Cross section for Compton scattering by polarized bound electrons

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The double-differential cross section for inelastic x-ray scattering by polarized bound electrons has been calculated within the so-called impulse approximation. In this way the analysis of Ribberfors [Phys. Rev. B **12**, 2067 (1975)] has been extended to the case of magnetic Compton scattering.

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It is well known that circularly polarized x rays couple to the electron spin, which accounts for a spin-dependent term of Compton scattering. Measuring the Doppler broadening of the scattered radiation allows the determination of the momentum distribution of unpaired electrons in ferro- or ferrimagnetic materials. Since the pioneering work of Sakai and Ono [1] in 1976 this technique has attracted increasing attention. This is mainly due to the fact that in recent years strong sources of circularly polarized x-ray radiation have become available with the advent of synchrotron radiation from modern lepton storage rings. Here, either the out-of-plane technique has been used or—rather recently—special insertion devices have been developed as elliptical multipole wigglers. A feature that makes Compton scattering so interesting as a probe of the electronic structure of matter is that, within the so-called impulse approximation [2], the double-differential cross section of the inelastically scattered photon becomes simply proportional to the Compton profile, which in the case of magnetic materials is a two-dimensional integration over the momentum density ρ_m of the unpaired electrons:

$$J_m(p_z)=\int\int \rho_m(\mathbf{p})dp_y dp_x, \tag{1}$$

where the z axis is parallel to the momentum transfer vector $\mathbf{q}$ (see below). Up to now it has been assumed that the proportionality factor is in essence the single-differential cross section for the scattering of polarized radiation from polarized electrons at rest. This cross section was derived by Lipps and Tolhoek [3] in 1954. The increasing accuracy of modern magnetic Compton profile measurements [4–9] makes it desirable to improve this approximation. In a series of papers Grotch and co-workers [10–12] have calculated cross sections for spin-dependent Compton scattering from *bound* electrons by an expansion of the quantum electrodynamic Hamiltonian by means of a generalized Foldy-Wouthuysen transformation. Inspired by its success we want to follow, in this contribution, the much simpler approach of Ribberfors [13] by extending the Lipps-Tolhoek cross section to moving electrons and applying the impulse approximation. Suppose a photon with four-momentum $k=(\mathbf{k},\omega)$ is scattered at a moving electron with $p=(\mathbf{p},E)$ resulting in the final four-momenta $k'=(\mathbf{k}',\omega')$ and $p'=(\mathbf{p}',E')$. Guided by the equivalent expressions for nonmagnetic scattering as developed by Ribberfors [13] we obtain for the magnetic double-differential cross section

$$\frac{d^2\sigma_m}{d\omega' d\Omega'}=\frac{\alpha^2}{2}\frac{\omega'}{\omega}\int d^3\mathbf{p}\,\frac{X_m\rho_m(\mathbf{p})}{EE'}\,\delta(E+\omega-E'-\omega'), \tag{2}$$

where $\rho_m=\rho_\uparrow-\rho_\downarrow$ is the difference of the momentum density for spin-up and spin-down electrons, and the cross-section function X_m reads

$$\begin{aligned}X_m&=P_3(f-1)(fk\cdot S+k'\cdot S)\\&=P_3(f-1)[f\mathbf{k}+\mathbf{k}'+(fh+h')\mathbf{p}]\cdot\mathbf{S},\end{aligned} \tag{3}$$

where

$$\begin{aligned}h&=\mathbf{k}\cdot\mathbf{p}/(E+1)-\omega,\\h'&=\mathbf{k}'\cdot\mathbf{p}/(E+1)-\omega',\end{aligned} \tag{4}$$

and $f=1+1/K-1/K'$ with $K=-k\cdot p$ and $K'=-k'\cdot p=K+k\cdot k'$. We use the so-called natural units $\hbar=m=c=1$; i.e., $e^2=\alpha$, the fine-structure constant. The spin four-vector S has the components

$$S=(\mathbf{S}+\mathbf{p}\cdot(\mathbf{p}\cdot\mathbf{S})/(E+1),\mathbf{p}\cdot\mathbf{S}) \tag{5}$$

and becomes a spacelike unit vector in the rest frame of the electron [14,15]. It is easy to show that in the electron rest frame $f=\cos\Theta$, where Θ is the photon scattering angle. P_3 in Eq. (3) is the Stokes parameter for circularly polarized x rays. Our sign convention means $P_3>0$ if the electric-field vector rotates clockwise for an observer looking in the $\hat{\mathbf{k}}$ direction. X_m is written in terms of invariants, i.e., it holds in any coordinate system. For instance, going to the rest frame of the electron, the cross-section function of Lipps and Tolhoek [3] is reproduced.

