First correction to the nonrelativistic Compton cross section in the impulse approximation

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A correction to the nonrelativistic double differential Compton cross section within the framework of the impulse approximation is discussed. An expression for a first correction is found. The expression explains the asymmetry that is obtained in experiments where the Compton profile is measured.

I. INTRODUCTION

Within the framework of the impulse approximation, the nonrelativistic double differential Compton cross section is proportional to the Compton profile.[1,2] The Compton profile $J(p_z)$ is a symmetric function with its maximum value centered on $p_z=0$. However, experiments show small deviations from this picture. Measurements of the Compton profile result in an asymmetry.[3–5] Theoretic attempts exist to explain this effect by an exact first Born approximation.[6,7] In the present paper we will use another method to explain this effect theoretically. The method is based on the idea of an operator expansion introduced by Eisenberger and Platzman.[2] The result of this method is then used to study the asymmetry in the Compton profile. The asymmetry can be defined as

$$[J(p_z)-J(-p_z)]/J(0) ,$$

where $p_z \geq 0$, and is of the order 1–2 % in the region 0–2 a.u.[3]

Section II takes a closer look at the validity of the use of plane waves in the final states of the electron. In Sec. III an expression for a first correction to the differential cross section is elaborated. In Sec. IV this expression is tested, using momentum transforms of wave functions for hydrogenlike systems. This test is performed on aluminum. In spite of the use of simple hydrogenlike wave functions, the result agrees quite well with experiments where the asymmetry is measured. Section V deals with the validity of the impulse approximation.[2] Section VI is a summary.

II. VALIDITY OF THE USE OF PLANE WAVES IN THE FINAL STATES OF THE ELECTRON

In this section, and throughout this paper, we will assume natural units, i.e., $c=1$ and $\hbar=1$. Compton scattering will involve an incident and a scattered photon. Let us denote the momentum and energy of the incident photon by $\mathbf{k}$ and ω, respectively. The momentum and energy of the scattered photon will be denoted by $\mathbf{k}'$ and ω', respectively. The nonrelativistic double differential Compton cross section can be written as[2]

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\sum_f |\langle \psi_f | e^{i\mathbf{q}\cdot\mathbf{r}} | \psi_i \rangle|^2 \times \delta(\varepsilon_f-\varepsilon_i+\omega'-\omega) , \quad (1)$$

where $|\psi_f\rangle$ represents the final and $|\psi_i\rangle$ the initial state of the electron, and ε_f and ε_i the energies of the electron in, respectively, the final and initial state. Furthermore, r_0 is the classical radius of the electron, θ' is the scattering angle, and $\mathbf{q}$ stands for $\mathbf{k}-\mathbf{k}'$. [The quantity $q=|\mathbf{q}|$ can be written as $(k^2-2kk'\cos\theta'+k'^2)^{1/2}$, or as $(\omega^2-2\omega\omega'\cos\theta+\omega^2)^{1/2}$, since $\mathbf{k}\cdot\mathbf{k}'=kk'\cos\theta'$.] Expression (1) may be rewritten. Since we assume wave functions in the central-field approximation, we can use the relation $\hat{H}\psi=\varepsilon\psi$, and write Eq. (1) as

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\sum_f \frac{1}{2\pi}\int_{-\infty}^{\infty} dt \langle \psi_i | e^{-i\mathbf{q}\cdot\mathbf{r}} | \psi_f \rangle \langle \psi_f | e^{i\hat{H}t} e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i\hat{H}t} | \psi_i \rangle e^{i(\omega'-\omega)t} , \quad (2)$$

where we have used the well-known integral representation of the δ function. Since we are dealing with Compton scattering of photons, $|\psi_f\rangle$ will stand for a continuum state. The continuum states form a complete set together with the bound states. This means that we can sum up the continuum states as follows:

$$\frac{d^2\sigma}{d\omega' d\Omega'} = \frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\frac{1}{2\pi}\int_{-\infty}^{\infty} dt \left[\langle \psi_i | e^{-i\mathbf{q}\cdot\mathbf{r}} e^{i\hat{H}t} e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i\hat{H}t} | \psi_i \rangle - \sum_j \langle \psi_i | e^{-i\mathbf{q}\cdot\mathbf{r}} | \psi_j \rangle \langle \psi_j | e^{i\hat{H}t} e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i\hat{H}t} | \psi_i \rangle \right] e^{i(\omega'-\omega)t} , \quad (3)$$

which can be rewritten as

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\,\langle\psi_i|e^{-i\mathbf{q}\cdot\mathbf{r}}e^{i\hat{H}t}e^{i\mathbf{q}\cdot\mathbf{r}}e^{-i\hat{H}t}|\psi_i\rangle e^{i(\omega'-\omega)t}\right.$$
$$\left.-\sum_j|\langle\psi_j|e^{i\mathbf{q}\cdot\mathbf{r}}|\psi_i\rangle|^2\delta(\varepsilon_j-\varepsilon_i+\omega'-\omega)\right], \tag{4}$$

where $|\psi_j\rangle$ stands for a bound state, and ε_j its energy. The last term in Eq. (4) can be removed, since $\omega'\leq\omega+\varepsilon_i=\omega-\varepsilon_B$ in the case of Compton scattering. (The energy ε_B is the binding energy of the electron in the initial state.) Thus the Compton cross section can be written as[2]

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\,\langle\psi_i|e^{-i\mathbf{q}\cdot\mathbf{r}}e^{i\hat{H}t}e^{i\mathbf{q}\cdot\mathbf{r}}e^{-i\hat{H}t}|\psi_i\rangle e^{i(\omega'-\omega)t}\,. \tag{5}$$

The essential feature of this expression is that we have eliminated the continuum states which is the essence of this work. The advantage one gains by eliminating the continuum states ought to be quite clear because of the difficulty of working with continuum states.

