Kwame Nkrumah University Of Science And Technology

Two-Electron Capture From Helium-Like Atomic Systems By Completely Stripped Projectiles

by

Augustine Larweh Mahu(BSc. Hons)

A Thesis Submitted To Department Of Mathematics

In Partial Fulfilment Of The Requirements For The Degree

Of

Master Of Science

College of Science

November 2010

Declaration

I hereby declare that this submission is my own work towards the Master of Science (MSc.) and that, to the best of my knowledge, it contains no material previously published by another person nor material which has been accepted for the award of any other degree of the University, except where due acknowledgement has been made in the text.

Augustine Larweh Mahu	....	....
Student	Signature	Date

Certified by:

F. T. Oduro (Dr.)	....	....
Supervisor	Signature	Date

Certified by:

S. K. Amponsah (Dr.)	....	....
Head of Department	Signature	Date

Abstract

Solution to four-body version of the boundary corrected first Born (CB1-4B) approximation has been solved by Dževad Belkić. We consider symmetric double-charge exchange in fast collisions of bare nuclei with helium-like atomic systems. We particularly are interested in the calculation of the four-body version of the boundary corrected second Born (CB2-4B) approximation with full account of the long-range Coulomb effects arising from the relative motion of the scattering aggregates. Using the formalism of Perturbation Theory in Quantum Mechanics, we employ Lippman-Schwinger Equation with free Green Function. We write the transition matrix elements for the second order contribution as a set of nine integrals. This makes use of unperturbed wavefunctions from the entrance and exit channels. We did not consider calculating the matrix elements.

Contents

List of Figures

Acknowledgements

I am particularly grateful to Dr. A. K. Agyei for his immense contribution to my understanding in Advanced Quantum Mechanics and General Relativity and Cosmology. His lucid approach to presentation and teaching has been a guiding light to success in Advanced Quantum Mechanics and General Relativity and Cosmology. Many thanks to my Supervisor, Dr. F. T Oduro, for guiding and directing the success of this thesis, and I am grateful for his support. It is important to recognize also, Rev. Dr. G. O. Lartey, for his earlier contribution to my Undergraduate Education in Quantum Mechanics and Special Relativity. To my friend Eric Neebo Wiah, for his encouragement saw me through this thesis. I am grateful to the Department of Mathematics, Kwame Nkrumah University of Science and Technology, for a part well played in my Education.

To my parents Mr. and Mrs. Mahu, and siblings; Ekow, Korleki, Dapaa, Atteh and Terpi; I thank you all for the love you've shown me through my entire studies. It has been the grace and mercies of God throughout my entire education and I am humbled by that.

Chapter 1

Introduction

1.1 Background

It is important for me to mention here that, the review of works in the area of *Four-body methods for high-energy ion-atom collision* techniques has a lucid write up by *Belkić et al.* [1], and this accounts for all the inputs made to the field.

Determination of the interactive dynamics of atomic systems is still among the most fundamental challenges in physics. Since the interaction potentials in atomic systems are exactly known, any discrepancy between experimental measurements and theories can be attributed to inappropriate theoretical models for describing many-particle systems or to unreliable experimental techniques. One of the central questions which arises in scattering problems involving many-electron systems concerns the influence of the electron-electron interaction on the overall dynamics in these collisional phenomena. Since the helium atom (or a heliumlike ion) is the simplest many-electron target where one can assess the importance of electronic correlations, its investigation has attracted most attention from both the theoretical and experimental sides. Collisional processes in which two nuclei and two electrons take part represent pure four-body problems [2][3][4][5]. A basic motivation for developing four body theories to treat ion (atom)-atom collisions is to more thoroughly understand the role of the electron-electron correlation and phase coherences in such important processes. In atomic physics, electronic correlation effects originate from pure Coulombic interactions between active electrons. Phase coherences are interference patterns for competing mechanisms in four-body collisional transitions.

In ion-atom collisions, there are two kinds of electronic correlations: static and dynamic. Static correlations are built into multi electron bound-state wave functions without any reference to collisions. Quantum-mechanical bound states are prepared without the presence of an incident beam. Several methods for obtaining bound-state wave functions and the corresponding eigenenergies for two-electron atomic systems have recently been reviewed [6]. The dynamic correlations describe interactions between two electrons in the exit channel, if we deal with $Z_P - (Z_T; e_1, e_2)_i$ collisions, or in the entrance channel, if $(Z_P, e_1)_{i_1} - (Z_T, e_2)_{i_2}$ process is considered. The electronic interactions alone are capable of causing a transition of the entire collisional system from an initial to a final state. Such a dynamical effect automatically possesses both radial and angular correlations through the inclusion of the interelectron Coulomb potential $\frac{1}{r_{12}}$ in the final interaction potential V_f appearing in the post form of the transition amplitude T_{if}^{+}, if the $Z_P - (Z_T; e_1, e_2)_i$ collisions are studied. The same potential $\frac{1}{r_{12}}$ appears in the initial perturbation potential V_i of the prior form of the transition amplitude T_{if}^{-}, if the $(Z_P, e_1)_{i_1} - (Z_T, e_2)_{i_2}$ collisions are investigated.

The majority of the theoretical studies that have considered the $Z_P - (Z_T; e_1, e_2)_i$ collisions employed the independent-particle model (IPM) ([7][8][9][10][11][12][13][14] [15][16][17][18][19][20][21][22][23][24][25][26][27] [28][29][30][31][32][33]). The basic feature of all these previous investigations within the IPM and its variants is the preservation of a pure three-body formalism, despite the fact that the studied four-body problems include two active electrons. Within the IPM itself, there are many ways of approximating the wave function of a heliumlike atomic system. An approach in which an active electron of a two electron atom or ion moves in an effective potential generated by the other nucleus and the passive electron has frequently been used. The term passive electrons is used here in the sense that their interactions with the active electrons do not contribute to the collisional process. Thus, in the IPM, the initial four-body problem is effectively reduced to a three-body problem. The main drawback of the IPM is that the dynamic correlation effect during the collisional phenomenon are completely ignored from the outset.

Hence, if we are to adequately assess the role of electron-electron correlations, we must deal with four-body problem from the beginning. Guided by this argument, various quatum-mechanical four-body methods have been proposed to study one-electron and two-electron transitions in scattering of completely stripped projectiles on heliumlike atomic systems or in collisions between two hydrogenlike atoms or ions. In addition to four-body theories, the role of electronic correlations in energetic ion-atom collisions has also been investigated elswhere [25][26][24][34].

The first formulation and implementation of the four-body continuum distorted-wave (CDW-4B) method for double-electron capture was carried out by [4][5]. The CDW-4B method obeys the asymptotic convergence criteria of [35][36] for Coulomb potentials. These initial computations of [4][5] on the formation of H^- in the $H^+ - He$ collisions yielded total cross sections that were in excellent agreement with available experimental data. Subsequently, the CDW-4B method was applied to other collisional systems [37][38][39][40][41], including double capture into singly and doubly excited final states by multiply charged projectile ions. Further, an adequate description of simultaneous transfer and ionization has been devised using the CDW-4B method [2][3][42][43]. Studies of transfer ionization by means of the CDW-4B method indicate that dynamic electronic correlations in perturbation potentials are more important than the static ones. The substantial improvement of the CDW-4B method over, e.g., the IPM has been attributed solely to the role of dynamic electron correlation effects.

Throughout this review, emphasis is placed on the adequate solutions of the asymptotic convergence problem [36][44] by requiring not only the correct asymptotic behaviours of all the scattering wave functions, but also their proper connections with the corresponding perturbation interactions. This strategy proves to be simultaneously fundamental (consistency of theory by reference to the first principles of physics), and practical (stringent scrutiny of theory through its systematic verification against experiment). A striking example which illustrates this issue is a four-body problem with single-electrom detachment from H^- by H^+. For this problem, the eikonal Coulomb-Born method has been proposed by [45] with the correct asymptotic behaviours of the initial and final scattering states. Yet, the ensuing total cross sections of this method overestimates the corresponding experimental data by some 2-3 orders of magnitude at all impact energies. As shown by [2][3], the reason for this discrepancy was the lack of the proper link between the initial scattering state and the perturbation potential in the entrance channel. When this link has properly been established for the same collisional problem, the modified Coulomb-Born method emerged [2][3], exhibiting excellent agreement with the experimental data at all impact energies. This latter approximation is a simplified version of the CDW method for ionization proposed by [46], who originally derived the scattering wave for the final state as the product of three full Coulomb functions (later called the C3 function) to satisfy the correct boundary condition for three charged particles in the exit channel. This C3 scattering wave function has repeatedly been rediscovered in subsequent studies [47][48]. Throughout the years, and especially more recently [49][50], it was conclusively established that the most successful theory for heavy-particle ion-atom ionization at high energies is the CDW method of [46] regarding both differential and total cross sections. Of late, the CDW method has been exported to neighboring research fields, such as medical physics for a more adequate description of the stopping power of multiply charged ions passing through matter, as encountered in applications to hadron radiotherapy [51].

The three-body reformulated impulse approximation (RIA-3B) of [52][53], after resolving a longstanding problem on the inadequacy of the corresponding impulse approximation (IA) for the total cross sections in the $\mathrm{H}^+ - \mathrm{H}$ charge exchange, has been extended to four-body collisions. Cross sections of the four-body reformulated impulse approximation (RIA-4B) of Belkić for transfer ionization (TI) in the $\mathrm{H}^+ - \mathrm{He}$ collisions have been reported in a joint theoretical and experimental study [54]. The total cross sections of the RIA-4B for the TI process have indicated a trend of the v^{-11} behavior at sufficiently large values of the impact velocity v. This asymptotic behavior, as the quantum-mechanical counterpart of the corresponding classical double scattering [55], has been confirmed on the same collision by two subsequent measurements [56][57].

As a further exploration of the CDW-4B method, simultaneous transfer and excitation (TE) have also been the subject of studies [58][59][60][61][62]. This process takes place when a target electron is captured by a non bare projectile, while the initial electronic structure of the latter is excited at the same time. For the process of TE, where a doubly excited autoionizing state is formed on the projectile, two modes have been identified and termed the resonant (RTE) and the nonresonant transfer excitation (NTE). In the RTE, excitation of the projectile is due to the dielectronic interaction between the projectile electron and the target electron, which is captured. In the NTE, a target electron is transferred and excitation of the projectile comes from the interaction with the rest of the target. In addition to these two-electron transitions, the CDW-4B method has also been applied to single-electron capture [63][64][43] in a number of processes, such as the $\mathrm{H}^+ - \mathrm{He}, \mathrm{H}^+ - \mathrm{Li}^+, \mathrm{He}^{2+} - \mathrm{He}$, and

Li^{3+} − He collisions. In the CDW-4B method, the electronic continuum intermediate states are included in both channels through the full Coulomb waves. Using this method, we emphasize the pivotal role of the dynamic electron correlations in differential cross sections. In particular, the CDW-4B method predicts two competing double scattering mechanisms leading to a double structure with the Thomas peak of the 1st $(P - e - T)$ and 2nd $(P - e - e)$ kind, where the former (standard) is a purely high-energy occurrence, whereas the latter novel systematically persists at all impact energies [65][66].

In the boundary-corrected four-body first Born approximation (CB1-4B) , pure electronic continuum intermediate states are not taken into account. Here the scattering state vectors are given by the product of unperturbed channel states and logarithmic distortion phase factors due to the Coulomb long-range remainders of the perturbation potentials. The CB1-4B method was initially formulated and applied to double-electron capture by [67][68]. This method has subsequently been used for describing single-charge exchange in energetic collisions between two hydrogenlike atoms or ions [69][70].

The four-body boundary-corrected continuum intermediate state (BCIS-4B) method of [71] and the four-body Born distorted-wave (BDW-4B) method of [37] have been introduced and used first for investigation of double-electron and then single-electron capture. These two methods, with the correct boundary conditions, can be applied and extended to any number of colliding particles, so that the more generic acronym BCIS and BDW can be used. Both methods employ the scattering wave functions from the CDW method in one of the two channels, in either the entrance or exit channel, for the initial or final state, depending on whether the prior or post form of the transition amplitudes is used. For the other channel, the BCIS and BDW methods use the corresponding wave functions of the CB1 method. As a result, the distorting potentials that cause the transitions from the initial to final states of the system are different in the BCIS and BDW methods. These latter potentials are the usual electrostatic Coulomb interactions in the BCIS method (shared by the CB1 method) , whereas they are the operator-type potentials $\vec{\nabla} \cdot \vec{\nabla}$ in the BDW method (shared by the CDW method). Thus, if one wishes to make these remarks more transparent, the original acronym BDW introduced by [37], and subsequently used by [72] and [73], could be relabeled as CDW-CB1. In particular, the notations for the post and prior BDW or, equivalently, CDW-CB1 can further be differentiated by highlighting the use of the boundary-corrected first-order Born initial and final states (BIS and BFS). This has led to yet another equivalent set of acronyms, CDW-BIS and CDW-BFS [74][75] for the post and prior versions of the BDW method of [37]. Using the BCIS and BDW methods, [71][37] has shown that double-charge exchange is sensitive to the inclusion of long-range Coulomb effects through electronic continuum states. These latter states play an important role even at those incident energies at which the Thomas double scattering is not apparent. By means of the mentioned hybrid four-body approximations, one can study various mechanisms that can produce the Thomas peaks in the differential cross sections. Even for single-charge exchange with heliumlike targets, these methods deal explicitly with two active electrons from the onset and, therefore, they preserve the four-body nature of the original problem. The post and prior BDW methods (or, equivalently, the CDW-BIS and CDW-BFS methods, respectively) have been employed to compute both differential and total cross sections for single-electron capture in collisions between bare projectiles and heliumlike atoms or ions [72][74][75][73].

