Quantum mechanical potentials and inactive electron effects in charge exchange collisions

A L Harris and A Plumadore

Physics Department, Illinois State University, Normal, IL 61790, United States of America

E-mail: alharri@ilstu.edu

Received 3 August 2018, revised 10 January 2019
Accepted for publication 23 January 2019
Published 12 February 2019

Abstract
Scattering angle differential cross sections for the He\(^+\) + He single electron capture process are studied using plane wave Born approximation models for projectile energies between 180 keV and 1.89 MeV. Within this simplistic framework, we study the effects of the frozen core approximation by performing a full 5-Body calculation that explicitly includes all particles in the collision and comparing it with a single bound state model that neglects the bound electron in the projectile and a double bound state model that neglects the inactive electron in the target atom. Results are compared with experiment and we show that inclusion of the inactive electron in the perturbation potential is more important than inclusion in the wave functions. We also introduce a semi-quantum mechanical (SQM) perturbation potential that treats the atomic electrons as a quantum mechanical electron cloud rather than point particles. The SQM perturbation removes the deep, unphysical minimum that exists in cross sections calculated with Born-type models, but also has the effect of greatly reducing the magnitude of the small scattering angle cross sections.

Keywords: electron capture, charge transfer, frozen core approximation

(Some figures may appear in colour only in the online journal)

1. Introduction
Electron capture processes play an important role in many physical systems, from fusion reactors to astrophysical processes. In an electron capture collision, an incident ion collides with a target atom, captures an electron, and leaves the collision as a bound state. Recent experimental results for heavy ion single electron capture at low projectile velocities exhibit features in the differential cross section that can be attributed to Fraunhofer diffraction effects [1–6]. At high velocities, the two-step Thomas mechanism becomes important in order to accurately describe the differential cross sections [7–9]. In the intermediate energy range, recent work has shown that projectile coherence effects can be important, especially when the collision target is a small molecule, such as H\(_2\) [10–14]. In electron capture collisions, it is common to neglect inactive electrons in what is known as the frozen core approximation. Some of our previous work has focused on the validity of the frozen core approximation in electron and heavy ion ionization collisions [15, 16]. Here, we extend this work to electron capture differential cross sections with dressed projectiles.

We introduce several plane wave Born approximation (PWBA) models that are used to explore the continuum distorted wave Born initial state (CDW BIS) effects of neglecting inactive electrons in the collision. We also introduce variants of these models that treat the interaction potential between the projectile and target atom semi-quantum mechanically rather than classically. All of the models are then compared to the experimental results of [17]. For the sake of clarity, and to make comparisons with recent experiments, we focus exclusively on the He\(^+\) + He single electron capture process with all bound electrons in the ground state. The experimental data sets with which we compare our models use a \(^3\)He projectile. From an experimental standpoint, the distinguishability of the projectile from the target is a clear advantage. The effect of the isotope on the theoretical models is minimal and only appears in the mass of the projectile.
There is no effect on the charges of the particles in the collision, and any effect on binding energies is so small it can be safely neglected.

The PWBA is the simplest perturbative model available and is well-known to overestimate the magnitude of the scattering cross sections. However, the use of such a simplistic model still holds value in qualitatively studying the physical effects in which we are interested, particularly at larger projectile velocities. The models presented here should be viewed as a guide for assessing the relative importance of certain physical effects and hopefully influence the development of more sophisticated models. Atomic units are used throughout unless otherwise stated.

2. Theory

We present results for angular differential cross sections from three different fully quantum mechanical PWBA models. In all models, the center of mass cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^3\mu_{pa}\mu_{pi}k_f}{k_i} |T_{fi}|^2, \quad (1)$$

where $\mu_{pa}$ is the reduced mass of the initial state projectile and target atom, $\mu_{pi}$ is the reduced mass of the scattered projectile and residual ion, $k_f$ ($k_i$) is the center of mass momentum of the scattered (incident) projectile, and $T_{fi}$ is the transition matrix given by

$$T_{fi} = \langle \Psi_f | V | \Psi_i \rangle. \quad (2)$$

The lab frame cross section is related to the center of mass cross section by

$$\frac{d\sigma}{d\Omega} = \left[ \frac{1 + 2\delta \cos \theta_c + \delta^2}{1 + \delta \cos \theta_c} \right] \frac{d\sigma}{d\Omega}, \quad (3)$$

where $\theta_c$ is the scattering angle of the projectile in the center of mass frame. The quantity $\delta$ is given by the ratio of the magnitude of the velocity of the center of mass of the entire collision system in the lab frame $V$ and the magnitude of the scattered projectile velocity in the center of mass frame $V_f$, such that $\delta = \frac{V}{V_f}$. The lab frame and center of mass frame scattering angles are related by

$$\tan \theta_L = \frac{\sin \theta_c}{\cos \theta_c + \delta}. \quad (4)$$

The form of the initial (final) wave function $\Psi_i$ ($\Psi_f$), and the perturbation $V_t$ are dependent upon the model used, although in each case, we assume independent electrons in the bound states. We also note that for simplicity in the derivation, the diagrams and equations used here describe distinguishable electrons, but our calculations properly account for the indistinguishability of the electrons in the target atom. Then, two-particle bound states are represented by a simple product variational wave function

$$\Phi_{He}(\vec{r}, \vec{y}) = \frac{\alpha^3}{\pi} e^{-\alpha \vec{r}} e^{-\alpha \vec{y}}$$

with $\alpha = 1.6875$ as the screening parameter. This choice of independent electron helium atom wave function neglects electron correlation within the atom, but it has been shown that for electron capture without excitation, electron correlation plays a minimal role in the cross sections [17, 18]. In all models, the motion of the initial and final state continuum projectiles are treated as plane waves and bound states involving only one active electron are purely hydrogenic. The 1s hydrogenic wave function with nuclear charge $Z$ is given by

$$\phi(\vec{x}) = \frac{Z^{3/2}}{\sqrt{\pi}} e^{-Z \vec{r}}. \quad (6)$$

Additionally, for the analytical calculations it is necessary to use the momentum space wave function for a 1s hydrogen-like atom with nuclear charge $Z$ given by

$$\phi^{PT}(\vec{p}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\vec{p}\cdot\vec{r}} \phi(\vec{x}) d\vec{x} = \frac{4Z^{5/2}}{\pi^{1/2} (Z^2 + p^2)^{3/2}}. \quad (7)$$

Equation (2) can then be written as an integral over the spatial coordinates of all particles included in the calculation. Because of the approximations made, most of the integrations can be performed analytically, with only a three-dimensional integral that is performed numerically.

