SINGLE-ELECTRON CAPTURE IN $p - \mathrm{He}^+$ COLLISIONS

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Abstract. Single-electron capture in collisions between fast protons p and helium ions $\mathrm{He}^+(1s)$ in the ground state is studied in the framework of the three-body boundary-corrected first Born approximation (CB1-3B). State-summed total cross sections are calculated by summing up the state-resolved total cross sections for principal quantum number values $n \leq 4$ according to the Oppenheimer scaling law. The obtained theoretical results are found to be in satisfactory agreement with the available experimental data.

1. INTRODUCTION

Electron capture processes in collisions between fast ionic projectiles with atomic targets have been a subject of non-diminished interest for decades. Computations of their corresponding cross sections carry both a fundamental, as well as a practical value. Electron capture cross sections play a crucial role in estimating the energy losses of ions during their passage through matter of varying kinds. As such, these cross sections databases find useful applications in both pure physics areas, such as plasma physics, astrophysics and heavy ion transport physics, as well as interdisciplinary areas, such as fusion energy research and medical physics.

In this work, we are interested in the process of single-electron capture in collisions between fast protons p and helium ions $\mathrm{He}^+(1s)$ in the ground state. This is a genuine three-body process, and as such poses a critical test to the validity of three-body theories. The cross sections are calculated in the framework of the boundary-corrected first Born approximation, often abbreviated as CB1-3B, which was first developed in the work of Belkić et al. 1979. The CB1-3B method represents the first order term in the perturbation expansion of the exact eikonal transition amplitude. Note that since the CB1-3B method employs the eikonal hypothesis, it is essentially a high energy theory. This method was successfully applied to a plethora of electron capture processes (Belkić et al. 1986, Belkić et al. 1987, Belkić et al. 1987b), as well as extended to a four-body theory, with the development of the four-body boundary-corrected first Born approximation, abbreviated as CB1-4B (Mačev et al. 2012). A systematic agreement with available measurements at intermediate and high energy values was found. The CB1-3B and CB1-4B approximations are fully quantum-mechanical approaches, which strictly preserve the correct boundary conditions in both the entrance and exit collision channels. In ion-atom collisions, boundary conditions should fully be taken into account, whenever the aggregates are charged in the asymptotic channels (Belkić 2004, Belkić 2008). Charge exchange in $p + \mathrm{He}^{+}(1\mathrm{s})$ collisions has been investigated by means of various methods, such as the hidden crossing theory within the framework of dynamical adiabatic approach (Grozdanov et al. 2018), the wave-packet convergent close-coupling method (Faulkner et al. 2019), the continuum distorted-wave approximation (Mukherjee et al. 1980), the boundary-corrected continuum intermediate state approximation (Samanta et al. 2010). Atomic units will be used throughout unless otherwise stated.

2. THEORY

We consider single-electron capture in collisions between fast protons and helium ions in the ground state according to process:

$$p + \mathrm{He}^{+}(1\mathrm{s}) \to \mathrm{H}(\Sigma) + \mathrm{He}^{2+}, \tag{1}$$

which can also be written in the following form:

$$Z_P + (Z_T, e)_{1s} \to (Z_P, e)_{\Sigma} + Z_T, \tag{2}$$

where $Z_P = 1$ and $Z_T = 2$ are the respective charges of the projectile P and target T, while the symbol Σ denotes the capture into all final states of the projectile. In order to actually calculate the state-summed total cross sections Q_{Σ} for process (2), we will first need to calculate the state-resolved total cross sections Q_{nlm} for capture into arbitrary final states, with $\{n, l, m\}$ being the usual triplet of quantum numbers. We first consider the following process:

$$Z_P + (Z_T, e)_{1s} \to (Z_P, e)_{nlm} + Z_T. \tag{3}$$

The prior form of the transition amplitude in the CB1-3B approximation for process (3) can be written in the following form:

$$T_{if}(\vec{\eta}) = Z_{\mathrm{P}} \int\int \mathrm{d}\vec{s}\mathrm{d}\vec{R}\varphi^{*}_{nlm}(\vec{s}) \left(\frac{1}{R} - \frac{1}{s}\right) \varphi_i(\vec{x}) \mathrm{e}^{i\vec{\beta}\cdot\vec{R} - i\vec{v}\cdot\vec{s}} (vR + \vec{v}\cdot\vec{R})^{i\xi}, \tag{4}$$

where $\vec{\beta} = -\vec{\eta} - \beta_z \hat{\vec{v}}$ is the momentum transfer (with $\beta_z = v/2 + \Delta E/v$), while $\Delta E = E_i - E_f$ is the difference between the initial (target and electron) and final (projectile and electron) bound state energies, and $\vec{v}$ is the projectile velocity. The transverse momentum transfer vector is denoted by $\vec{\eta} = (\eta\cos\phi_\eta, \eta\sin\phi_\eta, 0)$, and has the property $\vec{\eta}\cdot\vec{v} = 0$ for $\vec{v}$ along the $z-$axis. The position vectors of the electron relative to the projectile and target are denoted by $\vec{s}$ and $\vec{x}$, respectively, while $\vec{R}$ denotes the relative position vector of the projectile to the target. One-electron wave functions $\varphi_i(\vec{x})$ and $\varphi_{nlm}(\vec{s})$ are, respectively, the bound state wave functions of the target system $(Z_T, e)_{1s}$ before the collision (i.e. the He^{+} ground state wave function), and the projectile system $(Z_P, e)_{nlm}$ after the collision (i.e. the H arbitrary state wave function). Finally, we also introduced the following symbol $\xi = (Z_P - Z_T)/v$.

