ELECTRON IMPACT EXCITATION OF THE LOWEST AUTOIONIZING STATE INCESIUM USING DISTORTED WAVE METHOD

BY

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE AWARD OF THE DEGREE OF MASTER OF SCIENCE IN THEORETICAL PHYSICS IN THE SCHOOL OF PURE AND APPLIED SCIENCES OF KENYATTA UNIVERSITY

NOVEMBER 2015
DECLARATION

I declare that the work presented in this thesis is my original work and has not been presented for a degree in any other university or any other award.

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DEDICATION

TO

MY FAMILY
ACKNOWLEDGEMENT

I will forever be grateful to my supervisors, Dr. Singh C.S and Prof. Okumu J. for the material support, knowledge, skills and encouragement accorded to me during this research. I wish to extend my sincere gratitude to all the members of teaching and non teaching staff in the Physics department who have contributed in one way or another to the success of this research.

Special thanks to my family for the support, moral or otherwise accorded to me throughout the research period.

Above all else, all glory and honour be to God. It is through his grace that this has been possible.
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Abbreviation and meaning

EXPT - Experimental

RDW - Relativistic distorted wave

DWE - Distorted wave approximation including exchange

FBA - First Born Approximation

MFBA - Modified First Born Approximation
ABSTRACT

In previous studies made on electron impact excitation of lowest autoionizing state of cesium atom, there are discrepancies in the results obtained using theoretical and experimental methods. Even the theoretical results do not agree among themselves. So in this study, differential cross sections, integral cross sections, alignment parameter and angular correlation parameter (lambda) for electron impact excitation of the lowest autoionizing state in cesium have been calculated using Distorted Wave Method with the new distortion potential. We have applied a linear combination of static potentials of the target taken in both initial and final states as the final channel distortion potential and static potential in the initial state as the initial channel distortion potential. The wave functions used in this model are the double zeta wave functions. Numerical calculations have been performed using a modified DWBA1 program. Comparison of the present results with the available theoretical and experimental results shows that the present integral cross sections results at low energies (≤ 40 eV) are in better agreement with the experimental results compared to other theoretical results. Lambda and alignment parameters results have the same trend as other theoretical results even though the differential cross section results are in disagreement with the other theoretical result.
CHAPTER 1

INTRODUCTION

1.1 Background to the study

Most collision processes studied in Quantum Collision Theory involve collisions between a projectile (electrons, protons or fast moving atoms) and a target (molecules, atoms or ions). Electron-atom studies provide a tool for obtaining detailed information on the structure of the target atoms and molecules and final collision products. Analysis of collision phenomena plays a central role in almost all investigations into the structure of matter on the macroscopic scale. This is achieved through both experimental and theoretical models. The results of these experimental and theoretical models such as the total cross section, differential cross section, angular correlation parameters and alignment parameters are used to get a better insight into the collision processes.

In general, approaches into scattering problems fall under two broad categories, namely classical and quantal methods. Within the quantal methods, all the works falls under either close coupling approach (close coupling, R-matrix, variational methods) or perturbation series expansion (Born series, eikonal series, distorted wave series, many body theory).

Experiments involve counting of electrons and photons with particular energy, momentum and spin characteristics. The resulting probability distribution is described by Quantum Mechanics.

A schematic representation of a typical collision experiment is as shown in figure 1.1.

A beam of particles A, interacts with the target and the detectors record outgoing scattered particles in the asymptotic region. The incident beam should be well collimated and nearly mono energetic.
The incident beam should neither be too intense – so that the interaction between the incident particles maybe neglected—nor too weak, because one wants to observe a reasonable number of ‘events’ during the experiment.

During the collision several processes may occur, that is, elastic scattering, inelastic scattering and reactions.

In case of elastic scattering between a particle A of the incident beam and a scatterer B of the target, the two particles A and B are simply scattered without any change in their internal structures.

\[ A + B = A + B \]  \hspace{1cm} [1.1]

An inelastic scattering results in a change of internal quantum state for one or both the target and the projectile

\[ A + B = A' + B \text{ or} \]  \hspace{1cm} [1.2]

\[ A + B = A + B \text{ or} \]  \hspace{1cm} [1.3]
\[ A + B = A' + B' \]  \[1.4\]

Where \( A' \) and \( B' \) denote new internal states.

In case the interaction is a reaction type, the composite system \((A + B)\) splits into particles different from \( A \) and \( B \).

\[ A + B = c_1 + c_2 + \ldots + c_n \]  \[1.5\]

Where \( n \) is greater than two.

If the projectile energy is relatively high (energy greater than the ionization threshold) the target may ionize directly or may get excited to higher states above this threshold. The latter are called the autoionizing levels.

If the target is excited to any of these autoionizing states, they in principle decay via either (i) a radiative transition to a bound state of the atom below the ionization potential or (ii) by a non-radiative transition to the ground state or to one of the excited state of the ion. The non-radiative channel (autoionization) leads to emission of a fast electron whose kinetic energy equals the difference in energies between the autoionizing state and the ion.

In our study, electron impact excitation of the lowest autoionizing state in cesium, have been investigated. The transition probabilities, differential cross sections, integral cross sections, angular correlation parameter \( \lambda \) and alignment parameter \( A_{20} \), were evaluated using the distorted wave method.
This method has been found to be quite successful in explaining various features of an excitation process and in providing results which are in good agreement with experimental data for intermediate and high incident energy regions (Katiyar and Srivastava, 1988).

1.2 Statement of research problem

In this study we investigated electron impact excitation of the lowest autoionizing state in cesium using distorted wave method in the energy range 10-600 eV. Comparisons of our results have been made with available experimental and theoretical data.

1.3 Objectives of the research

1.3.1 General objective

The main objective of this research was to study the electron impact excitation of the lowest autoionizing state in cesium using First Order Distorted Wave Method.

1.3.2 Specific objectives

The specific objectives of this study were as follows:

(i) To formulate the problem and modify a DWBA1 program for the problem
(ii) To determine the differential and total cross sections for electron impact excitation of the lowest autoionizing state in cesium for the projectile energies ranging from the first excitation threshold up to 600eV.

(iii) To determine angular correlation parameter (\(\lambda\)) and alignment parameter (\(A_{20}\)), for the lowest autoionizing state in cesium.

(iv) To compare the results obtained with experimental and theoretical data available in literature.

(v) To determine the suitability of distorted wave method for calculation of the excitation of the lowest autoionizing state in cesium.

1.4 Rationale of the study

There are discrepancies between the theoretical distorted wave calculations and experimental results, available in literature for electron impact excitation of autoionizing state of cesium. Furthermore, discrepancies exist amongst theoretical results themselves. It is for this reason that the distortion potentials (in both initial and final channels) as well as the wave functions have been varied to see how the results would be affected.
CHAPTER 2

LITERATURE REVIEW

2.1 Introduction to autoionization

The alkali metal atoms have traditionally been a favourite subject of study by experimentalists and theorists because of their relatively simple electronic structure and spectra. Excitation through any collisional mechanism with photons, electrons, ions and fast moving atoms results in both direct ionization and auto-ionization. The processes of direct ionization and auto ionization are indistinguishable (Joachain, 1975).

Autoionization refers to the process by which atoms or molecules spontaneously emit one of the shell electrons, thus going from a state with Z electrons to a state with Z-1 electrons. A series of auto ionizing levels in atoms and molecules result from the excitation of the inner core electron or from the spontaneous excitation of the two electrons. Excitation of one inner-shell electron into an empty orbital leads to an autoionizing state. This is called core excitation. These levels are located above the first ionization potential. In cesium the lowest autoionizing level is located approximately 8eV above the first ionization potential at 3.9eV. These levels decays via either (i) a radiative transition to a bound state of the atom below the ionization potential or (ii) by a non radiative transition to the ground state or to one of the excited states of the ion.

The radiation-less transition mechanism is called autoionization. The non-radiative channel leads to the emission of a fast electron whose kinetic energy equals the difference in binding energies of the initial autoionizing state and that of the final state of the residue.
ion, that is, the difference in energies between the initial and final states (Hahn and Nygaard, 1971). In cesium one of the inner electrons (5p) in the 5p\(^6\) 6s ground state configuration becomes excited via electron impact and results in a bound state with electron configuration 5p\(^5\)6s\(^2\). This state \(^2P\) is located 8.41eV above the ground state of Cs\(^+\) and decays by ejecting a fast electron with kinetic energy of 8.41eV.

2.2 Electron impact excitation of autoionizing states of alkalis

Roy and Rai (1972), in their theoretical paper, studied the electron impact ionization of alkali metals using the symmetrical model as well as the correct Hartree-Fock Velocity distribution for the velocity of the bound electron to obtain single ionization cross-sections. They found that the autoionizing contribution to the total cross section would be significant for energies within 1eV of the respective threshold energies. However, the energies at which the auto ionization peaks occurred were not in absolute agreement with magnitudes in predicted theory.

