Four-Body Charge Transfer Processes in Heavy Particle Collisions

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Four-Body Charge Transfer Processes in Heavy Particle Collisions

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Abstract. Fully differential cross sections (FDCS) for proton + helium single capture and transfer-excitation collisions are presented using the Four-Body Transfer-Excitation (4BTE) model. This is a first order perturbative model that allows for any two-particle interaction to be studied. For single capture, the effect of the projectile-nuclear term in the perturbation is examined. It is shown that inclusion of this term results in an unphysical minimum in the FDCS, but is required to correctly predict the magnitude of the experimental results. For transfer-excitation, the role of electron correlation in the target helium atom is studied, and shown to be unimportant in the calculation of the FDCS.

1. Introduction

The few-body problem is one of the most fundamental unsolved problems in physics, and arises from the fact that the Schrödinger equation is not analytically soluble for more than two mutually interacting particles. As a result, theory must resort to approximations, the validity of which is determined by comparison with experiment.

There has been much work done on the three-body problem, and in many cases, theory and experiment agree very well [1, 2, 3, 4]. Recent advancements in experimental techniques and computing capabilities now allow for the study of more complicated collision systems, such as four-body collisions. One of the simplest four-body problems is a charged particle collision with a helium atom, in which both atomic electrons change state. This type of collision can result in many different outcomes, such as excitation-ionization, double excitation, and double ionization for either positively or negatively charged projectiles; as well as single charge transfer, double charge transfer, transfer-excitation, and transfer-ionization for positively charged projectiles. This paper will focus on single charge transfer and transfer-excitation for proton-helium collisions.

The process of single charge transfer (or single capture, SC) has been studied a great deal, beginning early in the 20th century. For the case of proton collisions, an incident proton collides with a target atom, captures a single electron, and leaves the collision as a neutral hydrogen atom. The first theoretical model for charge transfer was developed by Thomas [5] in 1927 for alpha particle collisions with hydrogen, and was strictly a classical calculation consisting of a two-step process. Soon after Thomas' model, Oppenheimer [6] and Brinkman and Kramers [7] performed the first quantum mechanical calculations for the SC process.

Most models treat the SC process as a three-body process using the independent particle model, regardless of the target being used. However, for low target nuclear charge, electron correlation can be important. For helium atoms, there have only been a couple of calculations that include the interaction of the passive electron through a correlated target wave function [8, 9]. In the case of four-body problems, this correlation is expected to be much more important. One such four-body problem is transfer-excitation (TE). In this case, not only is one electron captured by the projectile, but the remaining atomic electron is promoted to an excited state, making it a full four-body process.

Many of these calculations have been performed for total cross sections, but differential cross sections provide a much more stringent test of theory, and will be the focus of the work presented here. In this paper, theoretical differential cross sections for p + He single charge transfer and transfer-excitation will be presented using the Four-Body Transfer-Excitation model (4BTE). Atomic units are used unless otherwise noted.

2. 4BTE Theory

The FDCS for single charge transfer and transfer-excitation is differential only in projectile scattering angle, and is given by

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \mu_{pa}\mu_{pi}\frac{k_f}{k_i}\left|T_{fi}\right|^2, \tag{1}$$

where μ_{pa} is the reduced mass of the projectile and target atom, μ_{pi} is the reduced mass of the hydrogen atom and the residual He^+ ion, k_i is the momentum of the incident projectile, and k_f is the momentum of the scattered hydrogen atom.

In the 4BTE model [10], the transition matrix, T_{fi}, is given by

$$T_{fi} = \left\langle \chi_p^f \phi_H \psi_{He^+} \middle| V_i \middle| \chi_p^i \Phi_{He} \right\rangle, \tag{2}$$

where V_i is the initial state perturbation given by

$$V_i = \frac{Z_p Z_{nuc}}{r_1} + \frac{Z_p Z_e}{r_{12}} + \frac{Z_p Z_e}{r_{13}}. \tag{3}$$

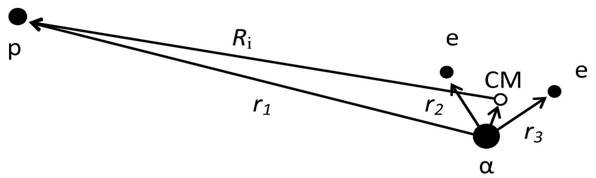

Figure 1. Jacobi coordinate system for the initial state projectile-helium atom system.

Here, Z_p, Z_e, Z_{nuc} are the charges of the projectile, electron, and target nucleus respectively; and $\vec{r}_1, \vec{r}_2, \vec{r}_3$ are the coordinates of the projectile and two atomic electrons with respect to the target nucleus. Also, $\chi_p^i \left(\chi_p^f\right)$ is the wave function for the incident (scattered) projectile, Φ_{He} is the wave function for the groundstate helium atom, ψ_{He^+} is the wave function for the final state He^+ ion, and ϕ_H is the wave function for the captured electron. Both ϕ_H and ψ_{He^+} are simply hydrogenic wave functions, and thus known exactly. The ground state helium atom wave function is given by either a 20-term Hylleraas wave function [11] that includes both radial and angular correlations or a Hartree-Fock wave function [12] that has no correlation.

