A DISTORTED WAVE METHOD APPLIED TO STUDY THE 2s AND 2p EXCITATION OF HELIUM ATOM BY ELECTRON IMPACT

BY

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A distorted wave method applied to
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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To my wife Alice, and our son Raphael Muriithi
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<tr>
<td>CCC</td>
<td>Convergent Close Coupling</td>
</tr>
<tr>
<td>CCC75</td>
<td>Convergent Close Coupling with 75 Target State</td>
</tr>
<tr>
<td>CCC85</td>
<td>Convergent Close Coupling with 85 Target State</td>
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<td>CPB</td>
<td>Coulomb-projected Born approximation</td>
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<tr>
<td>DCS</td>
<td>Differential Cross Section</td>
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<td>DW</td>
<td>Distorted wave</td>
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<td>DWM</td>
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<td>FOMBT</td>
<td>First Order Many Body Theory</td>
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ABSTRACT

Electron scattering by atoms and molecules has attracted considerable attention since the earliest days of quantum mechanics. This is because they form the basis of understanding of many experimental techniques in physics, for example Rutherford back scattering and atomic and molecular spectroscopy. Due to the demand for atomic collision data set in various fields of physics various experimental techniques and theoretical approaches have been developed. In this study the distorted wave method has been applied to calculate the differential and integral cross sections for $1^1S$-$2^3S$ and $1^1S$-$2^3P$ excitations of helium atom by electron impact in the energy range of 40-200 eV. The initial distortion potential was taken as the static potential of the helium (target) atom in the initial state ($1^1S$) while the final distortion potential was taken as the average of the initial- and final-state static potentials of helium atom. The distorted waves were determined by partial wave expansion method by expanding them in terms of spherical harmonics while the radial equation corresponding to distorted waves was evaluated using Numerov method. A computer program DWBA1 written for $e^-$-H scattering by Madison and Bartschat was modified to perform the numerical calculations for $e^-$-He scattering and the results for differential and total cross section were calculated and compared with experimental and theoretical results. The present distorted wave method results for $2^3P$ at all incident energies except for 40 eV compared well with most of the experimental and theoretical results than in the case of $2^3S$ where the agreement was good at lower scattering angles except for 200 eV. Therefore we can conclude that the present distorted wave method worked for well for excitations. However it worked better for $1^1S$-$2^3P$ transition than in the case of $1^1S$-$2^3S$ transition.
CHAPTER 1
INTRODUCTION

1.1 Background to the Study

Electron scattering by atoms and molecules has attracted considerable attention since
the earliest days of quantum mechanics. This is partly because these processes
provide a means of investigating the dynamics of many-particle systems at
fundamental level. For example, many important observations made in physics are
through analyzing the scattering of particles or waves. Some of these include the
Rutherford’s discovery of the atomic nucleus, atomic and molecular spectroscopy and
nuclear fusion among others. In addition a detailed understanding of collision
processes is required in many fields particularly in astrophysics, plasma physics and
laser physics among others.

The theory of atomic collision is a branch of quantum collision theory which is
concerned with collision between two atomic systems or between an atomic system
and an “elementary particle” such as electron, a positron or a proton. In the study of
atomic collision, a beam of particles (the projectile) prepared in the remote past is
made to interact with the target (atom) and in the far future, detector records the
scattered particles in the asymptotic region (figure 1.1). After the interaction between
the projectile and the target atom the target may remain in the same initial state (elastic
collision) or exchange of energy between the projectile and the target may occur
resulting in target excitation or ionization (inelastic collision) (McDaniel, 1989).
The need for detailed knowledge of atomic collision physics permeates many fields of science and technology. In nuclear physics for example, there is a need for information on stopping powers and on the state of energetic ions penetrating solids and gases. In condensed matter physics it can be applied on method of surface and near surface characterization and material modification. The range of atomic collisions involved in astrophysics covers the entire extent of energy this is because most of the knowledge we have about universe resides in the form of photons; to interpret the message they bring in their journey to us, we must reconstruct the events in which they participated. The processes which produce the photons and the processes which modify them belong to the domain of electronic, atomic and molecular physics (Dalgarno, 1989).
To understand these collision processes the knowledge about the differential and total cross sections are of great importance. Differential cross section is defined as transition probabilities per unit time, per unit target scatterer and per unit relative flux of the incident particles with respect to the target and given as

\[ \sigma_{\text{diff}} = \frac{d\sigma}{d\Omega}(\theta, \phi) \]  

while the total cross section is simply obtained by integrating the differential cross section over all the scattering angles. This is given below as

\[ \sigma_{\text{tot}} = \int_0^{2\pi} \int_0^\pi \frac{d\sigma}{d\Omega} \sin \theta d\theta d\phi \]  

It is misleading to judge the success of a theoretical method purely on the agreement of the total cross section with the experimental measurement. Differential cross section (DCS) is known to provide better insight into a collisional process than the total cross section and should be calculated for the reliable assessment of a theoretical method (Katiyar and Srivastava, 1989). The reason for this is that, DCSs reflect more clearly the characteristics of the interacting potential and are more dependent on the target wave functions and approximation used than the integral cross-sections (ICS) (Zhong et al., 1997)

Specifically electron collision processes involving helium are important in a large variety of systems and environment e.g. various discharge and laser systems, fusion plasmas, planetary and astrophysical environment. From an academic point of view; these collisions represent simple processes that are suitable for theoretical treatment and refined calculation schemes. If the differential cross section for particular
scattering process for helium is known accurately, then this may be used to normalize data pertaining to other collision processes involving complex atoms. Because helium is the simplest system with electron-electron interaction term and it is easily handled experimentally and theoretically, it has become the subject of several studies. It is because of this potential application that considerable importance is attached to the determination of accurate cross section for electron-helium scattering (Scott and Taylor, 1979; Bartschat, 1998).

1.4 Statement of the Research Problem

The variation in the distorted wave method, which was used in this study, has never been used for a process, which occurs only through exchange. This study tested its applicability to $1^1S-2^3S$ and $1^1S-2^3P$ excitations of helium atom by electron impact which occurs only through exchange when spin dependent interactions are neglected.

1.5 Objectives of the Research Project

1.5.1 Main Objective

The main objective was to study the electron impact excitation of $2^3S$ and $2^3P$ states of helium atom by electron impact using the distorted wave method.

1.5.2 Specific Objectives

The specific objectives of the study were:

(i) To calculate the differential and integral cross-sections for $1^1S-2^3S$ and $1^1S-2^3P$ excitation of helium atom by electron impact using the distorted wave method.
(ii) To compare the results obtained with other theoretical and experimental results available.

(iii) To test the suitability of the present variation of distorted wave method to the study of $^2\!^3\!^S$ and $^2\!^3\!P$ excitation of helium atom by electron impact.

1.4 Rationale of the Study

The field of atomic collisions has been a test ground for various theoretical as well as many experimental methods in atomic physics; it is of great importance in many fields of physics, for example, plasma physics, laser development, gaseous discharge, fluorescent lighting and upper atmosphere dynamics among others. These collisions represent simple processes that are suitable for theoretical treatment and for developing and refining calculation schemes. Therefore, the available database is continuously being assessed in order to provide the most reliable dataset needed, for example, in calculation of rate coefficient for transport processes (Bartschat, 1998), and any new method proposed is assessed for its suitability. It is in this view that the present study was done. The variation in the distorted wave method, which was used here, has never been used for a process, which occurs only through exchange. So, it was interesting to see how this works for $^1\!^S\!-2\!^3\!S$ and $^1\!^S\!-2\!^3\!P$ excitations of helium atom by electron impact since they occur through exchange when spin dependent interactions are neglected.

More specifically, the study involving helium atom as the target is of great interest since the two electrons of the helium atom permits inter-electron repulsions which are
encountered in more complex atoms and ions to be introduced in a realistic manner. At the same time reliable wave functions are available for helium. Experimental data and theoretical calculations are also more readily available on helium than for other complex atoms. Therefore, the cross sections for helium excitations by electron-impact are of undisputed interest in experimental measurements and theoretical calculations.
CHAPTER 2
LITERATURE REVIEW

2.1 Introduction

Though the study of atomic collisions started in 1930s, more work has been done from 1970s and as a result various approximation methods have been applied by several researchers to study collision processes involving various atomic and sub-atomic systems as well as molecules. This was due to an increasing demand for reliable data sets of collision cross sections to be used in other fields such as astrophysics, laser physics and plasma physics among others (Bartschat, 1998).

2.2 Related Studies for Electron Helium Excitation

Various theoretical methods and experimental measurements have been applied by various researchers to study the differential and integral cross sections for electron-impact excitation of helium atom at different incident energies. Some of these theoretical methods are: R-matrix method, convergence close coupling, variable charge Coulomb projected Born approximation, first order many body theory and distorted wave methods. Studies on electron-helium scattering using all these approximation methods and experimental measurements are discussed in this section except for distorted wave methods which is discussed in section 2.3.

2.2.1 The R-Matrix Method

Berrington et al. (1975) used the R-matrix method to solve equations describing the scattering of electrons by helium atoms. They calculated the elastic and inelastic
cross-sections for excitation to $2^1S$, $2^3S$, $2^1P$ and $2^3P$ states from ground state ($1^1S$) and compared the results obtained with experimental results and other theoretical results. Further, Fon et al. (1977) extended R-matrix method to calculate the electron excitation cross sections for $2^3S$, $2^1S$, $2^3P$, and $2^1P$ states of helium between $n=2$ and $n=3$ excitation thresholds and compared the results with other theoretical and experimental results which showed quite good agreement.

Fon et al. (1979) used R-matrix method to calculate the integral and differential cross-sections for electron-impact excitation of the ground state helium atom to the $2^3S$ and $2^3P$ states in the energy range ($21.4 \leq E \leq 30$ eV and $80 \leq E \leq 200$ eV). They compared these results with experimental measurement of Trajmar, (1973). The results were generally in good agreement and were an improvement on earlier calculations. More studies on the cross-sections were carried out by Fon et al. (1981) where they calculated the inelastic cross-sections for all transitions between the $1^1S$, $2^3S$, $2^1S$, $2^3P$, and $2^1P$ states of helium atom using the five states R-Matrix. Further Nakazaki et al. (1991) applied both 7-state and 11-state R-matrix to calculate the differential cross sections for the transitions $1^1S$ to $2^3S$ and $2^3P$ in helium by electron impact at incident energies 100 and 200 eV.

