{l,m_j+1/2}(\theta,\phi) \end{bmatrix} \tag{31}$$

when $j = l+1/2$ and

$$y_{jl}^{m_j}(\theta,\phi) = (2l+1)^{-1/2} \times \begin{bmatrix} -(l-m_j+1/2)^{1/2}Y_{l,m_j-1/2}(\theta,\phi) \\ (l+m_j+1/2)^{1/2}Y_{l,m_j+1/2}(\theta,\phi) \end{bmatrix} \tag{32}$$

when $j = l-1/2$. Here, $Y_{l,m_j-1/2}$ and $Y_{l,m_j+1/2}$ stand for the spherical harmonic function.

At this point we will define some expressions and show some relationships which will be useful later. The momentum transform of the initial wave function

$$\psi_i(\mathbf{p})=\left[\frac{1}{2\pi}\right]^{3/2}\int \psi_i(\mathbf{r})e^{-i\mathbf{p}\cdot\mathbf{r}}d^3r \tag{33}$$

will enter into the calculations. Here, the initial wave function $\psi_i(\mathbf{r})$ represents a relativistic central-field Hartree-Fock bound state, which can be written in the form given in Eq. (29). Owing to that, we define the following functions:

$$\chi^G_{nlj}(p)=4\pi\left[\frac{1}{2\pi}\right]^{3/2}\int_0^\infty G_{nlj}(r)j_l(pr)r\,dr \tag{34}$$

and

$$\chi^F_{nlj}(p)=4\pi\left[\frac{1}{2\pi}\right]^{3/2}\int_0^\infty F_{nlj}(r)j_{l'}(pr)r\,dr\ , \tag{35}$$

where $G_{nlj}(r)=rg_{nlj}(r)$ and $F_{nlj}(r)=rf_{nlj}(r)$. Here, $j_l$ and $j_{l'}$ stand for the spherical Bessel function. Using the spherical harmonic expansion of the function $e^{-i\mathbf{p}\cdot\mathbf{r}}$, which is well known,[10,11] and the wave function in Eq. (29), we can develop an expression for the momentum transform from Eq. (33). Due to the orthonormalization of the spherical harmonics, we are able to show that the momentum transform of the wave function in Eq. (29) can be written as

$$\psi_{nljm_j}(\mathbf{p})=\begin{bmatrix}(-i)^l\chi^G_{nlj}(p) & 0\\ 0 & (-i)^{l'}i\chi^F_{nlj}(p)\end{bmatrix}\begin{bmatrix}y^{m_j}_{jl}(\theta_p,\phi_p)\\ y^{m_j}_{jl'}(\theta_p,\phi_p)\end{bmatrix}, \tag{36}$$

where $p$, $\theta_p$, and $\phi_p$ are the spherical coordinates in momentum space. Using the addition theorem of spherical harmonics,[10,11] we are also able to show that the momentum density for a completely occupied shell can be written as follows:

$$\rho_{nlj}(p)=\sum_{m_j}\psi^\dagger_{nljm_j}(\mathbf{p})\psi_{nljm_j}(\mathbf{p})$$
$$=\frac{2j+1}{4\pi}[\,|\chi^G_{nlj}(p)|^2+|\chi^F_{nlj}(p)|^2\,], \tag{37}$$

where $m_j$ runs from $-j$ to $j$. This is the momentum density for bound states that ought to be used in Eq. (10). Let us leave this for the moment and proceed to the main problem.

In the Schrödinger theory, the coupling between the electron and the photon gives rise to a perturbation potential containing $\mathbf{A}^2$ and $\mathbf{p}\cdot\mathbf{A}$ terms plus spin-orbit coupling. In the Dirac theory, all this is reduced to $\boldsymbol{\alpha}\cdot\mathbf{A}$, where $\boldsymbol{\alpha}$ is a matrix and $\mathbf{A}$ refers to the quantized transverse electromagnetic field. If we use the notation used by Sakurai,[9] the perturbation or interaction potential can be written as

$$\hat{H}_I(t)=-e\boldsymbol{\alpha}\cdot\mathbf{A}(t)\ , \tag{38}$$

where

$$\boldsymbol{\alpha}=i\gamma_4\boldsymbol{\gamma}=i\gamma_4(\gamma_1,\gamma_2,\gamma_3)\ , \tag{39}$$

$$\mathbf{A}(t)=\sum_{\mathbf{k},\alpha}\left[\frac{1}{2V\omega}\right]^{1/2}(\hat{a}_{\mathbf{k}\alpha}\boldsymbol{\varepsilon}^{(\alpha)}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$
$$+\hat{a}^\dagger_{\mathbf{k}\alpha}\boldsymbol{\varepsilon}^{(\alpha)}e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)})\ , \tag{40}$$

$\gamma_\mu$ ($\mu=1,2,3,4$) stands for a gamma matrix, $V$ is the (normalization) volume, and $\boldsymbol{\varepsilon}^{(\alpha)}$ is the polarization vector of a transverse photon. The operators $\hat{a}_{\mathbf{k}\alpha}$ and $\hat{a}^\dagger_{\mathbf{k}\alpha}$ in Eq. (40) are, respectively, the usual annihilation and creation operators for a transverse photon.

In the Dirac theory, Compton scattering is described by second-order perturbation theory. The second-order transition amplitude $S^{(2)}_{fi}(\tau)$ can be written as[9]

$$S^{(2)}_{fi}(\tau)=-\sum_n\int_0^\tau dt\int_0^t dt'\langle f|\hat{H}_I(t)|n\rangle$$
$$\times\exp[i(\varepsilon_f-\varepsilon_n)t]$$
$$\times\langle n|\hat{H}_I(t')|i\rangle$$
$$\times\exp[i(\varepsilon_n-\varepsilon_i)t']\ , \tag{41}$$

where $|f\rangle$, $|n\rangle$, and $|i\rangle$ represent the final, intermediate, and initial states, respectively, and $\tau$ is the time during which the perturbation acts. Here, $\varepsilon_f$, $\varepsilon_n$, and $\varepsilon_i$ stand for the total relativistic energies of the electron system in the final, intermediate, and initial states, respectively.

The scattering process occurs instantly, and because of that, the nonscattered electrons are assumed to have the same states, i.e., wave functions, in the initial and the final states of the system. Evidently, we just have to consider the electron that is involved in the scattering process. Furthermore, the electron and the photon operate in different subspaces, which in this case means, so far as the photon is concerned, that we can ignore the intermediate states. If we make $\psi$ characterize a wave function of an electron, $|\gamma\rangle$ the initial photon state, and $|\gamma'\rangle$ the final photon state, we can write $|i\rangle$, $|n\rangle$, and $|f\rangle$ as $|\psi_i\rangle|\gamma\rangle$, $|\psi_n\rangle$, and $|\psi_f\rangle|\gamma'\rangle$, respectively. Letting $\hat{a}$ and $\hat{a}'^\dagger$ stand for the annihilation operator of the incoming photon and the creation operator of the scattered photon, respectively, the only contributions come then from the matrix elements $\langle\gamma'|\hat{a}\,\hat{a}'^\dagger|\gamma\rangle$ and $\langle\gamma'|\hat{a}'^\dagger\hat{a}|\gamma\rangle$, so far as the photon is concerned. Thus if we denote the polarization vectors of the incoming photon and the scattered photon by $\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}'$, respectively, we can readily formulate the second-order transition amplitude $S^{(2)}_{fi}(\tau)$ as

$$S_{fi}^{(2)}(\tau)=-\sum_n \int_0^\tau dt \int_0^t dt' \frac{e^2}{2V}\left[\frac{1}{\omega\omega'}\right]^{1/2} [\langle \psi_f \mid (\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}) e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \mid \psi_n \rangle \langle \psi_n \mid (\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}') e^{-i(\mathbf{k}'\cdot\mathbf{r}-\omega' t')} \mid \psi_i \rangle$$