An interesting point can be deduced from expression (5). Let us insert a complete set of plane-wave states in Eq. (5) as follows:

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\sum_{\mathbf{p}'}\frac{1}{V}\langle\psi_i|e^{-i\mathbf{q}\cdot\mathbf{r}}|e^{i\mathbf{p}'\cdot\mathbf{r}}\rangle\langle e^{i\mathbf{p}'\cdot\mathbf{r}}|e^{i\hat{H}t}e^{i\mathbf{q}\cdot\mathbf{r}}e^{-i\hat{H}t}|\psi_i\rangle e^{i(\omega'-\omega)t}\,. \tag{6}$$

Here, V is the normalization volume. The Hamiltonian of the electron $\hat{H}$ can be written as $\hat{H}=\hat{H}_0+V$, where $\hat{H}_0=\hat{\mathbf{p}}^2/2m$ is the Hamiltonian of a free electron, $\hat{\mathbf{p}}=-i\nabla$, and V the potential (which is isotropic in the central-field approximation). If we make use of the approximation

$$\exp(i\hat{H}t)=\exp(i\hat{H}_0t)\exp(iVt)\,,$$

which gives the approximation $\exp(-iVt)\exp(-iH_0t)$ of the operator $\exp(-i\hat{H}t)$, we can let the potential cancel out in Eq. (6), since $\exp(\pm iVt)$ and $\exp(\pm i\mathbf{q}\cdot\mathbf{r})$ commute.[2] If we do so, and use the relation

$$\hat{H}_0\exp(i\mathbf{p}\cdot\mathbf{r})=(p^2/2m)\exp(i\mathbf{p}\cdot\mathbf{r})\,,$$

expression (6) can approximately be written as

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\sum_{\mathbf{p}'}\frac{1}{V}|\langle e^{i\mathbf{p}'\cdot\mathbf{r}}|e^{i\mathbf{q}\cdot\mathbf{r}}|\psi_i\rangle|^2\delta\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}'-q^2/2m+\omega'-\omega\right]\,. \tag{7}$$

Let us now use the well-known rule

$$\lim_{V\to\infty}\frac{1}{V}\sum_{\mathbf{p}}=\left[\frac{1}{2\pi}\right]^3\int d^3p\,, \tag{8}$$

and perform the substitution $\mathbf{p}=\mathbf{p}'-\mathbf{q}$, and rewrite Eq. (7) as

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\int d^3p\,|\psi_i(\mathbf{p})|^2\delta\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}+q^2/2m+\omega'-\omega\right]\,, \tag{9}$$

where $\psi_i(\mathbf{p})$ is the momentum transform of $\psi_i(\mathbf{r})$, and can be written as

$$\psi_i(\mathbf{p})=\left[\frac{1}{2\pi}\right]^{3/2}\int d^3r\,\psi_i(\mathbf{r})e^{-i\mathbf{p}\cdot\mathbf{r}}\,. \tag{10}$$

The expression in Eq. (9) should be recognized as the usual expression for the nonrelativistic Compton cross section in the impulse approximation. The interesting point here is how we arrive at this result. The insertion of a complete set of plane waves in Eq. (5) is not an approximation. Consequently, when comparing Eqs. (2) and (6), the use of plane waves in the final states of the electron is obviously not an approximation. The potential cancellation, first introduced by Eisenberger and Platzman,[2] is the only approximation that has been carried out. The fact that one can, at least within the framework of the potential cancellation, choose final states of the electron in the form of plane waves without undertaking approximations, is entirely due to the completeness of the plane waves. The completeness of the plane waves would be the reason why the impulse approximation to a large extent works extremely well rather than the plane wave itself being a proper description of the final state of the electron. Because, if the plane wave is a proper description of the final state, i.e., a good approximation of the final state, one should get an accurate result only by replacing $\langle\psi_f|$ and ε_f in Eq. (1) with $(1/V)^{1/2}\langle e^{i\mathbf{p}'\cdot\mathbf{r}}|$ and $p'^2/2m$, respectively, and sum over $\mathbf{p}'$. However, this operation will give a less accurate result. This must be credited to the fact that the potential is not properly canceled out of the energy for the initial and final states.

Furthermore, one cannot say that a cancellation of the potential makes the plane wave become a good description of the final state as this argument would also justify a plane wave in the initial state of the electron. Thus the use of plane waves in the final states is entirely justified within the framework of the potential cancellation. The reason for this is not that the plane wave is a good approximation of the final state, although this seems to be a rather common view of the matter. The reason is apparently more subtle. However, the plane wave will, of course, be a proper description of the final state when the energy of the ejected electron is large compared with the binding energy of the active electron because the influence of the potential will be less important. This is also the requirement for the application of the impulse approximation. But here due to the fact that one takes into consideration a potential in the final state, it is apparently possible to allow the ejected electron to have energies for which the final state starts to be badly described by the plane wave.

III. FIRST CORRECTION TO THE DOUBLE DIFFERENTIAL CROSS SECTION

According to the preceding section, if we want to look for a correction term to the cross section in Eq. (9), it is only necessary to consider the approximation of

$$\exp(i\hat{H}t)\exp(i\mathbf{q}\cdot\mathbf{r})\exp(-i\hat{H}t)$$

in Eq. (6). However, we will start from expression (5), and consider the approximation of

$$\exp(-i\mathbf{q}\cdot\mathbf{r})\exp(i\hat{H}t)\exp(i\mathbf{q}\cdot\mathbf{r})\exp(-i\hat{H}t)$$

to try to find a correction to the usual nonrelativistic Compton cross section in Eq. (9).

