ELECTRON IMPACT DOUBLE EXCITATION OF (2s²) ¹S AND (2s2p) ¹P STATES OF HELIUM ATOM USING A DISTORTED WAVE METHOD

BY

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A thesis submitted in partial fulfillment of the requirements for the award of the degree of Master of Science in the school of pure and applied sciences of Kenyatta University.

APRIL, 2010
DECLARATION

This thesis is my original work and has not been presented for a degree in any other university or any other award.

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We confirm that the work reported in this thesis was carried out by the candidate under our supervision.

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DEDICATION

To Martha.
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<tr>
<td>BO</td>
<td>Born-Oppenheimer</td>
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<tr>
<td>BOR</td>
<td>Born-Oppenheimer-Rudge</td>
</tr>
<tr>
<td>CC</td>
<td>Close-Coupling</td>
</tr>
<tr>
<td>CCC</td>
<td>Convergent Close-Coupling</td>
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<td>CI</td>
<td>Configuration-Interaction</td>
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<td>COLTRIMS</td>
<td>Cold Target Recoil Ion Momentum Spectroscopy</td>
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<td>DCS</td>
<td>Differential Cross Section</td>
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<td>DW</td>
<td>Distorted Wave</td>
</tr>
<tr>
<td>DWM</td>
<td>Distorted Wave Method</td>
</tr>
<tr>
<td>DWPO</td>
<td>Distorted Wave Polarized Orbital</td>
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ABSTRACT

Cross section studies are important as they supply fundamental level researchers with necessary information and predictions for their experiments. Once experimental measurements agree with some prediction, the theoretical model yielding the prediction is then applied to other situations and finally validated. Very few studies have been made on electron impact double excitation of \((2s^2)^1S\) and \((2s2p)^1P\) states of helium and even the results obtained in these studies do not agree among themselves. It is on this ground that the cross sections for the excitation of the above states have been calculated using a modified distorted wave method. In this method, a linear combination of the static potentials of the helium atom in the initial and final states is taken as the final channel distortion potential and the initial state static potential of the helium atom is taken as the initial channel distortion potential. Analytic wave functions for the ground and excited states are used. Numerical calculations are performed using a modified DWBA1 computer program. It is noticed that the effect of the exchange is appreciable up to about 400 eV for the \((2s^2)^1S\) excitation and up to 200 eV for \((2s2p)^1P\) excitation. It is encouraging that the results obtained agree well with some of the theoretical and experimental data.
Chapter 1

INTRODUCTION

1.1 Background to the Study

Atomic collision theory has gained momentum in research areas in physical sciences due to it’s applicability in the investigation of the dynamics of many-particle systems at fundamental level. The importance of observations made in physics by analyzing the scattering of particles or waves can hardly be over exaggerated. Many of the most important discoveries have been made by collision experiments. They range from Rutherford’s discovery of the atomic nucleus, over atomic and nuclear spectroscopy, to nuclear fission and the discovery of properties of fundamental particles such as muons, pions and leptons. More discoveries are based on observations made by analysis of light scattering (Newton, 1966).

Growing interest in atomic collision studies was sparked off by a host of factors. These include: revelation by studies of planetary atmospheres and astrophysical phenomena that present knowledge of important atomic collisions is insufficient, possible exhaustion of conventional energy resources hence the search of an alternative such as controlled fusion of light nuclei in thermonuclear plasmas and the dependency of the development of many useful devices on acquisition of new information about many kinds of atomic
collisions. Some of the devices so developed include gas lasers, gas filled radiation detectors and ion sources which are important in industry and in scientific research (McDaniel, 1989).

The study of atomic collision involves the scattering of projectiles (usually electrons, positrons, protons, antiprotons, ions or neutrons) by targets (atoms, molecules or ions). Experimentally, a beam of free particles is prepared in the remote past and in the far future detectors record the scattered particles in the asymptotic region (see figure 1.1) (Joachain, 1975). The theoretical study can be done using semi classical methods or quantal approaches. Semi classical methods include semi classical impact parameter method, classical trajectory Monte Carlo method, classical impulse binary encounter approximation, Eikonal approximation, multi-channel Eikonal treatment and Glauber approximation. Quantal approaches are further classified into two branches; perturbative and non-perturbative methods. The non-perturbative methods include R-matrix, convergent close coupling and variational methods. Perturbative methods include Born series, Eikonal series, distorted wave series and many-body theory (Bartschat, 1998).
Correspondence between theory and experiment is essential. As experimental work produces new data, theory is tested against the data and used to normalize it. Sometimes a flash of theoretical insight leads to new experiments (Bohr’s theory of atomic spectra); at other times an experiment surprisingly produces new data that upsets currently accepted theories (black hole radiation). New theories and experiments are then developed to try and accommodate each other. It is in this quest that new methods of experimentation are put forward and new theories are formulated (McDaniel, 1989).

In the electron-helium collision, such as the one discussed here, an elastic or inelastic collision can occur. In case of an elastic collision, the target and the projectile energies are unaffected by the collision. In inelastic collision, there is
some energy transfer between the incident electron and the target. This results in either the target electrons moving to higher energy levels (excitation) or one of the (or both) electrons being lost (ionization). Double excitation occurs if two target electrons simultaneously draw sufficient energy from the incident electron to rise to other levels.

Most of the doubly excited states are autoionizing states, their energies lying above the first ionization threshold. This makes it difficult to obtain experimental data for double excitation processes. The lifetime of doubly excited autoionizing states is extremely short ($10^{-13}$-$10^{-14}$s). Some states are, however, stable against autoionization. These states have received more attention both theoretically and experimentally among the doubly excited states and are of the form $nl n'l' {}^{1,3}L$, so that $l + l' - L$ is odd (where $nl$ and $n'l'$ are the principle and orbital angular momentum quantum numbers of the two excited electrons and $^{1,3}L$ denotes the total orbital angular momentum L and the multiplicity of the doubly excited states). The decay of these states via electron emission is prohibited (Srivastava and Kumar, 1985). Comparatively, little has been done in the study of parity-favoured autoionizing states of helium, like $2s^2 {}^1S$ and $2s2p {}^1P$ considered here.
In this study, the two electrons, initially in the ground state, get excited to \((2s^2)^1S\) and \((2s2p)^1P\) states, both parity-favoured autoionizing states, by electron impact. Doubly excited states may later autoionize, singly or doubly, by ejection of one or two electrons respectively. The two steps involved in the autoionization are:

\[
e^{-} + \text{He} \rightarrow \text{He}^{**} + e^{-}
\]

\[
\text{He}^{**} \rightarrow \text{He}^{-} + e^{-}
\]

OR

\[
\text{He}^{**} \rightarrow \text{He}^{2-} + 2e^{-}
\]

The present study will dwell only on the excitation process. The differential cross sections (DCS) and integral cross sections (ICS) for the two excited states will be calculated. Results, thus obtained, will be compared with available experimental and other theoretical data. Distorted wave method (DWM) will be employed in this quest. This is due to the method’s flexibility and relative computational simplicity (Katiyar and Srivastava, 1989). A particular modification to the distorted wave method suggested by Singh (2004) will be used.
1.2 Statement of the Research Problem

In this study, differential and integral cross sections for the \((2s^2)^1S\) and \((2s2p)^1P\) double excitation of helium from its ground state by electron impact will be calculated using the distorted wave method.

1.3 Objectives of the Research Project

1.3.1 Main Objective

To study the electron impact double excitation of helium into the \((2s^2)^1S\) and \((2s2p)^1P\) autoionizing states.

1.3.2 Specific Objectives

(i) To determine the differential and integral cross sections for electron impact double excitation of helium into the \((2s^2)^1S\) and \((2s2p)^1P\) states.

(ii) To compare the results obtained with available experimental and theoretical data.

(iii) To test the suitability of the present variation of the distorted wave method to the study of \((2s^2)^1S\) and \((2s2p)^1P\) double excitation of helium by electron impact.
1.4 Rationale of the Study

Atomic collision literature has constantly grown since its inception (McConkey, 2005). Although receiving significant attention, double excitation studies are not very common when compared with ionization and single excitation processes. Not many studies (both theoretical and experimental) have been made on the electron impact excitation of \( (2s^2)^1S \) and \( (2s2p)^1P \) states of helium, and the results obtained in the few studies made do not agree among themselves. It is majorly in the pursuit of resolving this discrepancy and adding to the double excitation literature that this study is made.

Secondly, theoretical models do not absolutely resolve all collision processes. New approaches are constantly put forward in the attempt of resolving particular collision processes. Each suggested method is then subjected to several tests, varying projectiles and scatterers, to assess its suitability until such a method as is agreeable to all tests is found. Once an accurate model is found, it is then used to normalize data pertaining to other collision processes and to calibrate experimental apparatus. It is on this ground that we test the suitability of a new variation on the distorted wave method that has not been subjected to double excitation test before.
Chapter 2

LITERATURE REVIEW

2.1 Early Developments

The study of double excitation is almost as old as quantum mechanics. Buoyed by the quest to verify the identities of far ultraviolet helium lines as suggested by Compton and Boyce (1928) and by Kruger (1930) and Rosenthal’s (1934) theory of corona spectrum, Fender and Vinti (1934) and Wu (1934) performed calculations of the energy eigenvalues and spectral lines of various doubly excited helium states using hydrogenic wave functions. Later during a collision experiment in which electrons were scattered by helium, Whiddington and Priestley (1934) discovered a unique line they could explain only as originating from the \(2p^2\) state, a doubly excited state. Further calculations on doubly excited helium states were carried out by Massey and Mohr (1935). There have since been many experimental and theoretical investigations mainly on ionization energies and spectral lines by various doubly excited helium states.

