

Compton Scattering of Photons by Inner-Shell Electrons

T. Surić,^{(1),(2)} P. M. Bergstrom, Jr.,⁽²⁾ K. Pisk,⁽¹⁾ and R. H. Pratt⁽²⁾

⁽¹⁾*Ruder Bošković Institute, 41000 Zagreb, Yugoslavia*

⁽²⁾*Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260*
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We have developed an exact second-order S -matrix code for the relativistic numerical calculation of cross sections for Compton scattering of photons by bound electrons within the independent-particle approximation. We find good agreement with less exact treatments in regions where such theories are valid, recovering the impulse approximation and the soft-photon infrared divergence. We do not find agreement with an earlier calculation of Whittingham. We compare with recent scattering experiments in the regime $Z\alpha(\hbar\omega_i) \sim E_B$, where we find that the impulse approximation is not adequate.

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We have developed a code for calculating cross sections for Compton scattering of photons by bound electrons [1]. There has been considerable recent interest [2–5] in measuring the inelastic (Compton) scattering cross sections on bound atomic electrons, in circumstances in which the composite structure of the initial atomic state modifies the scattering from free particles. Accurate theoretical cross sections for Compton scattering by bound inner-shell electrons are needed as basic data with which experiments may be compared, to provide insight into the nature of the response of the composite system and to separate this process from others of experimental concern. Inelastic scattering from bound inner-shell electrons is important in astrophysical and laser plasmas where ions have only a few electrons remaining and in condensed-matter studies where an accurate knowledge of inner-shell electron Compton profiles permits their separation and so an accurate determination of the properties of valence electrons. The Compton scattering process is one of the few low-order photon-bound-electron interactions that has resisted a reasonably exact treatment. An accurate calculation of Compton scattering requires the evaluation of thousands of slowly converging integrals. Some of the spectra that we present here required several hours of time on a Cray Y-MP supercomputer; such calculations have only recently become feasible. Our approach is exact within the framework of the independent-particle approximation to second-order relativistic external-field quantum electrodynamics. Our calculations use spherically symmetric atomic potentials, both screened (self-consistent) and point Coulombic. We present comparisons with simpler, more approximate calculations, and with experiment. Differences from the widely used simpler approaches are often substantial.

The difficulty of performing such calculations of Compton scattering in the past has led to various more approximate theoretical treatments of the process. In the nonrelativistic domain, the interaction Hamiltonian for the electron-photon system is [6] $H_{\text{int}} = \frac{1}{2} e^2 A^2 - e\mathbf{p} \cdot \mathbf{A}$.

In this regime, two common approximations are used. One approach that is most widely used is based on the first term (A^2) in the nonrelativistic Hamiltonian [7–9]. The other is based on the second or $\mathbf{p} \cdot \mathbf{A}$ term in the non-

relativistic Hamiltonian [10]. The precise criterion of validity of these approaches is not known although it is clear that it should include both incoming and outgoing photon energy as well as scattering angle. Gavril's numerical results for the $\mathbf{p} \cdot \mathbf{A}$ term were obtained only within the dipole approximation and are valid throughout the spectrum in the point Coulombic potential for $Z\alpha \ll 1$, $Z\alpha\omega_i/E_B \ll 2$. This $\mathbf{p} \cdot \mathbf{A}$ term correctly predicts, however, the divergent character of the spectrum for soft scattered photons ($\omega_f \rightarrow 0$) present in any atomic potential. Several of the most commonly used approximations result from the use of the A^2 term. Among these approaches are the impulse approximation [8,11] (which leads to the incoherent scattering factor approximation [12]), the relativistic A^2 approximation [13], and the relativistic impulse approximation [14]. The A^2 term becomes more important for $Z\alpha\omega_f/E_B \geq 1$; in many cases only this relatively hard-final-photon part of the spectrum has been observed, and this is the situation to which the criterion of Eisenberger and Platzman [8] may be applied. We will demonstrate that in general both terms are important and must be included [15].

A more accurate treatment of Compton scattering by bound electrons requires a calculation based on relativistic external-field quantum electrodynamics. The only published attempt at such a calculation was reported by Whittingham [16], taking the external field as point Coulombic (unscreened), and including a limited number of partial waves and multipoles. Results were significantly larger than the predictions of more approximate methods for the cases that were considered; tests of the code and verification of known limiting cases were not reported. Our approach is made within the same general framework, but it allows the use of any spherically symmetric atomic potential within independent-particle approximation and utilizes different numerical techniques. We use point Coulombic potentials to compare with approximate theories which use such potentials and screened self-consistent potentials [17] when comparing with experiments; we describe our various tests of the code.