2.2.2 The Convergence Close Coupling (CCC) Method

Fursa and Bray, (1995) applied CCC method with 75 target states to calculate the differential and total cross-sections for electron-helium excitation from ground state to $2^1S$, $2^1P$, $2^3S$, $2^3P$, $3^1S$, $3^3S$ and $3^3P$ states at energy ranging from 1.5 to 500 eV. The
results obtained were in good agreement with experimental and other theoretical results. However, there was some discrepancy on the set of measurement at forward angles of the n\(^3\)P channel (n \(\leq 3\)) which they attributed to difficulties associated with measuring electron to forward angles. Roder et al. (1996) also applied the CCC method with 85 target states to calculate and experimentally measured the differential cross sections for 2\(^3\)P state of helium by electron impact at 30, 40 and 50 eV.

2.2.3 The Variable Charge Coulomb Projected Born Approximation (VCCPBA)

Studies of electron impact excitation cross-sections for 1\(^1\)S-2\(^3\)S transition of helium atom were done by Singh, (1983) using both the variable charge coulomb projected Born model as well as the 'modified' variable charge coulomb projected Born model. The results were compared with other distorted waves and other theoretical results available then. The results obtained in the variable charge Coulomb Born model were in a poor agreement with the results of other distorted wave models and also with other theoretical methods. However, results for 'modified' variable charge Coulomb Born model (Singh et al., 1984) were in close agreement with the experimental results of Trajmar, (1973).

2.2.4 Experimental Measurements

Zajonc et al. (1977) measured experimentally the differential cross-sections for inelastic process of helium atom (1\(^1\)S-2\(^3\)S) just above threshold and compared the results with theoretical as well as experimental results, which did not show a good agreement, and they proposed further study to be done. Trajmar et al. (1992) applied
first order many body theory (FOMBT) and experimentally measured differential and integral cross-sections for the n\(^3\)S, n\(^1\)S and n\(^3\)P (n=2, 3) states of helium by electron impact from ground state. The results were in a reasonable agreement with other experimental and theoretical results. Yagishita et al. (1976) experimentally measured the differential cross sections for excitation of the 2\(^3\)S and 2\(^3\)P states of helium atom by electron impact at incident energies from 50 to 500 eV and from 50 to 200 eV respectively. Trajmar, (1973) measured both the differential and integral cross sections for electron impact excitation of the 2\(^3\)S, 2\(^1\)S and 2\(^3\)P states of helium at 29.6 and 40.1 eV.

2.3 Distorted Wave methods

Different types of the distorted wave methods have been applied by various researchers to study various collision processes which include excitation, autoionization and ionization of atoms and molecules. The variants in the distorted wave methods depend on how the distortion of the incident and scattered electron is introduced. Some of these ways are as discussed below.

Scott and McDowell (1975) used the distorted wave polarized-orbital model of McDowell et al. (1974) to calculate the total and differential cross sections for 2\(^1\)S, 2\(^3\)S and 3\(^1\)S excitation of helium atom by electron impact at incident energies from 29.2 eV to 300 eV. Also Scott et al. (1976) calculated the differential cross sections of n\(^1\)P (n=2, 3, 4, 5) and 2\(^3\)P states of helium from ground state. In both cases, the distortion potential in
the initial and final channels included static potential, polarization potential and also the
distortion of the target by the dipole polarization.

The distorted wave method have been applied by Mathur et al. (1986) to calculate
differential and total cross-sections for electron impact excitation of helium atom from
metastable state $2^3S$ to $2^3P$, $3^3S$ and $3^3P$ states. The distortion potential used in the
initial and final channels was taken as the combination of the initial state static
potential and polarization potential. Further, Srivastava et al. (1989) applied the
distorted wave approximation with the distortion potential taken as the average of the
initial- and final-state static potentials $U = \frac{1}{2}(U_i + U_f)$ in both channels to calculate
the differential cross-sections and angular correlation parameters for $(1^1S-2^1P)$
excitation of helium by electron impact. The results obtained were compared with
experimental and theoretical results which showed excellent agreement.

The distorted wave method have been applied by Katiyar and Srivastava, (1988) to study
the differential and integral cross sections for electron- and proton-impact excitation of
helium atom from the ground state $(1^1S)$ and excited metastable state $(2^1S)$ to $2^1S$, $3^1S$
and $3^1P$ states. The distortion potential was taken as the combination of the ground state
static potential and polarization potential in the initial channel while in the final channel it
was taken as the sum of the final state static potential and the polarization potential. That
is

$$U_i = V_{stat}^i(r) + V_{pol}^i(r) \tag{2.3.1}$$

for initial channel and for the final channel
Srivastava and Itikawa, (1993) applied distorted wave method to calculate the differential cross section for electron-impact excitation of $1^1S - 2^3S$ transition in helium atom at incident energies 100 eV and 200 eV. The distortion potential used in the initial channel was taken as the sum of the initial state static, exchange and polarization potentials while for the final state distortion potential was taken as the linear combination of the final state static, exchange and polarization potentials. These are given as

\[ U_i = V_{stat}^i(r) + V_{ex}^i + V_{pol}^i(r) \]  

for initial state and

\[ U_f = V_{stat}^f(r) + V_{ex}^f + V_{pol}^f(r) \]  

for final state.

Chen and Madison, (2005) applied the second-order distorted wave method to calculate the triple differential cross sections for electron-impact ionization of helium with the residual ion left in the n=1 and 2 states at intermediate energies. The initial-state distortion potential was chosen as the spherical average over the initial atomic state $\phi_i$ which is defined as

\[ U_i(r_0) = \frac{1}{4\pi} \int \langle \phi_i(r_1, r_2) | V_i | \phi_i(r_1, r_2) \rangle d\mathbf{r}_0 \]

But, for the final state distortion potential for the ejected electron was chosen as the spherical average over the final ionic state given as
Recently, Singh (2005; 2004) used the distorted wave method to calculate the differential cross sections for $2^1S$ excitation of helium atom by electron impact (Singh, 2005) and calculated the magnetic sublevel differential cross sections for $2^1P$ excitation of helium atom by electron impact (Singh, 2004). The choice of the distortion potential was taken as the static potential of helium atom in the initial state ($^1S$) for initial channel and the final state distorted wave was generated by the average of the initial state static potential ($U_i$) and final state static potential ($U_f$) of helium atom. In both cases the results obtained were in reasonable agreement with other theoretical and experimental results.

The variation of distorted wave method that was applied to study $2^1S$ and $2^1P$ excitation of helium (Singh 2005; 2004) has not been applied to triplet transitions. So, through this study the suitability of this method was tested for triplet excitations and generally to the excitations where exchange processes are dominant.
CHAPTER 3

THEORETICAL BACKGROUND OF APPROXIMATION METHODS

3.1 Introduction

Due to the demand for atomic collision data set in various fields of physics, various experimental techniques and theoretical approaches have been developed in order to get reliable data set for atomic collision processes. Theoretical approaches proposed are either classified as perturbative or non-perturbative. The latter is based on close coupling approach that expands trial wave functions into a set of basic functions. Some of these approaches include: the close coupling method, the R-matrix and the convergent close coupling method among others. The former are based on the Born series expansion, some of them include: First Born approximation, distorted wave methods and many body theory among others (Bartschat, 1998). Some of the methods are briefly discussed in section 3.2.

3.2 Theoretical Approximation Methods

3.2.1 The Born Approximation

In the Born series expansion, the scattering amplitude is written as

\[
f = -\frac{1}{4\pi} \langle \psi_{kf} | U + UG_0^*U + UG_0^*UG_0^*U + \cdots | \psi_{ki} \rangle
\]  

(3.2.1)

Here \( \psi_{kf} \) is the product of final plane wave \( e^{i\mathbf{k}_f \cdot \mathbf{r}} \) of the projectile and the final target wave function \( \varphi_f \). \( \psi_{ki} \) is the product of the initial plane wave \( e^{i\mathbf{k}_i \cdot \mathbf{r}} \) of the incident particle and the initial atomic wave function \( \varphi_i \). \( U \) is the interaction potential and the function \( G_0^* \) is outgoing Green’s function given as

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\[ G_0^+(k,r,r') = -\frac{1}{4\pi} \frac{e^{i|r-r'|}}{|r-r'|} \]  

(3.2.2)

The first term in the series (3.2.1) is the first Born approximation to the scattering amplitude and is given as

\[ f_{B1} = -\frac{1}{4\pi} \langle \psi_{k_f} | U | \psi_{k_i} \rangle \]  

(3.2.3)

When the first two terms in the series (3.2.1) are taken then it is the second Born approximation \( f_{B2} \) and so on. The first Born approximation is valid generally for high impact energies when the interaction is for a very short duration and the projectile waves (incident and scattered) can be approximated as plane waves (Joachain, 1975).

### 3.2.2 The Coulomb-projected Born (CPB) approximation

The Coulomb-projected Born approximation consists basically of modifying the usual Born approximation by taking an explicit account of the Coulomb interaction between the projectile and the nucleus. The final state plane wave in the Born approximation is replaced by a Coulomb wave in the CPB method. Different ways of taking this Coulomb interaction into account has led to different CPB methods, for example CPB approximation by Geltman, (1971), Generalized CPB approximation by Stauffer and Morgan, (1975) and a variable charge CPB approximation by Schaub-shaver and Stauffer, (1980).

### 3.2.3 The R-Matrix Method

In this method the configuration space for the \((N+1)\) electron-atom system is divided into two regions depending on the relative distance \(r\) between the projectile electron and the
atomic nucleus. One is the internal region \((r<a)\) and the other is the external region \((r>a)\). In the internal region the interaction is strong and electron exchange is important while in the external region exchange can be neglected and the collision is described by coupled differential rather than integro-differential equations which often have an analytic solution or at least a solution which can be readily obtained by numerical method. In this method, the target eigenstates and pseudostates are written as linear sums of Slater orbitals and the incident electron wave function is expanded in terms of orthogonal orbitals which satisfy logarithmic boundary condition on the surface of the sphere. The Hamiltonian is then diagonalized in an appropriately chosen basis in the internal region and the cross sections calculated by solving the asymptotic problem in the external region (Burke et al., 1971).

3.2.4 The Optical Potential Method

The idea of this method is to analyze the elastic scattering of a particle from a complex target by replacing the complicated interactions between the projectile and the target particles by an optical potential or pseudo potential in which the incident particles moves. Once the optical potential is determined, the original many body problem reduces to a one-body situation. However, this reduction is in general a difficult task, and approximations are necessary. For the cases involving fast collisions a multiple scattering approach is often used since it is convenient (Joachain, 1975).
3.2.5 The Convergent Close Coupling (CCC) Method

The CCC method relies on the close coupling formalism for solving the coupled equations without approximations. The convergence is tested by including an ever increasing set of states in the close coupling formalism. The target states are obtained by diagonalising the target Hamiltonian in an orthogonal Laguerre basis which ensures that the completeness is approached as the basis size increases. The CCC treats both the discrete and continuum parts of the target space through the close coupling formalism; this allows the validity of the CCC method to be independent of the projectile energy or the transition of interest (Fursa and Bray, 1995).

