ELECTRON-IMPACT EXCITATION OF THE LOWEST AUTOIONIZING STATES OF ALKALIS USING A DISTORTED-WAVE METHOD

ERIC OUMA JOBUNGA (B.Ed (Sci))
156/10294/2006
DEPARTMENT OF PHYSICS

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

MARCH, 2009
Jobunga, Eric Ouma
Electron-impact excitation of the
DECLARATION

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

Sign  

Date  

Jobunga, Eric Ouma

Department of Physics,

Kenyatta University

We confirm that the candidate, under our supervision, carried out the work reported in this thesis

Sign  

Date  

Dr. C. S. Singh

Department of Physics

Kenyatta University

Prof. John Okumu

Department of Physics

Kenyatta University
DEDICATION

Dedicated to my loving wife Jacque, my jovial son Samuel Edward and my cheerful daughter Faith Winfrey.
ACKNOWLEDGEMENT

I am deeply indebted to my supervisors' Dr Singh C. S. and Prof. Okumu J. for the material support, encouragement, knowledge, skills and reliability that they accorded me in this research. I lack words to express my sincere gratitude to them. I am also grateful to Dr Ambusso for his guidance especially in computer programming. My appreciation goes also to all other members of teaching and non teaching staff in the Physics department. In one way or the other, each of them has contributed to the success of this research.

I extend my appreciation to my colleagues in the laboratory: Okiambe, Kebwaro, Zavani, Agumba, Ochillo, Wekunda and Karanja who provided moral support in times of need. In a special way, I thank James Mugambi who has always been both an inspiration and a challenge in the field of atomic and molecular physics.

I sincerely thank my employer, the TSC, for the two years study leave granted to me. It really helped me to concentrate in my academic work. Special thanks also to Kenyatta University for the partial scholarship I was awarded.

Last but not least, I am grateful to my wife Jacque, my mum and all my friends and relatives for the moral support they accorded me during my studies. At times, it was never smooth but it was good just to know that they were there for me.

Above all else, all glory and honour to God our Father who has given me strength, good health and a sound mind to do all this!
TABLE OF CONTENTS

DECLARATION ................................................................. ii
DEDICATION ................................................................. iii
ACKNOWLEDGEMENT ........................................................... iv
TABLE OF CONTENTS ............................................................ v
LIST OF TABLES ................................................................. vii
LIST OF FIGURES ............................................................... viii
LIST OF ABBREVIATIONS ........................................................ ix
Abbreviation and Meaning ...................................................... ix
ABSTRACT ........................................................................ x

CHAPTER 1 ........................................................................ 1
INTRODUCTION ................................................................. 1
  1.2 Statement of Research Problem ........................................... 5
  1.3 Objectives of the Research Project ....................................... 6
    1.3.1 Main Objective ......................................................... 6
    1.3.2 Specific Objectives .................................................... 6
  1.4 Rationale of the study ........................................................ 6

CHAPTER 2 ........................................................................ 7
LITERATURE REVIEW ........................................................ 7
  2.1 Introduction to Electron Impact Excitation of Autoionizing States of Alkalis ................................................................. 7
  2.2 Studies on Cross-sections Involving Experimental and Other methods ................................................................. 8
  2.3 Studies on Cross-sections using Distorted Wave Method (DWM) ................................................................. 10
  2.4 Summary of the Review ...................................................... 11

CHAPTER 3 ........................................................................ 12
THEORETICAL FRAMEWORK .............................................. 12
  3.1 Introduction to Theoretical Methods ....................................... 12
  3.2 Quantum mechanical Methods ............................................ 12
    3.2.1 The Born Approximation ............................................ 12
    3.2.2 The Coulomb-Projected Born (CPB) Approximation ........ 13
    3.2.3 The R-Matrix Method ............................................... 14
    3.2.4 The Optical Potential Method ...................................... 14
    3.2.5 The Convergent Close Coupling (CCC) Method .............. 15
    3.2.6 The Distorted Wave Methods (DWM) ............................ 15
  3.3 Distorted Wave Formula using Two-Potential Scattering Model ................................................................. 16

CHAPTER 4 ........................................................................ 20
METHODOLOGY ................................................................. 20
  4.1 The Distorted Wave Method ................................................ 20
  4.2 Distortion Potentials U^i and U^f .......................................... 22
  4.3 Evaluation of Static Potentials .............................................. 24
  4.4 Evaluation of Direct and Exchange Matrix Elements ............. 28
  4.5 Angular Correlation and Alignment Parameters \lambda and \lambda_0 ................................................................. 30
  4.6 Atomic Wave Functions ..................................................... 32
  4.7 Computer Code and Analysis ............................................. 38
CHAPTER 5...................................................................................................................... 39
RESULTS AND DISCUSSIONS...................................................................................... 39
  5.1 Introduction............................................................................................................. 39
  5.2 Excitation of $1s^22s - 1s2s^2S^2S$ state of lithium............................................. 40
    5.2.1 Integral cross sections.................................................................................... 40
    5.2.2 Differential cross sections............................................................................ 41
  5.3 Excitation of $2p^53s^2P$ state of Sodium............................................................ 49
    5.3.1 Integral Cross sections................................................................................... 49
    5.3.2 Differential Cross Sections.......................................................................... 50
    5.3.3 Alignment parameter $A_{20}$.......................................................................... 51
    5.3.4 Lambda $\lambda$ parameter............................................................................... 52
  5.4 Excitation of $3p^54s^2P$ state of Potassium......................................................... 66
    5.4.1 Integral Cross sections................................................................................... 66
    5.4.2 Differential Cross sections.......................................................................... 67
    5.4.3 Alignment Parameter $A_{20}$.......................................................................... 68
    5.4.4 Lambda $\lambda$ Parameter............................................................................... 68
  5.5 Summary of Results and Discussions................................................................... 83
CHAPTER 6...................................................................................................................... 84
CONCLUSIONS AND RECOMMENDATIONS................................................................. 84
  6.1 Conclusions........................................................................................................... 84
  6.2 Recommendations............................................................................................... 85
REFERENCES............................................................................................................... 86
LIST OF TABLES

