Photon-Atom Scattering Cross-sections of Atomic Hydrogen and Helium

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Synopsis We have developed an ab initio method for computing photon-atom scattering cross-sections in a single-shot calculation. Our method uses pseudostate information to compute the complex transition polarisabilities and the Rayleigh, Raman, Compton and photoionisation cross-sections for atomic hydrogen. Our method is simple and intuitive and can easily be adapted to higher-order scattering processes and other atoms. We also present the low energy scattering cross-sections of helium.

We present a quantitative description of the second-order photon-hydrogen scattering processes involving the absorption and emission of one photon. We introduce a method that allows us to compute the cross-sections of the Rayleigh, Raman, Compton and photoionisation process using complex transition polarisabilities. These scattering cross-sections have applications in fields such as astrophysics [1] or high-precision AMO experiments [2].

Rayleigh scattering refers to the elastic scattering process where a photon of frequency ω is absorbed and emitted. Raman and Compton scattering are inelastic processes where a photon of frequency ω is absorbed and a frequency of ω' is emitted. In the case of Raman scattering, the final state is a bound state that is not the initial state, whilst Compton scattering ionises the atom (final state is in the continuum).

Our method uses configuration interaction and an atom-in-a-box approach. As a result, the continuum is discretized and described by a set of discrete, positive energy states that we refer to as 'pseudostates'. These pseudostates allow us to compute the complex transition polarisabilities above the ionisation threshold, and allows us to avoid the infra-red divergence in the Compton cross-section calculation.

The complex transition polarisabilities are given by the Kramers-Heisenberg matrix elements and describe the process where an atom initially in state i transitions to state j through the absorption and emission of a photon. It should be noted that the transition polarisability has *two* imaginary terms where $\mathrm{Im}_0[\alpha_{ij}(\omega)]$ is related to the linewidth of each state and $\mathrm{Im}_1[\alpha_{ij}(\omega)]$ to the photoionisation. These complex transition polarisabilities are used to compute the second order scattering cross-sections, which are presented in Fig. 1 for atomic hydrogen.

Our cross-sections for Rayleigh and Raman transitions are in agreement with previous work, and the cross-sections in Figure 1 agree qualitatively with the scattering cross-sections from the FFAST database. However, our Compton cross-section is up to three orders of magnitude larger than previous results by Bergstrom et al. [3] and Drukarev et al. [4]. We have been able to resolve this large discrepancy by considering the contributions to the cross-section by states of different angular momentum and comparing the Compton differential cross-sections [5].

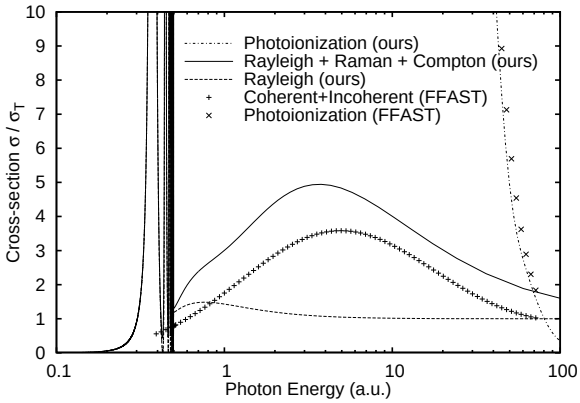

Figure 1. Plot of benchmark cross-sections for a photon scattered by atomic hydrogen, relative to the Thomson scattering cross-section σ_T. Various scattering cross-sections from the NIST databases (http://www.nist.gov/pml/data/) are also shown.

Our computational method has the advantage of being extremely versatile, as it can be extended to any atom in any initial state as well as to higher-order scattering processes. We will present the second-order hyperpolarisability at frequencies below and above the first ionisation threshold as well.

References

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