3.2.6 The Distorted Wave Methods

In the distorted wave approximation, the incident electron is taken to be elastically scattered by the initial state atomic potential. If the excitation of the atom is through the direct process, the incident electron makes a transition to a state in which it is being elastically scattered by final-state atomic potential. If the excitation of the atom is through the exchange process, the incident electron is captured into a bound state of the atom, while one of the initially bound electrons is ejected. In this case, the transition between the initial and final elastic state is calculated by a perturbation method. It is suitable for calculation of differential cross section for electron impact excitation of atoms at intermediate and high incident energies (Itikawa, 1986). Distorted wave methods have been one of the most successful perturbative methods used. Their advantage lies in the leading term of the perturbation series expansion such that the distorted wave series converges faster than Born series. Distorted wave method can be
comfortably applied to study electron-molecule collision, electron impact ionization of atoms and collision processes among heavy particles. Distorted wave methods have been applied in various collision processes; since it is quite successful in explaining various features of an excitation process for example distortion (Katiyar and Srivastava, 1988). However their limitation is that it gives poor results at low incident energies. Distorted wave methods are more conveniently discussed within the frame work of the two-potential formalism discussed in section 3.3.

3.3 Distorted Wave Formula Using Two-Potential Scattering Model

In this section, we shall describe the general formulation of the distorted wave approximation before specialising it to the particular case of electron helium scattering which will be discussed in chapter 4. The distorted wave methods are discussed within the framework of a two potential formalism where the interaction potential is broken in a physically meaningful way in two parts: one which is treated exactly, and the other which is handled in an approximate way (Joachain, 1975). That is,

\[ V_s = W_s + U_s \]  

(3.3.1)

where s=i or f for initial and final states respectively. It is also assumed that the equation

\[ (H_0 + U)\chi^\pm = E\chi^\pm \]  

(3.3.2)

can be solved exactly. In this equation \( H_0 \) denotes the unperturbed Hamiltonian (Hamiltonian of the target atom plus the non-interacting projectile), \( \chi \) is the product of 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 elements for any scattering problem is given as
\[ T_f = \langle \phi_f | V_f | \Psi_i^+ \rangle \]  \hspace{1cm} (3.3.3)

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

Making use of equation (3.3.1), it can now be written as

\[ T_f = \langle \phi_f | U_f + W_f | \Psi_i^+ \rangle \]  \hspace{1cm} (3.3.4)

Since

\[ | \chi_f^- \rangle = | \phi_f \rangle + \frac{1}{E_f - H_f - i\epsilon} U_f | \phi_f \rangle, \]  \hspace{1cm} (3.3.5)

here \( H_f = H_0 + U_f \) and this Hamiltonian satisfies equation (3.3.2), we can write

\[ \langle \phi_f | = \langle \chi_f^- | - \langle \phi_f | U_f \frac{1}{E_f - H_f + i\epsilon} \]  \hspace{1cm} (3.3.6)

Expanding equation (3.3.4) and making use of equation (3.3.6), the transition matrix elements can be written as

\[ T_f = \langle \phi_f | U_f | \Psi_i^+ \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle - \langle \phi_f | U_f \frac{1}{E_f - H_f + i\epsilon} W_f | \Psi_i^+ \rangle \]  \hspace{1cm} (3.3.7)

The third term on the right hand side of equation (3.3.7) can be transformed by making use of the relation

\[ | \Psi_i^+ \rangle = | \phi_i \rangle + \frac{1}{E_i - H + i\epsilon} V_i | \phi_i \rangle \]  \hspace{1cm} (3.3.8)

where \( \phi_i \) is the product of the initial atomic wave function and the initial plane wave for the projectile, as (on the energy shell \( E = E_i = E_f \)
and further making use of equation (3.3.6), we can write equation (3.3.9) as

\[ \langle \phi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f \Psi_i^+ \rangle = \langle \phi_f | U_f \frac{1}{E - H_f + i\varepsilon} W_f \phi_i \rangle \]

\[ + \langle \phi_f | U_f \frac{1}{E - H_f + i\varepsilon} W_f \frac{1}{E - H + i\varepsilon} V_i \phi_i \rangle \]

\[ \text{(3.3.9)} \]

Making use of the operator identity

\[ \frac{1}{B} (B - A) \frac{1}{A} = \frac{1}{A} - \frac{1}{B} \]

with \( A = E - H + i\varepsilon \), \( B = E - H_f + i\varepsilon \) and recalling that \( H - H_f = W_f \), we find that

\[ \langle \phi_f | U_f \frac{1}{E - H_f + i\varepsilon} W_f \frac{1}{E - H + i\varepsilon} V_i \phi_i \rangle = \langle \phi_f | U_f \frac{1}{E - H + i\varepsilon} V_i \phi_i \rangle - \langle \phi_f | U_f \phi_i \rangle \]

\[ \text{(3.3.11)} \]

If we make use of equations (3.3.6) and (3.3.8), equation (3.3.11) is reduced to

\[ \langle \phi_f | U_f \frac{1}{E - H_f + i\varepsilon} W_f \frac{1}{E - H + i\varepsilon} V_i \phi_i \rangle = \langle \phi_f | U_f \Psi_i^+ \rangle - \langle \phi_f | U_f \phi_i \rangle \]

\[ - \langle \chi_f^- | V_i \phi_i \rangle + \langle \phi_f | V_i \phi_i \rangle \]

\[ \text{(3.3.12)} \]

Substituting equations (3.3.10) and (3.3.12) in equation (3.3.7), we get

\[ T_{\text{eff}} = \langle \phi_f | U_f \Psi_i^+ \rangle + \langle \chi_f^- | W_f \Psi_i^+ \rangle - \langle \chi_f^- | W_f \phi_i \rangle + \langle \phi_f | W_f \phi_i \rangle \]

\[ - \langle \phi_f | U_f \Psi_i^+ \rangle + \langle \phi_f | U_f \phi_i \rangle + \langle \chi_f^- | V_i \phi_i \rangle - \langle \phi_f | V_i \phi_i \rangle \]

\[ \text{(3.3.13)} \]

Using the fact that on the energy shell

\[ \langle \phi_f | U_f + W_f \phi_i \rangle = \langle \phi_f | V_f \phi_i \rangle = \langle \phi_f | V_i \phi_i \rangle \]

equation (3.3.13) can be written as
\[ T_{\theta} = \langle \chi_f^- | V_i - W_f | \phi_i \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle \] (3.3.14)

It is simplified when we take \( V_i = V_f = V \). In this case,
\[ T_{\theta} = \langle \chi_f^- | U_f | \phi_i \rangle + \langle \chi_f^- | V - U_f | \Psi_i^+ \rangle \] (3.3.15)

This is the distorted wave formula obtained by two potential scattering model. When the potential \( U \) is taken as a linear combination of the static potential of the target states, the first term on the r.h.s of (3.3.15) vanishes due to the orthogonality of the target states and the T-matrix element takes the form
\[ T_{\theta} = \langle \chi_f^- | V - U_f | \Psi_i^+ \rangle \] (3.3.16)

So, it is this form of the transition matrix element which is used in the distorted wave calculations when any linear combination of the state potential of the target states is taken as the distortion potential for the initial and final states of the projectile.
4.0 Introduction

In the distorted wave approximation, the incident electron is taken to be elastically scattered by the initial state atomic potential. If the excitation of the atom is through the direct process, the incident electron makes a transition to a state in which it is being elastically scattered by final-state atomic potential. If the excitation of the atom is through the exchange process, the incident electron is captured into a bound state of the atom, while one of the initially bound electrons is ejected. In this case, the transition between the initial and final elastic state is calculated by a perturbation method. Distorted wave method can be comfortably applied to study electron-molecule collision, electron impact ionization of atoms and collision processes among heavy particles. Distorted wave methods have been applied in various collision processes; since it is quite successful in explaining various features of an excitation process, for example, distortion of the atomic wave function. However their limitation is that it gives poor results at low incident energies. In section 4.1 distorted wave method has been discussed as applied to the study of electron-helium collision.

4.1 Distorted Wave Method Applied to Electron-Helium Collision

The total Hamiltonian of the electron-helium system can be written as (Singh, 2004; Madison and Bartschat, 1996)

\[ H = H_A + T + V \]  

4.1.1
where $H_A$ is the Hamiltonian of the helium atom, $T$ is the kinetic energy of projectile electron and $V$ is the interaction potential between the incident electron and atom. They are given by

$$ T = -\nabla_o^2 $$

$$ V = \frac{2}{r_{01}} + \frac{2}{r_{02}} - \frac{2Z_n}{r_0} $$

Both $T$ and $V$ are in Rydberg’s units. The subscript 0 refers to the projectile electron and subscript 1 and 2 refers to the bound atomic electrons, $r_{01}$ and $r_{02}$ are the distances between the projectile electron and the atomic electrons 1 and 2 respectively and $Z_n$ is the nuclear charge which is equal to 2 for helium.

The general T-matrix in two potential approach for an electron colliding with an $N$-electron atom derived by (Madison and Bartschat, 1996)

$$ T_j = (N + 1) \langle \chi_j(0) \psi_j(1, ..., N) | V - U_j | A \Psi_i^* (0, ..., N) \rangle $$

$$ + \langle \chi_j(0) \psi_j(1, ..., N) | U_j | \psi_i(1, ..., N) \beta_i \rangle $$

where $\beta_i$ is the initial plane wave (eigenfunction for an isolated projectile) and $\Psi_i^*$ is the total wave function of the electron-atom system satisfying the Schrödinger equation

$$ H \Psi_i = E \Psi_i $$
with outgoing wave boundary conditions.

$\psi_i$ and $\psi_f$ are the properly antisymmetrised initial and final atomic wave functions for the isolated target atom, $A$ is the antisymmetrization operator which is generally expressed as

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

where $P_{\omega}$ is the operator that exchanges $i^{th}$ atomic electron and the projectile electron.