Initially, we have used our code to calculate the doubly differential cross section for the scattering of unpolarized

photons on spin-averaged bound electrons. We have checked the code against approximate treatments in their regions of validity. For example, at low (nonrelativistic) energies and low nuclear charge Z (in a region where $Z\alpha\omega_i/E_B \ll 1$ and the A^2 term can be neglected), comparisons were made between dipole calculations made with our code and the $\mathbf{p} \cdot \mathbf{A}$ calculations performed in the dipole approximation. For $Z=1$ and $1.05 \leq \omega_i/E_B \leq 5$ ($Z\alpha\omega_i/E_B < 0.04$) agreement with Gavril's calculations [10] was within at least 0.1% over the spectrum (including outgoing electron energies that approach but are not equal to zero). A comparison was also made with L -shell calculations with similar agreement [10]. We have compared, using additional photon multipoles and a Coulombic atomic potential, with the A^2 approximation [7,8] in high-energy- and low-energy-loss regimes where the $\mathbf{p} \cdot \mathbf{A}$ contribution should be unimportant, obtaining excellent agreement. Figure 1 shows a situation where neither approximation is valid at all angles and scattered photon energies and the effects of both terms in the nonrelativistic Hamiltonian are important ($Z\alpha\omega_f/E_B \leq 0.4$). Note the contribution of the A^2 term is negligible for forward scattering but not for backward scattering, indicating strong angular dependence of the precise criterion for the relative contributions of $\mathbf{p} \cdot \mathbf{A}$ and A^2 terms.

Checks of the code at higher energies were made by evaluating analytically the relativistic amplitude in the Born approximation. This corresponds to assuming a free propagator and free outgoing electron. The corresponding assumptions can be made with our code. In a wide range of incident photon energies (≈ 15 –600 keV) and elements the agreement of the approaches was always

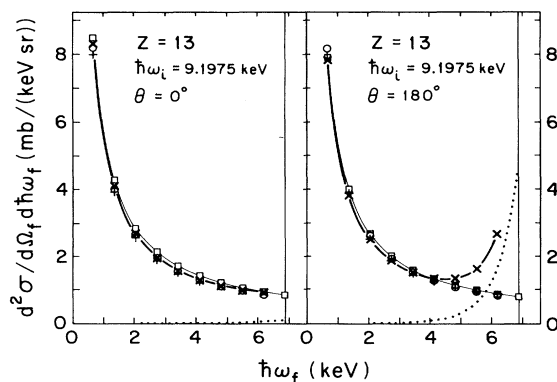


FIG. 1. Scattering of 9.1975-keV photons from the K -shell electrons of aluminum into a scattering angle of 0° (left panel) and 180° (right panel). Comparison between the nonrelativistic A^2 approximation (dotted line), the nonrelativistic $\mathbf{p} \cdot \mathbf{A}$ calculation (open circles), our code for the full multipole case (crosses), and results from photoeffect (squares). A point Coulomb potential is used in the calculations. Solid vertical lines represent the kinematic limit of our calculations. Lines through points have been drawn to aid the eye. Also shown are the results of our code in the dipole approximation (plusses).

better than 0.1%.

An additional test of our calculation is possible utilizing a low-energy theorem. In the soft outgoing-photon energy limit, the matrix element for Compton scattering is proportional to the matrix element for the photoeffect by this theorem. The unpolarized doubly differential cross section for Compton scattering can be written in terms of the unpolarized photoeffect differential cross section [10,18]. We present the values of this prediction, using photoeffect calculations within the same framework and the same potentials used in the Compton scattering calculations, and we will see that it is quite well verified in our numerical calculations.

There exist a fair number of experiments in high-photon-energy regimes where agreement with A^2 -approximation calculations is expected and obtained. We note several recent experiments involving x-ray [2–4] or γ -ray [5] scattering in which deviations from the commonly used A^2 approximation would be expected. There are two recent experiments on Zr ($Z=40$), one on the K shell [4] and the other on the L shell [3]. Manninen, Hamalainen, and Graeffe [4] used an incident photon energy of 59.54 keV; the momentum transfer is in a region where the impulse approximation is not expected to be valid. The authors compare with this approximation, however, and report agreement. We do find deviations from the impulse approximation in this case that correspond to the infrared behavior of the $\mathbf{p} \cdot \mathbf{A}$ term. Unfortunately, since the experiment is not absolute, it is not possible to discuss whether the authors were correct in subtracting all soft photons as due to bremsstrahlung background, or whether some, as we predict, should have been retained. A complete comparison with the recent experiments of Marchetti and Franck [2] and Simionivici *et al.* [3] will require an extension of our code to handle polarized sources. In the latter case we compared with the results of our L -shell calculations [19], which are similar to Gavril's Coulomb predictions, and confirm the expectation of Simionivici *et al.* that the inclusion of more multipoles and screening cannot resolve the discrepancy between theory and experiment.

