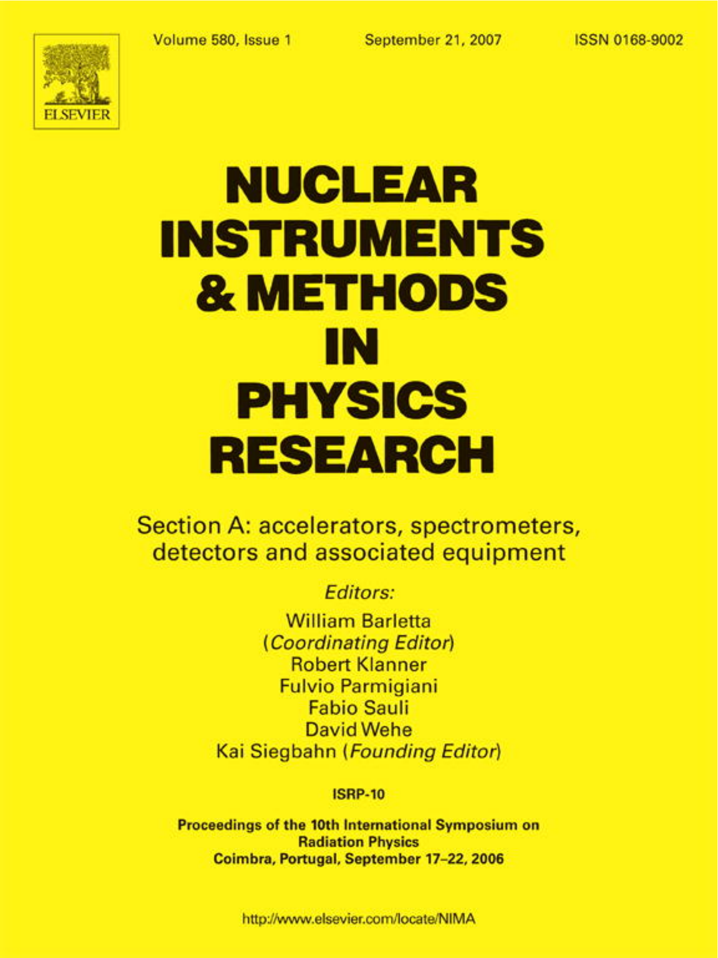

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NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH
Section A

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Asymmetry and the shift of the Compton profile

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Abstract

We show that the conventionally defined asymmetry of the Compton profile (CP) is, to a large extent, simply a shift of CP. Compton scattering is widely used in studying the electron momentum distribution (EMD) of complex systems. Extraction of information about the EMD is based on an impulse approximation (IA) description of the process. In IA the scattering from bound electrons is described as scattering from the EMD of free electrons. Most often the angular and energy distributions of scattered photons (doubly differential cross sections (DDCS)) is measured and presented in terms of CP, which is just the DDCS normalized by a kinematical factor. The deviations of measured CP from the IA results are conventionally described as an asymmetry of CP about the IA peak position. IA predicts CP to be symmetric. We have examined the discrepancy between IA predictions (and the corresponding relativistic version of IA, RIA) and more rigorous approaches (A^2 and S-matrix), using independent particle approximations for the description of the bound state of electrons. In the nonrelativistic region (in which many measurements of CP are performed) we find that the conventional asymmetry can largely be understood as the shift of the peak position. The true asymmetry with respect to the shifted peak position is in fact much smaller. RIA has similar properties to IA, except that for atoms with high nuclear charge the $\vec{p}\cdot\vec{A}$ interaction may modify the shift and limit the utility of description as a shift.

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Keywords: Compton scattering; Compton profile; Impulse approximation; Independent particle approximation; *S*-matrix; Asymmetry

The asymmetry of the Compton profile (CP) around the peak position which impulse approximation (IA) predicts (rather than asymmetry about the true peak) is conventionally used to describe deviations of measurements from the IA [1,2]. However we find that the conventionally defined asymmetry can, to a large extent, simply be understood as the shift of the true peak from the IA peak. We suggest using symmetric and antisymmetric deviations of a shifted CP from the IA predictions as more appropriate characterization. Within independent particle approximation (IPA) we have examined the deviation of IA [3], predictions (and the corresponding relativistic version of IA, RIA [4]) from more rigorous approaches: A^2 approximation, and the S-matrix approach [5,6], which allows study of the importance of the $\vec{p}\cdot\vec{A}$ interaction term (neglected in the A^2). RIA has similar properties to IA, but for atoms with high nuclear charge the $\vec{p}\cdot\vec{A}$ interaction may modify the shift and limit the utility of description as a shift.