2.2 Theoretical Studies on Double Excitation of Helium by Electron Impact

Becker and Dahler (1964) studied some of the parity unfavoured doubly excited states in helium by electron impact. In their study, they used the Born-Oppenheimer (BO), distorted wave (DW), and close coupling (CC) approximations to calculate both differential and total cross sections using simple
analytic wave functions. They then compared the results obtained using the various methods. Woollings and McDowell (1973) calculated some (nsmp) $^1P$ total cross sections to check the effect of the second Born correction to the first Born approximation while Gillespie (1973) performed elaborate calculations on similar states using multi-parameter Hylleraas-type wave functions for the ground-state and Vinti’s (1932) variational wave functions for the excited states. Roy and Sil (1976), motivated by the studies carried out by Becker and Dahler, tried the integral form of the close coupling approximation for the $^1S - ^3P$ excitations of helium. Hickerson et al. (1978) reviewed the work of Becker and Dahler using both BO and the Born-Oppenheimer-Rudge (BOR) approximations and applying the Hartree-Fock and correlated wave functions for the ground state in place of simple analytical radial wave-functions.

Disagreement with experimental data, later availed, led to more studies carried out in the aim of integrating experimental data with theory. These included Williamson et al. (1982) who performed calculations in Glauber-Ochkur approximation but the Glauber exchange amplitude they employed was later found to be unreliable and Srivastava and Kumar (1985) who used the distorted wave polarized orbital (DWPO) approach to obtain both differential and total cross sections for the excitation of some of the parity-unfavoured states, $(2p^2) ~^3P$, $(2p3p) ~^1P$ and $(2p3d) ~^{1,2}D$. Failure of their results to concur with experimental data led to
their recommendation for more absolute measurements of the double excitation processes in helium to supplement earlier tasks. More recently, Plottke et al. (2004) performed calculations for total excitation cross sections in the S-wave model from threshold to high energies. They used convergent close coupling (CCC) with configuration interaction (CI) wave functions in their calculations. Cross sections were obtained for various meta-stable states as the initial states besides the ground state excited to $2s2s \, ^1S$, $2s3s \, ^1S$ and $2s3s \, ^3S$ final doubly excited states. They compared the results with the various initial states excited to different final states.

### 2.3 Other Theoretical Studies on Double Excitation

Helium and other atoms, molecules and ions have received attention theoretically using other projectiles like protons, antiprotons, photons and other radiation. A few of these include Kulander and Dahler (1972) who considered the double excitation of lithium, beryllium, magnesium and carbon ions by electron impact, McGuire et al. (1992) who studied the double excitation of helium by fast charged particles and Griffin et al. (1992) who studied the double excitation autoionization due to electron impact of lithium ion by applying 11- and 37- state R matrix method. More recently, Malegat and Selles (2000) studied absolute differential cross-sections for the photo double ionization of helium using the hyperspherical R-matrix method with semi-classical outgoing waves. Bodea and Nagy (2000)
studied the double excitation of hydrogen molecule by fast charged particle impact and Gudonov et al. (2002) studied the double excitation of the autoionizing states (2s^2, 2s2p and 2p^2) of helium by proton impact.

2.4 Autoionization

The (2s^2) ^1S and (2s2p) ^1P states are autoionizing. The autoionization problem has abundantly been studied for helium and other atoms and molecules. Some of the more recent studies on autoionization include Pochat et al. (1982) who calculated double and triple differential cross sections for the electron impact autoionization of helium, Samardzic et al. (1994) who studied the autoionization of the (2s^2) ^1S, (2p^2) ^1D and (2s2p) ^1P states of helium and Horner et al. (2004) who calculated the S-wave model electron impact autoionization of helium.

2.5 Experimental Advances

Experiments on double excitation by electron impact could either track the scattered electron or the ejected electron following autoionization. Some of the experiments tracking the scattered electron include Spence’s (1975) electron impact excitation of (2s^2) ^1S and (2s2p) ^3P and Westerveld et al.’s (1979) electron impact excitation of (2p^2) ^3P. Progress has however been made on experimentation with other projectiles evolving from energy loss spectroscopy (Htwe et al., 1994) to very advanced techniques like cold target recoil ion momentum spectroscopy.
(COLTRIMS) as was used by Weber et al. (2004). Even presently, experimental results have not been fully matched with theoretical data.

2.6 Deduction

The theoretical results for \((2s^2)^1S\) and \((2s2p)^1P\) so far advanced agree neither with each other nor with experimental results available, hence the need for studying these states in an attempt of resolving the existing discrepancies.
Chapter 3

RESEARCH METHODOLOGY

3.1 Introduction

In this chapter, the approach to the evaluation of differential and integral cross sections is described. Since the distorted wave formula using the two-potential model is core to the development, the model is discussed in section 3.2. In section 3.3, the distorted wave method as applied to the double excitation of helium is discussed while in section 3.4 we give the atomic wave functions. In section 3.5 the distortion potentials are discussed and evaluated. The T-matrix elements are evaluated in section 3.6 and the computer code discussed in section 3.7.

3.2 Distorted Wave Formula Using the Two-Potential Scattering Model

If the interaction potential, $V$ between the projectile and the scatterer can be broken into two parts such that one can be exactly treated and the other approximated, then we have

$$V_s = W_s + U_s$$

(3.2.1)

where $s = i$ or $s = f$ for the initial and final channels respectively. The part that can be exactly solved is combined with the unperturbed Hamiltonian, $\mathcal{H}_0$ (Hamiltonian of the target atom and the non-interacting projectile) so that

$$(\mathcal{H}_0 + U_s)\chi^\pm = E\chi^\pm$$

(3.2.2)
where $\chi$ is a product of the target wave function and the projectile wave function within the interaction region (distorted wave) and $+ (-)$ refers to the outgoing (incoming) wave boundary conditions.

The transition matrix element for a scattering problem is given by

$$T_{if} = \langle \Phi_f | V_f | \Psi_i^+ \rangle$$  \hspace{1cm} (3.2.3)

where $\Phi_f$ is the product of the final target wave function and the final plane wave of the projectile in the asymptotic region and $\Psi_i^+$ is the total wave function of the system.

Putting (3.2.1) in (3.2.3) we have

$$T_{if} = \langle \Phi_f | U_f + W_f | \Psi_i^+ \rangle$$  \hspace{1cm} (3.2.4)

Now using the Lippmann-Schwinger equation, we can write

$$|\chi_f^-\rangle = |\Phi_f\rangle + \frac{1}{E_f - H_f - i\epsilon} U_f |\Phi_f\rangle$$  \hspace{1cm} (3.2.5)

where

$$H_f = H_0 + U_f$$  \hspace{1cm} (3.2.6)

Solving for $\Phi_f$ in (3.2.5) we can write

$$\langle \Phi_f | = \langle \chi_f^- | - \langle \Phi_f | U_f \frac{1}{E_f - H_f + i\epsilon}$$  \hspace{1cm} (3.2.7)

Putting (3.2.7) in (3.2.4) we have
Similarly $\Psi_i^+$ can be expanded in terms of the Lippmann-Schwinger equation as

$$|\Psi_i^+\rangle = |\phi_i\rangle + \frac{1}{E_i - H_i + i\varepsilon} V_i |\phi_i\rangle$$  \hspace{1cm} (3.2.9)$$

where $\phi_i$ is the product of the initial state atomic wave function and the initial plane wave for the projectile.

Now, on the energy shell, $E = E_i = E_f$. The third term of (3.2.8) on using (3.2.9) becomes

$$T_{if} = \langle \phi_f | U_f | \Psi_i^+ \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle - \left| \phi_f \right| U_f \frac{1}{E_f - H_f + i\varepsilon} W_f |\Psi_i^+(\Phi_i)\rangle$$

(3.2.8)

On using (3.2.7) on the first term of (3.2.10) we have
\[
\begin{align*}
\left\langle \Phi_f \left| U_f \frac{1}{E_f - H_f + i\varepsilon} W_f \right| \Psi_i^+ \rightangle \\
= \left\langle \chi_f^- \left| W_f \right| \phi_i \right\rangle - \left\langle \phi_f \left| W_f \right| \phi_i \right\rangle \\
+ \left\langle \Phi_f \left| U_f \frac{1}{E_f - H_f + i\varepsilon} W_f \frac{1}{E_f - H + i\varepsilon} V_i \right| \phi_i \rightangle \\
\end{align*}
\]

Using the operator identity, \( \frac{1}{B} (B - A)^{\frac{1}{A}} = \frac{1}{A} - \frac{1}{B} \), with \( A = E_f - H + i\varepsilon \) and \( B = E_f - H + i\varepsilon \) and recalling \( H - H_f = W_f \) we have the third term of (3.2.10) becoming

\[
\begin{align*}
\left\langle \Phi_f \left| U_f \frac{1}{E_f - H_f + i\varepsilon} W_f \frac{1}{E_f - H + i\varepsilon} V_i \right| \phi_i \rightangle \\
= \left\langle \Phi_f \left| U_f \frac{1}{E_f - H + i\varepsilon} V \right| \phi_i \rightangle \\
- \left\langle \Phi_f \left| U_f \frac{1}{E_f - H_f + i\varepsilon} V_i \right| \phi_i \rightangle \\
\end{align*}
\]

Using (3.2.7) and (3.2.9) in (3.2.12) we have
\[
\left( \Phi_f \left| \frac{1}{E_f - H_f + i\epsilon} W_f \frac{1}{E_f - H + i\epsilon} \right| \Phi_i \right) \\
= \langle \Phi_f | U_f | \Psi_i^+ \rangle - \langle \Phi_f | U_f | \Phi_i \rangle - \langle \chi_f^- | V_i | \Phi_i \rangle + \langle \Phi_f | V_i | \Phi_i \rangle
\]

(3.2.13)

Using (3.2.11) and (3.2.13) in (3.2.8) we have

\[
T_{if} = \langle \Phi_f | U_f | \Psi_i^+ \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle - \langle \chi_f^- | W_f | \Phi_i \rangle + \langle \Phi_f | W_f | \Phi_i \rangle \\
- \langle \Phi_f | U_f | \Psi_i^+ \rangle + \langle \Phi_f | U_f | \Phi_i \rangle + \langle \chi_f^- | V_i | \Phi_i \rangle - \langle \Phi_f | V_i | \Phi_i \rangle
\]

(3.2.14)

Hence

\[
\langle \Phi_f | U_f + W_f | \Phi_i \rangle = \langle \Phi_f | V_f | \Phi_i \rangle = \langle \Phi_f | V_i | \Phi_i \rangle
\]

(3.2.15)

Using (3.2.15) in (3.2.14) we have

\[
T_{if} = \langle \chi_f^- | V_i - W_f | \Phi_i \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle
\]

(3.2.16)

If \( V_i = V_f = V \) then

\[
T_{if} = \langle \chi_f^- | U_f | \Phi_i \rangle + \langle \chi_f^- | V - U_f | \Psi_i^+ \rangle
\]

(3.2.17)
which is the distorted wave formula for the two-potential model. If $U$ is some linear combination of the static potentials of the target states, the first term vanishes due to orthogonality of the target states. In this case the $T$-matrix element becomes

$$T_{if} = \langle \chi_f^- | V - U_f | \psi_i^+ \rangle$$  \hspace{1cm} (3.2.18)

Equation (3.2.18) is the form of transition matrix element used in the distorted wave method we shall be employing.