Below is a description of each of the models and table 1 includes a comparison of the wave functions and perturbations used in equation (2). Calculations are performed in the center of mass frame using Jacobi coordinates, however results are presented in the lab frame for comparison with experiment. The diagrams in figures 1 through 4 show the coordinate systems used for each of the models.

2.1. 5-Body model

The He$^+$ + He collision system is inherently a 5-body system, consisting of three electrons and two nuclei. Within the PWBA and independent electron model, it is possible to perform a complete 5-body calculation that includes all particles in the collision system and does not invoke the frozen core approximation. In this case, the incident projectile bound state is purely hydrogenic (equation (6)), while the target atom is a bound state represented by the product of two hydrogen-like orbitals (equation (5)). The initial state wave function is then given by

$$\Psi_i = \chi_i(\vec{R}_i) \phi_p(\vec{r}_{41}) \Phi_{He}(\vec{r}_2, \vec{r}_3), \quad (8)$$

where $\chi_i(\vec{R}_i)$ is the incident projectile plane wave, $\phi_p(\vec{r}_{41})$ is the incident projectile bound state, and $\Phi_{He}(\vec{r}_2, \vec{r}_3)$ is the target atom wave function.

After the collision, the scattered projectile is a bound state represented by the product of two hydrogen-like orbitals (equation (5)), while the residual ion is purely hydrogenic (equation (6)). The final state wave function is given by

$$\Psi_f = \chi_f(\vec{R}_f) \Phi_{pb}(\vec{r}_{41}, \vec{r}_{41}) \xi_{He}(\vec{r}_2), \quad (9)$$

where $\chi_f(\vec{R}_f)$ is the scattered projectile plane wave, $\phi_{pb}(\vec{r}_{41}, \vec{r}_{41})$ is the captured electron bound state, and $\xi_{He}(\vec{r}_2)$ is the residual ion wave function.
Table 1. Comparison of initial and final state wave functions and perturbations for the models as described in the text.

| Model   | $\Psi_i$ | $\Psi_f$ | $V_{J\Omega}^1$ | $V_{SQM}^1$ |
|---------|----------|----------|-----------------|-------------|
| S-Body  | $\chi_i(\overline{R}_i) \phi_p^{(\overline{r}_i)} \Psi_{He}(\overline{r}_i)$ | $\chi_f(\overline{R}_f) \phi_p^{(\overline{r}_f)} \Psi_{He}(\overline{r}_f)$ | $\frac{Z_a Z_i}{r_1} + \frac{Z_a Z_e}{r_2} + \frac{Z_a Z_e}{r_3} + \frac{Z_a Z_e}{r_4}$ | $2Z_a \alpha \left( e^{-2i\alpha r_1} + e^{-2i\alpha r_1} - \frac{1}{\alpha r_1} \right)$ |
|         |          |          | $\frac{Z_a Z_i}{r_1} + \frac{Z_a Z_e}{r_2} + \frac{Z_a Z_e}{r_3} + \frac{Z_a Z_e}{r_4}$ | $2Z_a \alpha \left( e^{-2i\alpha r_1} + e^{-2i\alpha r_1} - \frac{1}{\alpha r_1} \right)$ + $\frac{2Z_a \alpha}{r_1}$ |
| SBS     | $\chi_i(\overline{R}_i) \phi_p^{(\overline{r}_i)} \Psi_{He}(\overline{r}_i)$ | $\chi_f(\overline{R}_f) \phi_p^{(\overline{r}_f)} \Psi_{He}(\overline{r}_f)$ | $\frac{Z_a Z_i}{r_1} + \frac{Z_a Z_e}{r_2} + \frac{Z_a Z_e}{r_3} + \frac{Z_a Z_e}{r_4}$ | $2Z_a \alpha \left( e^{-2i\alpha r_1} + e^{-2i\alpha r_1} - \frac{1}{\alpha r_1} \right)$ |
|         |          |          | $\frac{Z_a Z_i}{r_1} + \frac{Z_a Z_e}{r_2} + \frac{Z_a Z_e}{r_3} + \frac{Z_a Z_e}{r_4}$ | $2Z_a \alpha \left( e^{-2i\alpha r_1} + e^{-2i\alpha r_1} - \frac{1}{\alpha r_1} \right)$ + $\frac{Z_a \alpha}{r_1}$ |
| DBS     | $\chi_i(\overline{R}_i) \phi_p^{(\overline{r}_i)} \Psi_{He}(\overline{r}_i)$ | $\chi_f(\overline{R}_f) \phi_p^{(\overline{r}_f)} \Psi_{He}(\overline{r}_f)$ | $\frac{Z_a Z_i}{r_1} + \frac{Z_a Z_e}{r_2} + \frac{Z_a Z_e}{r_3} + \frac{Z_a Z_e}{r_4}$ | $Z_a \left( e^{-2Z_0 r_1} + e^{-2Z_0 r_1} - \frac{1}{r_1} \right)$ |
|         |          |          | $\frac{Z_a Z_i}{r_1} + \frac{Z_a Z_e}{r_2} + \frac{Z_a Z_e}{r_3} + \frac{Z_a Z_e}{r_4}$ | $Z_a \left( e^{-2Z_0 r_1} + e^{-2Z_0 r_1} - \frac{1}{r_1} \right)$ + $\frac{Z_a}{r_1}$ |
| DBS-Y   | $\chi_i(\overline{R}_i) \phi_p^{(\overline{r}_i)} \Psi_{He}(\overline{r}_i)$ | $\chi_f(\overline{R}_f) \phi_p^{(\overline{r}_f)} \Psi_{He}(\overline{r}_f)$ | $\frac{Z_a Z_i}{r_1} + \frac{Z_a Z_e}{r_2} + \frac{Z_a Z_e}{r_3} + \frac{Z_a Z_e}{r_4}$ | $Z_a \left( e^{-2Z_0 r_1} + e^{-2Z_0 r_1} - \frac{1}{r_1} \right)$ |
|         |          |          | $\frac{Z_a Z_i}{r_1} + \frac{Z_a Z_e}{r_2} + \frac{Z_a Z_e}{r_3} + \frac{Z_a Z_e}{r_4}$ | $Z_a \left( e^{-2Z_0 r_1} + e^{-2Z_0 r_1} - \frac{1}{r_1} \right)$ + $\frac{Z_a}{r_1}$ |
In a traditional PWBA model, the perturbation includes all two particle Coulomb interaction terms between the incident projectile and the target atom and is given by