$$+\langle \psi_f \mid (\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}') e^{-i(\mathbf{k}'\cdot\mathbf{r}-\omega' t)} \mid \psi_n \rangle \langle \psi_n \mid (\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}) e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t')} \mid \psi_i \rangle]$$

$$\times \exp[i(\varepsilon_f-\varepsilon_n)t+i(\varepsilon_n-\varepsilon_i)t'] , \tag{42}$$

where $\varepsilon_f$, $\varepsilon_n$, and $\varepsilon_i$ are the total relativistic energies of the electron in the final, intermediate, and initial states, respectively. Using operators of the form $e^{i\hat{H}t}$, where $\hat{H}$ is the (relativistic) Hamiltonian of the electron, we can put the exponential energy factors inside the transition matrix elements and sum up the intermediate states. Due to the completeness of the intermediate states, this operation gives the following elaboration of Eq. (42):

$$S_{fi}^{(2)}(\tau)=-\frac{e^2}{2V}\left[\frac{1}{\omega\omega'}\right]^{1/2} \int_0^\tau dt \int_0^t dt' [C_0(\hat{H},\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')+C_0(\hat{H},-\mathbf{k}',-\mathbf{k},-\omega',-\omega,\boldsymbol{\varepsilon}',\boldsymbol{\varepsilon})] , \tag{43}$$

where

$$C_0(\hat{H},\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')=\langle \psi_f \mid e^{i\hat{H}t}(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}) e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} e^{-i\hat{H}t} e^{i\hat{H}t'} (\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}') e^{-i(\mathbf{k}'\cdot\mathbf{r}-\omega' t')} e^{-i\hat{H}t'} \mid \psi_i \rangle . \tag{44}$$

Knowing that the energy operator $\hat{H}$ can be represented by $\hat{H}_0+V(r)$, where $\hat{H}_0$ is the Hamiltonian of a free electron, and $V(r)$ the potential, we can make an approximation; the operator $e^{i\hat{H}t}$ can be approximated as follows:[10]

$$e^{i\hat{H}t}=\exp(i\hat{H}_0 t)\exp(iVt) . \tag{45}$$

This also implies that the approximation to $e^{-i\hat{H}t}$ ought to be written as $\exp(-iVt)\exp(-i\hat{H}_0 t)$. (The sequence of the operators is important.) Applying these approximations in Eq. (43), we are able to show that the potential vanishes. Since $e^{iVt}$, for instance, commutes with $e^{i\mathbf{k}\cdot\mathbf{r}}$, $e^{-i\mathbf{k}'\cdot\mathbf{r}}$, $(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})$, and $(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')$, we can make the potential cancel out. This is the central point in the impulse approximation. Thus Eq. (43) can approximately be written as

$$S_{fi}^{(2)}(\tau)=-\frac{e^2}{2V}\left[\frac{1}{\omega\omega'}\right]^{1/2} \int_0^\tau dt \int_0^t dt' [C_0(H_0,\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')+C_0(H_0,-\mathbf{k}',-\mathbf{k},-\omega',-\omega,\boldsymbol{\varepsilon}',\boldsymbol{\varepsilon})] , \tag{46}$$

where the matrix element $C_0$ is defined by Eq. (44). [Note: The interpretation $\hat{H}\psi=\varepsilon\psi$, where $\hat{H}=\hat{H}_0+V(r)$, is correct if the one-electron wave function $\psi$ stands for a wave function in the central-field approximation.]

The operators containing $H_0$ do not commute with $e^{i\mathbf{k}\cdot\mathbf{r}}$, $e^{-i\mathbf{k}'\cdot\mathbf{r}}$, $(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})$, or $(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')$, and therefore Eq. (46) will cause a problem. This problem can be solved using plane waves, resulting in the possibility of moving the exponential energy operators outside the transition matrix elements. This is realized by expanding the initial state of the electron in plane waves, inserting a complete set of plane waves as intermediate electron states, and then assuming that the final state of the electron is a plane-wave state. The first two steps are in no way approximations but the third step is. In the attempt to get reasonable calculations, we must approximate the final state by a plane wave. The error that might arise from this approximation ought to be more significant than the error due to the approximation in Eq. (45). This is so because the next term that will add to the approximation in Eq. (45) carries a factor $e^2$, since the Coulomb potential contains $e^2$.[10] However, the plane-wave approximation will be accurate when the energy transfer to the electron is large enough in comparison with the binding energy of the initial state. This is accomplished for $\gamma$ rays, except when the so-called $K$ edge is approached.

In accordance with the plane-wave exposition above, we will now introduce a plane-wave expansion of the initial state and plane waves as intermediate states. We will use the notation put forth by Sakurai.[9] The spinors to be used are the electron spinor $u^{(s)}(\mathbf{p})$ and the positron spinor $v^{(s)}(\mathbf{p})$, where $s=1,2$. We can also use the electron spinor $u^{(r)}(\mathbf{p})$, where $r$ runs from 1 to 4. Here, $u^{(3)}(\mathbf{p})$ and $u^{(4)}(\mathbf{p})$ refer to the negative-energy solutions. However, the first two spinors likely represent the physical picture better than the last two. Therefore, we expand initial state as follows:

$$\psi_i(\mathbf{r})=\sum_{\mathbf{p},s}\left[\frac{m}{VE}\right]^{1/2} [A_{ps}u^{(s)}(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{r}}+B_{ps}v^{(s)}(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{r}}] , \tag{47}$$

where

$$A_{ps}=\left[\frac{m}{VE}\right]^{1/2} \int d^3r\, u^{(s)\dagger}(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{r}}\psi_i(\mathbf{r}) , \tag{48}$$

$$B_{ps}=\left[\frac{m}{VE}\right]^{1/2} \int d^3r\, v^{(s)\dagger}(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{r}}\psi_i(\mathbf{r}) , \tag{49}$$

and $E$ is the relativistic energy of a free particle, i.e., $E=(m^2+p^2)^{1/2}$. The complete set of intermediate states would consist of the plane waves

$$(m/VE'')^{1/2}u^{(s'')}(\mathbf{p}'')\exp(i\mathbf{p}''\cdot\mathbf{r})$$

and

$$(m/VE'')^{1/2}v^{(s'')}(\mathbf{p}'')\exp(-i\mathbf{p}''\cdot\mathbf{r}) .$$

Here, in order to separate the energies, the momentums, and the spins, we use the notations $E''$, $\mathbf{p}''$, and $s''$ for the intermediate states. Returning to the final state of the electron, the final state is simply approximated by the plane wave $(m/VE')^{1/2}u^{(s')}(\mathbf{p}')\exp(i\mathbf{p}'\cdot\mathbf{r})$.

