Photon Absorption and Photon Scattering - What We Don't Know and Why It Matters

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Abstract

We examine some of the problems of theory and experiment that are limiting our understanding of photon absorption and photon scattering. Much of what we know and don't know is signified via simple models, whether: (i) in semi-classical non-relativistic dipole radiation of the hydrogen atom, treated as two quantum particles bound in a Coulomb potential, or; (ii) in full relativistic multipole radiation of an atom in independent particle approximation. Chaotic and singular features can already be recognised. The inconsistencies in a non-relativistic multipole description lead to spurious predictions for absorption and scattering, but even the full theory is not in agreement with experiment. Additionally, paradoxes associated with quantum entanglement are already present in these simple models. The more advanced approaches treating many particle interactions and field quantization lead to a more sophisticated description of states and fields and cross-sections, which can simplify to the simpler models in various sum rule approximations, by invoking limitations on experimental measurement. Advanced discussions include issues of correlations and consequences of infrared divergence. A further level of complexity is to recognize the inevitable presence of environments, whether in a cage, a solid or a plasma, with consequences of modifying isolated processes, and in the significances for coherence and decoherence, and loss of entanglement. We conclude by reviewing the current status of the agreement between theory and experiment for photon absorption and scattering.

I. Photons and atoms

A. The dominant processes

The dominant processes when photons of energies below an MeV are incident on atoms are photoeffect, Rayleigh scattering, and Compton scattering. These will be the primary subjects of this paper. At higher energies pair production also needs to be considered (Fig. 1). There are many other features that can be considered, including the Delbruck scattering contribution to elastic photon scattering (Delbruck, 1931), processes with ejection of multiple electrons from the atom (Aksela et al., 1988), and processes where more than one photon (as in a laser) is incident on the atom in its initial state (Bartels et al., 2000; Lewenstein et al., 1994). Processes with an electron incident on an atom or ion, as in bremsstrahlung or radiative recombination, are closely related to these processes, including via the Mott formula (Mott, 1966; Animalu, 1972; Mott, Davis, 1971).

Figs 1 and 2 illustrate the relative importance of the dominant processes, considered as a function of incident photon energy E (*keV)* and atom nuclear charge *Z.* At the lowest energies only elastic scattering is allowed. Once there is enough photon energy to ionize the atom, photoeffect dominates. At still higher energy the importance of inelastic scattering, with ionization accompanying scattering, becomes dominant. With increasing atomic number *Z,* this cross-over occurs at higher energy E.

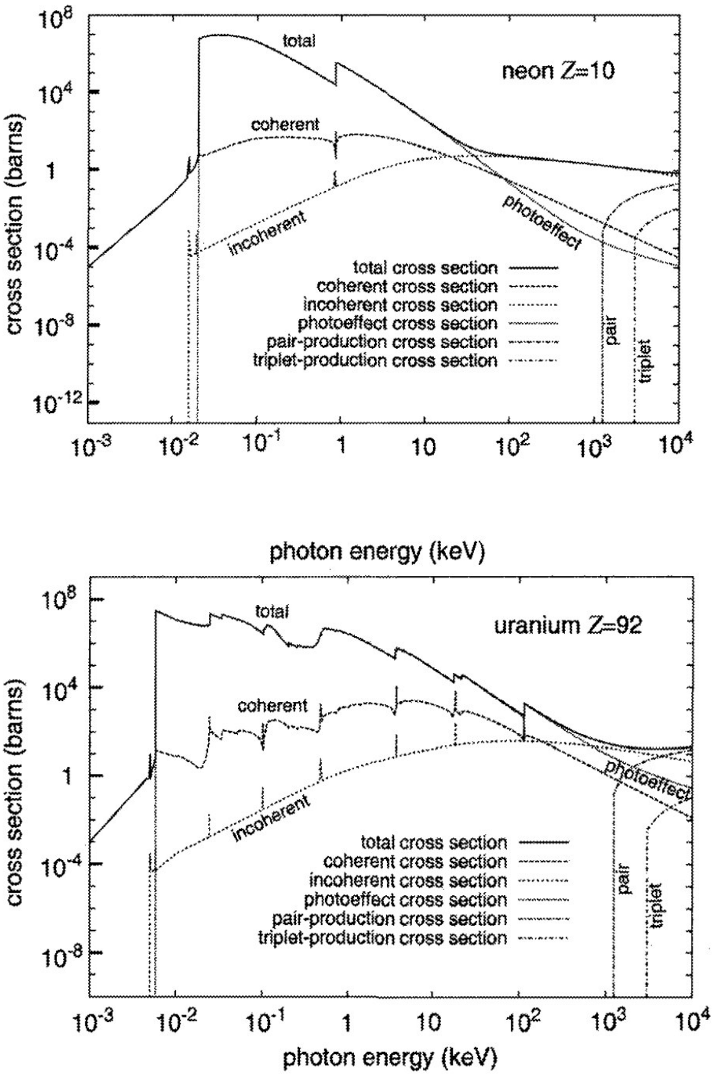

Figure 1. Total cross sections for various photon-atom processes, from Pratt (2000).

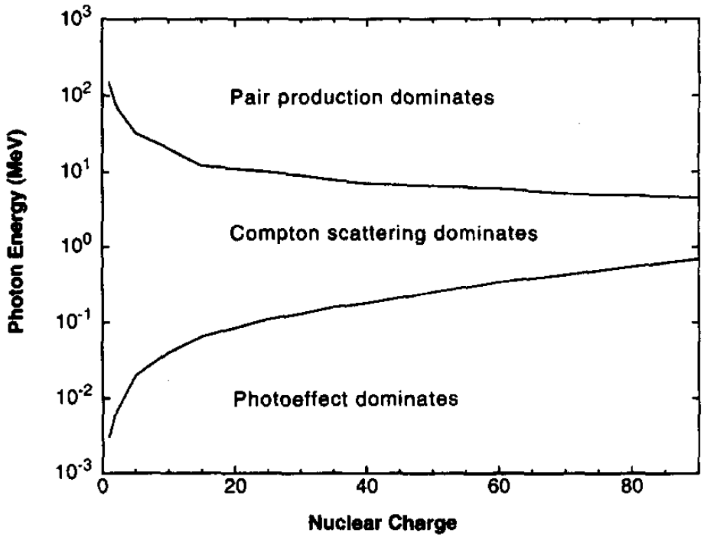

Figure 2. Relative importance of processes in total absorption cross sections as a function of photon energy and element. Below the lowest ionization threshold Rayleigh scattering will dominate. From Bergstrom (1997).

B. Observables

In describing a process we must specify the observables of the particles in the initial and final states. For electrons and photons these are energy and momentum (magnitude, direction), together with spin polarization. As an alternative prescription of observables to momentum, the angular momentum can be specified, and in particular, the multipolarity of matrix elements, electronic and atomic states can be presented in selection rules relating to the multipolarity of the photon interaction. Atoms and ions will be specified by their atomic states, including their excitation or ionization, and their orientation. In addition it needs to be specified whether these particles are isolated, or in environments; whether they are part of a target system, or a beam flux, and whether they are entangled with other particles.

In describing an experiment one must also specify its resolution, how precisely energy and angle are observed, and what particles may be present in the process but are unobserved. The non-integrability of low-energy photon flux (the infrared divergence) is an example of necessary theory relating to experimental detector methodology, leading to a low energy theorem. Sometimes it is possible to perform simple sums over unobserved particles or processes, leading to well-established sum rules. Simplified models, such as the independent particle approximation (IPA), are often helpful, as is the use of two-step process description (perhaps with a simplification of the definition of the intermediate state) where appropriate. In all cases, transitions between the same initial state *i* and the same final state *f* must be added coherently at the matrix element level, as for example for the Rayleigh and Delbruck amplitudes for elastic photon atom scattering. How this is done is limited by resolution and choice of observations.

