Radiation Physics and Chemistry 95 (2014) 4–13

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

journal homepage: www.elsevier.com/locate/radphyschem

Photon absorption and photon scattering—What we do not know and why it matters

R.H. Pratt

Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA

ARTICLE INFO

Available online 31 October 2013

Keywords:
Photon absorption
Photon scattering
Compton scattering
Rayleigh scattering

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 recognized. 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.

1. Photons and atoms

1.1. 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 and Garnow, 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 and 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.

1.2. 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

E-mail address: rpratt@pitt.edu

0969-806X/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.radphyschem.2013.10.018

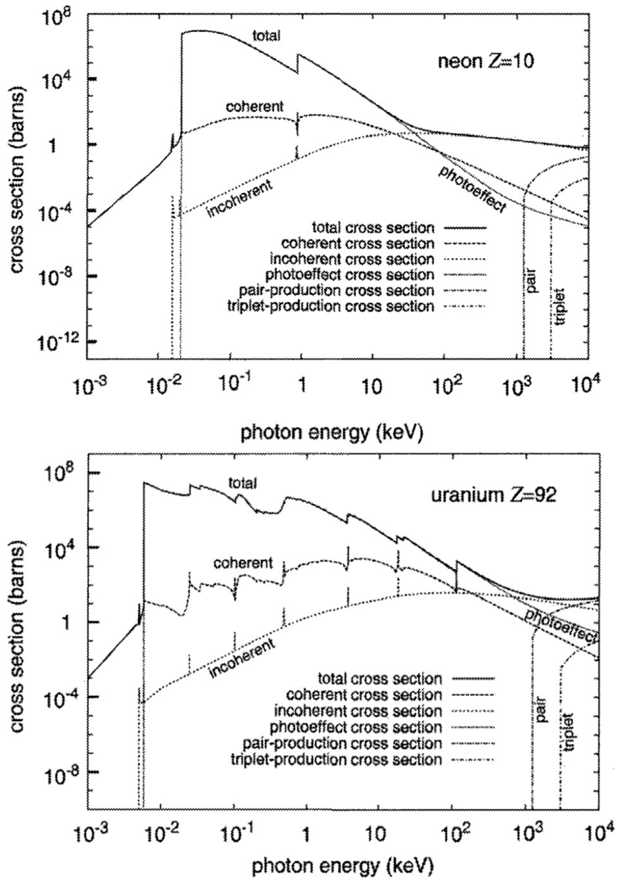

Fig. 1. Total cross sections for various photon–atom processes.
Reproduced with permission from the American Insitute of Physics (Pratt, 2000)

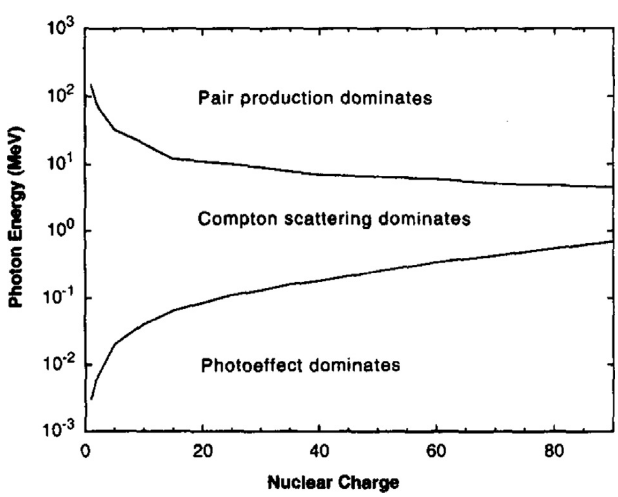

Fig. 2. Relative importance of processes in total absorption cross sections as a function of photon energy and element. Below the lowest ionization threshold Rayleigh scattering will dominate. .
Reproduced with permission from Elsevier (Bergstrom and Pratt, 1997)

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)

$$\sigma_{\rm pe} = \sigma_{\rm pe}\sum_{i,j}\xi_i\zeta_j \mathrm{C}_{i,j\ pe}$$

and for Rayleigh scattering (for incident and final photon)

$$\sigma_{\rm R} = \sigma_{\rm R}\sum_{i,j}\zeta_i\zeta_j \mathrm{C}_{i,j\ R}.$$

here σ 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 et al., 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.

2. 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 Fig. 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.

2.1. Total attenuation

We show in Figs. 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 5–60 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.