3.3 Application of the Distorted Wave Formula to Electron–Helium Collision

The total Hamiltonian, $\mathcal{H}$, of an electron-helium collision is given as

$$\mathcal{H} = \mathcal{H}_a + T + V$$  \hspace{1cm} (3.3.1)

where $\mathcal{H}_a$ is the isolated atom’s Hamiltonian while $T$ and $V$ are kinetic energy of the incident electron and the interaction potential between the incident electron and the atom, respectively, given by

$$T = -\nabla_0^2$$  \hspace{1cm} (3.3.2)

and

$$V = -\frac{2Z_p}{r_{01}} - \frac{2Z_p}{r_{02}} + \frac{2Z_pZ_n}{r_0}$$  \hspace{1cm} (3.3.3)

The units in equations (3.3.2) and (3.3.3) and hereafter are in Rydberg.
The subscript 0 refers to the incident electron while the subscripts 1 and 2 refer to the bound atomic electrons. \( r_{01} \) and \( r_{02} \) are the distances between the projectile electron and the bound electrons 1 and 2 respectively. \( Z_p \) is the projectile charge (-1 for the electron) and \( Z_n \) is the nuclear charge (2 for helium).

The T-matrix element for the electron—N-electron target collision in the two-potential approach is given by (Madison and Bartschat, 1996)

\[
T_{fi} = (N + 1) \langle \chi_f(0) \psi_f(1, ..., N) \mid V - U_f \mid A \psi_i^+(0, ..., N) \rangle \\
+ \langle \chi_f(0) \psi_f(1, ..., N) \mid U_f \mid \psi_i(1, ..., N) \beta_i \rangle
\]  

(3.3.4)

where \( \beta_i \) is the initial plane wave given as:

\[
\beta_i = \exp(ik_i, r_0)
\]  

(3.3.5)

\( \psi_i^+ \) is the total wave function of the electron—atom system satisfying the outgoing wave boundary conditions and is a solution of the Schrödinger equation:

\[
H \psi_i^+ = E \psi_i^+
\]  

(3.3.6)

\( \psi_i \) and \( \psi_f \) are, respectively, the initial and final wave functions of the helium atom.
$A$ is the antisymmetrization operator for the electron—atom system, generally given as

$$A = \frac{1}{N + 1} \left( 1 - \sum_{i=1}^{N} P_{i0} \right)$$

(3.3.7)

and with $N = 2$, for helium, the antisymmetrization operator so defined becomes

$$A = \frac{1}{3} (1 - P_{10} - P_{20})$$

(3.3.8)

where $P_{i0}$ is the operator that exchanges the $i^{th}$ atomic electron with the incident electron (labeled 0). $\chi_f^-$ is a solution of the wave equation:

$$\left( \nabla_0^2 - U_f + k_f^2 \right) \chi_f^- = 0$$

(3.3.9)

satisfying the incoming wave boundary conditions. $k_f$ is the final wave vector of the projectile electron ($k_f^2$ gives the kinetic energy, in Rydberg, of the projectile electron in the final channel). $U_f$ is an arbitrarily chosen potential, usually chosen as the static potentials of the target states, for the distortion of the final state projectile electron wave function.

Since we will be choosing $U_f$ as some combination of static potentials of the target states (which only depend on the co-ordinate of the projectile) then for the inelastic collision considered here, the second term on the right hand side of equation
(3.3.4) will vanish because of the orthogonality of the atomic wave functions. Equation (3.3.4) then becomes:

$$T_{fi} = \langle \chi_f^-(0) \psi_f(1,2) | V - U_f | (1 - P_{10} - P_{20}) \Psi^+_i(0,1,2) \rangle$$  \hspace{1cm} (3.3.10)

Since $\Psi^+_i$ can not be evaluated exactly, the first order distorted wave Born approximation will be employed, which requires $\Psi^+_i(0,1,2)$ to be approximated as follows:

$$\Psi^+_i(0,1,2) = \psi_i(1,2) \chi^+_i(0)$$  \hspace{1cm} (3.3.11)

where $\chi^+_i$ is the distorted wave function representing the projectile electron in the initial channel and is a solution to the wave equation

$$\left( \nabla^2_0 - U_i + k_i^2 \right) \chi^+_i = 0$$  \hspace{1cm} (3.3.12)

where $U_i$ is an arbitrarily chosen potential for the distortion of the initial state projectile electron wave function, $k_i$ is the initial wave vector of the projectile electron. Using equation (3.3.11) into equation (3.3.10) yields the transition matrix element, $T_{fi}$, in terms of the direct, $T_{fi}^d$, and exchange, $T_{fi}^{ex}$, scattering amplitudes as

$$T_{fi} = T_{fi}^d - T_{fi}^{ex}$$  \hspace{1cm} (3.3.13)
where

$$T^d_{fi} = \langle \chi_f^-(0) \psi_f(1,2) | V | \psi_i(1,2) \chi_i^+(0) \rangle$$

$$- \langle \chi_f^-(0) \psi_f(1,2) | U_f(0) | \psi_i(1,2) \chi_i^+(0) \rangle$$  \hspace{1cm} (3.3.14)$$

and

$$T^{ex}_{fi} = \langle \chi_f^-(0) \psi_f(1,2) | V | \psi_i(0,2) \chi_i^+(1) \rangle$$

$$+ \langle \chi_f^-(0) \psi_f(1,2) | V | \psi_i(1,0) \chi_i^+(2) \rangle$$

$$- \langle \chi_f^-(0) \psi_f(1,2) | U_f(0) | \psi_i(0,2) \chi_i^+(1) \rangle$$

$$- \langle \chi_f^-(0) \psi_f(1,2) | U_f(0) | \psi_i(1,0) \chi_i^+(2) \rangle$$  \hspace{1cm} (3.3.15)$$

In the direct term (equation 3.3.14), the second term will vanish because of the orthogonality of the target states and in the exchange term (equation 3.3.15) the two last terms will be neglected because the overlap integral between the continuum and bound electron wave functions will be negligible (Madison and Bartschat, 1996).

Substituting the value of $V$ (equation 3.3.3) into equations (3.3.14) and (3.3.15) we obtain:
\[ T_{fi}^d = -2Z_p \langle \chi_f^- (0) \psi_f (1,2) \left| \frac{1}{r_{01}} \right| \psi_i (1,2) \chi_i^+ (0) \rangle \]

\[ - 2Z_p \langle \chi_f^- (0) \psi_f (1,2) \left| \frac{1}{r_{02}} \right| \psi_i (1,2) \chi_i^+ (0) \rangle \]  \hspace{1cm} (3.3.16)

where the term with \( r_0 \) vanishes because of the orthogonality of the atomic wave functions and

\[ T_{fi}^{ex} = -2Z_p \langle \chi_f^- (0) \psi_f (1,2) \left| \frac{1}{r_{01}} \right| \psi_i (0,2) \chi_i^+ (1) \rangle \]

\[ - 2Z_p \langle \chi_f^- (0) \psi_f (1,2) \left| \frac{1}{r_{02}} \right| \psi_i (0,1) \chi_i^+ (2) \rangle \]  \hspace{1cm} (3.3.17)

where the terms with overlap integrals involving bound and continuum wave functions have been neglected.

The distorted waves \( \chi_i^+ \) and \( \chi_f^- \) for the projectile in the initial and final states are expanded in partial waves (Singh, 2005; Madison and Bartschart, 1996) as

\[ |\chi_i^+ \rangle = \sqrt{\frac{2}{\pi k_i r}} \sum_{l_i m_i} i^{l_i} \chi_{l_i} (k_i, r) Y_{l_i m_i} (\hat{\mathbf{r}}) Y_{l_i m_i}^* (\hat{\mathbf{k}}_i) \]  \hspace{1cm} (3.3.18)

and

\[ |\chi_f^- \rangle = \sqrt{\frac{2}{\pi k_f r}} \sum_{l_f m_f} i^{l_f} \chi_{l_f}^* (k_f, r) Y_{l_f m_f} (\hat{\mathbf{r}}) Y_{l_f m_f}^* (\hat{\mathbf{k}}_f) \]  \hspace{1cm} (3.3.19)
where \( Y_{lm} \) are spherical harmonics.