The original six-dimensional integral for the transition amplitude matrix elements T_{if} from Equation (4) can be reduced to a one-dimensional integral over a real variable in the interval $[0, 1]$. The state-resolved total cross sections become:

$$Q_{nml} \equiv Q_{if}(a_0^2) = \frac{1}{2\pi v^2} \int_0^{\infty} d\eta\eta |T_{if}(\vec{\eta})|^2. \tag{5}$$

Numerical integration of the two-dimensional integral in Equation (5) over the two real variables is performed using Gauss-Legendre quadrature. Our general program can calculate the state-resolved total cross sections for capture from the ground state ($1s$) of the target into arbitrary final states (n, l, m) of the projectile. The state-summed total cross sections for capture into all final states are then obtained by applying the Oppenheimer n^{-3} scaling law (Oppenheimer 1928) as:

$$Q \equiv Q_\Sigma = Q_1 + Q_2 + Q_3 + 2.561 Q_4, \tag{6}$$

where the state-resolved total cross sections Q_n and Q_{nl} are, respectively, calculated according to:

$$Q_n = \sum_{l=0}^{n-1} Q_{nl}, \quad Q_{nl} = \sum_{m=-l}^{+l} Q_{nlm}. \tag{7}$$

A preassigned convergence of at least two decimal places is achieved, with a total of 96 integration points along each of the two integration axes being used.

3. RESULTS AND DISCUSSION

The present theoretical results in the CB1-3B method, as well as the comparison with the available experimental data, are given in Figure 1. Theoretical results are

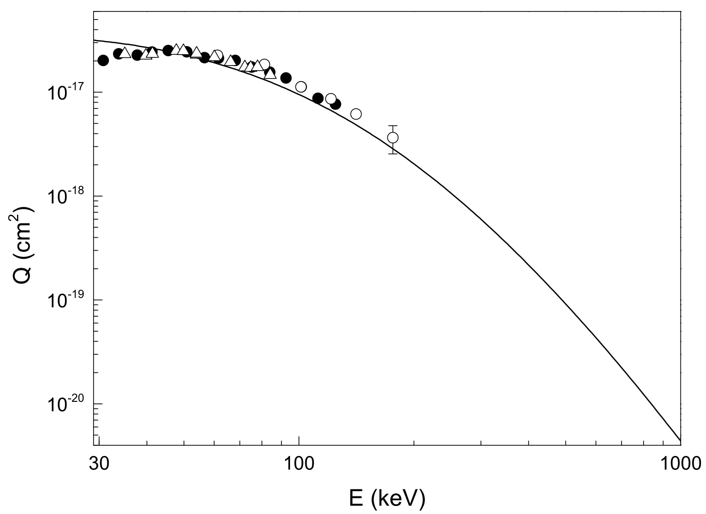

Figure 1: State-summed total cross sections as a function of impact energy E (keV) in the laboratory frame of reference for single-electron capture into all final bound states H(Σ) from the ground state of the helium ion He^+(1s) by protons. The full curve is present result in the CB1-3B method. Experimental data: △ Peart et al. 1983, • Rinn et al. 1985, ○ Watts et al. 1986.

presented in the energy range from 30 to 1000 keV in the laboratory frame of reference, while the measurements were made for energies up to 176 keV. Note that all experimental data sets Peart et al. 1983, Rinn et al. 1985, and Watts et al. 1986 are in good mutual accord. As can be seen in Figure 1, the present CB1-3B results exhibit a very good agreement with all the available measurements. There is a slight overestimation of the experimental data for energies below 40 keV, as well as a slight underestimation for energies between 60 keV and 140 keV. These discrepancies are, however, very slight, and for the highest energy data point of Watts et al. 1986 at $E = 176$ keV, the theory approaches the experimental value within the measurement error. Moreover, having in mind that CB1-3B is a high energy theory, and the available measurements are all in the intermediate energy range, some discrepancy was indeed natural. The agreement is nevertheless good, and is expected to improve even further for higher energy values.

4. CONCLUSION

The value of this work, besides providing us with useful total cross section values for the process of single-electron capture in collisions between protons p and helium ions He^+, is that it also represents a further critical test of the validity of the CB1-3B approximation. The CB1-3B method has provided very accurate reproductions of experimental results for many electron capture processes. After contrasting it with the experimental data for this genuinely three-body single-electron capture process (1), we can conclude that the agreement is indeed good, and the validity of the CB1-3B method is now even more strongly confirmed.

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