For electron-helium system the T-Matrix takes the form

$$T_{fi} = 3 \langle \chi_i^-(0) | \psi_f(1,2) | V - U_f | A \Psi_i^+(0,1,2) \rangle + \langle \chi_i^-(0) | \psi_f(1,2) | U_f | \psi_i(1,2) \exp(ik, r) \rangle$$

and

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

The potential $U_f$ in equation (4.1.4) is an arbitrary distortion potential for the projectile electron, which is used to calculate $\chi_f^-$ by solving the equation

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

where the $-$ superscript denotes the incoming wave boundary conditions. $k_f$ is the final state wave vector of the projectile electron and $k_f^2$ gives the kinetic energy (in Rydberg) of the projectile electron in the final state. Since we choose $U_f$ as some combination of static potentials of the target states, for inelastic collision (as we have considered) the second term on the right hand side of equation (4.1.7) will vanish. This
is due to the orthogonality of the atomic wave functions since $U_j$ depends only on the single coordinate of the projectile. Therefore, equation (4.1.7) reduces to:

$$T_{fi} = 3\left(\chi_f^-(0)\psi_f(1,2)|V - U_f|A\chi_i^+(0,1,2)\right)$$  \hspace{1cm} \text{(4.1.10)}$$

To evaluate equation (4.1.10) we will make some approximation due to the fact that $\Psi_i^+$ cannot be evaluated without making some approximation. In distorted-wave approach, $\Psi_i^+$ is expressed in terms of a product of an initial-state distorted wave $\chi_i^+$ and an initial state atomic wave function $\psi_i$. Thus in the first order distorted wave Born approximation, $\Psi_i^+(0,1,2)$ will be replaced by $\psi_f(1,2)\chi_i^+(0)$, where $\chi_i^+$ is a solution to the wave equation

$$(\nabla_0^2 - U_i + k_i^2)\chi_i^+ = 0$$  \hspace{1cm} \text{(4.1.11)}$$

where $U_i$ is an arbitrary potential chosen for the distortion of the initial state projectile electron wave function, $k_i$ is the initial wave vector of the projectile electron and $k_i^2$ gives the kinetic energy (in Rydberg units) of the projectile electron in the initial state. $\chi_i^+$ satisfies the outgoing wave boundary conditions.

Now the T-Matrix to be used will given by

$$T_{fi} = \langle \chi_f^-(0)\psi_f(1,2)|V - U_f|\{1 - P_{10} - P_{20}\}\psi_i(1,2)\chi_i^+\rangle$$  \hspace{1cm} \text{(4.1.12)}$$

Expanding equation (4.1.12) it gives

$$T_{fi} = T_{fi}^d - T_{fi}^{ex}$$  \hspace{1cm} \text{(4.1.13)}$$

where

$$T_{fi}^d = \langle \chi_f^-(0)\psi_f(1,2)|V|\psi_i(1,2)\chi_i^+(0)\rangle - \langle \chi_f^-(0)\psi_f(1,2)|U_f(0)|\psi_i(1,2)\chi_i^+(0)\rangle$$  \hspace{1cm} \text{(4.1.14)}$$

$$T_{fi}^{ex} = (1 - P_{10} - P_{20})\langle \chi_f^-(0)\psi_f(1,2)|\psi_i(1,2)\rangle$$
and

\[ T_{\mu}^{\alpha} = \langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (1,0) \chi_i^+(2) \rangle + \langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (0,2) \chi_i^+(1) \rangle \]

\[ - \langle \chi_f^-(0) | \nu_f, (1,2) | U_f, (0) | \psi_i, (1,0) \chi_i^+(2) \rangle - \langle \chi_f^-(0) | \nu_f, (1,2) | U_f, (0) | \psi_i, (0,2) \chi_i^+(1) \rangle \]  \hspace{1cm} 4.1.15

Since it is only the triplet states that are being considered the direct part \((T_{\mu}^{\alpha})\) of the T-matrix in equation 4.1.13 is zero since we are not considering the spin dependent interaction. In the exchange T-matrix \((T_{\mu}^{\alpha})\) the last two terms are neglected because the overlap integral of the continuum and the bound electron wave functions will be negligible. This is due to the oscillatory nature of the distorted wave which causes this integral to vanish, particularly when the distorted wave oscillates significantly more rapidly than the bound-state wave functions, which is the case for intermediate to high projectile energies (Madison and Bartschat, 1996). Thus equation 4.1.15 reduces to

\[ T_{\mu}^{\alpha} = \langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (1,0) \chi_i^+(2) \rangle + \langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (0,2) \chi_i^+(1) \rangle \]  \hspace{1cm} 4.1.16

Substituting the interaction potential in equation (4.1.16) we get

\[ T_{\mu}^{\alpha} = 2\langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (0,2) \chi_i^+(1) \rangle + 2\langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (0,2) \chi_i^+(1) \rangle \]

\[ - 2\langle \chi_f^-(0) | \nu_f, (1,2) | \chi_i^+(2) \rangle + 2\langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (1,0) \chi_i^+(2) \rangle \]

\[ + 2\langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (1,0) \chi_i^+(2) \rangle - 2\langle \chi_f^-(0) | \nu_f, (1,2) | \psi_i, (1,0) \chi_i^+(2) \rangle \]  \hspace{1cm} 4.1.17
On the same ground of the overlap integral of the bound state and the continuum wave functions we neglect the second, third, fourth and sixth terms in the above equation. So, we finally get the exchange matrix as

$$T_{fi}^{ex} = 2\langle \chi_f(0)|\psi_f(1,2)|\psi_i(0,2)\chi_i^*(1)\rangle + 2\langle \chi_f(0)|\psi_f(1,2)|\psi_i(1,0)\chi_i^*(2)\rangle$$  \hspace{1cm} 4.1.18

Before evaluating the T-matrix element, it is important to mention the atomic wave functions to be used and choice and evaluation of the static potentials

4.2 Atomic Wave Functions

For ground state ($1^1S$) of the helium atom, we used the Hartee-fock wave function of Byron and Joachain (1966). i.e.

$$\psi_i(r_1, r_2) = \phi_0(r_1)\phi_0(r_2)$$  \hspace{1cm} 4.2.1

where

$$\phi_0(r) = \frac{N_1}{\sqrt{4\pi}}(\exp(-pr) + c\exp(-qr))$$

with $N_1=2.60505$, $p=1.41$, $q=2.61$, and $c=0.799$

For the excited state ($2^3S$) we used the wave function of Bos (1969) given as

$$\psi_{2^3S}(r_1, r_2) = \frac{1}{4\pi}\left\{\phi_1(r_1)\phi_2(r_2) - \phi_1(r_2)\phi_2(r_1)\right\}$$  \hspace{1cm} 4.2.2

where

$$\phi_1(r) = \exp(-a_s r)$$

$$\phi_2(r) = N(\exp(-c_s r) - b r \exp(- b_s r))$$

With $a_s = 2.0$, $b_s = 0.61$, $c_s = 1.57$, $N=4.196$ and $b=0.340$
For the excited state \((2^3P)\) we used the wave function of Morse et al. (1935) given as

\[
\psi_{2^3p}(r_1, r_2) = \frac{1}{\sqrt{2}} \{ \phi_{1s}(Z, r_1)\phi_{2p}(Z', r_2) - \phi_{1s}(Z, r_2)\phi_{2p}(Z', r_1) \}
\]

where \(\phi_{n,l,m}(\xi, r)\) are the hydrogenic orbitals with nuclear charge \(\xi\), which are given by

\[
\phi_{1s}(r) = \left( \frac{Z}{a_o} \right)^{3/2} 2 \exp \left( -\frac{Zr}{a_o} \right) Y_{00}(r)
\]

and

\[
\phi_{2p_m}(r) = \left( \frac{Z'}{2a_o} \right) \frac{2}{\sqrt{3}} \exp \left( -\frac{Z'r}{2a_o} \right) Y_{l,m}(r)
\]

With \(Z = 1.99\), \(Z' = 1.1\) and \(a_o = 1\) and \(Y_{l,m}(r)\) are the spherical harmonics.

### 4.3 Distortion Potential

Though the choice of the distortion potential is arbitrary, the common choice is either the potential of the target atom in its initial or final state, or any linear combination of the two (Itikawa, 1986). In this study the distorted waves are generated as suggested by Singh, (2004). Here the initial state distorted wave is due to static potential of helium atom in the initial state \((1^1S)\) and the final state distorted wave will be generated by the average of the initial state static potential \((U_i)\) and final state \((2^3S\) or \(2^3P)\) static potential \((U_f)\) of helium atom as given below

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

and
The reason for this choice is that when the electron is in the initial state, for all the time it is in the field of the initial state of the target. Hence the distortion potential for the projectile electron in the initial state should be taken as the static potential of the target atom in the initial state. When the energy from the projectile electron is transferred to the target atom, the atom takes time (relaxation time) to go to the final state. Because of this time lag between the time of energy transfer and the instant when the atom reaches its final state, the projectile electron in its final state 'sees' a potential that is intermediate between the initial-state and final-state static potentials. Hence the final state distortion potential is taken as the average of the initial- and final-state static potentials of helium atom.

4.3.1 Evaluation of Static Potentials

4.3.1.1 Ground State Static Potential

The ground state static potential is given by

\[ U_{ss} = \left( |\psi_i, V | \psi_i, V \right) + \left( |\psi_f, V | \psi_f, V \right) \]

\[ U_{ss} = \langle \psi_i | \sum_{r1} \frac{2Z_p}{r_1} + \frac{2Z_p}{r_2} + \frac{2Z_N Z_p}{r_0} | \psi_i \rangle \]

Where \( \psi_i \) is the ground state wave function of the helium atom given by equation 4.2.1, and \( Z_p \) is the charge of the projectile, thus

\[ U_{ss} = \left( \frac{N_1}{\sqrt{4\pi}} e^{-pn_1} + c e^{-\eta n} \right) \left( \frac{N_1}{\sqrt{4\pi}} e^{-pn_2} + c e^{-\eta n} \right) - \frac{2Z_p}{r_0} - \frac{2Z_p}{r_0} + \frac{2Z_N Z_p}{r_0} \]

4.3.1
From equation 4.3.1 first we evaluate the term associated with \( \frac{2Z_p}{r_{01}} \) of the interaction potential.

\[
I = \left( \frac{N_1}{\sqrt{4\pi}} \left[ e^{-\mu_1} + ce^{-\eta_1} \right] \right) \left( \frac{N_1}{\sqrt{4\pi}} \left[ e^{-\mu_2} + ce^{-\eta_2} \right] \right) - \frac{2Z_p}{r_{01}} \left( \frac{N_1}{\sqrt{4\pi}} \left[ e^{-\mu_1} + ce^{-\eta_1} \right] \right) \left( \frac{N_1}{\sqrt{4\pi}} \left[ e^{-\mu_2} + ce^{-\eta_2} \right] \right)
\]

4.3.2

Performing integration over \( r_2 \) will give 1 since the wave functions are normalized.