Let us now use the plane-wave approach above to elaborate Eq. (46). Knowing that[9]

$$\hat{H}_0 u^{(s)}(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{r}}=Eu^{(s)}(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{r}} , \tag{50}$$

and

$$\hat{H}_0 v^{(s)}(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{r}}=-Ev^{(s)}(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{r}} , \tag{51}$$

the intermediate states properly used will give the following elaboration of Eq. (46):

$$S_{fi}^{(2)}(\tau)=-\frac{e^2}{2V}\left[\frac{1}{\omega\omega'}\right]^{1/2}\int_0^\tau dt\int_0^t dt'[C_1(\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')+C_1(-\mathbf{k}',-\mathbf{k},-\omega',-\omega,\boldsymbol{\varepsilon}',\boldsymbol{\varepsilon})] , \tag{52}$$

where

$$\begin{aligned}C_1(\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')=\sum_{\mathbf{p},s}\sum_{\mathbf{p}'',s''}\frac{m}{V}\left[\frac{1}{EE'}\right]^{1/2}\frac{m}{VE''}[&\langle u'e^{i\mathbf{p}'\cdot\mathbf{r}}|(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})e^{i\mathbf{k}\cdot\mathbf{r}}|u''e^{i\mathbf{p}''\cdot\mathbf{r}}\rangle\\ &\times\langle u''e^{i\mathbf{p}''\cdot\mathbf{r}}|(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')e^{-i\mathbf{k}'\cdot\mathbf{r}}|A_{ps}ue^{i\mathbf{p}\cdot\mathbf{r}}e^{-iEt'}\\ &+B_{ps}ve^{-i\mathbf{p}\cdot\mathbf{r}}e^{iEt'}\rangle e^{i(E'-\omega-E'')t}e^{i(E''+\omega')t'}\\ &+\langle u'e^{i\mathbf{p}'\cdot\mathbf{r}}|(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})e^{i\mathbf{k}\cdot\mathbf{r}}|v''e^{-i\mathbf{p}''\cdot\mathbf{r}}\rangle\\ &\times\langle v''e^{-i\mathbf{p}''\cdot\mathbf{r}}|(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')e^{-i\mathbf{k}'\cdot\mathbf{r}}|A_{ps}ue^{i\mathbf{p}\cdot\mathbf{r}}e^{-iEt'}\\ &+B_{ps}ve^{-i\mathbf{p}\cdot\mathbf{r}}e^{iEt'}\rangle e^{i(E'-\omega+E'')t}e^{i(-E''+\omega')t'}] .\end{aligned} \tag{53}$$

Here we have used the simpler notations $u$, $v$, $u'$, $u''$, and $v''$ instead of $u^{(s)}(\mathbf{p})$, $v^{(s)}(\mathbf{p})$, $u^{(s')}(\mathbf{p}')$, $u^{(s'')}(\mathbf{p}'')$, and $v^{(s'')}(\mathbf{p}'')$, respectively.

An integration over $t$ and $t'$ in Eq. (52) gives some Dirac $\delta$ functions if we let $\tau\to\infty$. The only $\delta$ function of these that will give a nonzero contribution is $\delta(E'+\omega'-E-\omega)$. Using the $\delta$-function representation

$$\delta(x)=\lim_{\tau\to\infty}\frac{\sin(\tau x)}{\pi x} , \tag{54}$$

we can do the approximation

$$\int_0^\tau dt\int_0^t dt'e^{i\omega t}e^{i\omega' t'}=\frac{\pi}{i\omega'}\left[\delta\left[\frac{\omega+\omega'}{2}\right]-\delta\left[\frac{\omega}{2}\right]\right] \tag{55}$$

if $\tau$ is large. Thus by integrating over $t$ and $t'$ the remaining part of Eq. (52) will eventually be

$$S_{fi}^{(2)}(\tau)=\frac{i\pi e^2}{2V}\left[\frac{1}{\omega\omega'}\right]^{1/2}[C_2(\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')+C_2(-\mathbf{k}',-\mathbf{k},-\omega',-\omega,\boldsymbol{\varepsilon}',\boldsymbol{\varepsilon})] , \tag{56}$$

where

$$C_2(\mathbf{k},\mathbf{k}',\omega,\omega',\varepsilon,\varepsilon')=\sum_{\mathbf{p},s}\sum_{\mathbf{p}'',s''}\frac{m}{V}\left[\frac{1}{EE'}\right]^{1/2}\frac{m}{VE''}\left[\frac{1}{\omega'+E''-E}\langle u'e^{i\mathbf{p}'\cdot\mathbf{r}}\mid(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})e^{i\mathbf{k}\cdot\mathbf{r}}\mid u''e^{i\mathbf{p}''\cdot\mathbf{r}}\rangle\right.$$
$$\times\langle u''e^{i\mathbf{p}''\cdot\mathbf{r}}\mid(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')e^{-i\mathbf{k}'\cdot\mathbf{r}}\mid A_{ps}ue^{i\mathbf{p}\cdot\mathbf{r}}\rangle$$
$$\left.+\frac{1}{\omega'-E''-E}\langle u'e^{i\mathbf{p}'\cdot\mathbf{r}}\mid(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})e^{i\mathbf{k}\cdot\mathbf{r}}\mid v''e^{-i\mathbf{p}''\cdot\mathbf{r}}\rangle\right.$$
$$\left.\times\langle v''e^{-i\mathbf{p}''\cdot\mathbf{r}}\mid(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')e^{-i\mathbf{k}'\cdot\mathbf{r}}\mid A_{ps}ue^{i\mathbf{p}\cdot\mathbf{r}}\rangle\right]$$
$$\times\delta\left[\frac{E'+\omega'-E-\omega}{2}\right], \tag{57}$$

The part that contained $B_{ps}$ has vanished, as it ought to have done. Strictly speaking, we cannot have a transition from a positron to an electron state.

Let us now take a look at the cross section. The transition probability $P$ can be written as

$$P=\frac{1}{\tau}\mid S_{fi}^{(2)}(\tau)\mid^2. \tag{58}$$

If we sum up all possible state that the scattered electron and the scattered photon can accept, we obtain the total transition probability

$$P=\sum_{\mathbf{p}',s'}\sum_{\mathbf{k}'}\frac{1}{\tau}\mid S_{fi}^{(2)}(\tau)\mid^2. \tag{59}$$

Here, we have for the moment ignored the possibility for the scattered photon to accept different polarization states. The total cross section can be obtained from Eq. (59) if we divide by the incoming flux. In this case, the flux is simply $1/V$.[4] Thus the total cross section can be expressed as follows:

$$\sigma=\sum_{\mathbf{p}',s'}\sum_{\mathbf{k}'}\frac{V}{\tau}\mid S_{fi}^{(2)}(\tau)\mid^2, \tag{60}$$

where $S_{fi}^{(2)}(\tau)$ is given in Eq. (56). Using Eq. (33) we can rewrite Eq. (48) as

$$A_{ps}=\left[\frac{m}{VE}\right]^{1/2}u^{(s)\dagger}(\mathbf{p})(2\pi)^{3/2}\psi_i(\mathbf{p}). \tag{61}$$

If we use this and the well-known integral representation of the $\delta$ function, we obtain the following expression for the cross section from Eq. (60):

$$\sigma=\frac{1}{V}\sum_{\mathbf{p}'}\frac{1}{V}\sum_{\mathbf{k}'}\sum_{s'}\frac{1}{\tau}\frac{2\pi^5e^4m^5}{\omega\omega'E'}\mid C_3(\mathbf{k},\mathbf{k}',\omega,\omega',\varepsilon,\varepsilon')+C_3(-\mathbf{k}',-\mathbf{k},-\omega',-\omega,\varepsilon',\varepsilon)\mid^2, \tag{62}$$

where

$$C_3(\mathbf{k},\mathbf{k}',\omega,\omega',\varepsilon,\varepsilon')=\frac{1}{V}\sum_{\mathbf{p}}\frac{1}{V}\sum_{\mathbf{p}''}\sum_{s,s''}(2\pi)^6\frac{1}{EE''}\left[\frac{1}{\omega'+E''-E}[u'^{\dagger}(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})u''][u''^{\dagger}(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')u]\delta(-\mathbf{p}'+\mathbf{k}+\mathbf{p}'')\right.$$
$$\times\delta(-\mathbf{p}''-\mathbf{k}'+\mathbf{p})+\frac{1}{\omega'-E''-E}[u'^{\dagger}(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})v''][v''^{\dagger}(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')u]$$
$$\left.\times\delta(-\mathbf{p}'+\mathbf{k}-\mathbf{p}'')\delta(\mathbf{p}''-\mathbf{k}'+\mathbf{p})\right]$$
$$\times[u^{\dagger}\psi_i(\mathbf{p})]\delta\left[\frac{E'+\omega'-E-\omega}{2}\right]. \tag{63}$$