The description of spin and polarization variables is relatively simple. A differential cross-section σ, in which electron spins ξ_i (in their rest frame) and photon polarizations ζ_j (Stokes parameters) are observed, is linear in ξ_i and ζ_j, where $i, j = 0,1,2,3$ and $\xi_0 = \zeta_0 = 1$. Thence for photoeffect (for incident photon and ejected final electron)

$$\sigma_{pe} = \underline{\sigma}_{pe} \sum_{i,j} \xi_i \zeta_j C_{i,j\,pe}$$

and for Rayleigh scattering (for incident and final photon)

$$\sigma_R = \underline{\sigma}_R \sum_{i,j} \zeta_i \zeta_j C_{i,j\,R} .$$

Here $\underline{\sigma}$ is the cross-section averaged over spin/polarization.

The $C_{i,j}$ are the *polarization correlations* ($C_{0,0} = 1$). Similar relations can be written for cross-sections with other numbers of observed particles. Note that these $C_{i,j}$ variables, while compact, are not the way experimentalists normally characterize their measurements of spin and polarization.
The $C_{i,j}$ for a process are not all independent, as there is a relation connecting them. This relation has been obtained in the Rayleigh scattering case (Roy, 1986), also for elastic electron scattering (Gursey, 1957). The corresponding relations for other processes - photoeffect, bremsstrahlung, Compton scattering - have not been known, but for photoeffect and bremsstrahlung they have now been investigated (Pratt and Surzhykov, 2012; Martin et al., 2012; Tashenov et al., 2013), and are similar in form.

II. Recent problems (two examples)

Many major results in radiation physics were obtained long ago, but with the new attention the field is now receiving it becomes clear that many major issues have not previously been considered. Here we describe two examples of these recent problems. (1) We focus on the recent experimental work of the Chantler group using XERT (the X-ray Extended Range Technique), measuring total attenuation due to the processes we have described above and displayed in Figure 1. There is substantial disagreement between these new experimental results, which are of much higher precision, and the best available theoretical predictions. Most likely better theory is needed. The data is needed in diverse determinations of structure, calibration of energies and amplitudes, and in probing advanced and developing theory of atomic and condensed matter physics. (2) In theoretical work it has recently been realized that the use of a non-relativistic treatment of electron kinematics, together with a full multipole treatment of radiation, can introduce spurious features, invalidating earlier work, particularly for total cross sections of the processes, even at relatively low energies. Yet for angular distributions, simpler approaches may still be valuable. These questions arise in relation to each of the processes we have described above.

A. Total attenuation

We show in Figures 3 - 7 some of the recent work of the Chantler group on total attenuation, published in Phys. Rev. A and Phys. Rev. Lett. over the decade 2001-2010. Measurements have been made for Si, Cu, Zn, Mo, Sn, Au, including the photon energy range 5 keV - 60 keV, with XERT, typically accurate to 0.1%-0.2% and with accuracies down to 0.02% (de Jonge et al., 2005) and 0.04% (de Jonge et al., 2007), far better than most previous measurements. The key idea of the technique is to use extended ranges on each parameter space to provide information on key systematics to reach below the previous 1%-10% accuracy limit (Chantler, 2010; Chantler et al., 2012).

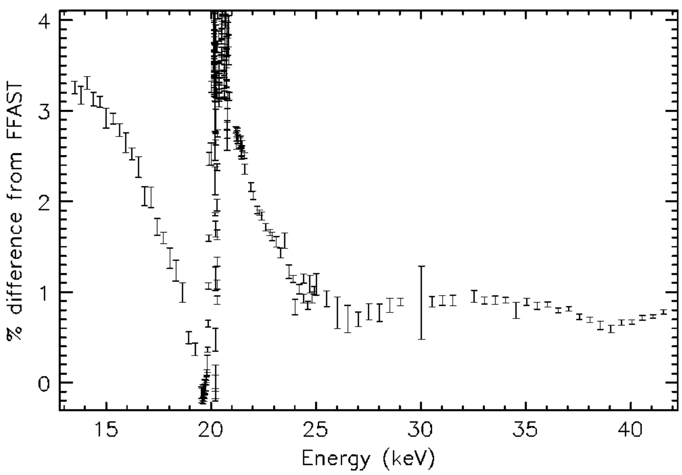

Figure 3. Total attenuation in Mo (Chantler group), from de Jonge (2005), relative to FFAST theory.

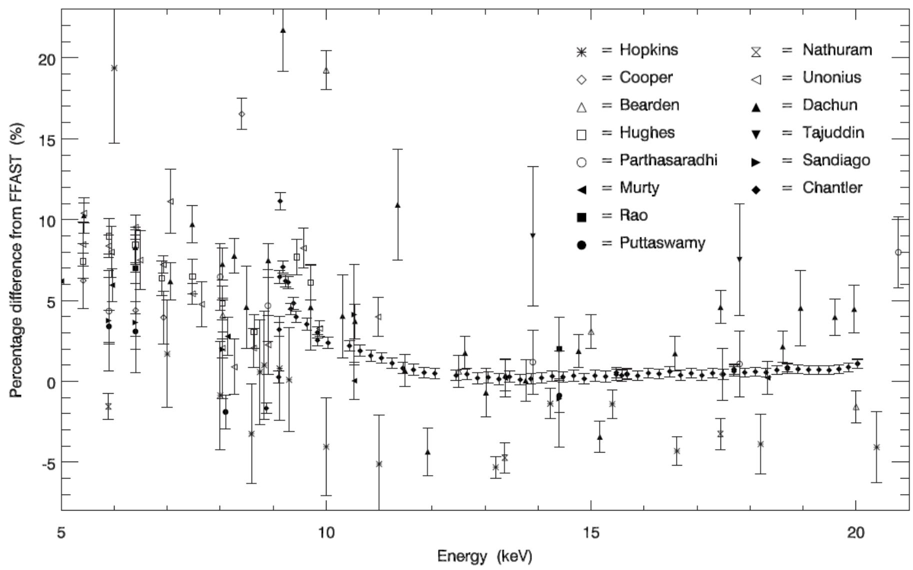

Figure 4. Total attenuation in Cu (Chantler group), from Glover (2008).

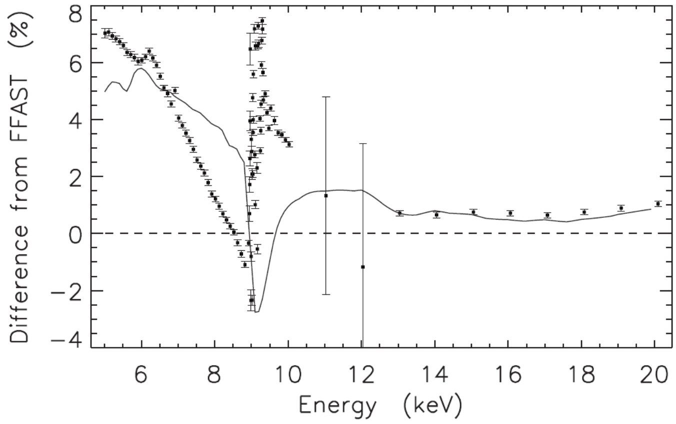

Fig. 5. Total attenuation in Cu (Chantler group), from Glover (2008).

