EFFECT OF EXCHANGE AND ABSORPTION POTENTIAL IN THE DISTORTED WAVE CALCULATION OF ELECTRON IMPACT EXCITATION OF AUTOIONIZING STATE OF CESIUM

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A thesis is submitted in the partial fulfillment of the requirements for the award of the degree of Masters of Science in the School of Pure and Applied Sciences of Kenyatta University

SEPTEMBER, 2017
DECLARATION

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

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DEDICATION

This work is dedicated to my loving wife Judith, my son Jordan, my brother Kevin, my niece Emma, my sister Sarah. I also want to dedicate this to my late mother; Rosemary and my late aunt Benta and all who passed on in a tragic road accident from my graduation ceremony (2009) in my heart your memories will live forever.
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ABBREVIATIONS

CCC - Convergent Close Coupling

Cs - Cesium

DCS - Differential Cross Section

DWBA1 - First order Distorted Wave Born Approximation

DWD - Distorted Wave Born method without exchange

DWE - Distorted Wave Born method with exchange

DWM - Distorted Wave Born method

ICS - Integral Cross Sections

MZ - Multi Zeta wave functions

RBA – Relativistic born approximation

$V^{\text{abs}}$ – Absorption potential

$V^{\text{exch}}$ - Exchange potential
Study of electron impact excitation of autoionizing states of alkali metal atom is very important because it can explain the near threshold features observed in the ionization curves of these atoms. Many theoretical methods, for example, R-matrix, close coupling and distorted wave methods, have been used for this study. In the distorted wave method no calculations have been performed for electron impact excitation of cesium atom using complex distortion potential. That is why in this study, I have used the distorted wave method to calculate differential cross sections and integral cross sections for the electron impact excitation of the lowest autoionizing level of cesium (Cs) atom using the complex distortion potential which comprises of, static, exchange and absorption potentials. I have applied a linear combination of the static potentials of the target atom in its initial and final states plus exchange and absorption potentials as the final channel distortion potential and the static potential of the target atom in its initial state plus exchange and absorption potentials as the initial channel distortion potential. I have used multizeta (MZ) wave function by Mclean and Mclean for cesium atom. Numerical calculations have been performed using modified computer code DWBA1 developed by Madison and Bartschart. The results of this study have been compared with previous experimental data and theoretical data available in literature. It is seen that the present differential cross section, integral cross section and angular correlation parameters are in reasonable agreement with the available theoretical and experimental results. Inclusion of absorption potential lowers the integral cross sections at intermediate energy region and brings them closer to the experimental results.
1

CHAPTER 1

INTRODUCTION

1.1 Background of the study

Atomic collision is a branch of physics which helps in the study of dynamical features of colliding particles i.e. electron, photon, atom, ion, and molecule. It involves a beam of projectiles directed to the target and the scattered particles are detected in an asymptotic region (Joachain, 1975). Figure 1.1 gives the schematic diagram of atomic scattering process. The collision of particles is classified into elastic and inelastic scattering. Elastic scattering is where the internal quantum state of the colliding particles (projectile and target) remains unchanged (McDaniel, 1989). In the inelastic scattering, there is exchange of energy between the projectile and the target which lead to change in quantum state (excitation) of both or one of the projectile and target.

In inelastic scattering, if the impact energy of the projectile (electron) is higher than the ionization threshold of the target atom, then there are two possibilities. One, the atom is ionized directly and second, the atom is excited to an energy level above the first ionization threshold called the autoionizing states. The excited atom then decays either through non-radiative transition to ground state where the excited atom emits an electron whose kinetic energy is equal to the difference in the energies of the excited atom and the ion of the atom formed after emission of electron in a process called auto ionization, or through radiative transition to the bound state of the atom below the ionization potential. In this process a photon is emitted and the atom comes to its ground state.
The study of atomic collision finds useful application in many fields like: astrophysics, planetary atmosphere, controlled fusion, laser spectroscopy, plasma dynamics, and laser development.

Detector

collimator

\theta

Beam of projectiles

Target

Direction of incident beam

Figure 1.1 Schematic diagram for atomic scattering process

The atomic collision process can be studied in the laboratory with high precision instruments or by use of theoretical methods. Due to the difficulties and cost associated with setting up and performing such experiment, theoretical physics aim at developing reliable and efficient computational methods which calculate the outcome of these collisions. This involves calculation of cross sections i.e differential cross section (DCS) and integral cross section (ICS) which describe the collision process. Due to the fact that the atomic wave functions and the distortion potentials are not precisely known and one cannot get the exact solution to the total wave function in the scattering problem, approximation methods are used to calculate these cross
These approximation methods are classified into semi classical and quantal methods. Quantal methods can further be classified into two categories: perturbative and non-perturbative methods. Non-perturbative methods are close coupling, R-matrix and variation methods. Perturbative methods are Born series, Eikonal Born series and distorted wave Born series. We have used one of the quantum perturbative approximation methods, that is distorted wave method (DWM) with complex distortion potential to study electron impact excitation of the lowest auto ionizing state of Cs. Use of complex distortion potential (static + exchange + absorption) will enable us find the effect of inclusion of exchange and absorption potential in the distortion potential.

1.2 Statement of the research problem

In this study I wish to investigate the effect of exchange and absorption potential on the electron impact excitation of the autoionizing state of Cs, using the Distorted Wave Method with different choices for static potentials in the initial and final channels (Singh, 2004). The energy range I have used extend from 13eV- 500eV. This energy range is above the excitation threshold of the first autoionizing state of cesium.
1.3 Objectives of the research project

1.3.1 General objective

The main objective of this research project is to study the effect of exchange and absorption potentials in electron impact excitation of the auto ionizing state of cesium.

1.3.2 Specific objectives

Following are the specific objectives:

(i) To formulate the T-matrix and modify DWBA1 program for electron impact excitation of the lowest autoionizing state of cesium.

(ii) To determine the differential and integral cross sections for electron impact excitation of the lowest autoionizing states of cesium at impact energy range 13eV - 500eV, using real distortion potential (static) in both the channels.

(iii) To determine the differential and integral cross sections for electron impact excitation of the autoionizing states of cesium at impact energy range 13eV - 500eV, using complex distortion potential, which includes static, exchange and absorption potentials.

(iv) To compare the results obtained using real (static) and complex distortion potentials to establish the effect of exchange and absorption potentials.

(v) To determine the angular correlation parameters.

(vi) To compare the results with available experimental and theoretical data to find the suitability of the present method.
1.4 Rationale of the study

Cesium is an alkali metal atom with simple electronic structure with the outer shell consisting of a single valence electron. This makes it a favourite test object for experimental and theoretical studies of different excitation and autoionization processes. Also, the study of electron impact excitation of the autoionizing levels of heavy alkali metal atoms, for example, Cs and Rb, is very important in the development of plasma devices, Laser physics, and astrophysics. The study of auto-ionizing states also provides information on the atomic structure and the dynamics of their state excitation. The main motivation in this study is driven by the fact that in all the studies that have been carried out on electron impact excitation of the heavy alkali metal atoms (in particular Cs) using distorted wave method (Pangantiwar and Srivastava, 1987; Kaur and Srivastava, 1999), it is either the static potential or static plus exchange potential which has been used as distortion potential. No calculation has been made with the inclusion of imaginary absorption potential in the distortion potential. The results reported are generally not in good agreement with the experimental data at the intermediate energy region. That is why I have introduced a complex distortion potential which includes static, exchange and absorption potentials to establish the effect.

I have chosen the Distorted Wave Method (DWM) because it is a high energy approximation method which is quite successful in explaining the various features of an excitation process. It also provides results that are in good agreement with the experimental data at intermediate and high impact energy excitation (Katiyar and Srivastava, 1988). DWM is also less expensive computationally as compared to other reliable theories like R-Matrix and close-coupling methods.
CHAPTER 2

LITERATURE REVIEW

2.1 Auto-ionization

Auto ionization refers to the process where an excited atom / molecule spontaneously emit one of the shell electrons and thus undergoes a transition from a state with $Z$ electrons to a state with $Z-1$ electrons. These ionized states are called autoionizing states. The excitation of the inner shell electron to some higher orbital leads to an autoionizing state. These levels are located above the first ionization potential and can decay by either radiative or non-radiative means. By radiative channel the atom makes transition to bound state below the ionization potential. On the other hand by non-radiative channel, the atom makes transition to the ground state or one of the excited state of the ion of the atom. This process leads to the emission of an electron from the atom whose kinetic energy is equal to the difference in the energy of the excited (autoionizing) state and the energy of the ion. In Cs the lowest autoionizing level is approximately 8.41eV above the ionization potential at 3.9eV. Excitation of inner –core electron may lead to discrete state beyond the first ionization limit i.e one of the inner core electrons (5p) in the 5p 6s ground state configuration is excited and it results into a bound excited state with electron configuration 5p 6s 2. This doublet state ( 3P ) is located 12.3eV above the ground state of the atom. It may decay through non radiative channel to state Cs+ (1S0) by ejecting an electron with kinetic energy 8.41eV. The study of autoionization levels in heavy alkali metals i.e K, Rb and Cs reveals new structures in the ionization curves of these metals (Roy and Rai, 1973).
2.2 Study on exchange and absorption potential

Staszewska et al. (1984) did an investigation on how the shape of absorption potential influences the absorption and differential cross sections. They found out that these cross sections are sensitive to the choice of absorption potentials at high energies.

Singh (2013) carried out a study on the effect of exchange and absorption potentials on the distorted wave calculation of the electron impact excitation of autoionizing state of lithium. He made calculation of DCS and ICS using different choices of potentials. He observed that the absorption potentials have a large effect on both DCS and ICS where the cross sections are reduced. The absorption potential of Staszewska et al. (1984) was found to work best for elastic scattering for mercury. The inclusion of exchange potentials of Furness and McCarthy (1973) improves the agreement between experimental and theoretical results on DCS.

2.3 Electron impact excitation of autoionizing states of alkali atoms

Borovik et al. (2013) did a study on electron impact excitation dynamics of lowest doublet and quartet autoionizing states in rubidium atom experimentally by measuring the ejected – electron excitation function for states \((4p^55s^2)\frac{2}{1}P_{3\frac{1}{2}}\) and \((4p^54d5s)\frac{4}{1}P_{3\frac{1}{2}},\frac{3}{2}\) individually and theoretically by performing fully relativistic B-spline R-matrix calculation. The data revealed a strong resonance of all states considered and the results for experiment and theory were in good agreement for the lowest \(2P_{3\frac{1}{2}}\) states. Pangantiwar and Srivastava (1987) studied the electron impact excitation of the lowest lying autoionizing levels in alkalis: lithium, sodium, potassium, rubidium and cesium using distorted wave calculations. They found out that the autoionization contribution of the lowest autoionization levels to ionization curve of alkalis is expressed by their cross sections. Srivastava et al. (1982) calculated the total cross sections for
electron impact excitation of the lowest autoionizing levels in Li, Na and K using Glauber approximation, method of Crothers and McCarrol and first Born approximation. They compared the results with earlier ones and found out that they converge only at higher energies.