The nonrelativistic CP is just the DDCS normalized by a kinematical term (units $\hbar = c = 1$ are used)

$$J(p_z,k) = \frac{(\mathrm{d}^2\sigma)/(\mathrm{d}\omega_f \mathrm{d}\Omega_f)}{(\alpha/m)^2(1/2)(1+\cos^2\theta)(\omega_f/\omega_i)(m/k)} \tag{1}$$

where ω_i (ω_f) is incoming (outgoing) photon energy, $\vec{k}$ is photon momentum transfer ($\vec{k} = \vec{k}_i - \vec{k}_f$) and θ is photon scattering angle, and p_z, which is fixed, is given as

$$p_z = \frac{k}{2} - \frac{m(\omega_i - \omega_f)}{k}. \tag{2}$$

Here, p_z may be understood (in IA) as the component of the initial state electron momentum in the direction of photon momentum transfer.

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The use of Compton scattering in studying the electron momentum distribution (EMD) of complex systems is based on IA [2,3]. In IA the scattering from bound electrons is described as scattering from the EMD of free electrons $\rho(\vec{p})$ where $\rho(\vec{p}) = |\psi(\vec{p})|^2$ and $\psi(\vec{p})$ is the Fourier transform of the coordinate space bound state wave function. In IA the CP is given by

$$J^{\mathrm{IA}}(p_z) = \int_{|p_z|}^{\infty} \rho(p) p \, \mathrm{d}p \tag{3}$$

which is a symmetric function around $p_z = 0$ with a peak at $p_z = 0$. For a H-like K-shell this is, for example, given by

$$J^{\mathrm{IA}}(p_z) = \frac{8a^5}{3\pi(a^2 + p_z^2)^3} \tag{4}$$

where $a = mZ\alpha$. The validity of IA increases with the increase in photon momentum transfer, and the corrections decrease as the ratio a/k becomes small. Although a fair agreement of the IA result for CP with experiment is found even for $a/k \approx 1$, there is some discrepancy between IA results and measurements even at quite large momentum transfers, which influence the interpretation of results. These deviations from the IA results are conventionally described utilizing the asymmetry A of the Compton peak about the IA peak position $p_z = 0$,

$$A(p_z, k) = \frac{J(p_z, k) - J(-p_z, k)}{J(0, k)}. \tag{5}$$

However, we find that the asymmetry A is, to a large extent, just a shift (i.e., there is little asymmetry about the true peak, which is shifted by an amount δ from the IA peak at $p_z = 0$). We obtain the same result at relativistic energies for low Z elements. Hence, we suggest making a new definition of asymmetry. The relative difference between a shifted CP J (shifted by δ so that its maximum is at $p_z = 0$) and the IA prediction J^{IA}, normalized by N to give the same peak value as J, can be partitioned into small symmetric S' and antisymmetric A' parts

$$\frac{J(p_z + \delta, k) - NJ^{\mathrm{IA}}(p_z)}{J(\delta, k)} = S'(p_z, k) + A'(p_z, k). \tag{6}$$

Here we define the true asymmetry A' of the CP, while S' is the main deviation from IA shape. (Note that if we had not shifted J we would obtain antisymmetric part which, due to the change in definition, would be just half of the conventional asymmetry A. There would also be a symmetric part.)

