Low-energy photon-alkali atom scattering cross-sections

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Synopsis We have developed an *ab-initio* computational method to calculate the fundamental cross-sections that describe how a photon is scattered by an atom. We compute the complete set of (complex) transition polarizabilities which are then used to compute the scattering cross-sections of photoionization, Rayleigh, Raman (ending in bound-states), and Compton (ending in continuum-states) processes. These are obtained from a single-shot atomic structure calculation, via a pseudostate-based discretisation of the continuum. We find cross-sections for atoms including hydrogen and helium that have orders-of-magnitude discrepancies against previous cross-sections. We present here total cross-sections for low-energy (sub-100 eV) photon scattering off hydrogenic systems, helium, metastable helium, and the alkali metals, along with two-photon ionisation cross-sections.

We have developed and applied a method to solve the photon-atom scattering problem using an atom-in-a-box by diagonalising the atomic Hamiltonian in a large Laguerre-orbital basis. We have solved the benchmark photon-hydrogen [1] and photon-helium scattering problems where we are able to observe the onset of the infra-red divergence that plagues analytic approaches to total Compton scattering. We report here a set of cross-sections for low-energy photon scattering off neutral alkali atoms. Our target photon energies are restricted to below ≈ 100 eV, where core-excitations are not explicitly allowed. This is the regime of many AMO physics experiments.

Our cross-sections for photon-helium scattering are shown in Fig. 1, up to 54 eV (ie. the middle of the extreme ultraviolet range) The calculations by Grosges *et al.* [2], using different computational methods to ours (Dalgarno-Lewis), predicts that helium behaves as if it is has 1000s of electrons through the extreme ultraviolet region, whereas we find only a couple. We also find no evidence for the strong oscillations in their cross-sections. Our configuration interaction calculations have up to 16,000 configurations, and are converged (except for the smallest Raman contribution around $\omega = 1.25$ a.u. where errors due to the pseudostate discretisation are evident).

We also find disagreement with the FFAST database [3], which predicted 1/10th of an electron in this energy range. The USA-based NIST has various Atomic and Molecular Physics databases as part of the Standard Reference Data program [4], including XCOM/XGAM, FFAST, XAAMDI. These databases, which focus on X-Ray through γ-Ray photon energies, find application through fundamental physics, materials sciences, and medical physics. The NIST calculations all resort to severe approximations which are not reliable at these energies.

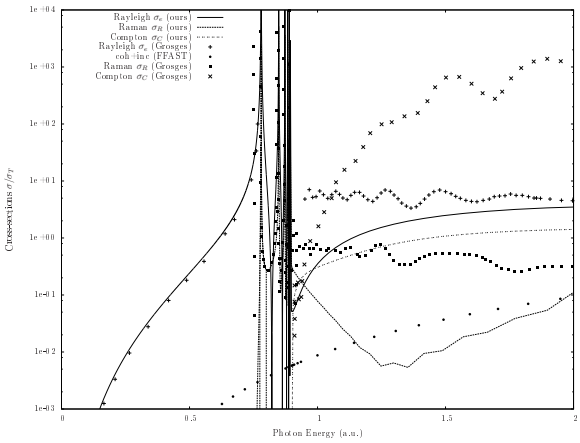

Figure 1. Total cross-sections σ/σ_T for photon-helium scattering (incoming photon energy in atomic units, i.e. up to 54 eV). Compared to previous calculations [2], and FFAST [3]. The Thomson cross-section $\sigma_T \equiv 6.65 \times 10^{-25}$ cm^2.

Our computational methods can be extended to any atom (or molecule) in any initial state, and enables quantitative insight into photon-atom scattering processes, especially for photon energies that can ionise the atom. Here we will present a smorgasbord of photon scattering cross-sections from hydrogenic systems, helium, metastable helium, and through to the alkali metals. We will also present recent work on adapting our methods towards calculating two-photon ionisation cross-sections of atomic systems.

References

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