\[ V_{\text{pert}} = \sum_{i} \frac{Z_e Z_{\alpha}}{r_i} + \frac{Z_e Z_{\alpha}}{r_{i+1}} + \frac{Z_e Z_{\alpha}}{r_{i+2}} + \frac{Z_e Z_{\alpha}}{r_{i+3}}, \]

where \( Z_e \) is the charge of the electron and \( Z_{\alpha} \) is the charge of the alpha particle. This perturbation contains terms based on classical, non-quantum mechanical point particles and will be referred to as a 'classical perturbation'. In addition to this classical perturbation, we also consider a perturbation in which the nucleus is a point particle but the electron charge cloud is treated quantum mechanically. The potential generated by the atom is then

\[ V_{\text{atom}}(r) = \sum_{i} \frac{Z_{\alpha}}{r_i} + V_e(r), \]

where \( V_e(r) \) is the potential of the atomic electron cloud. It can be found by integrating the electronic wave function to get the charge density, using Gauss’s law to find the electric field, and then calculating the potential. In the 5-Body model, this semi-quantum mechanical (SQM) perturbation is given by

\[ V_i = Z_{\alpha} V_{\text{atom}}(r_1) + Z_e V_{\text{atom}}(r_4), \]

For the variational wave function of equation (5), the target atom electronic potential is

\[ V_e(r) = 2\alpha \left( e^{-2\alpha r} + \frac{e^{-2\alpha r}}{\alpha r} - \frac{1}{\alpha r} \right). \]

Jacobi coordinates are used to calculate the center of mass \( T \)-matrix and are shown in figure 2. They are related to the lab coordinates of figure 1 by

\[ \overline{R_i} = \frac{m_p \overline{r_i}}{m_e + m_p} - \frac{m_e (\overline{r_3} + \overline{r_4})}{2m_e + m_{\alpha}} + \frac{m_e \overline{r_5}}{m_e + m_p}, \]

\[ \overline{R_f} = \frac{m_p \overline{r_1}}{2m_e + m_p} + \frac{m_e (\overline{r_3} + \overline{r_4})}{2m_e + m_{\alpha}} - \frac{m_e \overline{r_2}}{m_e + m_{\alpha}}, \]

\[ \overline{s} = \overline{r_3} - \frac{m_e \overline{r_2}}{m_e + m_{\alpha}}, \]

\[ \overline{t} = \overline{r_2}, \]

\[ \overline{u} = \overline{r_3} - \frac{m_p \overline{r_1}}{m_e + m_p} - \frac{m_e \overline{r_5}}{m_e + m_p}, \]

where \( m_e \) is the mass of the electron, \( m_{\alpha} \) is the mass of the alpha particle nucleus and \( m_p \) is the mass of the projectile nucleus. Note that in the initial state target atom wave function we have assumed \( \overline{s} \approx \overline{r_3} \) and in the final state scattered projectile wave function, we have assumed \( \overline{u} = \overline{r_3} \).

Inserting the wave functions from equations (8) and (9) along with the classical perturbation of equation (10) into (2)
yields the 5-Body model transition matrix

\[
T_{ij}^5 = \frac{256\alpha^5 Z_a^5 (Z_a + \alpha)^2}{\pi^3} \int \frac{d\beta}{(\alpha^2 + p^2)^2} \frac{1}{|\beta - \beta'|^2} \\
\times \left( \frac{Z_a}{[(Z_a + \alpha)^2 + D^2]^2} + \frac{Z_e}{[(Z_a + \alpha)^2 + |\beta - \beta'|^2]^2} \right) \\
\times \left( \frac{1}{|\alpha^2 + |\beta - \beta'|^2|^2} \right) \\
\times \left( \frac{Z_e}{[(Z_a + \alpha)^2 + B^2]^2} + \frac{Z_e}{[(Z_a + \alpha)^2 + |\beta - B|^2]^2} \right) \\
\times \left( \frac{Z_e}{[(Z_a + \alpha)^2 + \beta'|^2]^2} \right),
\]

where \( \bar{A}, \bar{B}, \bar{C} \) and \( \bar{D} \) are related to the center of mass momenta \( k_i \) and \( k_f \) by

\[
\bar{A} = \frac{m_p k_i}{m_e + m_p}, \quad \bar{B} = \frac{m_p k_f}{2m_e + m_a}, \quad \bar{C} = \frac{m_e k_i}{2m_e + m_a}, \quad \bar{D} = \frac{m_e k_f}{2m_e + m_p}.
\]