Kaur and Srivastava (1999) also studied electron impact excitation of the lowest autoionizing state of alkali metals, Na, K, Rb, and Cs using Relativistic Distorted Wave Method (RDW). From their results they note that effect of exchange is very important in the distorted wave calculations. Their results for the integral cross section for cesium are similar to those of rubidium, where they observed a peak in the ICS at near threshold. This was attributed to the distortion and exchange potentials as incorporated in the distorted wave approximation.

Borovik et al. (1999) measured the metastable excitation function and the near threshold energy loss spectrum in potassium corresponding to 3P⁶ core excitation over the energy range of 18 – 24 eV. They observed many structures in the excitation function and were able to determine the excitation threshold for the lowest – lying metastable autoionizing levels in potassium.

2.4 Electron impact excitation of autoionizing state of cesium

Borovik et al. (2011) studied excitation cross sections and spectroscopic classification of autoionizing levels in cesium atom. The results from this study reveals a characteristic feature of electron impact excitation of the 5P⁶ sub shell in cesium namely; effective formation of negative ion resonance at near threshold energies.

Borovik et al. (2009) studied the autoionization cross section of cesium atoms at an incident electron energy range from 5P⁶ lowest autoionization threshold at 12.3 eV up to 16.6 eV. The data shows that there is a strong negative ion resonance excitation and quartet states from 5p⁵5d6s configuration gives the bulk of the autoionization cross section which reaches
maximum value of $4.8 \times 10^{-16} \text{ cm}^2$ at 14.7 eV. Hahn and Nygaard (1971) studied electron impact ionization of the alkali metals and concluded that in Cs, the doublet autoionizing level approximately 12.3 eV above its ground state have very small lifetimes (of the order of $10^{-15}$ s). It is the excitation of these states that is responsible for the second peak observed in single ionization curve of Cs. Though a lot of researches have been done on alkali metals using the distorted wave, there is no study which has been done on cesium atom using distorted wave method with complex distortion potential do exist in literature. That is why in this study we focus on the inclusion of complex distortion potential.

From literature review, Kaur and Srivastavas (1999), a lot of studies have been done on heavy alkali metals particularly cesium atom using the Distorted wave method. The results obtained in these studies are not in perfect agreement with the experimental results. Furthermore no attempt has been made to include absorption potential in the distortion potential in these studies. Thus the main aim of this study is to include the absorption potential in the distortion potential and ascertain whether its inclusion may give results which are in reasonable agreement with the experimental results.
CHAPTER 3

THEORETICAL FRAMEWORK

3.1 Introduction

Atomic collision can be studied theoretically or experimentally. Theoretically the process is studied by use of approximation methods. These methods are classified into two namely: semiclassical and quantal approximation methods. Quantum mechanical methods uses quantum mechanics principles. The semi-classical methods includes Glauber approximation, method of Crothers and McCarroll, impact parameter method and many other theories. The quantal approximations are further subdivided into two namely: perturbative and non-perturbative methods. Examples of quantal methods are; close coupling, R-matrix, Born series, Eikonal Born series, distorted wave method and optical potential method. In the following sections we discuss some of these methods briefly.

3.2 The Optical Potential Method

This method is used to analyse elastic scattering of a particle from a composite target containing many scatterers by replacing the interaction between the projectile and target atom by an equivalent potential in which incident particle moves. This equivalent potential in which the incident particle moves is called the optical potential. This potential is also called pseudo-potential. This method reduces many body problem to a one body problem once the optical potential is determined.
3.3 Born Approximation Method

In this approximation method, scattering amplitude is written as:

\[ f = \frac{1}{4\pi} \langle \Psi_{k_f} \left| U + UG_0^+U + UG_0^+UG_0^+U + \cdots \right| \Psi_{k_i} \rangle \]  \hspace{1cm} (3.1)

Here \( \Psi_{k_s} \) is the product of the plane wave of the projectile and the target wave function in the initial and final channel where \( s = i \) for initial and \( s = f \) for final state. \( U \) is the interaction potential and \( G_0^+ \) is the outgoing Green’s function given as:

\[ G_0^+(k,r,r') = -\frac{1}{4\pi} \frac{e^{ik|r-r'|}}{|r-r'|} \]  \hspace{1cm} (3.2)

The first term in the series in (3.1) is the first Born approximation for the scattering amplitude and is given by:

\[ f_{B1} = -\frac{1}{4\pi} \langle \Psi_{k_f} \left| U \right| \Psi_{k_i} \rangle \] \hspace{1cm} (3.3)

When the first two terms are taken in series (3.1), we obtain the second Born approximation and when the first three terms are taken from the series we obtain the third Born approximation and so on. The Born approximation has been improved by inclusion of exchange amplitude term (Born-exchange approximation) which gives better results since exchange is taken care of.

3.4 The Coulomb – Projected Born (CPB) Approximation

This is an improved version of simple Born approximation method by taking an explicit account of Coulomb interaction term between projectile and nucleus of the target. In Born series the electron-nucleus interaction term do not make any contribution because of the
orthogonality constraint of the atomic wave function. In CPB, the electron – nucleus interaction term is included in the unperturbed Hamiltonian and thus makes contribution as below;

\[ H_0 = H_a - \frac{1}{2} \nabla^2 r - \frac{1}{r_2} \tag{3.4} \]

Where \( H_a \) is the Hamiltonian of the atom and \(-\frac{1}{r_2}\) is the electron- nucleus interaction term.

And the transition matrix in the CPB method takes the form;

\[ T_{i,f}^{CPB} = \langle \varphi_f(r_1) \chi_f(r_2) \left| \frac{1}{r_{12}} \right| \varphi_i(r_2) e^{ik_i r_i} \rangle \tag{3.5} \]

The electron- nucleus interaction has been taken into account in the CPB method through the Coulomb wave \( \chi_f \). This approximation give results which are in good agreement with the experimental results.

### 3.5 The R-matrix method

This method is only reliable at low projectile impact energies since it ignores long range interactions. The R-matrix principle relies on a division of the configuration space for the projectile-target system into internal and external regions of two radii from the centre of the target atom. In the external region interactions and exchange effects are negligible while in the internal region these effects are important. In the external region the collision process is represented by a set of coupled integro-differential equations solved numerically to obtain analytical solutions. Slater orbitals are summed up to obtain the target eigen states and the R–matrix is calculated in the internal region by a single diagonalization of the Hamiltonian in order to obtain the eigen energies and corresponding eigen solutions. The cross section is calculated by
solving the asymptotic problem in the external region (Burke et al., 1971).

3.6 Generalized Coulomb Projected Born Approximation (GCPB)

Stanffer and Morgan (1975) later argued that the incident electron never sees the bare nucleus as assumed in CPB approximation. They reason that the electron does not experience full nuclear charge but only see’s a partially screened nucleus. Thus the Hamiltonian is split into two i.e the unperturbed part and the interaction between the target and the projectile as below:

\[ H_o = H_a - \frac{1}{2} \nabla_r^2 - \frac{\bar{Z}}{r_2} \]  

(3.6)

Where \( \bar{Z} \) is the nuclear charge and \( 0 \leq \bar{Z} \leq 1 \) the interaction is given by:

\[ V = -\left( \frac{1-\bar{Z}}{r_2} \right) + \frac{1}{r_{12}} \]  

(3.7)

The corresponding transition matrix element takes the form:

\[ T_{i,f} = \langle \varphi_f(r_1)\chi_f(\bar{Z},r_2) \mid V \mid \varphi_i(r_2)e^{ikr_2} \rangle \]  

(3.8)

Where \( \chi_f \) is the coulomb wave describing the scattered electron in the field of a charge \( \bar{Z} \) situated at the position of the nucleus. This approximation reduces to simple Born approximation when \( \bar{Z} = 0 \) and when \( \bar{Z} = 1 \), it goes over to CPB approximation. The generalized Coulomb projected Born approximation is a form of distorted wave approximation where distortion by the nuclear charge is taken only in the final channel.

3.7 The Convergent Close Coupling Method
This method attempts to solve close coupled differential equations with much accuracy by utilizing the fact that the complete set of eigen states of the target atom (discrete plus continuum) forms a basis for expanding the three-body projectile-target wave function in terms of a complete set of target atom states. Expanding the Schrodinger equation by means of these target states converts it to an infinite system of coupled equations, which is formidable to solve directly because of the infinite sum over the discrete states and the integration over the continuum. This method treats both discrete and continuum parts of the target space through close coupling which allows its validity to be independent of the projectile energy or transition of interest. Convergence is tested by including the increasing set of target 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 achieved as the basis size increases. This method is suitable for both elastic and inelastic scattering at lower projectile impact energies (Fursa and Bray, 1995).

3.8 Distorted Wave Formula using Two – Potential Scattering Method

In the two potential scattering model, the interaction between the projectile and the target is split into two; one ($U$) treated exactly and the other ($W$) as a perturbation. That is,

$$V = U + W \quad (3.9)$$

The potential $U$ fits into the Schrodinger equation:

$$(H_0 + U) \chi^\pm = E \chi^\pm \quad (3.10)$$
Here, $H_0$ is the unperturbed Hamiltonian and $\chi^\pm$ is the product of the distorted wave of the projectile and the wave functions of the target in the collision region and $+\ (-)$ represent the outgoing (incoming) wave boundary conditions. This equation is solved exactly. The transition matrix elements is given as;

$$T_{i,f} = \langle \varphi_f | V_f | \Psi^+_i \rangle$$ (3.11)

Where $\varphi_f$ 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. For the two potential problem the transition matrix element takes the form as;

$$T_{i,f} = \langle \varphi_f | U_f + W_f | \Psi^+_i \rangle$$ (3.12)

Using the Lippmann Schwinger equation, given as;

$$\langle \chi^-_f \rangle = \langle \varphi_f \rangle + \frac{1}{E_f - H_f - i\epsilon} U_f \langle \varphi_f \rangle$$ (3.13)

And solving for $\varphi_i$ we obtain;

$$\langle \varphi_f \rangle = \langle \chi^-_f \rangle - \langle \varphi_f \rangle \frac{1}{E_f - H_f + i\epsilon}$$ (3.14)

Substituting in the transition matrix equation (3.12) we obtain;

$$T_{i,f} = \langle \varphi_f | U_f | \Psi^+_i \rangle + \langle \chi^-_f | W_f | \Psi^+_i \rangle - \langle \varphi_f \rangle U_f \frac{1}{E_f - H_f + i\epsilon} W_f \langle \Psi^+_i \rangle$$ (3.15)

Expanding $\Psi^+_i$ in terms of Lippmann Schwinger equation we get;

$$\langle \Psi^+_i \rangle = \langle \varphi_i \rangle + \frac{1}{E_i - H_i + i\epsilon} V_i \langle \varphi_i \rangle$$ (3.16)

On the energy shell, $E = E_i = E_f$, then substituting (3.16) in the third term of (3.15) we get;
\[
\langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f | \psi_i^+ \rangle 
\]

\[
= \langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f | \varphi_i \rangle + \langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f \frac{1}{E_f - H_f + i\varepsilon} | \varphi_i \rangle \quad (3.18)
\]

Making use of relation (3.14) we can write equation (3.18) as;

\[
\langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f | \psi_i^+ \rangle = \langle \chi_f^- | W_f | \varphi_i \rangle - \langle \varphi_f | W_f | \varphi_i \rangle
\]

\[
+ \left( \langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f | \varphi_i \rangle \right)
\]

\[
+ \left( \langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f \frac{1}{E_f - H_f + i\varepsilon} V_i | \varphi_i \rangle \right) \quad (3.19)
\]