Hence equation 4.3.2 will reduce to

\[
I = \left( \frac{N_1}{\sqrt{4\pi}} \left[ e^{-\mu_1} + ce^{-\eta_1} \right] \right) - \frac{2Z_p}{r_{01}} \left( \frac{N_1}{\sqrt{4\pi}} \left[ e^{-\mu_1} + ce^{-\eta_1} \right] \right)
\]

4.3.3

Performing angular integration over \( r_1 \) and expanding \( \frac{1}{r_{01}} \) in spherical harmonics as

\[
\frac{1}{r_{01}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \left( r_1 \right)^l Y_{lm}(r_0)Y_{lm}^*(r_1).
\]

4.3.4

equation 4.3.4 reduces to

\[
I = -2N_1^2 Z_p \int \left( e^{-\mu_1} + ce^{-\eta_1} \right)^2 \frac{1}{r_1} r_1^2 dr_1
\]

4.3.5

Breaking the integral in equation 4.3.5 into two parts we get

\[
I = -2N_1^2 Z_p \left[ \frac{1}{r_0} \int \left( e^{-\mu_1} + ce^{-\eta_1} \right)^2 r_1^2 dr_1 + \int \left( e^{-\mu_1} + ce^{-\eta_1} \right)^2 r_1 dr_1 \right]
\]

4.3.6

Evaluating equation 4.3.6 we get

\[
I = -2N_1^2 Z_p \left[ \left( -\frac{1}{4p^2} - \frac{1}{4p^3 r_0} \right) e^{-p\mu_6} + \frac{1}{4p^3 r_0} + c^2 \left( -\frac{1}{4q^2} - \frac{1}{4q^3 r_0} \right) e^{-q\eta_6} + \frac{1}{4q^3 r_0} \right]
\]

\[
+ 2c \left( -\frac{1}{(p+q)} + \frac{2}{(p+q)^3 r_0} \right) e^{-(p+q)\mu_7} + \frac{2}{(p+q)^3 r_0} \right)
\]

4.3.7
Because of the symmetry of the wave function between $r_1$ and $r_2$ coordinates the term associated with $\frac{-2Z_p}{r_{02}}$ in equation 4.3.1 will be the same as $I$ in equation 4.3.7. Now evaluating the term associated with $\frac{2Z_pZ_N}{r_0}$ we get it as $\frac{2Z_pZ_N}{r_0}$ since the ground state wave functions are normalized. Thus the ground state static potential will be given as

$$U_{\text{stat}} = 2I + \frac{2Z_NZ_p}{r_0}$$

4.3.1.2 Static Potential for $2^3P$ State

The static potential for the excited state ($2^3P$) will be given by

$$U_{2^3P} = \langle \psi_{2^3P} | V | \psi_{2^3P} \rangle$$

With $\psi_{2^3P}$ as given by equation (4.2.3). Hence

$$U_{2^3P} = \left\{ \frac{1}{\sqrt{2}} \left\{ \phi_{1s}(Z,r_1)\phi_{2p}(Z',r_2) - \phi_{1s}(Z,r_2)\phi_{2p}(Z',r_1) \right\} \right\} - \frac{2Z_p}{r_{01}} - \frac{2Z_p}{r_{02}} + \frac{2Z_NZ_p}{r_0}$$

4.3.8

Because of the symmetry of the wave function between $r_1$ and $r_2$ coordinates in equation 4.3.8, the term associated with $\frac{-2Z_p}{r_{02}}$ will have the same value as the term associated with $\frac{-2Z_p}{r_{01}}$. The term associated with $\frac{-2Z_p}{r_{01}}$ is given as
Expanding equation 4.3.9 results in four terms as

$$STP = \left( \frac{1}{\sqrt{2}} \{ \phi_{t_s}(Z, r_1) \phi_{2_p}(Z', r_2) - \phi_{t_s}(Z, r_2) \phi_{2_p}(Z', r_1) \} - \frac{2Z_p}{r_{01}} \right)$$

$$- \left( \frac{1}{\sqrt{2}} \{ \phi_{t_s}(Z, r_1) \phi_{2_p}(Z', r_2) \} - \frac{1}{\sqrt{2}} \phi_{t_s}(Z, r_2) \phi_{2_p}(Z', r_1) \right)$$

$$- \left( \frac{1}{\sqrt{2}} \{ \phi_{t_s}(Z, r_2) \phi_{2_p}(Z', r_1) \} - \frac{1}{\sqrt{2}} \phi_{t_s}(Z, r_2) \phi_{2_p}(Z', r_2) \right)$$

$$+ \left( \frac{1}{\sqrt{2}} \{ \phi_{t_s}(Z, r_2) \phi_{2_p}(Z', r_1) \} - \frac{1}{\sqrt{2}} \phi_{t_s}(Z, r_2) \phi_{2_p}(Z', r_2) \right)$$

The first term of the above equation is evaluated written as STP1

$$STP1 = -Z_p \phi_{t_s}(Z, r_1) \phi_{2_p}(Z', r_2) \frac{1}{r_{01}} \phi_{t_s}(Z, r_1) \phi_{2_p}(Z', r_2)$$

Integrating over \( r_2 \) will give 1 since \( \phi_{2_p}(Z, r_2) \) is normalized. Expanding equation 4.3.10 and using equation 4.3.4 it gives

$$STP1 = -Z_p \int_{r_{01}}^{r_{01}} r^2 \sin \theta \, d\theta \, d\phi \, dr$$

Where \( d\tau = r^2 \sin \theta \, d\theta \, d\phi \, dr \) is the volume element.

Performing angular integration over \( r_1 \) we get

$$STP1 = -Z_p \int_{r_{01}}^{r_{01}} (R_{1s}(Z, r_1))^2 \frac{1}{r^1} \, dr_1$$

$$\text{32}$$
Where \( R_{1S}(Z, r_1) = 2Z^2e^{-Zr} \) is the radial part of the atomic wave function.

Integrating equation 4.3.12 will give

\[
STP1 = -4Z \left[ \left( -\frac{1}{4Z^2} - \frac{1}{4Z^3 r_0} \right) e^{-2Zr_0} + \frac{1}{4Z^3 r_0} \right]
\]

The second term

\[
STP2 = \left( \frac{1}{\sqrt{2}} \left\langle \phi_{1s}(Z, r_1) \phi_{2p}(Z', r_2) \right\rangle \right) - \frac{2Z_p}{r_{01}} \left( \frac{1}{\sqrt{2}} \left\langle \phi_{1s}(Z, r_2) \phi_{2p}(Z', r_1) \right\rangle \right)
\]

and the third term

\[
STP3 = \left( \frac{1}{\sqrt{2}} \left\langle \phi_{1s}(Z, r_2) \phi_{2p}(Z', r_1) \right\rangle \right) - \frac{2Z_p}{r_{01}} \left( \frac{1}{\sqrt{2}} \left\langle \phi_{1s}(Z, r_1) \phi_{2p}(Z', r_2) \right\rangle \right)
\]

of equation 4.3.9 will vanish due to the orthogonality of \( \phi_{1s}(Z, r) \) and \( \phi_{2p}(Z', r) \).

Evaluating the fourth term of equation 4.3.9 we get

\[
STP4 = -Z_p \left\langle \phi_{1s}(Z, r_2) \phi_{2p}(Z', r_1) \right\rangle \frac{1}{r_{01}} \left\langle \phi_{1s}(Z, r_1) \phi_{2p}(Z', r_2) \right\rangle
\]

Now integrating over \( r_2 \) will give 1, since \( \phi_{1s}(Z, r_2) \) is normalized. Then after making the angular integration over \( r_1 \), we get.

\[
STP4 = -Z_p \sum_{\lambda_{max}} U_{1,0}^{1,0}(r) Y_{\lambda,0}
\]

Where

\[
U_{1,0}^{1,0}(r) = \left( \frac{4\pi}{2\lambda + 1} \right)^{1/2} C(1\lambda 1; 000)C(1\lambda 1; 000) \int_{r_3} R_{2p}^2(Z', r) \frac{r^4}{r_{\lambda+1}} r^2 dr
\]

33
Here \( C(l_1l_2l_3;m_1m_2m_3) \) is the Clebsh-Gordan coefficient and \( r_\alpha (r_\beta) \) is lesser or greater of \( r \). For our calculations we will use only the spherically symmetric part of the series 4.3.15 which corresponds to \( \lambda = o \) (Madison et al., 1991)

Hence

\[
STP4 = -Z_p [C(1\lambda 1;000)]^2 \int_0^\infty R_{2p}^2(Z',r) r^2 dr
\]

where \( R_{2p}(Z',r) \) is the Radial part of the hydrogenic wave function \( \phi_{2p}(Z',r) \).

On integration, equation 4.3.16 gives

\[
STP4 = -\frac{Z_p Z^5}{24} \left[ \left( -\frac{r_0^2}{Z^2} - \frac{6r_0}{Z^3} - \frac{18}{Z^4} - \frac{24}{Z^5 r_0} \right) + \frac{24}{Z^5 r_0} \right]
\]

Now evaluating the term associated with \( \frac{2Z_p Z_N}{r_0} \) we get it as \( \frac{2Z_p Z_N}{r_0} \) since the excited state wave functions are normalized. Thus the excited state static potential for \( 2^3P \) will be given as

\[
U_{2^3 P} = 2(STP1 + STP4) + \frac{2Z_p Z_N}{r_0}
\]

### 4.3.1.3 Static Potential for \( 2^3S \)

The static potential for the excited state \( 2^3S \) will be given by

\[
U_{2^3 S} = \langle \psi_{2^3 S} \mid \nabla \mid \psi_{2^3 S} \rangle
\]

where \( \psi_{2^3 S} \) is as given by equation 4.2.2. Hence

\[
U_{2^3 S} = \frac{1}{4\pi} \left\{ \phi_1 (r_1) \phi_2 (r_2) - \phi_1 (r_2) \phi_2 (r_1) \right\} - \frac{2Z_p}{r_{01}} - \frac{2Z_p}{r_{02}} + \frac{2Z_N Z_p}{r_0}
\]

34
\[
\left| \frac{1}{4\pi} \left\{ \phi_1(r_1)\phi_2(r_2) - \phi_1(r_2)\phi_2(r_1) \right\} \right| \]

From the symmetry of the wave function between \( r_1 \) and \( r_2 \) in the above equation the term associated with \( -\frac{2Z_p}{r_{01}} \) will have the same value as the term associated with \( -\frac{2Z_p}{r_{02}} \).