In the expansion of \( \chi_f \), the complex conjugate of the radial part \( \chi_{lf} \) is taken so that it satisfies the incoming boundary conditions. On substituting equations (3.3.18) and (3.3.19) into equations (3.3.9) and (3.3.12) we obtain the radial distorted waves to be solution of the following equation.

\[
\left( \frac{d^2}{dr^2} - \frac{l_s(l_s + 1)}{r^2} - U_s(r) + k_s^2 \right) \chi_{ls}(r) = 0 \tag{3.3.20}
\]

with \( s = i \) for the initial state and \( s = f \) for the final state distorted waves. In the asymptotic region, they will satisfy the boundary condition:

\[
\lim_{r \to \infty} \chi_{ls}(k_s, r) = j_{ls} + B_{ls}(\eta_{ls} + ij_{ls}) \tag{3.3.21}
\]

where \( j_l \) and \( \eta_l \) are the regular and irregular Ricatti–Bessel functions and \( B_l \) is given as:

\[
B_l = \exp(i\delta_l) \sin \delta_l \tag{3.3.22}
\]

where \( \delta_l \) is the elastic scattering phase shift.
The radial distorted wave equations (3.3.20) for initial and final states will be solved using Numerov method and the differential cross sections will be obtained using the relation

\[
\frac{d\sigma}{d\Omega} = 4\pi^4 \frac{k_f}{k_i} |T^d - T^{ex}|^2
\] (3.3.23)

which when integrated yields the total cross section, \(\sigma\), as

\[
\sigma = \int \frac{d\sigma}{d\Omega} d\Omega
\]

\[
= 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin \theta \, d\theta
\] (3.3.24)

This integration and all other integrations are numerically done by the Simpson’s three point method.

In the next two sections we discuss the wave functions we used and the distortion potentials before evaluating the transition matrix elements, \(T^d\) and \(T^{ex}\).

### 3.4 Atomic Wave Functions

For the ground state, \((1s^2)^1S\), of the helium atom we will use the Hartree-Fock wave function of Byron and Joachain (1966) given as:

\[
\psi_{1s^2} = \Phi_0(r_1)\Phi_0(r_2)
\] (3.4.1)
where

$$\psi_{2s^2} = \varphi_{2s}(\mathbf{r}_1)\varphi_{2s}(\mathbf{r}_2) \quad (3.4.3)$$

For (2s$^2$) $^1S$, a simple analytic wave function as suggested by Ma and Wu (1936) will be used.

$$\varphi_{2s}(\mathbf{r}) = \sqrt{4\alpha^3}(1 - \alpha r)\exp(-\alpha r)Y_{00}(\hat{\mathbf{r}}) \quad (3.4.4)$$

where $\alpha = 0.85$

For (2s2p) $^1P$, we will use the analytic wave function as suggested by Vinti (1932).

$$\psi_{2s2p} = \frac{1}{\sqrt{2}}\left\{\Phi_{2s}(z, \mathbf{r}_1)\Phi_{2p}(\beta, \mathbf{r}_2) + \Phi_{2s}(z, \mathbf{r}_2)\Phi_{2p}(\beta, \mathbf{r}_1)\right\} \quad (3.4.5)$$

Where $z = 2$ and $\beta = 1.58$. $\Phi_{nl}(\mathbf{r})$ are hydrogenic orbitals given as

$$\Phi_{2s}(2, \mathbf{r}) = 2(1 - r)e^{-r}Y_{00}(\hat{\mathbf{r}}) \quad (3.4.6)$$
and

\[ \phi_{2p}(\beta, r) = \phi_{2p}(2\xi, r) = \frac{2}{\sqrt{3}} \xi^2 \text{Re} e^{i\xi r} Y_{1,m}(\hat{r}), m = 0, \pm 1 \]  

(3.4.7)

where \( \xi = \frac{\beta}{2} = 0.79 \)

### 3.5 Distortion Potentials

#### 3.5.1 Introduction

The distortion potentials \( U_i \) and \( U_f \) could be arbitrarily picked but they are usually the static potentials of the target atom in its initial or final state or any linear combination of the two (Itikawa, 1986). The distortion potentials used here are those suggested by Singh (2004) where the initial distortion potential will be taken as the static potential of the target atom in its initial state while the final distortion potential will be taken as the simple average of target atom static potentials in its initial and final states. That is;

\[ U_i = \langle \psi_i | V | \psi_i \rangle \]  

(3.5.1)

and

\[ U_f = \frac{1}{2} \langle \psi_i | V | \psi_i \rangle + \frac{1}{2} \langle \psi_f | V | \psi_f \rangle \]  

(3.5.2)
The reason for taking the above choice is that when the projectile electron is in its initial state it ‘sees’ the initial state static potential of the target atom for all the time it is in its field. However, when the energy of the projectile electron is transferred to the target atom, it takes time (relaxation time) for the atom to go to its final state. That is there is a time lag between the time of transfer of energy and instant when the atom reaches the final state. Thus the projectile in it’s final state ‘sees’ a potential which is intermediate between the initial and the final-state static potentials of the target. The static potentials in equations 3.5.1 and 3.5.2 are evaluated in the following section.

3.5.2 Evaluation of the Static Potentials

3.5.2.1 The Ground State Static Potential

The ground state is the initial state and therefore gives the initial-state static potential.

\[ V_{1s^2} = \left\langle \phi_0(r_1) \phi_0(r_2) \right| \frac{2}{r_{01}} Z_p - \frac{2}{r_{02}} Z_p + \frac{2}{r_0} Z_p Z_N \left| \phi_0(r_1) \phi_0(r_2) \right\rangle \]

(3.5.3)

which simplifies to

\[ V_{1s^2} = -2Z_p \left[ \left( \phi_0(r_1) \right| \frac{1}{r_{01}} \phi_0(r_1) \right) + \left( \phi_0(r_2) \right| \frac{1}{r_{02}} \phi_0(r_2) \right) - \frac{Z_N}{r_0} \]

Since \( \left\langle \emptyset_0(r) \right| \emptyset_0(r) \right\rangle = 1 \)
\[ = 2Z_p \left( \frac{Z_N}{r_0} - 2 \left( \frac{1}{r_{01}} \right) \frac{\phi_0(r_1)}{\phi_0(r_1)} \right) \]  \hspace{1cm} (3.5.4)  

Since \( \left( \frac{1}{r_{0i}} \right), i = 1,2 \) are similar.

On substituting for \( \phi_0 \) we obtain

\[ V_{1s^2} = 2Z_p \left[ \frac{Z_N}{r_0} \right. \]

\[ - 2 \int \left( N_1 (\exp(-pr_1)) \right. \]

\[ + c \exp(-qr_1)) \right)^2 Y_{00}(\hat{r}_1) \left( \frac{1}{r_{01}} \right) Y_{00}(\hat{r}_1) \, dr_1 \]  \hspace{1cm} (3.5.5)  

Expanding \( \frac{1}{r_{01}} \) in terms of spherical harmonics as

\[ \frac{1}{r_{01}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} \frac{r_1^l}{r_{01}} Y_{lm}^*(\hat{r}_0) Y_{lm}(\hat{r}_1) \]  \hspace{1cm} (3.5.6)  

Therefore \( \frac{1}{r_{01}} \) is a tensor operator since it has spherical harmonics. This calls for the Wigner-Eckart theorem. There is only one viable term in the expansion, the
term in \( l = 0, m = 0 \). Therefore the static potential after angular integration becomes

\[
V_{1s^2} = 2Z_p \left[ \frac{Z_N}{r_0} - 2N_1^2 \int_0^\infty (e^{-pr_1} + ce^{-qr_1})^2 \frac{r_1^2}{r_>^2} \, dr_1 \right]
\]

which when evaluated yields

\[
V_{1s^2} = \frac{2Z_p}{r_0} \left[ Z_N + 2N_1^2 \left( \frac{e^{-2p}r_0}{4p^3} + \frac{c^2e^{-2qr_0}}{4q^3} \right) + \frac{2ce^{-(p+q)r_0}((p+q)r_0 + 2)}{(p+q)^3} \right] - 2
\]

3.5.2.2 The \( 2s^2 \) Static Potential

This yields one of the final-state static potentials

\[
V_{2s^2} = -2Z_p \left( \varphi_{2s}(r_1) \varphi_{2s}(r_2) \right) \left[ \frac{2}{r_{01}} - \frac{Z_N}{r_0} \varphi_{2s}(r_1) \varphi_{2s}(r_2) \right]
\]

which simplifies to

\[
V_{2s^2} = 2Z_p \left[ \frac{Z_N}{r_0} - \left( \varphi_{2s}(r_1) \right) \left[ \frac{2}{r_{01}} \varphi_{2s}(r_1) \right] \right]
\]
Expanding $\frac{1}{r_{01}}$ in spherical harmonics, retaining viable terms only (due to Wigner-Eckart theorem), and performing angular integration yields the static potential as

$$V_{2s^2} = 2Z_p \left[ \frac{Z_N}{r_0} - 8\alpha^3 \int_0^\infty (1 - 2\alpha r_1 + \alpha^2 r_1^2) e^{-2\alpha r_1} \frac{r_1^2}{r_>} dr_1 \right]$$  (3.5.10)

which when evaluated yields

$$V_{2s^2} = \frac{2Z_p}{r_0} \left[ Z_N + e^{-2\alpha r_0} (2\alpha^3 r_0^3 + 2\alpha^2 r_0^2 + 3\alpha r_0 + 2) - 2 \right]$$  (3.5.11)

3.5.2.3 The 2s2p $^1P$ Static Potential

The (2s2p) $^1P$ state is one of the final states and yields a final-state static potential.

$$V_{2s2p} = \left( \psi_{2s2p} \right| - \frac{2}{r_{01}} Z_p - \frac{2}{r_{02}} Z_p + \frac{2}{r_0} Z_p Z_N \left| \psi_{2s2p} \right)$$  (3.5.13)