Making use of the operator identity \( \frac{1}{B} (B - A) \frac{1}{A} = \frac{1}{A} - \frac{1}{B} \) where \( A = E_f - H + i\varepsilon \) and \( B = E_f - H_f + i\varepsilon \) and recalling that \( H - H_f = W_f \) hence the third term in (3.19) becomes

\[
\langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f \frac{1}{E_f - H_f + i\varepsilon} V_i | \varphi_i \rangle = 
\]

\[
\langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} V_i | \varphi_i \rangle - 
\]

\[
\langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} V_i | \varphi_i \rangle \quad (3.20)
\]

Making use of relation (3.13) and (3.16) in (3.20) we get;
Again making use of the relations (3.19) and (3.21) in (3.15) we obtain the transition matrix as;

\[
T_{i,f} = \langle \varphi_f | U_f | \Psi_i^+ \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle - \langle \chi_f^- | W_f | \varphi_i \rangle + \langle \varphi_f | U_f | \varphi_i \rangle
\]

\[
- \langle \varphi_f | U_f | \Psi_i^+ \rangle + \langle \varphi_f | W_f | \varphi_i \rangle + \langle \varphi_f | U_f | \varphi_i \rangle
\]

\[
+ \langle \chi_f^- | V_i | \varphi_i \rangle - \langle \varphi_f | V_i | \varphi_i \rangle
\]

(3.22)

Making use of the fact that on the energy shell;

\[
\langle \varphi_f | U_f + W_f | \varphi_i \rangle = \langle \varphi_f | V_f | \varphi_i \rangle = \langle \varphi_f | V_i | \varphi_i \rangle
\]

We can write the transition matrix (3.22) as ;

\[
T_{i,f} = \langle \chi_f^- | V_i - W_f | \varphi_i \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle
\]

(3.23)

This is the two potential formula of Gellman and Goldberger. It is simplified when;
\[ H_i = H_0 = H, \quad V_i = V_f = V, \quad U_i = U_f = U \quad \text{and} \quad W_i = W_f = W \]

Hence we get:

\[ T_{i,f} = \langle \chi_f^- | U | \varphi_i \rangle + \langle \chi_f^- | W | \Psi_i^+ \rangle \quad \text{(3.24)} \]

This is the distorted wave formula for the two-potential model. If the distortion potential \( U \) is taken as linear combination of the static potentials of the target states, the first term of (3.24) vanishes due to orthogonality of the target states. In this case the T-matrix element takes the form:

\[ T_{i,f} = \langle \chi_f^- | W | \Psi_i^+ \rangle \quad \text{(3.25)} \]

This is the transition matrix employed in our distorted wave method in the calculation of the scattering amplitude.
CHAPTER 4
RESEARCH METHODOLOGY

4.1 The distorted wave method

The problem I have considered is the scattering of an electron from a neutral cesium atom. The total Hamiltonian of the system is expressed as below (atomic units are being used);

\[ H = H_o + V \]  \hspace{1cm} (4.1)

where \( H_o \) is the unperturbed hamiltonian describing a free motion of the electron and atom, and is given by the expression below,

\[ H_o = h_a + k \]  \hspace{1cm} (4.2)

where \( k \) is the kinetic energy operator of the projectile electron given by;

\[ k = -\frac{1}{2} \nabla_i^2 \]  \hspace{1cm} (4.3)

and \( h_a \) is the hamiltonian of the \( Z \)-electron target atom given by;

\[ h_a = \sum_{i=1}^{Z} k_i + u \]  \hspace{1cm} (4.4)

where \( k_i = -\frac{1}{2} \nabla_i^2 \), \( u = \sum_{i>j} \frac{1}{r_{ij}} \).
V is the interaction potential between the projectile electron and the target atom given by the following equation:

\[ V = -\frac{Z}{r_0} + \sum_{i=1}^Z v_i (4.5) \]

where \( v_i = \frac{1}{r_{0i}} (4.6) \)

where \( r_0 \) is the position of the projectile electron (taking nucleus of the atom as the origin) and \( r_{0i} \) is the separation between the projectile electron and the \( i^{th} \) atomic electron. The initial state full scattering wave function \( \Psi_i^+ \) is a solution to the Schrödinger’s equation;

\[ (H - E)\Psi_i^+ = 0 (4.7) \]

where superscript + indicates the outgoing boundary conditions. The first order T-matrix in the two potential approach is given by (Madison and Bartschat, 1996);

\[
T_{i,f} = \\
(N + 1)(x_f^- (0) \psi_f (1 ... N) \mid V - U_f (0) \mid A \Psi_i^+ (0 ... N)) + \\
\langle x_f^- (0) \psi_f (1 ... N) \mid U_f (0) \mid \psi_i (1 ... N) \beta_i^+(0) \rangle (4.8)
\]

where \( \psi_{i,f} \) are the initial/final state atomic wave functions, \( U_f \) is the final state complex distorting potential, \( A \) is the antisymmetrizing operator given by;

\[ A = \frac{1}{N+1} (1 - \sum_{i=1}^N P_{i,0}) \quad (4.9) \]

where \( P_{i,0} \) is the operator that exchanges electrons 0 and \( i \), \( \beta_i \) is the initial state plane wave and \( x_f^- \) is the distorted wave in the final channel with incoming boundary conditions.
The T-matrix (4.8) can be used for both elastic and inelastic collision. For inelastic collision, the second term of equation (4.8) vanishes due to the orthogonality of initial and final state wave functions. We have taken the potential $U_f$ in equation (4.8) as a complex distortion potential in the final channel which include static, exchange and absorption potential. This complex distortion potential is used to calculate the final distorted wave $x_f^-$ by solving the Schrödinger equation below;

$$(\nabla_o^2 + k_f^2 - U_f)x_f^- = 0 \quad (4.10)$$

The superscript – indicates incoming wave boundary conditions, $k_f$ is the final state wave vector and its corresponding energy is given as $E_f = k_f^2$ (in Rydberg unit). $U_f$ can be any arbitrary potential as long as $x_f^-$ satisfies the appropriate boundary conditions.

In the first order distorted wave approximation, $\Psi_i^+$ in equation (4.8) is replaced by the product of initial state distorted wave $x_i^+$ and the initial state atomic wave function $\psi_i$ and then it takes the form (for excitation process);

$$T_{i,f} = (N + 1) \langle x_f^- (0) \psi_f (1, ... N) \mid V - U_f (0) \mid \frac{1}{N+1} (1 - \sum_{i=1}^{N} P_{i0}) x_i^+ (0) \psi_i (1, ... N) \rangle \quad (4.11)$$

The initial state distorted wave $x_i^+$ is a solution to the Schrödinger’s equation;

$$(\nabla_0^2 + k_i^2 - U_i)x_i^+ = 0 \quad (4.12)$$

where $U_i$ is arbitrary complex distorting potential in the initial channel, $k_i$ is the incident wave vector, which is connected to incident particle energy given as $E_i = \frac{1}{2} k_i^2$. Both the $U_i$ and $U_f$ appearing in equations 4.10 and 4.12 are all in Rydberg unit.
4.2 Distortion Potentials $U_i$ and $U_f$

The distortion potential we have used is complex in nature both in initial and final channel. The complex distortion potential includes static, exchange and absorption potentials;

$$U_{i,f} = V_{i,f}^{st}(r) + V_{i,f}^{exc}(r) + iV_{i,f}^{abs}(r) \quad (4.13)$$

In this study we choose the static potential of the target atom in its initial state plus the exchange and absorption potentials as the distorting potential for the initial state of the projectile electron and a linear combination of the static potentials of the target atom in its initial and final states plus the exchange and absorption potentials as the distorting potential for the final state of the electron. The reason behind these choices of the static potentials is that, in the initial state of the projectile, it only ‘sees’ the initial-state static potential of the target atom, but when the energy of the projectile is transferred to the atom, it takes some time before the atom goes to its final state. As a result, the projectile in its final state ‘sees’ an intermediate potential between the initial and final state static potentials of the target (Singh, 2004).

The initial state static potential is given as,

$$V_{i}^{st}(r_0) = \langle \psi_i \mid V(r_0,r_i) \mid \psi_i \rangle \quad (4.14)$$

The final state static potential is given as,

$$V_{f}^{st}(r_0) = \frac{1}{2} \langle \psi_i \mid V(r_0,r_i) \mid \psi_i \rangle + \frac{1}{2} \langle \psi_f \mid V(r_0,r_f) \mid \psi_f \rangle \quad (4.15)$$

Thus the distortion potentials in the initial and final channels respectively are given by:

$$U_i = \langle \psi_i \mid V(r,r_i) \mid \psi_i \rangle + V_{i}^{exc}(r) + iV_{i}^{abs}(r) \quad (4.16)$$
\[ U_f = \frac{1}{2} \langle \psi_i | V(r_0, r_i) | \psi_i \rangle + \frac{1}{2} \langle \psi_f | V(r_0, r_i) | \psi_f \rangle + V^{\text{exc}}(r) + iV^{\text{abs}}(r) \]  

(4.17)

where,

\[ V^{\text{exc}}(r) = \frac{1}{2} [E - V^{\text{st}}(r)] - \frac{1}{2} \left\{ [E - V^{\text{st}}(r)]^2 + 4\pi a_0 e^4 \rho(r) \right\}^{\frac{1}{2}} \]  

(4.18)

is the exchange potential (Furness and McCarthy, 1973), \( E \) is the incident particle energy, \( \rho(r) \) is target electron charge density, \( a_0 \) is Bohr radius. The exchange potential accounts for exchange effects between the projectile electron and bound atomic electron.

\[ V^{\text{abs}}(r) = \frac{1}{2} T_{\text{loc}} \rho(r) \sigma_b \]  

(4.19)

is the absorption potential (Staszewska et al. 1984),

where \( T_{\text{loc}} = \left[ 2(E - V_{se}) \right]^{\frac{1}{2}} \) is the local kinetic energy of the incident electron, \( V_{se} \) is the static + exchange potential and \( \sigma_b \) is the average binary collision cross section. This absorption potential account for removal of incident projectile from the channel being considered.

In the initial channel we have used initial state static potential plus the exchange and absorption potentials as the distorting potential given as below:

\[ U_i = \langle \psi_i | V | \psi_i \rangle + V^{\text{exc}}(r) + iV^{\text{abs}}(r) \]  

(4.20)

and in the final channel we have used the linear combination of static potentials of initial and final states of the atom with equal weight as the static potential and then add to it the exchange and absorption potential as follows:
\[
U_f = \frac{1}{2} \{ \langle \psi_i | V | \psi_i \rangle + \langle \psi_f | V | \psi_f \rangle \} + V^{\text{exc}}(r) + iV^{\text{abs}}(r) \quad (4.21)
\]

The calculation of DCS and ICS have been made by the following choices of distortion potential (Singh, 2013).

