J. At. Mol. Sci.
doi: 10.4208/jams.083112.091512a

Vol. 4 , No. 3 , pp. 193-209
August 2013

SDCS quantum mechanical flux formula revisited for electron-hydrogen ionization

L. U. Ancarani[a,*] and J. M. Randazzo[b]

[a] *Laboratoire de Physique Moléculaire et des Collisions, UMR CNRS 7565, Université de Lorraine, 57078 Metz, France*
[b] *División de Colisiones Atómicas, Centro Atómico Bariloche and CONICET, 8400 San Carlos de Bariloche, Río Negro, Argentina*

Received 31 August 2012; Accepted (in revised version) 15 September 2012
Published Online 28 June 2013

Abstract. Through a simple, classical, energy conservation analysis, we propose a finite distance reinterpretation of the standard energy fraction definition used for the single differential cross section (SDCS) for the electron-hydrogen S wave ionization process. The energy modification is due to the fact that, at finite distances from the nucleus, the continuum electrons have to overcome the remaining potential energy to be completely free. As a consequence, the flux formula for extracting - at finite distances - SDCS is also modified. Differently from the usual observations, the proposed corrections yield finite and well behaved SDCS values also at the asymmetrical situation where one of the continuum electrons carries all the energy while the other has zero energy. Results of calculations performed at various impact energies, for both singlet and triplet symmetry, are presented and compared favorably with benchmark theoretical data. Although we do not know how, we believe that finite distance effects should strongly affect the evaluation of the flux and consequently the SDCS, also in the full electron-hydrogen case.

PACS: 34.8.Dp, 03.65.Nk, 34.10.+x

Key words: ionization, flux formula, differential cross section

1 Introduction

The solution of the quantum three-body Coulomb break-up problem is notoriously difficult both from a scattering theory and a numerical point of view. In the last decade, several numerical approaches have been put forward [1–8] to deal, in particular, with

*Corresponding author. *Email address:* ancarani@univ-metz.fr (L. U. Ancarani)

the single ionization of atomic hydrogen by electron impact: remarkable good agreement between several theoretical results, and with the available experimental data, was observed.

The present work aims to investigate some issues related to the extraction of cross sections from the asymptotic part of the (numerically evaluated) scattered wave function. While numerical solutions of the Coulomb three-body problem are now available with different methods, they are generally restricted to finite regions of the configurations space; this is directly associated to the computer clusters size. The main difficulty is to ensure that the appropriate asymptotic behavior is reached, and this requires very large domains (several hundreds atomic units, see e.g. [7]). Besides, some difficulties occur because all the channels are entangled when solving the Schrödinger equation. In the particular case of the ionization of hydrogen by electron impact, the elastic, excitation, and the ionization channels are all present and coupled. Investigating and comparing extractions procedures is of interest also for more complicated break up problems, the e-H case serving as benchmark test.

Different strategies have been used to extract ionization cross sections from the computed solutions. One of them is based on the counting of particles by means of the quantum mechanical probability current designed by Peterkop and his coworkers [9–11]. This flux formula procedure has two main advantages. First of all, it is independent of the description of the electrons in the final state which, for long range interactions, has a certain arbitrariness. Secondly, since the flux formula corresponds to counting particles, it is adequate not only for infinite, but also, for finite domains (which is always the case for numerical solutions). The usual technique to extract differential cross sections consists in extrapolating to infinity the results obtained on a finite domain (the infinite domain corresponds to the exact solution, which can be compared with the experimental macroscopic domains). In spite of these advantages, the flux formula has been somehow abandoned because it yielded a bad e-H SDCS behavior for extreme unequal energy sharing [10]. This unphysical behavior has been associated [11] to the fact that the ionization flux at finite distances is contaminated by discrete –excitation– channels. Other procedures to calculate cross sections use integral formulae; they do not present any difficulties associated to the finite domains as they yield convergent results. For this reason, integral formulae have been favoured [12], and the flux formula has been finally discarded. In this contribution, we revisit the flux formula: in a specific, benchmark, case we will show that it can be successfully used if an appropriate finite distances' correction is taken into account, and that the contribution of discrete two-body channels (which indeed should be present and coupled to the ionization channel) is not, to our mind, responsible for the failure of the procedure.

The Temkin-Poet (TP) model [14, 15] of e-H scattering provides an ideal test of any method that aims to study the problem of ionization. This simplified S wave model, in which angular momentum is neglected (the electron-electron repulsion is spherically averaged), contains all the complexities of a three-body Coulomb problem, in particular the long range nature of the Coulomb interactions. The TP model has been systematically