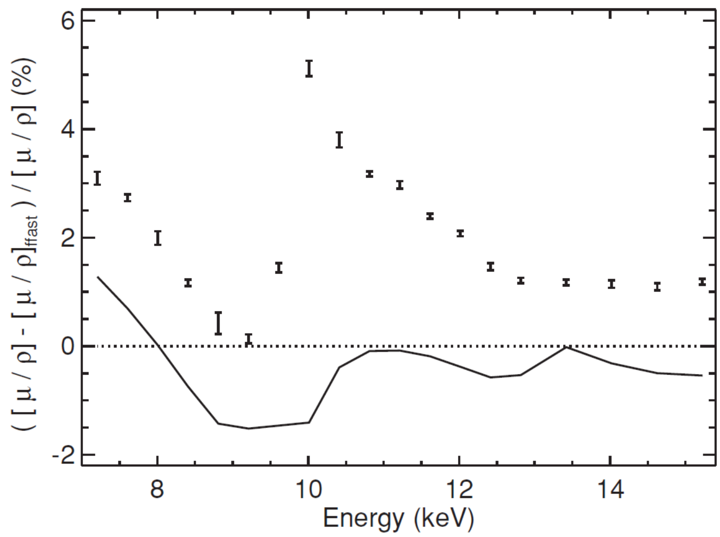

Figure 6. Total attenuation in Zn (Chantler group), from Rae (2010); compared to results of XCOM (solid line) and relative to FFAST (dotted line).

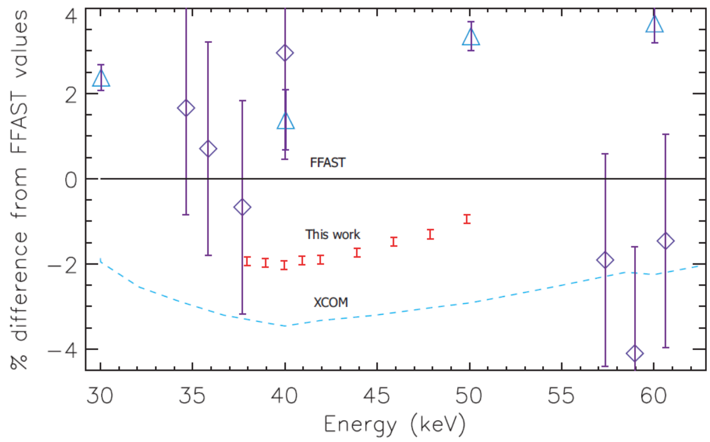

Figure 7. Total attenuation in Au (Chantler group), from Islam (2010)); compared to results of XCOM (dashed line) and relative to FFAST (zero line).

The results differ from tabulation (theory) by 1%-2%, even well above threshold, where isolated atom IPA predictions are presumed appropriate. For theory, inclusive calculations are required, summing over all processes. In the figures comparisons are made with two NIST theory tabulations (both IPA based): the more recent FFAST (Chantler 1995, 2000), and also the older XCOM (Berger 1987, Saloman 1988) in Figures 5 - 7. Earlier experimental work is also shown in Figures 4 and 7. Data in the figures is shown as differences from FFAST predictions.
The substantial scatter among previous experimental results is notable. At lower energies correlation effects will be important for edge positions, and condensed matter effects can become significant. There is a common tendency for XCOM to define edge positions relatively poorly (Fig. 5), and for convergence limitations of both theoretical frameworks to increase uncertainty for lower energies (below K edges or especially L-edges) above the anticipated high-energy uncertainty of order 1% (Chantler, 1995; Chantler, 2000). At the higher energies it is problematic to find

consistent positioning among the two present theory tabulations and the Chantler group experiments for the different elements. Fractional differences appear to become more stable at high energies, suggesting possible normalization issues (theoretical uncertainties here are anticipated to be about 1%, so indeed this may be within the uncertainties of theory).

Clearly in this situation there are two needs. (1) There should be independent confirmations of the Chantler group experimental approach and results. Indeed, the field ought to be moving in a direction where improved accuracy is expected, in order to give deeper insight to any patterns, and even comparisons of possible experimental issues at local beamlines. While some groups including Kodre (2006) and Ito (1998) have performed excellent investigations of atomic gases and vapours, the normal accuracy is quite understandably around 1%-10% and so does not easily address these questions – but indeed raises more. (2) A better theory of photoeffect and Compton scattering is needed, including correlation effects, consideration of higher shell contributions and relativistic effects. The importance of condensed matter effects at various energies needs to be investigated more closely.

B. Failure of nonrelativistic multipole description

We have recently noticed (Pratt and Florescu, 2012) that use of non-relativistic kinematics together with full multipole photons permits the prediction of spurious processes, revealing now the cause of such spurious features observed in predictions for photoeffect and photon scattering.

For example, for non-relativistic photon absorption by a free electron at rest, $k = p$, $ck = p^2/2m$, where k and p are magnitudes of photon and electron momentum. Hence $ck = k^2/2m$ with solutions $ck = 0$, $2mc^2$, i.e. a photon of energy $2mc^2$ could apparently be absorbed by an electron at rest ($k = 0$ means there is no process). However, in the dipole approximation the photon momentum is set to 0, so that there is no process permitting photon absorption by a free electron.

The corresponding full relativistic energy-momentum relations for absorption by a free electron in its rest frame of a photon are $k = p$, $(ck + mc^2)^2 = (cp)^2 + (mc^2)^2$. Substituting, the equation reduces to $2ck\ (2mc^2) = 0$ and thus there is indeed no process allowing absorption by a free electron.

With bound states rather than a free electron (as in photoeffect, Rayleigh or Compton scattering) the resulting spurious singularity moves off the real energy axis, but it impacts upon estimates of cross-sections even at and below 100 keV. The spurious terms in total cross sections are order $(Z\alpha)^2$ and p^2, in fact cancelled by relativistic terms of the same order. However, in angular distributions, multipole contributions lead to corrections of order $Z\alpha$ and p (which cancel in integration over angles), which are not affected by relativistic corrections. These are real and important multipole effects, not spurious. The same issue occurs in bremsstrahlung, where with non-relativistic kinematics a free electron (not in a field) can radiate a photon.

III. How we got here

A. Development of field

The idea of atoms goes back to the ancient Greeks, although it remained a less popular view at least until the time of Newton. We can associate the beginnings of a list of elements with Lavoisier in the 18th century. In the 19th century spectroscopy associated wave lengths of light with substances. Thomson identified the electron as the next century began. Bohr gave the beginnings of a quantum description of states and transitions, Rutherford gave our still recognizable model of the atom and its nucleus, and Einstein our concept of a photon.
We can trace the development of the field, which initially largely used independent particle approximation (IPA) in the description of atoms, used quantum mechanics and the quantum theory of radiation in the description of radiation processes. In some cases one could find useful simpler approaches. Later one went beyond IPA, describing correlations, recognizing the consequences of the various atomic environments. And for practical purposes one began to prepare tabulations of the cross sections for these processes.
We shall return to this development in the following section, but first we shall review a little of what the original workers in the field actually said. It is healthy to appreciate how where we now begin came about. In the following subsection we provide some fragmentary quotations, giving a little sense of our current starting point.

B. Some of the original ideas

(1) NEWTON Opticks, Book Three, Part I, Quest 30 and 31

Are not .. Bodies and Light convertible into one another, and may not Bodies receive much of their Activity from the Particles of Light.
Have not the small Particles of Bodies certain Powers, Virtues, or Forces, by which they act at a distance, not only upon the Rays of Light ... but also upon one another?... Bodies act one upon another by the Attractions of Gravity, Magnetism, and Electricity .. there may be more attractive powers than these... we must learn .. what bodies attract one another, and what are the Laws and Properties of the Attraction, before we enquire the Cause..The Attractions .. reach to very sensible distances... and there may be others which range to so small distances as hereto escape Observation..
The Parts of...hard bodies stick together very strongly...for explaining ...this.. some have invented hooked Atoms..others that bodies are glued together by rest ..by conspiring motions.. I infer that their particles attract one another by some force in immediate contact ..exceeding strong ..reaches not far from the Particles..
All bodies seem to be composed of hard Particles.. Even the Rays of Light seem to be hard bodies; for otherwise they would not retain different Properties in their different Sides...
And as in Algebra, where affirmative Quantities vanish and cease, there negative ones begin; so in Mechanicks, where Attraction ceases, there a repulsive Virtue ought to succeed. …
..Nature.. performing all the great Motions of the heavenly Bodies by the Attraction of Gravity.. and almost all the small ones of their Particles by some other attractive and repelling Powers .. The Vis inertiae is a passive Principle by which Bodies persist in their Motion or Rest, receive Motion in proportion to the Force impressing it, and

resist as much as they are resisted. …Some other Principle was necessary for putting Bodies in Motion; and now they are in Motion, some other principle is necessary for conserving the Motion.
All these things being consider'd, it seems probable to me, that God in the Beginning form'd Matter in solid, massy, hard, impenetrable, movable Particles, of such Shapes and Figures, and with such other Properties, and in such Proportion to Space, as most conduced to the End for which he form'd them;
Should they wear away, or break in pieces, the Nature of Things depending on them, would be changed... And therefore, that Nature may be lasting, the Changes of corporeal Things are to be placed only in the various Separations and new Associations and Motions of these permanent Particles...