In another study, Tiwarly and Rai (1975) calculated total cross sections for electron impact excitation of the lowest lying autoionizing levels in alkali metal atoms using FBA, MFBA and Vainshtein approximation (neglecting exchange). Their results were in good agreement with experimental results of Nygaard and Hahn (1973).

Pangantiwar and Srivastava (1987) performed distorted wave calculations for electron (and positron) impact excitation of lowest autoionizing levels in alkalis (Li, Na, K, Rb and Cs). They concluded that (among others) it is difficult to make any conclusive statement of the validity of any theory as far as comparison with experimental results is
concerned. Their results had a broad maximum and a small dip in the cross section, which however, disappeared on inclusion of exchange.

Kaur and Srivastava (1999) carried out RDW calculations for the electron impact excitation of the lowest autoionizing states \([np^5(n+1)s^2 2P]\) in K, Na and Cs alkali atoms from ground state \([np^6(n+1)s]\). They found that, indeed, autoionization processes contributes significantly to the ionization cross-sections of alkali metals—as earlier predicted by Roy and Rai (1972), Nygaard (1975) and Pangantiwar and Srivastava (1987).

Jobunga et al. (2010) calculated the electron impact excitation of the lowest autoionizing states of sodium using Distorted Wave Method and reproduced near threshold resonances observed in the experimental excitation of sodium.

2.3 Experimental studies on electron impact excitation of the autoionizing levels in alkalis

Nygaard (1975) studied (in a crossed beam apparatus) electron impact autoionization in heavy alkali metals (cesium and rubidium). He concluded that autoionization is significant in ionization curves.

Borovik and Kupliauskiene (2009) studied the autoionization cross section of cesium atoms in the incident energy range from \(5p^6\) lowest autoionization threshold at 12.3eV up to 16.6 eV. They found out that the dominant features of the autoionization function are
near threshold peak at 12.4eV. They postulated that this can be attributed to the presence of a group of efficiently excited autoionizing levels here.

Borovik et al. (2011) studied the electron impact excitation of the $5p^6$ sub-shell in cesium atom by measuring excitation cross section of lines in ejected electron spectra arising from the decay of the $5p^6n_1l_1n_2l_2$ autoionizing doublet and quartet levels. They found out that there is formation of negative-ion resonances at near threshold energies.

2.4 Summary of review

From the above studies discussed, no model gives results that are in perfect agreement with experimental data. Furthermore, discrepancies exist amongst theoretical results themselves. These points of departure between theoretical results and experimental results and amongst theoretical results themselves prompted us to carry out a study on electron impact excitation of the lowest autoionizing state in cesium using distorted wave method.

We have used an average of static potentials in the initial and final states of the atom as the distortion potential for the scattered electron wave function in the final state and static potential in the initial state of the atom as the distortion potential in the initial state of the incident electron.

We have used an approximate Roothan-Hartree Fock wave function (double zeta wave functions) in which a given electron orbital is described by two slater functions.
CHAPTER 3

THEORETICAL FRAMEWORK

3.1 Introduction

Over the years, both classical and quantal methods have been used to calculate scattering amplitudes. The quantal approaches fall under either close coupling technique (close coupling, R-matrix, variation methods e.t.c) or into the category of perturbation series expansions (Born series, distorted wave series, Eikonal series, many body theory).

In this chapter, a brief overview, of some quantum mechanical approaches have been discussed.

3.2 Quantum mechanical methods

3.2.1 Born approximation

Born series is a perturbation type expansion of the wave function or the scattering amplitude in powers of the interaction potential (Joachain, 1975).

The Lippmann-Schwinger equation, which is a replacement of the Schrödinger with the boundary condition

\[ \Psi_{k_1}(r)_{r \to \infty} = A(\exp(ik_r r) + f(\theta, \varphi) \frac{\exp(ik_r r)}{r}) \]

given as

\[ \Psi_{k_1}(r)_{r \to \infty} = (2\pi)^{\frac{3}{2}} \exp(ik_r r) + \int G_0^{(+)}(r, r') U(r') \Psi_{k_1}(r') dr' \]
where \( \psi_{k_1}^+ (r) \) is the exact scattering wave function, \( G_0^+ \) is the Green's function

\[
G_0^+ = \frac{1}{4\pi} \exp\left(\frac{ik|r-r'|}{r-r'}\right)
\]

[3.3]

can be solved iteratively starting with the plane wave, \( \phi_{k_1}(r) = 2\pi \frac{3}{2}\exp(ik_1 \cdot r) \) as the zero order approximation. A sequence of functions is obtained;

\[
\psi_0(r) = \phi_{k_1}(r)
\]

[3.4]

\[
\psi_1(r) = \phi_{k_1}(r) + \int G_0^+(r,r')U(r')\psi_{n-1}(r') \, dr'
\]

[3.5]

\[
\psi_n(r) = \phi_{k_1}(r) + \int G_0^+(r,r')U(r')\psi_{n-1}(r') \, dr'
\]

[3.6]

The function \( \psi_n(r) \) can be written in the form;

\[
\psi_n(r) = \sum_{m=0}^{n} \phi_m(r)
\]

[3.7]

Letting \( n \to \infty \), a Born series for the scattering wave function is obtained.

Replacing the exact scattering wave function \( \psi_{k_1}^+ (r) \) by the integral representation of the scattering amplitude,

\[
f = -2\pi^2 \langle \phi_{k_f} | U | \psi_{k_1}^+ \rangle
\]

[3.8]

where \( \phi_{k_f} \) is the plane wave corresponding to the final wave vector \( k_f \).
The sequence obtained;

\[ f_{B1} = -2\pi^2 \langle \varphi_{k_f} | U | \varphi_{k_i} \rangle \]  \hspace{1cm} [3.9]

\[ f_{B2} = -2\pi^2 \langle \varphi_{k_f} | U | \psi_1 \rangle \]  \hspace{1cm} [3.10]

\[ f_{Bn} = -2\pi^2 \langle \varphi_{k_f} | U | \psi_{n-1} \rangle \]  \hspace{1cm} [3.11]

where \( f_{Bn} \) is the \( n^{th} \) Born approximation to the scattering amplitude.

In first Born approximation, the differential cross section is given by;

\[ \left( \frac{d\sigma}{d\Omega} \right)_{B1} = \left| f_{B1} \right|^2 \]  \hspace{1cm} [3.12]

The total \( 1^{st} \) Born cross section is given by;

\[ \sigma_{tot}^{B1}(k) = \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin \theta \left| f_{B1}(k, \theta, \varphi) \right|^2 \]  \hspace{1cm} [\tau.13]

Born series does not always converge. However, when used as a practical method of computing amplitudes, it must converge so rapidly that only the first few terms provide a reliable approximation. In most cases, it is used only if the first term alone is dominant (Taylor, 1972). Nonetheless, at high energies or weak potentials, the series converge rapidly.

3.2.2 Optical potential
In this method, elastic scattering of a given projectile by a composite target containing several scatterers is conveniently analyzed by replacing the multiple interactions between the beam and the target by an optical potential (pseudopotential) in which the incident projectile moves (Joachain, 1975).
The optical potential is a complicated non-local, complex operator determined through approximation (MacCarthy, 1995). Once the optical potential is determined, the many body problem (interaction between the projectile and multiple scatterers of the target) is reduced to a one body situation, namely scattering of a particle by a potential.

3.2.3 R-matrix method

In this method, the (N+1)-electron collision problem is solved in a sphere of radius \( a \), which is chosen to be larger than the distance beyond which the radial orbitals of a chosen set of bound states becomes negligibly small. The solution is essentially a configuration-interaction method where the basis configurations consists of determinants of bound orbitals representing the N target electrons and continuum electron (MacCarthy, 1995).

The internal solutions, at \( r = a \), are matched to solutions of the scattering problem in the external region. Here it is a simple coupled-channels problem in which exchange and target-correlation terms are negligible. The matching matrix is the \( r \)-matrix.

3.2.4 The coulomb-projected Born approximation

Coulomb-projected Born approximation is a modification of the Born approximation by taking into account the coulomb interaction between the projectile and the nucleus. In this method, the final state plane wave in the Born approximation is replaced by a coulomb wave function corresponding to the nuclear charge. These approximations are useful in describing collisional mechanisms between the projectile and the target and gives better results than Born approximation.
3.3.5 Distorted wave approximations

Distorted wave methods have proved to be the most successful approaches for the theoretical calculations of electron-atom scattering. The results therein are in reasonable qualitative agreement with the experimental data (Madison et al., 1991), and are dependent on the type of approximation and the choice of distortion potential.

