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SCATTERING OF PHOTONS FROM ATOMIC ELECTRONS

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ABSTRACT

Validity of simpler approaches for elastic and inelastic photon scattering by atoms and ions is assessed by comparison with second-order S-matrix predictions. A simple scheme for elastic scattering based on angle-independent anomalous scattering factors has been found to give useful predictions near and below photoeffect thresholds. In inelastic scattering, major deviations are found from A^2-based calculations. Extension of free-atom and free-ion cross sections to the dense plasma regime is discussed.

1. Introduction

In many plasmas, atoms are not totally ionized, so that processes involving bound atomic electrons must be considered. Scattering of photons from bound electrons in plasmas has sometimes been neglected, or treated as though the electrons were free. A next level of approximation has utilized form factors for elastic scattering and incoherent scattering factors for inelastic scattering. These approximations still neglect most of the important electron-binding effects especially for photon energies near and below the photoeffect thresholds.

We have developed more sophisticated codes, based on the second-order S matrix in a central potential, which permit us to assess the usefulness of simpler approaches to scattering. We begin our assessment of simpler approaches with neutral, isolated atoms, and for ions. These results may be useful in plasmas,

especially at low densities. For scattering in dense plasmas, we start with ions and consider further modifications. In some cases, important differences exist between atomic models. Analysis of the physics of the process can indicate when differences in models are expected to be important.

2. Elastic Scattering

In many cases, elastic photon scattering by bound electrons (sometimes called coherent scattering, or Rayleigh scattering) has been ignored, considered as scattering from a free charge, included at the level of form factor approximation, or corrected for additional electron-binding effects through use of anomalous scattering factors. We can use our second-order S-matrix code (see the review of Kane et al.[1]) to assess the validity of these approximations.[2]

Classically, the scattering of a photon from a free point charge was studied by Thomson, and is called Thomson scattering. The unpolarized Thomson cross section, differential in scattering angle θ (the angle between the initial and scattered photon directions), is given as

$$\frac{d\sigma^T}{d\Omega} = \frac{r_o^2}{2} \left(1 + \cos^2\theta \right) , \tag{1}$$

and the total, angle-integrated Thomson cross section is

$$\sigma^T = \frac{8}{3} \pi r_o^2 , \tag{2}$$

where the classical electron radius is $r_C = e^2/mc^2 \approx 2.82 \times 10^{-15}$m.

A zeroth-order binding correction to the Thomson cross section is provided by the form-factor approximation, which models scattering from a charge distribution. In form-factor approximation, the differential cross section for unpolarized scattering is written as

$$\frac{d\sigma^{FF}}{d\Omega} = \frac{r_o^2}{2} |f(q)|^2 \left(1 + \cos^2\theta \right) , \tag{3}$$

where, the momentum transferred by the photon to the atom is $\hbar q = (2\hbar\omega/c)\sin(\theta/2)$. For a spherically-symmetric bound-electron charge distribution $\rho(r)$, the form factor is given by

$$f(q) = 4\pi \int_0^\infty \rho(r) \frac{\sin(qr)}{qr} r^2 \, dr . \tag{4}$$

The form-factor approximation breaks down badly when the photon energy is near or below the photoeffect threshold. Extensive tabulations of the form factor exist for neutral atoms.[3,4]

A modified relativistic form factor, g, has a further electron-binding correction that results in improved high-energy-limit values as compared with the form factor, f. In modified relativistic form-factor approximation, the differential elastic scattering cross section is

$$\frac{d\sigma^{MFF}}{d\Omega} = \frac{r_o^2}{2} |g(q)|^2 (1 + \cos^2\theta) , \quad (5)$$

where, for a for a spherically-symmetric bound-electron charge distribution for the i-th subshell, $\rho_i(r)$,

$$g(q) = 4\pi \sum_i \int_o^\infty \rho_i(r) \frac{\sin(qr)}{qr} \left[\frac{mc^2}{E_i - V(r)} \right] r^2 \, dr . \quad (6)$$

Like the form-factor approximation, the modified relativistic form-factor approximation breaks down badly when the photon energy is near or below the photoeffect thresholds. A tabulation of the modified relativistic form factor exists for all neutral atoms.[5]