The SQM perturbation still permits a mostly analytical calculation with the 5-Body SQM transition matrix given by

\[
T_{SQM}^5 = \frac{256\alpha^5 Z_a^5 (Z_a + \alpha)^2}{\pi^3 [((Z_a + \alpha)^2 + B^2]^2} \times \int d\beta \frac{1}{|\beta - \beta'|^2} \\
\times \left( \frac{Z_a}{[(Z_a + \alpha)^2 + D^2]^2} + \frac{Z_e}{[(Z_a + \alpha)^2 + |\beta - \beta'|^2]^2} \right) \\
\times \left( \frac{1}{|\alpha^2 + |\beta - \beta'|^2|^2} \right) \\
\times \left( \frac{Z_e}{[(Z_a + \alpha)^2 + B^2]^2} + \frac{Z_e}{[(Z_a + \alpha)^2 + |\beta - B|^2]^2} \right) \\
\times \left( \frac{Z_e}{[(Z_a + \alpha)^2 + \beta'|^2]^2} \right).
\]

The three-dimensional integrals over \( \beta \) are performed numerically using Gauss–Legendre quadrature.

### 2.2. Single bound state (SBS) model

In the SBS model, the incident projectile is treated using the frozen core approximation and is assumed to be structureless with a charge \( Z_a \) and mass \( m_e + m_p \). This model neglects any bound state effects of the incident He\(^+\) ion and is identical to that used in [19], except for the difference in mass of the projectile. The target helium atom is a two-electron atom. In this model, the initial state wave function is given by

\[
\Psi_i = \chi_i(\bar{R}_i) \Phi_{He}(\bar{r}_2, \bar{r}_3),
\]

where \( \chi_i(\bar{R}_i) \) is the incident projectile plane wave and \( \Phi_{He}(\bar{r}_2, \bar{r}_3) \) is the target atom wave function. The final state consists of a scattered one-electron bound state projectile and one-electron residual helium ion. The final state wave function is then given by

\[
\Psi_f = \chi_f(\bar{R}_f) \phi_p(\bar{r}_3) \xi_{He}(\bar{r}_2),
\]

where \( \chi_f(\bar{R}_f) \) is the scattered projectile plane wave, \( \phi_p(\bar{r}_3) \) is the captured electron bound state, and \( \xi_{He}(\bar{r}_2) \) is the residual ion wave function. We again consider classical and SQM perturbations. The classical perturbation consists of all two-particle interaction terms between the projectile and the two-electron helium target and in the SBS model it is given by

\[
V_i = \frac{Z_p Z_a}{r_1} + \frac{Z_p Z_e}{r_2} + \frac{Z_p Z_e}{r_3},
\]

where \( Z_p \) is the charge of the incident projectile. The SQM perturbation in the SBS model is

\[
V_i = Z_p V_{atom}(s),
\]

where \( V_{atom} \) is given by equation (11). The Jacobi coordinates for the SBS model are shown in Figure 3. Note that because the projectile is assumed structureless, there is no \( \bar{r}_2 \) coordinate in the SBS model.

The relationship between the lab frame coordinates and the Jacobi coordinates are given by

\[
\bar{R}_i = \frac{m_e + m_p}{m_e + m_a} \bar{r}_1 - \frac{m_p}{m_e + m_a} \bar{r}_3,
\]

\[
\bar{R}_f = \frac{m_e + m_p}{m_e + m_a} \bar{r}_3 + \frac{m_e}{m_e + m_a} \bar{r}_2,
\]

\[
\bar{s} = \bar{r}_3 - \frac{m_p}{m_e + m_a} \bar{r}_2.
\]
Note that again we have assumed that $\tilde{s} \approx \tilde{r}_3$. Inserting all of the wave function expressions and the two choices of perturbation for the SBS model into equation (2) yields the following expressions for the transition matrices

$$T_{ji}^p = \frac{8Z_{p}^{3/2}Z_{ii} Z_{pf}^{3/2}}{\pi^{3/2}} \times \int \frac{d\tilde{p}}{[Z_{pf}^{2} + p^{2}]^{2}} \left[ \frac{Z_{o}^{2} + (\alpha + Z_{o})^{2}}{(\alpha^{2} + |\tilde{A} - \tilde{p}|^{2})^{2}} + \frac{Z_{o}}{(\alpha^{2} + |\tilde{C} - \tilde{A} + \tilde{p}|^{2})^{2}} \right],$$

and

$$T_{ji}^{SQM} = \frac{64\alpha^{3}(Z_{o}^{2} + \alpha)^{3/2}Z_{o}^{3}Z_{pf}^{3}}{\pi^{3}[(Z_{o}^{2} + \alpha)^{2} + C_{e}^{2}]^{2}} \times \int \frac{d\tilde{p}}{[Z_{pf}^{2} + p^{2}]^{2}[(4\alpha^{2} + |\tilde{A} - \tilde{p}|^{2})^{2}]^{2}},$$

where now $\tilde{A} = \tilde{R}_{i} - \frac{m_{e}k_{i}^{2}}{m_{e} + m_{e}}$, $\tilde{B} = \frac{m_{e}k_{i}^{2}}{m_{e} + 2m_{e}} + \frac{m_{e}k_{i}^{2}}{m_{e} + m_{o}}$, and $\tilde{C} = \frac{m_{e}k_{i}^{2}}{m_{e} + 2m_{e}} + \frac{m_{e}k_{i}^{2}}{m_{e} + m_{o}}$.