In the standard first order distorted wave method (DWBA1), the coupling between the two states is assumed to be weak (negligible) and also the initial and final state distorting potentials are assumed to be spherically symmetric.

Distorted wave methods are more conveniently discussed within the framework of two-potential formalism. Within the two-potential model, the transition matrix is given as (Joachain, 1975);

\[ T_{1f} = \langle \chi_f^- | U_f | \phi_i^+ \rangle \langle \chi_f^- | V - U_f | \psi_i^+ \rangle \]  \[3.14\]

where \( \chi \) is the distorted wave, \( U \) is an arbitrary distorting potential for the projectile, experienced by the target atom in its final state, \( \phi_i \) is the product of the initial state target wave function and the plane wave of the projectile and \( \psi_i^+ \) is the total wave function of the system.

This is the model that we have used to evaluate the scattering parameters for electron impact excitation of the lowest autoionizing state in cesium atom. This method is discussed in detail in chapter 4.
CHAPTER 4

METHODOLOGY

4.1 The distorted wave method

The total Hamiltonian for the electro-(neutral) atom system can be written as (Madison and Bartschart, 1996);

\[ H = h_a + T + V \]

where \( h_a \) is the hamiltonian for an isolated system, \( T \) and \( V \) are respectively the kinetic and potential energies (in Rydberg unit) of the projectile electron and are given as;

\[ T = -\nabla_0^2 \]

\[ V = \frac{2z_p z_N}{r_0} - \sum_{i}^N \frac{2z_p}{r_{0i}} \]

where, \( r_0 \) is the projectile electron coordinate with respect to the nucleus, \( r_{0i} \) is the distance between the projectile electron and the \( i^{th} \) atomic electron, \( z_N \) is the charge of the nucleus and \( z_p \) is the charge of the projectile.

The initial full scattering wave function \( \Psi_i^+ \) is a solution of the Schrödinger equation;

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

where (+) indicates the outgoing wave boundary conditions. In this case, the projectile electron experiences either elastic or inelastic collision with an N-electron atom. The exact T-Matrix in the two potential approach (Madison and Bartschart, 1996) is given by;
\[ T_{if} = (N+1) \langle \chi_f^- (0) \psi_f (1, \ldots, N) \mid V - U_f \mid A \Psi_i^+ (0, \ldots, N) \rangle + \]

\[ \langle \chi_f^- (0) \psi_f (1, \ldots, N) \mid U_f \mid \Psi_i^+ (1, \ldots, N) \beta_i (0) \rangle \]  

where \( \beta_i \) is the initial state plane wave (eigen function for an isolated projectile).

A is antisymmetrizing operator for the N+1 electron system.

\( T_{if} \) is the exact T-Matrix for the case of the incoming and outgoing projectile being represented by plane waves. \( \psi_i \) and \( \psi_f \) are the properly antisymmetrized initial and final atomic wave functions for an isolated atom which diagonalize the atomic Hamiltonian \( h_\alpha \), according to;

\[ \langle \psi_n \mid h_\alpha \mid \psi_n \rangle = \epsilon_n \delta_{nn} \]  

If \( \Psi_i^+ (0, \ldots, N) \) is chosen to be the product of a projectile wave function (electron 0) and the antisymmetrized atomic wave function (electrons 1, \ldots, N) then;

\[ A = \frac{1}{N+1} (1 - \sum_i^n P_{i0}) \]  

where \( P_{i0} \) is the operator that exchanges electrons 0 and i.

\( U_f \) in equation 4.1.5, is the distorting potential for the projectile which is used to calculate \( \chi_f \) by solving;

\[ (V_0^2 - U_f + k_f^2) \chi_f^- = 0 \]

where (-) superscript designates incoming wave boundary conditions and \( E_f \) is the final state energy of the projectile. \( U_f \) is chosen to be spherically symmetric final state.
approximation of $V$ since it's the potential used to calculate the final state wave function for the projectile.

$U_f$ can be any potential provided $\chi_f$ satisfies the appropriate boundary condition

$k_f$ is the final state wave vector of the projectile.

Choosing $U_f$ as a linear combination of static potentials of the target states, for the inelastic collision, the second term vanishes due to orthogonality of atomic wave functions. On the other hand, for elastic scattering, the second term is the dominant term, since generally, $U_f$ is chosen such that the matrix elements of $V - U_f$ vanish.

The T-Matrix is evaluated by making approximations since $\Psi_i^+$ cannot be evaluated exactly. In distorted wave approach, $\Psi_i^+$ is expressed in terms of a product of an initial state distorted wave $\chi_i^+$ times an initial atomic wave function $\psi_i$ (Madison and Bartschart, 1996).

Initial state distorted wave, $\chi_i$ (distorted wave function representing the projectile) is a solution to the wave equation;

$$ (\nabla_0^2 - U_i + k_i^2)\chi_i^+ = 0 $$ \hspace{1cm} [4.1.9]

where $U_i$ is an arbitrary potential, chosen for the distortion of the initial state projectile electron wave function which vanishes asymptotically. $k_i$ is the initial wave vector of the projectile electron and is related to the incident energy by

$$ E_i = \frac{1}{2} k_i^2 $$ \hspace{1cm} [4.1.10]
The Lipmann Schwinger solution for $\Psi_i^+$ in terms of $\chi_i$ is given by;

$$\Psi_i^+ = (1 + G^+[V - U_i])\psi_i\chi_i^+ \tag{4.1.11}$$

where $\Psi_i^+$ is the total wave function (a product of an initial state distorted wave, $\chi_i$ times an initial atomic wave function $\psi_i$), $U_i$ is an arbitrary distortion potential. In this study, $U_i$ is the initial state static potential;

$$G^+ = (E - H + i\eta)^{-1} \tag{4.1.12}$$

is the full Green's function.

A series expansion of the full Green's function, $G^+$ in terms of the distorted Green's function $g^+$ defined as;

$$g^+ = (h_a - T - U + i\eta)^{-1} \tag{4.1.13}$$

can be written as;

$$G^+ = g^+ + G^+(V - U)g^+ \tag{4.1.14}$$

Equation [4.1.14] is then iterated to obtain the series expansion for the full Green's function as;

$$G^+ = g^+ + g^+(V - U)g^+ + g^+(V - U)g^+(V - U)g^+ \tag{4.1.15}$$

Using [4.1.11] in [4.1.5] along with [4.1.15], a series expansion of the transition matrix is obtained;

$$T_{If} = T_1 + T_2 + T_3 \tag{4.1.16}$$
where;

\[ T_1 = (N+1) \langle \chi_f^- (0) \psi_f (1,\ldots,N) \mid V - U_f \mid \chi_i^- (0) \rangle \]

\[ + \langle \chi_f^- (0) \psi_f (1,\ldots,N) \mid U_f \mid \chi_i^- (0) \rangle \beta_i (0) \] \quad [4.1.17]

\[ T_2 = (N+1) \langle \chi_f^- (0) \psi_f (1,\ldots,N) \mid (V - U_f) A g^+ (V - U_i) \mid \psi_i (1,\ldots,N) \rangle \]

\[ \chi_i^+ (0) \] \quad [4.1.18]

\[ T_3 = (N+1) \langle \chi_f^- (0) \psi_f (1,\ldots,N) \mid (V - U_f) A g^+ (V - U) g^+ (V - U_i) \mid \psi_i (1,\ldots,N) \rangle \]

\[ \chi_i^- (0) \] \quad [4.1.19]

where \( T_1, T_2 \) and \( T_3 \) are the first, second and third order distorted wave approximations.

### 4.2 Static potentials

The choice of distortion potentials is arbitrary, the common choice is either the static potential of the target atom in its initial or final state, or a linear combination of the two (Itikawa, 1986). In our study the initial state distorted wave is generated by a spherically symmetric distortion potential (Madison et al., 1991) given by;

\[ U_i = W_{nl}(r) = - \frac{2Z}{r} + \frac{u^0_{nl0} (r)}{\sqrt{\pi}} \] \quad [4.2.1]

where \( u^0_{nl0} = \frac{1}{4\pi^2} C (l0l; m0m) \times C (l0l; 000) \int R^2_{nl}(r) \frac{1}{r} \, dr \)
C \( l_1 l_2 l_3; m_1 m_2 m_3 \) is a Clebsch-Gordan coefficient and \( r_\geq \) is the greater of \( r \) and \( R \). The final state distorted wave is generated by a potential taken as the sum of one-half of the initial distortion potential \( w_{nl}(r) \) and one-half of the final state \( (5p^4 6s^2) \) static potential of cesium atom (Singh, 2004);

\[
U_f = \frac{1}{2} [w_{nl}(r) + \langle \psi_f | V | \psi_f \rangle] \quad [4.2.2]
\]

The subscripts \( f \) denotes final state and \( V \) is the projectile-target interaction. \( \psi_f \) is the target wave function in the final state. This choice of distortion potential (Singh, 2004) is necessitated by the reasoning that when the projectile is in the initial state, for all the time it is in the field of the initial state. When the energy from the projectile electron is transferred to the target atom, the atom takes time (relaxation time) to go to its final state. That is, there is a time lag between the time of transfer of energy and the instant when the atom reaches its final state. Thus the projectile electron in its final state ‘sees’ a potential which is intermediate between the initial and the final state static potentials of the target.