(a) Static potential only both in the initial and final channels

(b) Static potential plus exchange potential both in the initial and final channels

(c) Static potential plus absorption potential both in the initial and final channels

(d) Static potential plus exchange and absorption potentials both in the initial and final channels

4.3 Atomic wave functions

We have used multi zeta (MZ) wavefunctions as given by Mclean and Mclean (1981). They are based on the Roothan–Hartree–Fock (RHF) expansion technique. The total wave function for an N-electron atom is a Slater determinant given by;

\[
\Psi = A(\Phi_1^1 \ldots \ldots \Phi_n^n) \quad (4.22)
\]

A is the antisymmetrizing operator and n is the total number of electrons, while \( \Phi_i^j \) are the spin orbital (one electron function) which are assumed to be orthogonal to each other. These orbitals are characterized by an index \( \lambda \), which indicates the symmetry species (\( \lambda \) corresponds to the azimuthal quantum number \( l \)), by an index \( \eta \), which indicates the subspecies (the subspecies label the individual members of the degenerate set that transform according to the representation \( \lambda \)) and by an index \( i \), which refers to the \( i^{th} \) orbital of symmetry \( \eta \). The orbital \( \Phi_{i\eta\lambda} \) is expanded in terms of the basis functions according to;

\[
\Phi_{i\eta\lambda} = \sum_p \chi_{p\eta\lambda} C_{inp} \quad (4.23)
\]
where \( p \) is the basis function of symmetry \( \eta \). \( C_{i\eta p} \) is the expansion coefficients which depends on \( \eta, p \ and \ i \) and not \( \lambda \).

The basis function \( \chi_{p\eta\lambda} \) are Slater-type orbitals with integer quantum numbers given as;

\[
\chi_{p\eta\lambda} (r, \theta, \varphi) = R_{\eta p} (r) Y_{\eta\lambda} (\theta, \varphi) \tag{4.24}
\]

where \( R_{\eta p} (r) \) is the radial Slater-type basis function given by;

\[
R_{\eta p} (r) = N r^{n-1} e^{-\xi r} \tag{4.25}
\]

The normalization factor \( N \), takes the form;

\[
N_n = \frac{(2\xi)^n + \frac{1}{2}}{\sqrt{(2n)!}} \tag{4.26}
\]

where \( n \) and \( \xi \) are principal quantum number and orbital exponent zeta respectively. The initial state cesium 5p multi-zeta wave function is given as the sum of all basis function given in atomic data tables by Mclean and Mclean (1981);

\[
\Phi(5p) = \sum_p \chi_i C_i
\]

\[
\Phi(5p) = -0.00315\chi_1 - 0.078657\chi_2 + 0.053942\chi_3 + 0.302615\chi_4
\]

\[
-0.219290\chi_5 - 0.389365\chi_6 + 0.236781\chi_7
\]

\[
+ 0.643721\chi_8 + 0.284540\chi_9 \tag{4.27}
\]

where the basis functions in the initial channel are given as;

\[
\chi_1 = N_1 r^1 exp(-35.277273r) Y_{1,0}(\theta, \varphi)
\]

\[
\chi_2 = N_2 r^1 exp(-23.712551r) Y_{1,0}(\theta, \varphi)
\]

\[
\chi_3 = N_3 r^2 exp(-11.909618r) Y_{1,0}(\theta, \varphi)
\]
\[ \chi_4 = N_4 r^2 e^{-10.450074r} Y_{1,0} (\theta, \varphi) \]

\[ \chi_5 = N_5 r^3 e^{-10.006642r} Y_{1,0} (\theta, \varphi) \]

\[ \chi_6 = N_6 r^3 e^{-6.171388r} Y_{1,0} (\theta, \varphi) \]

\[ \chi_7 = N_7 r^4 e^{-4.133844r} Y_{1,0} (\theta, \varphi) \]

\[ \chi_8 = N_8 r^4 e^{-2.789953r} Y_{1,0} (\theta, \varphi) \]

\[ \chi_9 = N_9 r^4 e^{-1.801024r} Y_{1,0} (\theta, \varphi) \]

The normalization constants are given as below:

\[ N_1 = 8535.065989, \quad N_2 = 3161.659261, \quad N_3 = 2457.995864, \quad N_4 = 1555.451654, \]

\[ N_5 = 3574.146507, \quad N_6 = 406.066864, \quad N_7 = 58.30837242, \quad N_8 = 6.70758738, \quad N_9 = 0.604144339 \]

The final state \((6s)\) wave function for cesium atom is given by

\[ \Phi (6s) = \sum_p \chi_p C_p \]

\[ \Phi (6s) = -0.000121 \chi_1 - 0.009671 \chi_2 - 0.01431 \chi_3 + 0.045249 \chi_4 \\
+ 0.026484 \chi_5 - 0.099676 \chi_6 + 0.082486 \chi_7 + 0.055398 \chi_8 \\
- 0.149640 \chi_9 - 0.125989 \chi_{10} + 0.156234 \chi_{11} + 0.571532 \chi_{12} \\
+ 0.423044 \chi_{13} \]

(4.28)

The basis functions in the final channel are given by:

\[ \chi_1 = N_1 r^0 e^{-56.231412r} Y_{0,0} (\theta, \varphi) \]

\[ \chi_2 = N_2 r^0 e^{-37.677605r} Y_{0,0} (\theta, \varphi) \]

\[ \chi_3 = N_3 r^1 e^{-27.973164r} Y_{0,0} (\theta, \varphi) \]
\[ \chi_4 = N_4 r^1 \exp(-23.863798r) Y_{0,0}(\theta, \phi) \]

\[ \chi_5 = N_5 r^2 \exp(-16.001179r) Y_{0,0}(\theta, \phi) \]

\[ \chi_6 = N_1 r^2 \exp(-12.807302r) Y_{0,0}(\theta, \phi) \]

\[ \chi_7 = N_7 r^3 \exp(-7.762725r) Y_{0,0}(\theta, \phi) \]

\[ \chi_8 = N_8 r^3 \exp(-5.85833r) Y_{0,0}(\theta, \phi) \]

\[ \chi_9 = N_9 r^4 \exp(-3.958971r) Y_{0,0}(\theta, \phi) \]

\[ \chi_{10} = N_{10} r^4 \exp(-2.658013r) Y_{0,0}(\theta, \phi) \]

\[ \chi_{11} = N_{11} r^5 \exp(-1.914259r) Y_{0,0}(\theta, \phi) \]

\[ \chi_{12} = N_{12} r^5 \exp(-1.179036r) Y_{0,0}(\theta, \phi) \]

\[ \chi_{13} = N_{13} r^5 \exp(-0.755359r) Y_{0,0}(\theta, \phi) \]

The normalization constants are given as below:

\[ N_1 = 843.3318046, \quad N_2 = 462.54599992, \quad N_3 = 4778.849429, \quad N_4 = 3212.316133, \]

\[ N_5 = 6909.882764, \quad N_6 = 3169.86315, \quad N_7 = 1140.088656, \quad N_8 = 321.260474, \quad N_9 = 45.9712404, \]

\[ N_{10} = 5.138631958, \quad N_{11} = 0.281534112, \quad N_{12} = 0.012062919, \quad N_{13} = 0.0006676112442. \]

### 4.4 Evaluation of the static potentials \( U_i \text{and} U_f \)

The mathematical formulation of static potentials felt by the projectile electron in the field of cesium atom both in the initial and final channels is given as (Joachain 1975):

\[ U_S = \langle \Phi_s | V | \Phi_s \rangle \quad (4.29) \]
Where, \( s = i \) or \( f \) for initial or (final) state respectively. The initial atomic wave function is given as;

\[
\Phi_i = \Phi(5p) = \sum_p \chi_i C_i \tag{4.30}
\]

The final wave function (excited state) is given as;

\[
\Phi_f = \Phi(6s) = \sum_p \chi_f C_f \tag{4.31}
\]

\( V \) is the interaction potential between the target atom (cesium) and the projectile (electron) in atomic unit given as (with the value of \( V \) in Rydberg unit);

\[
V = -2Z_p \left( \frac{1}{r_{o,1}} - \frac{Z_N}{r_0} \right) \tag{4.32}
\]

Where \( Z_p = -1 \), is the charge of the projectile electron and \( Z_N = 1 \) is the charge of the target nucleus where cesium atom has been taken as one electron system. Considering 5p electron being excited to 6s orbital, the initial and final state static potentials are given by;

\[
U_{i,f} = \sum_n \sum_{n'} C_{i,f} C_{i,f} \langle \chi_{i,f} | V | \chi_{i,f} \rangle \tag{4.33}
\]

Obtained by substituting equations \( (4.30) \) and \( (4.31) \) in \( (4.29) \). When we substitute for the interaction potential \( V \) in the above equation \( (4.33) \) and expanding the term \( \frac{1}{r_{o,1}} \) in terms of spherical harmonics as;

\[
\frac{1}{r_{o,1}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{l,m} (\hat{r}_0) Y_{l,m}^* (\hat{r}_1) \tag{4.34}
\]

where \( r_< (r_> \) is the lesser (greater) between \( r_0 \) and \( r_1 \) and taking only the terms associated with \( l = 0 \) and \( m = 0 \) in the expansion \( 4.34 \) and since the non- spherical term contribution is very small
and hence negligible (Madison et al 1991), the static potential takes the form, after substituting $Y_{00} = \frac{1}{\sqrt{4\pi}}$,

$$U_{i,f} = 2 \sum_n \sum_{n'} C_{i,f}^n C_{i,f}^{n'} \left< \chi_{i,f} \left| \frac{1}{r_1} - \frac{1}{r_0} \right| \chi_{i,f} \right>$$

(4.35)

Also substituting the slater-type wave function as constructed from the RS and AD Mclean tables in equation (4.33) we obtain the static potentials both in the initial and final channels as;

$$U_{i,f} = 2 \sum_n \sum_{n'} N_n N_{n'} C_n C_{n'} \int_0^\infty r_1^{\mu_n + \mu_{n'}} e^{-(\xi_n + \xi_{n'})r_1} \left| \frac{1}{r_1} - \frac{1}{r_0} \right| dr_1$$

(4.36)

where $N_n$ is the normalization factor, $\mu_n$ is the principal quantum number, $\xi_n$ is orbital exponent and $C_n$ is the expansion coefficient.

Splitting the integral appearing in equation 4.36 as $\int_0^{r_0}$ and $\int_{r_0}^\infty$, and noting that $r_0 > r_1$ for the integral from 0 to $r_0$ and $r_1 > r_0$ for the integral from $r_0$ to $\infty$, the static potential takes the form;

$$U_{i,f} = 2 \sum_n \sum_{n'} N_n N_{n'} C_n C_{n'} \int_0^{r_0} r_1^{\mu_n + \mu_{n'}} e^{-(\xi_n + \xi_{n'})r_1} \left| \frac{1}{r_1} - \frac{1}{r_0} \right| dr_1$$

(4.37)

Since $\int_0^{r_0} r_1^{\mu_n + \mu_{n'}} e^{-(\xi_n + \xi_{n'})r_1} \left| \frac{1}{r_1} - \frac{1}{r_0} \right| dr_1 = 0$

Letting $\zeta = \xi_n + \xi_{n'}$, we can write static potential as;

$$V_{i,f} = 2 \sum_n \sum_{n'} N_n N_{n'} C_n C_{n'} \int_0^\infty r_1^{\mu_n + \mu_{n'}} e^{-\zeta r_1} \left| \frac{1}{r_1} - \frac{1}{r_0} \right| dr$$

(4.38)

The problem reduces to analytically calculating the integrals with respect to $r_1$. The analytical solutions to the static distortion potential elements for initial and final states are calculated below.
according to the principal quantum number which give the power of \( r_1 \) under the integral starting from \( r^2 \) when the principal quantum number \( n = l \) for the atomic wave functions.