(2) MAXWELL (1873) British Association at Bradford
Molecules

An atom is a body which cannot be cut in two....The doctrine of atoms (Democritus) and that of homogeneity (Anaxagoras) are .. in direct contradiction.
.. One may see the atom as a material point, invested and surrounded by potential forces. Another sees no garment of force, but only the bare and utter hardness of mere impenetrability.
The old atomic theory, as described by Lucretius and revived in modern times, asserts that the molecules of all bodies are in motion,...These flying molecules must beat against whatever is placed among them ... what is called the pressure of air.
The molecule, though indestructible, is not a hard rigid body, but is capable of internal movements, and when these are excited, it emits rays, the wave length of which is a measure of the time of vibration of the molecule. ..molecules from every specimen of hydrogen in our laboratories have the same set of periods of vibration, ..the same..is emitted from the sun and from the fixed stars .. molecules of the same nature ..exist in these distant regions.
Each molecule .. through the universe bears ..the stamp of a metric system .. No ..evolution can account for similarity of molecules, for evolution …implies continuous change.
None of the processes of nature .. have produced the slightest difference in the properties of any molecule. We are unable to ascribe either the existence of molecules or the identity of their properties to … any of the causes which we call natural.
On the other hand, the exact equality of each molecule to all others of the same kind gives it ... the essential characteristic of a manufactured object, and precludes the idea of its being eternal and self-existent.
..Science is arrested when she assures herself…that the molecule has been made, and …that it has not been made by any of the processes we call natural.

(3) EINSTEIN (1905)

In fact, it seems to me that the observations on “black-body radiation”, photoluminescence, the production of cathode rays by ultraviolet light and other phenomena involving the emission or conversion of light can better be understood on the assumption that the energy of light is distributed discontinuously in space.
According to the assumption considered here, when a light ray starting from a point is propagated, the energy is not continuously distributed over an ever increasing volume,

but it consists of a finite number of energy quanta, localized in space, which move without being divided and which can be absorbed or emitted only as a whole.

(4) N. BOHR, Philosophical Magazine, VI, 26, 1 (1913)
On the Constitution of Atoms and Molecules

Rutherford has given a theory. ….The atoms consist of a positively charged nucleus surrounded by a system of electrons kept together by attractive forces from the nucleus; the total negative charge of the electrons is equal to the positive charge of the nucleus. Further, the nucleus is assumed to be the seat of the essential part of the mass of the atom, and to have linear dimensions exceedingly small compared with the linear dimensions of the whole atom.
...We meet.. with difficulties of a serious nature arising from the apparent instability of the system of electrons
The way of considering ..this kind has…undergone essential alterations .. owing to the development of the theory of .. energy radiation…affirmation …found by experiments on very different phenomena such as specific heat, photoelectric effect, Röntgen-rays, andc.
…General acknowledgment of the inadequacy of the classical electrodynamics in describing the behavior of systems of atomic size. ... necessary to introduce …a quantity foreign to the classical electrodynamics, i.e. Planck's constant..
It will be shown that it is possible from the point of view taken to account in a simple way for the law of the line spectrum of hydrogen.
…The essential point in Planck's theory …is that the energy radiation from an atomic system does not take place in the continuous way assumed in the ordinary electrodynamics, but that it, on the contrary, takes place in distinctly separated emissions
..We are …led to assume the existence of a series of stationary configurations ...The configuration in which the greatest amount of energy is emitted ... we shall assume to be the permanent state of the system
…We may now…conclude that a bound electron -- also in cases in which there is no ionization -- will have an absorbing (scattering) influence on a homogeneous radiation…in perfect analogy with the assumption generally used that a free electron will have an absorbing (scattering) influence on light of any frequency.

(5) HIDEKI YUKAWA On the Interaction of Elementary Particles (1934)

…Interaction between elementary particles can be described by a field of force, just as interaction between charged particles is described by the electromagnetic field.
…This field should be accompanied by a new quantum, just as the electromagnetic field is accompanied by the photon,
The law of conservation of the electric charge demands that the quantum should have the charge either +e or -e. ..We obtain for m …200 times …the electron mass.
The interaction of such a quantum with the heavy particle should be far greater than with the light particle in order to account for the large interaction of the neutron and proton as well as the small probability of β-disintegration.

IV. What we do, and don't, know (Questions)

A. Description of atomic processes

In describing atomic processes one generally begins with independent particle approximation (IPA), in which all electrons move independently in a common central potential. In some cases simpler approaches are useful. But by now in many situations it is necessary to go beyond the IPA approach. And often it is also necessary to consider the environment in which the processes takes place, not taking the atom and the process as isolated.
Within the independent particle approximation (IPA) it is assumed that all electrons (bound and continuum) move in a common central potential V, not interacting with each other.
The potential V reflects the nuclear charge Z, perhaps also the charge distribution of the atomic electrons. The potential V is sometimes obtained self-consistently from the nuclear charge and the charge distribution of the atomic electrons. V is sometimes taken as $\propto 1/r$ at large distances r (a Latter tail), so that an atomic electron is not seeing its own potential. V can also include a local exchange approximation. Since there are no interactions among electrons, processes thus often only involve one "active" electron, the rest only present as "spectators". One uses quantum radiation theory, or (relativistic) quantum mechanics. Very rarely does anyone attempt to derive results using a bound-state (full) quantum electrodynamics (QED), and then primarily for a single-electron (hydrogenic) system. There is a relativistic full multipole version, obtaining elements of the relativistic S-matrix (in first or second order of perturbation theory for the atomic radiation processes). Many properties of the processes follow from the nature of the singularity of the potential V and the interactions in the process, particularly the high energy behavior of processes.
Simpler approaches can often be useful, although they must be used with care. The non-relativistic dipole approximation is often appropriate at low energies. Bound electrons can sometimes be replaced by a momentum distribution of free electrons, leading to:
(i) coherent scattering, with *form factors*, as in Rayleigh scattering, electron scattering, and bremsstrahlung, or; (ii) incoherent scattering, as in *impulse approximation* (IA) for Compton scattering. We may also mention *incoherent scattering factors*, representing sum rule integrations over IA to obtain differential Compton cross-sections.
In going beyond IPA a next level of complexity yields the Hartree-Fock approach (including non-local exchange). Proceeding to attempt to include correlations, many-body perturbation theory (MBPT) provides a systematic approach, but many other methods (such as the random phase approximation - RPA) have continued potential. Some processes impinge on fully relativistic structural approaches, including discussions of: (i) Delbrück scattering and (virtual) pair production; (ii) low-energy photons, and infrared divergence (IRD). New features also emerge in multiple processes, as in double ionization (with photoeffect and Compton contributions). Advanced approaches include relativistic MBPT (RMBPT) (Desclaux, 1973; Deslattes et al., 2003; Lindgren et al., 2006), multi-configuration Dirac-Fock (MCDF) (Grant et al., 1980; Chantler et al., 2009; Lowe et al., 2013), configuration interaction (CI) (Chen et al., 2001; Cheng et al., 2008) and (relativistic) convergent close-coupling (RCCC) (Bostock et al., 2009; Hoszowska et al., 2009) approaches, able to probe new processes.