### 4.3 Evaluation of static potentials

Static potential refers to the potential felt by the incident electron in the field of the target atom. It can be expressed mathematically as;

\[
V_{st}(r_0) = \langle \psi_n | V | \psi_n \rangle \quad [4.3.1]
\]

where;

\( \psi_n \) is the wave function of the target state,
n is the initial (final) state of the target;

\[ V = \frac{1}{r_{01}} - \frac{1}{r_0} \] is the interaction potential between the incident projectile (electron) and the valence target electron.

Double Zeta wave functions (Mclean and Mclean, 1981) (for both states) were used to evaluate static potential given by equation [4.3.1]. Double zeta wave function is an approximate Roothan-Hartre Fock atomic wave function in which a given electron orbital is described by two Slater functions (details given in section 4.6).

To evaluate equation [4.3.1], \( r_{01}^{-1} \) was first developed in terms of spherical harmonics, as;

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

where \( r_> \) is the greater of \( r_0 \) and \( r_1 \) and \( r_< \) is the lesser of them.

Substituting equation [4.3.2] in eq. [4.3.1], angular integrations were performed and only the 1st term on the right of equation [4.3.2] corresponding to \( I = m = 0 \), contributes to the integral and it reduces to;

\[ V_{st}(r_0) = 2c_n c_n^* \int_0^r d\bar{r}_1 \bar{r}_1^2 \varphi_n^* \varphi_n \left[ \frac{1}{r_>} \frac{1}{r_0} \right] \]  

We have used;

\[ |\psi_n\rangle = \sum_n c_n |\varphi_n\rangle \]  
\[ \langle \psi_n | = \sum_n c_n^* \langle \varphi_n | \]  
\[ Y_{0,0} = 4\pi \frac{1}{2} \]
Equation [4.3.3] was then broken into two integrals;

\[ \int_{0}^{\infty} = \int_{0}^{r_{0}} + \int_{r_{0}}^{\infty} \]

we then have;

\[ V_{st}(r_{0}) = 2c_{n}c_{n}^{*} \int_{r_{0}}^{\infty} dr_{1} r_{1}^{2} \varphi_{n^{*}} \varphi_{n} \left[ \frac{1}{r_{1}} - \frac{1}{r_{0}} \right] \]

Where \( c_{n} \) represents the expansion coefficient and \( \varphi_{n} \) are the slater type orbitals;

\[ \varphi_{n} = N_{n} r^{n-1} \exp(-\zeta r) Y_{l,m}(r) \]

where \( n \) is the principal quantum number of the \( n^{th} \) orbital of the basis set, \( \zeta \) is a constant and \( N_{n} \) is the normalization factor of the orbital, given as;

\[ N_{n} = \left[ (2n)! \right]^{-\frac{1}{2}} 2^{n-\frac{1}{2}} \]

Substituting eq. [4.3.9] in eq. [4.3.8] we got;

\[ V_{st}(r_{0}) = 2 \sum_{n} \sum_{n'} c_{n} c_{n'}^{*} N_{n} N_{n'}^{*} \int_{r_{0}}^{\infty} r_{1}^{(n+n')-1} \left( \frac{1}{r_{1}} - \frac{1}{r_{0}} \right) \exp[-(\zeta_{n} + \zeta_{n'}) r_{1}] dr_{1} \]

From equation [4.3.11], it can be seen that the total static potential is a summation of all the elements of a \( n \times n' \) matrix. The analytical solutions of each element of eq. [4.3.11] varies in form depending on the sum of the principal quantum numbers, \( n \) and \( n' \). For our initial state the sum varied from 2 to 8 whereas for the final state, it varied from 2 to 12.

Analytical solutions were evaluated and were found to be as given in the tables 1 and 2 below (for initial and final states respectively)
Table 4.1: Analytical solutions of static potentials for $5p^66s\,^2S_1$ state in cesium for different values of $(n + n')$ in $r^{n+n'}$.

| $n+n'$ | Distortion potential $\langle \Psi_n | V | \Psi_n \rangle$ |
|--------|--------------------------------------------------|
| 2      | $\beta \left( \frac{r^2}{\zeta^2} + \frac{6r}{\zeta^3} + \frac{18}{\zeta^4} + \frac{24}{r\zeta^5} \right)$ |
| 3      | $\beta \left( \frac{r^3}{\zeta^2} + \frac{8r^2}{\zeta^3} + \frac{36r}{\zeta^4} + \frac{96}{\zeta^5} + \frac{120}{r\zeta^6} \right)$ |
| 4      | $\beta \left( \frac{r^4}{\zeta^2} + \frac{10r^3}{\zeta^3} + \frac{6r^2}{\zeta^4} + \frac{240r}{\zeta^5} + \frac{720}{r\zeta^7} + \frac{600}{\zeta^8} \right)$ |
| 5      | $\beta \left( \frac{r^5}{\zeta^2} \frac{12r^4}{\zeta^3} + \frac{90r^3}{\zeta^4} + \frac{480r^2}{\zeta^5} + \frac{1800r}{\zeta^6} + \frac{5040}{r\zeta^8} + \frac{4320}{\zeta^9} \right)$ |
| 6      | $\beta \left( \frac{r^6}{\zeta^2} + \frac{14r^5}{\zeta^3} + \frac{126r^4}{\zeta^4} + \frac{840r^3}{\zeta^5} + \frac{4200r^2}{\zeta^6} + \frac{15120r}{\zeta^7} + \frac{40320}{r\zeta^9} + \frac{35280}{\zeta^{10}} \right)$ |
| 7      | $\beta \left( \frac{r^7}{\zeta^2} + \frac{16r^6}{\zeta^3} + \frac{160r^5}{\zeta^4} + \frac{1344r^4}{\zeta^5} + \frac{8300r^3}{\zeta^6} + \frac{40320r^2}{\zeta^7} + \frac{141120r}{r\zeta^9} + \frac{362880}{\zeta^{10}} + \frac{322560}{\zeta^{11}} \right)$ |
| 8      | $\beta \left( \frac{r^8}{\zeta^2} + \frac{19r^7}{\zeta^3} + \frac{216r^6}{\zeta^4} + \frac{2016r^5}{\zeta^5} + \frac{15120r^4}{\zeta^6} + \frac{90720r^3}{\zeta^7} + \frac{42336r^2}{\zeta^8} + \frac{1451520}{11\zeta^9} + \frac{3628800}{r\zeta^{10}} + \frac{3628800}{\zeta^{11}} \right)$ |

Where $\beta = -\text{ANCO} = -C_nC_{n'}N_nN_{n'}$
Table 4.2: Analytical solutions of static potentials for $5p^66s^2^2P$ state in cesium for different values of $(n + n')$ in $r^{n+n'}$.

