Calculation of differential cross sections for electron impact excitation of H and He^+

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Abstract. We present the distorted wave Born approximation (DWBA) for electron impact excitation and a method to calibrate the DWBA. With the calibrated DWBA, the differential cross sections (DCS) for excitation of H and He⁺ from 1s to 2s and 2p are calculated and the results are compared with the absolute experimental measurements for H at incident energies of 50 eV and 100 eV. It has been found that the theoretical results are in very good agreement with the experiment, which confirms the validity of the calibration procedure. This work prepares an efficient theoretical method for numerical simulations of non-sequential double ionization of He in strong laser pulse in which laser-induced electron impact excitation of He⁺ is involved.

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Key words: electron impact excitation, distorted wave Born approximation, differential cross sections, total cross sections

1 Introduction

The process of electron impact excitation of atoms and ions is one of the most basic and important processes in atomic physics. Theoretical investigations of such problems are of not only practical interest but also more fundamental interest. Numerous theoretical methods have been proposed for calculations of differential cross sections (DCS) for electron impact excitation, including the distorted wave Born approximation (DWBA) [1,2], the second-order distorted wave model [3], the convergent close-coupling (CCC) calculations [5], and the *R*-matrix method [4], among which the DWBA is the simplest. The sophisticated theoretical models, such as the CCC and the *R*-matrix method, are supposed to be able to reproduce accurate DCS in angular distribution and absolute magnitude as

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well at low incident energies. On the other hand, for high energies, both the total cross sections (TCS) and the DCS predicted by DWBA are in fairly good agreement with the absolute measurements. However, it has been well recognized that, at low energies, the TCS predicted by the DWBA substantially overestimates the experimental values. "Ideally, one could use the *R*-matrix approach for low energies, the DWBA for high energies, and the two theories would yield the same results for intermediate energies. Unfortunately, we do not live in an ideal world [6]."

The purpose of this work is to calibrate the DWBA for electron impact excitation of H and He⁺ at low energies by employing the empirical formula proposed by Tong *et al.* [7]. This calibration procedure has been previously applied to correct the overestimate of DWBA on the DCS for electron impact excitation of Ne and Ar [8].

Our ultimate objective is to apply the calibrated DWBA to simulate the correlated momentum distributions in nonsequential double ionization (NSDI) of He in strong laser fields [9,10].

The process of NSDI is one of the laser-induced rescattering processes, which still remains one of the most interesting and challenging topics in strong field physics. Both electron impact ionization and electron impact excitation of ions could be involved in NSDI. In the last two decades a lot of experimental measurements have been performed, particularly noteworthy are the correlated momentum distributions of the two outgoing electrons which were measured at the turn of this century [11]. In the meantime, a number of theoretical efforts have been devoted to this problem as well. In one of the theoretical models, which was developed by Chen et al. [12,13], the correlated two-electron momentum spectra can be treated as a product of the wave packet for laser-induced returning electrons and the differential cross sections for the laser-free electron impact excitation and/or ionization of the parent ion. In the practical simulations of the correlated electron momentum distributions for NSDI, one needs to evaluate the DCS for electron impact excitation of the parent ion to all possible excited states at all incident energies from threshold to the maximum returning electron energy which is usually less than 200 eV. Due to the heavy computational demand, relatively simple and efficient theoretical approaches are highly desired. Since the shape of the DCS predicted by DWBA is typically in fairly good agreement with the experimental measurements, once the overestimate of DWBA on the DCS is corrected, the calibrated DWBA can serve as a good candidate for such required theoretical tools.

The organization of this paper is as follows: In Section 2, the theory of DWBA for electron impact excitation is presented in detail and the method to calibrate DWBA is proposed. In Section 3, the normalization factors for DWBA at incident energies below 1000 eV are given for electron impact excitation of H and He⁺ from 1s to 2s and 2p, and the calibrated DCS of DWBA for H at 50 eV and 100 eV are compared with the experimental measurements. Furthermore, some calibrated DCS of DWBA for H and He⁺ at four different incident energies below 100 eV are analyzed. And finally some conclusions are drawn in Section 4.

Atomic units are used in this paper unless otherwise specified.