The quantity $\exp(-i\mathbf{q}\cdot\mathbf{r})\exp(i\hat{H}t)\exp(i\mathbf{q}\cdot\mathbf{r})\exp(-i\hat{H}t)$ in Eq. (5) can be rewritten. Using the operator relation

$$\hat{H}e^{i\mathbf{q}\cdot\mathbf{r}}=e^{i\mathbf{q}\cdot\mathbf{r}}\left[\frac{1}{m}\mathbf{q}\cdot\hat{\mathbf{p}}+q^2/2m+\hat{H}\right], \tag{11}$$

we are able to obtain

$$e^{-i\mathbf{q}\cdot\mathbf{r}}e^{i\hat{H}t}e^{i\mathbf{q}\cdot\mathbf{r}}e^{-i\hat{H}t}=\exp\left[i\left[\frac{1}{m}\mathbf{q}\cdot\hat{\mathbf{p}}+q^2/2m\right]t\right]\hat{X}, \tag{12}$$

where

$$\hat{X}=\exp(-i\mathbf{q}\cdot\hat{\mathbf{p}}t/m)\exp\left[i\left[\frac{1}{m}\mathbf{q}\cdot\hat{\mathbf{p}}+\hat{H}\right]t\right]e^{-i\hat{H}t}. \tag{13}$$

Here, we have used the fact that q^2 commutes with $\mathbf{q}\cdot\hat{\mathbf{p}}$ and $\hat{H}$. If we now use this, and

$$\psi_i(\mathbf{r})=\left[\frac{1}{2\pi}\right]^{3/2}\int d^3p\,\psi_i(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{r}}, \tag{14}$$

where $\psi_i(\mathbf{p})$ is the momentum transform of $\psi_i(\mathbf{r})$, we are able to write Eq. (5) as

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\left[\frac{1}{2\pi}\right]^4\int d^3p\int d^3p'\psi_i^\dagger(\mathbf{p})\psi_i(\mathbf{p}')\int_{-\infty}^{\infty}dt\,\langle e^{i\mathbf{p}\cdot\mathbf{r}}|\hat{X}|e^{i\mathbf{p}'\cdot\mathbf{r}}\rangle\exp\left[i\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}+W\right]t\right], \tag{15}$$

where $W=q^2/2m-(\omega-\omega')$. Our intention now is to find an approximation to $\hat{X}$. Expanding $\hat{X}$, the first three terms will be as follows:[8]

$$\hat{X}=1+\frac{it}{2!}\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,\hat{H}\right]+\frac{it}{3!}\left[\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,\hat{H}\right]\right]+\left[i\hat{H}t,\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,\hat{H}\right]\right]\right]+\cdots$$

$$=1+\frac{it}{2!}\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,V\right]+\frac{it}{3!}\left[\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,V\right]\right]+\left[\frac{it}{2m}\hat{\mathbf{p}}^2,\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,V\right]\right]\right]+\cdots, \tag{16}$$

where $[\,,\,]$ stands for the usual commutator. Here, we might just take the term $it[-i\mathbf{q}\cdot\hat{\mathbf{p}}t/m,V]/2!$ as a first correction to expression (9). [If we just put $\hat{X}=1$, we will, of course, obtain expression (9).] However, in this case, we have to consider a whole expansion series of $\hat{X}$ as a first correction, and the series is

$$\hat{X}_1=\frac{it}{2!}\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,V\right]+\frac{it}{3!}\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,V\right]\right]+\frac{it}{4!}\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t,V\right]\right]\right]+\cdots, \tag{17}$$

where higher-order terms would contribute. The reason why all the terms of this series would be important is the momentum transfer $q=|\mathbf{k}-\mathbf{k}'|$. Since we are only interested in a first correction term to expression (9), the impulse approximation is still assumed to work well, which ought to mean that the momentum transfer $q=|\mathbf{k}-\mathbf{k}'|$ must be large. Thus, in this case, we would look for an expansion to $\hat{X}$, where the first term contains the factor $1/q$, the second $(1/q)^2$, and so on. (The zeroth-order term is 1.)

Returning to Eq. (15), the time t that appears in the terms in the expansion of $\hat{X}$, can be eliminated by derivation with respect to W in expression (15), since W is a constant quantity. Assuming that $\mathbf{q}\cdot\mathbf{p}$ can be written as $-qp_z$, we will obtain the δ function $\delta(W-qp_z/m)$ in Eq. (15). Let us also assume that we can retain this δ function, until we are able to perform an integration, which removes the δ function. On the basis of these assumptions, after the integration, we are able to put $\partial/\partial W=(m/q)(\partial/\partial p_z)$. This last equation tells us that all

terms of $\hat{X}_1$ contribute in the first order with respect to $1/q$. The operator $\hat{X}_1$ can be rewritten into a more convenient form as follows:[8]

$$\hat{X}_1=\sum_{n=1}^{\infty}\frac{it}{(n+1)!}\left[\left[\frac{\partial}{\partial\lambda}\right]^n\exp\left[-i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t\lambda\right]\times V\exp\left[i\frac{\mathbf{q}\cdot\hat{\mathbf{p}}}{m}t\lambda\right]\right]_{\lambda=0}. \tag{18}$$

The term $[i\hat{\mathbf{p}}^2t/2m,[-\mathbf{q}\cdot\hat{\mathbf{p}}t/m,iVt]]/3!$ in Eq. (16) contributes in the second order with respect to $1/q$. This term belongs to a series, where all terms will contribute in the second order. The term $[i\hat{\mathbf{p}}^2t/2m,[-i\mathbf{q}\cdot\hat{\mathbf{p}}t/m,iVt]]3!$ is the only one that will be considered in this paper; see Sec. IV. Let us denote this term by $\hat{X}_2$. Since $[\mathbf{q}\cdot\hat{\mathbf{p}},\hat{\mathbf{p}}^2]=0$, we can rewrite $\hat{X}_2$ as

$$\hat{X}_2=-2\frac{it}{3!}\left[\frac{it}{2m}\right]^2[\mathbf{q}\cdot\hat{\mathbf{p}},[\hat{\mathbf{p}}^2,V]]\,. \tag{19}$$