Table 1: Analytical Solutions for the Distortion Potential Elements ...........................................(27)
Table 2: Integral Cross-section Results of Lithium .................................................................(42)
Table 3: Differential Cross section Results of Lithium ..............................................................(43)
Table 4: Integral Cross-section and Alignment Parameter ($A_{20}$) Results of Sodium ..........(53)
Table 5: Differential Cross-section Results of Sodium ............................................................(54)
Table 6: Lambda ($\lambda$) Parameter Results of Sodium ............................................................(55)
Table 7: Integral Cross-section and Alignment Parameter ($A_{20}$) Results of Potassium .......(70)
Table 8: Differential Cross-section Results of Potassium .........................................................(71)
Table 9: Lambda ($\lambda$) Parameter Results of Potassium .......................................................(72)
LIST OF FIGURES

Figure 1 : Graph of Integral Cross-sections of Lithium.................................(44)
Figure 2 : Graph of Differential Cross-sections of Lithium at 75 eV..................(45)
Figure 3 : Graph of Differential Cross-sections of Lithium at 100 eV..................(46)
Figure 4 : Graph of Differential Cross-sections of Lithium at 200 eV..................(47)
Figure 5 : Graph of Differential Cross-sections of Lithium at 300 eV..................(48)
Figure 6 : Graph of Integral Cross-sections of Sodium.................................(56)
Figure 7 : Graph of Differential Cross-sections of Sodium at 40 eV....................(57)
Figure 8 : Graph of Differential Cross-sections of Sodium at 70 eV....................(58)
Figure 9 : Graph of Differential Cross-sections of Sodium at 100 eV..................(59)
Figure 10: Graph of Differential Cross-sections of Sodium at 200 eV..................(60)
Figure 11: Graph of Alignment Parameter Results A2o of Sodium.......................(61)
Figure 12: Graph of Lambda (λ) Parameter Results of Sodium at 40 eV...............(62)
Figure 13: Graph of Lambda (λ) Parameter Results of Sodium at 70 eV...............(63)
Figure 14: Graph of Lambda (λ) Parameter Results of Sodium at 100 eV..............(64)
Figure 15: Graph of Lambda (λ) Parameter Results of Sodium at 200 eV............(65)
Figure 16: Graph of Integral Cross-sections of Potassium..............................(73)
Figure 17: Graph of Differential Cross-sections of Potassium at 24.3 eV.............(74)
Figure 18: Graph of Differential Cross-sections of Potassium at 40 eV...............(75)
Figure 19: Graph of Differential Cross-sections of Potassium at 70 eV...............(76)
Figure 20: Graph of Differential Cross-sections of Potassium at 100 eV.............(77)
Figure 21: Graph of Alignment Parameter (A2o) Results of Potassium..................(78)
Figure 22: Graph of Lambda (λ) Parameter Results of Potassium at 24.3 eV........(79)
Figure 23: Graph of Lambda (λ) Parameter Results of Potassium at 40 eV...........(80)
Figure 24: Graph of Lambda (λ) Parameter Results of Potassium at 70 eV...........(81)
Figure 25: Graph of Lambda (λ) Parameter Results of Potassium at 100 eV...........(82)
# LIST OF ABBREVIATIONS

**Abbreviation and Meaning**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCC</td>
<td>Convergent Close Coupling</td>
</tr>
<tr>
<td>CPB</td>
<td>Coulomb Projected Born approximation</td>
</tr>
<tr>
<td>DCS</td>
<td>Differential Cross-sections</td>
</tr>
<tr>
<td>DWBA</td>
<td>Distorted wave Born approximation</td>
</tr>
<tr>
<td>DWBE</td>
<td>Tiwary and Macek’s, (1985) Distorted wave method with exchange</td>
</tr>
<tr>
<td>DWD</td>
<td>Pangantiwar and Srivastava’s, (1987) Distorted wave method without exchange</td>
</tr>
<tr>
<td>DWE</td>
<td>Pangantiwar and Srivastava’s, (1987) Distorted wave method with exchange</td>
</tr>
<tr>
<td>DWM</td>
<td>Distorted wave method</td>
</tr>
<tr>
<td>DWMD</td>
<td>Present Distorted wave method without exchange</td>
</tr>
<tr>
<td>DWME</td>
<td>Present Distorted wave method with exchange</td>
</tr>
<tr>
<td>DWME-DZ</td>
<td>Present Distorted wave method using double zeta wavefunctions</td>
</tr>
<tr>
<td>GA</td>
<td>Glauber approximation</td>
</tr>
<tr>
<td>ICS</td>
<td>Integral Cross-sections</td>
</tr>
<tr>
<td>MCM</td>
<td>Method of Crothers and McCarol</td>
</tr>
<tr>
<td>PWBA</td>
<td>Plane wave Born approximation</td>
</tr>
<tr>
<td>RDW</td>
<td>Relativistic Distorted wave method</td>
</tr>
<tr>
<td>RHF</td>
<td>Roothan Hartree-Fock expansion</td>
</tr>
</tbody>
</table>
ABSTRACT

