(e, 3e) Test on e–e correlations in helium

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Abstract. The angular variations of the five-fold differential cross section obtained by using different wave functions of helium are compared with experimental data. It is found that in the coplanar geometry two kinematical arrangements, (i) equal energy sharing between the two ejected electrons with one of them ejected along the momentum transfer direction and the other along varying direction and (ii) the Bethe ridge condition with fixed sum of ejected electron energies and varying angle between them, are very sensitive to e–e correlations contained in the target wave function. This comparison has been used to show that open-shell class of wave functions better incorporate e–e correlations than the closed-shell class.

Keywords. Electron–electron correlation; differential cross section.

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1. Introduction

One of the main aims of (e, 3e) studies initiated and pioneered by Lahmam-Bennani and co-workers about ten years ago was to investigate electron–electron correlation in the target. The angular distribution of the five-fold differential cross section (FDCS) in the kinematically fully determined initial and final states carries that information. Earlier experiments [1,2] were performed on Kr and Ar and that prompted theoretical (e, 3e) studies on these systems. The interpretation of the results in a (e, 3e) process and extraction of correlation information is however made quite difficult by several complicating factors. One of the factors relates to the mechanism of double ionization: (i) the shake-off (SO) in which the projectile is assumed to interact only once with the target and ejects one of the target electrons. The ejection of the other target electron is caused only by their mutual correlation in the initial state and the relaxation of the residual ion after the first ejection. The ejection of the other target electron is caused only by their mutual correlation in the initial state and the relaxation of the residual ion after the first ejection. (ii) a two-step (TS1) process in which the incident particle ejects one target electron which then interacts with and ejects the second one and (iii) another two-step (TS2) process in which the incident particle interacts successively with the target electrons and ejects them one by one. A proper accounting of e–e correlation in the final state which contains three electrons in the field of the residual ion and eliminating its influence on FDCS angular distribution is another complicating factor. Then, there are complications due to the multielectronic
structure of the target and the residual ion. In order to better understand the process, several (e, 3e) studies have been done on helium [3–15]. Helium is the simplest target for (e, 3e) with no internal core and the residual He$^{+2}$ ion is a bare nucleus and so there are no complications due to the multielectronic structure of the residual ion in the final channel. The details of the angular distribution of FDCS have been analyzed in the coplanar geometry with symmetric and asymmetric energy sharing between the ejected electrons and in the Bethe ridge kinematics and have also been compared with $(\gamma, 2e)$ process. The calculations have been done at large incident energy $E_0 \sim 5$ keV, very small scattering angle and low ejected electron energies corresponding to the measurements of Lahmam-Bennani and co-workers.

Recent experiments [12–14] on helium have given a new dimension to (e, 3e) studies. A fairly large number of wave functions have been proposed over the years to describe the ground state of helium. It is now possible for the first time, due to the availability of (e, 3e) data, to "(e, 3e) test" them for internal electron–electron correlations and assess their suitability. These wave functions have been used in calculating various macroscopic quantities such as dielectric and magnetic susceptibility, van der Waals constant etc. and in various studies such as elastic scattering, inelastic scattering, single ionization, etc. The results are found to be essentially similar and the experimental data is not able to lead to any preference for one choice over the other [16]. This is understandable since the results depend on the density distribution or single electron momentum distribution. The criteria for the choice of the wave function therefore has been simple analytic structure for ease in calculations, easier interpretation, largest binding energy and satisfying electron–nucleus and electron–electron cusp conditions.

$$\left(\frac{1}{\phi_0} \frac{\partial \phi_0}{\partial r_1}\right)_{r_1 \to 0} = \left(\frac{1}{\phi_0} \frac{\partial \phi_0}{\partial r_2}\right)_{r_2 \to 0} = -Z,$$

$$\left(\frac{1}{\phi_0} \frac{\partial \phi_0}{\partial r_{12}}\right)_{r_{12} \to 0} = \frac{1}{2}.$$

These wave functions may be put in three broad groups: (i) Hartree–Fock wave function [17], its analytical fit by Byron–Joachain [18], Hylleraas zero order wave function and a recent one by Bhattacharyya et al [19]. These are sometimes called closed-shell (CS) type. (ii) Hylleraas higher order wave functions, those due to Silvermann et al [20], Mires [21], Srivastava and Bhaduri [22], Wu [23], Joachain and Vanderpoorten [24] and a recent one by Sech et al [25]. These are classified as open-shell (OS) type. (iii) Third group contains wave functions that are based on Feshbach–Rubinow [26,27] model, one due to Abott and Maslen [28] and another due to Tripathi et al [29]. The wave functions in the third group are a bit complicated and hence have not been used in any calculation. The Silvermann wave function [20], one-parameter Slater wave function and a Hylleraas-type wave function [30] have been used earlier [11,13,15]. In the present study we choose one wave function from the first group and the other from the second group and apply the (e, 3e) test. The former is closed-shell type and the latter is open-shell type.

2. Theory

We consider events in which fast electrons having energy $E_0$ are incident on helium and are inelastically scattered with energy $E_a$ into the solid angle $d\Omega_a$ in the direction $(\theta_a, \Phi_a)$