Let us approximate $\hat{X}$ with $\hat{X}=1+\hat{X}_1$, and try to elaborate a first correction to Eq. (9). The calculation will, in the present paper, be restricted to completely occupied shells. In the central-field approximation, the initial wave function $\psi_i(\mathbf{r})$ can be written as $R_{nl}(r)Y_{lm}(\theta,\phi)$, where n, l, and m are the usual quantum numbers, and Y_{lm} stands for the spherical harmonic function. The momentum transform of $\psi_i(\mathbf{r})$ can be defined as follows:

$$\psi_i(\mathbf{p})=\left[\frac{1}{2\pi}\right]^{3/2}\int d^3r\,\psi_i(\mathbf{r})e^{-i\mathbf{p}\cdot\mathbf{r}}=(-i)^l\chi_{nl}(p)Y_{lm}(\theta_p,\phi_p)\,, \tag{20}$$

where p, θ_p, and ϕ_p are the spherical coordinates in momentum space,

$$\chi_{nl}(p)=\left[\frac{2}{\pi}\right]^{1/2}\int_0^{\infty}r^2dr\,R_{nl}(r)j_l(pr)\,, \tag{21}$$

and j_l stands for the spherical Bessel function. If we now use Eq. (20), the addition theorem[8,9]

$$\sum_{m=-l}^{l}Y_{lm}^*(\theta_{p'},\phi_{p'})Y_{lm}(\theta_p,\phi_p)=\frac{2l+1}{4\pi}P_l(\mathbf{p}\cdot\mathbf{p}'/pp')\,, \tag{22}$$

where P_l stands for the Legendre polynomial of degree l, and set $\hat{X}=1+\hat{X}_1$, expression (15) can be written as

$$\frac{d^2\sigma}{d\omega'd\Omega'}=\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\frac{2l+1}{4\pi}\int d^3p\,|\chi_{nl}(p)|^2\delta\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}+W\right]+\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\frac{2l+1}{4\pi}\left[\frac{1}{2\pi}\right]^4\int d^3p\int d^3p'\chi_{nl}(p)\chi_{nl}(p')P_l(\mathbf{p}\cdot\mathbf{p}'/pp')\times\int_{-\infty}^{\infty}dt\langle e^{i\mathbf{p}\cdot\mathbf{r}}|\hat{X}_1|e^{i\mathbf{p}'\cdot\mathbf{r}}\rangle\exp\left[i\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}+W\right]t\right], \tag{23}$$

for a completely occupied shell. Here, the spin is not included. Let us define the usual Compton profile for a completely occupied shell as

$$J_0(p_z)=\frac{q}{m}\frac{2l+1}{4\pi}\int d^3p\,|\chi_{nl}(p)|^2\delta\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}+W\right]=\frac{2l+1}{4\pi}\int_{|p_z|}^{\infty}dp\,2\pi p\,|\chi_{nl}(p)|^2\,. \tag{24}$$

The first correction to J_0, which also will be a function of p_z, is now defined as

$$J_1(p_z)=\frac{q}{m}\frac{2l+1}{4\pi}\left[\frac{1}{2\pi}\right]^4\int d^3p\int d^3p'\chi_{nl}(p)\chi_{nl}(p')P_l(\mathbf{p}\cdot\mathbf{p}'/pp')\int_{-\infty}^{\infty}dt\langle e^{i\mathbf{p}\cdot\mathbf{r}}|\hat{X}_1|e^{i\mathbf{p}'\cdot\mathbf{r}}\rangle\exp\left[i\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}+W\right]t\right]\,. \tag{25}$$

The double differential Compton cross section can now be written in quite a simple form as follows:

$$\frac{d^2\sigma}{d\omega'd\Omega'}=\frac{r_0^2\omega'}{\omega}\frac{1+\cos^2\theta'}{2}\frac{m}{q}J(p_z)\,, \tag{26}$$

where

$$J(p_z)=J_0(p_z)+J_1(p_z)\,. \tag{27}$$

The last task now is to make $J_1(p_z)$ as simple as possible. Using Eq. (18) in expression (25), we are able to show the following:

$$J_1(p_z)=\sum_{n=1}^{\infty}\frac{1}{(n+1)!}\left[\left[\frac{\partial}{\partial\lambda}\right]^nC(\lambda)\right]_{\lambda=0}, \tag{28}$$

where

$$C(\lambda)=\frac{\partial}{\partial W}\frac{q}{m}\frac{2l+1}{4\pi}\left[\frac{1}{2\pi}\right]^4\int d^3p\int d^3p'\chi_{nl}(p)\chi_{nl}(p')P_l(\mathbf{p}\cdot\mathbf{p}'/pp')$$
$$\times\int_{-\infty}^{\infty}dt\langle e^{i\mathbf{p}\cdot\mathbf{r}}|V|e^{i\mathbf{p}'\cdot\mathbf{r}}\rangle\exp\left[i\frac{1}{m}\mathbf{q}\cdot(\mathbf{p}-\lambda\mathbf{p}+\lambda\mathbf{p}')t+iWt\right]. \tag{29}$$

Expression (28) can be rewritten in a more convenient form as follows:

$$J_1(p_z)=\sum_{n=2}^{\infty}\frac{1}{n!}\left[\left[\frac{\partial}{\partial\lambda}\right]^n\int_{\lambda_0}^{\lambda}C(\lambda')d\lambda'\right]_{\lambda=0}=\int_{\lambda_0}^{\lambda=1}C(\lambda')d\lambda'-\int_{\lambda_0}^{\lambda=0}C(\lambda')d\lambda'-C(0)$$
$$=\int_0^1 d\lambda\,C(\lambda)-C(0)\,, \tag{30}$$

where we have simply made an identification with a Taylor-series expansion. We will now focus our attention on a simplification of $C(\lambda)$. Using the momentum transform

$$V(\mathbf{p})=\left[\frac{1}{2\pi}\right]^{3/2}\int d^3r\,V(\mathbf{r})e^{-i\mathbf{p}\cdot\mathbf{r}}\,, \tag{31}$$

we promptly get

$$C(\lambda)=\frac{\partial}{\partial W}\frac{q}{m}\frac{2l+1}{4\pi}\left[\frac{1}{2\pi}\right]^{3/2}\int d^3p\int d^3p'\chi_{nl}(p)\chi_{nl}(p')P_l(\mathbf{p}\cdot\mathbf{p}'/pp')V(\mathbf{p}-\mathbf{p}')\delta\left[\frac{1}{m}\mathbf{q}\cdot(\mathbf{p}-\lambda\mathbf{p}+\lambda\mathbf{p}')+W\right], \tag{32}$$

from Eq. (29). In this case, the integration order is not important. Thus we can do the change $\mathbf{p}'-\mathbf{p}$ to $\mathbf{p}'$, and write Eq. (32) as

$$C(\lambda)=\frac{\partial}{\partial W}\frac{q}{m}\frac{2l+1}{4\pi}\left[\frac{1}{2\pi}\right]^{3/2}\int d^3p\int d^3p'\chi_{nl}(p)\chi_{nl}(|\mathbf{p}'+\mathbf{p}|)P_l\left[\frac{\mathbf{p}\cdot(\mathbf{p}'+\mathbf{p})}{p|\mathbf{p}'+\mathbf{p}|}\right]V(-\mathbf{p}')\delta\left[\frac{1}{m}\mathbf{q}\cdot(\mathbf{p}+\lambda\mathbf{p}')+W\right]. \tag{33}$$