2.3. Double bound state (DBS) model

In the DBS model, the electronic structure of the incident projectile is now included in the calculation. However, the target atom wave function is treated with the frozen core approximation and therefore modeled as a single active electron wave function for effective charge $Z_{et}$ and mass $m_{e} = m_{e} + m_{o}$. This results in the calculation not including the coordinate $\tilde{r}_2$. The initial state wave function is given by

$$\Psi_{i} = \chi_{i}(\tilde{R}_{i}) \Phi_{He}(\tilde{r}_{31}),$$

and the residual ion is a structureless point particle of charge $Z_{o}$. The final state wave function is given by

$$\Psi_{f} = \chi_{f}(\tilde{R}_{f}) \Phi_{pb}(\tilde{r}_{41}, \tilde{r}_{31}),$$

where $\chi_{i}(\tilde{R}_{i})$ is the scattered projectile plane wave and $\Phi_{pb}(\tilde{r}_{41}, \tilde{r}_{31})$ is the scattered projectile bound state wave function. The classical perturbation is given by

$$V = \frac{Z_{o}Z_{ii}}{r_{1}} + \frac{Z_{o}Z_{e}}{r_{3}} + \frac{Z_{e}Z_{e}}{r_{4}} + \frac{Z_{e}Z_{ii}}{r_{4}}.$$ (39)

The SQM perturbation is now

$$V_{c}(r) = Z_{o} \left[ \frac{e^{-2Z_{o}r}}{Z_{o}r} \right].$$ (41)

The Jacobi coordinates used for the DBS model are shown in figure 4.

The expressions linking the lab frame coordinates to the Jacobi coordinates are

$$\tilde{R}_{i} = \frac{m_{p} \tilde{r}_{i}}{m_{e} + m_{p}} - \frac{m_{e} \tilde{r}_{3}}{2m_{e} + m_{o}} + \frac{m_{e} \tilde{r}_{4}}{m_{e} + m_{p}}$$

$$\tilde{R}_{f} = \frac{m_{p} \tilde{r}_{i}}{2m_{e} + m_{p}} + \frac{m_{e} (\tilde{r}_{3} + \tilde{r}_{4})}{2m_{e} + m_{p}}$$

$$\tilde{u} = \tilde{r}_{3} - \frac{m_{p} \tilde{r}_{i}}{m_{e} + m_{p}} - \frac{m_{e} \tilde{r}_{4}}{m_{e} + m_{p}}$$

$$\tilde{v} = \tilde{r}_{3} + \tilde{r}_{4}$$

As before, we make the approximation that $\tilde{u} \approx \tilde{r}_{31}$. 

![Figure 4](image-url)
Inserting all of the wave functions and the two choices of perturbation for the DBS model into equation (2) yields

\[
T^l_{\beta} = \frac{2(Z_{\alpha} + \alpha) \alpha Z Z^{3/2}_{\alpha} Z^{3/2}_{\alpha}}{\pi^1} \int d\beta \left[ \frac{Z_{\alpha}}{(\alpha^2 + p^2)^2 |\vec{D} - \vec{p} - \vec{G}|^2} + \frac{Z_{\alpha}}{((\alpha + Z_{\alpha})^2 + |\vec{D} - \vec{p}|^2)^2} \right]
\]

and

\[
T^{SQM}_{\beta} = \frac{32\alpha Z Z^{5/2}_{\alpha} Z^{5}_{Z}(Z_{\alpha} + \alpha)}{\pi^4} \int d\beta \left[ \frac{1}{[\alpha^2 + p^2]|Z^2_{\alpha} + |\vec{p} - \vec{F}|^2|} \times \frac{Z_{\alpha}}{|(Z_{\alpha} + \alpha)^2 + |\vec{D} - \vec{p}|^2|^2} + \frac{Z}{4Z^2_{\alpha} + |\vec{D} - \vec{p} - \vec{G}|^2 + |\vec{D} - \vec{p}|^2|^2} \right] \tag{47}
\]

where \( \vec{D} = \frac{m_h}{m_h + m_\gamma} - \frac{m_\gamma}{m_h + m_\gamma} \) and \( \vec{F} = \frac{m_h}{2m_h + m_\gamma} + \frac{m_\gamma}{2m_h + m_\gamma} \).

Finally, we introduce one additional variant of the DBS model in which the potential of the target atom frozen core is modeled with a screened Coulomb (Yukawa) potential. In this case, the classical perturbation of the DBS model is modified such that the two-particle interaction between the projectile constituents and the target nucleus is multiplied by a screening term, with screening parameter \( \beta \). In this DBS-Yukawa (DBS-Y) model, the perturbation is

\[
V_{\gamma} = \frac{Z_{\alpha}Z_{\alpha}e^{-\beta t}}{r_1} + \frac{Z_{\alpha}Z_{\alpha}}{r_{13}} + \frac{Z_{\alpha}Z_{\alpha}}{r_{13}} + \frac{Z_{\alpha}Z_{\alpha}e^{-\beta t}}{r_1}. \tag{49}
\]

If \( \beta = 0 \), this perturbation reduces to that of the classical DBS perturbation. The DBS-Y transition matrix is given by

\[
T^l_{\beta} = \frac{32\alpha Z Z^{3/2}_{\alpha} Z^{3/2}_{\alpha}}{\pi^4} \int d\beta \left[ \frac{Z_{\alpha}}{[\alpha^2 + p^2]|\vec{D} - \vec{p} - \vec{G}|^2[Z^2_{\alpha} + |\vec{D} - \vec{p}|^2]^2} + \frac{Z_{\alpha}}{|(Z_{\alpha} + \alpha)^2 + |\vec{D} - \vec{p}|^2|^2} \right]
\]

For a comparison of the classical, SQM, and Yukawa perturbations used, figure 5 shows \( V_{\text{atom}} \) for the SBS-SQM, DBS-SQM, Coulomb, and Yukawa potentials, as well as the charge enclosed \( Q(r) \) as a function of radial distance. Note that the Coulomb and Yukawa potentials shown are those of the target atom nucleus only and do not include the electronic potential. However, the curves for \( V_{\text{atom}} \) include both the electronic and nuclear potentials. From figure 5, it can be seen that other than the Coulomb nuclear potential, the Yukawa nuclear potential decays most slowly. This results in the Yukawa nuclear charge distribution being the broadest. The SMS SQM charge enclosed is two at the origin, while the DBS SQM charge enclosed is one at the origin. This difference is due to the use of the frozen core approximation in the target atom wave function in the DBS model, and leads to the DBS charge enclosed having a greater range than the SBS charge.