The function $\delta[(E'+\omega'-E-\omega)/2]$ is obtained from the $\delta$-function representation in Eq. (54). Let us consider the function $\mid\delta[(E'+\omega'-E-\omega)/2]\mid^2$. According to Eq. (54), we can do following approximation:

$$\left|\delta\left[\frac{E'+\omega'-E-\omega}{2}\right]\right|^2=\left[\pi\frac{E'+\omega'-E-\omega}{2}\right]^{-2}\sin^2\left[\tau\frac{E'+\omega'-E-\omega}{2}\right] \tag{64}$$

when $\tau$ is large. The $\delta$ function can also be represented by

$$\delta(x)=\lim_{\tau\to\infty}\frac{\tau}{\pi}\left[\frac{\sin(\tau x)}{\tau x}\right]^2, \tag{65}$$

which gives following approximate form of Eq. (64):

$$\left|\delta\left[\frac{E'+\omega'-E-\omega}{2}\right]\right|^2=\frac{\tau}{\pi}\delta\left[\frac{E'+\omega'-E-\omega}{2}\right]=2\frac{\tau}{\pi}\delta(E'+\omega'-E-\omega)\ . \tag{66}$$

(Note: If 2 had been placed outside the $\delta$ function earlier, i.e., in Eq. (64), we would not have received the correct approximation of $|\delta[(E'+\omega'-E-\omega)/2]|^2$ in Eq. (66).) Let us now use Eq. (66), and the well-known rule

$$\lim_{V\to\infty}\frac{1}{V}\sum_{\mathbf{p}}=\left[\frac{1}{2\pi}\right]^3\int d^3p \tag{67}$$

for an elaboration of the cross section in Eq. (62). Due to Eq. (67), we receive one integral over $\mathbf{p}$ and one over $\mathbf{p}''$. Thus, using Eq. (67), after an integration over $\mathbf{p}$ and $\mathbf{p}''$, we can use Eq. (66) and obtain the following result:

$$\sigma=\int d^3k'\int d^3p'\frac{e^4m}{16\pi^2\omega\omega'E^2E'}\sum_{s'}|C_4(\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')+C_4(-\mathbf{k}',-\mathbf{k},-\omega',-\omega,\boldsymbol{\varepsilon}',\boldsymbol{\varepsilon})|^2\delta(E'+\omega'-E-\omega)\ , \tag{68}$$

where

$$C_4(\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')=\sum_{s,s''}\frac{m^2}{E''}\left[\frac{1}{\omega'+E''-E}[u^{(s')\dagger}(\mathbf{p}')(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})u^{(s'')}(\mathbf{p}'')][u^{(s'')\dagger}(\mathbf{p}'')(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')u^{(s)}(\mathbf{p})]\right.$$
$$\left.+\frac{1}{\omega'-E''-E}[u^{(s')\dagger}(\mathbf{p}')(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})v^{(s'')}(-\mathbf{p}'')][v^{(s'')\dagger}(-\mathbf{p}'')(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}')u^{(s)}(\mathbf{p})]\right]$$
$$\times[u^{(s)\dagger}(\mathbf{p})\psi_i(\mathbf{p})]\ , \tag{69}$$

$\mathbf{p}=\mathbf{p}'+\mathbf{k}'-\mathbf{k}$, and $\mathbf{p}''=\mathbf{p}-\mathbf{k}'$.

The quantity $C_4(\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')$ can be simplified if we make use of the trace techniques put forth by Sakurai.[9] If we also make use of the identities $\boldsymbol{\alpha}=i\gamma_4\boldsymbol{\gamma}$ and $\mathbf{p}''=\mathbf{p}-\mathbf{k}'$, we can show that

$$C_4(\mathbf{k},\mathbf{k}',\omega,\omega',\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}')$$
$$=u^{(s')\dagger}(\mathbf{p}')\left[\frac{m^2}{\pi\cdot\kappa'}\gamma_4(\boldsymbol{\gamma}\cdot\boldsymbol{\varepsilon})\left[B+\frac{i\gamma\cdot\kappa'}{2m}\right]\right.$$
$$\left.\times(\boldsymbol{\gamma}\cdot\boldsymbol{\varepsilon}')B\gamma_4\right]\psi_i(\mathbf{p})\ , \tag{70}$$

where $B=(m-i\gamma\cdot\pi)/2m$. Here, $\gamma$, $\pi$, and $\kappa'$ stand for the four-vectors $(\boldsymbol{\gamma},\gamma_4)$, $(\mathbf{p},iE)$, and $(\mathbf{k}',i\omega')$, respectively. Thus knowing that $d^3k'=\omega'^2d\omega'd\Omega'$ and using Eq. (70) we can elaborate the following differential cross section from Eq. (68):

$$\frac{d^2\sigma}{d\omega'd\Omega'}=\frac{r_0^2\omega'}{\omega}\int d^3p'\frac{m^3}{E^2E'}\sum_{s'}|u^{(s')\dagger}(\mathbf{p}')NB\gamma_4\psi_i(\mathbf{p})|^2$$
$$\times\delta(E'+\omega'-E-\omega)\ , \tag{71}$$

where

$$N=\frac{m^2}{\pi\cdot\kappa'}\gamma_4(\boldsymbol{\gamma}\cdot\boldsymbol{\varepsilon})\left[B+\frac{i\gamma\cdot\kappa'}{2m}\right](\boldsymbol{\gamma}\cdot\boldsymbol{\varepsilon}')$$
$$-\frac{m^2}{\pi\cdot\kappa}\gamma_4(\boldsymbol{\gamma}\cdot\boldsymbol{\varepsilon}')\left[B-\frac{i\gamma\cdot\kappa}{2m}\right](\boldsymbol{\gamma}\cdot\boldsymbol{\varepsilon})\ , \tag{72}$$

$\kappa$ stands for the four-vector $(\mathbf{k},i\omega)$, and $r_0$ for the classical radius of the electron. In line with the trace techniques, we can show the following:[9]

$$\sum_{s'}|u^{(s')\dagger}(\mathbf{p}')NB\gamma_4\psi_i(\mathbf{p})|^2=\mathrm{Tr}[\Psi_i(\mathbf{p})M]\ , \tag{73}$$

where

$$M=(NB\gamma_4)^\dagger B'\gamma_4NB\gamma_4\ , \tag{74}$$

and $\Psi_i(\mathbf{p})$ is simply the matrix $\psi_i(\mathbf{p})\psi_i^\dagger(\mathbf{p})$. Here, $B'$ stands for $(m-i\gamma\cdot\pi')/2m$, where $\pi'$ is the four-vector $(\mathbf{p}',iE')$. Thus using Eq. (73) we can write the differential cross section as

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{r_0^2 \omega'}{\omega} \int d^3p \frac{m^3}{E^2 E'} \mathrm{Tr}[\Psi_i(\mathbf{p}) M] \times \delta(E' + \omega' - E - \omega) , \tag{75}$$

owing to Eq. (71). Here, we have used $\mathbf{p}' = \mathbf{p} + \mathbf{k} - \mathbf{k}'$, allowing $d^3p'$ to be replaced with $d^3p$, since $\mathbf{k}$ and $\mathbf{k}'$ are constant during the integration.

