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INITIAL-STATE CORRELATION EFFECTS IN LOW-ENERGY PROTON IMPACT IONIZATION

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Abstract. In this paper, we will report on fully differential cross sections (FDCS) for single ionization of helium by 75 keV proton impact for fixed ejected electron energies and different momentum transfers. These measurements show major discrepancies in the absolute magnitude between experiment and the theoretical, 3DW (three-distorted-wave) model. The 3DW model treats the collision as a three-body process (projectile, ion, ejected electron), and for the scattering plane it has accurately predicted the FDCS for higher energy C^{6+} impact ionization of helium. The lack of agreement between the 3DW model and experiment for low energy collisions suggests that a three-body model may not be appropriate for lower collision energies. We will present a four-body model that includes full initial-state correlation.

Keywords: ground states; wave functions; ion-atom collisions, ionization, helium neutral atoms
PACS: 34.10.+x, 34.85.+x, 03.65.Nk, 34.50.Fa

INTRODUCTION

Recent fully differential cross section (FDCS) measurements, using the COLTRIMS technique, have been reported for kinematical conditions previously unstudied for low energy (75 keV) proton impact ionization of helium [1-2]. Initially, it was thought that at large projectile energies theoretical models like the three-distorted-wave (3DW) model or even the less sophisticated first-Born-approximation-Hartree-Fock (FBA-HF) should produce an accurate FDCS for single ionization of helium by proton impact in the scattering plane. The FBA-HF approximation varies from the standard FBA model in the choice of the final state wavefunction for the ejected electron. The FBA-HF approximation uses an ejected electron wavefunction that is calculated as an eigenfunction of the Schrödinger equation using a Hartree-Fock potential for the ion. Thus, the effective charge seen by the ejected electron varies from two close to the nucleus to unity asymptotically. The FBA-HF model treats the projectile as a plane wave in both the initial and final state. The use of the Hartree-Fock wavefunction for the ionized electron has been shown to provide much better agreement with the magnitude for the absolute FDCS for 100 MeV/u C^{6+} ionization of helium [3]. Both the FBA-HF and the 3DW models employ Hartree-Fock initial state wavefunctions for the helium atom. For the cases of 100 MeV/u and 2 MeV/u C^{6+} ionization of helium, both the FBA-HF and 3DW models were able to

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reproduce the overall magnitude of the experimental data accurately. The 3DW approach is an improved fully quantum mechanical version of the standard CDW (continuum-distorted-wave) approximation [4-8] that has been used successfully for decades to study single and double differential cross sections for heavy ion collisions.

A rough measure of the accuracy of using the first term in a perturbation theory expansion is the ratio between the projectile's charge, Z_p, to the incoming projectile velocity, v_a. The charge-to-velocity ratios for the 100 MeV/u and 2 MeV/u C^{6+} are 0.1 and 0.7, respectively. For 75 keV protons, the charge-to-velocity ratio is 0.6. By this measure, one would expect that the 3DW models should yield satisfactory results for 75 keV protons similar to the 2 MeV/u C^{6+} results.

Figure 1 compares the absolute experimental data of Hasan et al. [2] and Maydanyuk et al. [1] with the 3DW and FBA-HF calculations. In figure 1, the ejected electron

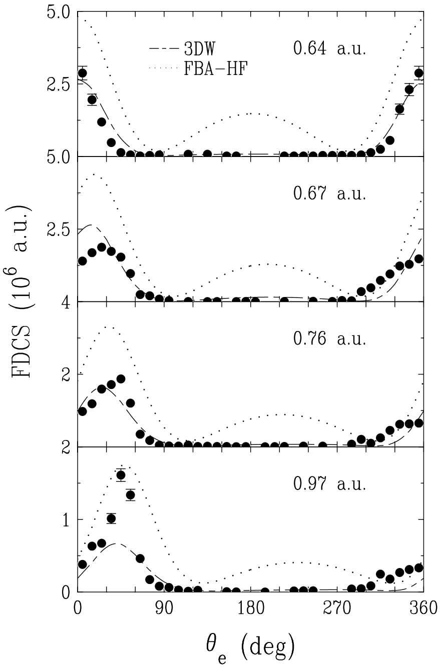

FIGURE 1. Fully differential cross sections for 75 keV p^+ impact ionization of helium in the scattering plane. All of the experimental data are absolute values in the centre of mass frame. The ejected electron energy E_e is 5.5 eV and the magnitude of the momentum transfer, |q|, is indicated in each part of the figure. The emission angle θ_e of the ejected electron in the scattering plane is measured clockwise from the beam direction. The solid circles are the absolute measurements and the theoretical curves: dotted line FBA-HF, and long dash short dashed line 3DW model multiplied by a factor of 0.25 line.