The next step is to do the change $\mathbf{p}+\lambda\mathbf{p}'$ to $\mathbf{p}$, which results in

$$C(\lambda)=\frac{\partial}{\partial W}\frac{q}{m}\frac{2l+1}{4\pi}\left[\frac{1}{2\pi}\right]^{3/2}\int d^3p\,\delta\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}+W\right]\int d^3p'\chi_{nl}(|\mathbf{p}-\lambda\mathbf{p}'|)\chi_{nl}(|\mathbf{p}'+\mathbf{p}-\lambda\mathbf{p}'|)$$
$$\times P_l\left[\frac{(\mathbf{p}-\lambda\mathbf{p}')\cdot(\mathbf{p}'+\mathbf{p}-\lambda\mathbf{p}')}{|\mathbf{p}-\lambda\mathbf{p}'||\mathbf{p}'+\mathbf{p}-\lambda\mathbf{p}'|}\right]V(-\mathbf{p}')\,. \tag{34}$$

Let us now use the fact that the potential V is isotropic in the central-field approximation, i.e., $V(\mathbf{r})=V(r)$, and $V(\mathbf{p})=V(p)$. Since we integrate over the whole $\mathbf{p}'$ space in Eq. (34), we are able to make the choice $\mathbf{p}\cdot\mathbf{p}'=pp'\cos\theta$. Utilizing this choice, we can show the following:

$$C(\lambda)=\frac{\partial}{\partial W}\frac{q}{m}\frac{2l+1}{4\pi}\left[\frac{1}{2\pi}\right]^{1/2}\int d^3p\,\delta\left[\frac{1}{m}\mathbf{q}\cdot\mathbf{p}+W\right]\int_{-1}^{1}dt\int_0^{\infty}p'^2dp'\chi_{nl}(p_1')\chi_{nl}(p_2')P_l[(p_1'^2+p_2'^2-p'^2)/2p_1'p_2']V(p')\,, \tag{35}$$

where

$$p_1'=(p^2+\lambda^2p'^2-2\lambda pp't)^{1/2}\,, \tag{36}$$

and

$$p_2'=[p^2+(1-\lambda)^2p'^2+2(1-\lambda)pp't]^{1/2}\,. \tag{37}$$

Now, since we also integrate over the whole $\mathbf{p}$ space, it is possible to make the choice $\mathbf{q}\cdot\mathbf{p}=-qp_z$, and obtain

$$C(\lambda)=\frac{\partial}{\partial W}\frac{2l+1}{4\pi}(2\pi)^{1/2}\int_{|p_z|}^{\infty}p\,dp\int_{-1}^{1}dt\int_0^{\infty}p'^2dp'\chi_{nl}(p_1')\chi_{nl}(p_2')P_l[(p_1'^2+p_2'^2-p'^2)/2p_1'p_2']V(p')\,, \tag{38}$$

where

$$p_z=\frac{m}{q}W=\tfrac{1}{2}q-\frac{m}{q}(\omega-\omega') \ . \tag{39}$$

The definition of p_z in Eq. (39) is the one usually chosen. Using this definition, we can perform the derivation regarding W in expression (38), and finally get

$$C(\lambda)=-p_z\frac{m}{q}\frac{2l+1}{4\pi}(2\pi)^{1/2}\int_{-1}^{1}dt\int_0^\infty p^2dp\ V(p)\chi_{nl}(p_1)\chi_{nl}(p_2)P_l[(p_1^2+p_2^2-p^2)/2p_1p_2] \ , \tag{40}$$

where

$$p_1=(p_z^2+\lambda^2p^2-2\lambda p_zpt)^{1/2} \ , \tag{41}$$

and

$$p_2=[p_z^2+(1-\lambda)^2p^2+2(1-\lambda)p_zpt]^{1/2} \ . \tag{42}$$

Here, we have simply used the notation p instead of p', since p_z replaces p after the derivation in Eq. (38). The expression in Eq. (40) is the important one in this paper, together with Eq. (30). These expressions make it possible to calculate a first correction to the double differential Compton cross section in the impulse approximation.

IV. ASYMMETRY

The expression in Eq. (40) is asymmetric with respect to p_z. How one defines p_z is therefore very important. [Besides the definition in Eq. (39), we are able to define p_z as $p_z=(m/q)(\omega-\omega')-(q/2)$.] If we want to study the asymmetry in the Compton profile, the sign in the asymmetry will depend on how we define p_z. Thus, considering the asymmetry, one must always clearly state what definition of p_z is being used. In this paper we will always use the definition in Eq. (39). In order to test the asymmetry, arising from expression (40), we consider hydrogenlike wave functions. The material that we will focus our interest on is aluminum. Hence, if the three outermost electrons of aluminum are treated as a Fermi-Dirac gas, we are able to use the momentum transforms of $1s$, $2s$, and $2p$ electrons for a hydrogenlike system as the momentum transforms of the $1s$, $2s$, and $2p$ electrons of aluminum, respectively. Thus we need the functions $\chi_{10}(p)$, $\chi_{20}(p)$, and $\chi_{21}(p)$, defined by Eq. (21), for a hydrogenlike system. Using Eq. (21) for hydrogenlike wave functions, these three functions can be written as

$$\chi_{10}(p)=\left[2\frac{\varepsilon}{\pi}\right]^{1/2}\frac{4\varepsilon^2}{(\varepsilon^2+p^2)^2} \ , \tag{43}$$

$$\chi_{20}(p)=32\varepsilon^2\left[\frac{\varepsilon}{\pi}\right]^{1/2}\frac{4p^2-\varepsilon^2}{(\varepsilon^2+4p^2)^3} \ , \tag{44}$$

and

$$\chi_{21}(p)=64\varepsilon^2\left[\frac{4\varepsilon}{3\pi}\right]^{1/2}\frac{\varepsilon^3p}{(\varepsilon^2+4p^2)^3} \ , \tag{45}$$

where $\varepsilon=\alpha mZ$; α is the fine-structure constant, and Z is the atomic number. The potential for a hydrogenlike system can be written as

$$V(r)=-\frac{\varepsilon}{mr} \ , \tag{46}$$

which gives the momentum transform

$$V(p)=\left[\frac{1}{2\pi}\right]^{3/2}\int d^3r\ V(r)e^{-i\mathbf{p}\cdot\mathbf{r}}$$
$$=-\left[\frac{2}{\pi}\right]^{1/2}\frac{\varepsilon}{mp^2} \ . \tag{47}$$