If the initial momentum $\mathbf{p}$ of the electron is small, i.e., $p\ll 1$, as holds for valence electrons in magnetic materials, one can consider only linear corrections in $\mathbf{p}$ to the Lipps-Tolhoek cross section. Direct expansion of Eq. (3) yields

$$X_m\cong X_{m0}+X_{m1}, \tag{6}$$

with

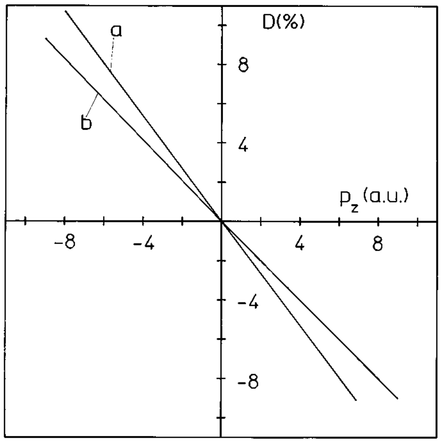

FIG. 1. The relative deviation of the cross section of Eq. (8) from that of Lipps and Tolhoek [3]. Curve *a*: ω=48 keV, Θ=160°, $\phi_S=\pi$, Ref. [9]; curve *b*: ω=129 keV, Θ=145°, Θ_S=30°, ϕ_S=0°, Ref. [16].

$$X_{m0}=P_3(\cos\Theta-1)(\mathbf{k}\cos\Theta+\mathbf{k}')\cdot\mathbf{S},$$
$$X_{m1}=P_3\{(1-\cos\Theta)(\omega\cos\Theta+\omega')\mathbf{p}+\eta[(2\cos\Theta-1)\mathbf{k}+\mathbf{k}']\}\cdot\mathbf{S}, \tag{7}$$

where

$$\eta=\frac{\mathbf{p}\cdot\mathbf{k}}{\omega^2}-\frac{\mathbf{p}\cdot\mathbf{k}'}{\omega'^2}-\frac{\mathbf{p}\cdot\mathbf{q}}{\omega\omega'}.$$

Following the analysis of Ribberfors [13] we obtain from Eq. (2), within a good approximation, the cross section in its factorized form

$$\frac{d^2\sigma_m}{d\omega' d\Omega'}=\frac{\alpha^2}{2}\frac{\omega'}{q\omega}\tilde{X}_m J_m(p_z), \tag{8}$$

with

$$\tilde{X}_m=\tilde{X}_{m0}+\tilde{X}_{m1}, \tag{9}$$

where

$$\tilde{X}_{m0}=P_3(\cos\Theta-1)(A\cos\Theta+B),$$
$$\tilde{X}_{m1}=P_3p_z\{(1-\cos\Theta)(\omega\cos\Theta+\omega')C+\tilde{\eta}[(2\cos\Theta-1)A+B]\}/q. \tag{10}$$

Using the notation

$$A=\omega\cos\Theta_S,$$
$$B=\omega'(\sin\Theta\sin\Theta_S\cos\phi_S+\cos\Theta\cos\Theta_S),$$
$$C=\cos\Theta_S(\omega-\omega'\cos\Theta)-\omega'\sin\Theta\sin\Theta_S\cos\phi_S, \tag{11}$$
$$\tilde{\eta}=(1+\cos\Theta)[2-(\omega/\omega'+\omega'/\omega)],$$

q is the modulus of the momentum transfer $q=|\mathbf{k}-\mathbf{k}'|=(\omega^2+\omega'^2-2\omega\omega'\cos\Theta)^{1.2}$. From kinematics the p_z component of the initial electron momentum is

$$p_z\equiv\mathbf{p}\cdot\mathbf{q}/q=[\omega-\omega'-\omega\omega'(1-\cos\Theta)]/q. \tag{12}$$

Note that the sign of p_z is important. In Eq. (11) it is assumed that **S** is a unit vector whose direction is given by the polar angle Θ_S that **S** makes with **k** and the azimuthal angle ϕ_S that is counted from the $(\mathbf{k},\mathbf{k}')$ scattering plane. For a coplanar arrangement ($\phi_S=0$ or π) and electrons at rest ($p_z=0$), Eq. (9) reduces to the cross-section function

$$\tilde{X}_m(p_z=0)=-P_3(1-\cos\Theta)(\omega\cos\Theta\cos\Theta_S+\omega'\cos\alpha) \tag{13}$$

that is frequently used in the analysis of magnetic Compton profiles [5,9,16]. Here, α is the angle between $\mathbf{k}'$ and **S**, which becomes either $\alpha=\Theta-\Theta_S$ for $\phi_S=0$ or $\alpha=\Theta+\Theta_S$ for $\phi_S=\pi$. In Fig. 1 we have plotted the relative difference of the p_z-dependent cross section of Eq. (8) to that with $p_z=0$, i.e., the Lipps-Tolhoek cross section

$$D=100\times[d^2\sigma_m(p_z)-d^2\sigma_m(0)]/d^2\sigma_m(0). \tag{14}$$

The two curves correspond to the experimental situation of Ref. [9] (curve *a*) and Ref. [16] (curve *b*). It is seen that deviations up to $\pm10\%$ are observed, which means that corrections due to cross-section effects should be taken into account. It is also seen that the deviation D does not become larger with increasing photon energy ω or, conversely is rather strong at photon energies as low as 48 keV.

It is readily seen from Eqs. (2) and (3) that also in the case of moving electrons the magnetic part of the cross section is proportional to the spin three-vector **S** and the proportionality factor being independent of **S**. Therefore, the magnetic Compton profile $J_m(p_z)$ can be isolated by reversing the direction of magnetization and subtracting the spin-up and spin-down signals. The resulting count rate is proportional to the cross section of Eq. (2). We remark that our more general result [Eqs. (8)–(11)] becomes identical to Eq. (33) of Grotch *et al.* [10] if one assumes in the $\tilde{X}_{m1}$ term of Eq. (10) vanishing inelasticity, i.e., $\omega'=\omega$, which implies $\tilde{\eta}=0$. The result of Ref. [10] has been used very recently for the correction of experimental magnetic Compton profile measurements [17].

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