| n+n' | Distortion potential $\langle \Psi_n | V | \Psi_n \rangle$ |
|------|--------------------------------------------------|
| 2    | $\beta \ast \left( \frac{1}{\zeta} + \frac{2}{r^n \zeta^2} \right)$ |
| 3    | $\beta \ast \left( \frac{r}{\zeta^2} + \frac{4}{\zeta^3} + \frac{6}{r^2 \zeta^5} \right)$ |
| 4    | $\beta \ast \left( \frac{r^2}{\zeta^2} + \frac{6r^2}{\zeta^3} + \frac{18}{r^3 \zeta^5} + \frac{24}{r^5 \zeta^7} \right)$ |
| 5    | $\beta \ast \left( \frac{r^3}{\zeta^2} + \frac{8r^3}{\zeta^3} + \frac{36r^2}{r^4 \zeta^6} + \frac{120}{r^5 \zeta^8} + \frac{96}{r^7 \zeta^{10}} \right)$ |
| 6    | $\beta \ast \left( \frac{r^4}{\zeta^2} + \frac{10r^4}{\zeta^3} + \frac{60r^4}{r^4 \zeta^6} + \frac{240r^3}{r^5 \zeta^8} + \frac{720}{r^6 \zeta^{10}} + \frac{60}{r^8 \zeta^{12}} \right)$ |
| 7    | $\beta \ast \left( \frac{r^5}{\zeta^2} + \frac{12r^5}{\zeta^3} + \frac{90r^5}{r^4 \zeta^6} + \frac{480r^4}{r^5 \zeta^8} + \frac{1800r^3}{r^6 \zeta^{10}} + \frac{5040}{r^7 \zeta^{12}} \right)$ |
| 8    | $\beta \ast \left( \frac{r^6}{\zeta^2} + \frac{14r^6}{\zeta^3} + \frac{126r^6}{r^4 \zeta^6} + \frac{840r^5}{r^5 \zeta^8} + \frac{4200r^4}{r^6 \zeta^{10}} + \frac{15120r^3}{r^7 \zeta^{12}} + \frac{40320}{r^8 \zeta^{14}} + \frac{35280}{r^9 \zeta^{16}} \right)$ |
| 9    | $\beta \ast \left( \frac{r^7}{\zeta^2} + \frac{16r^7}{\zeta^3} + \frac{165r^7}{r^4 \zeta^6} + \frac{1344r^6}{r^5 \zeta^8} + \frac{8300r^5}{r^6 \zeta^{10}} + \frac{40320r^4}{r^7 \zeta^{12}} + \frac{141120r^3}{r^8 \zeta^{14}} + \frac{322560}{r^9 \zeta^{16}} + \frac{322560}{r^{10} \zeta^{18}} \right)$ |
| 10   | $\beta \ast \left( \frac{r^8}{\zeta^2} + \frac{18r^8}{\zeta^3} + \frac{216r^8}{r^4 \zeta^6} + \frac{2016r^7}{r^5 \zeta^8} + \frac{15120r^6}{r^6 \zeta^{10}} + \frac{90720r^5}{r^7 \zeta^{12}} + \frac{423360r^4}{r^8 \zeta^{14}} + \frac{1451520r^3}{r^9 \zeta^{16}} + \frac{3628800}{r^{10} \zeta^{18}} + \frac{3265920}{r^{11} \zeta^{20}} \right)$ |
| 11   | $\beta \ast \left( \frac{r^9}{\zeta^2} + \frac{20r^9}{\zeta^3} + \frac{270r^9}{r^4 \zeta^6} + \frac{2880r^8}{r^5 \zeta^8} + \frac{25200r^7}{r^6 \zeta^{10}} + \frac{181440r^6}{r^7 \zeta^{12}} + \frac{1058400r^5}{r^8 \zeta^{14}} + \frac{4858400r^4}{r^9 \zeta^{16}} + \frac{16329600r^3}{r^{10} \zeta^{18}} + \frac{39916800}{r^{11} \zeta^{20}} + \frac{3628800}{r^{12} \zeta^{22}} \right)$ |
| 12   | $\beta \ast \left( \frac{r^{10}}{\zeta^2} + \frac{22r^{10}}{\zeta^3} + \frac{330r^{10}}{r^4 \zeta^6} + \frac{3960r^9}{r^5 \zeta^8} + \frac{39600r^8}{r^6 \zeta^{10}} + \frac{332640r^7}{r^7 \zeta^{12}} + \frac{2328480r^6}{r^8 \zeta^{14}} + \frac{13305600r^5}{r^9 \zeta^{16}} + \frac{59875200r^4}{r^{10} \zeta^{18}} + \frac{199584000r^3}{r^{11} \zeta^{20}} + \frac{479001600}{r^{12} \zeta^{22}} + \frac{439084800}{r^{13} \zeta^{24}} \right)$ |
4.4 Evaluation of direct and exchange matrix elements

The excitation process was treated as shown;

\[ e^+ Q [np^5(n+1)s^2]_2 S \rightarrow e^+ Q [np^5(n+1)s^2]_2 P \]  \[ (4.4.1) \]

For cesium \( n=5 \) in equation (4.5.1), and \( 5p^56s^2 \ 2P \) is lowest autoionizing state of cesium. \( Q \) can be any alkali atom.

Similar to the approximations made earlier, (Srivastava et al., 1982; Tiwarly et al., 1985; Pangantiwar and Srivastava, 1987), the transition \( np \leftrightarrow (n+1)s \) was treated as behaving like a one electron system.

The direct transition matrices in general for a one electron system making transition from an initial state \( i \) to a final state \( f \) by electron impact is expressed in atomic units as;

\[ T_{dir} = (\psi_f^-(r_0) \psi_f(r_1) | V(r_0, r_1) | \chi_i^+(r_0) \psi_i(r_1)) \]  \[ (4.4.2) \]

and for exchange excitation;

\[ T_{ex} = (\chi_f^-(r_0) \psi_f(r_1) | V(r_0, r_1) | \chi_i^+(r_0) \psi_i(r_0)) \]  \[ (4.4.3) \]

where \( \psi_{i(f)} \) are the initial (final) state wave functions of the cesium atom.

\( V(r_0, r_1) \) is the projectile electron –cesium atom interaction potential;

\[ V(r_0, r_1) = \frac{1}{r_0} + \frac{1}{r_{01}} \]  \[ (4.4.4) \]
\( \mathbf{r}_0 \) is the position vector of the incident projectile. \( \mathbf{r}_1 \) is the position vector of the atomic electron undergoing the transition. \( \mathbf{r}_{01} \) is the column vector between the projectile and the target electron.

To evaluate the direct (equation 4.5.2) and exchange (equation 4.5.3) scattering amplitudes, the distorted waves \( \chi_i^+ \) and \( \chi_f^- \) are expanded in terms of the partial waves as (Madison and Bartschart, 1996);

\[
|\chi_i^+\rangle = \frac{1}{\sqrt{\pi k_i r}} \sum_{l m_i} i^{l m_i} \chi_i^+(k_i, r) Y_{l m_i}(r) Y_{l m_i}^*(k_i) \tag{4.4.5}
\]

\[
|\chi_f^-\rangle = \frac{1}{\sqrt{\pi k_f r}} \sum_{l f m_f} i^{l f m_f} \chi_f^-(k_f, r) Y_{l f m_f}(r) Y_{l f m_f}^*(k_f) \tag{4.4.6}
\]

where, \( Y_{l m} \) is a spherical harmonic. In the expansion of \( \chi_f^- \) the complex conjugate of the radial part \( \chi_f \) is taken so that to achieve the incoming wave boundary conditions. Substituting the above partial expansions of the distorted waves [4.5.5] and [4.5.6], we find that the radial distorted waves are solutions of the following equation;

\[
\left( \frac{d^2}{dr^2} - \frac{i s}{r^2} (l_s + 1) - U_s(r) + k_s^2 \right) \chi_{l s}(r) = 0 \tag{4.4.7}
\]

where, \( s = i \) for initial state and \( s = f \) for final state distorted waves.

In the asymptotic region, they satisfy the boundary condition;

\[
\lim_{r \to \infty} \chi_{l s}(k_s, r) = j_{l s} + B_l (-\eta_{l s} + i j_{l s}) \tag{4.4.8}
\]

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

\[
B_l = \exp(i \delta_l) \sin \delta_l \tag{4.4.9}
\]
where $\delta_l$ is the elastic scattering phase shift.

The radial distorted wave equations [4.5.7] for initial (final) states are solved using Numerov method and the differential cross sections are obtained using the relation (Joachain, 1975);

$$
\frac{d\sigma}{d\Omega}_{5p\rightarrow 6s} = \frac{1}{4\pi^2 k_f} \left\{ \left( \frac{1}{4} \right) T_{5p\rightarrow 6s}^{dir} + T_{5p\rightarrow 6s}^{ex} \right\}^2 + \frac{3}{4} \left\{ T_{5p\rightarrow 6s}^{dir} - T_{5p\rightarrow 6s}^{ex} \right\}^2 \right\} ,
$$

[4.4.10]

The total cross section is obtained as;

$$
\sigma = \int_0^\pi \int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin \theta d\theta d\varphi
$$

[4.4.11]

### 4.5 Angular correlation parameter ($\lambda$) and alignment parameter ($A_{20}$)

Most theoretical and experimental models endeavour to calculate differential and total cross sections for the collisional excitation of the autoionizing states in neutral atoms. However, these two parameters cannot give a deeper insight into atomic structure and the dynamics of the excitation process.

Data from anisotropic emission of electrons relative to the incident particle beam, gives explicit details of the collision process. This is due to the fact that any collisional excitation of a state by particle impact leads to an alignment of the excited state, that is, the magnetic substates ($\mid m_l \mid$) are populated differently (Pangantiwar and Srivastava, 1987).
In this work, alignment parameter \( A_{20} \), which is the measure of angular anisotropy of the autoionizing electrons from the \( ^2P \) state is reported and was evaluated using the relation (Pangantiwar and Srivastava, 1987);

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

[4.5.1]

Where \( \sigma_0 \) and \( \sigma_1 \) give the total excitation of a \( np_m \) electron to an \( (n+1)s \) state with \( m=0 \) and \( 1 \) respectively.