The remaining task now is to calculate the trace in Eq. (75). In the present paper we restrict the calculation to completely occupied shells. Thus, letting $\psi_i(\mathbf{p})$ stand for the momentum transform of a relativistic central-field Hartree-Fock bound state given in Eq. (36), we are able to sum up $m_j$. Hence, we must consider the following trace:

$$\sum_{m_j} \mathrm{Tr}[\Psi_i(\mathbf{p}) M] = \sum_{m_j} \mathrm{Tr}[\Psi_i(\mathbf{p}) (NB\gamma_4)^\dagger B' \gamma_4 NB\gamma_4] = \mathrm{Tr}\left[ \gamma_4 NB\gamma_4 \left[ \sum_{m_j} \psi_{nljm_j}(\mathbf{p}) \psi^\dagger_{nljm_j}(\mathbf{p}) \right] \times \gamma_4 B^\dagger N^\dagger B' \right] . \tag{76}$$

Using the expansions given by Merzbacher (Ref. 10, p. 187) we can show that

$$\sum_{m_j} \Psi_i(\mathbf{p}) = \sum_{m_j} \psi_{nljm_j}(\mathbf{p}) \psi^\dagger_{nljm_j}(\mathbf{p}) = \frac{1}{4} \frac{2j+1}{4\pi} \left[ |\chi^G_{nlj}(p)|^2 (1+\gamma_4) + |\chi^F_{nlj}(p)|^2 (1-\gamma_4) \pm \frac{2}{p} \chi^G_{nlj}(p) \chi^F_{nlj}(p) i(\boldsymbol{\gamma}\cdot\mathbf{p}) \gamma_4 \right] , \tag{77}$$

where the positive sign is valid when $j = l + 1/2$, and the negative when $j = l - 1/2$. By using Ref. 9 we can show that $B^\dagger = \gamma_4 B \gamma_4$, $BB = B$, $B\gamma_4 B = (E/m)B$, and $B\gamma_4 B\gamma_4 B = (E/m)^2 B$. If we use this, Eq. (77), and the identity $i(\boldsymbol{\gamma}\cdot\mathbf{p}) = m + \gamma_4 E - 2mB$, we obtain the following from Eq. (76):

$$\sum_{m_j} \mathrm{Tr}[\Psi_i(\mathbf{p}) M] = \frac{1}{4} \frac{2j+1}{4\pi} \left[ \left( \frac{E}{m} + 1 \right) |\chi^G_{nlj}(p)|^2 + \left( \frac{E}{m} - 1 \right) |\chi^F_{nlj}(p)|^2 \pm \left( -2\frac{p}{m} \right) \chi^G_{nlj}(p) \chi^F_{nlj}(p) \right] \times \mathrm{Tr}(\gamma_4 NB\gamma_4 N^\dagger B') . \tag{78}$$

The fact that $p^2$ can be written as $E^2 - m^2$ allows us also to write Eq. (78) as

$$\sum_{m_j} \mathrm{Tr}[\Psi_i(\mathbf{p}) M] = \frac{1}{2} \frac{2j+1}{8\pi} \frac{E}{m} \left[ \left( 1 + \frac{m}{E} \right)^{1/2} \chi^G_{nlj}(p) \pm (-1) \left( 1 - \frac{m}{E} \right)^{1/2} \chi^F_{nlj}(p) \right]^2 \mathrm{Tr}(\gamma_4 NB\gamma_4 N^\dagger B') . \tag{79}$$

The matrix $\gamma_4 NB\gamma_4 N^\dagger B'$ involves several $\gamma$ products. The trace evaluation of this matrix requires the use of some tricks.[9] We are also able to use the identities $\mathbf{p}' + \mathbf{k}' - \mathbf{p} - \mathbf{k} = 0$ and $E' + \omega' - E - \omega = 0$ to simplify the evaluation. Here, however, we simply introduce the result, which is

$$\mathrm{Tr}(\gamma_4 NB\gamma_4 N^\dagger B') = X(\mathbf{p}, \mathbf{p}') = \frac{1}{2} \left( \frac{K}{K'} + \frac{K'}{K} \right) - 1 + 2 \left[ (\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}') + \frac{(\boldsymbol{\varepsilon}\cdot\mathbf{p})(\boldsymbol{\varepsilon}'\cdot\mathbf{p}')}{K} - \frac{(\boldsymbol{\varepsilon}\cdot\mathbf{p}')(\boldsymbol{\varepsilon}'\cdot\mathbf{p})}{K} \right]^2 , \tag{80}$$

where $K = -\pi\cdot\kappa$ and $K' = -\pi\cdot\kappa'$. Thus, owing to Eqs. (75), (79), and (80), the differential cross section for a completely occupied shell can be written as

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{r_0^2 \omega'}{2\omega} \int d^3p \frac{m^2}{EE'} X(\mathbf{p}, \mathbf{p}') \frac{2j+1}{8\pi} \times \left[ \left( 1 + \frac{m}{E} \right)^{1/2} \chi^G_{nlj}(p) \pm (-1) \left( 1 - \frac{m}{E} \right)^{1/2} \chi^F_{nlj}(p) \right]^2 \times \delta(E' + \omega' - E - \omega) . \tag{81}$$

When the polarizations of the photons are not observed, we must sum up the final polarization directions and average over the initial polarization directions. By

doing this in Eq. (81), we get another so-called $X$ factor, instead of $X(\mathbf{p},\mathbf{p}')$ above, and that will be precisely the $X$ factor $\bar{X}(K,K')$ given in Eq. (5).[6] The only angle dependence in Eq. (81) comes from the $X$ factor, which we now interpret as the factor $\bar{X}(K,K')$. Owing to that, we can repeat the calculation of Ribberfors,[7] which resulted in expression (10). Hence, proceeding from Eq. (81), we can immediately write a corresponding expression which reads as follows:

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{m^2r_0^2\omega'}{2\omega q}\int_{|p_z|}^{\infty}\frac{\bar{X}_{\rm int}(p)}{E(p)}2\pi\frac{2j+1}{8\pi}\left[\left[1+\frac{m}{E}\right]^{1/2}\chi^G_{nlj}(p)\pm(-1)\left[1-\frac{m}{E}\right]^{1/2}\chi^F_{nlj}(p)\right]^2 p\,dp\ , \tag{82}$$

where $q$, $\bar{X}_{\rm int}(p)$, and $|p_z|$ are given in Eqs. (12), (13), and (19), respectively. As before, the positive sign is valid when $j=l+1/2$, and the negative sign is valid when $j=l-1/2$. The expression in Eq. (82) is the important one in the present work. It allows us to calculate differential cross sections for arbitrary completely occupied shells. To obtain this expression, which is more general but just as simple as those previously used, we simply apply the so-called impulse approximation.

Let us complete this section with some remarks concerning incompletely occupied shells. The outermost electrons in an atom usually form an incompletely occupied shell. Expression (82) is valid only for completely occupied shells. However, we can make use of the knowledge that an electron outermost in an atom has a small binding energy, and due to that, a widely spread probability density $|\psi(\mathbf{r})|^2$ in coordinate space. If the probability density $|\psi(\mathbf{r})|^2$ is widely spread in coordinate space, the corresponding momentum density $|\psi(\mathbf{p})|^2$ will be well localized in momentum space. This means, for instance, that the Compton profile for outermost electrons is bigger than the Compton profile for innermost electrons near $p_z=0$, i.e., the Compton line. Near the so-called $K$ edge, the opposite is true. This fact allows us to treat the outermost electrons more freely. Previously used forms for the differential cross section have proved to work very well near the Compton line.[8,12] This will also be the case for our expression, i.e., (82), as will be shown indirectly in Sec. IV. Equation (82) differs very little from expression (10) near the Compton line. Since all forms for the cross section contain the momentum transform or density, the contribution to the total cross section from the outermost electrons will just be important near the Compton line. Consequently, so far as the outermost electrons are concerned, we are able to freely choose a method that only needs to work well near the Compton line. Furthermore, due to the small binding energies of these electrons, we are also able to choose a nonrelativistic momentum transform and density. If we consider metals, for instance, we can use expression (10) and assume a nonrelativistic Fermi distribution. We can also use the expression for the relativistic differential cross section for anisotropic systems, elaborated by Ribberfors.[13] If we are dealing with materials other than metals, the last expression for anisotropic systems will be the one that we ought to consider.