After substitution of the wave function, expansion and integration over $r_2$ and using the orthonormality of the hydrogenic orbitals we get
Expanding $\frac{1}{r_{01}}$ in spherical harmonics and retaining viable terms only, in accordance to Wigner-Eckart theorem, and performing angular integration we obtain on making the substitution $\beta = 2\xi$ in the wave function

\[ V_{2s2p} = 2Z_p \left( \frac{Z_N}{r_0} - \left[ \langle \phi_{2s} (r_1) \| \frac{1}{r_{01}} \| \phi_{2s} (r_1) \rangle + \langle \phi_{2p} (r_1) \| \frac{1}{r_{01}} \| \phi_{2p} (r_1) \rangle \right] \right) \]

(3.5.14)

which is evaluated to yield

\[ V_{2s2p} = \frac{2Z_p}{r_0} \left\{ Z_N + e^{-2r_0} \left( r_0^3 + r_0^2 + \frac{3r_0}{2} + 1 \right) \right. \\
+ \left. e^{-2\xi r_0} \left( \frac{\xi^3 r_0^3}{3} + \xi^2 r_0^2 + \frac{3\xi r_0}{2} + 1 \right) - 2 \right\} \]

(3.5.16)
3.6 Evaluation of the T-Matrix

3.6.1 1s\(^2\)–2s\(^1\)S Transition

3.6.1.1 Direct Amplitude

Due to the symmetry of the initial and final wave functions, the two terms in equation 3.3.16 are similar. Hence

\[ T_{fi}^d = -4Z_p \left\langle \chi_f^-(0) \psi_f(1,2) \right| \frac{1}{r_{01}} \right| \psi_i(1,2) \chi_i^+(0) \right\rangle \] (3.6.1)

After substituting in equation (3.6.1) the appropriate wave functions from equations (3.4.1) and (3.4.3), we have

\[ T_{fi}^d = -4Z_p \left\langle \chi_f^-(0) \varphi_{2s}(r_1) \varphi_{2s}(r_2) \right| \frac{1}{r_{01}} \right| \Phi_0(r_1) \Phi_0(r_2) \chi_i^+(0) \right\rangle \] (3.6.2)

which simplifies to

\[ T_{fi}^d = -4Z_p \left\langle \varphi_{2s}(r_2) \right| \Phi_0(r_2) \right\rangle \left\langle \chi_f^-(0) \varphi_{2s}(r_1) \right| \frac{1}{r_{01}} \right| \Phi_0(r_1) \chi_i^+(0) \right\rangle \] (3.6.3)

Using (3.4.2) and (3.4.4) in (3.6.3) and then evaluating \( \left\langle \varphi_{2s}(r_2) \right| \Phi_0(r_2) \right\rangle \) analytically we have
\[ T_{fi}^d = -16N_1 \alpha^2 Z_p \left[ \frac{1}{(\alpha + p)^3} + \frac{c}{(\alpha + q)^3} - \frac{3\alpha}{(\alpha + p)^4} \right. \]
\[ \left. - \frac{3ac}{(\alpha + q)^4} \right| \chi_f^-(0) \varphi_{2s}(r_1) \right| \frac{1}{r_{01}} \left| \phi_0(r_0) \chi_i^+(0) \right\rangle \] (3.6.4)

### 3.6.1.2 Exchange Amplitude

Here again the two terms in equation (3.3.17) are similar so that

\[ T_{fi}^{ex} = -4Z_p \left( \chi_f^-(0) \psi_f(1,2) \right| \frac{1}{r_{01}} \left| \psi_i(0,2) \chi_i^+(1) \right\rangle \] (3.6.5)

Substituting into (3.6.3) the appropriate wave functions and simplifying we have

\[ T_{fi}^{ex} = -4Z_p \langle \varphi_{2s}(r_2) | \phi_0(r_2) \rangle \left( \chi_f^-(0) \varphi_{2s}(r_1) \right| \frac{1}{r_{01}} \left| \phi_0(r_0) \chi_i^+(1) \right\rangle \] (3.6.6)

which when \( r_2 \) integral is evaluated analytically yields

\[ T_{fi}^{ex} = -16N_1 \alpha^2 Z_p \left[ \frac{1}{(\alpha + p)^3} + \frac{c}{(\alpha + q)^3} - \frac{3\alpha}{(\alpha + p)^4} \right. \]
\[ \left. - \frac{3ac}{(\alpha + q)^4} \right| \chi_f^-(0) \varphi_{2s}(r_1) \right| \frac{1}{r_{01}} \left| \phi_0(r_0) \chi_i^+(1) \right\rangle \] (3.6.7)
3.6.2 1s²—2s2p ¹P Transition

3.6.2.1 Direct Amplitude

Proceeding as in section 3.6.1.1 and using 3.4.1 and 3.4.5 as the initial and final state wave functions, respectively, in equation (3.3.16) we have

\[
T_{fi}^d
= -\frac{4Z_p}{\sqrt{2}} \left[ \langle \chi_f^- (0) \phi_{2s} (2, r_1) \phi_{2p} (\beta, r_2) \mid \frac{1}{r_{01}} \mid \phi_0 (r_1) \phi_0 (r_2) \chi_i^+ (0) \rangle \right. \\
+ \left. \langle \chi_f^- (0) \phi_{2s} (2, r_2) \phi_{2p} (\beta, r_1) \mid \frac{1}{r_{01}} \mid \phi_0 (r_1) \phi_0 (r_2) \chi_i^+ (0) \rangle \right]
\]  \hspace{1cm} (3.6.8)

which on using orthogonality property of wave functions simplifies into

\[
T_{fi}^d
= -2\sqrt{2}Z_p \langle \phi_{2s} (2, r_2) \mid \phi_0 (r_2) \rangle \langle \chi_f^- (0) \phi_{2p} (\beta, r_1) \mid \frac{1}{r_{01}} \mid \phi_0 (r_1) \chi_i^+ (0) \rangle
\]

\hspace{1cm} (3.6.9)

After analytical evaluation of \( r_2 \) integral, we obtain

\[
T_{fi}^d = -8\sqrt{2}N_1 Z_p \left[ \frac{1}{(1 + p)^3} + \frac{c}{(1 + q)^3} - \frac{3}{(1 + p)^4} - \frac{3c}{(1 + q)^4} \right]
\]

\[
\langle \chi_f^- (0) \phi_{2p} (\beta, r_1) \mid \frac{1}{r_{01}} \mid \phi_0 (r_1) \chi_i^+ (0) \rangle
\]
3.6.2.2 Exchange Amplitude

Similarly the exchange term (equation 3.3.17) for this excitation becomes

\[
T_{fi}^{ex} = -2\sqrt{2}Z_p \langle \phi_{2s}(2, r_2) | \phi_0(r_2) \rangle \langle \chi_f(0) \phi_{2p}(\beta, r_1) | \frac{1}{r_{01}} | \phi_0(r_0) \chi_i^+(1) \rangle
\]

which is evaluated to yield

\[
T_{fi}^{ex} = -8\sqrt{2}N_1 Z_p \left[ \frac{1}{(1 + p)^3} + \frac{c}{(1 + q)^3} - \frac{3}{(1 + p)^4} \right]
\]
\[
- \frac{3c}{(1 + q)^4} \langle \chi_f(0) \phi_{2p}(\beta, r_1) | \frac{1}{r_{01}} | \phi_0(r_0) \chi_i^+(1) \rangle
\]

3.7 The Computer Code

The direct and exchange T-matrix elements obtained in the forms given by equations (3.6.4) and (3.6.7) for (2s\(^3\) \(^1\)S excitation and equations (3.6.10) and (3.6.12) for (2s2p) \(^1\)P excitation are to be numerically evaluated. This requires a computer code.
Madison and Bartschart (1996) developed a code to evaluate integrals similar to ours. Their expressions were

\[
f = -2Z_p \left\langle \chi_f^- (0) \psi_f (1) \frac{1}{r_{01}} \left| \psi_i (1) \chi_i^+ (0) \right. \right\rangle
\]  

(3.7.1)

and

\[
g = -2Z_p \left\langle \chi_f^- (0) \psi_f (1) \frac{1}{r_{01}} \left| \psi_i (0) \chi_i^+ (1) \right. \right\rangle
\]  

(3.7.2)

for direct and exchange amplitudes for 2s and 2p excitations of hydrogen atom by electron or positron impact.

By comparing these two expressions with our expressions we need to multiply their amplitudes with a factor, \(K\). This modification was made and wave functions and distortion potentials were changed to adapt their code to our problem. These comparisons led to two constants \(K_1\) and \(K_2\) corresponding to \(2s^2\) \(^1\)S and \((\text{2s2p})^1\)P excitations, respectively, as follows

\[
K_1 = 8N_1 \alpha^2 \left[ \frac{1}{(\alpha + p)^3} + \frac{c}{(\alpha + q)^3} - \frac{3\alpha}{(\alpha + p)^4} - \frac{3\alpha c}{(\alpha + q)^4} \right]
\]  

(3.7.3)

and
\[ K_2 = 4\sqrt{2}N_1 \left[ \frac{1}{(1+p)^3} + \frac{c}{(1+q)^3} - \frac{3}{(1+p)^4} - \frac{3c}{(1+q)^4} \right] \quad (3.7.4) \]
Chapter 4

NUMERICAL TECHNIQUE

4.1 Introduction

The differential equation (3.3.20) and the integrations (equations 3.3.16, 3.3.17 and 3.3.24) are difficult to evaluate exactly. A numerical technique is required to estimate these values. The DWBA1 program developed by Madison and Bartschat (1996) was adapted for the present problem. The changes made in the program, besides that mentioned in section 3.7, are discussed in section 4.2. In section 4.3 the radial mesh is discussed while the transfers of the wave functions and the static potentials into the radial mesh are discussed in sections 4.4 and 4.5, respectively.