### Analytical solution of static distortion potentials

<table>
<thead>
<tr>
<th>Terms with</th>
<th>Distortion potential elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r^2 )</td>
<td>(- \frac{ANCO_2}{\zeta^3 r_0} (\zeta r_0 + 2) e^{-(kr_0)} )</td>
</tr>
<tr>
<td>( r^3 )</td>
<td>(- \frac{ANCO_3}{\zeta^4 r_0} (\zeta^2 r_0^2 + 4\zeta r_0 + 3!) e^{-(kr_0)} )</td>
</tr>
<tr>
<td>( r^4 )</td>
<td>(- \frac{ANCO_4}{\zeta^5 r_0} (\zeta^3 r_0^3 + 6\zeta^2 r_0^2 + 18\zeta r_0 + 4!) e^{-(kr_0)} )</td>
</tr>
<tr>
<td>( r^5 )</td>
<td>(- \frac{ANCO_5}{\zeta^6 r_0} (\zeta^4 r_0^4 + 8\zeta^3 r_0^3 + 36\zeta^2 r_0^2 + 96\zeta r_0 + 5!) e^{-(kr_0)} )</td>
</tr>
<tr>
<td>( r^6 )</td>
<td>(- \frac{ANCO_6}{\zeta^7 r_0} (\zeta^5 r_0^5 + 10\zeta^4 r_0^4 + 60\zeta^3 r_0^3 + 240\zeta^2 r_0^2 + 600\zeta r_0 + 6!) e^{-(kr_0)} )</td>
</tr>
</tbody>
</table>
\begin{align*}
\alpha^n & = \frac{\text{ANCO}_n}{\zeta^n r_0} \left( \sum_{i=0}^{n} a_i \zeta^i r_0^i \right) + \left( n! \right) e^{-(kr_o)} \\
& = \frac{\text{ANCO}_n}{\zeta^n r_0} \left( \sum_{i=0}^{n} a_i \zeta^i r_0^i \right) + \left( n! \right) e^{-(kr_o)}
\end{align*}
The ANCO values is the product of normalization factor and the expansion coefficient obtained from Mclean and Mclean (1981) data tables.

**The initial 5p state ANCO values for static potential elements**

<table>
<thead>
<tr>
<th>Terms with</th>
<th>ANCO VALUES</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r^4$</td>
<td>$(N_1 C_1 + N_2 C_2)^2$</td>
</tr>
<tr>
<td>$r^5$</td>
<td>$2(N_1 C_1 + N_2 C_2)(N_3 C_3 + N_4 C_4)$</td>
</tr>
<tr>
<td>$r^6$</td>
<td>$2(N_1 C_1 + N_2 C_2)(N_5 C_5 + N_6 C_6) + (N_3 C_3 + N_4 C_4)^2$</td>
</tr>
<tr>
<td>$r^7$</td>
<td>$2(N_1 C_1 + N_2 C_2)(N_7 C_7 + N_8 C_8 + N_9 C_9) + 2(N_3 C_3 + N_4 C_4)(N_5 C_5 + N_6 C_6)$</td>
</tr>
<tr>
<td>$r^8$</td>
<td>$2(N_3 C_3 + N_4 C_4)(N_7 C_7 + N_8 C_8 + N_9 C_9) + (N_5 C_5 + N_6 C_6)^2$</td>
</tr>
<tr>
<td>$r^9$</td>
<td>$2(N_5 C_5 + N_6 C_6)(N_7 C_7 + N_8 C_8 + N_9 C_9)$</td>
</tr>
<tr>
<td>$r^{10}$</td>
<td>$(N_7 C_7 + N_8 C_8 + N_9 C_9)^2$</td>
</tr>
</tbody>
</table>

The final 6s state ANCO values for the static potential elements
<table>
<thead>
<tr>
<th>Terms with</th>
<th>ANCO VALUES</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r^2$</td>
<td>$(N_1C_1 + N_2C_2)^2$</td>
</tr>
<tr>
<td>$r^3$</td>
<td>$2(N_1C_1 + N_2C_2)(N_3C_3 + N_4C_4)$</td>
</tr>
<tr>
<td>$r^4$</td>
<td>$2(N_1C_1 + N_2C_2)(N_5C_5 + N_6C_6) + (N_3C_3 + N_4C_4)^2$</td>
</tr>
<tr>
<td>$r^5$</td>
<td>$2(N_1C_1 + N_2C_2)(N_7C_7 + N_8C_8) + 2(N_3C_3 + N_4C_4)(N_5C_5 + N_6C_6)$</td>
</tr>
<tr>
<td>$r^6$</td>
<td>$2(N_1C_1 + N_2C_2)(N_9C_9 + N_{10}C_{10}) + 2(N_3C_3 + N_4C_4)(N_7C_7 + N_8C_8)$</td>
</tr>
<tr>
<td></td>
<td>$+ (N_5C_5 + N_6C_6)^2$</td>
</tr>
<tr>
<td>$r^7$</td>
<td>$2(N_1C_1 + N_2C_2)(N_{11}C_{11} + N_{12}C_{12} + N_{13}C_{13})$</td>
</tr>
<tr>
<td></td>
<td>$+ 2(N_3C_3 + N_4C_4)(N_9C_9 + N_{10}C_{10})$</td>
</tr>
<tr>
<td></td>
<td>$+ 2(N_5C_5 + N_6C_6)(N_7C_7 + N_8C_8)$</td>
</tr>
<tr>
<td>$r^8$</td>
<td>$2(N_3C_3 + N_4C_4)(N_{11}C_{11} + N_{12}C_{12} + N_{13}C_{13})$</td>
</tr>
<tr>
<td></td>
<td>$+ 2(N_7C_7 + N_8C_8)(N_9C_9 + N_{10}C_{10}) + (N_7C_7 + N_8C_8)^2$</td>
</tr>
<tr>
<td>$r^9$</td>
<td>$2(N_5C_5 + N_6C_6)(N_{11}C_{11} + N_{12}C_{12} + N_{13}C_{13})$</td>
</tr>
<tr>
<td></td>
<td>$+ 2(N_7C_7 + N_8C_8)(N_9C_9 + N_{10}C_{10})$</td>
</tr>
<tr>
<td>$r^{10}$</td>
<td>$2(N_7C_7 + N_8C_8)(N_{11}C_{11} + N_{12}C_{12} + N_{13}C_{13}) + (N_9C_9 + N_{10}C_{10})^2$</td>
</tr>
<tr>
<td>$r^{11}$</td>
<td>$2(N_9C_9 + N_{10}C_{10})(N_{11}C_{11} + N_{12}C_{12} + N_{13}C_{13})$</td>
</tr>
<tr>
<td>$r^{12}$</td>
<td>$(N_{11}C_{11} + N_{12}C_{12} + N_{13}C_{13})^2$</td>
</tr>
</tbody>
</table>

### 4.5 Evaluation of direct and exchange T-matrix elements

The excitation process that we have consider for our calculation using cesium atom is given by (Pangantiwar and Srivastava, 1987);
\[ e^- + \text{Cs}(5p^66s)^2S_1 \rightarrow e^- + \text{Cs}(5p^56s^2)^2P_{1/2} \]

The system is taken as one electron system excited from initial state 5p to final state 6s. The transition matrices for direct and exchange processes are expressed as (using equation (4.8)) and neglecting terms associated with \( U_f(0) \) because of the orthogonality of the atomic wave functions and orthogonality of bound and continuum wavefunctions;

\[
T^{\text{dir}} = (x^-_f(r_0)\psi_f(r_1) | V(r_0, r_1) | x^+_i(r_o)\psi_i(r_1)) \quad (4.39)
\]

\[
T^{\text{exc}} = (x^-_f(r_0)\psi_f(r_1) | V(r_0, r_1) | x^+_i(r_1)\psi_i(r_0)) \quad (4.40)
\]

where \( V(r_0, r_1) = \frac{1}{r_{o1}} - \frac{1}{r_o} \), is the interaction potential between the projectile electron and target atom. \( r_o \) is the position vector for the projectile electron, \( r_1 \) is the position vector of an atomic electron undergoing transition relative to the nucleus of the target atom (cesium), \( r_{o1} \) is the displacement vector between the projectile and the target electron.

To evaluate scattering amplitude (4.39) and (4.40), the distorted waves \( x^+_i \) and \( x^-_f \) are expanded in terms of partial waves (Singh, 2004, Madison and Bartschart, 1996);

\[
|x^+_i> = \frac{\sqrt{2}}{\pi k_{i|r}} \sum i_{l_i m_i} i^{l_i} x_{l_i}(k_{i}, r) Y_{l_i m_i}(r) Y_{l_i m_i}^*(k_{i}) \quad (4.41)
\]

\[
|x^-_f> = \frac{\sqrt{2}}{\pi k_{f|r}} \sum i_{l_f m_f} i^{l_f} x_{l_f}^*(k_{f}, r) Y_{l_f m_f}(r) Y_{l_f m_f}^*(k_{f}) \quad (4.42)
\]

In the above equations (4.41) and (4.42), \( Y_{lm} \) is the spherical harmonics. In the expansion of equation (4.42), the complex conjugate of the radial \( x_{l_f} \) is taken so that it satisfies the incoming wave boundary condition.
The radial part of the initial / final state distorted waves is obtained by substituting the partial wave expansions of the distorted wave in equations (4.41) and (4.42) into Schrödinger equations (4.12) and (4.10) respectively. The radial distorted waves $x_{li}$, $x_{lf}$ are the solutions of the following equation;

$$x_{ls}''(r) + \left[ k_s^2 - \frac{l_s(l_s+1)}{r^2} - U_r(r) \right] x_{ls}(r) = 0 \quad (4.43)$$

where the prime denotes derivatives with respect to $r$, $l$ is partial wave angular momentum. $s = i, f$ indicating initial/ final channels respectively. This radial equation (4.43) is solved using Numerov method. In the asymptotic region the radial distorted waves satisfy the following boundary conditions;

$$\lim_{r \to \infty} x_{ls}(k_s, r) = j_{ls} + \beta_{ls} (ij_{ls} - \eta_{ls}) \quad (4.44)$$

where $j_l and \eta_l$ are regular and irregular Rucatti- Bessel function.

$$\beta_l = \exp(i\delta_l) \sin \delta_l$$, where $\delta_l$ is the elastic scattering phase shift.