Further electron-binding corrections are given by the anomalous-scattering-factor approximation

$$\frac{d\sigma^{MFWAC}}{d\Omega} = \frac{r_o^2}{2} |F|^2 (1 + \cos^2\theta) , \quad (7)$$

where the scattering factor can be written in terms of g and angle-independent corrections g' and g" as

$$F = g(q) + g'(\omega) + i\, g''(\omega) . \quad (8)$$

The real and imaginary parts of the energy-dependent corrections are related by the dispersion relation

$$g'(\omega) = \frac{2}{\pi} P \int_o^\infty \frac{\omega' \, g''(\omega')}{\omega'^2 - \omega^2} d\omega' , \quad (9)$$

and g" is obtained from the optical theorem:

$$g''(\omega) = - \frac{\alpha}{4\pi} \left(\frac{\hbar\omega}{mc^2}\right) \left[\frac{\sigma_{PE}(\omega) - \sigma_{BPP}(\omega)}{r_o^2} \right] - \frac{\pi}{2} \sum_{n,m} \omega_{nm} f_{nm} \delta(\omega - \omega_{nm}) . \quad (10)$$

Here, σ_{PE} is the photoeffect cross section, σ_{BPP} is the bound pair-production cross section (the electron of the pair is created in a bound state), and f_{nm} is the oscillator strength for the transition from the occupied bound state n to the unoccupied bound state m. (Although σ_{BPP} is zero for photon energies below

about $2mc^2$, its contribution is important at x-ray energies and below because it is required for convergence of the dispersion integral. Also, it affects results at low energy through an overall constant.)

In Fig. 1 we show a comparison of our S-matrix predictions with those of modified-form-factor approximation and angle-independent anomalous-scattering-factor predictions. We have concluded[2,6,7,8,9] that, in comparison to S-matrix predictions in the same potential, angle-independent anomalous-scattering-factor predictions can be expected to be accurate at about the 15% level or better for neutral atoms, for all Z, for photon energies near and below the K-shell photoeffect threshold. The accuracy of this approximation improves considerably for smaller Z and lower energies.

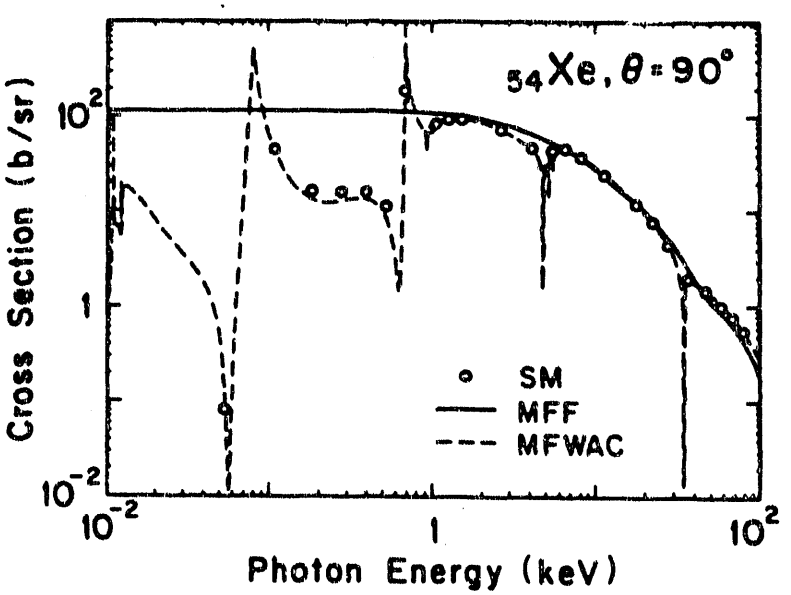

Fig. 1. Comparison of S-matrix predictions (SM) with those of modified relativistic form-factor approximation (MFF) and MFF with angle-independent anomalous scattering factors (MFWAC) for neutral xenon.

We also have verified that this prescription of using angle-independent anomalous scattering factors can be extended to ions.[10,11,12] But, the importance of the bound-bound contribution increases as the degree of ionization increases because larger values of f_{nm} for increasingly inner-shell transitions m will be included in g" and consequently in g'. In Fig. 2 we display cross section for various degrees of ionization of neon.