Atomic collisions involve scattering of projectiles by some target. The scattering can be done experimentally under certain laboratory conditions or modeled theoretically using known and reliable methods. From scattering a lot of information about the target and also the dynamics of the collision process can be obtained through determination of cross sections, alignment parameters and the angular correlation parameters. These information find application in various branches of physics, for instance, laser physics, biophysics and plasma physics. In this study, integral cross-sections, differential cross-sections, alignment and lambda parameters for electron-impact excitation of the lowest autoionizing states of Li, Na and K have been calculated using Distorted-Wave method. We have applied a linear combination of static potentials of initial and final target states as the final channel distortion potential and the static potential of the initial target state as the initial channel distortion potential. The wave functions used in this model are the multi zeta and the double zeta Hartree-Fock single electron wave functions. Numerical calculations have been performed using a modified program. The results of this study are compared with experimental and theoretical data available in literature. Incase of sodium, our results predict the near threshold resonance which is observed in the experimental results.
CHAPTER 1
INTRODUCTION

1.1 Background to the Study

Studies on atomic collisions basically involve scattering of projectiles which can be electrons, positrons, protons, photons, ions or neutrons by a target in the form of an atom, a molecule or an ion. The parameters of interest in scattering are mainly cross sections which can be differential or integral, alignment and angular correlation parameters. These studies can either be done through experiment using high precision instruments under certain laboratory conditions or by applying known theoretical models. In these collision processes, a beam of free particles (projectiles), prepared in the remote past, interacts with the target and in the far future the detectors record the scattered particles in the asymptotic region. These kinds of experiments find application in many branches of physics for example astrophysics, laser spectroscopy, electrical discharges, chemical kinetics, and biophysics amongst others.

Theoretically, scattering is approached by attempting to solve the Schrödinger’s equations which are differential equations that govern the interaction between the targets and the projectiles. It is important to note that it is impossible to obtain exact solutions for these atomic collision problems. This is because, in most instances, the requisite wave functions are not known with complete accuracy and that the approximate wave functions on which we must rely are frequently not orthogonal (McDaniel, 1989). To worsen the situation, the structure of the equations to be solved is such that approximate methods must be employed
even if the necessary wave functions are completely and exactly known, as is the case of the hydrogen atom.

The range of validity of these approximations depends to a considerable degree on the masses of the colliding structures. For example, collisions between free electrons differ significantly from heavy particle collisions because the masses of atomic systems are so much greater than the mass of an electron. Also, relative velocity, rather than energy, is the parameter that generally determines which of the prospective approximation must be used if it is to be satisfactory in terms of its results.

These approximations can be classified as either quantum mechanical techniques or semi-classical techniques. Quantum mechanical techniques can be categorised into two broad approaches. One of these is the close coupling approach which involves R matrix, convergent close coupling and variational methods. The other approach is a perturbative series expansion used in Born series, eikonal Born series, distorted wave Born series, many body theory and many others. Semi-classical approximations include semi-classical impact parameter method, classical trajectory Monte Carlo method, classical impulse-binary encounter approximation, eikonal approximation, multi channel eikonal treatment, Glauber approximation, and semi-classical S-matrix method (McDaniel, 1989).

During collision, the interaction between the projectile and the target can lead to either elastic scattering, where the state of the target is unchanged, or inelastic scattering which leads to excitation of the target to any of its higher energy states (Joachain, 1975). If the impact energy of the projectile is relatively high, it can lead to direct ionization of the target
provided that the ionization threshold is exceeded. Alternatively, the target can be excited to higher states above this threshold, and then it undergoes self ionization by ejecting an electron. This process is known as autoionization and these higher energy bound states are known as autoionizing states (levels).

If the target is excited to any of these autoionizing states, they can in principle decay via a radiative transition to a bound state of the system below the first ionization limit or by non-radiative transition (autoionization) to the ground state or to one of the excited states of the corresponding ion (Rai and Srivastava, 1984). In the latter, there is emission of an electron whose kinetic energy equals the difference between the energies of the excited state of the target and that of the resulting ion. Schematically, this process of autoionization may be thought of as a two-step process involving the following two stages:

\[
e^{-} + A \rightarrow A^{*} + e^{-}
\]
\[
A^{*} \rightarrow A^{+} + e^{-}
\]

In the first step the target \( A \) is excited by electron impact, while in the next step the excited target \( A^{*} \) autoionizes by ejecting an electron. If autoionization takes place in a negative ion it may produce a neutral atom. This effect is referred to as autodetachment.