Coincidence parameter \( \lambda \), was calculated using the relation;

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

[4.5.2]

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

The differential cross sections are related to their scattering amplitude \( f_i(\theta, \varphi) \) by;

\[
\sigma_i(\theta, \varphi) = \frac{k_f}{k_i} |f_i(\theta, \varphi)|^2
\]

[4.5.3]

The scattering amplitude is directly connected to the transition matrix using the relation;

\[
f_i(\theta, \varphi) = -2\pi^2 T_{if}(i)
\]

[4.5.4]

\( T_{if}(i) \) is the T-matrix for the excitation process expressed by equation 4.5.11.
\[ R_{\lambda p} = \left[ \frac{1}{(2\pi)^{3/2}} \int \frac{1}{(2\xi_{\lambda p})^{n_{\lambda p}+1/2}} x^{(n_{\lambda p}-1)} e^{(n_{\lambda p} r)} \right] \]

and \( Y_{\lambda\alpha}(\theta, \varphi) \) are normalized spherical harmonics.

The initial state of cesium (5P) considered in this study has 8 basis functions and for the final state (6S) there are 12 basis functions.

(i) For the initial state;

\[
\psi_{5p} = -0.003420X_1 - 0.078771X_2 + 0.109103X_3 + 0.168978X_4 - 0.218935X_5 + 0.651059X_6 + 0.92544X_8
\]

Where \( X_i \) is the \( i \)th slater function associated with \( p \)th orbital.

The basis functions for the initial state (5p-state) were as follows:

\[
X_1 = N_1 r e^{-\zeta_1 r_1} Y_{0,0}(\theta, \varphi)
\]

\[
X_2 = N_2 r e^{-\zeta_2 r_2} Y_{0,0}(\theta, \varphi)
\]

\[
X_3 = N_3 r^2 e^{-\zeta_3 r_3} Y_{0,0}(\theta, \varphi)
\]

\[
X_4 = N_4 r^2 e^{-\zeta_4 r_4} Y_{0,0}(\theta, \varphi)
\]

\[
X_5 = N_5 r^3 e^{-\zeta_5 r_5} Y_{0,0}(\theta, \varphi)
\]

\[
X_6 = N_6 r^3 e^{-\zeta_6 r_6} Y_{0,0}(\theta, \varphi)
\]

\[
X_7 = N_7 r^4 e^{-\zeta_7 r_7} Y_{0,0}(\theta, \varphi)
\]

\[
X_8 = N_8 r^4 e^{-\zeta_8 r_8} Y_{0,0}(\theta, \varphi)
\]
Table 4.3: Values of zeta and normalizing factors used for the initial $5p^56s^2\ ^2S$ state in cesium.

<table>
<thead>
<tr>
<th>Subscript ($i$)</th>
<th>Zeta ($\zeta_i$)</th>
<th>Normalizing constant, $N_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>34.7735</td>
<td>1.76680x10^7</td>
</tr>
<tr>
<td>2</td>
<td>23.628775</td>
<td>2.4631980x10^6</td>
</tr>
<tr>
<td>3</td>
<td>12.658736</td>
<td>6.2168x10^7</td>
</tr>
<tr>
<td>4</td>
<td>10.663267</td>
<td>1.256300971x10^{10}</td>
</tr>
<tr>
<td>5</td>
<td>8.126391</td>
<td>7.613758485x10^8</td>
</tr>
<tr>
<td>6</td>
<td>5.572441</td>
<td>3.256306403x10^6</td>
</tr>
<tr>
<td>7</td>
<td>3.333120</td>
<td>2.703398811x10^8</td>
</tr>
<tr>
<td>8</td>
<td>2.018224</td>
<td>3.970086423x10^6</td>
</tr>
</tbody>
</table>

(ii) For the excited state:

$$\psi_{6s} = -0.000285\chi_1 - 0.009399\chi_2 - 0.018142\chi_3 + 0.049666\chi_4 + 0.013953\chi_5 - 0.086381\chi_6 + 0.101009\chi_7 + 0.035248\chi_8 - 0.205988\chi_9 - 0.035690\chi_{10} + 0.502926\chi_{11} + 0.606831\chi_{12} \ [4.6.6]$$

where $\chi_i$ is the $i^{th}$ slater function associated with $p^{th}$ orbital.

The basis functions for the final state (6s-state) were as follows:

$$\chi_1 = N_1r e^{-\zeta_1 r} Y_{0,0}(\theta, \phi)$$

$$\chi_2 = N_2r e^{-\zeta_2 r} Y_{0,0}(\theta, \phi)$$

$$\chi_3 = N_3 r e^{-\zeta_3 r} Y_{0,0}(\theta, \phi)$$
\[ X_4 = N_4 r^2 e^{-\zeta_4 r^4} Y_{0,0}(\theta, \varphi) \]
\[ X_5 = N_5 r^3 e^{-\zeta_5 r^5} Y_{0,0}(\theta, \varphi) \]
\[ X_6 = N_6 r^3 e^{-\zeta_6 r^6} Y_{0,0}(\theta, \varphi) \]
\[ X_7 = N_7 r^4 e^{-\zeta_7 r^7} Y_{0,0}(\theta, \varphi) \]
\[ X_8 = N_8 r^4 e^{-\zeta_8 r^8} Y_{0,0}(\theta, \varphi) \]
\[ X_9 = N_9 r^5 e^{-\zeta_9 r^9} Y_{0,0}(\theta, \varphi) \]
\[ X_{10} = N_{10} r^5 e^{-\zeta_{10} r^{10}} Y_{0,0}(\theta, \varphi) \]
\[ X_{11} = N_{11} r^6 e^{-\zeta_{11} r^{11}} Y_{0,0}(\theta, \varphi) \]
\[ X_{12} = N_{12} r^6 e^{-\zeta_{12} r^{12}} Y_{0,0}(\theta, \varphi) \]
Table 4.4: Values of zeta and normalizing factors for the final state, $5p^56s^2\ 2p$ in cesium

<table>
<thead>
<tr>
<th>Subscript($i$)</th>
<th>Zeta ($\zeta_i$)</th>
<th>Normalizing($N_i$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>56.219117</td>
<td>1.776855 x10^3</td>
</tr>
<tr>
<td>2</td>
<td>37.566991</td>
<td>5.301749 x10^4</td>
</tr>
<tr>
<td>3</td>
<td>27.460490</td>
<td>3.122995 x10^7</td>
</tr>
<tr>
<td>4</td>
<td>23.778942</td>
<td>1.5205217 x10^6</td>
</tr>
<tr>
<td>5</td>
<td>16.977234</td>
<td>2.29348 x10^9</td>
</tr>
<tr>
<td>6</td>
<td>12.653157</td>
<td>2.7693 x10^8</td>
</tr>
<tr>
<td>7</td>
<td>7.456744</td>
<td>1.140415 x10^9</td>
</tr>
<tr>
<td>8</td>
<td>5.377117</td>
<td>6.012642 x10^7</td>
</tr>
<tr>
<td>9</td>
<td>3.721135</td>
<td>9.698390 x10^7</td>
</tr>
<tr>
<td>10</td>
<td>2.423665</td>
<td>8.6789755 x10^5</td>
</tr>
<tr>
<td>11</td>
<td>1.393434</td>
<td>1.274280387 x10^4</td>
</tr>
<tr>
<td>12</td>
<td>0.823743</td>
<td>1.372253 x10^1</td>
</tr>
</tbody>
</table>
4.7 Computer code and analysis

We have applied the computer program DWAI which was originally developed by Madison and Barstchart (1996), in fortran language, to calculate the direct and exchange amplitudes for both elastic and inelastic scattering. The program was originally written for electron and positron scattering from hydrogen or any atom with one electron outside a closed shell configuration. Exponents and constants for initial and final atomic wave functions were read in. Other modifications included; changes in sub routines POTENT and FHYD (for static potentials and wave functions respectively), changes to allow for p→s transition and changes in the declarations.

The parameter NDS was also adjusted accordingly, to obtain a finer radial mesh for evaluation of differential equations and for the program to run at energies higher than 200eV. Changes were also made to calculate λ and A₀ parameters.
5.1 Introduction

We have applied first order distorted wave method—which produces results which are reliable at intermediate and higher energy regions, to calculate integral cross sections, differential cross sections, angular correlation parameter($\lambda$) and alignment parameter($A_{20}$) for electron impact excitation of the lowest autoionizing state in cesium.

These calculations were done- for energies from near threshold 12.3eV to 600eV, for differential cross sections, integral cross sections and angular correlation parameter($\lambda$). Alignment parameter ($A_{20}$) was calculated for the energy range, 12.3eV - 900eV.