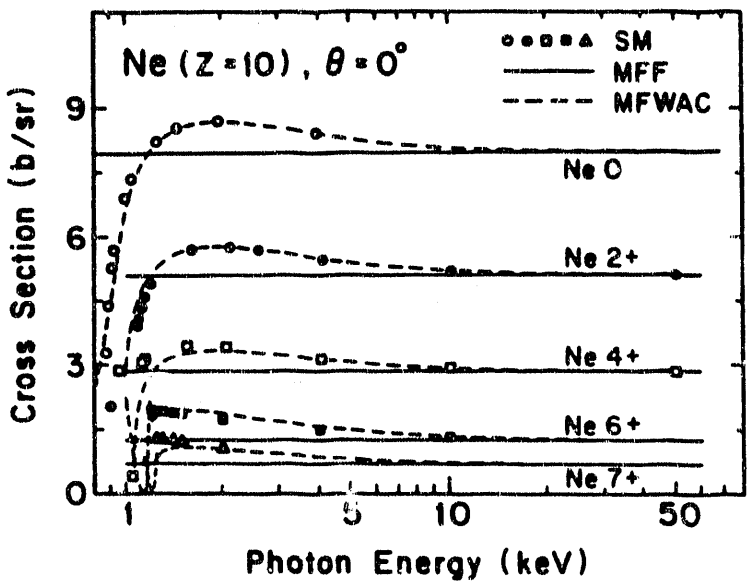

Fig. 2. Comparison of S-matrix predictions (SM) with those of modified relativistic form-factor approximation (MFF) and MFF with angle-independent anomalous scattering factors (MFWAC) for various degrees of ionization of neon.

3. Inelastic Scattering

As in the case of elastic scattering, inelastic photon scattering (also called incoherent scattering, bound-electron Compton scattering, or simply Compton scattering) has been ignored, considered as scattering from free electrons, or included at the level of the A^2 term in the nonrelativistic Hamiltonian (such as the incoherent-scattering-factor approximation, S(q)). Our first S-matrix results for inelastic scattering of photons from K- and L-shell electrons are just now becoming available.[13] They show that, for photon energies a few times electron binding or less, the usual A^2 approximation is inadequate, sometimes underestimating the cross section by an order of magnitude. Generally, we expect approximations based on the A^2 term to give reasonable result only when both the incident and scattered photon energy are large compared to electron binding.

An accurate evaluation of inelastic scattering exhibits some important features that are missing in simpler approaches but that are shown in the nonrelativistic hydrogenic results of Gavrila.[14] Cross sections show an infrared divergence for the case of a soft outgoing (scattered) photon. This is a well-known result for scattering processes involving free electrons and the emission of soft photons. In this case, the matrix element grows with the inverse power of the soft photon energy, and is proportional to the process in which the soft photon is absent (ie, photoeffect). Experimental verification of the infrared divergence is not conclusive. Some experiments[15] have failed to observe the effect while others[16] have measured significantly more scattering than is predicted by theory.

Another feature is that resonances appear in the cross section for photon energies in the neighborhood of energy differences of electron binding energies. Sometimes called resonant Raman scattering, this situation is not true Raman scattering (where electrons are not ejected from the atom) but simply the resonant part of bound-electron Compton scattering (where an electron is ejected from the atom).

Several previous attempts to obtain S-matrix predictions for bound-electron Compton scattering have been made, most notably those due to Whittingham.[17] Comparisons of our new results with those of Whittingham show serious disagreement. We feel reasonably confident in our results as we recover both the soft-photon divergent results of Gavrila and the hard-photon A^2 result; Whittingham's results appear inconsistent with these limiting cases.

In Fig. 3 we display our S-matrix results as compared with results of Gavrila, Whittingham and the A^2 approximation. Note that our results exhibit the proper soft-photon behavior and tend toward Gavrila's result, and also exhibit the correct hard-photon behavior and tend toward the A^2 result. Also note the significant disagreement of both our results and more approximate predictions with the earlier S-matrix results of Whittingham.[17]