Thus we are going to evaluate the term associated with \( -\frac{2Z_p}{r_{01}} \) and multiply it by two.

\[
I = \left( \frac{1}{4\pi} \left| \phi_1(r_1)\phi_2(r_2) - \phi_1(r_2)\phi_2(r_1) \right| - \frac{2Z_p}{r_{01}} \left| \frac{1}{4\pi} \left( \phi_1(r_1)\phi_2(r_2) - \phi_1(r_2)\phi_2(r_1) \right) \right| \right) \]

Expanding equation 4.3.20 will give four terms as,

\[
I = \left( \frac{1}{4\pi} \left| \phi_1(r_1)\phi_2(r_2) \right| - \frac{2Z_p}{r_{01}} \left| \frac{1}{4\pi} \left( \phi_1(r_1)\phi_2(r_2) \right) \right| \right) \]

\[
- \left( \frac{1}{4\pi} \left| \phi_1(r_1)\phi_2(r_2) \right| - \frac{2Z_p}{r_{01}} \left| \frac{1}{4\pi} \left( \phi_1(r_1)\phi_2(r_2) \right) \right| \right) \]

\[
- \left( \frac{1}{4\pi} \left| \phi_2(r_2)\phi_1(r_1) \right| - \frac{2Z_p}{r_{01}} \left| \frac{1}{4\pi} \left( \phi_2(r_2)\phi_1(r_1) \right) \right| \right) \]

\[
+ \left( \frac{1}{4\pi} \left| \phi_2(r_2)\phi_1(r_1) \right| - \frac{2Z_p}{r_{01}} \left| \frac{1}{4\pi} \left( \phi_2(r_2)\phi_1(r_1) \right) \right| \right) \]

We evaluate the first term of equation above as

\[
I_1 = -\frac{2Z_p}{(4\pi)^2} \left| \phi_1(r_1)\phi_2(r_2) \right| \frac{1}{r_{01}} \left| \phi_1(r_1)\phi_2(r_2) \right| \]

Integrating over \( r_2 \) we get a constant C that is

\[
C = \int \phi_2(r_2)\phi_2(r_2) dr_2 \]

This on integration will give
Making angular integration over $r_1$ and using

\[
\frac{1}{r_{01}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \left( \frac{r_1}{r} \right)^l Y_{lm}(r_0) Y_{lm}^*(r_1)
\]

Equation 4.3.21 reduces to

\[
I_1 = -2CZ_p \int (R_1(r_1))^2 \frac{1}{r_1} r_1^2 dr_1
\]

Where $R_1(r_1)$ is the Radial part of the wave function $\phi_1(r_1)$.

This on integration will give

\[
I_1 = -2CZ_p \left[ -\frac{1}{4a_n^2} - \frac{1}{4r_0a_n^3} \right] e^{-2a_n r_0} + \frac{1}{4r_0a_n^3}
\]

The second and the third terms given as

\[
I_2 = -\frac{2Z_p}{(4\pi)^2} \langle \phi_1(r_1) \phi_2(r_2) \rangle \frac{1}{r_{01}} \langle \phi_1(r_2) \phi_2(r_1) \rangle
\]

and

\[
I_3 = -\frac{2Z_p}{(4\pi)^2} \langle \phi_1(r_2) \phi_2(r_1) \rangle \frac{1}{r_{01}} \langle \phi_1(r_2) \phi_2(r_1) \rangle
\]

respectively will be equal, thus we evaluate $I_2$ and multiply it by two

\[
I_2 = -\frac{2Z_p}{(4\pi)^2} \langle \phi_1(r_1) \phi_2(r_2) \rangle \frac{1}{r_{01}} \langle \phi_1(r_2) \phi_2(r_1) \rangle
\]

On integrating over $r_2$ will give $C_1$ given as

\[
C_1 = \int \phi_1(r_2) \phi_2(r_2) dr_2 = N \left[ -\frac{2}{(a_n + c_n)^3} - \frac{6b}{(a_n + b_n)^4} \right]
\]
Integrating over $r_1$ and using
\[
\frac{1}{r_{01}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} (r_{0})^{2l+1} Y_{lm}(r_0) Y_{lm}^*(r_1)
\]
Equation 4.3.26 reduces to
\[
I_2 = 2Z_p C_1 \int R_1(r_1) R_2(r) \frac{1}{r_2} r_1^2 dr_1
\]

Where $R_1(r_1)$ and $R_2(r)$ are the radial part of the wave functions $\phi_1(r_1)$ and $\phi_2(r)$ respectively.

Evaluating equation 4.3.24 it gives
\[
I_2 = 2C_1 Z_p \left[ \left\{ -\frac{1}{(a_n + c_n)^2} - \frac{2}{(a_n + c_n) r_0} \right\} e^{-(a_n + c_n)} + \frac{2}{(a_n + c_n)^2 r_0} \right]
\]
\[- b \left\{ -\frac{r_0}{(a_n + b_n)^2} - \frac{4}{(a_n + b_n)^2 r_0} - \frac{6}{(a_n + b_n)^2} e^{-(a_n + b_n)} \frac{6}{(a_n + b_n)^2 r_0} \right\}
\]

Now evaluating the fourth term as
\[
I_2 = -\frac{2Z_p}{(4\pi)^2} \left( \phi_1(r_2) \phi_2(r_1) \frac{1}{r_{01}} |\phi_1(r_2) \phi_2(r_1)| \right)
\]

On integrating equation 4.3.26 over $r_2$ we get a constant $C_2$ given by
\[
C_2 = \int \phi_1(r_2) \phi_2(r_2) dr_2 = \frac{1}{4a_n^3}
\]

Performing angular integration over $r_1$ and using
\[
\frac{1}{r_{01}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} (r_{0})^{2l+1} Y_{lm}(r_0) Y_{lm}^*(r_1)
\]
Equation 4.3.26 reduces to
\[ I_4 = -2C_2 N^2 Z_p \int_{r_0}^{\infty} (R_2(r)) \frac{1}{r_i} r_i^2 dr_i \] 

4.3.27

Where \( R_2(r) \) is the Radial part of the wave function \( \phi_2(r) \).

This on integration will give

\[ I_2 = -2C_1 N^2 Z_p \left[ \left( -\frac{1}{4a_n^2} - \frac{1}{4r_0 a_n^3} \right) e^{-2a_n r_0} + \frac{1}{4r_0 a_n^3} \right] \]

\[ -2b \left[ \frac{r_0}{(b_n + c_n)^2} - \frac{4}{(b_n + c_n)^3} - \frac{6}{(b_n + c_n)^4} \right] e^{-(b_n + c_n)} \]

\[ + \frac{6}{(b_n + c_n)^4 r_0} \right] + b^2 \left[ \left( \frac{r_0^2}{4b_n^2} - \frac{3r_0}{4b_n^3} - \frac{9}{8b_n^4} - \frac{3}{4r_0 b_n^5} \right) e^{-2b_n r_0} \right] \] 

3.3.28

Now evaluating the term associated with \( \frac{2Z_p Z_N}{r_0} \) we get it as \( \frac{2Z_p Z_N}{r_0} \) since the excited state wave functions are normalized. Thus the excited state (2\( ^3S \)) static potential will be given as

\[ U_{2S} = 2(I_1 + 2I_2 + I_4) + \frac{2Z_p Z_N}{r_0} \] 

4.3.29

4.4 Evaluation of the T-Matrix

4.4.1 1\( ^1S \)-2\( ^3P \) Transition

Because of the symmetrical nature of both the initial \( \psi_i(r_1, r_2) \) and final \( \psi_f(r_1, r_2) \) wave functions, with respect to \( r_1 \) and \( r_2 \), given by equations 4.2.1 and 4.2.3, the two terms in the T-matrix \( T_{fi}^{ex} \) (given by equation 4.1.18) will be equal. Thus, we evaluate the first term of equation 4.1.18 by substituting the atomic wave functions given in equations 4.2.1 and 4.2.3 as follows
Expanding the right hand side of 4.4.1 we get it as

\[
2\langle \chi_j (0) \psi_j (1,2) \rvert \frac{1}{r_{01}} \rvert \psi_i (0,2) \chi_i^+ (1) \rangle = 2\left\langle \chi_j (r_0) \frac{1}{\sqrt{2}} [\phi_{1a} (Z, r_i) \phi_{2p} (Z', r_i) - \phi_{1a} (Z, r_i) \phi_{2p} (Z', r_i)] \right\rvert \frac{1}{r_{01}} \right. 
\]

\[
\left. \frac{N_1}{\sqrt{4\pi}} [e^{-\rho_0} + ce^{-\rho_0} ] \frac{N_1}{\sqrt{4\pi}} [e^{-\rho_1} + ce^{-\rho_1} ] \chi_i^+ (1) \right]\ 4.4.1
\]

Expanding the right hand side of 4.4.1 we get it as

\[
= \frac{2}{\sqrt{2}} \left\langle \chi_j (r_0) \phi_{1a} (Z, r_i) \phi_{2p} (Z', r_i) \right\rvert \frac{1}{r_{01}} \frac{N_1}{\sqrt{4\pi}} [e^{-\rho_0} + ce^{-\rho_0} ] \frac{N_1}{\sqrt{4\pi}} [e^{-\rho_1} + ce^{-\rho_1} ] \chi_i^+ (1) \right\rvert \frac{1}{r_{01}} \right. 
\]

\[
- \frac{2}{\sqrt{2}} \left\langle \chi_j (r_0) \phi_{1a} (Z, r_i) \phi_{2p} (Z', r_i) \right\rvert \frac{1}{r_{01}} \frac{N_1}{\sqrt{4\pi}} [e^{-\rho_0} + ce^{-\rho_0} ] \frac{N_1}{\sqrt{4\pi}} [e^{-\rho_2} + ce^{-\rho_2} ] \chi_i^+ (1) \right\rvert \frac{1}{r_{01}} \right. 
\]

\[
4.4.2
\]

The first term of 4.4.2 will be zero because of the orthogonality of \( \phi_{2p} \) and \( \phi_0 \).