## IV. VALIDITY OF THE MOMENTUM-DENSITY APPROACH

In this section we compare our expression in Eq. (82) with the Ribberfors expression in Eq. (10). The comparison carried out will concern hydrogenlike systems (in the ground states). For that purpose we need the momentum transform of a hydrogenlike system. The relativistic wave function of such a system, and its momentum transform, can be found elsewhere.[14] Here, due to Eqs. (34), (35), and (37), we define only the radial part of the momentum transform, which reads as follows:

$$\chi^G_{1,0,\frac{1}{2}}(p)=\frac{1}{p}\chi(p)\sin[(\gamma+2)x]\ , \tag{83}$$

$$\chi^F_{1,0,\frac{1}{2}}(p)=\chi(p)\frac{\gamma}{\alpha Zp}\left[\frac{1/p}{\gamma+1}(\beta^2+p^2)^{1/2}\sin[(\gamma+1)x]-\cos[(\gamma+2)x]\right]\ , \tag{84}$$

where

$$\chi(p)=8\pi C_N\left[\frac{\beta}{2\pi}\right]^{3/2}\beta^\gamma\Gamma(\gamma+2)(\beta^2+p^2)^{-(\gamma+2)/2}\ , \tag{85}$$

$$C_N=2^\gamma\left[\frac{\gamma+2}{\Gamma(2\gamma+3)}\right]^{1/2}\ , \tag{86}$$

$$\gamma=[1-(\alpha Z)^2]^{1/2}-1\ , \tag{87}$$

$\beta=m\alpha Z$, $x=\arctan(p/\beta)$, $Z$ is the atomic number, and $\alpha$ stands for the fine-structure constant. Thus the momentum transform above belongs to the radial wave function for a hydrogenlike $1s$ state. The binding energy $\varepsilon_{\rm gd}$ of this (ground) state is simply $\varepsilon_{\rm gd}=m(\gamma+1)$. This energy indicates the so-called $K$ edge of the $1s$ electron.

If we use the momentum transform above in Eq. (10) and (82), we obtain results that differ very little for moderate values in $|p_z|$, smaller than or comparable to approximately 100 a.u. This can be seen in Fig. 1. The figure shows the difference between expression (82) and (10), when compared to our method. In other words, it shows the relative deviation of expression (10) from expression (82). The relative deviation (in percent) is here

presented as a function of the scattered photon energy $\omega'$. Furthermore, we have here chosen a common energy of the incoming photon. (A choice of a lower energy will, by and large, just squeeze together the curves along the energy axis.) The values of $Z$ correspond to lead and copper.

Figure 1 shows a remarkably small deviation near the $K$ edge. On the other hand, it shows a quite large deviation for small energies of the scattered photon below the Compton line, i.e., for large negative values in $p_z$ below $-100$ a.u. Here, our expression gives a lower value than does the Ribberfors expression. Theoretically, this indicates that use of our expression is advantageous, at least below the Compton line. In particular, our expression ought to be useful for small scattering angles. The entire spectrum or curve will, to a large extent, appear below the Compton line when small angles are concerned [see Figs. 1(c) and 1(d)]. However, at present, few experiments have been carried out below the Compton line. The reason can be credited to problems associated with measurements in this area. The cross section is very weak here, which makes it difficult to correct the raw

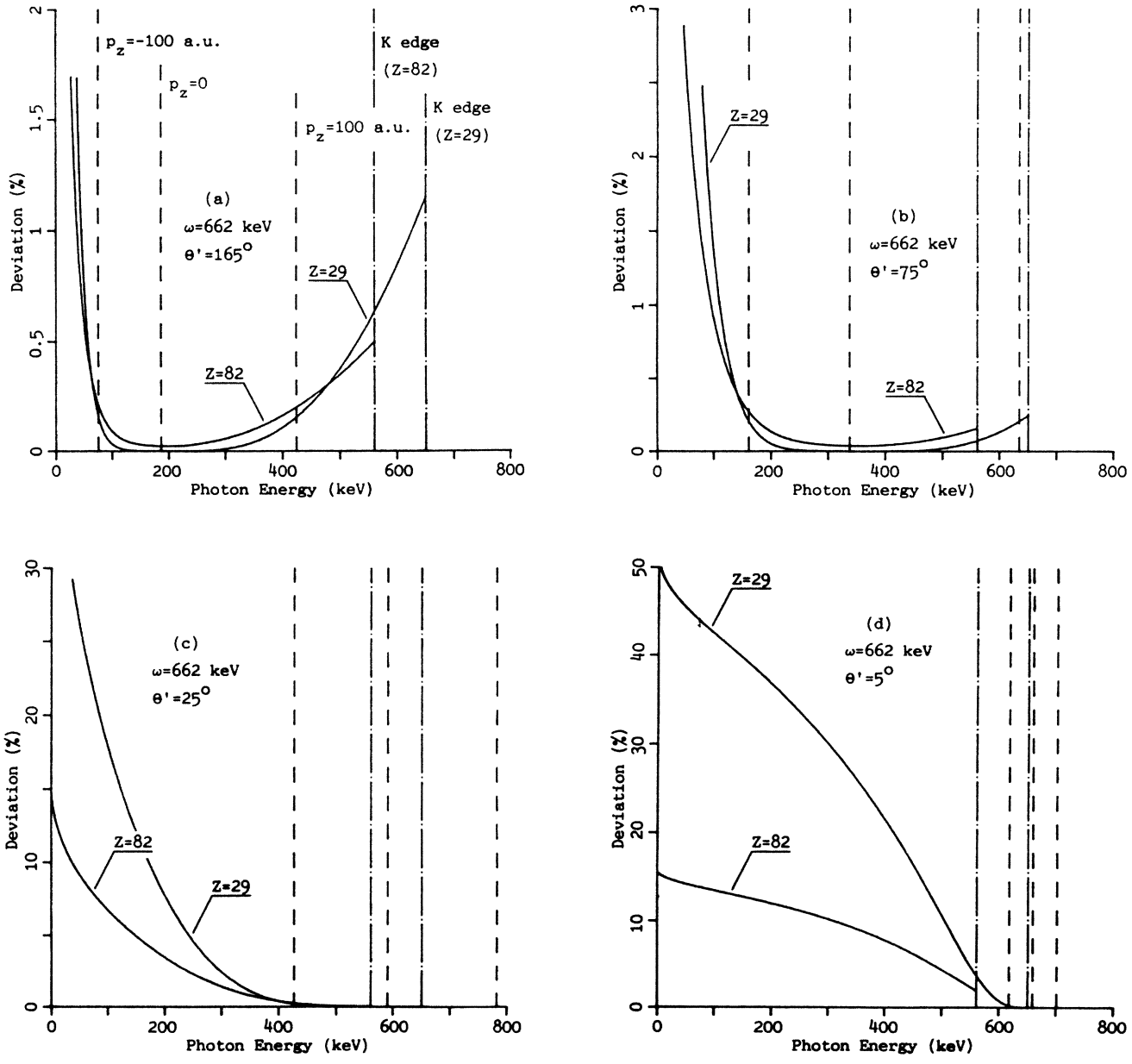


FIG. 1. Relative deviation of the Ribberfors expression (10) from expression (82) for a hydrogenlike system in the ground state as a function of the scattered photon energy $\omega'$. Here, the energy of the incoming photon $\omega$ is 662 keV. The choices of scattering angles are $\theta'=165°$, $\theta'=75°$, $\theta'=25°$, and $\theta'=5°$. The values $p_z=-100$ a.u., $p_z=0$, and $p_z=100$ a.u. are indicated as dashed straight lines, according to Eq. (20). The $K$ edges are indicated as straight dashed-dotted lines.

data. For this reason, expression (10) would be accurate enough for most purposes.