For a complete analysis of the models presented here, it is necessary to discuss the screening of the nuclear charge. Because all of the models contain some approximations to the two-electron bound states, some screening of the nuclear charge is possible. Thus, we have a choice in the values of \( Z_{\alpha} \) and \( Z_{\gamma} \), which will affect the binding energies used in the calculation. Table 2 contains a list of the values used for the results shown below. A qualitative discussion of their effects is contained in section 3.

3. Results

3.1. Classical perturbation models

As mentioned above, we consider the collision process of a \( ^3\text{He}^+ \) projectile colliding with neutral \( ^4\text{He} \). Results from all of the models discussed above are compared with the experimental data of [17] and we begin by comparing the results of the classical perturbation models with experiment. Despite the PWBA models’ shortcomings, comparison with experiment provides useful information about whether a specific approximation results in better or worse agreement with experiment. In general, perturbative models, such as the PWBA, are expected to work well when the perturbation parameter \( \eta = \frac{Z_{\alpha}}{\gamma} \) is less than 1. For the energies presented in figure 6, the perturbation parameters range from \( \eta = 0.64 \) (180 keV) to \( \eta = 0.2 \) (1.89 MeV), and are therefore within the range of validity of a perturbative model.

The most notable observation from figure 6 is that the differential cross sections for the models with the classical perturbation all show a deep minimum. This is commonly known to be caused by a cancellation of terms in the perturbation potential [17, 18, 20–23] and appears in other first order perturbative models, but is not present in second order or non-perturbative models. This minimum is also less severe when theory is convoluted over experimental angular and energy resolution [24]. For example, calculations using the more sophisticated first order CDW BIS model [17, 25] show similar deep minima at high energies, but at different
scattering angles than our SBS, DBS, or 5-Body models. The CDW BIS model is most similar to our SBS model, which treats the projectile as a structureless particle. However, the CDW BIS model includes distortion of the projectile wave in both the initial and final state, and this results in some differences in the cross sections of the two models, particularly the deep minimum location and a peak structure located near the Thomas peak region in the CDW BIS model. As in [25], we note that the changing of minimum location between models is due to the different perturbations. For the models presented here, a comparison shows that the SBS model has the minimum at the largest scattering angle, while the DBS model has it at the smallest scattering angle. The 5-Body model minimum appears between those of the SBS and DBS models because it contains the target atom bound state of the SBS model and the projectile bound state of the DBS model. Therefore, the 5-Body perturbation contains terms similar to the sum of the SBS and DBS models. For all models, the minimum appears at smaller scattering angles as projectile energy increases. The peak structure in the CDW BIS model is attributed to interference between the projectile distorted waves and is obviously not observed in our PWBA models.

In general, all of the classical perturbation models accurately predict the cross section magnitude at small scattering angles, where projectile-nuclear effects are less important. However, for large scattering angles, the 5-Body model is one to two orders of magnitude larger than the SBS or DBS models. Also, at the largest projectile energy, the 5-Body model is larger than the SBS and DBS models at all scattering angles.

One might instinctively assume that the 5-Body model should be more accurate since it does not make any simplifying assumptions about the inactive electron in the collision. However, it is not clear from figure 6 that the 5-Body model is any more accurate at predicting experiment than the SBS or DBS models. In general, the experimental data are best described by the DBS model at both large and small scattering angles, with the exception of the unphysical minimum. While none of the classical perturbation models are able to accurately predict the shape of the experimental data, the SBS model does a particularly poor job. The unphysical minimum occurs at a large scattering angle, and the model overestimates the cross section at small angles, while underestimating it at large angles. Contrary to this, the DBS and 5-Body models are able to predict the experimental results at scattering angles

Table 2. Charges and binding energies used to produce the results of section 3. The binding energies are: \( B_{ai} \) initial state target atom, \( B_{pi} \) incident projectile, \( B_{af} \) residual ion, \( B_{pf} \) scattered projectile.

| Model | \( Z_{pi} \) | \( Z_{ti} \) | \( B_{ai} \) (eV) | \( B_{pi} \) (eV) | \( B_{af} \) (eV) | \( B_{pf} \) (eV) |
|-------|-------------|-------------|-----------------|-----------------|-----------------|-----------------|
| 5-Body| NA          | NA          | −79.0           | −54.4           | −54.4           | −79.0           |
| SBS   | 1           | NA          | −79.0           | NA              | −54.4           | −13.6           |
| DBS   | NA          | 1           | −13.6           | −54.4           | NA              | −79.0           |

Figure 5. Model potentials used in the classical, SQM, and Yukawa perturbations. The top panel shows the potential versus radial distance from the nucleus and the bottom panel shows charge enclosed in a sphere of radius \( r \). The parameters used were \( \alpha = 1.6875 \), \( \beta = 1 \), \( Z_{pi} = 1 \), and \( Z_{ti} = 1 \). For the Coulomb potential \( V(r) = \frac{1}{r} \) and for the Yukawa potential \( V(r) = \frac{1}{r} e^{-br} \). Note that the Coulomb and Yukawa potentials shown are those of the target atom nucleus only and do not include the electronic potential. However, the curves for \( V_{\text{internal}} \) include both the electronic and nuclear potentials.
smaller than where the elbow in the experimental data occurs. This indicates that projectiles with electronic structure cannot be treated as point particles using the frozen core approximation. Their electronic structure must be included in the wave function and their interaction with the target atom needs to be included in the perturbation. Given that the electronic structure of the projectile is important, it is surprising that the 5-Body model does so poorly. This is primarily a result of the location of the minimum, which, like the SBS model, occurs at too large of a scattering angle. The structure of the projectile is included in the calculation in two ways: the wave function and the perturbation. Both the 5-Body and DBS models have the same projectile bound electron wave functions, but their perturbations are different. Therefore, the poor performance of the 5-Body model seems to indicate that it is the perturbation that is more important than the wave function. This is consistent with previous work that examined the effect of the frozen core approximation in ionization collisions [15, 16].