Furthermore, for a hydrogenlike system, the energy of an electron is

$$E_{nl}=-\frac{\varepsilon^2}{2mn^2} \ , \tag{48}$$

where n and l are quantum numbers. This equation makes it also possible to write ε as

$$\varepsilon=n(2m|E_{nl}|)^{1/2} \ . \tag{49}$$

To get proper energies, one can use Eq. (49) to calculate "effective" values in ε. Using binding energies of the $1s$, $2s$, and $2p$ shells of aluminum one simply replaces $|E_{nl}|$ with the corresponding binding energy of aluminum. However, we will use another method which gives proper momentum transforms, i.e., proper wave functions, rather than proper energies. Using tabulated Compton profiles,[10] we put $J_0(0)$ equal to the tabulated value, and calculate an effective value in ε. Let us make a comment here. If we calculate effective values in ε according to Eq. (49), we will get a result, i.e., an asymmetry, that differs from the result where the values in ε are calculated according to $J_0(0)$ being equal to the tabulated value. However, no matter how we choose to calculate ε, the tendency of the result is the same. [Using Eq. (49) to calculate the values in ε, we will get a larger asymmetry than what is deduced in this paper, but with the same feature.] The problem here is that we cannot get a proper wave function and a proper potential at the same time. In this paper we have made the choice that is likely the most correct one, i.e., calculated the effective values in ε according to $J_0(0)$ being equal to the tabulated value. For knowledge about problems closely related to the above, one may consult Issolah *et al.*[11]

We are now able to derive $J_0(p_z)$ for completely occupied $1s$, $2s$, and $2p$ shells. The evaluation of the integrals

is straightforward. Using Eqs. (43)–(45) in Eq. (24), we can show that the expressions of $J_0(p_z)$ for the $1s$, $2s$, and $2p$ shells are

$$J_0^{1s}(p_z)=\frac{8\varepsilon^5}{3\pi(\varepsilon^2+p_z^2)^3}\ , \tag{50}$$

$$J_0^{2s}(p_z)=(\varepsilon^4-10\varepsilon^2p_z^2+40p_z^4)\frac{128\varepsilon^5}{15\pi(\varepsilon^2+4p_z^2)^5}\ , \tag{51}$$

and

$$J_0^{2p}(p_z)=(\varepsilon^2+20p_z^2)\frac{64\varepsilon^7}{5\pi(\varepsilon^2+4p_z^2)^5}\ , \tag{52}$$

respectively. [Note: Here, the spin is not considered, i.e., expressions (50) and (51) include one s electron, and expression (52) three p electrons.] Considering the derivation of the quantity $J_1(p_z)$, here, the integral evaluations will be more extensive. Putting Eq. (40) in (30), we have to solve one double and one triple integral. However, it is possible to solve the resulting integrals, and obtain a result for $J_1(p_z)$ that corresponds to the one for $J_0(p_z)$. The result will be as follows:

$$J_1^{1s}(p_z)=J_0^{1s}(p_z)\frac{1}{q}[2\varepsilon\arctan(p_z/\varepsilon)-\tfrac{3}{2}p_z]\ , \tag{53}$$

$$J_1^{2s}(p_z)=J_0^{2s}(p_z)\frac{1}{q}\left[2\varepsilon\arctan(2p_z/\varepsilon)-\frac{5}{4}\frac{\varepsilon^4+48p_z^4}{\varepsilon^4-10\varepsilon^2p_z^2+40p_z^4}p_z\right], \tag{54}$$

and

$$J_1^{2p}(p_z)=J_0^{2p}(p_z)\frac{1}{q}\left[2\varepsilon\arctan(2p_z/\varepsilon)-\frac{2}{3}\frac{10\varepsilon^2+60p_z^2}{\varepsilon^2+20p_z^2}p_z\right]. \tag{55}$$

Here, expression (53) and (54) include one s electron, and expression (55) three p electrons. Note: This result is almost the same as that derived by Gasser and Tavard[6] using an exact first Born approximation. However, we have received another result for the $2s$ shell.

The asymmetry is defined as $[J(p_z)-J(p_z)]/J(0)$, where $p_z\geq 0$. The asymmetry will be due to $J_1(p_z)$, since $J(p_z)=J_0(p_z)+J_1(p_z)$, and $J_0(p_z)$ is symmetric. Considering Eqs. (53)–(55), $J_1(p_z)$ will be small compared to $J_0(p_z)$ when $|p_z|/q$ is small. The next term that is added to $J(p_z)$ contains the factor $(1/q)^2$. If q is large, this term should be smaller than $J_1(p_z)$. In the next section we will take a closer look at such problems. However, let us state here that $J_1(p_z)$ is a good first correction to $J_0(p_z)$ when $|p_z|/q\ll 1$ and $\varepsilon/q\ll 1$. Consequently, the expression

$$[J(p_z)-J(-p_z)]/J(0)=[J_1(p_z)-J_1(-p_z)]/J_0(0)$$

for the asymmetry is accurate when $|p_z|/q\ll 1$ and $\varepsilon/q\ll 1$. The condition $|p_z|/q\ll 1$ is no problem, since the asymmetry is only important near $p_z=0$, due to its definition. But we might meet with difficulties owing to