In many more complex applications the atomic environment is crucial. It may be a molecule, a Fullerene cage, a cluster, a solid, a surface, or a plasma. The incoming projectile may be an intense photon beam (laser). Entanglement issues may arise, as also with the final state.

B. Standard approaches

Here we mention the standard long used simpler approaches to the radiation processes with which we are concerned.

Photoeffect

In the non-relativistic dipole approximation (Hulme), the matrix element is

$$M \sim \int \Psi^{*}_{f}\, r\, \Psi_{i}\, \mathrm{d}^{3}r$$

Rayleigh scattering

In a form factor approximation

$$M \sim f_{0}(q) \sim \int \rho(r)\, e^{i\, q\cdot r}\, d^{3}r,$$

which is the coherent part of Thomson scattering off the charge distribution ρ(r).
As the form factor is complex, it must include coherent and incoherent processes in any full definition, and indeed include anomalous dispersion.

Compton scattering

In the impulse approximation for scattering from a distribution of free electrons - DuMond obtained the Compton profile

$$d^{2}\sigma \propto \mathrm{J}(\mathrm{p}_{z}) \propto \int_{\mathrm{p}_{z}}^{\infty} d\mathrm{p}_{x} d\mathrm{p}_{y}\, \mathrm{p}\, \rho(\mathrm{p})$$

where p_z is the initial free electron momentum along the photon momentum transfer required by free-particle energy momentum conservation, and ρ(p) is the atomic charge density in momentum space.

C. Photoeffect - newer issues

Continuing issues in atomic photoeffect involve low-energy photons (visible and VUV), and also higher-energy photons (X-rays). The issues include correlation effects among atomic electrons, but also the higher multipole effects of the radiation. Final states may involve more particles, as in multiple ionization. Observations may be more differential, and they may also include spin and polarization variables. Cross sections exhibit various kinds of structures, including resonances associated with intermediate states, shape resonances associated with scattering, and minima associated with matrix element zeroes at particular energies.

Correlation effects are very important at low energies and can drastically modify the magnitudes and behaviors of cross sections. Figure 8 shows an example, comparing an IPA total cross section (RHFSL type) for Ar 3s with a cross section including correlations (RRPA type). In the past most such calculations were performed within dipole approximation, but it is now appreciated that even at low energies higher multipoles (at least quadrupole) are often important, at least for angular distributions. Figure 9 shows the experimental determination of the deviations from a dipole angular distribution for Kr, and that they are well predicted by an IPA calculation in a screened central potential, but not for a point Coulomb potential.

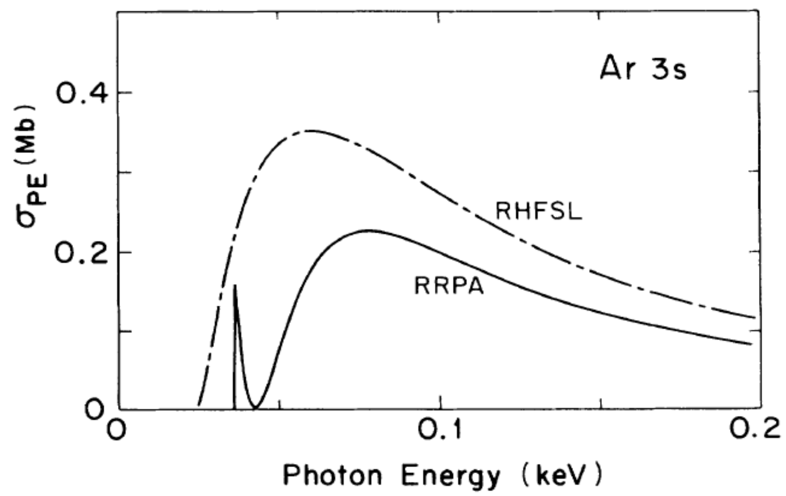

Figure 8. Photoionization total cross section of the Ar 3s subshell, dashed line in the RHFSL model (IPA) and solid line in an RRPA calculation (with correlations). From Zhou (1992).

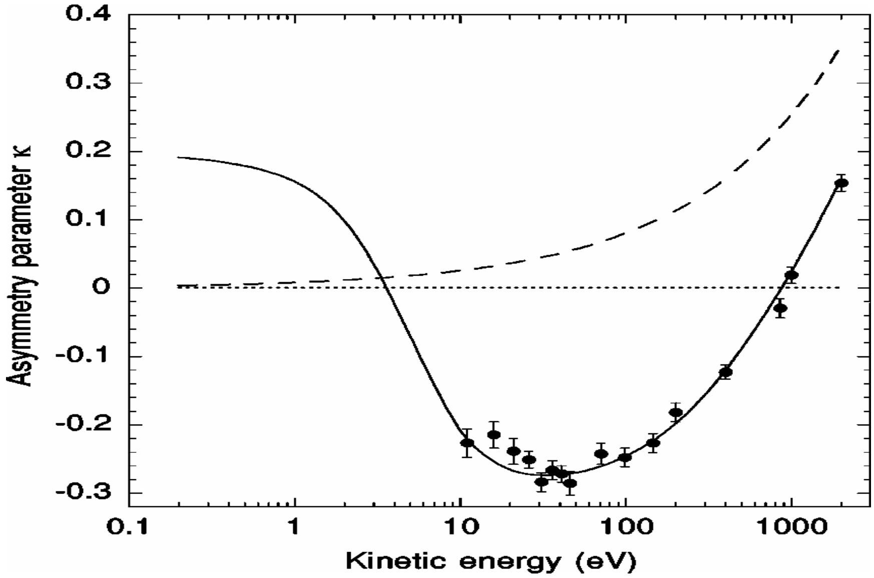

Figure 9. Retardation assymetry parameter κ for Kr 1s photoelectrons. Measurements (solid circles) are compared with screened IPA calculations (solid curve) and with the *4(v/c)* prediction of the point-Coulomb model (dashed curve). From Krassig (2003).

At higher energies (X-ray energies and above) full multipole calculations have always been used, but in the past it had been assumed that correlation effects became unimportant at high energies. Now it is realized that some correlation effects persist, even in the high-energy limit. Figure 10 illustrates the energy dependence of such effects observed in an experiment on Ne, comparing the ratio of 2s and 2p total cross sections in an experiment and with uncoupled and correlated calculations.

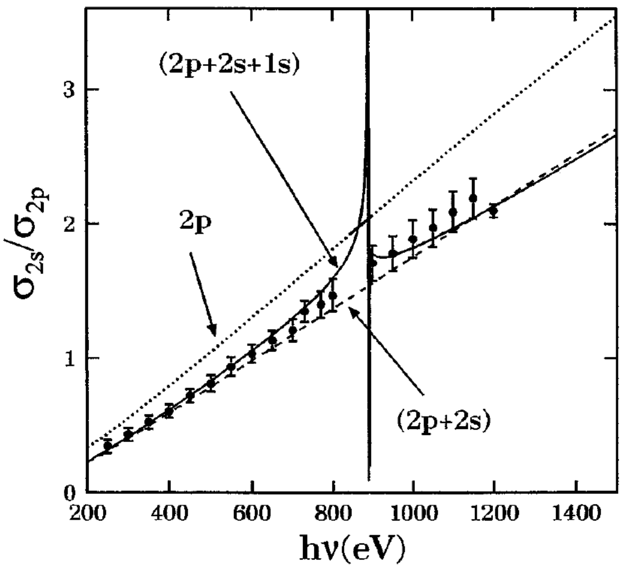

Figure 10. Ratio of 2s to 2p total photoionization cross sections for Ne, comparing experiment with RRPA calculations (1) with 2p, 2s and 1s channels coupled (solid curve), (2) with 2p and 2s channels coupled (dashed curve) and (3) with 2p and 2s channels uncoupled (dotted curve). From Dias (1997).