The calculations are performed in the center of mass frame, using the Jacobi coordinates shown in figures 1 and 2. Here, $\vec{R_i}$ is the relative vector between the projectile and the center of mass of the helium atom, and $\vec{R_f}$ is the relative vector between the center of mass of the hydrogen atom and the center of mass of the He^+ ion. They are given by

$$\vec{R_i} = \vec{r_1} - \frac{m_e}{m_a + 2m_e}(\vec{r_2} + \vec{r_3}) \tag{4}$$

and

$$\vec{R_f} = \frac{m_e\vec{r_2} + m_p\vec{r_1}}{m_p + m_e} - \frac{m_e}{m_e + m_a}\vec{r_3}, \tag{5}$$

where m_e, m_a, and m_p are the masses of the electron, alpha particle, and projectile respectively.

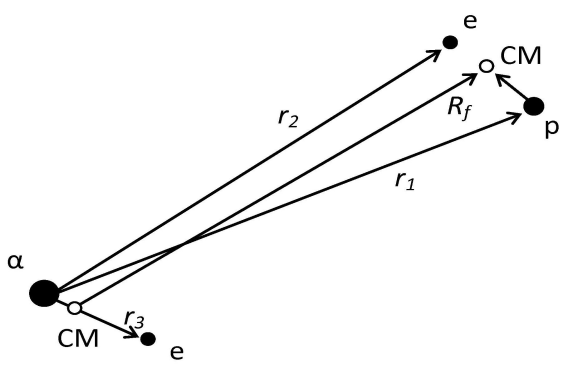

Figure 2. Jacobi coordinate system for the final state hydrogen-helium ion system.

The incident projectile wave function is represented by a plane wave given by

$$\chi_p^i = \frac{e^{i\vec{k}_i \cdot \vec{R}_i}}{(2\pi)^{3/2}}, \tag{6}$$

and the scattered projectile wave function is a Coulomb wave given by

$$\chi_p^f = \frac{e^{i\vec{k}_f \cdot \vec{R}_f}}{(2\pi)^{3/2}} e^{-\pi\gamma/2}\Gamma(1 - i\gamma)_1F_1\left(i\gamma, 1, -ik_f(r_1 + z_1)\right). \tag{7}$$

Here, $\gamma = 1/v_H$, $\Gamma(1 - i\gamma)$ is the gamma function, ${}_1F_1\left(i\gamma, 1, -ik_f(r_1 + z_1)\right)$ is a confluent hypergeometric function, and v_H is the speed of the hydrogen atom.

3. Results

3.1. Single Capture

There are many sets of experimental results for SC, and the calculations shown in figure 3 were performed for only a small subset of these. These results exhibit some well-known features and trends. The unphysical minimum seen in the calculation with the full perturbation is a result of cancellation of the terms in the perturbation [13]. Note that this minimum becomes deeper and shifts to smaller angles as the projectile energy increases, as was previously observed by Band [14] and Sil *et al.* [15]. The removal of the projectile-nuclear term in the perturbation results in the removal of this minimum, and an increase in the overall magnitude of the cross section, something seen by Belkić and Salin [13].

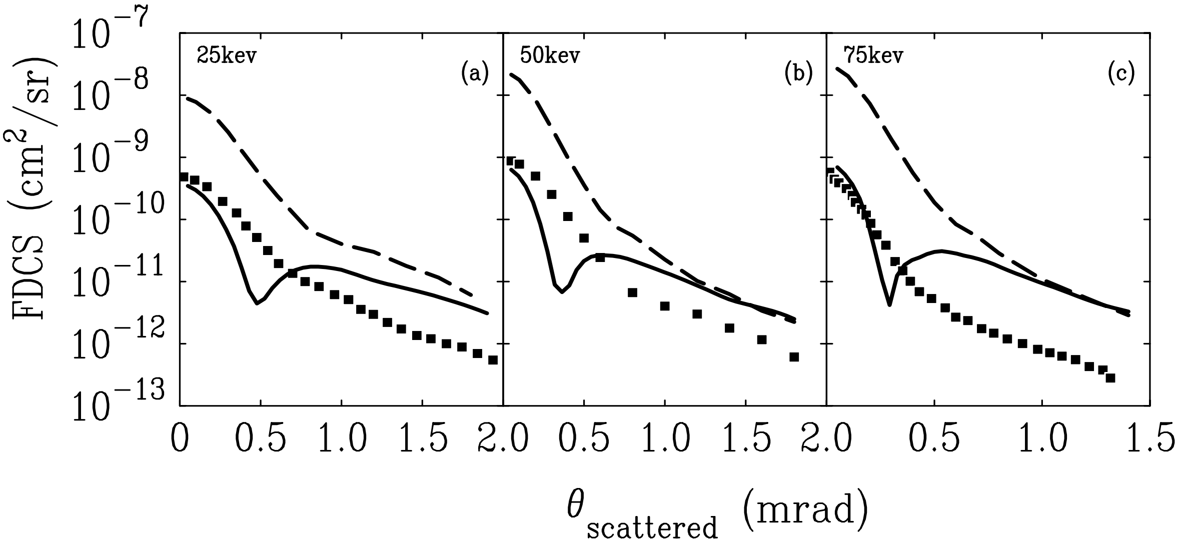

Figure 3. FDCS as a function of projectile scattering angle for p + He SC. The squares are the experimental results of Schulz, *et al.* [16] for the incident projectile energies shown in the figure. Both theoretical curves are from the 4BTE model with a plane wave for the incident projectile, Hylleraas wave function for the helium atom, and Coulomb wave for the scattered projectile. The solid line was calculated with all three terms in the perturbation, and the dashed line was calculated without the projectile-nuclear term in the perturbation.