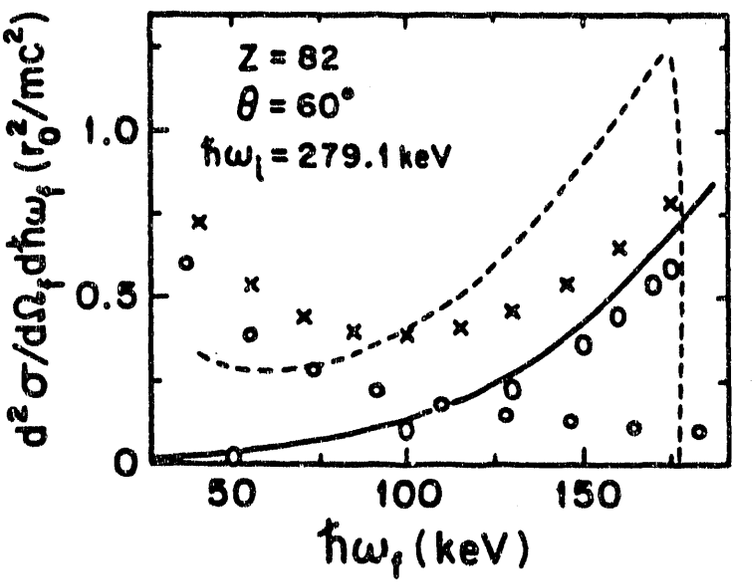

Fig. 3. Comparison between relativistic Coulomb S-matrix predictions (x), Gavrila's nonrelativistic Coulomb dipole results (o), relativistic A^2 approximation (O), nonrelativistic A^2 approximation (solid line), and Whittingham's relativistic Coulomb S-matrix results (dashed line). From Reference 13, with permission.

4. Dense-Plasma Potentials

These predictions for photon scattering have concentrated on isolated atoms and ions. Such results have immediate application in tenuous plasmas such as those found in stellar atmospheres and tokamak plasmas. In dense plasmas, free atom and ion scattering cross sections are modified, due to changes in the atomic potential. There are also important differences between a detailed configuration accounting (DCA) approach and the average atom (AA) approach which is most commonly used. These matters have been examined for elastic photon scattering,[18] utilizing techniques developed earlier for photoeffect[19] and now applied to bremsstrahlung.[20]

In Fig. 4 we show the charge densities within the ion sphere used in these studies; in Fig. 5 and 6 the resulting potentials are shown. Some insight into these questions may be developed by examining potentials calculated to reflect the various physical assumptions. Fig. 5 is an example of a low-density plasma where an NLTE approach (NLTEAA - non-local thermodynamic equilibrium average atom) is necessary and a simple Thomas-Fermi LTE theory (TFAA - Thomas Fermi average atom) is inadequate. Note that the isolated-ion potentials with the same total bound charge predicted in the NLTE approach (NLION - NLTE ion) and the LTE approach (TFION - Thomas Fermi ion) model the atomic potential fairly well in the interior of the ion, but fail at large distances where screening due to the stripped continuum electrons is not present. The neutral atom potential (NEUT) is too heavily screened throughout the atom due to additional bound electrons. In Fig. 6, at a much higher density, the predictions of the LTE and NLTE approaches show

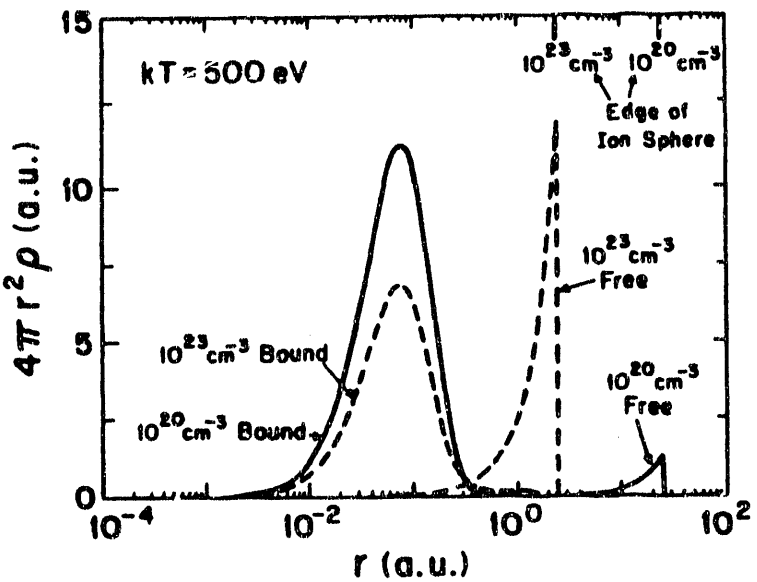

Fig. 4. Bound and free charge densities in aluminum plasmas at kT = 500 eV and densities of 10^{20} ions cm^{-3} (solid curves) and at 10^{23} ions cm^{-3} (dashed curves). From Reference 20, with permission.