Comparisons between differential cross sections for magnetic sub-states $m=0$ and $m=1$ are done in tabular form for various impact energies (table 6). Results for integral cross sections, differential cross sections summed over all magnetic sub-levels for various energies, and alignment parameter($A_{20}$) have been graphically presented (Figures 5.1, 5.2 and 5.3). Results for angular correlation parameter have also been graphically presented (Figures 5.4, 5.5, 5.6, 5.7 and 5.8).

The point of departure of our model from other distorted wave models is in the choice of distortion potentials and the wave functions. We have used an average of static potentials for initial and final states as the final channel distortion potential and initial state static potential as the initial channel distortion potential.
We have used an approximate Roothan-Hatree Fock wave function (double zeta wave functions) in which a given electron orbital is described by two slater functions.

Pangantiwar and Srivastava (1987) used ground state static potential as the distortion potential in the initial channel and the static potential due to the final state as the distortion potential in the final channel. Furthermore, they used accurate multizeta-type Roothan-Hatree Fock Wave functions from Clement et al. (1967). Kaur and Srivastava (1999), had relativistic distorted wave calculations where they used Dirac-Fock atomic wave functions.

5.2 Electron impact excitation of $5p^56s^2 \, ^2P$ state of cesium

5.2.1 Integral cross sections

Figure 5.1 shows our integral cross section results for the electron impact excitation of the lowest autoionizing state of cesium compared with distorted wave with exchange (DWE) results of Pangantiwar and Srivastava (1987), Relativistic Distorted Wave (RDW) results of Kaur and Srivastava (1999), experimental results by Borovik et al. (2011).

From figure 5.1, it can be seen that our results predict the near threshold resonance as observed experimentally. The near threshold peaks can correctly be attributed to the inclusion of the exact exchange amplitude in the transition matrix.

It can also be seen that, at low impact energies, our results are within the same range with the experimental results by Borovik et al. (2011). Our result predicts the same structure as the experimental results but differs in magnitude and the position of the peaks. At high impact energies, the present results are close to the theoretical results of Pangantiwar and
Srivastava. We deduce that, our choice of distortion potentials; static potential in the initial state as the distortion potential in the initial channel and an average of static potentials due to initial and final states as the distortion potential in the final channel is more appropriate, since it is giving better results at low energies.

Table 5, gives the integral cross sections for different impact energies ranging from low to relatively high energies.
Table 5.1: Integral cross sections for electron impact excitation of $5p^56s^2\ ^2P$ state in cesium.

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>Cross section ($\pi a_0^2$) x $10^{-2}$</th>
<th>Energy (eV)</th>
<th>Cross section ($\pi a_0^2$) x $10^{-2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>33.81</td>
<td>220</td>
<td>4.45</td>
</tr>
<tr>
<td>20</td>
<td>11.41</td>
<td>240</td>
<td>4.15</td>
</tr>
<tr>
<td>40</td>
<td>13.5</td>
<td>260</td>
<td>3.88</td>
</tr>
<tr>
<td>60</td>
<td>9.75</td>
<td>300</td>
<td>3.45</td>
</tr>
<tr>
<td>80</td>
<td>8.46</td>
<td>350</td>
<td>3.03</td>
</tr>
<tr>
<td>120</td>
<td>6.73</td>
<td>400</td>
<td>2.7</td>
</tr>
<tr>
<td>140</td>
<td>6.07</td>
<td>450</td>
<td>2.66</td>
</tr>
<tr>
<td>160</td>
<td>5.51</td>
<td>500</td>
<td>2.07</td>
</tr>
<tr>
<td>180</td>
<td>5.12</td>
<td>550</td>
<td>1.8</td>
</tr>
<tr>
<td>200</td>
<td>4.47</td>
<td>600</td>
<td>1.8</td>
</tr>
</tbody>
</table>
Figure 5.1: Integral cross sections for electron impact excitation of $5p^56s^2\,^2P$ state in cesium. Curve 1, present results; curve 2, DWE results (Pangantiwar and Srivastava, 1987); curve 3, Experimental results (Borovik et al., 2011); curve 4, RDW results (Kaur and Srivastava, 1999).
5.2.1 Differential cross section

Figure 5.2 shows our differential cross section results at energies 16, 30, 40 and 70eV. These results are compared with the results of Pangantiwar and Srivastava (1987).

From figure 5.2, it can be seen that lower scattering angles contribute more to the integral cross sections, since the differential cross sections there are generally higher than at the high scattering angles.

At lower scattering angles our results are lower in magnitude than DWE results of Pangantiwar and Srivastava (1987) for all impact energies. At intermediate and high scattering angles, our cross sections are higher in magnitude. Moreover, there is an increase in differential cross sections at impact energies of up to 40eV at intermediate and high scattering angles. This variation can be attributed to the choice of distortion potential and the method of evaluating the exchange amplitude in the transition matrix. In DWE results of Pangantiwar and Srivastava (1987), an approximate exchange T matrix by Ochkur-Bonham (Bonham 1962, Ochkur 1964) was used whereas in the present study, the exchange amplitude is evaluated exactly without employing any approximation.

From figure 5.2, we deduce that, the probability of scattering a particle into a given solid angle falls off rapidly with increasing scattering energy and angles. There are no experimental results to compare with.
Table 5.2: Differential cross sections for electron impact excitation of $5p^56s^2\ ^2P$ state in cesium for different magnetic sub-states and scattering angles in units of $\alpha_0^2/\text{sr}$ (Bohr radius squared per steradian)

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>15</th>
<th>100</th>
<th>200</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>M=0</td>
<td>M=1</td>
<td>M=0</td>
</tr>
<tr>
<td>0</td>
<td>1.1451E-01</td>
<td>0.0000E+00</td>
<td>4.7697E+00</td>
</tr>
<tr>
<td>20</td>
<td>8.9163E-02</td>
<td>1.1737E-04</td>
<td>1.7516E-03</td>
</tr>
<tr>
<td>40</td>
<td>4.9529E-02</td>
<td>3.3713E-04</td>
<td>6.5304E-04</td>
</tr>
<tr>
<td>60</td>
<td>1.8862E-02</td>
<td>5.5395E-04</td>
<td>3.0409E-05</td>
</tr>
<tr>
<td>80</td>
<td>2.8649E-03</td>
<td>7.1080E-04</td>
<td>2.2265E-05</td>
</tr>
<tr>
<td>100</td>
<td>4.2252E-03</td>
<td>7.2796E-04</td>
<td>6.9070E-06</td>
</tr>
<tr>
<td>120</td>
<td>1.9753E-02</td>
<td>5.7817E-04</td>
<td>2.0788E-05</td>
</tr>
<tr>
<td>140</td>
<td>4.1645E-02</td>
<td>3.2514E-04</td>
<td>1.0155E-04</td>
</tr>
<tr>
<td>179</td>
<td>6.7843E-02</td>
<td>2.4374E-07</td>
<td>2.2802E-04</td>
</tr>
</tbody>
</table>
Table 5.3: Differential cross sections summed over magnetic sublevels in units of $a_0^2 / \text{sr}$ (Bohr radius squared per steradian)

<table>
<thead>
<tr>
<th>ENERGY(EV)</th>
<th>15</th>
<th>30</th>
<th>60</th>
<th>90</th>
<th>120</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANGLE(DEG)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>2.4028E+00</td>
<td>4.2697E+00</td>
<td>6.3457E+00</td>
</tr>
<tr>
<td>20</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>1.5715E-02</td>
<td>4.1537E+00</td>
<td>1.7149E+00</td>
</tr>
<tr>
<td>40</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>2.6945E-03</td>
<td>1.6183E-03</td>
<td>9.8918E-04</td>
</tr>
<tr>
<td>60</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>8.9867E-04</td>
<td>3.4950E-04</td>
<td>1.5802E-04</td>
</tr>
<tr>
<td>80</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>2.6502E-04</td>
<td>1.4056E-04</td>
<td>5.5109E-05</td>
</tr>
<tr>
<td>100</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>2.1359E-04</td>
<td>6.3282E-05</td>
<td>1.8639E-05</td>
</tr>
<tr>
<td>120</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>3.4185E-04</td>
<td>3.0825E-05</td>
<td>3.3235E-05</td>
</tr>
<tr>
<td>140</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>4.0326E-04</td>
<td>9.1467E-05</td>
<td>7.6585E-05</td>
</tr>
<tr>
<td>179</td>
<td>5.9778E-06</td>
<td>9.2285E-04</td>
<td>4.4828E-04</td>
<td>2.2872E-04</td>
<td>1.2691E-04</td>
</tr>
</tbody>
</table>
Figure 5.2: Differential cross sections summed over all magnetic sub-levels results for electron impact excitation of $5p^56s^2 \, ^2P$ state in cesium, for different impact energies. ........ Pangantiwar and Srivastava (1987) result, ——— present result.
5.2.3 Alignment parameter, $A_{20}$

Figure 5.3 shows the present alignment parameter results for the excitation of $5p^56s^2\,^2P$ state in cesium compared with RDW results of Kaur and Srivastava (1999) and DWE results of Pangantiwar and Srivastava (1987).