3.2. Transfer-Excitation

Currently, only two sets of experimental data for fully differential cross sections for TE collisions are available [17, 18]. Experimentally, it is known that the outgoing hydrogen atom is in the ground state, and the residual helium ion is in an excited state. However, the exact excited state is not determined experimentally. Therefore, the cross sections must be summed over all possible excited states. Calculations have shown that contributions from excited states above $n = 4$ are negligible, as are contributions from higher angular momentum states. Because of this, the present results include only s and p excited states for $2 \leq n \leq 4$.

In figure 4, the effect of initial state correlation is shown [10]. One would be inclined to think that correlation would play an important role in the first order model of a four body process because the only interactions included in the perturbation are between the projectile and each individual electron, as well as the projectile-nuclear interaction. Thus, in order for two electrons to change state, some correlation should be required. However, figure 4 shows this expectation to be incorrect. Two calculations are shown in figure 4; one using a fully correlated Hylleraas wave function and the other using an uncorrelated Hartree-Fock wave function [12]. There is very little difference between the results of these two calculations, indicating that correlation is not important in this process.

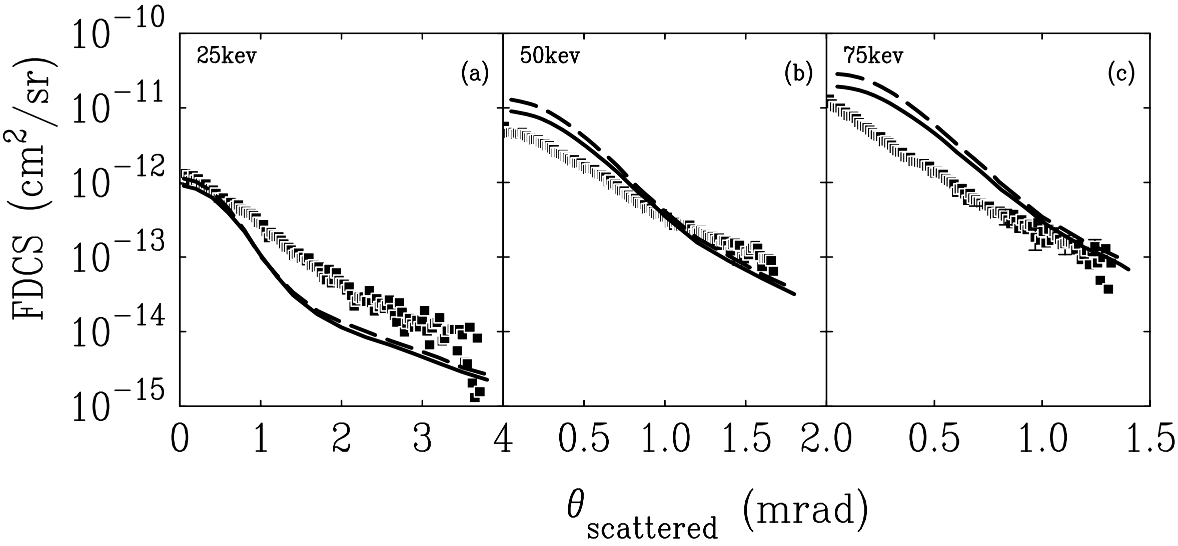

Figure 4. FDCS as a function of scattering angle for p + He TE showing the effect of electron correlation in the target atom wave function. The squares are the experimental results of Hasan, *et al.* [17] for the incident projectile energies shown in the figure. The solid line is the 4BTE model with a plane wave for the incident projectile, Hylleraas wave function for the helium atom, and Coulomb wave for the scattered projectile. The dashed line is the 4BTE model with a plane wave for the incident projectile, Hartree-Fock wave function for the helium atom, and Coulomb wave for the scattered projectile.

4. Conclusion

Results have been presented here for SC and TE in p + He collisions. The SC results exhibit the expected behavior of a first order perturbative model. A pronounced minimum in the FDCS is observed when all three terms in the perturbation potential are included in the calculation, and this minimum is removed when the projectile-nuclear term is excluded from the perturbation. However, using the full perturbation potential gives results closer to the magnitude of the experiment for small scattering angles.

The role of initial state electron correlation was explored for the TE process. It was expected that correlation in the ground state helium atom would play an important role in TE. However, results with and without correlation were nearly identical, showing that electron correlation has a negligible effect in the TE process.

Acknowledgments

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