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Double Ionization of Molecular Hydrogen by Fast Electron Impact

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Abstract. We propose a theoretical model of the double ionization of homonuclear diatomic targets by fast electron impact. By application of two-effective-center continuum waves to describe the ejected electrons in the exit channel and by use of Nordsieck-type integrals, an expression has been obtained by an analytical treatment for the five-fold differential cross section, the relevant quantity to describe the kinematically complete collisions in the coplanar geometry. The correlate motion of the ejected electrons is taken into account by means of adequate Sommerfeld parameters.

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Key words: Hydrogen, collision, ionization, analytical method.

1 Introduction

Ionization of atoms and molecules by electron impact is one of the fundamental processes of atomic physics, whose comprehension becomes important in many domains such as plasma physics and nuclear fusion devices [1]. In particular, the study of kinematically complete double ionization experiments by electron impact provides a straightforward and powerful tool to understand the role of the electron-correlation effects as well as the projectile-target interaction during the collision process.

The first theoretical studies of double ionization of atoms by electron impact by Byron and Joachain [2], Smirnov *et al.* [3] and Neudatchin *et al.* [4] appealed for experiments, which were carried out several years later by Lahmam-Bennani *et al.* [5, 6]. However, the development of kinematically complete double ionization experiments by electron impact rapidly turned out to be very challenging. On the one hand, the need for using triple-coincidence techniques, to detect energies and angles of the electrons produced

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by the reaction, is a serious experimental limitation. On the other hand, an additional complication for measurements arises from the low intensity of the double ionization cross section.

Nevertheless, the technical advances achieved in the area of high sensitivity detection and the emergence over the last few years of a new generation of sophisticated spectrometers [7–9] have renewed the interest for the experimental study of double ionization by electron impact [10].

From the theoretical point view, only few models have been proposed to describe kinematically complete double ionization on atomic targets [11, 12]. In the case of diatomic targets, the description of the continuum electrons in the field of two Coulomb or distorted centers is much more difficult. The use of the solutions of the two-center Schrödinger equation in prolate spheroidal coordinates to determine the multiply differential cross section results with such computational difficulties that their direct application turns out rapidly to a purely numerical problem relevant to the computer science field.

In the present study, we propose a theoretical model of the double ionization of homonuclear diatomic molecules by fast electron impact. A two-effective-center approach (TEC), which has shown to successfully reproduce experiments on molecular hydrogen targets [13, 14], is applied to describe the ejected electrons in the exit channel. By use of Nordsieck-type integrals [15] and dynamic Sommerfeld parameters [16], an expression has been obtained by an analytical approach for the fivefold differential cross section (5DCS), which is the relevant quantity to describe the kinematically complete collisions in the coplanar geometry. As an illustration of our theoretical treatment, we present 5DCS results for the double ionization of H_2 at an incident energy of 1099 eV and under symmetric kinematics for the two ejected electrons, which have an identical energy of 10 eV. For the sake of comparison with the (e,3e) experimental results for helium reported in Ref. [10], both the so-called *fixed ejected angle* and *symmetric geometry* modes are investigated in this work.

Atomic units are used throughout unless otherwise stated.

2 Theory

Let us consider the dissociative double ionization reaction of the hydrogen molecule in its electronic ground state by electron impact, i.e.,

$$e^- + H_2(^1\Sigma_g^+) \rightarrow 3e^- + H^+ + H^+. \tag{2.1}$$

The collision is described in the laboratory system, whose origin coincides with the center of mass of the molecular hydrogen target, and the longitudinal z-axis is chosen parallel to the direction of the wave vector $\mathbf{k}_i$ of the incident electron. In the case of fast electron impact collisions where the TEC approximation is valid (typically of the order of several