Table 7 gives the results of alignment parameter at various impact energies for the electron impact excitation of $5p^56s^2\,^2P$ state in cesium.

From figure 5.3, it can be seen that our results are comparable to RDW results of Kaur and Srivastava (1999) and DWE results of Pangantiwar and Srivastava (1987) in the sense that they are showing the same trend but are lower in magnitude for lower and intermediate impact energies. This can be attributed to (as mentioned in integral cross section results) the choice of atomic wave function-double zeta wave function.

From figure 5.3, the results by Pangantiwar and Srivastava (1987) show that the alignment parameter decreases at impact energies beyond about 300eV while the present study shows an increase in the values calculated. This can be attributed to inclusion of exact exchange amplitude in the transition matrix.

From figure 5.3, we deduce, from the definition of $A_{20}$ given by equation 4.6.1 in chapter 4, at lower and intermediate impact energies, the ground magnetic sub state ($m=0$) was more populated than the magnetic sub state, $m=1$ after the scattering, because at those energies, $\sigma_0$ is greater than $\sigma_1$. 
Table 5.4: Alignment parameter for the excitation of $5p^56s^2 \, ^2P$ state in cesium.

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>Alignment parameter ( A_{20} )</th>
<th>Energy (eV)</th>
<th>Alignment parameter ( A_{20} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>-0.8638</td>
<td>500</td>
<td>-0.2543</td>
</tr>
<tr>
<td>50</td>
<td>-0.6746</td>
<td>550</td>
<td>-0.2036</td>
</tr>
<tr>
<td>100</td>
<td>-0.5704</td>
<td>600</td>
<td>-0.1516</td>
</tr>
<tr>
<td>250</td>
<td>-0.4715</td>
<td>650</td>
<td>-0.0981</td>
</tr>
<tr>
<td>300</td>
<td>-0.4426</td>
<td>750</td>
<td>0.008025</td>
</tr>
<tr>
<td>400</td>
<td>-0.3557</td>
<td>800</td>
<td>0.05785</td>
</tr>
<tr>
<td>450</td>
<td>-0.3052</td>
<td>900</td>
<td>0.1467</td>
</tr>
</tbody>
</table>
Figure 5.3: Alignment parameter for the excitation of $5p^56s^2\,^2P$ state in cesium.
Curve 1, Pangantiwar and Srivastava(1987) result; curve 2, kaur and Srivastava(1999) result; curve 3, present result.
5.3.4 Lambda parameter

In addition to alignment parameter \((A_{20})\), angular correlation parameter \((\lambda)\) was also evaluated for electron impact excitation of the lowest autoionizing state in cesium.

Table 9, shows the angular correlation results at various energies for electron impact excitation of \(5p^56s^2\ 2P\) state in cesium.

Figure 5.4, shows our results for lambda at 70eV compared with DWE results of Pangantiwar and Srivastava (1987). It can be seen that our results are higher in magnitude than DWE results of Pangantiwar and Srivastava (1987) at lower and higher scattering angles. At intermediate scattering angles, our results are lower in magnitude. This can be attributed to the choice of distortion potential.

At incident energies 40eV and 30eV (figures 5.5 and 5.6), our results are higher in magnitude at all scattering angles. However, at low scattering angles both results have the same trend.

A comparison of the angular correlation results (figures 5.5 and 5.6), shows that the second dip reported by Pangantiwar and Srivastava (1987) at an angle of about 120° is less pronounced in the present results for impact energy of 40eV. The dip flattens out at impact energy of 30eV. This can be attributed to the choice of distortion potential and inclusion of exact exchange amplitude in the transition matrix.

Figure 5.7 shows our results at 16eV, compared with DWE results of Pangantiwar and Srivastava. The two results have a huge variation. The variation in the results can be attributed to the choice of distortion and the method of calculating the exchange
amplitude as mentioned earlier in this work. Because at low impact energies, the projectile takes more time in the field of the target, thus various interactions may take place. This results in variations of the results due to different choice of physical parameters.

From figure 5.8, which gives results for lambda parameter at different energies, we deduce that the probability of excitation of the ground magnetic sub state m=0, and m=1 vary with the scattering angle and with the impact energy.

From the relation 4.6.2 for lambda given in chapter 4, it is clear that if $\lambda$ is greater than 0.33, it means probability of excitation to m=0 level is higher than the probability of excitation to m=1 and if it is less than 0.33, it means probability of excitation to m=0 level is less than the probability of excitation to m=1 level.

So from figure 5.8, we can say that at low and high scattering angles, at all impact energies $\sigma_0(\theta, \varphi)$ is greater than $\sigma_1(\theta, \varphi)$ and at intermediate angles at the places where $\lambda$ is less than 0.33, $\sigma_1(\theta, \varphi)$ is greater than $\sigma_0(\theta, \varphi)$. 
Table 5.5: Lambda parameter for the excitation of $5p^56s^2\ 2P$ state in cesium at various impact energies.

<table>
<thead>
<tr>
<th>Angle(deg)/energy (eV)</th>
<th>15</th>
<th>100</th>
<th>200</th>
<th>300</th>
<th>600</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>9.552E-01</td>
<td>5.043E-01</td>
<td>1.191E-01</td>
<td>6.351E-02</td>
<td>3.166E-01</td>
</tr>
<tr>
<td>100</td>
<td>7.775E-01</td>
<td>1.821E-01</td>
<td>1.315E-01</td>
<td>3.713E-02</td>
<td>5.183E-02</td>
</tr>
<tr>
<td>179</td>
<td>10.00E+00</td>
<td>10.00E+00</td>
<td>9.996E-01</td>
<td>9.999E-01</td>
<td>5.911E-01</td>
</tr>
</tbody>
</table>
Figure 5.4: Angular correlation results for excitation of $5p^56s^22P$ state in cesium at 70eV. 

--- Present result; .......... Pangantiwar and Srivastava (1987) result.
Figure 5.5: Angular correlation results for excitation of $5p^5 6s^2 \, ^2P$ state in cesium at 40eV.

--- Present result; .......... Pangantiwar and Srivastava (1987) result.
Figure 5.6: Angular correlation results for excitation of $5p^56s^2\,^2P$ state in cesium at 30eV.  
- present result; .......... Pangantiwar and Srivastava (1987) result.
Figure 5.7: Angular correlation results for excitation of $5p^3 6s^2 2P$ state in cesium at 16eV.

-------- Pangantiwar and srivastava (1987) result:  ----- present result.
Figure 5.8: Angular correlation parameter ($\lambda$) results, for the excitation of $5p^56s^22p$ state in cesium for incident energies 16, 30, 40 and 70 eV.

$\lambda$ Pangantiwar and Srivastava (1987) result. $\lambda$ present results
CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

Integral cross sections, differential cross sections, alignment parameter ($A_{20}$) and angular correlation parameter ($\lambda$) have been calculated for electron impact excitation of the lowest autoionizing state in cesium using first order distorted wave method.

Double zeta wave functions were used. The initial state static potential was used as the distortion potential for the initial channel and an average of static potentials in the initial and final states as the distortion potential in the final channel.

Our integral cross section results exhibits the same structure as the experimental results at low scattering energies but differs in magnitude and the position of the peaks. This can be attributed to the inclusion of the exact exchange amplitude in the transition matrix and an appropriate choice of distortion potential.

Our results for alignment parameter are in qualitative agreement with DWE results of Pangantiwar and Srivastava (1987) and also RDW results of Kaur and Srivastava (1999) but differed in magnitude. Our results are lower at all energies.

Our results for angular correlation parameter $\lambda$ and differential cross section results generally show the same trend but differ in magnitude when compared with the results of Pangantiwar and Srivastava (1987).
The main success of the present method is in giving the good integral cross section results at low impact energies which are very close to the experimental results of Borovik et al. (2009). Present results shows the same structure as the experimental results at low impact energies but differs in magnitude and position of the peaks. This shows that the method used in this study-distorted wave method, is also suitable for calculation of excitation of the lowest autoionizing state in cesium.

6.2 Recommendations

i) More studies should be done using this method with distortion potentials inclusive of exchange, polarization and absorption effects.

ii) This formalism should be extended to higher autoionizing states in alkali and alkaline earth metals.

iii) More experimental and theoretical results should be made available especially for differential cross sections, angular correlation parameter and alignment parameter for purposes of comparison with our present work.
REFERENCES


