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Compton scattering cross section for inner-shell electrons in the relativistic impulse approximation

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ABSTRACT

Total Compton scattering cross sections and inelastic scattering factors for bound electron states of several elements have been evaluated in the framework of the relativistic impulse approximation (RIA). The accuracy of different approximate expressions for the singly differential cross section within the RIA is discussed. Accurate evaluations of bound state scattering factors require the use of the full RIA expression. Compton scattering from K-shell electrons dominates over the photoelectric absorption at higher energies. Energy values at which the Compton interaction become the main process of creation of K-shell vacancies are assessed. The role of binding effects in Compton processes at lower energies are clearly evidenced by the computed total cross sections. Calculated K-shell ionization total cross sections, defined as the sum of the photoelectric absorption and the Compton scattering cross sections, are in good agreement with available experimental data. The total Compton cross section for the 2s atomic orbital exhibits a shoulder-like structure, which can be traced back to the node structure of the 2s wave function.

1. Introduction

The inelastic X-ray scattering spectroscopy in the regime of large energy and momentum transfers, the so-called Compton regime, has proved to be a powerful technique to investigate ground state properties of valence electrons in condensed matter [1,2]. In this sense, synchrotron radiation-based Compton experiments with high momentum-space resolution have been applied to Fermiology studies on a large variety of systems, among them simple metals [3], substitutional alloys [4] and high T_c superconductors [5].

Provided that the energy transfer is larger than electron binding energies, Compton events may occur with the tightest electrons, and thus, give rise to vacancies in deep atomic orbitals. In some situations, the vacancy generated can be the most interesting consequence of the scattering event rather than the inelastically scattered photon. Inner-shell vacancies will be then filled by radiative (X-ray fluorescence emission) or non-radiative (Auger transition) processes. This way, Compton scattering by core electrons provides an additional channel for the creation of inner-shell vacancies, besides photoelectric absorption. As Compton scattering is the main interaction process for X-rays of several hundreds of keV in a wide range of atomic numbers, Compton processes involving bound electrons may play an important role in many areas. In radiology and radiation therapy, Compton collisions with K-shell electrons could significantly contribute to the absorbed dose [6]. Calculations of experimental dose limits in macromolecular crystallography showed that Compton scattering should be taken into account for incident energies above 20 keV [7]. In biomolecular imaging, where short radiation pulses from X-ray free electron lasers are planed to be used, the Compton scattering along with the photoelectric absorption should be the primary source of sample damage [8,9]. Several studies suggested a correlation between cell inactivation and inner-shell ionizations of DNA atoms [10–12], where Compton scattering of hard X-rays may be responsible for the cell damage during X-ray irradiation.

Experiments concerning Compton scattering from bound electrons have been performed for elements of medium and high atomic numbers using coincidence techniques. Most of the experiments focused on scattering from K-shell electrons and aimed to yield experimental data for the doubly differential cross section or, in a few cases, for the singly differential cross section at some selected scattering angles. These experimental works have been summarized and discussed in several reviews by Kane [13–15].

Theoretical aspects of the Compton scattering from bound electrons have been reviewed by Pratt et al. [16]. Different theoretical approaches have been developed and mainly applied to calculate doubly differential cross sections for K-shell electrons. A new theoretical contribution in this field has been made by Drukarev et al. [17], but this work is focused on low photon energies and provides scattering cross sections in a nonrelativistic treatment and only for hydrogen-like atoms.

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Studies on the total cross section for Compton scattering by inner-shell electrons are very scarce and are limited to a few experimental works [15]. Reported measured values were interpreted on the basis of the simple Klein–Nishina theory for free electrons. It is the aim of this work to compute total Compton cross sections for inner-shell electrons and to evaluate to which extent Compton processes contribute to inner-shell ionizations as compared to photoelectric absorption. Compton cross sections for 1s-, 2s- and 2p-electrons will be obtained from the doubly differential scattering cross section in the framework of the relativistic impulse approximation (RIA) [18,19]. This theoretical approach allows both electron binding effects and the electron momentum density distribution to be taken into account in a rather simple way. The dependence of the singly differential cross section for K-shell electrons on the incident photon energy, atomic number and scattering angle will also be discussed.

2. Basic relations

Several expressions for the doubly differential cross section (DDCS) for Compton scattering were derived in a relativistic treatment by Eisenberger and Reed [18] and Ribberfors [19] under several simplifying assumptions within the limits of the impulse approximation for photon–electron interactions [20]. Ribberfors [19] succeeded in obtaining a simple expression for the relativistic DDCS, which is valid for all scattering angles, factorizing it into a kinematical factor and a scattering system-dependent function (the Compton profile). In this framework, the DDCS for electrons of the *nlj* atomic level and for an unpolarized incident photon beam can be written as

$$\frac{d^2\sigma_{nlj}}{d\Omega dE'} = \frac{r_0^2}{2}\left(\frac{E'}{E}\right)\frac{(mc)^2}{q}\frac{1}{\left[(cp_z)^2+(mc^2)^2\right]^{1/2}} (R,R')\,Z_{nlj}J_{nlj}(p_z)\,\Theta(E-E'-E_{nlj}), \quad (1)$$

where r_0 is the classical electron radius, m the electron mass, c the velocity of light and q the magnitude of the scattering vector:

$$q = |\hbar\vec{k}' - \hbar\vec{k}| = \frac{1}{c}\left(E'^2 + E^2 - 2EE'\cos\theta\right)^{1/2} \quad (2)$$