Additionally, there are other hybrid-type approximations with the correct boundary conditions known as the continuum distorted wave eikonal initial state (CDW-EIS) and the continuum distorted wave eikonal final state (CDW-EFS) methods [76][77][78][79]. The CDW-EIS method was originally introduced by [76] for ionization of hydrogenlike atomic systems by nuclei treated as a pure three-body problem. In the work of [78], the CDW-EIS and CDW-EFS methods for single-electron capture from a two-electron target are reduced to a one-electron process. Here, the active captured electron was described by a self-consistent field orbital. The other noncaptured electron is passive, since it is considered as frozen in its initial state during the collision. Therefore, such versions of the CDW-EIS and CDW-EFS methods [77][78][79] belong to the category of three-body approximations. As to pure four-body collisions with two active electrons, the four-body continuum distorted wave eikonal initial state (CDW-EIS-4B) method has also been introduced and applied to double capture from helium by alpha particles [41], but without any success. The CDW-EIS and CDW-EFS methods differ from the CDW-BIS and the CDW-BFS methods, since EIS and EFS are different from BIS and BFS, respectively. Specifically, the difference is in the independent variables in asymptotic states {EIS, EFS} and {BIS, BFS}.

The dominant feature of most of the quoted quantum-mechanical four-body approximations is that they show systematic agreement with the corresponding experimental data at intermediate and high impact energies. This is striking in view of the fact that the impact parameter versions of the investigated approximations often fail (and do so dramatically in some cases) in their attempts to reproduce experimental data. The first indication on the breakdown of the IPM for double-electron capture has been given by [4]. The clear implication of this is that dynamic correlation effects are of critical importance for two-electron transitions. One of the tasks is to highlight this latter feature and to assess its overall significance for energetic ion-atom collisions with two actively participating electrons. The major goal is to critically evaluate the efficiency and overall utility of the leading methods within the realm of four-body quantum-mechanical scattering theory. For validation purposes, we shall formulate the necessary theoretical criteria that adequate four-body methods are expected to satisfy. Intermediate and high nonrelativistic energies permit a consistent extension of rigorous pure three-body distorted-wave methods to their pure four-body counterparts without any significant additional approximation. This represents an excellent opportunity to estimate the relevance of the well-known asymptotic convergence problem from formal scattering theory for Coulomb potentials when more than three particles are actively involved. Such an opportunity will presently be seized by building on the past successful experience with the similar challenges encountered in simpler three-body ion-atom rearrangement collisions for which, [44] have conclusively established the critical importance of the correct Coulomb boundary conditions in the most general case with the exact eikonal transition amplitude. Subsequent detailed numerical computations, with dramatic improvements relative to experimental data, expecially for the boundary corrected three-body first-order approximation of this exact eikonal T matrix [80][81][82][83][84], confirmed the validity of this theoretical concept, which was then widely accepted and reviewed in several articles and books on the subject [85][86][87][88][89][65][66][51].

1.2 Problem

We consider a projectile nucleus (bare nucleus), Z_P, approaching a target helium-like atomic sytem with nucleus Z_T from inifity. The occurence of scattering ensures that the projectile nucleus capture the two orbiting electrons and leaves the target nucleus bare. In this senario, we are required to formulate a theory that account for coulombic interaction at great distances between the projectile and the target nuclei. This occur in the entrance and the exit channels. Of great importance is the behaviour of the system when the projectile nucleus, Z_P, flies close to the target nucleus Z_T. Figure 2.1 and Figure 2.2 inlustrate this description.

1.3 Objectives

In this work we attempt to correctly

1. define boundary conditions of the unperturbed wavefunction in both the entrance and exit channels.

2. Solve the resulting Schrödinger equation governing the unperturbed states analytically.

3. Write the matrix elements of the second order contribution to the Second Born Approximation.

1.4 Methodology

The problem at hand will be divided in two parts, the entrance and exit channels. In the entrance channel, we write explicitly the Hamiltonian with the correct boundary conditions accounted for via introduction of the perturbation potential at infinity. The associated Schrödinger wave equation is solved to obtain the unperturbed wavefunction $\Phi_i^+ \equiv \Phi_i^c(\vec{r}_i \to \infty)$. Similarly, we obtain the unperturbed wavefunction to the exit channel state as $\Phi_f^- \equiv \Phi_f^c(\vec{r}_f \to \infty)$.

Next we introduce the formalism of Perturbation Theory of Quantum Mechanics [90] to write explicitly the matrix elements of the second order contribution to the Second Born Approximation.

Atomic units will be used throughout unless otherwise stated.

1.5 Justification of Problem

In principle the study is abstract and more theoretical and unrealistic in everyday life application. To many it is more pronounced in its applications to theoreticians. Now, such investigation as this has huge impact in Medical Sciences for treating patients in hospitals. Below are some of the methods and techniques employed.

1. Hadrontherapy; utilizes beams of light ions of atomic number around $Z = 6$. Better control slow growing radioresistant tumours which represents about 20% of all irradiated tumours [91].

2. A new application of great importance is the development of **X-ray Emitting Free Electron Lasers**. Availability of these intense sources will allow even to 'see' moving microstructures of angstrom dimensions. A project is under way in USA [91].

3. Cyclotrons are used to produce the medical isotopes used for *Positron Emission Tomography* (PET) and *Single Photon Emission Computed Tomography* (SPECT). Still, in **diagnostics**, about 80% of all examinations use isotopes (in particular Technetium 99m) produced at old reactors [91].

1.6 Structure of the Thesis

This thesis is in the three major phases. The first comprise chapter one, which basically reviews all the literature on the subject till 2008 [1]. It also clearly states the problem at hand , objectives and the justification of the study especially to the benefit of society.

The second part comprise chapter two. In this chapter the problem is described in terms of the standard four-body formalism and the approach to solving it is in two phases. Thus, we derive the unperturbed wavefunctions of the entrance and exit channel states in both asymptotic form and series solutions to the resulting transformed Schrödinger wave equation. Here we ensure correct boundary conditions for the unperturbed wavefunctions. The associated perturbation terms V_i^c and V_f^c are correctly stated.

The last part including chapter three, makes use of Perturbation Theory of Quantum Mechanics [90]. We put together results in chapter two and the T Matrix of the Second Born Approximation to produce matrix elements of the second order contribution. The first order contribution having already been computed by Dževad Belkić [92]. This is the result stated in chapter four. Finally, chapter five comprise discussion of results and conclusion.

Chapter 2

General Theory Of The Four-Body Formalism

2.1 Introduction

We are interested in ion-atom collisions in which two electrons take part. Such processes involve scattering between a bare nucleus (projectile) P of charge Z_P and a heliumlike atomic system consisting of two electrons e_1 and e_2 initially bound to the target nucleus T of charge Z_T, i.e the $Z_P - (Z_T; e_1, e_2)_i$ collisions, where the parentheses indicate the bound states. Specifically, we examine here double–electron capture in a colliding heliumlike projectiles:

$$Z_P + (Z_T; e_1, e_2)_i \rightarrow (Z_P; e_1, e_2)_f + Z_T \tag{2.1}$$

were indices i, f represents the collective labels for the set of quantum numbers needed to describe the initial and final bound states.

Let the position vectors of the projectile nucleus, the target nucleus, and electrons $e_{1,2}$ relative to an arbitary coordinate frame be, respectively, denoted by $\vec{r}_1$, $\vec{r}_2$, $\vec{r}_3$

and $\vec{r}_4$. Then the kinetic energy operator is given by

$$H_0 = -\frac{1}{2M_P}\nabla^2_{r_1} - \frac{1}{2M_T}\nabla^2_{r_2} - \frac{1}{2}\nabla^2_{r_3} - \frac{1}{2}\nabla^2_{r_4} \tag{2.2}$$

where M_P and M_T are the masses of the projectile and target, respectively. The position vectors of electrons $e_{1,2}$ relative to Z_P and Z_T are denoted by $\vec{s}_{1,2}$ and $\vec{x}_{1,2}$, respectively. We denote by $\vec{R}$, the position vector of the projectile Z_P relative to Z_T and by r_{12} the interelectron distance.

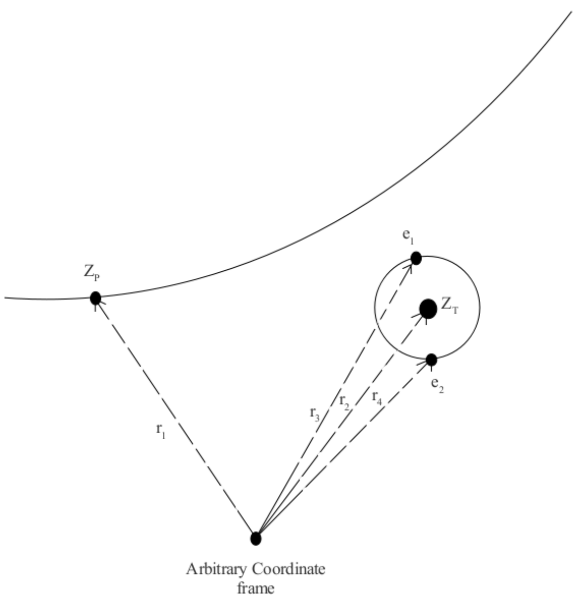

Figure 2.1: Arbitrary Coordinate Frame.

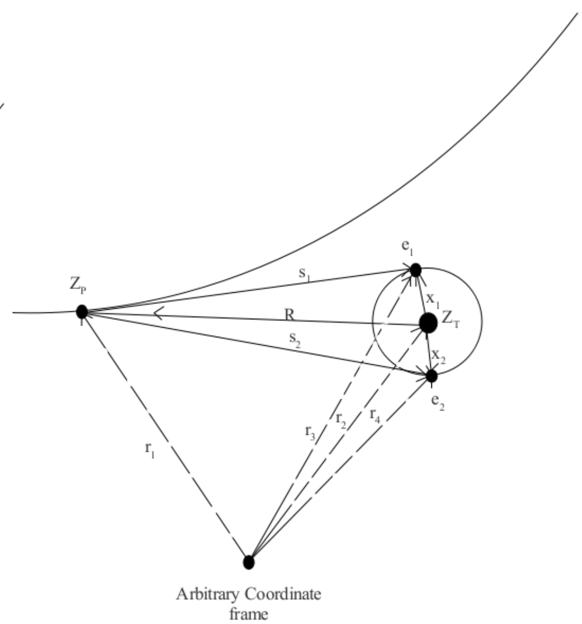

Figure 2.2: Relative vectors between (Z_P and Z_T), (Z_P and e_12), and (Z_T and e_12).

2.2 The entrance channel

We concentrate on the collisions of completely stripped projectiles with heliumlike targets, i.e, the Z_P-$(Z_T; e_1, e_2)_i$ collisions. Introducing $\vec{r}_i$ as a relative vector of Z_P

with respect to the center of mass of $(Z_T; e_1, e_2)_i$ we have

$$\vec{r}_i = \vec{r}_1 - \frac{\vec{r}_3 + \vec{r}_4 + M_T \vec{r}_2}{M_T + 2}.$$

As a matter of convenience we express the Hamiltonian $\hat{H}_0$ alternatively via a set of independent variables $(\vec{x}_1, \vec{x}_2, \vec{r}_i)$

$$\hat{H}_0 = -\frac{1}{2\mu_i}\nabla^2_{r_i} - \frac{1}{2b}\nabla^2_{x_1} - \frac{1}{2b}\nabla^2_{x_2} - \frac{1}{M_T}\vec{\nabla}_{x_1} \cdot \vec{\nabla}_{x_2} \tag{2.3}$$

where

$$\mu_i = \frac{M_P(M_T + 2)}{M_P + M_T + 2}$$

and

$$b = \frac{M_T}{M_T + 1}.$$

The last term in equation (2.3) is the so-called *mass polarization* term, which can be neglected for heavy particles beacuse $M_T \gg 1$.

The total Hamiltonian of the system under study in the center-of-mass frame for the whole system is given by

$$\hat{H} = \hat{H}_0 + V \tag{2.4}$$

where V represents the interaction potential operator

$$V = \frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} + \frac{1}{r_{12}} \tag{2.5}$$

Now, rearranging collisions, the complete Hamiltonian from equation (2.4) can be split into the following form

$$\hat{H} = \hat{H}_i + V_i \tag{2.6}$$

where $\hat{H}_i$ and V_i are the Hamiltonian and the perturbation potential in the entrance channel

$$\begin{aligned} \hat{H}_i &= \hat{H}_0 - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} + \frac{1}{r_{12}}, \\ V_i &= \frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}. \end{aligned} \tag{2.7}$$

The unperturbed channel state Φ_i is defined by

$$(\hat{H}_i - E_i)\Phi_i = 0,$$
$$\Phi_i = \varphi_i(\vec{x}_1, \vec{x}_2)e^{i\vec{k}_i.\vec{r}_i}. \tag{2.8}$$

The function $\varphi_i(\vec{x}_1, \vec{x}_2)$ represents the two-electron bound-state wave funtion of the atomic system $(Z_T; e_1, e_2)_i$, whereas $\vec{k}_i$ is the initial wave vector. This latter wave function satisfies the following eigenproblem

$$(\hat{h}_i - \epsilon_i)\varphi_i(\vec{x}_1, \vec{x}_2) = 0$$
$$\hat{h}_i = -\frac{1}{2b}\nabla^2_{x_1} - \frac{1}{2b}\nabla^2_{x_2} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} + \frac{1}{r_{12}}, \tag{2.9}$$

where $\hat{h}_i$ is the electronic Hamiltonian and ϵ_i is the electronic binding energy. The total energy of the four-body system is given by

$$E = E_i = \frac{k_i^2}{2\mu_i} + \epsilon_i$$

and it is conserved during the scattering event.

The wave functions of two-electron atomic systems have been the subject of extensive studies [93][6]. In the case of helium, the variational estimate $\epsilon_i = -2.903724377034105$ [94] via a fully correlated Hylleraas wave function, with explicit allowance for the interelectron coordinate r_{12} (through some 600 expansion terms), could be treated as practically the exact value.