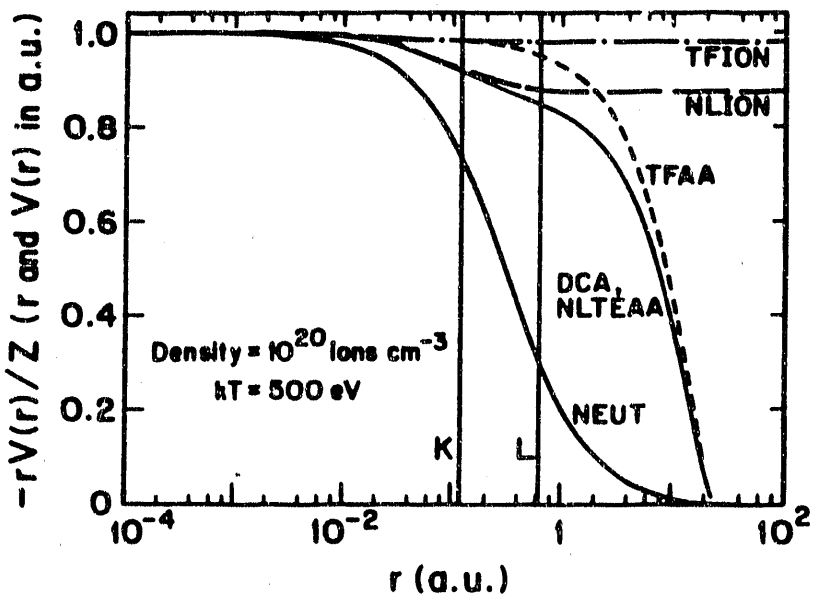

Fig. 5. Potentials for an aluminum plasma of density 10^{20} ions cm^{-3} and kT = 500 eV. The average radii of K- and L-shell orbits are indicated. See the text for a description of the labels. From Reference 20, with permission.

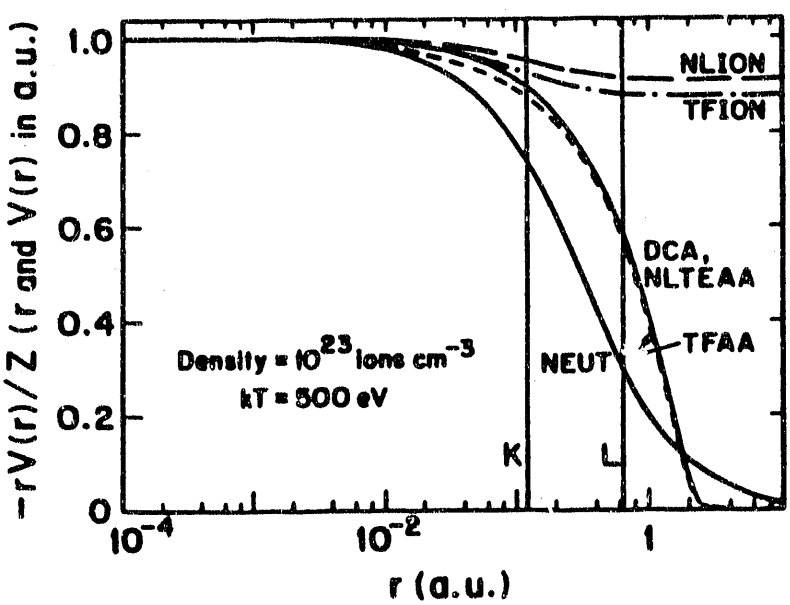

Fig. 6. Potentials for an aluminum plasma of density 10^{23} ions cm^{-3} and kT = 500 eV. The average radii of K- and L-shell orbits are indicated. See the text for a description of the labels. From Reference 20, with permission.

relatively good agreement as this is a regime where LTE thermodynamics is nearly valid. The ionic potentials are less adequate here. The neutral atom potential in this case is still inadequate but is nearer to the plasma potentials than in the low-density case. This reflects the confinement of the continuum electrons in the plasma approaches to ever smaller distances with increasing density. This confinement is most clearly evident at large distances where the plasma potentials are more screened than the neutral atom potential because a larger portion of the continuum charge is confined within the outermost bound charge in the isolated neutral atoms. The differences between a DCA approach and an average atom approach is highly process dependent. In general, differences are most clearly visible for processes with resonances and thresholds where the effects of the varying configurations of bound charge can not be adequately represented by a single average atom.

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