The study of the non-radiative (autoionizing) transitions is very important in atomic and molecular physics. For example, they are useful in the current methods for generating atomic wave functions since their transition probabilities are very sensitive to detailed nature of the atomic wave functions. Secondly, the knowledge of these autoionizing transition rates and associated excitations is also vital in a variety of measurements in nuclear and atomic physics, that is, laser spectroscopy, and auger electron spectroscopy. The other aspect of
autoionization which is of great astrophysical significance is the extremely short lifetime
($\approx 10^{-14}$ sec) and consequently large width of some of these levels. Finally the presence of
these autoionizing levels close to the ionization threshold in a number of atoms (ions) and
excitation to these levels contributes significantly to the total ionization cross-sections. The
excitation cross-sections for the autoionizing levels must therefore be added to the ionization
cross-section assuming that all such excitations lead to ionization (Rai and Srivastava, 1984).

This research is focussed on electron impact excitation of lowest autoionizing states of alkali
metals but focussing on Li, Na and K. Alkalis are elements with a single electron in their
valence shells. In their structure, they comprise a mixture of closed shells and an open
(valence) shell containing only one electron. The simplest among them in terms of the
atomic wave function and the electron-electron interaction term is lithium. In order to gain
useful insight into the details of the collision mechanism, we will need to determine the
collision cross sections and other scattering parameters. For example, differential cross
sections (DCSs) in comparison with integral cross section (ICS) reflect more clearly the
characteristics of the interaction potential and are more critically dependent on the target
wave function and the approximate method employed in the calculation (Zhong et al., 1997).

Also DCS for one particular scattering process if known accurately may be used to normalise
data pertaining to other collision processes and calibration of apparatus for general electron-
atom scattering (Scott and Taylor, 1979).

The Distorted Wave Method (DWM) is the technique we chose to evaluate the above
mentioned collision cross sections. This is because it 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). This method employs an arbitrary distortion potential in the calculation of the distorted waves and also in the evaluation of the transition matrices. This choice of the distortion potentials is one of the features that differentiate this study from previous studies which used distorted wave methods. It is also important to note that these transition matrices can not be evaluated exactly without making some approximations. The approximations made in this study range from the total wave function where we considered only first order term without regard for spin, also in evaluating the distortion potential the non spherical parts of the interaction potentials have not been used. In calculating the cross sections, the excitation energies of the targets are required. We used 56.39 eV, 30.77 eV and 18.72 eV for the excitation of the lowest autoionizing states of lithium, sodium and potassium respectively from their ground states. The further details of this method are given in chapter 3 and 4.

1.2 Statement of Research Problem

In this study, we investigated the effect of a Distorted Wave Method (DWM) with a variation on electron impact excitation of the lowest-lying autoionizing levels of alkalis particularly lithium, sodium, and potassium, in the energy range of 60-600 eV for lithium, 31 -1500 eV for sodium and 19-1000 eV for potassium. We also investigated the effect of double zeta wave functions on these excitations.
1.3 Objectives of the Research Project

1.3.1 Main Objective

The main objective of this research was to study the effect of a variant distortion potential on electron impact excitation of the lowest autoionizing levels of lithium, sodium, and potassium.

1.3.2 Specific Objectives

The specific objectives of this study were as follows:

(i) To determine differential and total cross-sections for electron-impact excitation of the lowest-lying autoionizing states of lithium, sodium and potassium at impact energies above the first excitation threshold up to 600 eV for lithium, 1500 eV for sodium and 1000 eV for potassium.

(ii) To determine angular correlation and alignment parameters $\lambda$ and $A_{20}$ respectively for sodium and potassium.

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

1.4 Rationale of the study

The theoretical results available for electron impact excitation of lowest autoionizing states of Li, Na and K are not in very good agreement between themselves and with reported experimental results. So it would be interesting to see how the change in the distorted wave method and also the change in the wave functions affect the results.
CHAPTER 2
LITERATURE REVIEW

2.1 Introduction to Electron Impact Excitation of Autoionizing States of Alkalis

Several aspects of excitation of autoionizing states have been investigated experimentally and theoretically. Borovik and Krasilinec, (1999) studied the ejected-electron functions of the lowest lying autoionizing states in lithium atom measured at an angle of 54.7° for the electron-impact energy range of up to 600 eV and observed strong influence of negative-ion resonances for all the states just above the excitation threshold.

In another study, Kupliauskiene et al. (2006) studied the role of cascade processes in electron-impact excitation of the \((3p^5 4s^2)^2P_{1/2, 3/2}\) autoionizing levels in potassium using experimental method and confirmed the enhancement of the apparent excitation cross-section for the lowest autoionizing state at 22 eV as predicted by Feuerstein et al. (1999).

Borovik et al. (1999) measured the metastable excitation function and the near-threshold energy loss spectrum in potassium, corresponding to \(3p^6\) core excitation, over the energy range 18-24 eV. They observed many structures in the excitation function and were also able to determine the excitation thresholds for the lowest-lying metastable autoionizing levels in potassium.