For a better understanding of the physical mechanisms involved in each of the models, we now turn to a comparison of the models themselves. In particular, comparison of the 5-Body model with the SBS model shows the effect of the inactive electron of the projectile, while comparison of the 5-Body model with the DBS model shows the effect of the inactive electron in the target atom. With the exception of the unphysical minimum, at all scattering angles the 5-Body model predicts a larger cross section than the SBS model, and the difference in magnitude increases as projectile scattering angle increases. The difference in magnitude between the 5-Body and SBS models also increases as projectile energy increases. The primary difference between the two models is the screening of the projectile nucleus. In the SBS model, the projectile is always fully screened by its bound electron, while in the 5-Body model, this screening changes with projectile location. Because the differences between the two models increase with both projectile energy and scattering angle, it indicates that projectile screening is more influential for close collisions. This can be understood using a classical scattering approach. For a given scattering angle, as the projectile energy increases, the impact parameter decreases. Therefore, larger projectile velocities require a closer collision in order to have the same scattering angle. Also, for a given energy, a smaller impact parameter is required for larger scattering. Therefore, both faster projectiles and larger scattering angles require a close collision, and this is when screening of the projectile has a larger effect on the cross section.

A comparison of the DBS model to the 5-Body model provides information about the screening of the target atom, and the results of figure 6 show that as projectile energy increases, the models become less similar. The models also become less similar as scattering angle increases. As in the case of projectile screening, this indicates that target atom screening is most important for close collisions.

Finally, a comparison of the SBS and DBS models shows that their differential cross sections become asymptotically similar for large scattering angles at all energies. Also, the magnitude of the cross section at zero scattering angle becomes more similar as projectile energy increases. These are the two regimes that correspond to close collisions, and the similarities of the SBS and DBS models in these two regions indicate that screening of either nucleus results in the same effects in the differential cross section.

Figure 6. Lab frame differential cross sections using the PWBA classical perturbation models described in section 2. Current models are compared to the experimental results of [17].
As mentioned above, in the SBS and DBS models, the values of the projectile charge and target nuclear charge can be varied to account for screening by the inactive electron. Variation of these charges will then affect the binding energies used in the calculations. The results shown in figure 6 do not include any screening effects in the charges (see table 2 for values used), however adjustment of the charges has some effect on the differential cross section. To simulate a decrease in screening of the projectile nucleus in the SBS model, we increased $Z_p i$ from 1 to 1.6875, which should result in the SBS model behaving more like the 5-Body model. It was observed that the SBS model with increased $Z_p i$ resulted in the deep minimum appearing at a larger scattering angle and the overall magnitude of the cross sections increasing by about one order of magnitude. The increase in magnitude is more similar to the 5-Body model, but the minimum appearing at larger scattering angle is contrary to the prediction.

In the DBS model, to test the effect of target nucleus screening, we increased $Z_t i$ from 1 to 1.6875 and found that the deep minimum moved to smaller scattering angles and the overall magnitude of the cross sections increased by about one order of magnitude. Again, the increase in magnitude makes the DBS model more similar to the 5-Body model, but the change in location of the minimum was in the opposite direction as what would be needed for the DBS model to more resemble the 5-Body model. However, the effect of the screening charges in both the SBS and DBS models indicate that the full nuclear screening is responsible for the difference in magnitude between the 5-Body, SBS, and DBS models. Because the 5-Body model consistently overestimates the experimental data compared to the SBS and DBS models, it can be concluded that some screening of the nuclei needs to be included.

3.2. SQM perturbation models

Because the deep minimum in the cross section is known to come from a cancellation of terms in the potential, we also consider the SQM perturbation described in section 2 in which the atomic electrons are not considered point particles, but rather a quantum mechanical electron cloud. This SQM perturbation softens the projectile-target electron interaction and removes the cancellation of terms in the potential. Results for the SQM models are shown in figure 7 and it can be seen that the effect of the SQM perturbation on the cross section is to dramatically lower the magnitude of the cross section at small scattering angles, while only minimally altering it at large scattering angles. Again, from a classical perspective, small angle scattering occurs for large impact parameters, or when the interaction between the projectile and target is weak. Because the SQM perturbation has the effect of smearing out the electron charge cloud, it produces a less localized interaction. This then results in a decreased probability of capture at small scattering angles and a smaller cross section. At large scattering angles, the dominant interaction is between the projectile and target nucleus, which is modeled as Coulombic in both classical and SQM perturbations. Therefore, the large scattering angle cross sections are similar for both types of models. In comparison to experiment, the SQM models generally do a poor job of predicting experiment at small scattering angles, but show good agreement for angles larger than the elbow in the experimental data. This pronounced elbow in the experimental results, where the slope of the cross section changes to become more gradual with increasing scattering angle, is due to different capture mechanisms dominating the small and large angle scattering regimes. For small angle scattering, the dominant capture mechanism is momentum transfer to the electron, while for large angle...
scattering, momentum transfer between the nuclei is dominant [26–28]. Because the SQM models have a less localized electron charge, when momentum transfer to the electron is dominant, the models underestimate experiment. The ability of the SQM models to accurately predict the large angle dominant, the models underestimate experiment. The ability electron charge, when momentum transfer to the electron is scattering, momentum transfer between the nuclei is dominant.

To further explore the effect of softening the potential in the perturbation, figure 7 also shows the differential cross section calculated using the DBS-Y model. In this model, the target nuclear interaction terms are softened by introducing a screening function. Unlike the SQM models, this screening of the nucleus does not remove the unphysical minimum in the cross section, but alters its location. In general, the DBS-Y and DBS models are very similar. Recall that as the screening parameter goes to zero, the DBS-Y model is identical to the DBS model. Results in figure 7 are shown for β = 1, however we examined other values of the screening parameter. As β increased, the magnitude of the cross section did not change, but the location of the minimum moved to larger scattering angles. This trend persisted, regardless of the energy of the projectile.