The main concern is to examine the effect of exchange and absorption potentials on DCS and ICS. The DCS summed over magnetic sub levels is obtained using the following formula;

$$\left( \frac{da}{d\Omega} \right)_{5p \to 6s} = (4\pi)^4 \frac{k_f}{k_i} \left[ \frac{1}{4} \left| T_{5p \to 6s}^{dir} + T_{5p \to 6s}^{exc} \right|^2 + \frac{3}{4} \left| T_{5p \to 6s}^{dir} - T_{5p \to 6s}^{exc} \right|^2 \right] (4.45)$$

The integral or total cross section is obtain by summing up the differential cross section given by the following relation;
\[ \sigma = \int_0^{2\pi} \int_0^\pi \sin\theta \frac{d\sigma}{d\Omega} \ d\theta \ d\varphi \]  

(4.46)

### 4.6 Angular correlation parameters

Angular correlation parameters between the scattered electron when the atom is excited from np→(n+1)s state and the emitted photon released from transition (n+1)s →np after excitation, are measured in order to obtain information regarding population of magnetic sub-states. These electron–photon coincidence parameter \( \lambda \) is expressed as:

\[ \lambda = \frac{\sigma_0(\theta, \varphi)}{\sigma_0(\theta, \varphi) + 2\sigma_1(\theta, \varphi)} \quad 0 \leq \lambda \leq 1 \]  

(4.47)

where \( \sigma_0(\theta, \varphi) \) and \( \sigma_1(\theta, \varphi) \) are the differential cross sections for \( np_m \rightarrow (n + 1)s \) transition where \( m = 0 \) or \( 1 \).

The alignment parameter or the anisotropy parameter \( A_{20} \) is the measure of the angular anisotropy of the autoionizing electron from the autoionizing state. It is given by the following relation for unresolved fine structure state:

\[ A_{20} = \frac{\sigma_1 - \sigma_0}{\sigma} \]  

(4.48)

\( \sigma_0 \) and \( \sigma_1 \) are integral cross sections for magnetic sublevels \( m=0 \) and \( m=1 \) respectively.

### 4.7 Computer code and data analysis
In order to evaluate the above mentioned collision parameters, for example T-matrix element, cross sections and radial distorted wave, angular correlation parameters, we have modified Fortran computer program (DWBA1) developed by Madison and Barstchart (1996) for electron–hydrogen scattering. We have modified it for electron–cesium scattering with a complex distortion potential. The following are the modifications done on the program to generate data for electron–cesium scattering:

a) In the main program, we have made several modifications to generate results for our study. Since the original program is for $s \rightarrow p$ transition, the main program was changed for $p \rightarrow s$ transition, that is, $5p \rightarrow 6s$. This involved changing parameters such as spin, orbital and magnetic quantum numbers for the initial and final states.

b) Also in the main program we changed all declarations parameters for the real distortion potentials to complex distortion potential to enable us include the imaginary absorption part.

c) The subroutine FHYD for hydrogen wave functions was modified to generate cesium wave functions for initial (5p) and final (6s) states as constructed from Mclean and Mclean (1981) tables.

d) The subroutine POTENT for hydrogen static potentials was modified to generate static potentials and complex distortion potentials for cesium atom both in the initial and final channels.

e) The main program has been modified to calculate $\lambda$ parameter and alignment parameter $A_{20}$ as described by the above relations (4.6.1) and (4.6.2) respectively.

The Microcal-Origin version 7 computer software was used to analyse data which includes generation of graphs of cross sections and angular correlation parameters.
CHAPTER 5

RESULTS AND DISCUSSIONS

5.1 Introduction

In this study, complex distortion potential has been used both in the initial and final channels. This includes static potential, exchange potential (Furness and McCarthy 1973) and absorption potential (Staszewska et al; 1984).

The static potential has been varied such that initial state static potential plus exchange and absorption potential is the distortion potential in the initial channel, while a linear combination of the initial and final state static potential plus exchange and absorption is the distortion potential in the final channel. In this work I have used HF multi-zeta wave function.

I have compared our results amongst themselves for establishing the effects of exchange and absorption. I have also compared our results with theoretical results of Pangantiwar and Srivastava (1987) and Kaur and Srivastava (1999), and experimental results of Borovik et al. (2011) for electron impact excitation of the lowest autoionizing state of cesium. The Kaur and
Srivastava(1999) results were obtained through relativistic distorted wave calculation method, while the results of Pangantiwar and Srivastava (1987) is a calculation using the distorted wave method where the initial state static potential is the initial channel distortion potential while the final state static potential is the final channel distortion potential.

5.2 Integral cross section

The present integral cross section results (figure 5.1) for electron impact excitation of the $5p^56s^2$ state of cesium atom obtained with variations in the distortion potentials, are compared amongst themselves. The results are further compared with the experimental work of Borovik et al (2011) and theoretical work of Kaur and Srivastava (1999) and Pangantiwar and Srivastava (1987).

In figure 5.1, the present integral cross section results obtained using static potential and static plus exchange potential experience a sharp increase in the cross section just around the excitation threshold (negative ion resonances) a phenomenon that is attributed to the formation of negative ion when the projectile electron is left with very little energy after exciting the target atom. This can also be caused by the longer time of interaction between the projectile electron and the target at excitation threshold leading to an enhanced cross section.

The present results using static potential only in both the initial and final channels are in good qualitative agreement with the experimental results of Borovik et al 2011 in the lower energy region around excitation threshold ($< 15eV$) and upper energy region ($300eV$). In the intermediate energy regime there is disparity, our results are higher than the experimental results. On inclusion of the absorption potential (Staszewska et al; 1984), the results are brought closer to the experimental results, that is between (19-40)eV. Inclusion of absorption potential improves our results at intermediate energy range.
The present results with exchange potential included in the distortion potential reduces the integral cross section drastically in the lower impact energies (around excitation threshold). This indicates that exchange potential model (Furness and McCarthy, 1973) which we are using in this study is not appropriate for heavy alkali metals like cesium where relativistic effects like spin-orbit coupling and multi-configuration mixing effects are very dominant.

It is seen that the inclusion of the absorption potential either to the static potential or to the static plus exchange potential, lowers the cross section. This is expected since absorption potential account for the possibility of projectile to be removed from the channel under consideration (excitation to the autoionizing state). Thus the total cross section is reduced.

My results (Figure 5.1) are in qualitative agreement with the theoretical result of Pangantiwar and Srivastava (1987) at higher impact energies. The disparity in lower impact energy is attributed to the difference in distortion potentials used since this is the energy region where effect of the potential is highly seen as the projectile takes more time interacting with the target atom. Our results also compares well with relativistic distorted wave (RDW) results of Kaur and Srivastava (1999) in the higher projectile energy region.
Table 5.1: Present integral cross section results in $a_0^2$ for electron impact excitation of the lowest autoionizing state of cesium using different distortion potentials.

<table>
<thead>
<tr>
<th>IMPACT ENERGY (eV)</th>
<th>STATIC</th>
<th>STATIC+EXCH</th>
<th>STATIC+ABSORP</th>
<th>STATIC+EXCH +ABSORP</th>
</tr>
</thead>
<tbody>
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<td>9.605E00</td>
<td>3.398E-01</td>
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<td>7.094E-01</td>
<td>3.951E-01</td>
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<td>3.362E-01</td>
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<td>4.599E-01</td>
<td>3.033E-01</td>
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<td>2.817E-01</td>
<td>2.810E-01</td>
</tr>
</tbody>
</table>
Figure 5.1 Integral cross section results for electron impact excitation of the lowest autoionizing state of cesium using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
5.3 Differential Cross Sections

The differential cross sections (DCS) in this study have been calculated at 16, 20, 30, 40, 70, 100, and 300eV, and scattering angles ranging from $\theta = 0^\circ$ to $\theta = 180^\circ$ with variations of the distortion potentials in the initial and final channels. The results of this study for the differential cross sections have been compared amongst themselves and with the theoretical results of Pangantiwar and Srivastava (1987) from excitation threshold to 300eV.

Figures (5.2-5.8) give the differential cross section results at different electron impact energies. The differential cross sections have maximum value at small scattering angles and they reduce as the angles increase except at very low impact energy. This means that more particles are scattered at small scattering angles and less at large angles. As the projectile energy increases, the particle encounters less interaction with the target atom, hence it is scattered at a small angle.

At low impact energies (just above the excitation threshold), the projectile electron has more interaction with the target atom (cesium) since this impact energy is around the excitation threshold and after the excitation of the atom, the projectile electron is left with very little energy. The projectile scattering at this energy region is therefore being determined more by the potential of the target atom (cesium). The projectile therefore has equal chances of being scattered in any direction. That is what we see in figure 5.2 which gives the differential cross section at 16eV electron impact energy.
The inclusion of the exchange and absorption potential lowers the differential cross section across the energy range of the study but does not change the trend. As the impact energy increases, the agreement between our present results improves. This is because as the impact energy increases, the difference in the distortion potentials become less important.

All the differential cross sections at all energies are large at small scattering angles. The differential cross sections (DCS) results obtained in this study and the study of Pangantiwar and Srivastava (1987) have a similar trend at all impact energies, slight variations are due to the different choices of distortion potentials.

At lower impact energies, the absorption potential has little effect on the DCS. This is because very few other channels are open at this energy. That explain why the inclusion of absorption potential at impact energies 16eV and 20eV (Figures 5.2 and 5.3) does not change the DCS at these energies. But as the impact energy increases, more channels are open and the inclusion of absorption potential shows its effect as we see at 30eV and 40eV electron impact energies (Figures 5.4 and 5.5). The present DCS at 100eV and 300eV (Figures 5.7 and 5.8) are in good agreement amongst themselves though there are no experimental or theoretical data available in literature for comparison.
Table 5.2: Present differential cross section results in \( \alpha_0^2 sr^{-1} \) for electron impact excitation of the lowest autoionizing state of cesium at 16eV using different distortion potentials.

<table>
<thead>
<tr>
<th>ANGLE (( \Theta )) IN DEGREES</th>
<th>STATIC ONLY</th>
<th>STATIC EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
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Table 5.3: Present differential cross section results in \( \alpha_0^2 sr^{-1} \) for electron impact excitation of the lowest autoionizing state of cesium at 20eV using different distortion potentials.

<table>
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<tr>
<th>ANGLE (( \Theta )) IN DEGREES</th>
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<th>STATIC EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
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**Table 5.4:** Present differential cross section results in $a_0^2 sr^{-1}$ for electron impact excitation of the lowest autoionizing state of cesium at 30eV using different distortion potentials.

<table>
<thead>
<tr>
<th>ANGLE ($\theta$) IN DEGREES</th>
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<th>STATIC + EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
</tr>
</thead>
<tbody>
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<td>1.6059E00</td>
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</tr>
<tr>
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<td>1.1360E-01</td>
</tr>
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<td>3.4256E-02</td>
</tr>
<tr>
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<td>5.682E-02</td>
<td>1.0221E-02</td>
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<td>2.2454E-02</td>
</tr>
<tr>
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<td>1.4162E-02</td>
<td>1.1988E-02</td>
<td>8.1129E-03</td>
<td>6.2680E-04</td>
</tr>
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<td>9.5599E-03</td>
<td>8.933E-03</td>
<td>3.4862E-03</td>
<td>2.605E-04</td>
</tr>
<tr>
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<td>4.4890E-03</td>
<td>4.745E-03</td>
<td>1.8287E-03</td>
<td>1.5591E-04</td>
</tr>
<tr>
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<td>3.638E-03</td>
<td>1.8029E-03</td>
<td>1.3450E-04</td>
</tr>
<tr>
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<td>6.106E-03</td>
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<td>1.4971E-04</td>
</tr>
<tr>
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<td>9.492E-03</td>
<td>2.0049E-03</td>
<td>1.462E-04</td>
</tr>
<tr>
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<td>1.1039E-02</td>
<td>1.9414E-03</td>
<td>1.3830E-04</td>
</tr>
</tbody>
</table>

**Table 5.5:** Present differential cross section results in $a_0^2 sr^{-1}$ for electron impact excitation of the lowest autoionizing state of cesium at 40eV using different distortion potentials.