Rassi et al. (1977) observed experimentally the ejected-electron spectrum of lithium at 75° with respect to an incident electron beam of energy: 80 eV, 200 eV and 500 eV. A total of 39 autoionizing levels were observed in the energy range 56 eV to 65 eV.
2.2 Studies on Cross-sections Involving Experimental and Other methods

Feuerstein et al. (1999) measured electron impact excitation cross sections of the inner shell excited lowest autoionizing state of potassium for incident energy range from 37.2 eV to 1000 eV. The absolute cross section measurements were normalized to a PWBA calculation at 500 eV. Negative ion resonances were observed at near threshold. In their PWBA calculation, they used different types of wave functions for the ground and the excited states respectively. In the ground state they used multi zeta Hartree-Fock wave functions and for the excited state they used multi-configuration intermediate-coupling wave functions. With this mixing, the cross sections reported were generally high.

Feuerstein et al. (1998) also measured relative electron impact excitation cross sections for the lowest lying autoionizing state 2p\(^5\)3s\(^2\)2P of sodium in the energy range of 1.5 keV down to the threshold (30.77 eV). Just as for potassium, the absolute cross sections obtained were normalized at 1.5 keV to the theoretical PWBA. Besides the experiment, they also performed a 26-state R-matrix calculation near the excitation threshold up to 50 eV. Both results revealed negative ion resonances near the excitation threshold.

Matterstock et al. (1995) measured the alignment parameter \(A_{20}\) for \(K^+ (3p^54s^{22}P^{1/2})\) and also the ratio of cross sections for fine structure states of \(K^+ (3p^54s^{22}P^{3/2,1/2})\) for electron impact excitation in the incident energy range of 31.4-500 eV and the results were compared to other theoretical results.
Borovik et al. (2008) measured the ejected-electron excitation functions of the fine structure components of $2p^53s^22P$, leading autoionizing doublet in sodium atoms, at an incident electron energy resolution of 0.25 eV over the incident electron energy range from the lowest excitation threshold up to 36 eV and observed strong near threshold structures. They also performed 56-state R-matrix calculation in the same energy range and classified the near threshold resonances as negative ion resonances.

Grum-Grzhimailo et al. (1999) using R-matrix method from threshold up to 80 eV predicted structures, likely due to negative-ion resonances, in the electron-induced alignment of the $Na^*(2p^53s^2)^2P_{3/2}$ autoionizing state near the excitation threshold. These predictions were supported by measurements of alignment via the anisotropic emission of the autoionization electrons in the impact energy range from threshold to 100 eV.

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 and then compared them with other earlier results. These results only converge at higher incident energies.

Srivastava and Rai, (1977) studied electron impact excitation of autoionizing levels in alkali atoms using the method of Crothers and McCarrol. They compared their total cross section results with the work of Tiwary and Rai, (1975) who used first Born, modified Born and Vainshtein approximations. In a separate study, Pejcev et al. (1977) obtained excitation functions for the lower autoionizing states of lithium by measuring the intensity of ejected
electrons at $75^\circ$ to the incident electron beam. The maximum incident electron energy was 550 eV.

2.3 Studies on Cross-sections using Distorted Wave Method (DWM)

Besides the experimental method, Feuerstein et al. (1998; 1999) and Matterstock et al. (1995) also performed various distorted wave calculations at intermediate and high energy range using different distortion potentials. Except for potassium when exchange potential is included in the distortion potential taken as the static potential of the target atom in the final state, the results obtained were not in good agreement with experimental results.

Kaur and Srivastava, (1998) carried out relativistic distorted-wave (RDW) calculations for the electron impact excitation of the lowest autoionizing states $np^5(n+1)s^2 3p_3/2$ in sodium ($n=2$), potassium ($n=3$), rubidium ($n=4$) and caesium ($n=5$) alkali atoms from the ground $np^6(n+1)s^2 S_1/2$ state using spin resolved Dirac-Fock wave functions. The total cross sections and alignment parameter results are reported in the range of near threshold to 1.5keV incident electron energies. The results obtained were not in very good agreement with the other previously reported results.

Pangantiwar and Srivastava, (1987) also studied the electron and positron impact excitation of autoionizing levels in alkalis using Distorted Wave approach for incident particle energy varying above the threshold energy of the atom to 600 eV. In this study, they used multi-zeta HF wave functions (Clementi and Roetti, 1974) and the initial-and final-state static potentials
as the distortion potentials for the initial and final distorted waves respectively. The results were only in good agreement with the experimental results at higher incident energies.

2.4 Summary of the Review

From the above studies, it is clear that so far there is no study that can claim perfect agreement with experimental results at intermediate and high energy region. It is on this basis that we have conducted a study on electron-impact excitation of the lowest autoionizing levels of alkalis (i.e. Li, Na and K) by using Distorted Wave method. This study employs an average of initial- and final-state static potentials as the final channel distortion potential and the initial-state static potential as the initial channel distortion potential. The wave functions that we have used are Roothan-Hartree-Fock (RHF) multi zeta wave functions and the Double-zeta (DZ) wave functions (Clementi and Roetti, 1974). The results obtained are compared with previous experimental and theoretical results.
CHAPTER 3
THEORETICAL FRAMEWORK

3.1 Introduction to Theoretical Methods

Just as mentioned in the introduction, theoretical approaches to scattering can be basically categorised into two approaches, that is, quantum mechanical approaches and semi-classical approaches. Quantum mechanical approaches which use the principles of quantum mechanics exclusively are also further classified into perturbative methods and close coupling methods. The semi-classical approaches use the principles borrowed from both classical and quantum mechanics. Some of the examples of these methods are Glauber approximation, the method of Crothers and McCarol and the impact parameter method. Similarly, the examples of perturbative methods are the Born series, Coulomb Projected Born approximations, and the Distorted wave series while close coupling methods include convergent close coupling, close coupling optical method and R-matrix. In this chapter, we have briefly discussed some of these quantum mechanical approaches.