The initial state Φ_i is distorted even at infinity, due to the presence of the asymtotic Coulomb repulsive potential $V_i^\infty = \frac{Z_P(Z_T-2)}{R}$ between the projectile and screened target nucleus. Notice that V_i^∞ is the asymtotic value of the perturbation V_i.

$$V_i = \frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} \rightarrow \frac{Z_P(Z_T-2)}{R} = V_i^\infty \tag{2.10}$$

as $r_i \rightarrow \infty$, $s_1, s_2 \rightarrow R$. Bearing in mind the long-range nature of the Coulomb interaction, the Hamiltonian $\hat{H}$ can be decomposed according to

$$
\begin{aligned}
\hat{H} &= \hat{H}_i^c + V_i^c, \\
\hat{H}_i^c &= -\frac{1}{2\mu_i}\nabla_{r_i}^2 + \frac{Z_P(Z_T-2)}{r_i} - \frac{1}{2b}\nabla_{x_1}^2 - \frac{1}{2b}\nabla_{x_2}^2 \\
&\quad - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} + \frac{1}{r_{12}}, \\
V_i^c &= \frac{Z_P Z_T}{R} - \frac{Z_P(Z_T-2)}{r_i} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}.
\end{aligned}
\tag{2.11}
$$

The potential V_i^c exhibits short-range behaviour when $R \to \infty$. The difference $\frac{1}{R} - \frac{1}{r_i}$ is by a factor δ smaller than $\frac{\vec{R}.(\vec{x}_1+\vec{x}_2)}{R^3}$, where $\delta = \frac{1}{M_T+2}$, as can be checked using Taylor series expansion. Thus, neglecting the terms of the order of $\frac{1}{M_T}$, we have that $r_i \simeq R$, so that V_i^c can be approved as

$$
V_i^c = \frac{2Z_P}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}. \tag{2.12}
$$

Obviously, V_i^c tends to $O(\frac{1}{R^2})$ as $R \to \infty$. It should be emphasized that the perturbation V_i^c depends only on the interaction between electrons and the projectile. The term $\frac{2Z_P}{R}$ in equation (2.12), despite its form, is not related to the internuclear potential, but originates solely from the electron-projectile interaction. The asymtotic tail of the potential $-\frac{Z_P}{s_1}$ is $-\frac{Z_P}{R}$, since $s_1 \to R$ as $R \to \infty$. This can be seen by utilizing a Taylor expansion for $\frac{Z_P}{s_1}$ around R. The small value of the x_1 coordinate in the entrance channel justifies this development. The same statement also holds true for the potential $-\frac{Z_P}{s_2}$. It is important to note that, unlike the channel perturbation V_i^c, the corresponding perturbation V_i from equation (2.7) contains the internuclear interaction $\frac{Z_P Z_T}{R}$. With the Hamiltonian $\hat{H}_i^c$ from equation (2.11), the eigenproblem in the entrance channel reads

$$
(\hat{H}_i^c - E_i)\Phi_i^c = 0. \tag{2.13}
$$

This is the counterpart of equation (2.8) when there is a remaining Coulomb potential in the asymtotic region. Using equations (2.9),(2.11) and substituting into equation (2.13) we have;

$$
\left(-\frac{1}{2\mu_i}\nabla_{r_i}^2 + \frac{Z_P(Z_T-2)}{r_i} + \hat{h}_i\right)\Phi_i^c = E_i\Phi_i^c \tag{2.14}
$$

We consider the wavefunction of the electronic Hamiltonian $\varphi_i(\vec{x}_1, \vec{x}_2)$ to be independent of the wavefunction generated by the projectile nucleus as follows;

$$\Phi_i^c = \phi_i(\vec{r}_i)\varphi_i(\vec{x}_1, \vec{x}_2) \tag{2.15}$$

Hence, substituting equation (2.15) into (2.14)

$$\left(-\frac{1}{2\mu_i}\nabla^2_{r_i} + \frac{Z_P(Z_T-2)}{r_i} + \hat{h}_i\right)\phi_i(\vec{r}_i)\varphi_i(\vec{x}_1, \vec{x}_2) = E_i\phi_i(\vec{r}_i)\varphi_i(\vec{x}_1, \vec{x}_2),$$

gives two sets of independent second order differential equations as,

$$\hat{h}_i\varphi_i(\vec{x}_1, \vec{x}_2) = \epsilon_i\varphi_i(\vec{x}_1, \vec{x}_2), \tag{2.16}$$

$$\left(-\frac{1}{2\mu_i}\nabla^2_{r_i} + \frac{Z_P(Z_T-2)}{r_i}\right)\phi_i(\vec{r}_i) = E_i\phi_i(\vec{r}_i). \tag{2.17}$$

We proceed to calculate the wavefunction of equation (2.17).

$$\left(\nabla^2_{r_i} + 2\mu_i E_i - \frac{2\mu_i Z_P(Z_T-2)}{r_i}\right)\phi_i(\vec{r}_i) = 0$$

$$\left(\nabla^2_{r_i} + k_i^2 + \frac{2\gamma_i k_i}{r_i}\right)\phi_i(\vec{r}_i) = 0. \tag{2.18}$$

$$where, \quad k_i^2 = 2\mu_i E_i, \quad -\gamma_i k_i = Z_P(Z_T-2)\mu_i \quad and \quad \mu_i = \frac{M_P(M_T+2)}{M_P+M_T+2}.$$

Note that $\gamma_i < 0$ corresponds to repulsion. As long as we are interested in a pure Coulomb field, it is possible to write our solution $\phi_i(\vec{r}_i)$ to equation (2.18) as

$$\begin{aligned}\phi_i(\vec{r}_i) &= e^{i\vec{k}_i.\vec{r}_i}\chi_i(\upsilon_i). \\ \upsilon_i &= ik_i r_i(1-\cos\theta) \\ \upsilon_i &= ik_i(r_i - z_i) = ik_i w_i.\end{aligned} \tag{2.19}$$

We note that $w_i = r_i - z_i$ and $\vec{k}_i.\vec{r}_i = k_i z_i$. The separation of variables for $\phi_i(\vec{r}_i)$ in equation (2.19) is plausible if we recognize;

1. that the solution will not involve the azimuthal angle because of the axial symmetry of the problem and.

2. since $\phi_i(\vec{r}_i)$ represents the complete Coulomb-wave function (incident plus scattered wave), terms must exist in its dominant asymptotic form that contains $e^{i\vec{k}_i.\vec{r}_i}$ and $r^{-1}e^{ik_i.r_i}$. We demonstrate that, with the choice of indenpendent variables we are about to make, this will indeed be the case [95].

Let us choose independent variables (z_i, w_i, λ_i) where $w_i = r_i - z_i$ and λ_i can be taken as the azimuthal angle, on which the solution $\phi_i(\vec{r}_i)$ does not depend. In changing from our Cartesian coordinates (x, y, z) to (z_i, w_i, λ_i), we use chain rule expressions such as [95]

$$\begin{aligned}
\frac{\partial}{\partial x} &= \frac{\partial w_i}{\partial x}\frac{\partial}{\partial w_i} + \frac{\partial z_i}{\partial x}\frac{\partial}{\partial z_i} + \frac{\partial \lambda_i}{\partial x}\frac{\partial}{\partial \lambda_i}, \\
&= \frac{\partial w_i}{\partial x}\frac{\partial}{\partial w_i} + \frac{\partial \lambda_i}{\partial x}\frac{\partial}{\partial \lambda_i}, \qquad (2.20)\\
\frac{\partial}{\partial y} &= \frac{\partial w_i}{\partial y}\frac{\partial}{\partial w_i} + \frac{\partial z_i}{\partial y}\frac{\partial}{\partial z_i} + \frac{\partial \lambda_i}{\partial y}\frac{\partial}{\partial \lambda_i}, \\
&= \frac{\partial w_i}{\partial y}\frac{\partial}{\partial w_i} + \frac{\partial \lambda_i}{\partial y}\frac{\partial}{\partial \lambda_i}, \qquad (2.21)\\
\frac{\partial}{\partial z} &= \frac{\partial w_i}{\partial z}\frac{\partial}{\partial w_i} + \frac{\partial}{\partial z_i} + \frac{\partial \lambda_i}{\partial z}\frac{\partial}{\partial \lambda_i}, \qquad (2.22)
\end{aligned}$$

Note that because $e^{ik_iz_i}\chi(\upsilon_i)$ is independent of λ_i, the operation $\frac{\partial}{\partial \lambda_i}$ makes no contribution. We recognize that

$$\begin{aligned}
z_i &= r_i \cos\theta, \\
r_i &= \sqrt{x^2 + y^2 + z^2}, \\
\frac{\partial w_i}{\partial x} &= \frac{x}{r_i}, \quad \frac{\partial w_i}{\partial y} = \frac{y}{r_i} \quad \textit{and} \quad \frac{\partial w_i}{\partial z} = -\frac{w_i}{r_i}.
\end{aligned}$$

We take the second derivative with respect to the x variable as

$$\begin{aligned}
\frac{\partial^2}{\partial x^2} &= \frac{x}{r_i}\frac{\partial}{\partial x}\left(\frac{\partial}{\partial w_i}\right) + \frac{\partial}{\partial x}\left(\frac{x}{r_i}\right)\frac{\partial}{\partial w_i}, \\
&= \frac{x}{r_i}\frac{\partial w_i}{\partial x}\frac{\partial}{\partial w_i}\left(\frac{\partial}{\partial w_i}\right) + \frac{\partial}{\partial x}\left(\frac{x}{\sqrt{x^2+y^2+z^2}}\right)\frac{\partial}{\partial w_i}, \qquad (2.23)\\
&= \frac{x^2}{r_i^2}\frac{\partial^2}{\partial w_i^2} + \left(\frac{1}{r_i} - \frac{x^2}{r_i^3}\right)\frac{\partial}{\partial w_i}.
\end{aligned}$$

Similarly, we have

$$\frac{\partial^2}{\partial y^2} = \frac{y^2}{r_i^2}\frac{\partial^2}{\partial w_i^2} + \left(\frac{1}{r_i} - \frac{y^2}{r_i^3}\right)\frac{\partial}{\partial w_i}. \tag{2.24}$$

We obtain the second order derivative with respect to the z variable as

$$\frac{\partial^2}{\partial z^2} = \frac{w_i^2}{r_i^2}\frac{\partial^2}{\partial w_i^2} + \left(\frac{w_i}{r_i^2} - \frac{w_i^2}{r_i^3}\right)\frac{\partial}{\partial w_i} - \frac{2w_i}{r_i}\frac{\partial^2}{\partial z_i \partial w_i} + \frac{w_i}{r_i^2}\frac{\partial}{\partial w_i} + \frac{\partial^2}{\partial z_i^2}. \tag{2.25}$$

Using equations (2.23),(2.24) we have

$$\begin{aligned}
\Phi_i(\vec{r}_i) &= e^{i\vec{k}_i\cdot\vec{r}_i}\chi(\upsilon_i) = e^{ik_iz_i}\chi(\upsilon_i), \\
I_1 &= \frac{\partial}{\partial w_i}\Phi_i(\vec{r}_i) = \frac{\partial}{\partial w_i}\left(e^{ik_iz_i}\chi(\upsilon_i)\right), \\
&= \frac{\partial}{\partial w_i}\left(e^{ik_i(r_i-w_i)}\right)\chi(\upsilon_i) + e^{ik_i(r_i-w_i)}\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i}\frac{\partial \upsilon_i}{\partial w_i}, \\
&= -ik_i\chi(\upsilon_i)e^{ik_i(r_i-w_i)} + ik_i\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}e^{ik_i(r_i-w_i)} \\
&= ik_ie^{ik_i(r_i-w_i)}\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right).
\end{aligned} \tag{2.26}$$

where $\frac{\partial \upsilon_i}{\partial w_i} = ik_i$. Now we let

$$\begin{aligned}
I_2 &= \frac{\partial}{\partial w_i}(I_1) = \frac{\partial}{\partial w_i}\left(-ik_i\chi(\upsilon_i)e^{ik_iz_i} + ik_i\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}e^{ik_iz_i}\right), \\
&= -ik_i\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}\frac{\partial\upsilon_i}{\partial w_i}e^{ik_iz_i} + (ik_i)^2\chi(\upsilon_i)e^{ik_iz_i} + ik_i\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}\frac{\partial\upsilon_i}{\partial w_i}e^{ik_iz_i} \\
&\quad - (ik_i)^2\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}e^{ik_iz_i}, \\
&= (ik_i)^2\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}e^{ik_iz_i} - 2(ik_i)^2\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}e^{ik_iz_i} + (ik_i)^2\chi(\upsilon_i)e^{ik_iz_i}, \\
&= -k_i^2e^{ik_i(r_i-w_i)}\left(\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2} - 2\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} + \chi(\upsilon_i)\right).
\end{aligned} \tag{2.27}$$

Substituting equations (2.26) and (2.27) into equation (2.23) we obtain

$$\begin{aligned}
\frac{\partial^2\Phi_i(\vec{r}_i)}{\partial x^2} &= -k_i^2\frac{x^2}{r^2}\left(\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2} - 2\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} + \chi(\upsilon_i)\right)e^{ik_i(r_i-w_i)} \\
&\quad + ik_i\left(\frac{1}{r_i} - \frac{x^2}{r_i^3}\right)\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right)e^{ik_i(r_i-w_i)},
\end{aligned} \tag{2.28}$$

and similary we obtain by substituting equation (2.26) and (2.27) into equation (2.24)

$$\begin{aligned}\frac{\partial^2\Phi_i(\vec{r}_i)}{\partial y^2} &= -k_i^2\frac{y^2}{r^2}\left(\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2} - 2\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} + \chi(\upsilon_i)\right)e^{ik_i(r_i-w_i)} \\ &\quad + ik_i\left(\frac{1}{r_i} - \frac{y^2}{r_i^3}\right)\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right)e^{ik_i(r_i-w_i)}.\end{aligned} \tag{2.29}$$