Multiple ionization is another consequence of correlation, and can sometimes be approximated within shakeup or shakeoff models. Figure 11 shows calculations of double and single ionization cross sections of He as a function of photon energy. Data is shown both for photoeffect and for Compton scattering.

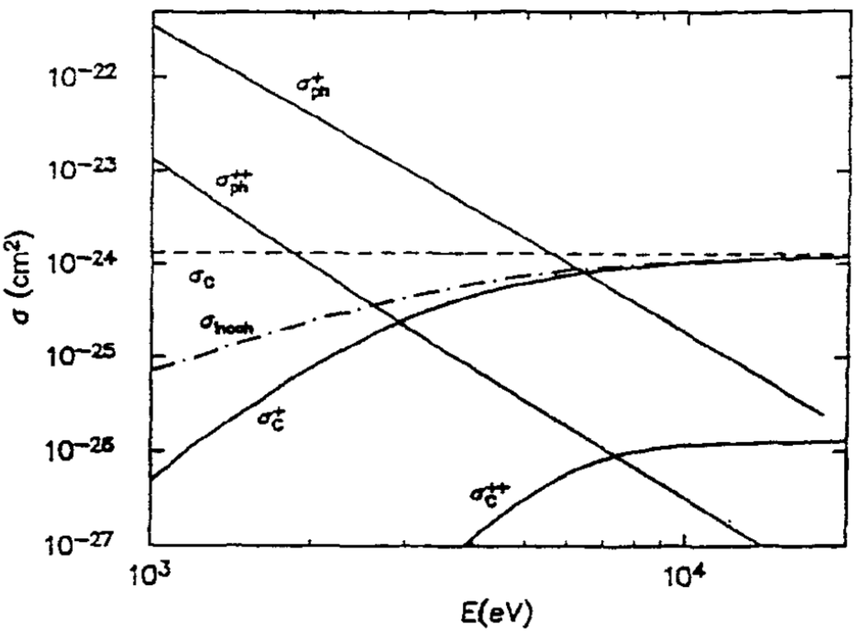

Figure 11. Theoretical total cross sections for double and single ionization of He by photoabsorption and by Compton scattering. Also shown are Compton scattering from two free electrons and total incoherent scattering (including Raman scattering). Note that σ_{incoh} is actually σ_{inel}, the inelastic contribution (σ_{ph} is also inelastic and incoherent). From Pratt (2000).

The minima in cross sections due to zeroes in dipole matrix elements, called Cooper minima (CM), have been known for some time. Their positions have been tabulated. The number of such minima is understood, but not yet their positions. Reduced matrix elements are analytic functions of energy, and in some cases the positions of zeroes are at negative energies, corresponding to the bound state regime. There are also CM associated with zeroes in quadrupole and higher multipole matrix elements. Effects of quadrupole CM have been observed in angular distributions. However, going beyond CM, it is now known that there are four different kinds of matrix element zeroes: (i) Cooper minima (CM), occuring in the 1 - 500 eV photon energy range, (ii) non-relativistic Coulomb minima (NRC) present even in the Coulomb potential, not allowed for dipole matrix elements, occuring at 500 eV - 50 keV, (iii) relativistic Coulomb minima (RC), only found in relativistic calculations, at 50 keV - 2 MeV, and (iv) high Z relativistic minima (HZR), found for Z > 128 near threshold. Situations in which these might be observed have been discussed.

D. Rayleigh scattering - newer issues

Form factor approximations give a good initial estimate of the differential cross-section for Rayleigh scattering in most situations. The contributions from the separate subshells, which add coherently, are shown in Figure 12 for C and Pb. Note that all subshells contribute at forward angles, but only inner subshells contribute at the larger angles. The resulting cross-sections, forward peaked at high energy and increasingly angle-independent at low energy, are shown in Figure 13.

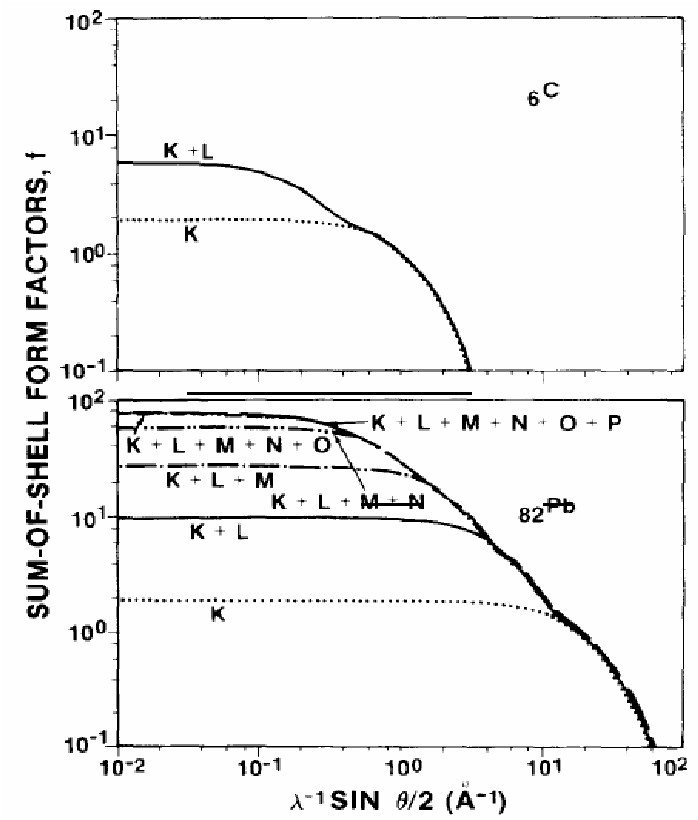

Figure 12. Atomic shell form factors as a function of momentum transfer, for C and Pb, from Kissel (1985).

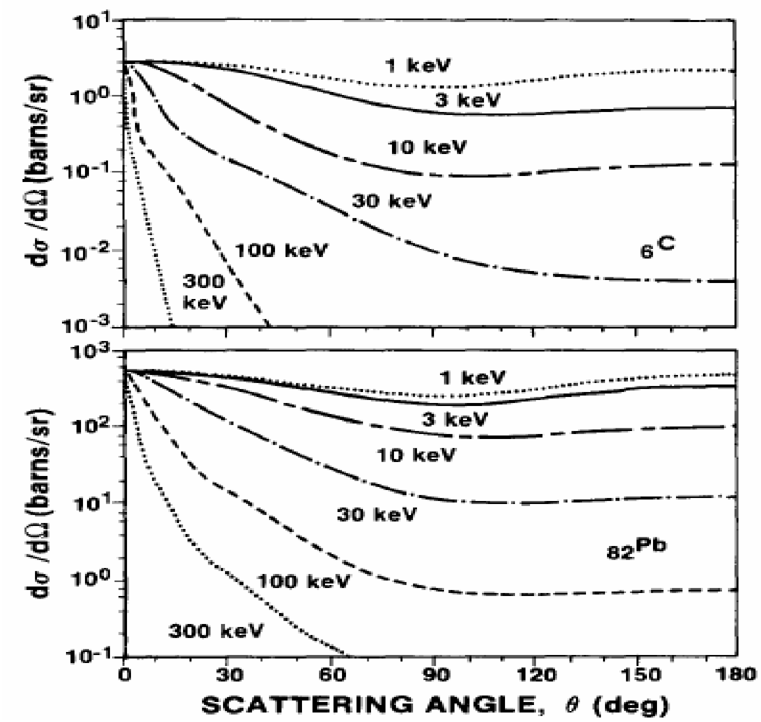

Figure 13. Differential elastic photon-atom scattering cross-sections, from the amplitudes for nuclear Thomson scattering and Rayleigh scattering in form factor approximation, for C and Pb, from Kissel (1985).