4.2 Adaptation of the DWBA1 Program

4.2.1 The Energies of the states

The ground state, \( 2s^2 \, ^1S \) state and \( 2s2p \, ^1P \) state energies are, respectively, \(-5.80534\text{Ry}, -4.29194\text{Ry}, \) and \(-4.24768\text{Ry} \) (Lindroth, 1994). These energy replacements were made in the main of the program.

4.2.2 The Atomic Wave Functions

The wave functions (defined in equations 3.4.2, 3.4.4 and 3.4.7) appearing in equations (3.6.4), (3.6.7), (3.6.10) and (3.6.12) replace the hydrogen wave functions in the subroutine, FHYD.
4.2.3 The Distortion Potentials

The calculated static potentials from section 3.5 are different from the hydrogen static potentials in the program. Appropriate replacement for these static potentials are made in the subroutine POTENT (see table 4.1). The averaging of the ground state static potential and the final state static potential to obtain the final channel distortion potential is incorporated by the pre-multiplication by the constants CSTF1 and CSTF2 (both read in as 0.5). The initial channel distortion potential is obtained by pre-multiplication of the static potentials by the constants CSTI1 and CSTI2 (read in as 1 and 0, respectively).

<table>
<thead>
<tr>
<th>STATE</th>
<th>ORIGINAL (HYDROGEN)</th>
<th>PRESENT (HELIUM)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Equation</td>
<td>Equation</td>
</tr>
<tr>
<td>Ground state</td>
<td>( \text{UCENTR}(I) = -2 \times \exp(X2M \times \text{ONE}+X) )</td>
<td>Equation ( (3.5.8) )</td>
</tr>
<tr>
<td>Excitation to 2s state</td>
<td>( \text{UCENTR}(I) = 2 \times \exp(-X) \times (X3/24.0D0 +XX/FOUR+0.75D0*X+\text{ONE}) )</td>
<td>Equation ( (3.5.12) )</td>
</tr>
<tr>
<td>Excitation to 2p state</td>
<td>( \text{UCENTR}(I) = 2 \times \exp(-X) \times (X3/8.0D0 +XX/FOUR+0.75D0*X+\text{ONE}) )</td>
<td>Equation ( (3.5.16) )</td>
</tr>
</tbody>
</table>

Table 4.1: An illustration of the changes made to the DWBA1 program. The 2s and 2p states in helium are \( (2s^2)^1S \) and \( (2s2p)^1P \) respectively.

4.2.4 The Differential Cross Sections

The differential cross section for hydrogen is given by
A change was made in the main program to cater for the difference between the expression above and the expression (3.3.23).

4.3 Radial Discretization

A radial mesh is necessary to solve the differential equation (3.3.20) and to perform integrations numerically. The radial mesh used in the program is an adaptation of the Herman-Skillman mesh in which a constant step size is used for 40 points then the step size is doubled for the next 40 points. This is repeated until a step size that can not be doubled without loss of numerical accuracy is obtained.

A constant step size is then maintained to the last point in the mesh. In the program 2720 points are used. The last doubling of the step size occurs after the 200\textsuperscript{th} mesh point (see figure 4.1 below).
4.4 Transfer of Wave Functions into the Radial Mesh

The integrations in section 3.6 for the direct and exchange amplitudes require the values of the atomic wave functions at various mesh points. The values of the analytical ground state and excited state wave functions at each mesh point were calculated and some are graphically presented in figure 4.2 below. The wave functions fall off rapidly so that the contribution of higher mesh points is negligible.
Figure 4.2: r-multiplied initial wave function, $\phi_{1s}$, and final wave functions ($\phi_{2s}$ and $\phi_{2p}$) on each mesh point.

4.5 Transfer of the Static Potentials into the Radial Mesh

The differential equation (3.3.20) requires the distortion potentials to be evaluated at every radial point. The static potentials are plotted at every mesh point in figure 4.3 and 4.4 for the $2s^2 \, ^1S$ and $2s2p \, ^1P$ excitations, respectively. The initial channel distortion potential is just the initial state static potential while the final channel distortion potential is the average of the initial state static potential and the final state static potential. The final state distortion potential is plotted together with the static potentials. The potentials fall off rapidly and the final state for the $2s2p \, ^1P$
falls off more rapidly than the $2s^2\,^1S$ state. The intermediate final state distortion potential nears the final state distortion potential with increase in radial distance.

Figure 4.3: The $r$-multiplied static potentials corresponding to the ground state (VSTi) and the $2s^2\,^1S$ state (VSTf) with the intermediate final channel distortion potential (Vd). The second graph shows how rapidly the potentials fall off.
Figure 4.4: Same as in Figure 4.3 for 2s2p \(^1\)P final state.

4.6 The Distorted Waves

4.6.1 The Numerov Method

Equation 3.3.20 can be rewritten, for a given state and \(l\)-value, as

\[
\frac{d^2\chi(r)}{dr^2} = F(r)\chi(r) \tag{4.6.1}
\]

where

\[
F(r) = \frac{v(r) + l(l + 1)}{r} - k^2 \tag{4.6.2}
\]

\(v(r)\) is the \(r\)-multiplied distortion potential given as
\[ v(r) = rU(r) \quad (4.6.3) \]

The Numerov method is suitable for solving second order differential equations, such as 4.6.1, in which the first derivative is absent. Since we will be calculating the distorted waves at every mesh point, we denote \( \chi(r) \), \( \chi(r + h) \) and \( \chi(r - h) \) by \( \chi_n \), \( \chi_{n+1} \) and \( \chi_{n-1} \) respectively. \( h \) is a constant step size. Then, by Taylor series expansion of \( \chi(r + h) \) and \( \chi(r - h) \) around \( \chi(r) \), we have

\[
\begin{align*}
\chi_{n+1} &= \chi_n + h\chi'_n + \frac{h^2\chi''_n}{2!} + \frac{h^3\chi'''_n}{3!} + \frac{h^4\chi^{(iv)}_n}{4!} + \cdots \\
\chi_{n-1} &= \chi_n - h\chi'_n + \frac{h^2\chi''_n}{2!} - \frac{h^3\chi'''_n}{3!} + \frac{h^4\chi^{(iv)}_n}{4!} - \cdots
\end{align*}
\]

(4.6.4)

On summing up the pair of equations 4.6.4 and rearranging we obtain

\[
\chi_{n+1} = 2\chi_n - \chi_{n-1} + h^2\chi''_n + \frac{h^4\chi^{(iv)}_n}{12} + \cdots 
\]

(4.6.5)

But from equation 4.6.1 we can write

\[
\chi''_n = F_n\chi_n
\]

(4.6.6)

and

\[
\chi^{(iv)}_n = \frac{d^2}{dr^2}(F_n\chi_n)
\]

(4.6.7)
Using the central difference formula similar to equation 4.6.5, and truncating after the second derivative term, equation 4.6.7 can be rewritten as

\[
\chi_n^{(iv)} = \frac{F_{n+1}\chi_{n+1} - 2F_n\chi_n + F_{n-1}\chi_{n-1}}{h^2}
\]  

(4.6.8)

Putting 4.6.6 and 4.6.8 into 4.6.5 and rearranging we have

\[
\chi_{n+1} = \frac{2\left(1 - \frac{h^2F_n}{12}\right)\chi_n - \left(1 - \frac{h^2F_{n-1}}{12}\right)\chi_{n-1} + h^2F_n\chi_n}{\left(1 - \frac{h^2F_{n+1}}{12}\right)}
\]  

(4.6.9)

which is the recurrence relation used in obtaining the distorted waves at various mesh points and for given \(l\)-values.

With the above recurrence relation we need the first two points to start off the Numerov integration. In the next section we discuss the first two points for this problem.

### 4.6.2 Distorted Waves for the First Two Points

The fact that the projectile can not propagate into the nucleus sets the initial condition that the distorted wave should collapse at \(r = 0\). Therefore \(\chi_0 = 0\). To obtain \(\chi_1\) we assume a polynomial fit of the form
Then

\[ \chi = Pr^{l+1} \quad (4.6.10) \]

Further differentiation of (4.6.12) yields

\[ \chi'' = P''r^{l+1} + \frac{2(l + 1)}{r} P'r^{l+1} + \frac{l(l + 1)}{r^2} Pr^{l+1} \quad (4.6.11) \]

Equating the right hand sides of (4.6.11) and (3.3.20) we obtain

\[ rP'' + 2(l + 1)P' = v - k^2r \quad (4.6.12) \]

Further differentiation of (4.6.12) yields

\[ \begin{align*}
    rP'''' + (2l + 3)P''' &= (v - k^2r)P' + (v' - k^2)P \\
    rP^{(iv)} + (2l + 4)P''' &= (v - k^2r)P'' + 2(v' - k^2)P' + v''P \\
    rP^{(v)} + (2l + 5)P^{(iv)} &= (v - k^2r)P'' + 3(v' - k^2)P'' + 3v''P' + v'''P
\end{align*} \quad (4.6.13) \]

Now \( P \) is a polynomial in \( r \) given as

\[ P = 1 + a_1r + a_2r^2 + a_3r^3 + a_4r^4 + \cdots \quad (4.6.14) \]

On differentiating (4.6.14) five times and using (4.6.13) we obtain the coefficients as
Using the forward difference method $v$ and its derivatives were found to be

\[
\begin{align*}
a_1 &= \frac{v}{2l + 2} \\
a_2 &= \frac{a_1 v + v' - k^2}{4l + 6} \\
a_3 &= \frac{a_2 v + a_1 (v' - k^2) + \frac{v''}{2}}{6l + 12} \\
a_4 &= \frac{a_3 v + a_2 (v' - k^2) + \frac{a_1 v''}{2} + \frac{v'''}{6}}{6l + 12}
\end{align*}
\]

(4.6.15)

The distorted waves are therefore solved for the first two points. Other points are obtained using the Numerov recurrence relation.

\[
\begin{align*}
v &= v_1 - \Delta v_1 + \Delta^2 v_1 - \Delta^3 v_1 + \Delta^4 v_1 \ldots \\
v' &= \frac{1}{h} \left( \Delta v_1 - \frac{3\Delta^2 v_1}{2} + \frac{11\Delta^3 v_1}{6} - \frac{50\Delta^4 v_1}{24} \ldots \right) \\
v'' &= \frac{1}{h^2} \left( \Delta^2 v_1 - \Delta^3 v_1 + \frac{33\Delta^4 v_1}{24} \ldots \right) \\
v''' &= \frac{1}{h^3} \left( \Delta^3 v_1 - \frac{10\Delta^4 v_1}{24} \ldots \right)
\end{align*}
\]

(4.6.16)

The distorted waves are therefore solved for the first two points. Other points are obtained using the Numerov recurrence relation.