In the same manner, we substitute equation (2.26) and (2.27) into equation (2.25) as follows

$$\begin{aligned}\frac{\partial^2\Phi_i(\vec{r}_i)}{\partial z^2} &= -k_i^2\frac{w_i^2}{r_i^2}\left(\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2} - 2\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} + \chi(\upsilon_i)\right)e^{ik_i(r_i-w_i)} \\ &\quad + (ik_i)\left(\frac{w_i}{r_i^2} - \frac{w_i^2}{r_i^3}\right)\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right)e^{ik_i(r_i-w_i)} \\ &\quad - (ik_i)\frac{2w_i}{r_i}\frac{\partial}{\partial z_i}\left(\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i}\right) \\ &\quad + (ik_i)\frac{w_i}{r_i^2}\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i} + \frac{\partial^2}{\partial z_i^2}\left(e^{ik_iz_i}\chi(\upsilon_i)\right).\end{aligned} \tag{2.30}$$

We set

$$I_3 = \frac{\partial}{\partial z_i}\left(\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i}\right) \tag{2.31}$$

$$I_4 = \frac{\partial^2}{\partial z_i^2}\left(e^{ik_iz_i}\chi(\upsilon_i)\right). \tag{2.32}$$

From equations (2.31) and (2.32) we have that

$$\begin{aligned}I_3 &= (ik_i)\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i} + \left(\frac{\partial\upsilon_i}{\partial z_i}\frac{\partial}{\partial\upsilon_i}\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}\right)\right. \\ &\quad \left. - \frac{\partial\upsilon_i}{\partial z_i}\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}\right)e^{ik_iz_i}, \\ &= (ik_i)\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i} + \left(-(ik_i)\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2} + (ik_i)\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}\right)e^{ik_iz_i}, \\ &= -(ik_i)\left(\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2} - 2\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i} + \chi(\upsilon_i)\right)e^{ik_iz_i}.\end{aligned} \tag{2.33}$$

$$
\begin{aligned}
I_4 \quad &= \tfrac{\partial}{\partial z_i}\left(ik_i\chi(\upsilon_i)e^{ik_iz_i} + \tfrac{\partial \upsilon_i}{\partial z_i}\tfrac{\partial \chi(\upsilon_i)}{\partial \upsilon_i}e^{ik_iz_i}\right), \\
&= ik_i\tfrac{\partial}{\partial z_i}\left(\chi(\upsilon_i)e^{ik_iz_i} - \tfrac{\partial \chi(\upsilon_i)}{\partial \upsilon_i}e^{ik_iz_i}\right), \\
&= -k_i^2\left(\tfrac{\partial^2 \chi(\upsilon_i)}{\partial \upsilon_i^2} - 2\tfrac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} + \chi(\upsilon_i)\right)e^{ik_iz_i}.
\end{aligned}
\tag{2.34}
$$

Thus, by equations (2.33) and (2.34), equation (2.30) becomes

$$
\begin{aligned}
\frac{\partial^2 \Phi_i(\vec{r}_i)}{\partial z^2} &= -k_i^2\frac{w_i^2}{r_i^2}\left(\frac{\partial^2 \chi(\upsilon_i)}{\partial \upsilon_i^2} - 2\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} + \chi(\upsilon_i)\right)e^{ik_iz_i} \\
&\quad + (ik_i)\left(\frac{w_i}{r_i^2} - \frac{w_i^2}{r_i^3}\right)\left(\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i} \\
&\quad - k_i^2\frac{2w_i}{r_i}\left(\frac{\partial^2 \chi(\upsilon_i)}{\partial \upsilon_i^2} - 2\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} + \chi(\upsilon_i)\right)e^{ik_iz_i} \\
&\quad + (ik_i)\frac{w_i}{r_i^2}\left(\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i} \\
&\quad - k_i^2\left(\frac{\partial^2 \chi(\upsilon_i)}{\partial \upsilon_i^2} - 2\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} + \chi(\upsilon_i)\right)e^{ik_iz_i}, \\
&= -k_i^2\left(1 + \frac{2w_i}{r_i} + \frac{w_i^2}{r_i^2}\right)\left(\frac{\partial^2 \chi(\upsilon_i)}{\partial \upsilon_i^2} - 2\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} + \chi(\upsilon_i)\right)e^{ik_iz_i} \\
&\quad + (ik_i)\left(\frac{2w_i}{r_i^2} - \frac{w_i^2}{r_i^3}\right)\left(\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i},
\end{aligned}
$$

Finally we obtain

$$
\begin{aligned}
\frac{\partial^2 \Phi_i(\vec{r}_i)}{\partial z^2} &= -k_i^2\left(1 + \frac{w_i}{r_i}\right)^2\left(\frac{\partial^2 \chi(\upsilon_i)}{\partial \upsilon_i^2} - 2\frac{\partial \chi_i(\upsilon_i)}{\partial \upsilon_i} + \chi(\upsilon_i)\right)e^{ik_iz_i} \\
&\quad + (ik_i)\left(\frac{2w_i}{r_i^2} - \frac{w_i^2}{r_i^3}\right)\left(\frac{\partial \chi(\upsilon_i)}{\partial \upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i}.
\end{aligned}
\tag{2.35}
$$

Now adding equations (2.28), (2.29) and (2.35) produces

$$
\begin{aligned}
\nabla^2_{r_i}\Phi_i(\vec{r}_i) = &\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Phi_i(\vec{r}_i),\\
&= -k_i^2 A\Bigg(\frac{\partial^2\chi(\upsilon_i)}{\partial \upsilon_i^2} - 2\frac{\partial\chi(\upsilon_i)}{\partial \upsilon_i} + \chi(\upsilon_i)\Bigg)e^{ik_iz_i}\\
&\quad + ik_iB\Bigg(\frac{\partial\chi(\upsilon_i)}{\partial \upsilon_i} - \chi(\upsilon_i)\Bigg)e^{ik_iz_i},
\end{aligned}
\tag{2.36}
$$

where A and B are defined;

$$
\begin{aligned}
A &= \left(\frac{x^2}{r_i^2}+\frac{y^2}{r_i^2}+\left(1+\frac{w_i}{r_i}\right)^2\right)\\
B &= \left(\frac{2}{r_i}-\frac{x^2}{r_i^3}-\frac{y^2}{r_i^3}+\frac{2w_i}{r_i^2}-\frac{w_i^2}{r_i^3}\right).
\end{aligned}
$$

Thus, for $w = r - z$, we have

$$
\begin{aligned}
A &= \frac{x^2}{r_i^2}+\frac{y^2}{r_i^2}+\left(2-\frac{z_i}{r_i}\right)^2\\
&= \frac{x^2}{r_i^2}+\frac{y^2}{r_i^2}+\frac{y^2}{r_i^2}+4-4\frac{z_i}{r_i}\\
&= 1+\frac{4w_i}{r_i}.
\end{aligned}
\tag{2.37}
$$

$$
\begin{aligned}
B &= \frac{2}{r_i}-\frac{x^2}{r_i^3}-\frac{y^2}{r_i^3}+\frac{2w_i}{r_i^2}-\frac{(r_i-z_i)^2}{r_i^3}\\
&= \frac{2}{r_i}-\frac{x^2}{r_i^3}-\frac{y^2}{r_i^3}+\frac{2w_i}{r_i^2}-\frac{(r_i^2-2r_iz_i+z_i^2)}{r_i^3}\\
&= \frac{1}{r_i}+\frac{2w_i}{r_i^2}+\frac{2z_i}{r_i^2}-\frac{1}{r_i}\left(\frac{x^2}{r_i^2}+\frac{y^2}{r_i^2}+\frac{z_i^2}{r_i^2}\right)\\
&= \frac{2(r_i-z_i)}{r_i^2}+\frac{2z_i}{r_i^2}\\
&= \frac{2}{r_i}.
\end{aligned}
\tag{2.38}
$$

$$
\begin{aligned}
\nabla^2_{r_i}\Phi_i(\vec{r}_i) = &-k_i^2\left(1+\frac{4w_i}{r_i}\right)\left(\frac{\partial^2\chi(\upsilon_i)}{\partial \upsilon_i^2} - 2\frac{\partial\chi(\upsilon_i)}{\partial \upsilon_i} + \chi(\upsilon_i)\right)e^{ik_iz_i}\\
&+\frac{2ik_i}{r_i}\left(\frac{\partial\chi(\upsilon_i)}{\partial \upsilon_i} - \chi(\upsilon_i)\right)e^{ik_iz_i}.
\end{aligned}
\tag{2.39}
$$

Equation (2.39) is obtained by substituting equations (2.37) and (2.38) into equation (2.36).

Now, putting the bits and pieces together in equation (2.18) we have,

$$
\begin{aligned}
-k_i^2\left(1+\frac{4w_i}{r_i}\right)&\left(\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}-2\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}+\chi(\upsilon_i)\right)e^{i\vec{k}_i\cdot\vec{r}_i}\\
&+\frac{2ik_i}{r_i}\left(\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}-\chi(\upsilon_i)\right)e^{i\vec{k}_i\cdot\vec{r}_i}+k_i^2\chi(\upsilon_i)e^{i\vec{k}_i\cdot\vec{r}_i}\\
&+\frac{2\gamma_i k_i}{r_i}\chi(\upsilon_i)e^{i\vec{k}_i\cdot\vec{r}_i}=0,
\end{aligned}
$$

$$
\begin{aligned}
-k_i^2\left(1+\frac{4w_i}{r_i}\right)\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}&+\left(2k_i^2\left(1+\frac{4w_i}{r_i}\right)+\frac{2ik_i}{r_i}\right)\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}\\
&+\left(-k_i^2\left(1+\frac{4w_i}{r_i}\right)-\frac{2ik_i}{r_i}+k_i^2+\frac{2\gamma_i k_i}{r_i}\right)\chi(\upsilon_i)=0.
\end{aligned}
\tag{2.40}
$$

Using the fact that $\upsilon_i = ik_iw_i$, it follows that $ik_i = \frac{\upsilon_i}{w_i}$ and $k_i^2 = -\frac{\upsilon_i^2}{w_i^2}$, thus,

$$
\begin{aligned}
\frac{\upsilon_i^2}{w_i^2}\left(1+\frac{4w_i}{r_i}\right)\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}&+\left(-\frac{2\upsilon_i^2}{w_i^2}\left(1+\frac{4w_i}{r_i}\right)+\frac{2\upsilon_i}{r_iw_i}\right)\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}\\
&+\left(\frac{\upsilon_i^2}{w_i^2}\left(1+\frac{4w_i}{r_i}\right)-\frac{2\upsilon_i}{r_iw_i}-\frac{\upsilon_i^2}{w_i^2}-\frac{2i\gamma_i\upsilon_i}{r_iw_i}\right)\chi(\upsilon_i)=0,
\end{aligned}
$$

$$
\begin{aligned}
\upsilon_i\left(\frac{1}{w_i}+\frac{4}{r_i}\right)\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}&+\left(-2\upsilon_i\left(\frac{1}{w_i}+\frac{4}{r_i}\right)+\frac{2}{r_i}\right)\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}\\
&+\left(\upsilon_i\left(\frac{1}{w_i}+\frac{4}{r_i}\right)-\frac{2}{r_i}-\frac{\upsilon_i}{w_i}-\frac{2i\gamma_i}{r_i}\right)\chi(\upsilon_i)=0,
\end{aligned}
$$

$$\upsilon_i\left(\frac{1}{w_i}+\frac{4}{r_i}\right)\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}+\left(\frac{2}{r_i}-2\upsilon_i\left(\frac{1}{w_i}+\frac{4}{r_i}\right)\right)\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}$$
$$+\left(\frac{4\upsilon_i}{r_i}-\frac{2}{r_i}-\frac{2i\gamma_i}{r_i}\right)\chi(\upsilon_i)=0,$$

$$\upsilon_i\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}+\left(\frac{2w_i}{r_i+4w_i}-2\upsilon_i\right)\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}+\frac{2w_i}{r_i+4w_i}\left(2\upsilon_i-1-i\gamma_i\right)\chi(\upsilon_i)=0,$$

$$\upsilon_i\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}+\left(\frac{2r_i}{5r_i-4z_i}-\frac{2z_i}{5r_i-4z_i}-2\upsilon_i\right)\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}$$
$$+\left(\frac{2w_i}{r_i+4w_i}(2\upsilon_i-1)-\left(\frac{2r_i}{r_i-4z_i}\right)i\gamma_i\right)\chi(\upsilon_i)=0. \tag{2.41}$$

Now for $r\to\infty$ equation (2.41) is represented as follows,

$$\upsilon_i\frac{\partial^2\chi(\upsilon_i)}{\partial\upsilon_i^2}+\left(\frac{2}{5}-2\upsilon_i\right)\frac{\partial\chi(\upsilon_i)}{\partial\upsilon_i}-\frac{2}{5}i\gamma_i\chi(\upsilon_i)=0$$

Thus, absorbing the coefficients of $2\upsilon_i\rightsquigarrow\upsilon_i$, $\frac{2}{5}\gamma_i\rightsquigarrow\gamma_i$ and setting $\rho=\frac{2}{5}$ the results above become

$$\upsilon_i\frac{\partial^2\chi_i(\upsilon_i)}{\partial\upsilon_i^2}+(\rho-\upsilon_i)\frac{\partial\chi_i(\upsilon_i)}{\partial\upsilon_i}-i\gamma_i\chi_i(\upsilon_i)=0 \tag{2.42}$$

We solve the second order differential equation above by considering the asymptotic case-that is, solusions for large r_i-z_i (away from the forward direction, since $r_i-z_i=r_i(1-\cos\theta)=0$ for $\theta=0$). Considering the two solutions (1) $\chi\sim\upsilon_i^\lambda$ and (2) $\chi\sim e^{\upsilon_i}$, we substitute the first part into equation (2.42) as

$$\upsilon_i\left(\lambda(\lambda-1)\upsilon_i^{\lambda-2}\right)+\lambda(\rho-\upsilon_i)\upsilon_i^{\lambda-1}-i\gamma_i\upsilon_i^\lambda=0$$
$$\lambda(\lambda-1+\rho)\upsilon_i^{\lambda-1}+(-\lambda-i\gamma_i)\upsilon_i^\lambda=0.$$