3.2 Quantum mechanical Methods

3.2.1 The Born Approximation

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

$$f = -\frac{1}{4\pi} \langle \Psi_{k_f} | U + UG_0^*U + UG_0^*UG_0^*U + \ldots | \Psi_{k_i} \rangle$$

(3.1)

Here $\Psi_{k_f}$ is the product of final plane wave $e^{ik_f \cdot r}$ of the projectile and the final target wave function $\phi_f$. $\Psi_{k_i}$ is the product of the initial plane wave $e^{ik_i \cdot r}$ of the incident particle and the
initial atomic wave function $\varphi_i$. U is the interaction potential and the function $G^+_0$ is outgoing Green's function given as
\[
G^+_0(k,r,r') = -\frac{1}{4\pi} \frac{e^{i|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \tag{3.2}
\]
The first term in the series (3.1) is the first Born approximation to the scattering amplitude and is given as
\[
f_{B1} = -\frac{1}{4\pi} \langle \Psi_{ki} | U | \Psi_{ki} \rangle \tag{3.3}
\]
When the first two terms in the series (3.1) are taken then it is the second Born approximation $f_{B2}$ and so on. The first Born approximation is valid generally for high impact energies when the interaction is for a very short duration and the projectile waves (incident and scattered) can be approximated as plane waves (Joachain, 1975). The Born approximations have been further improved by including the exchange amplitude. This was originally approximated by Born-Oppenheimer approximation, Born-Ochkur approximation, and Born-exchange approximation but currently the exchange amplitude can be evaluated exactly.

3.2.2 The Coulomb-Projected Born (CPB) Approximation

The Coulomb-projected Born approximation consists basically of modifying the usual Born approximation by taking an explicit account of the Coulomb interaction between the projectile and the nucleus. The final state plane wave in the Born approximation is replaced by a Coulomb wave functions corresponding to the nuclear charge. Different ways of taking this Coulomb interaction into account has led to different CPB methods, for example CPB approximation by Geltman, (1971), Generalized CPB approximation by Stauffer and
Morgan, (1975) and a variable charge CPB approximation by Schaub-shaver and Stauffer, (1980). These approximations are useful in describing collisions of electrons and ions with target atoms and ions and give results better than Born approximation results.

3.2.3 The R-Matrix Method

In this method the configuration space for electron-atom system is divided into two regions. For scattering of electrons from an atom, exchange can be neglected outside some radius \( r_o \). Hence for \( r>r_o \), the collision is described by coupled differential equations that often have analytical solutions easily obtainable by numerical methods. The basic problem, then, is to calculate the R-matrix in the internal region \((r<r_o)\) where the interaction is strong and electron exchange is important. In this method, the target eigen states and pseudo states are written as linear sums of Slater orbitals and the incident electron wave function is expanded in terms of orthogonal orbitals which satisfy logarithmic boundary condition on the surface of the sphere \((\text{of radius } r_o)\). The Hamiltonian is then diagonalized in an appropriately chosen basis in the internal region and the cross section calculated by solving the asymptotic problem in the external region \((\text{Burke et al., 1971})\). R-matrix is mainly suitable in different types of electron-molecule collisions but for electron-atom collisions, it is only convenient at lower projectile energies.

3.2.4 The Optical Potential Method

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

3.2.5 The Convergent Close Coupling (CCC) Method

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

3.2.6 The Distorted Wave Methods (DWM)

In the distorted wave approximation, the incident electron is taken to be elastically scattered by the initial state atomic potential. If the excitation of the atom is through the direct process, the incident electron makes a transition to a state in which it is being elastically scattered by final-state atomic potential. If the excitation of the atom is through the exchange process, the incident electron is captured into a bound state of the atom, while one of the
initially bound electrons is ejected into an elastic-scattering state. In this case, the transition between the initial and final elastic state is calculated by a perturbation method. This method is suitable for calculation of differential cross section for electron impact excitation of atoms at intermediate and high incident energies (Itikawa, 1986). Distorted wave methods have been one of the most successful perturbative methods used especially at intermediate and high impact energies of projectiles. Its advantage lies in the leading term of the perturbation series expansion such that the distorted wave series converges faster than Born series. Distorted wave method can be comfortably applied to study electron-molecule collision, electron impact ionization of atoms and collision processes among heavy particles. Distorted wave methods have been applied in various collision processes since it is quite successful in explaining various features of an excitation process for example the effect of a particular distortion potential (Katiyar et al., 1988). Distorted wave methods are more conveniently discussed within the frame work of the two-potential formalism discussed in the next section. However, these methods are unreliable at lower impact energies although some times they have been successful in predicting near threshold structures.