Our finding that A is to a large extent due to the shift in δ means that A' is small. This is illustrated in Fig. 1 for the scattering of 10 keV photons from the K-shell of Beryllium, for the scattering angle $\theta = 165°$. In Eq. (4), we have chosen an effective charge $Z_{\mathrm{eff}} = 2.86$ to have a realistic binding energy and profile for the K-shell of the Be atom. For this situation, $a/k = 0.54$. The figure shows Coulombic (with Z_{eff}) predictions (full line) and IA predictions (dotted line). One can see that the positions of the peaks in the two approaches differ by some amount $\delta(a/k)$, with the position of the peak of J^{IA} at $p_z = 0$. The heights of the peaks are also different, and we denote their ratio $J(\delta)/J^{\mathrm{IA}}(0) = N(a/k)$. Since experiments usually measure only relative cross-sections, the experimental data are often normalized to theoretical values, and the remaining difference between IA predictions and measured values are discussed in terms of the asymmetry A.

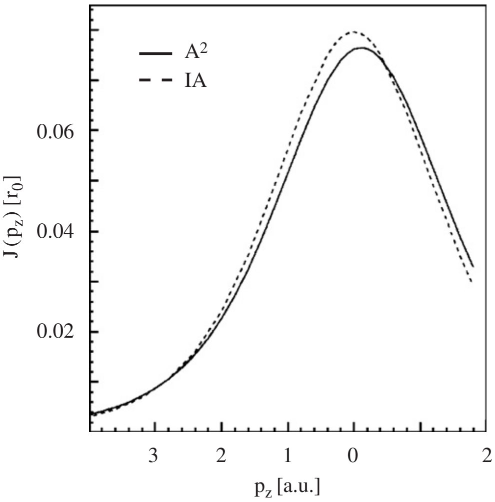

Fig. 1. Compton profile as a function of p_z for fixed $a/k = 0.54$, for a Be K-shell electron in a Hydrogenic model. We have chosen an effective charge $Z_{\mathrm{eff}} = 2.86$ in both IA and A^2 calculations to have a realistic binding energy and profile for the K-shell of Be atom.

An example of the asymmetry A obtained for the Beryllium atom (whole atom scattering) by Huotari et al. [1], scattering 10 keV photons into $\theta = 165°$, is shown in Fig. 2a, together with our K-shell S-matrix predictions (using screened initial state and final state wave functions) and Coulombic A^2 Z_{eff} predictions. [Huotari et al. found experimentally that contributions from valence electrons to the asymmetry $A(p_z)$ are negligible.] The overall magnitude and behavior are reasonably well represented by Coulombic K-shell Z_{eff} calculations, but S-matrix results give much better agreement with the experiment. In Fig. 2b, we show S' and A' for the case of Fig. 2a. Fig. 2b shows that both S' and A' are small, A' being about 0.2% at the largest p_z at which the experiment (Fig. 2) was performed, S' is about 2%. (We note again that if in our definition in Eq. (6), we do not use shifted J, we obtain an asymmetric part which, due to the change in definition, is half the conventional asymmetry, therefore large in this example, while the corresponding symmetric part is of similar magnitude.) With the finding that the shifted CP is in fact much closer to the IA prediction, the interpretation of measurements in terms of the EMD can be extended (e.g., in Eq. (4), one can use $p_z - \delta$ instead of p_z, where δ is a measured shift).

In the relativistic region we have used the S-matrix approach, taking into account the full electron–photon interaction at the IPA level. (IA and A^2 neglect the $\vec{p} \cdot \vec{A}$ interaction term, which is part of the full relativistic interaction.) We find that the revised description of deviations from IA in term of (δ, N) is also applicable at