Thus, λ values are computed as follows,

$$(-\lambda-i\gamma_i)\upsilon_i^\lambda\simeq 0\qquad and\qquad \lambda=-i\gamma_i \tag{2.43}$$
$$\lambda(\lambda-1+\rho)\upsilon_i^{\lambda-1}\simeq 0\qquad and\qquad \lambda=0.\qquad \lambda=1-\rho. \tag{2.44}$$

Of interest to us is the case where $\lambda = -i\gamma_i$ and hence we have the relation,

$$\begin{aligned}
\chi(\upsilon_i) &\sim \upsilon_i^{\lambda} \sim e^{-i\gamma_i \ln k_i(r_i - z_i)} \\
\upsilon_i &= ik_i(r_i - z_i) = i(k_i r_i - \vec{k}_i \cdot \vec{r}_i) \\
\chi(\upsilon_i) &\sim \upsilon_i^{\lambda} \sim e^{-i\gamma_i \ln(k_i r_i - \vec{k}_i \cdot \vec{r}_i)}. \qquad (2.45)
\end{aligned}$$

Substituting equation (2.45) into (2.19), the resulting wavefunction to the differential equation (2.18) is given by

$$\phi_i(\vec{r}_i) = e^{i\vec{k}_i . \vec{r}_i - i\gamma_i \ln(k_i r_i - \vec{k}_i \cdot \vec{r}_i)} \qquad (2.46)$$

Finally, the asymptotic solution to the differential equation governing the entrance channel (2.14) will be given in the form,

$$\Phi_i^+ \equiv \Phi_i^c(r_i \to \infty) = \varphi_i(\vec{x}_1, \vec{x}_2) e^{i\vec{k}_i . \vec{r}_i - i\gamma_i \ln(k_i r_i - \vec{k}_i \cdot \vec{r}_i)}. \qquad (2.47)$$

Alternatively, the second order differential equation (2.42) has a regular singular point and thus, we can resort to the Frobenius power series method of solution for $\chi_i(\upsilon_i)$. Assuming a solution of the type

$$\chi_i(\upsilon_i) = \upsilon_i^{\beta} \sum_{n=0}^{\infty} a_n \upsilon_i^n = \sum_{n=0}^{\infty} a_n \upsilon_i^{\beta+n} \qquad (2.48)$$

the corresponding derivatives are as follows;

$$\begin{aligned}
\frac{d\chi_i(\upsilon_i)}{d\upsilon_i} &= \sum_{n=0}^{\infty} (\beta + n) a_n \upsilon_i^{\beta+n-1} \qquad (2.49) \\
\frac{d^2\chi_i(\upsilon_i)}{d\upsilon_i^2} &= \sum_{n=0}^{\infty} (\beta + n)(\beta + n - 1) a_n \upsilon_i^{\beta+n-2} \qquad (2.50)
\end{aligned}$$

We substitute equations (2.48) – (2.50) into equation (2.42),

$$\sum_{n=0}^{\infty} (\beta + n)(\beta + n - 1) a_n \upsilon_i^{\beta+n-1} + (\rho - \upsilon_i) \sum_{n=0}^{\infty} (\beta + n) a_n \upsilon_i^{\beta+n-1} \\
- i\gamma_i \sum_{n=0}^{\infty} a_n \upsilon_i^{\beta+n} = 0,$$

$$\sum_{n=0}^{\infty}(\beta + n)(\beta + n + \rho - 1)a_n\upsilon_i^{\beta+n-1} - \sum_{n=0}^{\infty}(\beta + n + i\gamma_i)a_n\upsilon_i^{\beta+n} = 0,$$

$$\beta(\beta+\rho-1)a_0\upsilon_i^{\beta-1} + \sum_{n=1}^{\infty}(\beta+n)(\beta+n+\rho-1)a_n\upsilon_i^{\beta+n-1} - \sum_{n=0}^{\infty}(\beta+n+i\gamma_i)a_n\upsilon_i^{\beta+n} = 0,$$

$$\beta(\beta+\rho-1)a_0\upsilon_i^{\beta-1} + \sum_{n=0}^{\infty}\Big[(\beta+n+1)(\beta+n+\rho)a_{n+1} - (\beta+n+i\gamma_i)a_n\Big]\upsilon_i^{\beta+n} = 0. \tag{2.51}$$

Equating the coefficients of υ_i and higher order terms to zero we have respectively the indicial and recurrence equations as follows;

$$\beta(\beta+\rho-1)a_0 = 0, \quad \textit{implies} \quad \textit{that} \quad \beta = 0 \quad \textit{and} \quad \beta = 1-\rho, \tag{2.52}$$

$$(\beta+n+1)(\beta+n+\rho)a_{n+1} - (\beta+n+i\gamma_i)a_n = 0$$

$$a_{n+1} = \frac{(\beta+n+i\gamma_i)}{(\beta+n+1)(\beta+n+\rho)}a_n. \tag{2.53}$$

We are particularly interested in the case when $\beta = 0$, and setting $\eta_i = i\gamma_i$ gives the recurrence formula,

$$a_{n+1} = \frac{(\eta_i+n)}{(n+1)(\rho+n)}a_n. \tag{2.54}$$

$$\begin{aligned}
a_1 &= \frac{\eta_i}{1!\rho}a_0, \quad for \quad n=0,\\
a_2 &= \frac{\eta_i(\eta_i+1)}{2!\rho(\rho+1)}a_0, \quad for \quad n=1,\\
a_3 &= \frac{\eta_i(\eta_i+1)(\eta_i+2)}{3!\rho(\rho+1)(\rho+2)}a_0, \quad for \quad n=2,\\
&\vdots\\
a_n &= \frac{\eta_i(\eta_i+1)(\eta_i+2)\cdots(\eta_i+n-1)}{n!\rho(\rho+1)(\rho+2)\cdots(\rho+n-1)}a_0.
\end{aligned}$$

Thus, solution is represented as follows;

$$\begin{aligned}\chi_i(\upsilon_i) &= a_0 + a_0 \sum_{n=0}^{\infty} \frac{\eta_i(\eta_i+1)(\eta_i+2)\cdots(\eta_i+n-1)}{n!\rho(\rho+1)(\rho+2)\cdots(\rho+n-1)}\upsilon_i^n, \\ &= a_0\left(1+\frac{\eta_i}{1!\rho}\upsilon_i+\frac{\eta_i(\eta_i+1)}{2!\rho(\rho+1)}\upsilon_i^2+\frac{\eta_i(\eta_i+1)(\eta_i+2)}{3!\rho(\rho+1)(\rho+2)}\upsilon_i^3+\cdots\right) \quad (2.55)\end{aligned}$$

It is obvious that $\chi_i(\upsilon_i)$ is a solution of the confluent hpergeometric series described by ${}_1F_1(\eta_i, \rho; \upsilon_i)$ [96].

$${}_1F_1(\eta_i,\rho;\upsilon_i) = M(\eta_i,\rho;\upsilon_i) = a_0\left(1+\frac{\eta_i}{1!\rho}\upsilon_i+\frac{\eta_i(\eta_i+1)}{2!\rho(\rho+1)}\upsilon_i^2+\cdots\right). \quad (2.56)$$

The wavefunction governing the unperturbed state in equation (2.15) becomes,

$$\begin{aligned}\phi_i(\vec{r}_i) &= e_1^{i\vec{k}_i.\vec{r}_i}F_1(\eta_i,\rho;\upsilon_i), \\ &= a_0e^{i\vec{k}_i.\vec{r}_i}\left(1+\frac{\eta_i}{1!\rho}\upsilon_i+\frac{\eta_i(\eta_i+1)}{2!\rho(\rho+1)}\upsilon_i^2+\cdots\right),\end{aligned}$$

$$\Phi_i^c(\vec{r}_i\to\infty) = a_0\varphi_i(\vec{x}_1,\vec{x}_2)e^{i\vec{k}_i\cdot\vec{r}_i}\left(1+\frac{\eta_i}{1!\rho}\upsilon_i+\frac{\eta_i(\eta_i+1)}{2!\rho(\rho+1)}\upsilon_i^2+\cdots\right). \quad (2.57)$$

2.3 The exit channel

In this section we discuss the exit channel in respect of section 2.1. In analogy to the vector $\vec{r}_i$ introduced earlier, we can also consider $\vec{r}_f$ as the position vector of T with respect to the center of mass of the system $(Z_P; e_1, e_2)_f$ via

$$\vec{r}_f = \vec{r}_2 - \frac{\vec{r}_3+\vec{r}_4+M_P\vec{r}_1}{M_P+2}.$$

With this, the Hamiltonian $\hat{H}_0$ can be written in terms of the independent variables $(\vec{s}_1, \vec{s}_2, \vec{r}_f)$ as

$$\hat{H}_0 = -\frac{1}{2\mu_f}\nabla_{r_f}^2 - \frac{1}{2a}\nabla_{s_1}^2 - \frac{1}{2a}\nabla_{s_2}^2 - \frac{1}{M_P}\vec{\nabla}_{s_1}\cdot\vec{\nabla}_{s_2} \quad (2.58)$$

where

$$\mu_f = \frac{M_T(M_P+2)}{M_P+M_T+2}.$$

The mass polarization term $\frac{1}{M_P}\vec{\nabla}_{s_1}\cdot\vec{\nabla}_{s_2}$ can be omitted in accordance with the mass limit $M_P \gg 1$ for heavy particles. As a matter of convenience we write the total Hamiltonian in a separate form as

$$\hat{H} = \hat{H}_f + V_f,$$

where the channel Hamiltonian H_f and the corresponding perturbation V_f are defined via

$$\begin{aligned}
\hat{H}_f &= \hat{H}_0 - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} + \frac{1}{r_{12}}, \\
V_f &= \frac{Z_P Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2}.
\end{aligned} \tag{2.59}$$

We introduce the unperturbed state Φ_f in the exit channel for double-charge exchange as the solution of the eigenproblem

$$\begin{gathered}
\left(\hat{H}_f - E_f\right)\Phi_f = 0, \\
\Phi_f = \varphi_f(\vec{s}_1, \vec{s}_2)e^{-i\vec{k}_f.\vec{r}_f},
\end{gathered} \tag{2.60}$$

where $\varphi_f(\vec{s}_1, \vec{s}_2)$ is the bound state of the heliumlike atom or ion $(Z_P; e_1, e_2)_f$. This function statisfies the eigenproblem

$$\left(\hat{h}_f - \epsilon_f\right)\varphi_f(\vec{s}_1, \vec{s}_2) = 0$$

or, explicitly,

$$\left(-\frac{1}{2a}\nabla^2_{s_1} - \frac{1}{2a}\nabla^2_{s_2} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} + \frac{1}{r_{12}} - \epsilon_f\right)\varphi_f(\vec{s}_1, \vec{s}_2) = 0 \tag{2.61}$$

where ϵ_f is the binding energy of the final state. Conservation of energy of the entire four-body system requires

$$E_f = \frac{k_f^2}{2\mu_f} + \epsilon_f = E_i = E$$

where $\vec{k}_f$ is the final wave vector.

The final state is distorted even at asymptotically large separations due to the presence of an overall repulsive long-range Coulomb interaction between the target nucleus and the screened projectile $V_f^\infty = \frac{Z_T(Z_P-2)}{R}$. This suggests that the Hamiltonian should be written in the following additive form

$$\begin{aligned}
\hat{H} &= \hat{H}_f^c + V_f^c, \\
\hat{H}_f^c &= -\frac{1}{2\mu_f}\nabla_{r_f}^2 + \frac{Z_T(Z_P-2)}{r_f} - \frac{1}{2a}\nabla_{s_1}^2 - \frac{1}{2a}\nabla_{s_2}^2 - \frac{Z_P}{s_1} \\
&\quad - \frac{Z_P}{s_2} + \frac{1}{r_{12}}, \\
V_f^c &= \frac{Z_P Z_T}{R} - \frac{Z_T(Z_P-2)}{r_f} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2}.
\end{aligned} \tag{2.62}$$

Neglecting the terms of the order of $\frac{1}{M_P}$, we have $\vec{r}_f \simeq -\vec{R}$ or $r_f \simeq R$, so that V_f^c is reduced to

$$V_f^c = \frac{2Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} \tag{2.63}$$

The potential V_f^c is of a short-range, since it tends to $\vartheta(\frac{1}{R^2})$ when $R \to \infty$. We recall that

$$V_f = \frac{Z_P Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} \to \frac{Z_T(Z_P-2)}{R} = V_f^\infty \tag{2.64}$$

as $r_f \to \infty$.

$$\begin{aligned}
\left(\nabla_{r_f}^2 + 2\mu_f E_f - \frac{2\mu_f Z_T(Z_P-2)}{r_f}\right)\phi_f(\vec{r}_f) = 0 \\
\left(\nabla_{r_f}^2 + k_f^2 + \frac{2\gamma_f k_f}{r_f}\right)\phi_f(\vec{r}_f) = 0.
\end{aligned} \tag{2.65}$$

$$where, \quad k_f^2 = 2\mu_f E_f, \quad -\gamma_f k_f = Z_T(Z_P-2)\mu_f \quad and \quad \mu_f = \frac{M_T(M_P+2)}{M_P+M_T+2}.$$

Similarly, the solution to the eigenproblem $(\hat{H}_f^c - E_f)\Phi_f^c = 0$ is given by

$$\begin{aligned}
\Phi_f^c(\vec{r}_f) &= \varphi_f(\vec{s}_1, \vec{s}_2)\phi_f(\vec{r}_f), \\
\phi_f(\vec{r}_f) &= e^{-i\vec{k}_f\cdot\vec{r}_f}\chi(\upsilon_f),
\end{aligned}$$

and so we have the asymptotic wavefunction in the entrance channel as

$$\Phi_f^- \equiv \Phi_f^c(r_f \to \infty) = \varphi_f(\vec{s}_1, \vec{s}_2) e^{-i\vec{k}_f.\vec{r}_f - i\gamma_f \ln(k_f r_f - \vec{k}_f \cdot \vec{r}_f)}, \tag{2.66}$$

and its series analog solution is

$$\Phi_f^c(\vec{r}_f \to \infty) = a_0 \varphi_f(\vec{s}_1, \vec{s}_2) e^{i\vec{k}_f \cdot \vec{r}_f} \left(1 + \frac{\eta_f}{1!\rho} \upsilon_f + \frac{\eta_f(\eta_f + 1)}{2!\rho(\rho + 1)} \upsilon_f^2 + \cdots \right). \tag{2.67}$$

This obeys the correct boundary conditions in the exit channel.