is emitted into the scattering plane (i.e. the plane that contains the initial and final projectile momentum, $\mathbf{k_i}$ and $\mathbf{k_f}$) with an energy E_e of 5.5 eV and momentum transfers of 0.64 a.u., 0.67 a.u., 0.76 a.u., and 0.97 a.u. respectively. The peak between 0° and 90° is the binary peak and the peak between 180^0 and 270° is the recoil peak. While the qualitative agreement between the 3DW and the experiment for the shape of the

FDCS is good, the absolute magnitudes are in very poor agreement (factor of 4 greater than experiment). The FBA-HF model is actually in better agreement with the magnitude of the measurements than the 3DW results (factor of 1.6 greater than experiment). On the other hand, it is also seen that the experimental and 3DW results only have a binary peak while the FBA-HF approximation predicts both a binary and recoil peak. Thus, both models do not provide an adequate description of the data! We have therefore developed a new model which accounts for the four-body dynamics, i.e. the passive electron is treated as a separate particle.

ANALYSIS

The T-Matrix for single ionization of the helium atom is given by

$$T_{fi} = \langle \chi_f^-(r_1,r_2,r_3) | V_i | \psi_i(r_1,r_2,r_3) \rangle \quad (1)$$

Here V_i is the initial channel interaction potential between the projectile and helium atom,

$$V_i = 2/r_1 - 1/r_{12} - 1/r_{13} \quad (2)$$

The initial-state wavefunction ψ_i is a product of a plane wave for the projectile and a correlated initial-state wavefunction for the helium atom. Thus

$$\psi_i = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_1)\phi(\mathbf{r}_2,\mathbf{r}_3) \quad (3)$$

where $\phi(\mathbf{r}_2,\mathbf{r}_3)$ is the correlated ground state wavefunction for the helium atom (correlation refers to the electron-electron interaction). Calculations have been performed using three types of correlated initial-state wavefunctions: a 20-parameter Hylleraas wavefunction [9], the Le Sech wavefunction [10] and the Pluvinage wavefunction [11]. The 20-parameter Hylleraas wavefunction is considered the benchmark wavefunction for the helium atom because of the precision to which the ground-state energy of helium can be calculated (equal to the exact ground-state energy to six significant digits - see Hart and Herzberg [12] for the specific values of the parameters). However, the Hylleraas wavefunction does not satisfy the Kato cusp condition [13]. In order for the cusp condition to be met, the local energy must be a constant as $r_{23} \to 0$. For the Hylleraas wavefunction, the local energy is infinite as $r_{23} \to 0$. The second correlated initial-state wavefunction tested was the Le Sech [10] wavefunction. The Le Sech wavefunction is a three parameter analytic wavefunction that does meet the cusp conditions requirements and yields the helium ground-state energy to within three significant digits. The final correlated initial-state wavefunction was the Pluvinage wavefunction [11]. The Pluvinage wavefunction is also satisfies the Kato cusp conditions, but is the simplest wavefunction, and as a result, the ground state energy of helium is not as accurate as the previous two wavefunctions (~1% off the exact value). One of the attractive features of the Pluvinage wavefunction is the bound state equivalent to 3DW final state wavefunction. There is growing evidence that this is important treatment of the T-Matrix [13]. In a previous study of double ionization of helium, the Pluvinage wavefunction in conjunction with a final-state equivalent wavefunction yielded better agreement with experiment than calculations using a more accurate Hylleraas wavefunction [13-14].