Integrating the second term analytically over \( r_2 \) we get a constant K. Hence the T-matrix will be

\[
T_{ji} = -2\sqrt{2} K \left\langle \chi_j (r_0) \phi_{2p} (Z, r_i) \right\rvert \frac{1}{r_{01}} \frac{N_1}{\sqrt{4\pi}} [e^{-\rho_0} + ce^{-\rho_0} ] \chi_i^+ \right\rvert \right. 
\]

\[
4.4.3
\]

where

\[
K = \int \phi_{1a} (Z, r_2) \frac{N_1}{\sqrt{4\pi}} [e^{-\rho_1} + ce^{-\rho_2} ] dr_2
\]

4.4.2 \( 1^1S-2^3S \) Transition

Similarly because of the symmetrical nature of both the initial \( \psi_i (r_1, r_2) \) and final \( \psi_j (r_1, r_2) \) wave functions with respect to \( r_1 \) and \( r_2 \), given by equation 4.2.1 and 4.2.2, the
two terms in the T-matrix $T_{fi}^{\text{ex}}$ (given by equation 4.1.18) will be equal. Thus, we evaluate the first term of equation 4.1.18 by substituting the atomic wave functions given in equations 4.2.1 and 4.2.2 as follows

$$2\left\langle \chi_f^- (0) \psi_f (1, 2) \right| \frac{1}{r_{01}} \left| \psi_i (0, 2) \chi_i^+ (1) \right\rangle = 2\left\langle \chi_f^- (r_0) \right| \frac{1}{4\pi} \left[ \phi_1 (r_1) \phi_2 (r_2) - \phi_1 (r_2) \phi_2 (r_1) \right] \frac{1}{r_{01}}$$

$$\left[ \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_0}} + ce^{-q_{r_0}} \right] \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_2}} + ce^{-q_{r_2}} \chi_i^+ (1) \right\rangle$$

on expansion, the right hand side gives two terms

$$= 2\left\langle \chi_f^- (r_0) \right| \frac{1}{4\pi} \phi_1 (r_1) \phi_2 (r_2) \left| \frac{1}{r_{01}} \left[ \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_0}} + ce^{-q_{r_0}} \right] \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_2}} + ce^{-q_{r_2}} \chi_i^+ (1) \right\rangle$$

$$-2\left\langle \chi_f^- (r_0) \right| \frac{1}{4\pi} \phi_1 (r_2) \phi_2 (r_1) \left| \frac{1}{r_{01}} \left[ \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_0}} + ce^{-q_{r_0}} \right] \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_2}} + ce^{-q_{r_2}} \chi_i^+ (1) \right\rangle \quad 4.4.5$$

Now integrating analytically over $r_2$ we get constant $K_1$ for the first term and $K_2$ for the second term thus the T-matrix will be

$$T_{fi}^{\text{ex}} = 2K_1 \left\langle \chi_f^- (r_0) \right| \frac{1}{4\pi} \phi_1 (r_1) \left| \frac{1}{r_{01}} \left[ \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_0}} + ce^{-q_{r_0}} \right] \chi_i^+ (1) \right\rangle -$$

$$2K_2 \left\langle \chi_f^- (r_0) \right| \frac{1}{4\pi} \phi_2 (r_2) \left| \frac{1}{r_{01}} \left[ \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_0}} + ce^{-q_{r_0}} \right] \chi_i^+ (1) \right\rangle \quad 4.4.6$$

where $K_1$ and $K_2$ are given by the following equations

$$K_1 = 2 \int \frac{1}{4\pi} \phi_2 (r_2) \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_0}} + ce^{-q_{r_0}} dr_2$$

and

$$K_2 = 2 \int \frac{1}{4\pi} \phi_1 (r_1) \frac{N_1}{\sqrt{4\pi}} e^{-p_{r_0}} + ce^{-q_{r_0}} dr_2$$
The distorted waves $\chi^+_i$ and $\chi^-_f$ for the projectile in initial and final states respectively appearing in the T-matrix will be determined by partial wave expansions (Singh, 2005, 2004; Madison and Bartschat, 1996) given as:

$$|\chi^+_i\rangle = \sqrt{\frac{2}{\pi i k_i r}} \sum_{l,m} i^l m l_i(k_i, r) Y_{l,m_i}(r) Y^*_{l,m_i}(k_i)$$ 4.4.7

and

$$|\chi^-_f\rangle = \sqrt{\frac{2}{\pi i k_f r}} \sum_{l,m} i^l m l_i(k_f, r) Y_{l,m_i}(r) Y^*_{l,m_i}(k_f)$$ 4.4.8

where $Y_{l,m}$ is a spherical harmonics.

In the expansion of $\chi^-_f$, the complex conjugate of radial part $\chi^-_f$ is taken so that it will satisfy the incoming boundary wave conditions. When expansions 4.4.7 and 4.4.8 are substituted in equations 4.1.11 & 4.1.9 respectively, we get the radial distorted waves equation as

$$\left( \frac{d^2}{dr^2} - \frac{l_s(l_s + 1)}{r^2} - U_s(r) + k_s^2 \right) \chi_s(r) = 0$$ 4.4.9

with $s=i$ for initial state and $s=f$ for final state distorted waves. In the asymptotic region the waves satisfies the boundary conditions

$$\lim_{r \to \infty} (\chi^-_i, r) = j_{i_s} + B_i (-\eta_i + i j_{i_s})$$ 4.4.10

where $j_i$ and $\eta_i$ are regular and irregular Riccatti-Bessel functions, and $B_i$ is a complex number related to the phase shift for elastic scattering. It is given as:
\[ B_i = \exp(i\delta_i) \sin \delta_i \]  

where \( \delta_i \) is the elastic scattering phase shift.

Equation 4.4.9 was solved using Numerov method and the differential cross-section for the triplet state for helium atom were obtained using the relation

\[ \frac{d\sigma}{d\Omega} = 4\pi^4 \frac{k_f}{k_i} |T_{fi}^{\text{ex}}|^2 \]  

\( k_i \) and \( k_f \) are initial and final wave vectors respectively and \( T_{fi}^{\text{ex}} \) is the T-matrix given in equation 4.4.3 and 4.4.6 for \( 2^3P \) and \( 2^3S \) transitions respectively. The total cross section is calculated using the formulae

\[ \sigma = \int_0^{\pi} \int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin \theta d\theta d\phi \]  

4.5 The Computer Code

The computer code DWBA1 for electron-hydrogen scattering written by Madison and Bartschat, (1996) was modified to fit the problem of electron helium scattering. The areas modified include: Main program where the following Sections dealing with the input data, transition matrix, and distortion potential, differential and total cross sections were modified to fit our problem.

The following subroutines were also modified: subroutine FHYD- This is the subroutine dealing with atomic wave functions. The hydrogen atom wave functions were replaced by helium atom wave functions. Subroutine POTENT- This subroutine
was dealing with the distortion potentials. The analytically evaluated distortion potentials for helium were used to replace the distortion potentials for hydrogen and Subroutine EXCHGE—this subroutine dealt with evaluation of the exchange transition matrix. After the above changes were done the program was run and the results for differential and total cross sections were obtained.
5.1 Introduction

Distorted wave method (present model) have been applied to calculate the differential and total cross sections for the spin forbidden transitions

\[ e + \text{He} (1^1S) \rightarrow e + \text{He} (2^3S) \]

and

\[ e + \text{He} (1^1S) \rightarrow e + \text{He} (2^3P) \]

at impact energies ranging from 40 to 200 eV. This energy range was chosen in order to make suitable comparison with other results available in literature. The present differential cross sections results for \( 1^1S-2^3S \) and \( 1^1S-2^3P \) transition were compared with the experimental measurements and theoretical calculations in figures 5.1 to 5.5 and figures 5.6 to 5.10 respectively. The total cross sections are in figure 11 and figure 12 for \( 1^1S-2^3S \) and \( 1^1S-2^3P \) transition respectively. The present results for differential cross sections are also given in tables 5.1 and 5.2 for \( 1^1S-2^3S \) and \( 1^1S-2^3P \) transition respectively and the integral cross section are in table 5.3.

5.2 Differential Cross Sections

5.2.1 \( 1^1S-2^3S \) Transition

At 40 eV (figure 5.1) the present distorted wave method (DWM) results are compared with experimental results of Trajmar (1973) and theoretical results: first order many body theory (FOMBT) (Trajmar et al., 1992) and convergent close coupling with 75 target states (CCC75) (Fursa and Bray, 1995). The present results show a close agreement with
the experimental and CCC75 results at lower scattering angles up to 80°. The CCC75 results (Fursa and Bray, 1995) are in good agreement with the experimental results (Trajmar, 1973) at all scattering angles as expected. The FOMBT results (Trajmar et al., 1992) are in agreement in shape with the present DWM results but the FOMBT results are generally lower than the other results. Both the present and FOMBT results have a dip at 70° whereas the experimental and CCC75 results have minima at 100°.

At 50 eV (figure 5.2) the present DWM results are compared with experimental results of Trajmar et al. (1992) and theoretical results: FOMBT (Trajmar et al., 1992) and CCC75 (Fursa and Bray, 1995). The present results show a close agreement with the experimental and CCC75 results at lower scattering angles up to around 60°. The present DWM results show an agreement in shape with the FOMBT results of Trajmar et al. (1992), but the present results are higher than the FOMBT results as is the case at 40 eV. FOMBT and present DWM results have a dip at around 60° while the experimental and CCC75 results have a deep at 90° and 80° respectively.

At 80 eV (figure 5.3) the present DWM results are compared with the experimental results of Yagishita et al. (1976) and theoretical results: R-matrix (Fon et al., 1979), FOMBT (Trajmar et al., 1992) and CCC75 (Fursa and Bray, 1995). Present DWM results are in a good agreement with the experimental, R-matrix and CCC75 results at low scattering angles up to around 40°. At higher scattering angles (>50°) all the results are in disagreement. The present, R-matrix, CCC75 and experimental results all show a dip at around 45°.
At 100 eV (figure 5.4) the present DWM results are compared with the experimental results of Trajmar et al. (1992) and theoretical results: R-matrix (Fon et al., 1979), FOMBT (Trajmar et al., 1992), DW (Srivastava et al., 1993) and CCC75 (Fursa and Bray, 1995). The present DWM results show a close agreement with CCC75 and experimental results at lower scattering angle up to 40°. The experimental and present DWM results have a dip at 40° while other results have a dip at around 30°.

At 200 eV (figure 5.5) the present DWM results are compared with the experimental results of Yagishita et al. (1976) and Sakai et al. (1991) which however are restricted to \(0 \leq 20^\circ\) and theoretical results: 11-state R-matrix (Nakazaki et al., 1991), FOMBT (Trajmar et al., 1992), DW (Srivastava et al., 1993) and CCC75 (Fursa and Bray, 1995). Both the experimental results are in good agreement with the present DWM results. The theoretical results show a good agreement in shape with the present results. However, the present results are slightly higher. All the results display a dip, with the present and experimental results being at 25° while others is at 15°.

Generally the agreement of the present DWM results with both the experimental and theoretical results is good for \(1^1S-2^3S\) transition at lower scattering angles for all electron incident energies. At higher scattering angles its agreement is not so good, but at 200 eV impact energy present result are in good qualitative agreement with the experimental results throughout the range of \(0^\circ \leq \theta \leq 120^\circ\). At all incident energies results of this study
and those from experiments have a dip which becomes shallower and shifts towards the lower scattering angles as the incident energy increases.