4.6.3 Normalization of the Distorted Waves

The code is written to check for overflows and underflows and normalize the distorted waves appropriately. The distorted waves obtained are real and unnormalized. Upon normalization, the distorted waves are complex. The complex
normalization constant is obtained by equating the logarithmic derivatives of the calculated distorted waves and the asymptotic boundary condition (3.3.21). Below is a short table of the distorted waves obtained for $2s^2 \, ^1S$ excitation for 100 eV impact energy for $l = 4$.

<table>
<thead>
<tr>
<th>MESH POINT</th>
<th>UNNORMALIZED $\chi$</th>
<th>NORMALIZED $\chi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.32E-14</td>
<td>6.65E-15</td>
</tr>
<tr>
<td>2</td>
<td>1.70E-12</td>
<td>2.13E-13</td>
</tr>
<tr>
<td>3</td>
<td>1.29E-11</td>
<td>1.62E-12</td>
</tr>
<tr>
<td>4</td>
<td>5.46E-11</td>
<td>6.83E-12</td>
</tr>
<tr>
<td>5</td>
<td>1.67E-10</td>
<td>2.09E-11</td>
</tr>
<tr>
<td>10</td>
<td>5.36E-09</td>
<td>6.70E-10</td>
</tr>
<tr>
<td>20</td>
<td>1.73E-07</td>
<td>2.16E-08</td>
</tr>
<tr>
<td>40</td>
<td>5.60E-06</td>
<td>7.01E-07</td>
</tr>
<tr>
<td>60</td>
<td>1.83E-04</td>
<td>2.29E-05</td>
</tr>
<tr>
<td>80</td>
<td>1.40E-03</td>
<td>1.75E-04</td>
</tr>
<tr>
<td>100</td>
<td>1.79E-02</td>
<td>2.24E-03</td>
</tr>
<tr>
<td>500</td>
<td>5.64E+00</td>
<td>7.05E-01</td>
</tr>
<tr>
<td>1000</td>
<td>-6.21E+00</td>
<td>-7.77E-01</td>
</tr>
<tr>
<td>1500</td>
<td>-3.91E+00</td>
<td>-4.89E-01</td>
</tr>
<tr>
<td>2000</td>
<td>7.56E+00</td>
<td>9.47E-01</td>
</tr>
<tr>
<td>2500</td>
<td>1.13E+00</td>
<td>1.42E-01</td>
</tr>
</tbody>
</table>

Normalization constant $a_l = 0.1251$

Phase $e^{i\delta l} = 1 - 0.008259i$

Table 4. 2: Table showing the initial channel distorted waves for $(2s^2) \, ^1S$ excitation and for $l = 4$ using Numerov method.

4.7 Simpson’s Three-Point Integration

The integration required to obtain the transition matrix elements and total cross sections are performed using Simpson’s three point method that requires
\[ \int_{x_j}^{x_{j+2}} f(x) \, dx = \frac{h}{3} \left( f(x_j) + 4f(x_{j+1}) + f(x_{j+2}) \right) \]  

(4.7.1)

where

\[ h = x_{j+1} - x_j \]  

(4.7.2)

On applying 4.7.1 with smaller \( h \), the numerical approximation to the integral improves. Below is a graph of the integral cross section obtained on integrating the differential cross section using the Simpson’s three point rule.

![Graph of integral cross section](image)

Figure 4.5: Numerical integration of the differential cross section using Simpson’s three-point rule.
Chapter 5

RESULTS AND DISCUSSION

5.1 Introduction

The present model of the distorted wave method has been applied in the calculation of the total and differential cross sections for the doubly excited transitions

\[ e + \text{He} \, (1s^2) \rightarrow \text{He}^{**} \, (2s^2 \, 1S) + e \]

and

\[ e + \text{He} \, (1s^2) \rightarrow \text{He}^{**} \, (2s2p \, 1P) + e \]

from threshold to high energies. In section 5.2 the \((2s2p) \, 1P\) results are discussed while in section 5.3 the \((2s^2) \, 1S\) results are discussed. In both excitations the discussion of the total cross sections precedes the differential cross section discussion. This is so as differential cross sections will be discussed at various energies corresponding to the total cross sections features. Comparisons with available experimental and theoretical results are made.

5.2 1s^2 \(\rightarrow\) (2s2p) \(1P\) Transition

5.2.1 Total Cross Section

The results obtained for the total cross sections are tabulated in table 5.1 then graphed in figure 5.1. The present distorted wave results with exchange (Pexc+)
and without exchange (Pexc-) are compared with the first Born (1st Born) and second Born with higher terms correction (WMcD) results of Woollings and McDowell (1973), the 1.58 (Gill 1.58) and 1.8 (Gill 1.8) excited state wave function screening constants results of Gillespie (1973) and the first Born (M&M) results of Massey and Mohr (1935). The present results are in good agreement with both results of Woollings and McDowell but in poor agreement with the results of Gillespie and Massey and Mohr. The present exchange results show a resonance at 70 eV and a dip at 100 eV. Exchange enhances cross sections up to 90 eV but does not there after. It is observed that the exchange contribution diminishes at high energies.

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>70</th>
<th>100</th>
<th>200</th>
<th>300</th>
<th>400</th>
<th>500</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma \left(10^{-4}\pi a_0^2\right)$ Pexc+</td>
<td>9.132</td>
<td>5.419</td>
<td>1.453</td>
<td>17.60</td>
<td>17.78</td>
<td>16.93</td>
<td>12.88</td>
</tr>
<tr>
<td>$\sigma \left(10^{-4}\pi a_0^2\right)$ Pexc-</td>
<td>1.248</td>
<td>7.840</td>
<td>1.851</td>
<td>19.68</td>
<td>19.19</td>
<td>17.66</td>
<td>12.97</td>
</tr>
</tbody>
</table>

Table 5.1: Total cross sections for 1s$^2$ $\rightarrow$ (2s2p) $^1$P excitation of helium by electron impact
Figure 5.1: Total cross sections for $1s^2 \rightarrow (2s2p) \, ^1P$ excitation of helium by electron impact. Pexc+ (present results with exchange), Pexc- (present results without exchange), Gill 1.58 and Gill 1.8 (Gillespie’s (1973) results using 1.58 and 1.8 as wave function screening constants, respectively), 1st Born and WMcD (Woollings and McDowell’s (1973) first Born and Second Born with higher terms corrections results, respectively) and M&M (Massey and Mohr’s (1935) first Born results).
5.2.2 Differential Cross Sections

The differential cross sections are calculated at 70 eV, 90 eV, 100 eV, 200 eV and 400 eV electron impact energies and the contribution of exchange is discussed. At 200 eV and 400 eV, differential cross sections due to Massey and Mohr (1935) are available. The present results at these energies are compared with them. The present distorted wave results are tabulated in table 5.2 and graphed in figures 5.2—5.6. Discussions are based on the graphs.

The exchange contribution to the differential cross sections is appreciable at low energies and is largely responsible for the resonance at 70 eV (figure 5.2). This is so as the cross section with exchange is higher than the direct (without exchange) cross section from around 20°. There is a slight hump registered at around 60° by the exchange cross section. At 90 eV, the energy about which the integral cross section with exchange and without exchange coincides, the exchange contribution enhances cross sections after 50° (figure 5.3). This happens at a region of a lower power of 10 compared to the region where exchange inhibits cross sections so that even if the direct cross sections are higher for a shorter range of angles, the effect cancels out in the integral cross section. There is a shallow dip registered at around 30° by the cross section with exchange.
<table>
<thead>
<tr>
<th>Energy</th>
<th>70eV</th>
<th>90eV</th>
<th>100 eV</th>
<th>200 eV</th>
<th>400 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Angle (deg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>1.79E-04</td>
<td>1.213E-03</td>
<td>2.889E-03</td>
<td>4.81E-02</td>
<td>1.79E-01</td>
</tr>
<tr>
<td>10</td>
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<td>8.291E-04</td>
<td>1.909E-03</td>
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<tr>
<td>20</td>
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<td>7.65E-06</td>
<td>1.81E-06</td>
</tr>
<tr>
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<td>2.573E-04</td>
<td>1.558E-04</td>
<td>1.045E-04</td>
<td>5.06E-06</td>
<td>1.03E-06</td>
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<td>1.434E-04</td>
<td>9.536E-05</td>
<td>3.58E-06</td>
<td>6.23E-07</td>
</tr>
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<td>8.717E-05</td>
<td>2.71E-06</td>
<td>3.93E-07</td>
</tr>
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<td>110</td>
<td>2.104E-04</td>
<td>1.220E-04</td>
<td>8.021E-05</td>
<td>2.15E-06</td>
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Table 5.2: Differential cross sections for $1s^2$ – (2s2p) $^1P$ excitation (with exchange) in $a_0^2$/sr.
Figure 5.2: Differential cross sections for $1s^2 \rightarrow (2s2p)^1P$ excitation of helium by electron impact at 70 eV. Pexc+ (present results with exchange) and Pexc- (present results without exchange).
Figure 5.3: Differential cross sections for $1s^2 \rightarrow (2s2p)\,^1P$ excitation of helium by electron impact at 90 eV. Pexc+ (present results with exchange) and Pexc- (present results without exchange).
At 100 eV (figure 5.4), the direct cross section is higher than the cross section with exchange up to 60° after which the cross section with exchange is higher. This, however, happens at low values (two powers of ten lower) and hence the integral direct cross section is higher at this energy. A shallow dip is registered at 30° by the exchange cross section. At 200 eV (figure 5.5), cross sections with exchange and without exchange are very close. The direct cross sections are slightly higher up to 110° after which the results with exchange are higher. This happens at very low powers of 10 so that the integral direct cross sections are higher. At 400 eV (figure 5.6), both results (with exchange and without exchange) are very close at lower angles (up to 90°) but at higher angles cross sections with exchange are lower than cross sections without exchange. At this energy exchange contribution is negligible as is expected. At 200 eV and 400 eV, the present results are in good agreement with the results of Massey and Mohr. However, there is a big discrepancy between our results and theirs in the total cross sections.
Figure 5.4: Differential cross sections for $1s^2\rightarrow (2s2p)\,^1P$ excitation of helium by electron impact at 100 eV. Pexc+ (present results with exchange) and Pexc- (present results without exchange).
Figure 5.5: Differential cross sections for $1s^2 \rightarrow (2s2p)^1P$ excitation of helium by electron impact at 200 eV. Pexc+ (present results with exchange), Pexc- (present results without exchange) and M&M (Massey and Mohr’s (1935) first Born results).
Figure 5.6: Differential cross sections for $1s^2 \rightarrow (2s2p)^1P$ excitation of helium by electron impact at 400 eV. Pexc+ (present results with exchange), Pexc- (present results without exchange) and M&M (Massey and Mohr’s (1935) first Born results).
5.3 $1s^2 - (2s^2)^1S$ Transition

