Ab-initio simulations of strong field processes based on R-matrix theory

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Electron-ion re-collisions [1] are at the heart of most attosecond phenomena. An electron removed from an atom or molecule by a strong laser field oscillates and comes back to re-collide with the parent ion initiating a range of processes from high harmonic generation to double ionization and electron diffraction. These effects originate from electron–ion recombination or elastic/inelastic scattering in the presence of the strong laser field. It is commonly assumed that the strong laser field does not affect electron-ion recombination and scattering [2]. However, the situation may change in the presence of structured continua, as has been recently shown theoretically [3] and demonstrated experimentally [4]. We aim at developing an *ab initio* approach to investigate electron-ion collisions in the presence of the strong laser field. We will present our first proof-of-principle results for the H_2 molecule.

Our approach is based on the R-matrix method. The R-matrix method consists of partitioning the space into a complicated inner region containing all the electron-electron interactions ($r < a$), and a greatly simplified outer region ($r > a$) far enough from the atom or molecule, such that only the target long range potential and the laser interacts with the scattered electron. For *ab initio* simulations, we use the UK R-matrix suite developed by Tennyson *et al*. [5]. In order to adapt the UK R-matrix suite to the investigation of strong field physics, Harvey *et al*., developed the module CDENPROP which calculates the dipole transitions between continuum-continuum and continuum-bound states [6]. In this work, we describe the module STCFLD, which includes the quasi-static laser field to the UK R-matrix codes.

As an application of our methods, we study the photoionization of H_2 molecules in the low scattering energy regime (up to 40eV). Our preliminary calculations show the appearance of new resonances in the partial photoionization cross sections. Here, we will study and characterize these resonances for different intensities of the laser field.

References:

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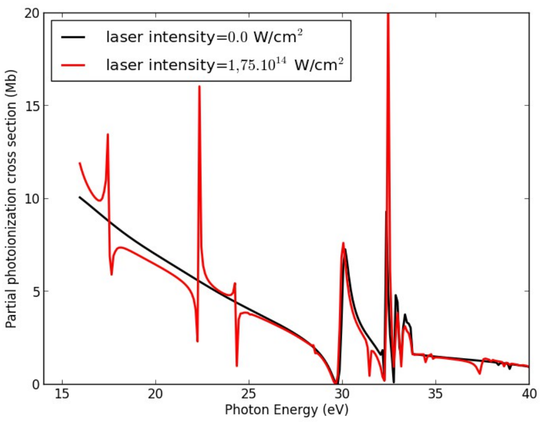

Figure 1: Partial differential cross section of H_2 with (red) and without (black) the quasi-static laser source.