The final state wavefunction that we have used for this study is a plane wave for the projectile, a Hartree-Fock distorted wave for the ejected electron and a bound state for the passive electron.

$$\chi^{-}_{final} = (2\pi)^{-3} \exp(i\mathbf{k_f} \cdot \mathbf{r_1})\ \phi^{-}_{e}(\mathbf{k_2}, \mathbf{r_2})\ \psi_{1s}(r_3) \qquad (4)$$

Here $\psi_{1s}(r_3)$ is the bound state wavefunction for the passive electron which is modeled as a hydrogenic wave function with the full nuclear charge of two. The Hartree-Fock distorted wave [15] ϕ^{-}_{e} for the ejected-electron-helium-ion subsystem is a numerical solution of the Schrödinger equation

$$\left(-\frac{1}{2}\nabla^2_{r_2} - U_{ion}(r_2) + \frac{k_2^2}{2} \right) \phi^{-}_{e}(\mathbf{k_2}, \mathbf{r_2}) = 0 \qquad (5)$$

where U_{ion} is the static Hartree-Fock potential for the helium ion.

To investigate the importance of initial state correlation effects between the ionized electron and an atomic passive electron for single ionization of helium by the impact of a 75 keV proton, figure 2 compares three different FBA-HF FDCS calculations using the various initial-state wavefunctions: FBA-HY (long dashed line), FBA-LS (dotted line), and FBA-PL (short dashed line) with the absolute experimental data (solid dots) (Maydanyuk et al. 2005, Hasan et al. 2004). For figure 2, the electron is ejected into the scattering plane with an energy, E_e, equal to 5.5 eV and four different momentum transfer values (|**q**| = 0.64 a.u., 0.67 a.u., 0.76 a.u., and 0.97 a.u.). The most distinctive feature of all three of the theoretical curves is the large

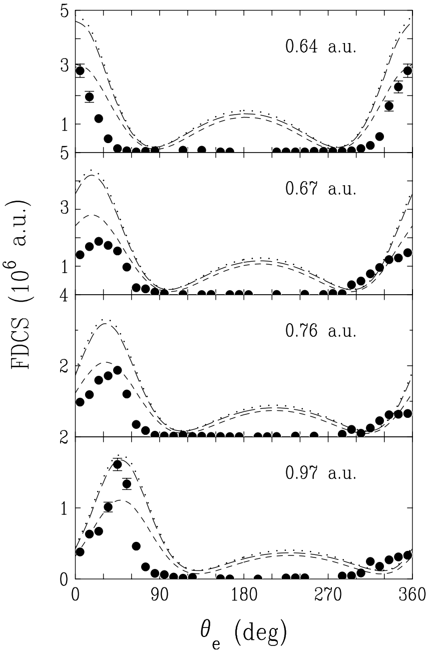

FIGURE 2. Same kinematical conditions as figure 1, the solid circles are the absolute measurements and the theoretical curves: dotted line FBA-LS, long dashed line FBA-HY model, and short dashed line FBA-PL.

recoil peak in the backward direction. In the FBA model, the recoil peak is always at about 180^0 from the binary peak and is understood as a double scattering event – the projectile interacts with the active electron and then the active electron backscatters from the ion. Since the final state distorted wave for the ejected electron is an elastic scattering wavefunction for the ejected electron in the field of the ion, the FBA-HF approach contains the physics necessary for a recoil peak and all the FBA calculations predict a recoil peak whereas no recoil peak is seen in the experimental data. Consequently, some additional physical effects not in the FBA-HF must suppress the recoil peak. For the binary peak, both, the FBA-HY and the FBA-LS results are virtually identical in both shape and scale. This observation suggests that satisfying the Kato cusp condition is not important for the initial state since the Hylleraas wavefunction does not satisfy the cusp condition whereas the Le Sech wavefunction does. Interestingly, the FBA-PL results are nearly a factor of 1.5 lower in absolute magnitude and in closer agreement with the absolute measurements. For the case of double ionization of helium, it was suggested that the Pluvinage wavefunction gave better agreement with experiment due to the fact that the initial and final states were then treated symmetrically. However, that is not the case here with a HF final state. On the other hand, the final state contains no direct correlation at all. To better understand the results of figure 2, a similar study of the effects of correlation on the final state is needed and we are currently in the process of performing such a study. In conclusion, these results indicate that the passive electron may play a more important role than previously assumed. However, a detailed study of final state correlation effects is needed before a definite conclusion can be drawn.

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