Chapter 3

Perturbation theory

3.1 Perturbation series with the correct boundary conditions

We are more careful to impose the proper Coulomb boundary conditions on the entrance and exit channels for ion-atom collisions. Disregarding this requirement, can lead to serious problems, and such models are inadequate for a description of experimental findings.

The dynamics of the entire four-body system are described by means of the Schrödinger equation

$$(\hat{H} - E)\Psi^{\pm} = 0,$$

where $\Psi^{\pm}$ are the full scattering states with the outgoing or incoming boundary conditions

$$\Psi^{+} \to \Phi_i^{+}(r_i \to \infty), \quad \Psi^{-} \to \Phi_i^{-}(r_i \to \infty). \tag{3.1}$$

The exact transition amplitude with the correct boundary conditions can be written in the *post*(+) and *prior*(−) [1] forms as

$$T_{if}^{+} = \langle \Phi_f^{-} | V_f^{c} | \Psi_i^{+} \rangle, \quad T_{if}^{-} = \langle \Psi_f^{-} | V_i^{c} | \Phi_i^{+} \rangle \tag{3.2}$$

Both forms are equivlent to each other on the energy shell, i.e; the exact expressions are equal, $T_{if}^{+} = T_{if}^{-}$, for transitions for which the total energy is conserved [66].

Solving a scattering problem in which four bodies take part (two nuclei and two electrons) is extremely difficult. As usual, at intermediate and high impact energies, the perturbation procedure is frequently employed. It is convenient to convert Schrödinger equation for a four-body problem into its corresponding integral representation such as the *Lippman-Schwinger* equations.

3.2 The Lippman-Schwinger equations for four-body collisions

The notation used here can be traced to [1] for the standard formalism of the Lippman-Schwinger Equations. We introduce the function

$$\Psi_i^{+} \equiv i\epsilon G^{+}\Phi_i^{+} \tag{3.3}$$

where Φ_i^{+} is the wave function defined by Equation (2.47). Here ϵ is an infinitesimally small positive number. In addition to the total Green's function $G^{\pm}$ in Equation (3.3), we also define the initial $G_i^{\pm}$, the final $G_f^{\pm}$, and the free Green's functions $G_0^{\pm}$ as

$$G^{\pm} = (E - \hat{H} \pm i\epsilon)^{-1}; \quad G_i^{\pm} = (E - \hat{H}_i \pm i\epsilon)^{-1}$$
$$G_f^{\pm} = (E - \hat{H}_f \pm i\epsilon)^{-1}; \quad G_0^{\pm} = (E - \hat{H}_0 \pm i\epsilon)^{-1}$$

These propagators are interrelated by the following Lippman-Schwinger integral equations for the total Green's functions.

$$\begin{aligned} G^{\pm} &= G_i^{\pm} + G_i^{\pm} V_i^c G^{\pm}, \\ G^{\pm} &= G_f^{\pm} + G_f^{\pm} V_f^c G^{\pm}, \\ G^{\pm} &= G_0^{\pm} + G_0^{\pm} V^c G^{\pm}. \end{aligned} \tag{3.4}$$

Thus, for $G^{\pm} = G_i^{\pm} + G_i^{\pm} V_i^c G^{\pm}$ we multiply from the left by $E - \hat{H}_i^c \pm i\epsilon$ and simultaneously from the right by $E - \hat{H} \pm i\epsilon$. It follows that $E - \hat{H}_i^c \pm i\epsilon = E - \hat{H} \pm i\epsilon + V_i^c$, is in agreement with Equation (3.3). We apply iteration procedures to Equation (3.4) to obtain the following expansions for the total Green's function in terms of G_0^+, G_i^+ and G_f^+.

$$
\begin{aligned}
G^+ &= G_0^+ + G_0^+ V G^+ \\
&= G_0^+ + G_0^+ V [G_0^+ + G_0^+ V G^+] \\
&= G_0^+ + G_0^+ V G_0^+ + G_0^+ V G_0^+ V G^+ \\
&= G_0^+ + G_0^+ V G_0^+ + G_0^+ V G_0^+ V [G_0^+ + G_0^+ V G^+] \\
&= G_0^+ + G_0^+ V G_0^+ + G_0^+ V G_0^+ V G_0^+ + G_0^+ V G_0^+ V G_0^+ V G_0^+ \ldots
\end{aligned}
\tag{3.5}
$$

Similarly, we obtain for G_i^+ and G_f^+;

$$
G^+ = G_i^+ + G_i^+ V_i^c G_i^+ + G_i^+ V_i^c G_i^+ V_i^c G_i^+ + G_i^+ V_i^c G_i^+ V_i^c G_i^+ V_i^c G_i^+ \ldots \tag{3.6}
$$

and

$$
G^+ = G_f^+ + G_f^+ V_f^c G_f^+ + G_f^+ V_f^c G_f^+ V_f^c G_f^+ + G_f^+ V_f^c G_f^+ V_f^c G_f^+ V_f^c G_f^+ \ldots \tag{3.7}
$$

Now, inserting $G^{\pm}$ from Equation (3.5) into (3.3), we have

$$
\begin{aligned}
\Psi_i^+ = i\epsilon G^+ \Phi_i^+ &= i\epsilon [G_i^+ + G_i^+ V G^+] \Phi_i^+ \\
&= i\epsilon G_i^+ \Phi_i^+ + G_i^+ V_i^c i\epsilon G^+ \Phi_i^+ \\
&= i\epsilon G_i^+ \Phi_i^+ + G_i^+ V_i^c \Psi_i^+
\end{aligned}
\tag{3.8}
$$

where we write the first term as $i\epsilon G_i^+ \Phi_i^+ = \Phi_i^+$. This can be directly verified if $\frac{i\epsilon}{E - \hat{H}_i^c + i\epsilon} \Phi_i^+ = \Phi_i^+$ is multiplied from the left by $E - \hat{H}_i^c + i\epsilon$. Thus, we have $i\epsilon \Phi_i^+ = (E - \hat{H}_i^c + i\epsilon) \Phi_i^+$, in agreement with Equation (3.3). By this, we obtain the Lippman-Schwinger equation for total scattering wave function in the case of a four-body problem.

$$
\begin{aligned}
\Psi_i^+ &= \Phi_i^+ + G_i^+ V_i^c \Psi_i^+, \\
&= \Phi_i^+ + \frac{1}{(E - \hat{H}_i \pm i\epsilon)} V_i^c \Psi_i^+.
\end{aligned}
\tag{3.9}
$$

This is an inhomogeneous integral equation, since it contains explicitly the incident wave Φ_i^+. The integral equation (3.9) can formally be solved iteratively as

$$\begin{aligned}
\Psi_i^+ &= \Phi_i^+ + G_i^+ V_i^c \Psi_i^+ \\
&= \Phi_i^+ + G_i^+ V_i^c [\Phi_i^+ + G_i^+ V_i^c \Psi_i^+] \\
&= \Phi_i^+ + G_i^+ V_i^c \Phi_i^+ + G_i^+ V_i^c G_i^+ V_i^c \Psi_i^+ \\
&= \Phi_i^+ + G_i^+ V_i^c \Phi_i^+ + G_i^+ V_i^c G_i^+ V_i^c [\Phi_i^+ + G_i^+ V_i^c \Psi_i^+] \\
&= \Phi_i^+ + G_i^+ V_i^c \Phi_i^+ + G_i^+ V_i^c G_i^+ V_i^c \Phi_i^+ + G_i^+ V_i^c G_i^+ V_i^c G_i^+ V_i^c \Psi_i^+ \\
&= (1 + G_i^+ V_i^c + G_i^+ V_i^c G_i^+ V_i^c + G_i^+ V_i^c G_i^+ V_i^c G_i^+ V_i^c \dots) \Phi_i^+ \\
&= \left(1 + \sum_{n=1}^{\infty} (G_i^+ V_i^c)^n\right) \Phi_i^+ = (1 + G^+ V_i^c) \Phi_i^+. \qquad (3.10)
\end{aligned}$$

This is the case because, if we multiply Equation(3.5) by V_i^c, we obtain

$$\begin{aligned}
G^+ V_i^c &= G_i^+ V_i^c + G_i^+ V_i^c G_i^+ V_i^c + G_i^+ V_i^c G_i^+ V_i^c G_i^+ V_i^c \dots \\
&= \sum_{n=1}^{\infty} (G_i^+ V_i^c)^n. \qquad (3.11)
\end{aligned}$$

Hence, the formal solution of the Lippman-Schwinger equation [90] in terms of the total Green's function G^+ is

$$\Psi_i^+ = \Phi_i^+ + G^+ V_i^c \Phi_i^+ = (1 + G^+ V_i^c) \Phi_i^+. \qquad (3.12)$$

3.3 The Born expansions with the correct boundary conditions for four-body collisions

Inserting the formal solution equation (3.12) into Equation (3.2) for the post form of the transition amplitude, it follows that

$$\begin{aligned} T_{if}^{+} &= \langle \Phi_f^- | V_f^c | \Psi_i^+ \rangle \\ &= \langle \Phi_f^- | V_f^c | (1 + G^+ V_i^c) \Phi_i^+ \rangle \\ &= \langle \Phi_f^- | V_f^c (1 + G^+ V_i^c) | \Phi_i^+ \rangle \end{aligned} \tag{3.13}$$

Thus, by substituting G^+ from Equation (3.5) into Equation (3.13), we can write several different versions of the Born expansion with the correct boundary conditions as

$$\begin{aligned} T_{if}^{+} &= \langle \Phi_f^- | V_f^c (1 + G_0^+ V_i^c + G_0^+ V G_0^+ V_i^c + \ldots) | \Phi_i^+ \rangle \\ &= \langle \Phi_f^- | V_f^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_0^+ V_i^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_0^+ V G_0^+ V_i^c | \Phi_i^+ \rangle + \ldots \\ &= T_{if}^{(CB1)+} + \langle \Phi_f^- | V_f^c G_0^+ V_i^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_0^+ V G_0^+ V_i^c | \Phi_i^+ \rangle + \ldots \end{aligned}$$

$$\begin{aligned} T_{if}^{+} &= \langle \Phi_f^- | V_f^c (1 + G_i^+ V_i^c + G_i^+ V_i^c G_i^+ V_i^c + \ldots) | \Phi_i^+ \rangle \\ &= \langle \Phi_f^- | V_f^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_i^+ V_i^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_i^+ V_i^c G_i^+ V_i^c | \Phi_i^+ \rangle + \ldots \\ &= T_{if}^{(CB1)+} + \langle \Phi_f^- | V_f^c G_i^+ V_i^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_i^+ V_i^c G_i^+ V_i^c | \Phi_i^+ \rangle + \ldots \end{aligned}$$

$$\begin{aligned} T_{if}^{+} &= \langle \Phi_f^- | V_f^c (1 + G_f^+ V_i^c + G_f^+ V_f^c G_f^+ V_i^c + \ldots) | \Phi_i^+ \rangle \\ &= \langle \Phi_f^- | V_f^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_f^+ V_i^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_f^+ V_f^c G_f^+ V_i^c | \Phi_i^+ \rangle + \ldots \\ &= T_{if}^{(CB1)+} + \langle \Phi_f^- | V_f^c G_f^+ V_i^c | \Phi_i^+ \rangle + \langle \Phi_f^- | V_f^c G_f^+ V_f^c G_f^+ V_i^c | \Phi_i^+ \rangle + \ldots \end{aligned}$$

Here $T_{if}^{(CB1)+}$ is the post form of the *First Born-Approximation* with the correct boundary conditons for four-body collisions, i.e the CB1-4B method. It is easily seen that, the term $T_{if}^{(CB1)+}$ is identical in all versions. In other words, the CB1-4B method is obtained by replacing the total wave function Ψ_i^+ by the asymptotic channel state Φ_i^+. Two methods for an explicit calculation of the matrix elements in the CB1-4B method for double-charge exchange have been devised and implemented in [67][68].

Likewise, the n^{th} Born approximation with the correct boundary conditions (CBn-4B) may be obtained by keeping the first n terms in the expansion. Of great interest is the four-body second Born approximation (CB2-4B). It is obtained this way

$$T_{if;0}^{(CB2)+} = T_{if}^{(CB1)+} + \langle \Phi_f^- | V_f^c G_0^+ V_i^c | \Phi_i^+ \rangle, \tag{3.14}$$

$$T_{if;i}^{(CB2)+} = T_{if}^{(CB1)+} + \langle \Phi_f^- | V_f^c G_i^+ V_i^c | \Phi_i^+ \rangle, \tag{3.15}$$

$$T_{if;f}^{(CB2)+} = T_{if}^{(CB1)+} + \langle \Phi_f^- | V_f^c G_f^+ V_i^c | \Phi_i^+ \rangle. \tag{3.16}$$

We note that Equation (3.14) in terms of G_0^+ is recognized as an extension of the corresponding three-body second Born approximation with the correct boundary conditions (CB2-3B) of Belkić [97][98][66]. Of course, many other versions of the Born exapnsion can be formulated by utilizing various possible iterative solutions for G^+. In other words, a unique Born series of the transition amplitude T_{if}^+ does not exist.