<table>
<thead>
<tr>
<th>ANGLE ($\theta$) IN DEGREES</th>
<th>STATIC ONLY</th>
<th>STATIC + EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.5158E00</td>
<td>3.970E00</td>
<td>4.1947E00</td>
<td>4.1163E00</td>
</tr>
<tr>
<td>10</td>
<td>1.3884E00</td>
<td>1.2006E00</td>
<td>1.3585E00</td>
<td>1.1860E00</td>
</tr>
<tr>
<td>20</td>
<td>1.5547E-01</td>
<td>1.1553E-01</td>
<td>1.5749E-01</td>
<td>1.0809E-01</td>
</tr>
<tr>
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<td>1.6431E-02</td>
<td>9.8820E-03</td>
<td>1.4241E-02</td>
<td>8.782E-03</td>
</tr>
<tr>
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<td>1.4161E-02</td>
<td>1.1531E-02</td>
<td>1.2512E-02</td>
<td>1.1336E-02</td>
</tr>
<tr>
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<td>8.524E-03</td>
<td>8.4619E-03</td>
<td>8.271E-03</td>
</tr>
</tbody>
</table>
Table 5.6: Present differential cross section results in \( \alpha^2_0 s \) \( \text{sr}^{-1} \) for electron impact excitation of the lowest autoionizing state of cesium at 70eV using different distortion potentials.

<table>
<thead>
<tr>
<th>ANGLE (( \Theta )) IN DEGREES</th>
<th>STATIC ONLY</th>
<th>STATIC + EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
</tr>
</thead>
<tbody>
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<td>1.0163E01</td>
</tr>
<tr>
<td>10</td>
<td>1.1314E00</td>
<td>1.0122E00</td>
<td>1.1061E00</td>
<td>9.9627E-01</td>
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<tr>
<td>20</td>
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<td>1.796E-02</td>
<td>2.7093E-02</td>
<td>1.7517E-02</td>
</tr>
<tr>
<td>30</td>
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<td>1.0201E-02</td>
<td>1.1291E-02</td>
<td>1.0260E-02</td>
</tr>
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<td>8.780E-03</td>
<td>8.426E-03</td>
<td>8.5176E-03</td>
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<td>1.268E-03</td>
<td>1.1150E-03</td>
<td>1.1280E-03</td>
</tr>
<tr>
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<td>3.274E-04</td>
<td>2.4163E-04</td>
<td>2.795E-04</td>
</tr>
<tr>
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<td>2.886E-04</td>
<td>2.4109E-04</td>
<td>2.619E-04</td>
</tr>
<tr>
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<td>2.118E-04</td>
<td>1.7949E-04</td>
<td>1.951E-04</td>
</tr>
<tr>
<td>140</td>
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<td>1.217E-04</td>
<td>9.6559E-05</td>
<td>1.105E-04</td>
</tr>
<tr>
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<td>7.408E-05</td>
<td>5.3230E-05</td>
<td>6.551E-05</td>
</tr>
<tr>
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<td>4.742E-05</td>
<td>4.6830E-05</td>
<td>4.090E-05</td>
</tr>
</tbody>
</table>

Table 5.7: Present differential cross section results in \( \alpha^2_0 s \) \( \text{sr}^{-1} \) for electron impact excitation of the lowest autoionizing state of cesium at 100eV using different distortion potentials.

<table>
<thead>
<tr>
<th>ANGLE (( \Theta )) IN DEGREES</th>
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<th>STATIC + EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
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<td>1.5869E01</td>
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<tr>
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<td>6.154E-01</td>
<td>5.636E-01</td>
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<tr>
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<td>4.201E-03</td>
<td>5.192E-03</td>
<td>4.408E-03</td>
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<tr>
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<td>1.099E-02</td>
<td>1.066E-02</td>
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<tr>
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<td>3.484E-03</td>
<td>3.572E-03</td>
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<tr>
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<td>2.323E-04</td>
<td>2.643E-04</td>
</tr>
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<td>1.644E-04</td>
</tr>
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<td>ANGLE (θ) IN DEGREES</td>
<td>STATIC ONLY</td>
<td>STATIC + EXCHANGE</td>
<td>STATIC + ABSORPTION</td>
<td>STATIC+EXCHANGE + ABSORPTION</td>
</tr>
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<td>----------------------</td>
<td>-------------</td>
<td>-------------------</td>
<td>---------------------</td>
<td>-----------------------------</td>
</tr>
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<td>5.2071E00</td>
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<tr>
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<td>9.827E-06</td>
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<td>6.530E-06</td>
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<td>4.4997E-06</td>
<td>4.836E-06</td>
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<td>3.645E-06</td>
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<tr>
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<tr>
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<td>1.510E-06</td>
<td>1.3077E-06</td>
<td>1.415E-06</td>
</tr>
</tbody>
</table>

Table 5.8: Present differential cross section results in $a_0^2 sr^{-1}$ for electron impact excitation of the lowest autoionizing state of cesium at 300eV using different distortion potentials.
Figure 5.2 Differential cross section results for electron impact excitation of the lowest autoionizing state of cesium at 16eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption). The graph of present static plus absorption is mounted on graph of present static only while the graph of present static, exchange plus absorption is mounted on the graph of present static plus exchange.
Figure 5.3 Differential cross section results for electron impact excitation of the lowest autoionizing state of cesium at 20eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption). The graph of present static plus absorption is mounted on graph of present static only while the graph of present static, exchange plus absorption is mounted on the graph of present static plus exchange.
Figure 5.4 Differential cross section results for electron impact excitation of the lowest autoionizing state of cesium at 30eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
Figure 5.5 Differential cross section results for electron impact excitation of the lowest autoionizing state of cesium at 40eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
Figure 5.6 Differential cross section results for electron impact excitation of the lowest autoionizing state of cesium at 70eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
Figure 5.7 Differential cross section results for electron impact excitation of the lowest autoionizing state of cesium at 100eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
Figure 5.8 Differential cross section results for electron impact excitation of the lowest autoionizing state of cesium at 300eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
5.4 **Alignment Parameter (A\textsubscript{20})**

The present alignment parameter results (figure 5.9) are compared amongst themselves and with the theoretical work of Kaur and Srivastava (1999) from above excitation threshold up to 500eV.

The present alignment results are in good qualitative agreement amongst themselves and at higher impact energies they converge closer, a phenomenon that is also noticed in the integral cross section at high impact energies. The present results are in qualitative agreement with the work of Kaur and Srivastava (1999), though their relativistic Born approximation (RBA) results are a bit higher than ours at all energies. Between (60-150) eV, our results for static and static plus absorption as the distortion potentials are in very close agreement with the relativistic distorted wave (without exchange) results (RDWD) of Kaur and Srivastava (1999).

From the formula of alignment parameter, when A\textsubscript{20} is negative indicates that \(\sigma\)\textsubscript{0} is greater than \(\sigma\)\textsubscript{1}. This means that most of the excitations are taking place from the magnetic substate \(m = 0\) and when A\textsubscript{20} is positive, it means that \(\sigma\)\textsubscript{1} is greater than \(\sigma\)\textsubscript{0} and the most of the excitations are taking place from \(m = 1\) magnetic substate. In our study (figure 5.9), from above excitation threshold up to around 350eV, alignment parameter is negative indicating that most of the incident electrons are scattered from the magnetic substate \(m = 0\), compared to magnetic substate \(m = 1\).
Table 5.9: Present alignment parameter results for electron impact excitation of the lowest autoionizing state of cesium atom using different distortion potentials.

<table>
<thead>
<tr>
<th>ENERGY (eV)</th>
<th>STATIC</th>
<th>STATIC+ EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>-0.9779</td>
<td>-0.9985</td>
<td>-0.9779</td>
<td>-0.9985</td>
</tr>
<tr>
<td>15</td>
<td>-0.9187</td>
<td>-0.9293</td>
<td>-0.9417</td>
<td>-0.9293</td>
</tr>
<tr>
<td>17</td>
<td>-0.8103</td>
<td>-0.8475</td>
<td>-0.8103</td>
<td>-0.8475</td>
</tr>
<tr>
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<td>-0.6390</td>
<td>-0.7100</td>
</tr>
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<td>-0.5520</td>
<td>-0.6172</td>
</tr>
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</tr>
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</tr>
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<td>-0.2570</td>
</tr>
<tr>
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<td>-0.2453</td>
<td>-0.1988</td>
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</tr>
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</tr>
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</tr>
<tr>
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<td>-0.06490</td>
<td>-0.1171</td>
</tr>
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<td>-0.0849</td>
<td>-0.05754</td>
<td>-0.08344</td>
</tr>
<tr>
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<td>-0.04627</td>
</tr>
<tr>
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<td>-0.01142</td>
</tr>
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</tr>
<tr>
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<td>0.1423</td>
<td>0.1259</td>
<td>0.14279</td>
<td>0.1263</td>
</tr>
</tbody>
</table>
Figure 5.9 Alignment parameter results for electron impact excitation of the lowest autoionizing state of cesium using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
5.5 Lambda parameter ($\lambda$)

Results for lambda parameter are presented at 16 eV, 30 eV, 40 eV and 70 eV projectile energies. These results are compared with lambda parameter results for $2p_{3/2}$ for cesium atom by Pangantiwar and Srivastava (1987). Tables 5.10-5.13 give present lambda parameter results for electron impact excitation of the lowest autoionizing state in cesium atom at various incident energies. Figures 5.10-5.13 show the lambda parameter results at different impact energies using different distortion potentials. At 16eV which is closer to the excitation threshold, our results are in close agreement with the results of Pangantiwar and Srivastava (1987) at lower and upper scattering angles, with disparity at intermediate scattering angles (30°-140°). At 30eV, 40eV, 70eV, the present lambda results are in good qualitative and quantitative agreement at lower scattering angles, while in upper scattering angles there is disparity which is associated to different distortion potential used in the initial and final channels. In the present study I am calculating the lambda parameter for the unresolved state. Pangantiwar and Srivastava (1987) only studied the lambda parameter for fine structure state (\(^{2}P_{3/2}\)) for cesium atom. It is clear that when $\lambda = 1$, then $\sigma_{0}(\theta,\varphi) \gg \sigma_{1}(\theta,\varphi)$ from the formula for lambda parameter. This shows that most of the particles are scattered from the magnetic substate $m = 0$ as indicated in lower and upper scattering angles in our present lambda parameter results for all the impact energies. We see from these figures 5.10 – 5.13, that as the impact energy increases most of the particles scattered at intermediate angles are scattered from $m = 1$ magnetic sublevel, since the lambda parameter value is less than 0.3 ($\lambda < 0.3$). When $\lambda = 0.3$, then the particles are evenly scattered from the two states.
Table 5.10: Present Lambda parameter results for electron impact excitation of the lowest autoionizing state of cesium at 16eV using different distortion potentials