5.3.1 Total Cross section

The present results, with exchange ($P_{\text{exc}+}$) and without exchange ($P_{\text{exc}-}$) are compared with the experimental results (Spence) of Spence (1975) and the theoretical results of Plottke (2004) on using 2 and 3 as the frozen core level (Plottke $n_c=2$ and Plottke $n_c=3$ respectively) and Massey and Mohr (1935) (M&M) (figure 5.7). The present results are in good agreement with the experimental results of Spence, which are available for a very short energy range above threshold but in poor agreement with the two theoretical results available. The results of Massey and Mohr are not only in disagreement with our results but also with the general trend that at higher energies cross sections should be lower. Their cross sections increase with energy. Our results and the experimental results of Spence are higher than the results of Massey and Mohr and the results of Plottke. Here, again the exchange contribution diminishes with increase in energy.

It is observed that the total cross sections for this transition are lower than those of the $(2s2p)^1P$ transition. This is in accordance with the Laporte rule that requires the $(2s^2)^1S$ transition to be an optically forbidden transition and $(2s2p)^1P$ to be optically allowed. Optically allowed transitions generally have higher cross sections than optically forbidden ones. Further, exchange enhances cross sections
up to 100 eV and is responsible for the resonance at 75 eV. Table 5.3 gives the total cross sections for this transition with a corresponding graph in figure 5.7.

<table>
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<tr>
<th>Energy (eV)</th>
<th>75</th>
<th>100</th>
<th>200</th>
<th>300</th>
<th>400</th>
<th>500</th>
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<td>$\sigma \left(10^{-4}\pi a_0^2\right)$ Pexc+</td>
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<td>5.742</td>
<td>2.248</td>
<td>2.036</td>
<td>1.766</td>
<td>1.541</td>
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<td>$\sigma \left(10^{-4}\pi a_0^2\right)$ Pexc-</td>
<td>1.653</td>
<td>3.450</td>
<td>3.762</td>
<td>2.868</td>
<td>2.240</td>
<td>1.839</td>
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Table 5.3: Total cross sections for 1s$^2$ $\rightarrow$ (2s$^2$) $^1$S excitation of helium by electron impact.
Figure 5.7: Total cross sections for $2s^2 \rightarrow (2s^2)^{1}S$ excitation of helium by electron impact. Pexc+ (present results with exchange), Pexc- (present results without exchange), Plotcke n=2 and Plotcke n=3 (Plotcke’s (2004) results using 2 and 3 as the frozen core level) Spence (Spence’s (1975) experimental results) and M&M (Massey and Mohr’s (1935) first Born results).
5.3.2 Differential Cross Sections

Differential cross sections have been calculated at 100 eV, 120 eV, 175 eV, 200 eV and 400 eV electron impact energies. We did not find other differential cross sections with which to compare ours. We will only study the exchange contribution to the cross section at these energies. The differential cross sections are first tabulated in table 5.4 before being graphed in figures 5.8—5.12.

At 100 eV, the energy at which the total cross section with and without exchange coincide, differential cross sections are presented in figure 5.8. At this energy the cross sections without exchange are higher up to 60° after which the cross sections with exchange are higher. Although the cross sections with exchange are higher for a longer range of angles, the direct cross sections are higher in the higher value region, hence a cancellation effect. There is a shallow dip at around 40° for the exchange cross section.

At 120 eV (figure 5.10), the direct cross section is higher than the cross sections with exchange up to 70°. The exchange cross sections are higher at a lower power of ten, hence, overall, direct cross sections are higher at this energy. The dip for the cross section with exchange deepens. At 175 eV (figure 5.11), the direct cross section is higher up to 90°. The cross section with exchange at large angles (above 90°) although higher than the direct cross section, it is smaller in magnitude.
Hence, overall, the direct cross section (without exchange) is higher. The dip observed at 120 eV for the cross section with exchange further deepens at 175 eV.

<table>
<thead>
<tr>
<th>Energy Angle (deg)</th>
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<th>120eV</th>
<th>175eV</th>
<th>200eV</th>
<th>400</th>
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Table 5.4 Differential cross sections for 1s$^2$ — (2s$^2$) 1S excitation (with exchange) in a$^2$/sr.
Figure 5. 8: Differential cross sections for $1s^2 - (2s^2)^1S$ excitation of helium by electron impact at 100 eV. Pexc+ and Pexc- (present results with and without exchange respectively).
Figure 5.9: Differential cross sections for $1s^2 - (2s^2)^1S$ excitation of helium by electron impact at 120 eV. $P_{exc}^+$ and $P_{exc}^-$ (present results with and without exchange respectively).
Figure 5. 10: Differential cross sections for $1s^2 \rightarrow (2s^2)^1S$ excitation of helium by electron impact at 175 eV. Pexc+ and Pexc- (present results with and without exchange respectively).
Figure 5.11: Differential cross sections for $1s^2 \rightarrow (2s^2)^1S$ excitation of helium by electron impact at 200 eV. Pexc+ and Pexc- (present results with and without exchange respectively).

At 200 eV (figure 5.12), the cross section without exchange is higher at higher powers of ten and up to $100^0$, hence the integral direct cross section is higher at
this energy. The dip grows shallower. At 400 eV, the result with exchange and that
without exchange are very close throughout the angular range. This means the
exchange contribution is negligible as is expected at high energies.

Figure 5. 12: Differential cross sections for 1s$^2$—(2s$^2$) $^1$S excitation of helium by
electron impact at 400 eV. Pexc+ and Pexc- (present results with and without
exchange respectively).
Chapter 6

CONCLUSION AND RECOMMENDATIONS

6.1 Conclusion

The differential and integral cross sections for the electron impact double excitation of helium atom from the ground state to the \((2s^2) \, ^1S\) and \((2s2p) \, ^1P\) states have been calculated from threshold to high energies. Deductions shall be confined more on the total cross sections as there are more results available on these.

Though there were not many reported theoretical or experimental results, the agreement between the present \((2s^2) \, ^1S\) results and the only available experimental measurement (Spence, 1975), is encouraging. However, the range for which these results were reported is too short to draw unambiguous conclusions. Even so, it can, loosely, be said that the present model was a success in predicting the cross sections for \((2s^2) \, ^1S\) excitation of helium atom. The disagreement of the present results with the results of Massey and Mohr (1935) is not only in magnitude but also in trend.

To further support the present model is the good agreement between the present results and the results of Woollings and McDowell (1973) for the \((2s2p) \, ^1P\) excitation. Even though the present results are in poor agreement with the results of Gillespie (1973) and Massey and Mohr (1935), the differential cross section
results of Massey and Mohr at 200 eV and 400 eV are in close agreement with the present results.

More so, the cross sections obtained by this method obey general trends. These include:

i. The $(2s2p)^1P$ excitation cross section is nearly 10 times higher as compared to the $(2s^2)^1S$ excitation cross sections. This is in accordance to the Laporte rule which requires the transition to the $(2s^2)^1S$ excited state to be optically forbidden and the transition to the $(2s2p)^1P$ excited state be optically allowed.

ii. The cross sections decrease with increase in impact energy since the probability of interaction decreases with increase in projectile energy.

iii. The exchange contribution to the cross section decreases with increase in projectile energy since the ‘knock off’ process is more unlikely to occur at high energies without leading to ionization.

6.2 Recommendations

Due to the success of this method in obtaining the differential and integral cross sections for the $(2s^2)^1S$ and $(2s2p)^1P$ doubly excited states, the following recommendations are made:
i. More experimental measurements with wider ranges of energies to be made on the doubly excited autoionizing states.

ii. Further studies to be carried out to find the effect of including the neglected terms while evaluating the T-matrix elements.

iii. The present model to be extended to the study of other doubly excited states e.g. (2s2p) $^3P$ state for which Spence provided experimental measurements.

iv. The present model be adopted with superior wave functions to those used in this study.
REFERENCES