For relativistic energies we may compare with the results reported by Whittingham [16] and with the measurements reported by Lad, Basavaraju, and Kane [5]. We begin with the comparisons with Whittingham, presented in Fig. 2. All of these calculations are made for scattering from the K -shell electrons in a Coulombic potential. We also show nonrelativistic and relativistic A^2 -approximation results [20] and results calculated from Gavril's nonrelativistic theory [10]. It is clear that our results approach $\mathbf{p} \cdot \mathbf{A}$ and A^2 behavior at the two ends of each spectrum. Additional confidence in our calculations comes from comparison with the soft-final-photon prediction from the photoeffect. From Fig. 2 it can be seen that for soft outgoing photons our results approach this prediction and for $\omega_f = \omega_i/10$ the agreement is within 10%. Note, however, the lack of agreement of the Whitting-

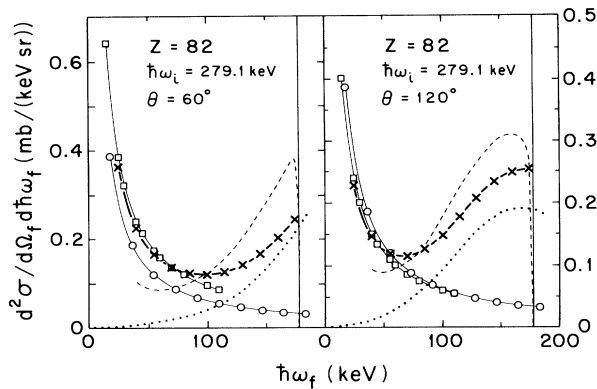


FIG. 2. Scattering of 279.1-keV photons from the K -shell electrons of lead into a scattering angle of 60° (left panel) and 120° (right panel). Same quantities as Fig. 1; also shown are Whittingham's results [16] (dashed line).

ham calculations both with our calculations and with the predictions of more approximate methods.

In Fig. 3 we present comparisons with recent experimental results of Lad, Basavaraju, and Kane [5] for 320-keV γ rays scattered by the K -shell electrons of holmium. The unpolarized doubly differential cross section was measured. Our calculation was performed in a screened potential. Agreement between theory and experiment is not impressive. At the high-energy end of the spectrum, the experimental points for holmium at 115° are consistent with the A^2 approximation within 2 standard deviations while our results are higher by 3 or more standard deviations. At 45° for holmium these measurements, unlike those reported in whole atom Compton profile experiments [21], are much smaller than all of the theoretical predictions for the high-energy end of the spectrum. Because of large experimental errors attributed to bremsstrahlung the authors do not present results in the infrared regime. We present results in this regime for reference. The obvious infrared divergence in our calculations is in quantitative agreement with results obtained using the low-energy theorem and in qualitative agreement with the nonrelativistic $\mathbf{p} \cdot \mathbf{A}$ treatment.

Our calculations of Compton scattering from bound electrons show unambiguously that the common approximations that follow from the use solely of the A^2 term in the nonrelativistic Hamiltonian generally do not describe the entire scattered photon spectrum, and we have seen the persistence of importance of inclusion of the $\mathbf{p} \cdot \mathbf{A}$ term through much of the spectrum. The complete relativistic treatment contains terms corresponding to the nonrelativistic $\mathbf{p} \cdot \mathbf{A}$ term that dominates the soft-outgoing-photon part of the spectrum. In this region, both the full relativistic treatment and a complete nonrelativistic treatment predict an infrared divergence. This divergent character in the doubly differential cross section means that the differential cross section singly differential in scattered photon angle (often calculated in terms of in-

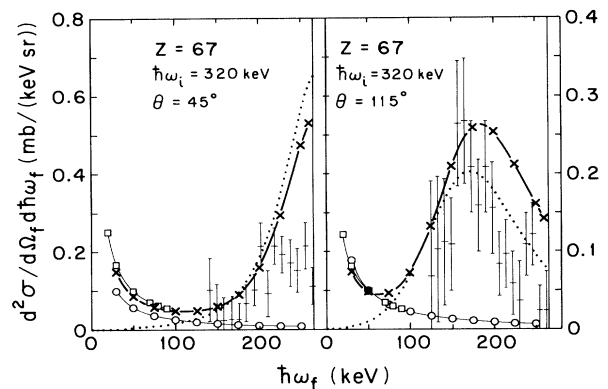


FIG. 3. Scattering of 320-keV photons from the K -shell electrons of holmium into a scattering angle of 45° (left panel) and 115° (right panel). Same quantities as Fig. 1 except that results from our code and photoeffect data are in a screened potential. Also shown are the results of Lad, Basavaraju, and Kane [5] (points with error bars).

coherent scattering factors) is undefined unless a detector efficiency for soft photons is included. In the higher-energy regime we do not confirm the results earlier reported by Whittingham, which are generally taken as the reference points in comparisons with experimental work. The tests that we have described here do give us confidence in our results, within second-order S -matrix theory, and in comparison to simpler, more approximate calculations and to calculations that have the same starting point. It is apparent that further, more precise measurements of the Compton scattering doubly differential cross section would be welcome in confirming our calculations. It is also apparent that further calculations should be performed, and we are in the process of obtaining further results which can serve as a basis for a more systematic discussion of the process.

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