New numerical techniques to determine ionization cross sections: series representation for r_{12}^{-1} integrals and Bohm's velocity field

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Synopsis Given an *ab initio* calculation of a three-body scattering wave function in spherical coordinates, we present a combination of new numerical tools for the evaluation of ionization cross sections.

In the last years we have developed an innovative tool to deal with three body scattering problems, based on a direct solution of the Schrödinger equation with appropriate flux boundary conditions [1]. The method uses a Generalized Sturmian Function (GSF) expansion of the three body wave function, in terms of two of the inter-particle coordinates of the problem. By using spherical coordinates, a partial wave series is performed both for the wave functions and the representation of the Coulomb interaction which depends on the third inter-particle coordinate, usually named r_{12}. The r_{12}^{-1} interaction is the only one not considered by the basis, as generally done in atomic calculations with not explicitly correlated basis functions.

Once all partial wave terms of the scattering wave function are evaluated, one may use integral formulas to extract the scattering amplitude. This is the case, for example, for the triple differential cross sections for double photoionization of Helium or for electron-Hydrogen ionization; from a practical point of view, this approach provides a good overall agreement with experimental results [1, 2]. However, such formulas have a major disadvantage since the integrals involve continuum wave functions and, besides, present some arbitrariness in the definition of the asymptotic final channels (see Ref. [3], for the discussion in the electron-hydrogen case).

In an attempt to overcome these difficulties, we recently proposed a new method [3] to recover the flux formula for ionization amplitudes [4] which was discarded after observation of apparently unphysical behaviors [5]. Our method, based on the use of Bohm's velocity field, has been applied successfully to s-wave electron-hydrogen ionization. In this contribution, we use it to deal with the ionization process in its full dimensionality, i.e., including the partial wave terms which are necessary for convergence.

Furthermore, we will combine this approach with a not so new technique to deal with the r_{12}^{-1} partial wave expansion. The idea, proposed in atomic calculations [6], is based on using a Taylor series in $\cos\theta_{12}$ instead of the usual Legendre polynomial expansion; the technique provides several alternatives as different series can be used for different angular regions. The method introduces a significant improvement when calculating atomic bound state energies; this can be understood as a more efficient representation of the potential for a given number of partial waves included in the expansion. We test this approach, for the first time here, for electron-hydrogen ionization and double photoionization of Helium.

References

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