We may embark on a similar procedure employed for the prior form of the transition amplitude. That is, the time independent wave function of the whole system in the exit channel is given by the following integral form.

$$\Psi_f^- = \Phi_f^- + G^- V_f^c \Psi_f^- = (1 + G^- V_f^c)\Phi_f^-.$$

The corresponding prior form of the transition amplitude is given as

$$T_{if}^- = \langle \Phi_f^- | (1 + G^+ V_f^c) V_i^c | \Phi_i^+ \rangle.$$

Chapter 4

Calculation

4.1 The CB1-4B method

Several investigations and comparisons have confirmed that the CB1-3B method is an accurate theory for rearrangement of intermediate and high impact energies. However, it is natural to extend this approximation to four-body collisions. Belkić [68] through the introduction of CB1-4B method has solved the problem of double-charge exchange which is in conformity with experiment. The transition amplitudes in the CB1-4B method for double-charge exchange within the prior (T_{if}^{-}) and post (T_{if}^{+}) forms are given by

$$T_{if}^{-} = \langle \Phi_f^{-} | V_i^c | \Phi_i^{+} \rangle \qquad T_{if}^{+} = \langle \Phi_f^{-} | V_f^c | \Phi_i^{+} \rangle.$$

We refer to Φ_i^{+} and Φ_f^{-} defined by Equations (2.47), (2.66) and V_i^c ,V_f^c respectively by Equations (2.12) and (2.63). Calculation of the transition amplitudes [1] are as follows;

$$
\begin{aligned}
T_{if}^{+} &= \langle \Phi_f^{-} | V_f^c | \Phi_i^{+} \rangle \\
&= \int\int\int \varphi_f^*(\vec{s}_1, \vec{s}_2) e^{i\vec{k}_f.\vec{r}_f + i\nu_f ln(k_f r_f - \vec{k}_f.\vec{r}_f)} \left(\frac{2Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} \right) \\
&\quad \times \varphi_i(\vec{x}_1, \vec{x}_2) e^{i\vec{k}_i.\vec{r}_i + i\nu_i ln(k_i r_i - \vec{k}_i.\vec{r}_i)} \, d\vec{R} \, d\vec{x}_1 \, d\vec{x}_2 \\
&= Z_T \int\int\int \varphi_f^*(\vec{s}_1, \vec{s}_2) e^{i\vec{k}_f.\vec{r}_f + i\vec{k}_i.\vec{r}_i} e^{i\nu_f ln(k_f r_f - \vec{k}_f.\vec{r}_f) + i\nu_i ln(k_i r_i - \vec{k}_i.\vec{r}_i)} \\
&\quad \times \left(\frac{2}{R} - \frac{1}{x_1} - \frac{1}{x_2} \right) \varphi_i(\vec{x}_1, \vec{x}_2) \, d\vec{R} \, d\vec{x}_1 \, d\vec{x}_2 \\
&= Z_T \int\int\int \varphi_f^*(\vec{s}_1, \vec{s}_2) e^{-2i\vec{q}_P.\vec{R} - i\vec{\varphi}.(\vec{x}_1, \vec{x}_2)} e^{i\nu_f ln(k_f r_f - \vec{k}_f.\vec{r}_f) + i\nu_i ln(k_i r_i - \vec{k}_i.\vec{r}_i)} \\
&\quad \times \left(\frac{2}{R} - \frac{1}{x_1} - \frac{1}{x_2} \right) \varphi_i(\vec{x}_1, \vec{x}_2) \, d\vec{R} \, d\vec{x}_1 \, d\vec{x}_2 \\
&= \int d\vec{R} e^{-2i\vec{q}_P.\vec{R}} e^{i\nu_f ln(k_f r_f - \vec{k}_f.\vec{r}_f) + i\nu_i ln(k_i r_i - \vec{k}_i.\vec{r}_i)} \\
&\quad \times Z_T \int\int d\vec{x}_1 \, d\vec{x}_2 \varphi_f^*(\vec{s}_1, \vec{s}_2) e^{-i\vec{\varphi}.(\vec{x}_1, \vec{x}_2)} \left(\frac{2}{R} - \frac{1}{x_1} - \frac{1}{x_2} \right) \varphi_i(\vec{x}_1, \vec{x}_2)
\end{aligned}
$$

Thus we have,

$$
\begin{aligned}
T_{if}^{+} &= \int d\vec{R} e^{-2i\vec{q}_P.\vec{R}} e^{i\nu_f ln(k_f r_f - \vec{k}_f.\vec{r}_f) + i\nu_i ln(k_i r_i - \vec{k}_i.\vec{r}_i)} F^{+}(\vec{R}) \\
F^{+}(\vec{R}) &= Z_T \int\int d\vec{x}_1 \, d\vec{x}_2 \varphi_f^*(\vec{s}_1, \vec{s}_2) e^{-i\vec{\varphi}.(\vec{x}_1, \vec{x}_2)} \left(\frac{2}{R} - \frac{1}{x_1} - \frac{1}{x_2} \right) \\
&\quad \times \varphi_i(\vec{x}_1, \vec{x}_2)
\end{aligned} \tag{4.1}
$$

4.2 The CB2-4B method

In order to perform the explicit calculations of the matrix elements, we shall presently choose the bound-state wave functions $\varphi_{i,f}$ in the form of the one-parameter Hylleraas orbitals [99],

$$\begin{aligned}\varphi_i(\vec{x}_1,\vec{x}_2) &= \psi_\alpha(\vec{x}_1)\psi_\alpha(\vec{x}_2),\\ \varphi_f(\vec{s}_1,\vec{s}_2) &= \psi_\beta(\vec{s}_1)\psi_\beta(\vec{s}_2),\end{aligned} \tag{4.2}$$

with the corresponding appropriate binding energies $\epsilon_i = -\alpha^2$, $\epsilon_f = -\beta^2$, and

$$\psi_\alpha(\vec{x}_j) = \left(\frac{\alpha^3}{\pi}\right)^{1/2} e^{-\alpha x_j}, \quad \psi_\beta(\vec{s}_j) = \left(\frac{\beta^3}{\pi}\right)^{1/2} e^{-\beta s_j}, \quad (j=1,2) \tag{4.3}$$

where $\alpha = Z_T - a$, $\beta = Z_P - b$, $a = b = \frac{5}{16} = 0.3125$.
Parameters α and β are the effective charges of the target and projectile nucleus defined by (4.3) in terms of $Z_{T,P}$ and the inner Slater sreening $a_s = b_s = 0.3125$.

Now, following the wavefunctions of the the unperturbed Hamiltonian in both the entrance and exit channels

$$\Phi_i^+ = \varphi_i(\vec{x}_1,\vec{x}_2)e^{i\vec{k}_i\cdot\vec{r}_i + i\gamma_i ln(k_i r_i - \vec{k}_i\cdot\vec{r}_i)} \tag{4.4}$$

$$\Phi_f^- = \varphi_f(\vec{s}_1,\vec{s}_2)e^{-i\vec{k}_f\cdot\vec{r}_f - i\gamma_f ln(k_f r_f - \vec{k}_f\cdot\vec{r}_f)} \tag{4.5}$$

and their corresponding series analogs

$$\Phi_i^+ = a_0\varphi_i(\vec{x}_1,\vec{x}_2)e^{i\vec{k}_i\cdot\vec{r}_i}\left(1 + \frac{\eta_i}{1!\rho}\upsilon_i + \frac{\eta_i(\eta_i+1)}{2!\rho(\rho+1)}\upsilon_i^2 + \cdots\right), \tag{4.6}$$

$$\Phi_f^- = a_0\varphi_f(\vec{s}_1,\vec{s}_2)e^{i\vec{k}_f\cdot\vec{r}_f}\left(1 + \frac{\eta_f}{1!\rho}\upsilon_f + \frac{\eta_f(\eta_f+1)}{2!\rho(\rho+1)}\upsilon_f^2 + \cdots\right). \tag{4.7}$$

The perturbing potentials for the entrance and exit channels and the Green's function G_0^+ are given as follows,

$$V_i^c = \frac{2Z_P}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} \tag{4.8}$$

$$V_f^c = \frac{2Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} \tag{4.9}$$

$$G_0^+ = \frac{1}{E - H_0 \pm i\epsilon}. \tag{4.10}$$

Considering the second term on the right hand side of equation (3.14) and substituting equations (4.8) and (4.9) we obtain,

$$\begin{aligned}\langle\Phi_f^-|V_f^c G_0^+ V_i^c|\Phi_i^+\rangle = {}& \langle\Phi_f^-|\left(\frac{2Z_T}{R}\right)G_0^+\left(\frac{2Z_P}{R}\right)|\Phi_i^+\rangle + \langle\Phi_f^-|\left(\frac{2Z_T}{R}\right)G_0^+\left(\frac{-Z_P}{s_1}\right)|\Phi_i^+\rangle + \\ & \langle\Phi_f^-|\left(\frac{2Z_T}{R}\right)G_0^+\left(\frac{-Z_P}{s_2}\right)|\Phi_i^+\rangle + \langle\Phi_f^-|\left(\frac{-Z_T}{x_1}\right)G_0^+\left(\frac{2Z_P}{R}\right)|\Phi_i^+\rangle + \\ & \langle\Phi_f^-|\left(\frac{-Z_T}{x_1}\right)G_0^+\left(\frac{-Z_P}{s_1}\right)|\Phi_i^+\rangle + \langle\Phi_f^-|\left(\frac{-Z_T}{x_1}\right)G_0^+\left(\frac{-Z_P}{s_2}\right)|\Phi_i^+\rangle \\ & + \langle\Phi_f^-|\left(\frac{-Z_T}{x_2}\right)G_0^+\left(\frac{2Z_P}{R}\right)|\Phi_i^+\rangle + \langle\Phi_f^-|\left(\frac{-Z_T}{x_2}\right)G_0^+\left(\frac{-Z_P}{s_1}\right)|\Phi_i^+\rangle \\ & + \langle\Phi_f^-|\left(\frac{-Z_T}{x_2}\right)G_0^+\left(\frac{-Z_P}{s_2}\right)|\Phi_i^+\rangle.\end{aligned} \tag{4.11}$$

$$\begin{aligned}\langle\Phi_f^-|V_f^c G_0^+ V_i^c|\Phi_i^+\rangle = {}& 4Z_T^*Z_P\langle\Phi_f^-|\frac{1}{R}G_0^+\frac{1}{R}|\Phi_i^+\rangle - 2Z_T^*Z_P\langle\Phi_f^-|\frac{1}{R}G_0^+\frac{1}{s_1}\Phi_i^+\rangle + \\ & - 2Z_T^*Z_P\langle\Phi_f^-|\frac{1}{R}G_0^+\frac{1}{s_2}|\Phi_i^+\rangle - 2Z_T^*Z_P\langle\Phi_f^-|\frac{1}{x_1}G_0^+\frac{1}{R}|\Phi_i^+\rangle + \\ & Z_T^*Z_P\langle\Phi_f^-|\frac{1}{x_1}G_0^+\frac{1}{s_1}|\Phi_i^+\rangle + Z_T^*Z_P\langle\Phi_f^-|\frac{1}{x_1}G_0^+\frac{1}{s_2}|\Phi_i^+\rangle \\ & - 2Z_T^*Z_P\langle\Phi_f^-|\frac{1}{x_2}G_0^+\frac{1}{R}|\Phi_i^+\rangle + Z_T^*Z_P\langle\Phi_f^-|\frac{1}{x_2}G_0^+\frac{1}{s_1}|\Phi_i^+\rangle \\ & + Z_T^*Z_P\langle\Phi_f^-|\frac{1}{x_2}G_0^+\frac{1}{s_2}|\Phi_i^+\rangle.\end{aligned} \tag{4.12}$$

$$\begin{aligned}\langle\Phi_f^-|V_f^c G_0^+ V_i^c|\Phi_i^+\rangle = {}& \frac{(4\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{1,1} - \frac{(2\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{1,2} - \frac{(2\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{1,3} \\ & - \frac{(2\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{2,1} + \frac{(\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{2,2} + \frac{(\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{2,3} \\ & - \frac{(2\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{3,1} + \frac{(\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{3,2} + \frac{(\beta^*\alpha)^3}{\pi^2}Z_T^*Z_P I_{3,3}.\end{aligned} \tag{4.13}$$

where,

$$I_{1,1} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{R}G_0^+\frac{1}{R}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

$$I_{1,2} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{R}G_0^+\frac{1}{s_1}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

$$I_{1,3} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{R}G_0^+\frac{1}{s_2}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

$$I_{2,1} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{x_1}G_0^+\frac{1}{R}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

$$I_{2,2} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{x_1}G_0^+\frac{1}{s_1}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

$$I_{2,3} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{x_1}G_0^+\frac{1}{s_2}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

$$I_{3,1} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{x_2}G_0^+\frac{1}{R}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

$$I_{3,2} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{x_2}G_0^+\frac{1}{s_1}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

$$I_{3,3} = \langle e^{-\beta(2\vec{R}-(x_1+x_2))-i\vec{k}_f\cdot\vec{r}_f-i\gamma_f ln(k_f r_f-\vec{k}_f\cdot\vec{r}_f)}|\frac{1}{x_2}G_0^+\frac{1}{s_2}|e^{-\alpha(x_1+x_2)+i\vec{k}_i\cdot\vec{r}_i+i\gamma_i ln(k_i r_i-\vec{k}_i\cdot\vec{r}_i)}\rangle$$

These are nine matrix elements which effect transition of states, from the entrance channel to the exit channel. We note that the Dirac Bra and Ket notation has integral representation in three dimensional form.