More advanced form factor approximations are important at all energies. Most significant is the situation at low energy, where the contribution from a given subshell in fact turns off for photons below the energy for (virtual) excitation or ionization of that subshell. Thus the Rayleigh cross-sections at low energy are much smaller than values based upon f_0. This is of concern for energies low enough that Rayleigh scattering is becoming dominant in total attenuation. In general the deviations from the basic form factor approximations may be characterized by anomalous scattering factors in the amplitudes. The imaginary part of the anomalous amplitude at forward angle is determined from the photoeffect total cross section; the real part can then be obtained from a dispersion relation. It is a moderately good approximation to take these scattering factors as angle independent, but this assumption can be poorest for high-Z inner shells. Naïve form factor approximations also omits the resonances of the full Rayleigh amplitude associated with the (virtual) excitations and ionizations of the bound electrons. All these effects can be included in more advanced form factor developments, including for example the modified form factor approximation MFF.
Rayleigh scattering, usually tabulated for neutral atoms in their ground state, naturally depends on the atomic configuration, and so differs depending on the state of excitation or ionization of the atom. This can be crucial in plasma investigations. An example of dependence on configuration is shown in Figure 14, which also illustrates that associated with resonance regions are also minima in cross sections.

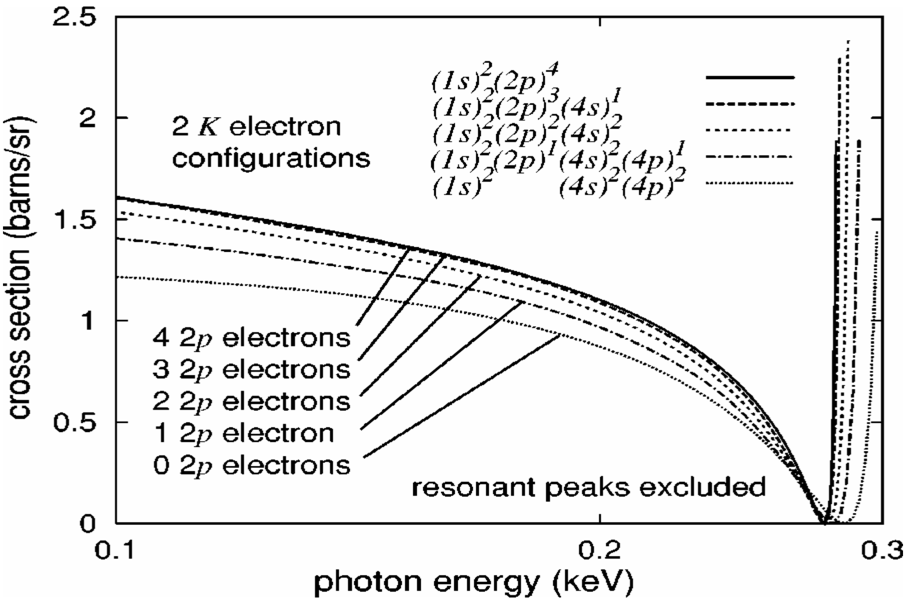

Figure 14. Forward-angle Rayleigh scattering cross-section in carbon below the resonance region for various configurations, from Carney (2000)

Rayleigh scattering in fact is simply one component of the total elastic scattering amplitude; it must be added coherently with all other components, most usually including nuclear Thomson scattering. The components are not physically distinguishable processes. There has been much discussion of the Delbrück amplitude, corresponding to scattering of a photon off a virtual electron/positron pair in the atomic field. This component of elastic scattering becomes important by gamma ray energies, and its contribution has probably been observed, although calculations have been uncertain.

E. Compton scattering - newer issues

In discussing Compton scattering there are two quite different situations, depending upon whether one is interested in the total scattering off the atom, or in scattering off a definite (inner) shell. Except for the lowest energies and lightest elements, the total scattering off the atom may be dominated by the scattering off the outer electrons, and which can be approximated by scattering off free electrons. Low energy light element scattering and high-energy scattering off high-Z inner shells are however very important and complex, and we will concentrate on the last of these. Further, studies of the triply differential cross section (observing the ejected electron) are very limited, and we will mainly discuss the doubly differential cross section, observing the energy and scattering angle of the outgoing photon.

In Figure 15 we show this spectrum at fixed scattering angle. It has three distinct features: (i) an infrared divergence for soft outgoing photons; (ii) resonances connected with resonant Raman scattering, present except for K shell scattering, and; (iii) a broad Compton peak reflecting the momentum distribution of bound electron charge, corresponding to the peak in scattering off a free electron. The infrared rise of the spectrum for soft final photons is shown in Figure 16. This cross-section is proportional to the corresponding photoeffect cross section (low energy theorem). It is divergent, and therefore the total cross-section for Compton scattering is not defined, without that one specifies an allowed energy resolution. Resonant Raman scattering also requires a separate treatment. Only the third feature, the Compton peak, is obtained in the impulse approximation.

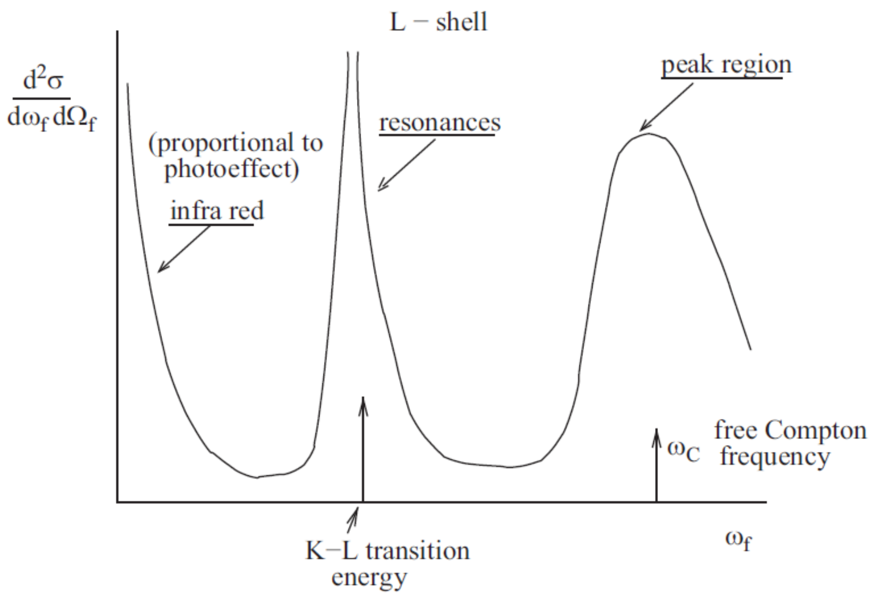

Figure 15. Schematic presentation of spectral features in Compton scattering of an outgoing photon energy, at a particular scattering angle, and for an incident photon energy, illustrating infra-red divergent behaviour for low-energy outgoing photons, resonant behaviour near characteristic X-ray energies (resonant Raman), and a broad Compton peak for high-energy outgoing photons. From Pratt (2010).