3.3 Distorted Wave Formula using Two-Potential Scattering Model

In the two-potential scattering model, the interaction may be broken in a physically meaningful way in two parts: one which is treated exactly, and the other which is handled in an approximate way. That is,

\[ V = U + W \]  

(3.4)

and it is assumed that the equation

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

(3.5)
can be solved exactly. In this equation $H_0$ denotes the unperturbed Hamiltonian, $\chi$ is the product of the target wave function and the projectile wave function within the interaction region (distorted wave) and $+ (-)$ refers to the outgoing (incoming) wave boundary conditions.

The transition matrix elements for any scattering problem is given as

$$ T_{y} = \langle \varphi_f | V_f | \Psi_i^+ \rangle \quad (3.6) $$

where $\varphi_f$ is the product of the final state target wave function and the final plane wave function of the projectile in the asymptotic region and $\Psi_i^+$ is the total wave function of the system. Making use of equation (3.4), equation (3.6) can now be written as

$$ T_{y} = \langle \varphi_f | U_f + W_f | \Psi_i^+ \rangle \quad (3.7) $$

The total wave function with incoming boundary conditions can be expressed as

$$ | \chi^-_f \rangle = | \varphi_f \rangle + \frac{1}{E_f - H_f - i\varepsilon} U_f | \varphi_f \rangle \quad (3.8) $$

where $H_f = H_0 + U_f$ and this Hamiltonian satisfies equation (3.5). Equation (3.8) can also be written as

$$ \langle \varphi_f | = \langle \chi^-_f | - \langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} $$

Expanding equation (3.7) and making use of equation (3.9), we can write the transition matrix element as

$$ T_{y} = \langle \varphi_f | U_f | \Psi_i^+ \rangle + \langle \chi^-_f | W_f | \Psi_i^+ \rangle - \langle \varphi_f | U_f \frac{1}{E_f - H_f + i\varepsilon} W_f | \Psi_i^+ \rangle \quad (3.10) $$
The third term on the right hand side of equation (3.10) can be transformed by making use of the relation
\[ \langle \psi_i^+ \rangle = \phi_i + \frac{1}{E_i - H + i\epsilon} V_i | \phi_i \rangle \] (3.11)
as (on the energy shell \( E=E_i=E_f \))

\[ \langle \phi_f | U_f \frac{1}{E_f - H_f + i\epsilon} W_f | \psi_i^+ \rangle = \langle \phi_f | U_f \frac{1}{E - H_f + i\epsilon} W_f | \phi_i \rangle \]
\[ + \langle \phi_f | U_f \frac{1}{E - H_f + i\epsilon} W_f \frac{1}{E - H + i\epsilon} V_i | \phi_i \rangle \] (3.12)

and further making use of equation (3.9), we can write equation (3.12) as
\[ \langle \phi_f | U_f \frac{1}{E - H_f + i\epsilon} W_f | \psi_i^+ \rangle = \langle \chi_f^- | W_f | \phi_i \rangle - \langle \phi_f | W_f | \phi_i \rangle \]
\[ + \langle \phi_f | U_f \frac{1}{E - H_f + i\epsilon} W_f \frac{1}{E - H + i\epsilon} V_i | \phi_i \rangle \] (3.13)

Using the operator identity
\[ \frac{1}{B - A} \frac{1}{A - \frac{1}{B}} = \frac{1}{A - B} \quad \text{with} \quad A = E - H + i\epsilon \quad \text{and recalling that} \quad H - H_f = W_f, \]
we find that
\[ \langle \phi_f | U_f \frac{1}{E - H_f + i\epsilon} W_f \frac{1}{E - H + i\epsilon} V_i | \phi_i \rangle = \langle \phi_f | U_f \frac{1}{E - H + i\epsilon} V_i | \phi_i \rangle \]
\[ - \langle \phi_f | U_f \frac{1}{E - H_f + i\epsilon} V_i | \phi_i \rangle \] (3.14)

If we make use of equations (3.9) and (3.11), then equation (3.14) is reduced to
\[ \langle \phi_f | U_f \frac{1}{E - H_f + i\epsilon} W_f \frac{1}{E - H + i\epsilon} V_i | \phi_i \rangle = \langle \phi_f | U_f | \psi_i^+ \rangle - \langle \phi_f | U_f | \phi_i \rangle \]
\[ - \langle \chi_f^- | V_i | \phi_i \rangle + \langle \phi_f | V_i | \phi_i \rangle \] (3.15)

Substituting equations (3.13) and (3.15) in equation (3.10), we get
\[ T_{if} = \langle \varphi_f | U_f | \Psi_i^+ \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle - \langle \chi_f^- | W_f | \varphi_i \rangle + \langle \varphi_f | W_f | \varphi_i \rangle - \langle \varphi_f | U_f | \Psi_i^+ \rangle + \langle \varphi_f | U_f | \varphi_i \rangle + \langle \chi_f^- | V_i | \varphi_i \rangle - \langle \varphi_f | V_i | \varphi_i \rangle \] (3.16)

Using the fact that on the energy shell

\[ \langle \varphi_f | U_f + W_f | \varphi_i \rangle = \langle \varphi_f | V_i | \varphi_i \rangle = \langle \varphi_f | V_i | \varphi_i \rangle \] we can write equation (3.16) as

\[ T_{if} = \langle \chi_f^- | V_i - W_f | \varphi_i \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle \] (3.17)