The small difference between expressions (10) and (82) that Fig. 1 clearly shows can be explained in a more theoretical way. This can be done by reviewing the definition of the wave function, and then upon only the radial part. The radial parts $G_{nlj}(r)=rg_{nlj}(r)$ and $F_{nlj}(r)=rf_{nlj}(r)$ of the relativistic wave function are connected to each other by two differential equations. Omitting the $nlj$ index, these can be written as[9]

$$\frac{dF}{dr}\pm\frac{1}{r}(j+\tfrac{1}{2})F(r)=-[\varepsilon-V(r)-m]G(r)\ , \tag{88}$$

and

$$\frac{dG}{dr}\pm(-1)\frac{1}{r}(j+\tfrac{1}{2})G(r)=[\varepsilon-V(r)+m]F(r)\ , \tag{89}$$

where $\varepsilon$ is the total relativistic energy of the bound electron, $V(r)$ is the potential, the positive sign is valid when $j=l+\frac{1}{2}$, and the negative sign is valid when $j=l-\frac{1}{2}$. [In a case where we make $G(r)$ and $F(r)$ characterize the radial parts of an atom other than a hydrogenlike one, the potential $V(r)$ has to be seen as some "effective" potential, consistent with the radial parts of the central-field Hartree-Fock wave function.] Now we interpret $\varepsilon$ as $E+V(r)$, which gives the equations

$$\frac{dF}{dr}\pm\frac{1}{r}(j+\tfrac{1}{2})F(r)=-(E-m)G(r) \tag{90}$$

and

$$\frac{dG}{dr}\pm(-1)\frac{1}{r}(j+\tfrac{1}{2})G(r)=(E+m)F(r) \tag{91}$$

from the differential equations above. The recent interpretation or approximation of $\varepsilon$, which causes the potential to cancel out, will give an interesting result.

We are now able to find some approximate relations between $\chi^G(p)$ and $\chi^F(p)$, and for the sake of simplicity only one case at a time will be considered. The first will be the case when $j=l+\frac{1}{2}$, and $l'=l+1$ [see Eq. (30)]. The spherical Bessel function $j_{l+1}(pr)$ can be written as[11]

$$j_{l+1}(pr)=\frac{l}{pr}j_l(pr)-\frac{1}{p}\frac{d}{dr}j_l(pr)\ . \tag{92}$$

Returning to Eq. (35), if we use Eq. (92), we can write expression (35) as

$$\chi^F(p)=4\pi\left[\frac{1}{2\pi}\right]^{3/2}\times\int_0^\infty dr\,rF(r)\left[\frac{l}{pr}j_l(pr)-\frac{1}{p}\frac{d}{dr}j_l(pr)\right]\ . \tag{93}$$

A partial integration properly used in Eq. (93) gives the following:

$$\chi^F(p)=4\pi\left[\frac{1}{2\pi}\right]^{3/2}\int_0^\infty\frac{1}{p}\left[\frac{dF}{dr}+\frac{1}{r}(j+\tfrac{1}{2})F(r)\right]\times j_l(pr)r\,dr\ , \tag{94}$$

due to the fact that we are dealing with bound states. According to Eqs. (34) and (90), we can write Eq. (94) as

$$\chi^F(p)=-\frac{E-m}{p}\chi^G(p)\ , \tag{95}$$

which also can be written as

$$\chi^G(p)=-\frac{E+m}{p}\chi^F(p)\ , \tag{96}$$

due to the identity $p^2=E^2-m^2$. Considering the case when $j=l-\frac{1}{2}$, and $l'=l-1$ [see Eq. (30)], in like manner we can show that $\chi^G(p)=[(E+m)/p]\chi^F(p)$ and $\chi^F(p)=[(E-m)/p]\chi^G(p)$. Here, we have to use Eq. (91) instead of (90). Evidently, we can formulate the following two approximate relations:

$$\chi^F_{nlj}(p)=\pm(-1)\frac{E-m}{p}\chi^G_{nlj}(p) \tag{97}$$

and

$$\chi^G_{nlj}(p)=\pm(-1)\frac{E+m}{p}\chi^F_{nlj}(p)\ , \tag{98}$$

where the positive sign is valid when $j=l+\frac{1}{2}$ and the negative sign is valid when $j=l-\frac{1}{2}$. If we now use these relations in Eq. (82), the square inside the integral can be rewritten as $2[\,|\chi^G_{nlj}(p)|^2+|\chi^F_{nlj}(p)|^2]$. With Eq. (37) in mind, the result will precisely be expression (10). This is the reason for the small difference between expressions (10) and (82). Thus the momentum-density approach of Eisenberger and Reed is not only adequate, but obviously a very good one.

The interpretation of $\varepsilon$ as $E+V(r)$ will make the potential cancel out in Eqs. (88) and (89). After some algebra, this interpretation results in the Ribberfors expression, i.e., Eq. (10). The central point in the impulse approximation will be that the potential cancels out. Thus we can indeed say that the "heuristic" approach of Eisenberger and Reed,[5] resulting in expression (10),[7] is "in the spirit of the impulse approximation."

## V. CONCEPT OF A COMPTON PROFILE AND ITS VALIDITY IN A RELATIVISTIC CONTEXT

In Sec. IV we show that expression (10) ought to be accurate enough for most purposes. In this section we are able to test the validity of Eq. (24), in other words, to find if the Compton profile is a well-defined concept also in a relativistic context. The interesting thing about the Compton profile is its direct relation to the momentum density, see Eqs. (1) and (25). It can give information about the electronic structure of a material. For this reason, researchers frequently present empirical results as Compton profiles. Thus it seems important to investigate the validity of expression (24). To study its validity, we will use the momentum transform for a hydrogenlike system defined in Sec. IV.

If we now repeat, with certain exceptions, the calculations from Sec. IV, using Eqs. (24) and (82), we obtain larger differences than before. Expression (24) gives a larger cross section than (82). This is stated by the curves in Fig. 2. The figure shows the relative deviation of expression (24) from expression (82), i.e., the difference be-

tween expressions (24) and (82), when compared to our method. As before, the relative deviation (in percent) is presented as a function of the scattered photon energy $\omega'$.

According to Fig. 2, the expressions differ very much for small energies below the Compton line. This is, by and large, also the case for energies near the $K$ edge. Even near the Compton line, we obtain major differences. [If Eq. (10) had been used instead of Eq. (82) the results would have been almost the same.] Equation (24) is obviously, to a large extent, invalid provided our intent is not simply to study the cross section near the Compton line for an electron with a small binding energy, i.e., a small value in $Z$ (see Fig. 3). Thus expression (24) cannot be used for the $K$ electrons of an atom unless we are dealing with a light element near the Compton line. A light element will, in such a case, be defined as an atomic number smaller than or comparable to 15.