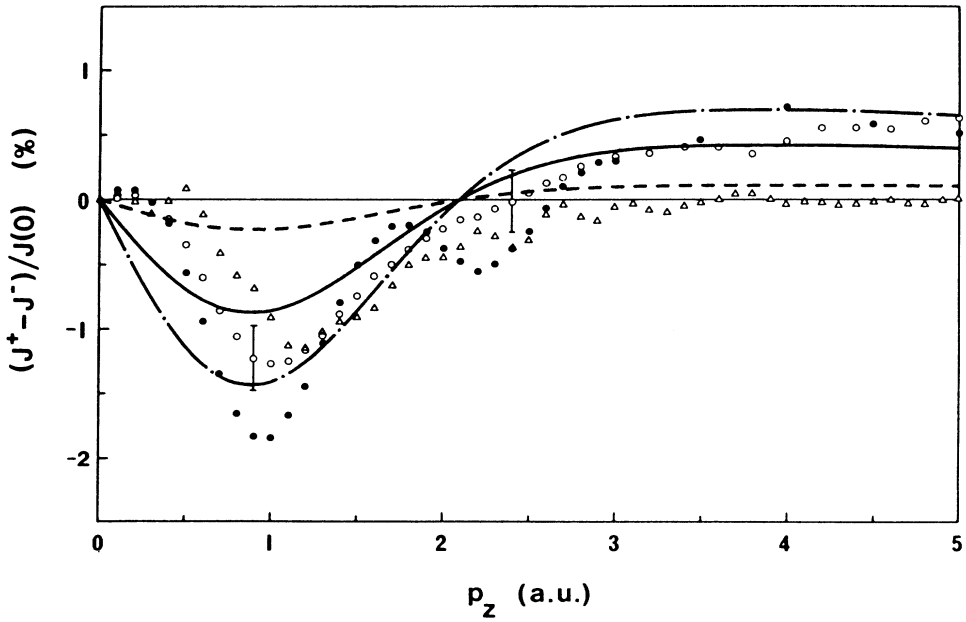

FIG. 1. The asymmetry $(J^+-J^-)/J(0)$ expressed in percent of $J(0)$ for aluminum. J^+ is the value of the profile on the high-energy (low-momentum-transfer) side. The scattering angle θ' is 170°. The experimental results for sample thicknesses of 0.6 mm (Δ), 0.25 mm (○), and 0.025 mm (●), are obtained using 59.54 keV photons. The dashed, the solid, and the dashed-dotted curves are the theoretical results for the photon energies 279.1, 59.54, and 35 keV, respectively.

the quantity ε/q. (Under typical experimental conditions, the quantity ε/q is not particularly small for a $1s$ electron of an atom with many electrons.) However, we can make an exception for an atom with many electrons. In fact, we might allow ε/q to be close to 1 for the innermost electrons, even if this means that the first correction $J_1(p_z)$, and maybe also the impulse approximation, do not work well for these electrons. The reason is simply that the Compton profile for the outermost electrons is bigger than the Compton profile for the innermost electrons near $p_z=0$, and that the asymmetry is only important near $p_z=0$. Thus the asymmetry seems to be an adequate test of our correction term $J_1(p_z)$.

Let us now compare our result with experiments. Figure 1 shows a comparison between experiments and theory for aluminum. Here, we have simply put our theoretical results in a figure, which shows experiments in aluminum for the energy 59.54 keV of the incident photon and scattering angle 170°. The figure is taken from Ref. 3. (Note: Here, we have used the simpler notation $(J^+-J^-)/J(0)$, taken from Ref. 3, instead of $[J(p_z)-J(-p_z)]/J(0)$.) We have put three theoretical curves in the figure. Two of them, the dashed one which shows the theoretical result for the energy 279.1 keV and the angle 170°, and the dashed-dotted one which shows the theoretical result for 35 keV and 170°, have been added to illustrate the energy dependence of the asymmetry. The solid curve, which shows the theoretical result for the energy 59.54 keV and the angle 170°, corresponds to the experiments. This curve seems also to be the one that gives the best agreement between theory and experiments. On the whole, the agreement is very good.

The comparison between theory and experiments for aluminum in Fig. 1 is the important matter in this paper. However, one can make out an interesting point for beryllium. Figure 2 shows theoretical results for beryllium. (Here, we have assumed a Fermi-Dirac gas for the $2s$ electrons.) The solid curve is the result for the energy

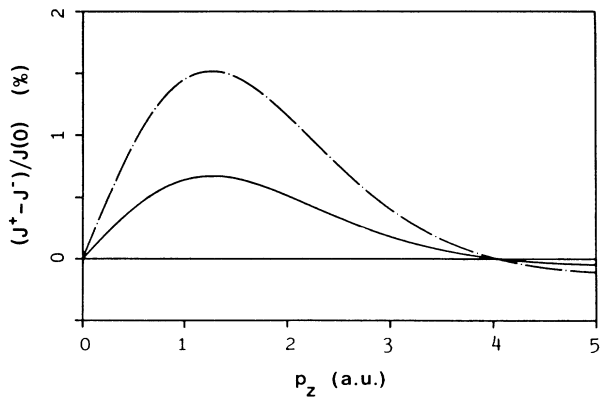

FIG. 2. The asymmetry $(J^+-J^-)/J(0)$ in percent of $J(0)$ for beryllium. The solid curve shows the theoretical result for the energy 59.54 keV and the angle 170°. The dashed-dotted curve is the result for 25 keV and 170°.

59.54 keV and the angle 170°, and the dashed-dotted curve is the result for 25 keV and 170°. The interesting thing here is that the asymmetry has changed sign. Furthermore, the asymmetry is not particularly large for the energy 59.54 keV, which may be the reason why Manninen and co-workers[3,4] failed to reveal any asymmetry for beryllium.