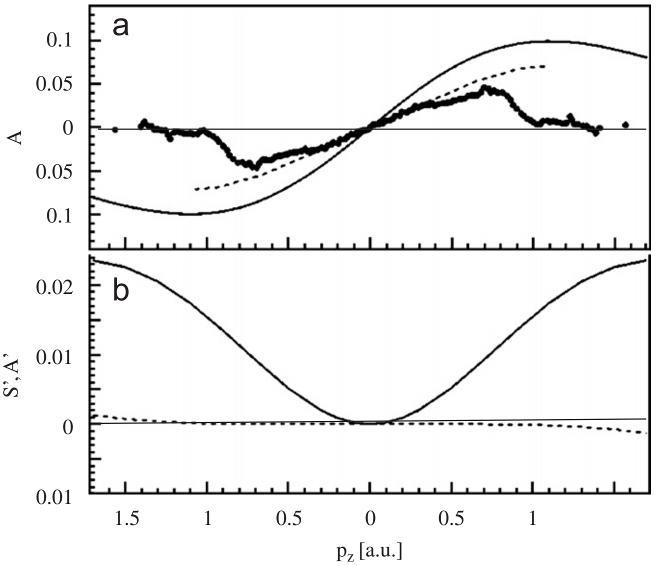

Fig. 2. (a) The measured asymmetry A(p_z, k) for the Compton profile of Be [1] (bold circles), together with the theoretical asymmetry obtained with the *S*-matrix approach using screened wave functions (dashes), and using a Coulombic A^2 approach (solid line). (b) The asymmetry A' (p_z, k) (dashes) of the exact Compton profile (A^2 results from Fig. 1) around its peak and the symmetric part $S'(p_z, k)$ (solid line).

relativistic energies, except however for high Z K-shell Compton scattering. The difference in this case can be understood as due to the contribution of the $\vec{p}\cdot\vec{A}$ interaction term (neglected also in RIA), in the peak region for $a/k \approx 1$, which becomes important for high Z [7].

The high Z behavior of CP is illustrated in Fig. 3 for scattering of 450 keV photons from the K-shell of Uranium ($Z = 92$) into 90° (panel a) and 180° (panel b). The profiles are obtained using the definition of Ribberfors (Eq. (54) of Ref. [4]). The figure shows that the infrared behavior (rise of the profile as p_z becomes increasingly negative, which corresponds to $\omega_f \to 0$), for high Z is not separated from the peak region, which illustrates that the importance of the $\vec{p}\cdot\vec{A}$ term is large in this case in which $a/k \approx 1$. However, with increasing photon momentum transfer k so that $a/k \ll 1$, one will obtain a situation similar to the low Z cases for $a/k \approx 1$, i.e., the $\vec{p}\cdot\vec{A}$ contribution in the peak region decreases. For $a/k \approx 1$ the $\vec{p}\cdot\vec{A}$ contribution in the peak region decreases roughly as Z^3 with decreasing Z, according to a very crude estimate [7]. This means that the $\vec{p}\cdot\vec{A}$ contribution is important only for the K-shell of high Z atoms.

In summary, we have examined the discrepancy between IA predictions (and the corresponding relativistic version of IA, RIA) and more rigorous approaches (A^2 and *S*-matrix approach) within IPA. We have shown that the conventionally defined asymmetry of CP can be, to a large extent, understood as a shift, and we therefore suggest characterizing deviations from IA as a shift, together with small symmetric and antisymmetric deviations of a so shifted profile from IA. Based on our *S*-matrix approach we have found that RIA has similar properties to IA except that for atoms with high nuclear charge the $\vec{p}\cdot\vec{A}$ interaction may modify the shift and limit the validity of such a description.

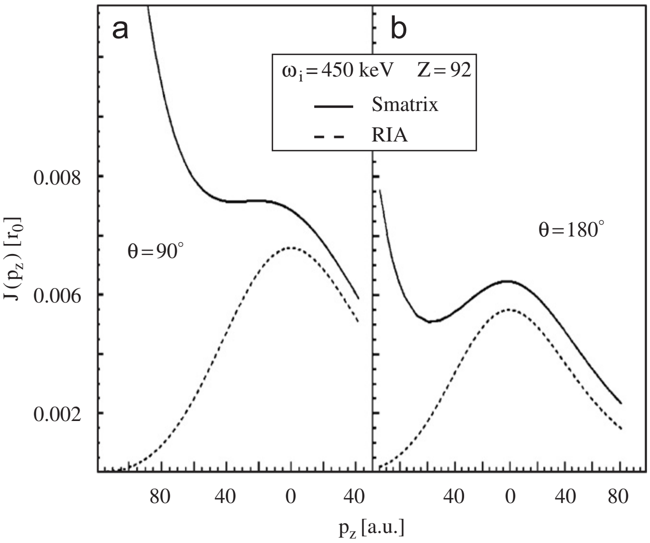

Fig. 3. Compton profile for scattering of 450 keV photons from the K-shell of Uranium ($Z = 92$) into 90° (Panel a) and 180° (Panel b). The figure shows that the infrared behavior for high Z is not separated from the peak region.

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