<table>
<thead>
<tr>
<th>ANGLE ((\theta)) IN DEGREES</th>
<th>STATIC ONLY</th>
<th>STATIC + EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1.000</td>
<td>1.000</td>
</tr>
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<td>0.955</td>
<td>0.9521</td>
</tr>
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</tr>
<tr>
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<td>0.7958</td>
</tr>
<tr>
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<td>0.8099</td>
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</tr>
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</tr>
<tr>
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<td>0.9190</td>
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</tr>
<tr>
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<td>0.8737</td>
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</tr>
<tr>
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</tr>
<tr>
<td>140</td>
<td>0.9583</td>
<td>0.9672</td>
<td>0.9583</td>
<td>0.9672</td>
</tr>
<tr>
<td>160</td>
<td>0.9898</td>
<td>0.9919</td>
<td>0.9898</td>
<td>0.9919</td>
</tr>
<tr>
<td>180</td>
<td>0.9997</td>
<td>0.9999</td>
<td>0.9997</td>
<td>0.9999</td>
</tr>
</tbody>
</table>

Table 5.11: Present Lambda parameter results for electron impact excitation of the lowest autoionizing state of cesium at 30eV using different distortion potentials

<table>
<thead>
<tr>
<th>ANGLE ((\theta)) IN DEGREES</th>
<th>STATIC ONLY</th>
<th>STATIC + EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>10</td>
<td>0.6774</td>
<td>0.6839</td>
<td>0.5572</td>
<td>0.5592</td>
</tr>
<tr>
<td>20</td>
<td>0.2785</td>
<td>0.2760</td>
<td>0.0200</td>
<td>0.0689</td>
</tr>
<tr>
<td>30</td>
<td>0.4772</td>
<td>0.4775</td>
<td>0.6034</td>
<td>0.6451</td>
</tr>
<tr>
<td>40</td>
<td>0.8216</td>
<td>0.8820</td>
<td>0.8213</td>
<td>0.7629</td>
</tr>
<tr>
<td>60</td>
<td>0.1395</td>
<td>0.1722</td>
<td>0.2708</td>
<td>0.3875</td>
</tr>
<tr>
<td>80</td>
<td>0.04151</td>
<td>0.2511</td>
<td>0.8117</td>
<td>0.7432</td>
</tr>
<tr>
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<td>0.00257</td>
<td>0.3279</td>
<td>0.6856</td>
<td>0.6729</td>
</tr>
<tr>
<td>120</td>
<td>0.4275</td>
<td>0.5239</td>
<td>0.8025</td>
<td>0.7332</td>
</tr>
<tr>
<td>140</td>
<td>0.9045</td>
<td>0.9196</td>
<td>0.9008</td>
<td>0.8739</td>
</tr>
<tr>
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<td>0.9895</td>
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<td>0.9559</td>
</tr>
<tr>
<td>180</td>
<td>0.9998</td>
<td>0.9999</td>
<td>0.9989</td>
<td>0.9998</td>
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</tbody>
</table>
Table 5.12: Present Lambda parameter results for electron impact excitation of the lowest autoionizing state of cesium at 40eV using different distortion potentials

<table>
<thead>
<tr>
<th>ANGLE (θ) IN DEGREES</th>
<th>STATIC ONLY</th>
<th>STATIC EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
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<td>1.000</td>
</tr>
<tr>
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</tr>
<tr>
<td>20</td>
<td>0.2022</td>
<td>0.1456</td>
<td>0.1456</td>
<td>0.1665</td>
</tr>
<tr>
<td>30</td>
<td>0.8034</td>
<td>0.8919</td>
<td>0.7883</td>
<td>0.8957</td>
</tr>
<tr>
<td>40</td>
<td>0.4590</td>
<td>0.4863</td>
<td>0.3884</td>
<td>0.5159</td>
</tr>
<tr>
<td>60</td>
<td>0.0396</td>
<td>0.0714</td>
<td>0.0688</td>
<td>0.09372</td>
</tr>
<tr>
<td>80</td>
<td>0.00936</td>
<td>0.0311</td>
<td>0.0707</td>
<td>0.08369</td>
</tr>
<tr>
<td>100</td>
<td>0.3796</td>
<td>0.4309</td>
<td>0.1902</td>
<td>0.2144</td>
</tr>
<tr>
<td>120</td>
<td>0.8926</td>
<td>0.8956</td>
<td>0.7706</td>
<td>0.7528</td>
</tr>
<tr>
<td>140</td>
<td>0.9822</td>
<td>0.9827</td>
<td>0.9627</td>
<td>0.9623</td>
</tr>
<tr>
<td>160</td>
<td>0.9943</td>
<td>0.9974</td>
<td>0.9940</td>
<td>0.9882</td>
</tr>
<tr>
<td>180</td>
<td>0.9988</td>
<td>0.9999</td>
<td>0.9999</td>
<td>0.9976</td>
</tr>
</tbody>
</table>

Table 5.13: Present Lambda parameter results for electron impact excitation of the lowest autoionizing state of cesium at 70eV using different distortion potentials

<table>
<thead>
<tr>
<th>ANGLE (θ) IN DEGREES</th>
<th>STATIC ONLY</th>
<th>STATIC EXCHANGE</th>
<th>STATIC + ABSORPTION</th>
<th>STATIC+EXCHANGE + ABSORPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>10</td>
<td>0.1775</td>
<td>0.2006</td>
<td>0.7879</td>
<td>0.1927</td>
</tr>
<tr>
<td>20</td>
<td>0.3397</td>
<td>0.3044</td>
<td>0.3316</td>
<td>0.3133</td>
</tr>
<tr>
<td>30</td>
<td>0.2616</td>
<td>0.3439</td>
<td>0.2431</td>
<td>0.3439</td>
</tr>
<tr>
<td>40</td>
<td>0.0587</td>
<td>0.0978</td>
<td>0.5238</td>
<td>0.0941</td>
</tr>
<tr>
<td>60</td>
<td>0.0269</td>
<td>0.0518</td>
<td>0.0228</td>
<td>0.0448</td>
</tr>
<tr>
<td>80</td>
<td>0.1911</td>
<td>0.1911</td>
<td>0.2036</td>
<td>0.2006</td>
</tr>
<tr>
<td>100</td>
<td>0.4461</td>
<td>0.4376</td>
<td>0.4634</td>
<td>0.4411</td>
</tr>
<tr>
<td>120</td>
<td>0.5376</td>
<td>0.5652</td>
<td>0.4992</td>
<td>0.5568</td>
</tr>
<tr>
<td>140</td>
<td>0.5534</td>
<td>0.5919</td>
<td>0.5616</td>
<td>0.5771</td>
</tr>
<tr>
<td>160</td>
<td>0.8322</td>
<td>0.8475</td>
<td>0.8049</td>
<td>0.8371</td>
</tr>
<tr>
<td>180</td>
<td>0.9974</td>
<td>0.9877</td>
<td>0.9956</td>
<td>0.9861</td>
</tr>
</tbody>
</table>
Figure 5.10 Lambda parameter results for electron impact excitation of the lowest autoionizing state of cesium at 16eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption). The graph of present static plus absorption is mounted on graph of present static only while the graph of present static, exchange plus absorption is mounted on the graph of present static plus exchange.
Figure 5.11 Lambda parameter results for electron impact excitation of the lowest autoionizing state of cesium at 30eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
Figure 5.12 Lambda parameter results for electron impact excitation of the lowest autoionizing state of cesium at 40eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
Figure 5.13 Lambda parameter results for electron impact excitation of the lowest autoionizing state of cesium at 70eV using different distortion potentials (static only; static plus exchange; static plus absorption; static plus exchange plus absorption)
5.6 Summary on results and discussions

From the above results for electron impact excitation of the autoionizing states of cesium, it is seen that the inclusion of absorption and exchange potentials both lowers the differential and integral cross sections.

The present results for integral cross section compares well with the experimental results of Borovik (2011) around excitation threshold when we use real distortion potentials but with disparity at intermediate energy region. When the imaginary absorption potential (Staszewska 1984) is included, the results are improved at the intermediate energies (our present results are brought closer to the experimental results). The exchange potential (Furness and McCarthy 1973) drastically reduces the integral cross section around the excitation threshold. The change is very big and this suggests that this model of exchange potential is not correct for heavy alkali metals such as cesium.

The present differential cross section results are in qualitative agreement with that of Pangantiwar and Srivastava (1987) at all impact energies considered. Though there are few discrepancies which are attributed to different distortion potentials used in both the initial and final channels and also the different method of calculation of the transition matrix.

The present alignment parameter results are in good qualitative agreement with the theoretical work of Kaur and Srivastava (1999). It is seen from the present results for lambda parameter, that as the impact energy increases, most of the particles scattered at intermediate angles are scattered from $m = 1$ substate.
6.1 Conclusions

The following are the conclusions from my study:

(i) The DWM integral cross section (ICS) results for electron impact excitation of the lowest autoionizing state of cesium obtained in the present study using static potential only and the experimental results of Borovik et al. (2011) are in good agreement at near threshold and higher energies, but there is disagreement at intermediate energies. When absorption potential is included in the distortion potential the present results are brought closer to the experimental results at around (20-50eV). This suggests that inclusion of absorption potential improves results at intermediate energies.

(ii) The inclusion of exchange potential (Furness and McCarthy 1973) drastically lowers the ICS results around the excitation threshold. This indicates that this exchange potential model is not suitable for heavy target like cesium where relativistic effects are dominant.

(iii) The near threshold strong negative ion resonance (Formation of negative ion) at impact energies close to excitation threshold is the cause of sharp rise in the ICS near the impact energies close to threshold.

(iv) The alignment parameter results indicate that above excitation threshold up to 350eV, the integral cross section for m = 0 magnetic sub-level is greater than integral cross section for magnetic sub level m = 1, above this energy range, the reverse is true. This condition is valid for all the distortion potentials considered in the present study.

(v) The present study results for ICS, DCS and angular correlation parameters are in reasonable qualitative agreement with the theoretical results of Pangantiwar and Srivastava (1987) and Kaur and Srivastava (1999). The small disagreement may be attributed to the different choice of the
distortion potential and the different method used to calculate the transition matrix. In the present study we have calculated exchange T-matrix exactly without approximation while Pangantiwar and Srivastava used Ochkur approximation. So it can be said that the present method is suitable for the process considered.

6.2 Recommendations

The present study was a great success though there was no any experimental research reported in literature on the differential cross sections and angular correlation parameters for comparison purposes. Furthermore the exchange potential model we used in this study drastically reduces the integral cross section around the excitation threshold of cesium. In view of these we make the following recommendations:

i. There is need for experimental research on the angular correlation parameters, DCS and ICS for electron impact excitation of the lowest autoionizing state of Cs

ii. There is need for a more accurate model of exchange potential to be developed for heavy target atoms like cesium.

iii. There is need for both theoretical and experimental study on positron impact excitation of the auto ionizing state of Cs for comparison.

iv. There is need to develop and include polarization potential for Cs as part of distortion potential in the future study in calculations of the distorted waves in order to determine its effect on the cross sections.
REFERENCES


Kaur, S. and Srivastava, R. (1999). Excitation of the lowest autoionizing $np^5(n+1)s^2, \ ^2p_{3/2}$ states of Na (n = 2), K (n = 3), Rb (n = 4) and Cs (n = 5) by electron impact. *Journal for Physics B: Atomic, Molecular and Optical Physics, 32*: 2323-2342.