4. Conclusion

We have presented results from three different PWBA models using two types of perturbations. In all models, the incident and scattered projectiles were treated as plane waves and any two-particle bound states were approximated as product wave functions within the independent particle model. While these are very simple models, they show qualitatively some important physical effects. In the 5-Body model, all particles in the collision system were explicitly included in the calculation, while in the SBS and DBS models, either the incident projectile electron or inactive target atom electron was neglected, respectively. The differences between the 5-Body and SBS or DBS models showed the effect of the frozen core approximation. When a classical perturbation was used, all models showed an unphysical minimum due to a cancellation in the terms in the perturbation. Comparison of the 5-Body, SBS, and DBS models revealed that the neglect of inactive electrons in the perturbation had the most significant effect on the shape of the cross section. In particular, screening of either the projectile or target nucleus had a significant effect on the magnitude of the differential cross sections. This effect was most important for close collisions. A reduction in screening through a change in the projectile or target nucleus charge resulted in an increase in magnitude of the cross section. This change in charges also affected the location of the unphysical minimum in the differential cross sections, as did the inclusion of a Yukawa screening term in the target nuclear potential.

The deep minimum in the cross section with the classical perturbation prompted us to develop a SQM perturbation potential in which the atomic electrons are modeled as a quantum mechanical electron cloud rather than point particles. Use of the SQM perturbation removed the unphysical minimum, but it also lowered the magnitude of the cross section at small scattering angles. This was attributed to the smearing out of the electron probability density, which reduces the small angle capture probability. Both the SQM and classical perturbation models produced good agreement with experiment at large scattering angles, where nuclear–nuclear interaction is dominant.

While the results presented here come from rudimentary models, they provide important physical insights regarding the role of inactive electrons and nuclear screening in the single electron capture process and the classical versus quantum mechanical description of the projectile-electron interaction. We anticipate that more sophisticated quantum mechanical models will be able to more accurately predict experimental results on a quantitative level.

Acknowledgments

We gratefully acknowledge the support of the NSF under Grant Nos. PHY-1505217 and PHY-1838550.

ORCID iDs

A L Harris https://orcid.org/0000-0003-2689-982X

References

[1] Guo D L et al 2017 Phys. Rev. A 95 012707
[2] Gao J W, Wu Y, Wang J G, Sisouarat N and Dubois A 2018 Phys. Rev. A 97 052709
[3] van der Poel M, Nielsen C V, Gearba M-A and Andersen N 2001 Phys. Rev. Lett. 87 123202
[4] Wang Q, Ma X, Zhu X L and Zhang S F 2012 J. Phys. B: At. Mol. Opt. Phys. 45 025202
[5] Leredde A, Cassimi A, Flec'hard X, Hennecart D, Jouin H and Pons B 2012 Phys. Rev. A 85 032710
[6] Agueny H 2015 Phys. Rev. A 92 012702
[7] Abufager P N, Fainstein P D, Martínez A E and Rivarola R D 2005 J. Phys. B: At. Mol. Opt. Phys. 38 11
[8] Briggs J S, Greenland P T and Koebach L 1982 J. Phys. B: At. Mol. Phys. 15 3085
[9] Rivarola R D, Pacentini R D, Salin A and Belkic D 1980 J. Phys. B: At. Mol. Phys. 13 2601
[10] Egodapitiya K N, Sharma S, Hasan A, Laforte A C, Madison D H, Moshammer R and Schulz M 2011 Phys. Rev. Lett. 106 153202
[11] Sharma S, Hasan A, Egodapitiya K N, Arthanayaka T P, Sakhelelashvili G and Schulz M 2012 Phys. Rev. A 86 022706
[12] Schneider K, Schulz M, Wang X, Kelkar A, Grieser M, Krantz C, Ulrich J, Moshhammer R and Fischer D 2013 Phys. Rev. Lett. 110 113201
[13] Sarkadi L, Fabre I, Navarrete F and Barrachina R O 2016 Phys. Rev. A 93 032702
[14] Kouzakov K A 2017 Eur. Phys. J. D 71 63
[15] Harris A L 2015 J. Phys. B: At. Mol. Opt. Phys. 48 115203
[16] Harris A L and Morrison K 2013 J. Phys. B: At. Mol. Opt. Phys. 46 145202
[17] Schöfler M S, Titze J, Schmidt L P H, Jahnke T, Neumann N, Jagutzki O, Schmidt-Böcking H, Dörner R and Mančev I 2009 Phys. Rev. A 79 064701
[18] Ghanbari-Adivi1 E and Ghavaminia H 2015 Chin. Phys. B 24 033401
[19] Harris A L and Madison D H 2014 Phys. Rev. A 90 022701
[20] Belkić D and Salin A 1978 J. Phys. B: At. Mol. Phys. 11 3905
[21] Omidvar K 1975 Phys. Rev. A 12 911
[22] Band Y B 1973 Phys. Rev. A 8 2857
[23] Sil N C, Saha B C, Saha H P and Mandal P 1979 Phys. Rev. A 19 655
[24] Vinitsky P S, Popov Y V and Chuluunbaatar O 2005 Phys. Rev. A 71 012706
[25] Milojević N, Mančev I and Belkić D 2017 Phys. Rev. A 96 032709
[26] Mergel V et al 1995 Phys. Rev. Lett. 74 2200
[27] Kamber E Y, Cocke C L, Cheng S and Varghese S L 1988 Phys. Rev. Lett. 60 2026
[28] Dörner R, Ulrich J, Schmidt- Böcking H and Olson R E 1989 Phys. Rev. Lett. 63 147