E and $\hbar\vec{k}$ (E' and $\hbar\vec{k}'$) are the energy and momentum of the incident (scattered) photon. The angle θ is the polar scattering angle measured from the incidence direction.

p_z is the projection of the electron momentum in the initial state on the direction of the scattering vector:

$$p_z = \frac{\vec{p}\cdot\vec{q}}{q} = \frac{EE'(1-\cos\theta) - mc^2(E-E')}{c^2 q} \quad (3)$$

In the last expression the relativistic energy of the electron was approximated by its rest energy mc^2 [18].

The factor $X(R,R')$ in Eq. (1) is defined by

$$X(R,R') = \frac{R}{R'} + \frac{R'}{R} + 2m^2c^4\left(\frac{1}{R}-\frac{1}{R'}\right) + m^4c^8\left(\frac{1}{R}-\frac{1}{R'}\right)^2, \quad (4)$$

where R and R' are given by

$$R = E\left\{\left[(cp_z)^2 + (mc^2)^2\right]^{1/2} + (E - E'\cos\theta)\frac{p_z}{q}\right\} \quad (5)$$

and

$$R' = R - EE'(1-\cos\theta) \quad (6)$$

The function $J_{nlj}(p_z)$ is the Compton profile of electrons of the *nlj* atomic orbital, defined as

$$J_{nlj}(p_z) = \iint \rho_{nlj}(\vec{p})\,dp_x\,dp_y, \quad (7)$$

$\rho_{nlj}(\vec{p}) = |\chi_{nlj}(\vec{p})|^2$ being the electron momentum density distribution and $\chi_{nlj}(\vec{p})$ the momentum-space wave function for the *nlj* atomic orbital. An isotropic electron momentum distribution was assumed in Ref. [19] in the derivation of Eq. (1). Anisotropy and polarization effects were introduced by Ribberfors in Ref. [21]. The normalization condition

$$\int_{-\infty}^{+\infty} J_{nlj}(p_z)\,dp_z = 1 \quad (8)$$

on the orbital Compton profiles is assumed.

The step function $\Theta(E-E'-E_{nlj})$ accounts for the possibility of exciting an electron of the *nlj* orbital only if the transferred energy is larger than its binding energy E_{nlj}. The occupancy of the orbital is considered through Z_{nlj} .

The DDCS in the framework of the RIA is a quite realistic description of inelastic scattering processes in the Compton regime since it accounts for electron binding effects and also for Doppler broadening of the Compton line through the Compton profile. This cross section has been widely used in the analysis of experimental Compton spectra [2] since it provides a simple connection between the DDCS and the Compton profile, from which valuable ground state information of valence electrons can be obtained. On the other hand, Eq. (1) is of practical interest because the simple relationship of the DDCS to a target-dependent function allows systematic evaluations of integrated cross sections for any atomic orbital using tabulated values for $J_{nlj}(p_z)$.

The validity of the factorization of the DDCS in a relativistic context was investigated by Holm [22]. Deviations of only a few percent around the peak center ($p_z \sim 0$) were found for high scattering angles, except for high Z atoms, for which the deviations could be somewhat higher. These discrepancies diminish for smaller scattering angles. The accuracy of the relativistic impulse approximation was the object of several works [23–26]. Tests were made by comparing RIA cross sections with exact S-matrix calculations in the independent particle approximation [27,28]. Despite same small deviations in the peak region, which is primarily a shift of the spectrum, Pratt et al. [16,25] argued that the RIA should be adequate to perform calculations of doubly differential Compton cross sections for bound electrons. Since this work is concerned with integrated Compton cross sections, those discrepancies should not affect the final results to a large extent. Contributions of the $\vec{p}\cdot\vec{A}$ interaction term (not considered in the RIA) in the peak region, would be appreciable only for scattering from high Z K-shells [16,25].

In order to compute singly differential and total cross sections for bound electrons under the RIA, some approximated expressions have been proposed. These will be briefly discussed in the next sections.

3. Results

3.1. Singly differential cross section. Scattering factor

Singly differential cross sections (SDCS) for Compton scattering by electrons of a given atomic orbital are obtained by integrating the DDCS over the allowed range of scattered energies

$$\frac{d\sigma_{nlj}}{d\Omega} = \int_0^{E-E_{nlj}} \frac{d^2\sigma_{nlj}}{d\Omega dE'}\,dE' \quad (9)$$

Several simplifying assumptions have been proposed to evaluate singly differential cross sections in the RIA formalism. Since the Compton profile has a maximum at $p_z = 0$ and tends to zero as $p_z \to \pm\infty$, only those electrons with values of p_z close to zero contribute mostly to the DDCS. Under this assumption, Ribberfors and Berggren [29] made the simplifications $p_z = 0$ and, corre-