Table 5.1: Differential cross sections (cm$^2$/sr) for $1^1S-2^2S$ transition

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Figure 5.1: Differential cross section for $^1S-^2S$ excitation of helium by electron impact at 40eV. Theoretical results: — Present DWM, — — — CCC75 (Fursa and Bray, 1995), — — — FOMBT (Trjmar et al., 1992), ■ Experimental results of Trajmar (1973).
Figure 5.2: Differential cross section for $^1S$-$^2S$ excitation of helium by electron impact at 50 eV. Theoretical results: — Present DWM, — — — CCC75 (Fursa and Bray, 1995), — — — FOMBT (Trajmar et al., 1992), • Experimental results of Trajmar et al. (1992).
Figure 5.3: Differential cross section for $1^1S-2^3S$ excitation of helium by electron impact at 80 eV. Theoretical results: — Present DWM, ——— CCC75 (Fursa and Bray, 1995), ——— FOMBT (Trajmar et al., 1992), ———— R-Matrix (Fon et al., 1979), and ▼ Experimental results of Yagishita et al. (1976).
Figure 5.4: Differential cross section for $1^1S-2^3S$ excitation of helium by electron impact at 100 eV. Theoretical results: — Present DWM, --- CCC75 (Fursa and Bray, 1995), ---- FOMBT (Trajmar et al., 1992), """" DW (Srivastava et al., 1993), "" R-Matrix (Fon et al., 1979), • Experimental results of Trajmar et al (1992).
Figure 5.5: Differential cross section for $1^1S$-$2^3S$ excitation of helium by electron impact at 200 eV. Theoretical results: --- Present DWM, --- CCC75 (Fursa and Bray, 1995), ---- FOMBT (Trajmar et al., 1992), 11-State R-matrix (Nakazaki et al., 1991), •••••• DW (Srivastava et al., 1993), ▽ Experimental results of Yagishita et al (1976), □ Experimental results of Sakai et al. (1991).
5.2.2 $1^1S-2^3P$ Transition

At 40 eV (figure 5.6) the present DWM calculations were compared with the experimental results of Trajmar (1973) and Roder et al. (1996) and theoretical calculations for CCC75 (Fursa and Bray, 1995). Present calculations are in qualitative agreement in shape with both experimental measurements and theoretical calculation, but not in quantitative agreement. This discrepancy may be attributed to the fact that first order distorted wave methods do not give good results at lower incident energies. The present result has a peak at around 60° while other results have a peak at 40°.

At 50 eV (figure 5.7) the present results were compared with same theoretical results as for 40 eV and with the experimental results of Roder et al. (1996) and Trajmar et al. (1992). The present results are in best agreement with the experimental results of Trajmar et al. (1992). The close coupling results are not in good agreement with the experimental results at intermediate scattering angles (40°-120°). The present result shows a peak at 50°, experimental results (Trajmar et al., 1992) have a peak at 40° while other results have a peak at around 45°.

At 80 eV (figure 5.8) the results of this study were compared with the experimental results of Yagishita et al. (1976) and theoretical calculations: R-matrix (Fon et al., 1979), CCC75 (Fursa and Bray, 1995) and FOMBT (Trajmar et al., 1992). The present results are in a close agreement with the experimental results of Yagishita et al. (1976). All the results have peaks at around 25°.
At 100 eV (figure 5.9) the present results are compared with experimental results of Yagishita et al. (1976) and Trajmar et al. (1992) and theoretical results; R-matrix (Fon et al., 1979), 11-state R-matrix (Nakazaki et al., 1991) and CCC75 (Fursa and Bray, 1995). Present results are in reasonably good agreement with experimental results as well as theoretical results. The present results are in best agreement with the experimental results of Trajmar et al. (1992) for scattering angles ≥110°. Both the present and other theoretical results have a peak at around 20°.

At 200 eV (figure 5.10) the present results are compared with experimental results of Yagishita et al. (1976) and theoretical results: 11-state and 7-state R-matrix (Nakazaki et al., 1991), R-matrix (Fon et al., 1979), FOMBT (Trajmar et al., 1992) and CCC75 (Fursa and Bray, 1995). The present results agree qualitatively with other theoretical calculations and experimental results. Both the present results, experimental results and all theoretical calculations have a peak at around 10°.

In general the present DWM results for 1S-2p transition are in good agreement with most theoretical calculations and experimental results at all electron incident energies except at 40 eV. Also, the experimental and theoretical results have a peak which shifts towards the left (lower scattering angles) with the increase of incident electron energy. If we ignore the 40 eV results for 2p excitation, the present differential cross section results for 1S-2p transition are in better agreement with the corresponding theoretical and experimental results than the present results for 1S-2S transition when compared with other theoretical and experimental results.
Table 5.2: Differential cross sections (cm\(^2\)/sr) for \(^{1}S-2^{3}P\) transition

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Figure 5.6: Differential cross section for $^1S - ^3P$ excitation of helium by electron impact at 40eV. Theoretical results: -- Present DWM, ---CCC75 (Fursa and Bray, 1995) Experimental results: ■ Trajmar (1973), ◊ Roder et al. (1996).
Figure 5.7: Differential cross section for $^1S-2^3P$ excitation of helium by electron impact at 50 eV. Theoretical results: — Present DWM, --··CCC75 (Fursa and Bray, 1995) ○ Experimental results of Roder et al. (1996) and • Experimental results of Trajmar et al., (1992)
Figure 5.8: Differential cross section for $1^1S-2^3P$ excitation of helium by electron impact at 80 eV. Theoretical results: — Present DWM, - - - - CCC75 (Fursa and Bray, 1995) ———— R-Matrix (Fon et al., 1979), - - - - FOMBT (Trajmar et al., 1992), ▽ Experimental results of Yagishita et al. (1976)
Figure 5.9: Differential cross section for $^1S$-$^2P$ excitation of helium by electron impact at 100 eV. Theoretical results: — Present DWM, -----CCC75 (Fursa and Bray, 1995) --------- R-Matrix (Fon et al., 1979), —— FOMBT (Trajmar et al., 1992), ——— 11- state R- matrix (Nakazaki et al., 1991), Experimental results: • Trajmar et al., (1992) and ▼ Yagishita et al. (1976)
Figure 5.10: Differential cross section for $^1S-^2P$ excitation of helium by electron impact at 200 eV. Theoretical results: — Present DWM, --- CCC75 (Fursa and Bray, 1995) (1996), ······ R-Matrix (Fon et al., 1979), ···· FOMBT (Trajmar et al., 1992), —Δ— 7-State R-matrix (Nakazaki et al., 1991). ▼ Experimental results of Yagishita et al (1976),
5.3 Integral Cross Sections

5.3.1 1^1S-2^3S Transition

As shown in figure 11 the present integral cross sections results for 1^1S-2^3S transition are compared with experimental results of de Heer et al. (1994) and theoretical calculations: CCC75 (Fursa and Bray, 1995), R-matrix (Fon et al., 1979), DW (Baluja and McDowell 1979) and FOMBT (Trajmar et al., 1992). The present results together with CCC75 results are in close agreement with the experimental results. The FOMBT results generally disagree with the experimental and all the other theoretical results.

5.3.2 1^1S-2^3P Transition

The present integral cross sections result (figure 12) for 1^1S-2^3P transition are compared with the experimental results of de Heer et al. (1992) and theoretical results: CCC75 (Fursa et al., 1995), FOMBT (Trajmar et al., 1992) and R-matrix (Fon et al., 1979). The present results show a close agreement with the R-matrix in the energy range of 40-80 eV but for energies greater or equal to 100 eV, the present results are higher than the experimental and other theoretical results.

Generally the present DWM has produced better results for the integral cross sections for 1^1S-2^3S transition than for 1^1S-2^3P transition. Incase of differential cross sections present results for 1^1S-2^3P transition at almost all energies agree well with other theoretical and experimental results than in of case 1^1S-2^3S transition. But since it is the differential cross section results which give the better test of a method, we can say that the present
distorted wave method works better in case of \(1^1S-2^3P\) transition than in case of \(1^1S-2^3S\) transition.

**Table 5.3 Integral cross sections (cm\(^2\))**

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Figure 5.11: Total cross sections for $1^1S-2^3S$ excitation of helium by electron-impact. Theoretical results; — Present DWM, — — — CCC75 (Fursa & Bray, 1995), —— R-Matrix (Fon et al., 1979), ——— FOMBT (Trajmar et al., 1992), --Δ-- DW (Baluja et al., 1979), Δ Experimental results of de Heer et al. (1992).
Figure 5.12: Total cross sections for $^{1}S-^{2}S$ excitation of helium by electron-impact. Theoretical results: — Present DWM, -- -- -- CCC75 (Fursa & Bray, 1995), ----- R-Matrix (Fon et al., 1979), ------ FOMBT (Trajmar et al., 1992) and ▲ Experimental results of de Heer et al. (1992).
CHAPTER 6

CONCLUSION AND RECOMMENDATIONS

6.1 Conclusion

In this study, the differential and integral cross sections calculations for electron-impact excitation of helium atom from $1^1S$ to $2^3S$ and $2^3P$ states using the distorted wave method (Singh, 2004) have been done for the energy range 40 to 200 eV.

The present differential cross section results for $1^1S-2^3S$ transition show a good agreement with the experimental measurements and theoretical results at lower scattering angles for all electron incident energies. At higher scattering angles its agreement is not so good except for 200 eV impact energy which show a good qualitative agreement with the experimental results throughout the scattering angles in the range $0^0 \leq \theta \leq 120^0$. At all incident energies all the results have a dip which becomes shallower and shifts towards the lower scattering angles as the incident energy increases. Unlike the differential cross section, total cross sections for $1^1S-2^3S$ transition are in good agreement with other theoretical and experimental results.

In case of $1^1S-2^3P$ transition the present differential cross section results are in good agreement with most theoretical calculations and experimental results at all electron incident energies greater or equal 50 eV. But, for incident energy 40 eV the agreement is no so good. This may be attributed to the fact that the first order distorted wave method does not produce good results at low incident energies. All the results have a peak which shifts towards the lower scattering angles with the increase of incident electron energy.
The total cross section show a good agreement with most of theoretical and experimental results at incident energies less or equal to 100 eV but they are higher for energies greater than 100 eV.

If we ignore the 40 eV results for $2^3P$ excitation the present differential cross section results for $1^1S-2^3P$ transition are in better agreement with the corresponding theoretical and experimental results than the present results for $1^1S-2^3S$ transition when compared with other theoretical and experimental results. Since it is the differential cross section results which give a better test of any theoretical method because DCSs reflect more clearly the characteristics of the interacting potential and are more dependent on the target wave functions and approximation method used than the integral cross-sections, we can say that the present distorted wave method works better in case of $1^1S-2^3P$ transition than in case of $1^1S-2^3S$ transition.

### 6.2 Recommendations

Looking at the performance of this method for $1^1S-2^3S$ and $1^1S-2^3P$ excitation in helium by electron impact, we recommend the following:

(i) Further studies to be carried out to find the effect of including the terms which were neglected while evaluating the T-matrix elements, on the ground that these terms involved the overlap integral of bound and continuum wave functions.

(ii) The present method to be extended to study excitation of atoms to higher l-states e.g. D-state.
(iii) The present method to be extended in the study of excitation from an excited state e.g. metastable state \((2^1S\) or \(2^3S\)) to other excited states.
REFERENCES