Chapter 5

Discussion of results and Conclusion

5.1 Results

It is important to note here that, all our effort was geared towards correctly deducing the unperturbed wavefunctions of the entrance and exit channels of the four body system $Z_P + (Z_T; e_1, e_2)_i \to (Z_P; e_1, e_2)_i + Z_T$, with boundary corrected conditions [67][68] proposed by Belkić. Following the correct forulation of the theory, rigorous solutions to the unperturbed Hamiltonian is obtained as a result of coordinate transformations from cartesian coordinates (x, y, z) to (z_i, w_i, λ_i). Solutions to the resulting differential equation in equation(2.42) assumes asymtotic form, $\chi \sim \upsilon_i^{\lambda}$ of the system. Equations (2.47) and (2.66) are the corresponding general solutions to the entrance and exit channels respectively. The second approach employed Frobenius series solution method to singular differential equations. The resulting solution ${}_1F_1(\eta_i, \rho; \upsilon_i)$, is a confluent hypergeometric series which is in complete agreement with the first method. Equations (2.57) and (2.67) are respectively the entrance and exit channel general solutions to the unperturbed Hamiltonian. The literature on the Formal Theory of Scattering [90], provides the framework for constructing a perturbation theory to which the Socond Born Approximation matrix elements $T^{(CB2)+}_{if;0} = T^{(CB1)+}_{if} + \langle \Phi^-_f | V^c_f G^+_0 V^c_i | \Phi^+_i \rangle$ is employed. The result is what we have written down in equation(4.13).

We recommend for further studies, explicit calculations of the matrix elements in section 4.2. The following difficulties are expected;

1. Each matrix element represent tripple integrals with a singularity inherent in the Lippman-Schwinger representation of the free Green Function $G^+_0 = \frac{1}{E - H_0 \pm i\epsilon}$.

2. The representation of the unperturbed wavefunctions Φ^-_f , Φ^+_i of Co-ordinate Space in Momentum Space. There are two known methods for doing this; Using the Standard Fourier Transform,

$$\tilde{f}(\vec{p}) \;=\; (2\pi)^{-3} \int dr e^{i\vec{p}\cdot\vec{r}} f(\vec{r}) \qquad f(\vec{r}) = (2\pi)^{-3} \int dp e^{-i\vec{p}\cdot\vec{r}} \tilde{f}(\vec{p}),$$

   and the other is by completely reformulating the problem in momentum space in which case the solution can be used direclty. Nontheless, this approach is also plagued with singularities in the coulomb potential. It is crucial to do calculations in momentum space because we have direct access to the observables.

5.2 Conclusion

We have investigated the problem of double-charge exchange in collisions between bare ions and two-electron atomic systems and correctly written out the unperturbed wavefunctions of the entrance and exit channels and their corresponding matrix element representation of the Second Born Approximation. The analysis is carried out by means of the boundary corrected Second Born(CB2) theory. Collisons involving two-electron capture is heteronulcear in nature and we can at the same time obtain homonuclear case if we consider the projectile to be an alpha particle. In which case both initial and fianl configurations of the target particle being the ground states described by fully uncorrelated one-parameter Hylleraas wavefunctions [99].

Bibliography

[1] Belkić Dž., I. Mančev and J. Hanssen: 2008, Rev. Mod. Phys. **80**,249.

[2] Belkić Dž., 1997a, Nucl. Instrum. Methods Phys. Res. B **124**, 365.

[3] Belkić Dž., 1997b, J. Phys. B **30**, 1731.

[4] Belkić Dž., and I. Mančev 1992, Phys. Scr. **45**, 35.

[5] Belkić Dž., and I. Mančev 1993, Phys. Scr. **46**, 18.

[6] Tanner G., K. Richter, J. M. Rost, 2000, Rev. Mod. Phys. **72**, 497.

[7] Hansteen J. M., and O. Mosebekk, 1972, Phys. Rev. Lett. **29**, 1361.

[8] Mukherjee S. C., K. Roy, and N. Sil, 1973, J. Phys. B **6**, 467.

[9] Biswas S., K. Bhadra, and D. Basu, 1977, Phys. Rev. A **15**, 1900.

[10] McGuire J. H., and L. Weaver, 1977, Phys. Rev. A **16**, 41.

[11] Lin C. D., 1979, Phys. Rev. A **19**, 1510.

[12] Theisen T., and J. H. McGuire, 1979, Phys. Rev. A **20**, 1406.

[13] Gayet R., R. Rivarola, and A. Salin, 1981, J. Phys. B **14**, 2421.

[14] Gayet R., J. Hanssen, A. Martínez, and R. Rivarola, 1991, Z. Phys. D: At., Mol. Clusters **18**, 345.

[15] Gayet R., and A. Salin, 1987, J. Phys. B **20**, L571.

[16] Gayet R., J. Phys.(Paris), Colloq. **50**, C1-53.

[17] Olso R. E., J. Phys. B **15**, L163.

[18] Olso R. E., A. Wetmore, and M. McKenzie, 1986, J. Phys. B **19**, L629.

[19] Brandt D., 1983, Phys. Rev. A **27**, 1314.

[20] Ghosh M., C. Mandal, and S. Mukharjee, 1985, J. Phys. B **18**, 3797.

[21] Ghosh M., C. Mandal, and S. Mukharjee, 1987, Phys. Rev. A **35**, 5259.

[22] Sidorovich V., V. Nikolaev, and J. McGuire, 1985, Phys. Rev. A **31**, 2193.

[23] McGuire J., 1987, Phys. Rev. A **36**, 1114.

[24] McGuire J., 1987, Adv. At., Mol., Opt. Phys. **29**, 217.

[25] Stolterfoht N., 1990, Phys. Scr. **42**, 192.

[26] Stolterfoht N., 1993, Phys. Rev. A **48**, 2980.

[27] Deco G., and N. Grün, 1991, Z. Phys. D: At., Mol., Clusters **18**, 339.

[28] Jain A., R. Shingal, and T. Zouros, 1991, Phys. Rev. A **43**, 1621.

[29] Shingal R., and C. D. Lin, 1991, J. Phys. B **24**, 251.

[30] Martínez A., R. Gayet, J. Hanssen, and R. Rivarola, 1994, J. Phys. B **27**, L375.

[31] Martínez A., H. Busnengo, R. Gayet, J. Hanssen, and R. Rivarola, 1997,Nucl. Instrum. Methods Phys. Res. B **132**, 344.

[32] McCartney M., 1997, J. Phys. B **30**, L155.

[33] Zerarka A., 1997, Phys. Rev. A **55**, 1976.

[34] McGuire J. H., 1997, *Electron Correlation Dynamics in Atomic Collisions* (Cambridge University Press, Cambridge, England).

[35] Dollard J. D., 1963, Ph.D. thesis(University of Michigan).

[36] Dollard J. D., 1964, J. Math. Phys. **5**, 729.

[37] Belkić Dž,1994, Nucl. Instrum. Methods Phys. Res. B **86**, 62.

[38] Belkić Dž., I. Mančev, and M. Mudrinić, 1994, Phys. Rev. A **49**, 3646.

[39] Gayet R., J. Hanssen, A. Martínez, and R. Rivarola, 1994a, Nucl. Instrum. Methods Phys. Res. B **86**, 158.

[40] Gayet R., J. Hanssen, L. Jacqui, A. Martínez, and R. Rivarola, 1996, Phys. Scr. **53**, 549.

[41] Martínez A., R. Rivarola, R. Gayet, J. Hanssen,1999, Phys. Scr. **T80**, 124.

[42] Mančev I., 1999b, Nucl. Instrum. Methods Phys. Res. B **154**, 291.

[43] Mančev I., 2001, Phys. Rev. A **64**, 012708.

[44] Belkić Dž., R. Gayet, and A. Salin, 1979, Phys. Rep. **56**, 279.

[45] Gayet R., R. Janev, and A. Salin, 1973, J. Phys. B **6**, 993.

[46] Belkić Dž., 1978, J. Phys. B **11**, 3529.

[47] Garibotti C. R., and J. E. Miraglia, 1980, Phys. Rev. A **21**, 572.

[48] Brauner M., J. S. Briggs, and H. Klar, 1989, J. Phys. B **22**, 2265.

[49] Gulyás L., and P. D. Fainstein, 1998, J. Phys. B **31**, 3297.

[50] Ciappina M. F., W. R. Cravero, and C. R. Garibotti, 2003, J. Phys. B **36**, 3775.

[51] Belkić Dž., 2009. *Quantum Theory of High-Energy Ion-Atom Collisions*, Taylor & Francis Group,LLC.

[52] Belkić Dž., 1995, Nucl. Instrum. Methods Phys. Res. B **99**, 218.

[53] Belkić Dž., 1996, Phys. Scr. **53**, 414.

[54] Mergel V., R. Dörner, M. Achler, Kh. Khayyat, S. Lencinas, J. Euler, O. Jagutzki, S. Nüttgens, M. Unverzagt, L Spielberger, W. Wu, R. Ali, J. Ullrich, H. Cederquist, A. Salin, C. Wood, R. Olson, Dž. Belkić, C. Cocke, and H. Schmidt-Böcking, 1997, Phys. Rev. Lett. **79**, 387.

[55] Thomas L., 1927, Proc. R. Soc. London, Ser. A **114**, 561.

[56] Schmidt H. T., A. Fardi, R. Schuch, S. Schwartz, H. Zettergren, H. Cederquist, L. Bagge, H. Danared, A. Källberg, J. Jensen, K. Rensfelt, V. Mergel, L. Schmidt, C. Cocke, and H. Schmidt-Böcking, 2002, Phys. Rev. Lett. **89**, 163201.

[57] Schmidt H. T., J. Jensen, P. Reinhed, R. Schuch, K. Stϕchkel, H. Zettergren, H. Cederquist, L. Bagge, H. Danared, A. Källberg, H. Schmidt-Böcking, and C. Cocke, 2005, Phys. Rev. A **72**, 012713.

[58] Bachau H., R. Gayet, J. Hanssen, and A. Zerarka, 1992, J. Phys. B **25**, 839.

[59] Gayet R., J. Hanssen, 1992, J. Phys. B **25**, 825.

[60] Gayet R., J. Hanssen, L. Jacqui, 1995, J. Phys. B **28**, 2193 [J. Phys. B **30**, 1619 (1997)(corrigenda)].

[61] Gayet R., J. Hanssen, L. Jacqui, and M. Ourdane, 1997, J. Phys. B **30**, 2209.

[62] Ourdane M., H. Bachau, R. Gayet, and J. Hanssen, 1999, J. Phys. B **32**, 2041.

[63] Belkić Dž., R. Gayet, J. Hanssen, I. Mančev, and A. Nu$\tilde{n}$ez, 1997, Phys. Rev. A **56**, 3675

[64] Mančev I., 1999a, Phys. Rev. A **60**, 351.

[65] Belkić Dž., 2001, J. Comput. Methods Sci. Eng. **1**, 1.

[66] Belkić Dževad, 2004. *Principles of Quantum Scattering Theory*(Institute of Physics, Bristol).

[67] Belkić Dž., 1993a, Phys. Rev. A **47**, 189.

[68] Belkić Dž., 1993b, J. Phys. B **26**, 497.

[69] Mančev I., 1995, Phys. Scr. **51**, 762.

[70] Mančev I., 1996, Phys. Rev. A **54**, 423.

[71] Belkić Dž., 1993c, Phys. Rev. A **47**, 3824.

[72] Mančev I., 2003, J. Phys. B **36**, 93.

[73] Mančev I., V. Mergel, and L. Schmidt, 2003, J. Phys. B **36**, 2733.

[74] Mančev I., 2005a, J. Comput. Methods Sci. Eng. **5**, 73.

[75] Mančev I., 2005b, Europhys. Lett. **69**, 200.

[76] Crothers D. S. F., and J. F. McCann, 1983, J. Phys. B **16**, 3229.

[77] Busnengo H. F., A. Martínez, and R. Rivarola, 1995, Phys. Scr. **51**, 190.

[78] Busnengo H. F., A. Martínez, and R. Rivarola, 1995, J. Phys. B **29**, 4193.

[79] Galassi M., P. Abufager, A. Martínez, R. Rivarola, and P. D. Fainstein, 2002, J. Phys. B **35**, 1727.

[80] Belkić Dž., R. Gayet, J. Hanssen, and A. Salin, 1986, J. Phys. B **19**, 2945.

[81] Belkić Dž., H. Taylor, and S. Saini, 1986, Z. Phys. D: At., Mol. Clusters **3**, 59.

[82] Belkić Dž., H. Taylor, and S. Saini, 1987, Phys. Rev. A **36**, 1601.

[83] Belkić Dž., and H. Taylor, 1987, Phys. Rev. A **35**, 1991.

[84] Dewangan D., and J. Eichler, 1986, J. Phys. B **19**, 2939.

[85] Bransden B. H., and D. P. Dewangan, 1988, Adv. At. Mol. Phys. **25**,343.

[86] Bransden B. H., and M. R. C. McDowell, 1992, *Charge Exchange and the Theory of Ion-Atom Collisions*(Clarendon Press, Oxford).

[87] Crothers D. S. F., and L. J. Dubé, 1993, Adv. At. Mol., Opt. Phys. **30**, 287.

[88] Dewangan D., and J. Eichler, 1994, Phys. Rep. **247**, 59.

[89] Bransden B. H., and C. J. J. Joachain, 2003, *Physics of Atoms and Molecules*, 2nd ed. (Prentice Hall, New York).

[90] Merzbacher Eugene, 1998, *Quantum Mechanics*, John Wiley and Sons, Inc.

[91] Proceedings of EPAC, 2000, Vienna, Austria.

[92] Belkić Dž., 1993, J. Physics B: At. Mol. Opt.Phys. **26**, 497.

[93] Bethe H., and E. Salpeter, 1977, *Quantum Mechanics of One and Two Electron Atoms*(Plenum, New York).

[94] Drake G., 1988, Nucl. Instrum. Methods Phys. Res. B **31**,7.

[95] Sakurai J. J., 1994, *Modern Quantum Mechanics*, Addison-Wesley, Reading.

[96] Beard R. E, M.B.E, F.I.A, F.S.S, A.S.A, JIA 86, 296-307 (1960).

[97] Belkić Dž., Europhys. Lett. **7**, 323.

[98] Belkić Dž., 1991, Phys. Rev. A **43**, 4571.

[99] Hylleraas E., 1929, Z. Phys. **54**, 347.