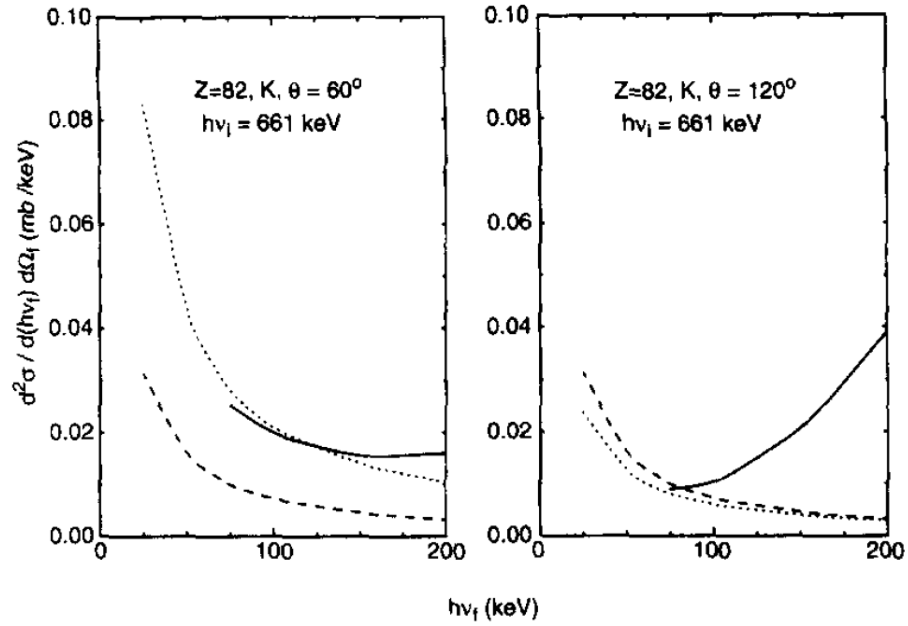

Figure 16. Low scattered photon photon energy part of the spectrum of the previous sketch, for 661 keV photons scattered from the K shell of copper into 60° and 90°. The solid curve is the S-matrix result, the dotted curve obtained using the low energy theorem, and the dashed curve using nonrelativistic *p.A* theory. From Bergstrom (1997).

The impulse approximation (IA) can be justified when the momentum transfer in scattering is large in comparison to the average bound state electron momentum. However IA is often found to be adequate even when they are comparable, although there are corrections for high Z. In Figure 17 we show a study of the validity of the impulse approximation, comparing it with full S matrix (SM) calculations. We see in this case that IA poorly represents the full triply differential cross section, but it does quite well for the integrated doubly differential cross section. Proof of this cancellation of errors has been attempted, but it has not yet been achieved.

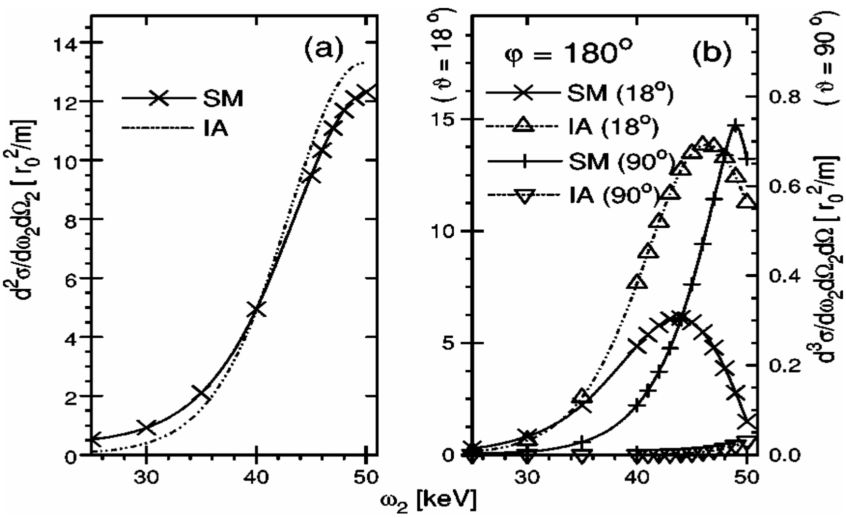

Figure 17. Validity of the impulse approximation, compared with S-matrix calculations, for scattering of a 59.32 keV photon from the K shell of Cu into 140°, (a) for the doubly differential crooss section, with good agreement, and (b) for two

outgoing electron angles of the triply differential cross section, displaying very poor agreement, frrom Kaliman (1998).

At high energies a relativistic impulse approximation (RIA) is needed (Ribberfors), as shown in Fig. 18. Relativistic kinematics in the factor multiplying the Compton profile leads to a large change in the magnitude of the peak; relativistic kineatics for *p* leads to a large change in the angular position of the peak. In high *Z* elements using a relativistic momentum density leads to some change in the magnitide of the peak. However, in comparison with SM, deviations from RIA can still be important in some cases, as illustrated in Fig. 19. Here LET (low energy theorem) deviations, describing the IR region, when added to RIA will remedy the soft photon region, but a deviation from SM remains in the peak region.

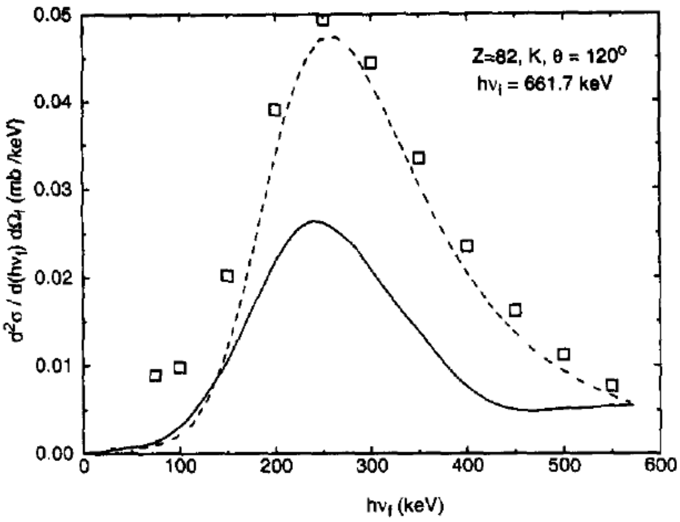

Figure 18. Comparison of relativistic impulse approximation (RIA, dashed line), nonrelativistic impulse approxomation (IA, solid line), and S-matrix calculations (boxes), for the scattering of an unpolarized beam of 662 keV photons from the K shell of lead into 120°, from Bergstrom (1997).

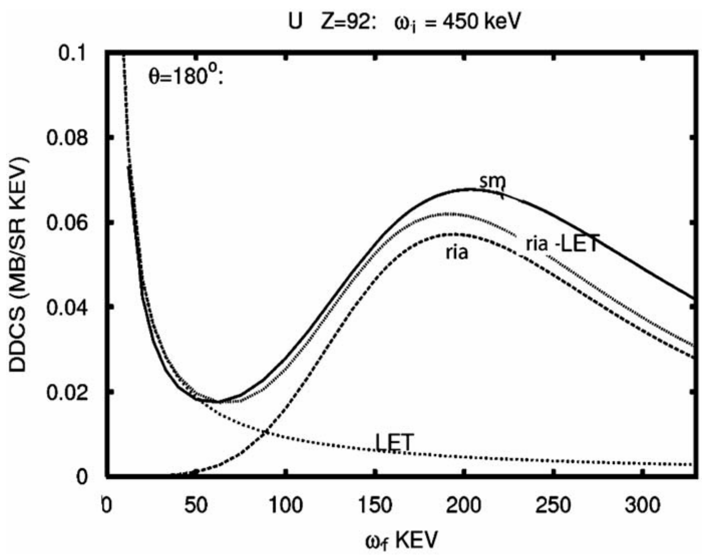

Figure 19. Compton scattering at 450 keV from the K shell of U at 180°, showing S-matrix calculations and contributions from the low energy theorem (LET) and relativistic impulse approximation (RIA). From Pratt (2010).

V. Summary

Total photon-atom cross sections and angular distributions of moderate accuracy are available for many situations. Predictions for more detailed observations or of higher precision are often uncertain. It is often not known how to do better.
In photoeffect the main uncertainty is in determining the role of correlations. Rayleigh scattering is most uncertain in threshold regions, but also in high Z elements, at high energies, and at large angles. The main uncertainties in Compton scattering are for inner shell contributions.
There is a lack of systematic high accuracy experimental and theoretical data. It remains unclear how to appropriately characterize, present, and tabulate data, even more so for more differential data.

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