V. VALIDITY OF THE IMPULSE APPROXIMATION

Let us start this section by considering a second correction term to J_0 for a hydrogenlike $1s$ electron. A second correction term can be found by using expression (19) for the operator $\hat{X}_2$ in Eq. (25), instead of $\hat{X}_1$. For a $1s$ electron, we can show that this term, denoted by J_2^{1s}, can be written as

$$J_2^{1s}(p_z)=J_0^{1s}(p_z)\left[\frac{1}{q}\right]^2\left[-4\varepsilon p_z\arctan(p_z/\varepsilon)+\frac{6\varepsilon^2p_z^2}{\varepsilon^2+p_z^2}+\tfrac{3}{4}p_z^2-\tfrac{1}{4}\varepsilon^2\right]. \quad (56)$$

We cannot be certain using J_2^{1s} as a second correction term, since this term belongs to an infinite series, where all terms contribute in second order with respect to $1/q$. However, the interesting point here is that ε/q, and $|p_z|/q$ as well, must be small, if J_2^{1s} shall be smaller than J_0^{1s}. (Considering J_1^{1s}, it is enough to require that $|p_z|/q$ is small.) Thus, to be sure that $J_1(p_z)$ is a good first correction to $J_0(p_z)$, we have to stipulate that $|p_z|/q\ll1$ and $\varepsilon/q\ll1$. We can always choose a region where $|p_z|/q$ is small. The critical quantity is ε/q. When ε/q is close to 1, we must consider more correction terms to $J_0(p_z)$ than $J_1(p_z)$. Of course, if we choose a region where $|p_z|/q$ is close to 1, we must also consider more terms than $J_1(p_z)$, even if $\varepsilon/q\ll1$. This can be an overwhelming task. It might be better to only consider $J_0(p_z)$, since the impulse approximation has turned out to work extremely well. In other words, one cannot say for sure that the impulse approximation is bad, when ε/q is close to 1, and/or $|p_z|/q$ is close to 1. However, when the impulse approximation works badly, either $|p_z|/q$ or ε/q must be close to 1. On the other hand, when $|p_z|/q\ll1$ and $\varepsilon/q\ll1$, the impulse approximation must work well.

The critical quantity is apparently ε/q. Figure 3 shows the maximal deviation in percent of $J(0)$ between the exact expression derived by Eisenberger and Platzman,[2] and the impulse approximation. The figure shows practically a straight line. The maximal deviation in percent of $J(0)$ can be written as about $10\varepsilon/q$. Furthermore, it also turns out that the maximal deviation was practically independent of the energy of the incident photon and scattering angle. However, the curve in Fig. 3 is the result for the energy 59.54 keV and the angle 90°. If we make the same calculation for our first $1s$-correction term, i.e., calculate the maximal deviation between the first $1s$-correction term and the impulse approximation, the maximal deviation in percent of $J(0)$ can also in this case be written as about $10\varepsilon/q$. (Note: The maximal de-

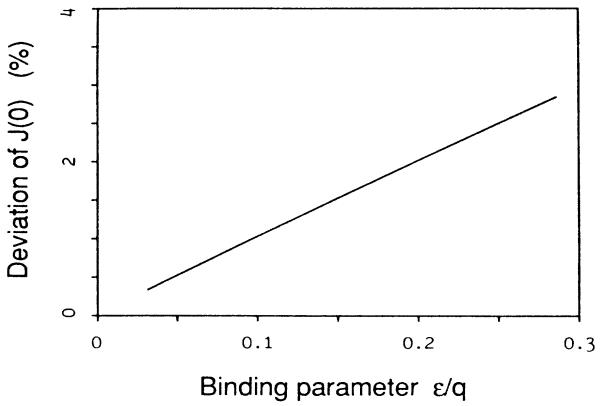

FIG. 3. The maximal deviation expressed in percent of $J(0)$ between the exact expression derived by Eisenberger and Platzman, and the impulse approximation as a function of the binding parameter ε/q. (Here, the choices of the energy of the incident photon and scattering angle θ' are, respectively, 59.54 keV and 90°.)

viation for our first $2s$-correction and $2p$-correction terms are approximately $20\varepsilon/q$ and $-20\varepsilon/q$, respectively.) Thus the magnitude of ε/q ought to be an adequate quantity to study if one wants to know the accuracy of the impulse approximation.

Let us complete this section by mentioning the Compton defect,[11–13] i.e., the deviation of the Compton profile maximum from the prediction of the impulse approximation. If we calculate the Compton defect for our first $1s$-correction term, we obtain the deviation $\varepsilon_B/6$ towards higher (photon) energies with ε_B as the ionization energy for the $1s$ electron. This result is in agreement with earlier calculated results.[12] [Note: In this case, we have assumed that ε can be written as $\varepsilon=(2m\varepsilon_B)^{1/2}$, i.e., that Eq. (49) is valid. The reason is simply that we can express the Compton defect in the binding or ionization energy. Of course, if we calculate ε according to $J_0(0)$ being equal to the tabulated value,[10] we will get a Compton defect that differs from $\varepsilon_B/6$. In Ref. 11 one can also deduce that different Compton defects are obtained for screened hydrogenlike wave functions and Hartree-Fock wave functions.] The result $\varepsilon_B/6$ may be rewritten as $\Delta\lambda=\lambda^2\varepsilon_B/6hc$ with $\Delta\lambda$ as the shift in wavelength between the two Compton profile maxima. Here, λ is the wavelength for the incident photon, and h and c are, respectively, Planck's constant and the velocity of light.

VI. SUMMARY

We have made an operator expansion of the nonrelativistic double differential cross section for Compton scattering of photons for hydrogenlike wave functions. The basic tools are commutator combinations between the potential $V(\mathbf{r})$ and $i\mathbf{q}\cdot\hat{\mathbf{p}}t/m$ with $\hat{\mathbf{p}}$ equal to the momentum operator and $\mathbf{q}$ equal to the scattering vector for the photons. Results for the asymmetry are calculated for aluminum and beryllium. Good agreement is achieved for aluminum when compared with experimental results.[3] For beryllium we predict an overall positive asymmetry. We also obtain a simple rule for the maximal deviation between our calculated differential cross section and the impulse approximation. This maximal deviation is proportional to ε/q. The practical result of this is that the maximal error when using the impulse approximation is proportional to the square root of the binding energy divided by the absolute value of the scattering vector. This relationship is valid for $1s$, $2s$, and $2p$ hydrogenlike wave functions and is expected to be valid approximately even for an arbitrary wave function.

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