Equation (24) seems to work well near the Compton line for electrons with small binding energies. This means if we view the total differential cross section for an atom, that expression (24) would be accurate enough in this area, since the Compton profile is larger here for the

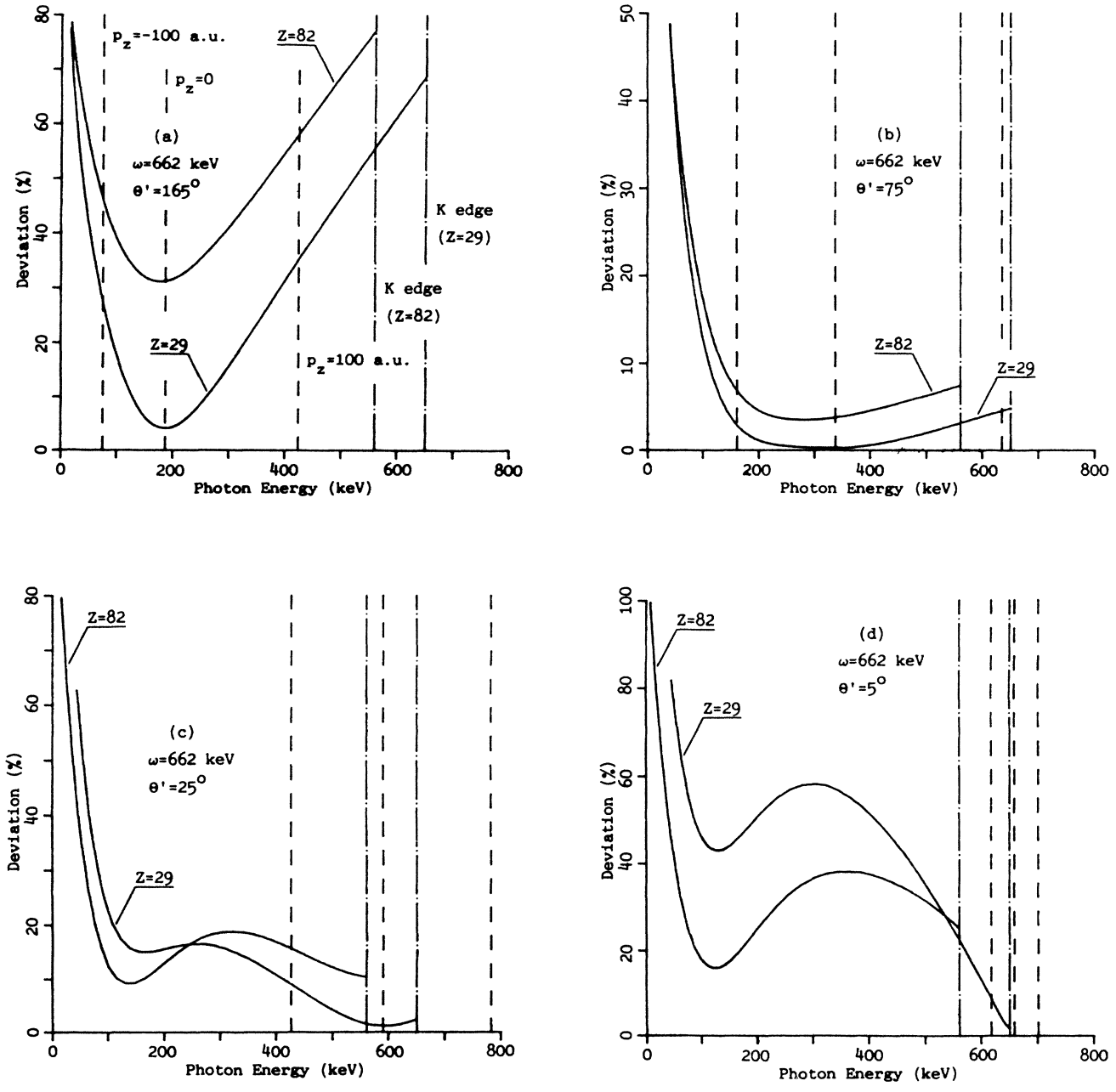


FIG. 2. Relative deviation of the expression (24) from expression (82) for hydrogenlike systems in the ground states as a function of the scattered photon energy $\omega'$.

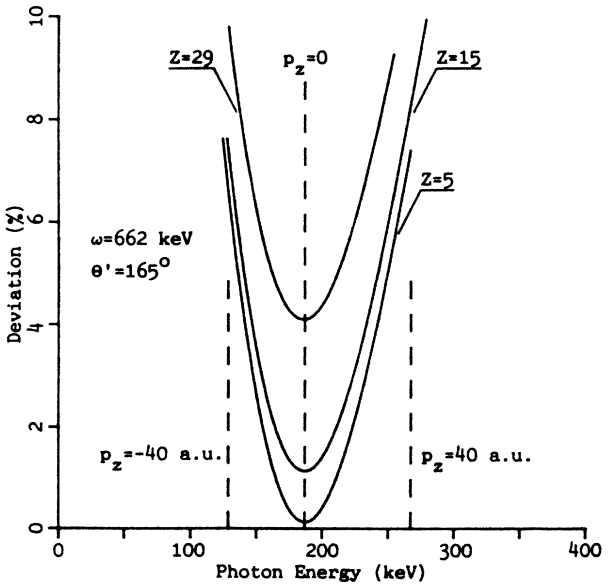


FIG. 3. Relative deviation of expression (24) from expression (82) for atomic numbers $Z=29$, $Z=15$, and $Z=5$. The choice of scattering angle $\theta'$ is 165°. The values of $p_z=-40$ a.u., $p_z=0$, and $p_z=40$ a.u. are indicated as dashed straight lines, according to Eq. (20).

outermost electrons than for innermost. In other words, the contribution to the total cross section from the outermost electrons dominates near the Compton line, which makes Eq. (24) accurate enough for the calculation of the total differential cross section in this area.

## VI. SUMMARY

We have considered the differential cross section for Compton scattering against completely occupied shells. Starting with general relativistic central-field Hartree-Fock wave functions, we have derived an expression for the differential cross section in the impulse approximation. Our new form for the cross section is quite as simple as those previously used but is more general. It is reminiscent of the one derived by Ribberfors. The difference between the two expressions is very slight near the Compton line, and all the way to the $K$ edge. On the other hand, the difference turns out to be several percent for small energies of the scattered photon below the Compton line. Here, the expression derived by us gives a smaller differential cross section than does the Ribberfors expression. Thus, theoretically, our formula should replace the previous formulas, at least below the Compton line. This means, in particular, that our expression ought to be used for small scattering angles. However, so far as completely occupied shells are concerned, the essential point with this work would be that Compton scattering has been entirely investigated within the impulse approximation. Deviations that might appear between theory and experiment have to be due to the impulse approximation, provided the contribution from higher-order terms can be neglected.

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[1]B. Williams, *Compton Scattering* (McGraw-Hill, New York, 1977).
[2]J. W. H. Dumond, Phys. Rev. **33**, 643 (1929); **36**, 146 (1930).
[3]P. Eisenberger and P. M. Platzman, Phys. Rev. A **2**, 415 (1970).
[4]A. I. Achieser and W. B. Berestezki, *Quantum-Electrodynamik* (Tuebner, Leipzig, 1962).
[5]P. Eisenberger and W. A. Reed, Phys. Rev. B **9**, 3237 (1974).
[6]J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Springer-Verlag, New York, 1980), pp. 228–235.
[7]R. Ribberfors, Phys. Rev. B **12**, 2067 (1975).
[8]A. Reineking, R. Wenskus, A. Baumann, D. Schaupp, P. Rullhusen, F. Smend, and M. Schumacher, Phys. Lett. **95A**, 29 (1983); M. V. Heller and J. R. Moreira, Phys. Rev. B **31**, 4146 (1985).
[9]J. J. Sakurai, *Advanced Quantum Mechanics* (Addison-Wesley, Reading, MA, 1982).
[10]E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970).
[11]P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).
[12]M. J. Cooper, Adv. Phys. **20**, 453 (1971).
[13]R. Ribberfors, Phys. Rev. B **12**, 3136, 1975.
[14]T. Mukoyama, J. Phys. B **15**, L785 (1982).