This is the two-potential formula of Gellmann and Goldberger (Joachain, 1975). It is simplified when we take \( V_i = V_f = V \) and \( W_f = V - U_f \). In this case, we can rewrite the T-matrix as

\[ T_{if} = \langle \chi_f^- | U_f | \varphi_i \rangle + \langle \chi_f^- | V_i - U_f | \Psi_i^+ \rangle \] (3.18)

This is the model that we used to evaluate the scattering parameters and it is discussed in detail in the next chapter with specific application to the electron impact excitation of the lowest autoionizing levels of lithium, sodium and potassium.
4.1 The Distorted Wave Method

The problem considered in this study is the scattering of an electron by a neutral atom. In this case the total Hamiltonian for the system is expressed as (atomic units are used unless otherwise stated)

\[ H = H_a - \frac{1}{2} \nabla_0^2 + V \]  
(4.1)

\( H_a \) is the Hamiltonian for an isolated atom, the second term is the kinetic energy \((T)\) operator for an isolated projectile, and \( V \) is the interaction potential between the projectile electron and the target and it is given by.

\[ V = -\frac{N}{r_0} + \sum_{i=1}^{N} \frac{1}{r_{0i}} \]  
(4.2)

where \( \frac{N}{r_0} \) and \( \frac{1}{r_{0i}} \) are the projectile electron-target nuclear interaction term and projectile electron-target electron interaction term respectively.

The initial-state full scattering wave function \( \Psi_i \) is a solution of Schrödinger's equation.

\[ (H - E) \Psi_i^+ = 0 \]  
(4.3)

where the + 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 Bartschat, 1996) is given by

\[ T_{ij} = (N+1) \langle \chi_f^- (0) \psi_f (1, \ldots, N) | V - U_f | A \Psi_i^+ (0, \ldots, N) \rangle 
+ \langle \chi_f^- (0) \psi_f (1, \ldots, N) | U_f | \psi_i (1, \ldots, N) \varphi_i (0) \rangle \]  
(4.4)
In equation 4.4, \( \psi_i \) and \( \psi_f \) are the properly antisymmetrized initial and final atomic wave functions for an isolated atom, which diagonalized the atomic Hamiltonian \( H_a \) according to
\[
\langle \psi_n^* | H_a | \psi_n \rangle = w_n \delta_{nn}.
\] (4.5)

Furthermore, \( \phi_i \) is an initial-state plane wave (Eigen function for an isolated projectile) and
\( A \) is the antisymmetrizing operator for the \( N+1 \) electrons. If \( \Psi^\dagger(0,...,N) \) is chosen to be a product of a projectile wave function (electron 0) and an antisymmetrized atomic wave function (electrons 1,..., N), then antisymmetrization operator may be expressed as
\[
A = \frac{1}{N+1}(1 - \sum_{i=1}^{N} P_{i0})
\] (4.6)

where \( P_{i0} \) is the operator that exchanges electrons 0 and \( i \). The potential \( U_j \) in equation (4.4) is an arbitrary distorting potential for the projectile, which is used to calculate \( \chi_f^- \) by solving the equation
\[
\left(-\frac{1}{2} \nabla_0^2 - \frac{1}{2} k_f^2 + U_f\right) \chi_f^- = 0
\] (4.7)

where the – superscript designates incoming wave boundary conditions and \( k_f \) is the final-state wave vector of the projectile. Generally the distortion potential \( U_f \) is chosen to be any linear combination of initial- and final-state static potential of the target atom. In principle, however, \( U_f \) can be any potential as long as \( \chi_f^- \) satisfies the appropriate boundary conditions.

For inelastic scattering, the second part of the transition matrix in equation (4.4) vanishes for orthogonal atomic wave functions since \( U_f \) depends only on the single co-ordinate of the projectile. But for elastic scattering, this second part of the same equation is the dominant
term; in fact, it is generally the only contributing term if $U_f$ is chosen such that the matrix elements of $V - U_f$ vanish.

The total wave function $\Psi_i^+$ in the expression of the transition matrix in equation 4.4 takes the form of Lippmann-Schwinger solution and it is expressed as

$$\Psi_i^+ = [1 + G^+(V - U_i)]\Psi_i^+ \chi_i^+$$

(4.8)

where $G^+$ is the full Green's function given by

$$G^+ = (E - H + i\varepsilon)^{-1}$$

(4.9)

But since $\Psi_i^+$ can not be evaluated without making approximations, in the distorted wave approach $\Psi_i^+$ is expressed in terms of a product of an initial-state distorted wave $\chi_i^+$ and an initial state atomic wave function $\Psi_i$ (first order approximation of equation (4.8)). For energy $E_i$ of the incident projectile, the initial-state distorted wave is a solution of the Schrödinger's equation

$$\left(-\frac{1}{2} \nabla_0^2 - \frac{1}{2} k_i^2 + U_i\right)\chi_i^+ = 0$$

(4.10)

for an arbitrary distorting potential $U_i$ which vanishes asymptotically. $k_i$ is the incident wave vector and it is related to the incident energy $E_i$ by

$$E_i = \frac{1}{2} k_i^2$$

(4.11)

4.2 Distortion Potentials $U_i$ and $U_f$

The choice of the distortion potential to be used in the above framework is arbitrary. It can either be the static potential of the target atom in its initial- or final-state, or any linear
combination of the two (Itikawa, 1986; Srivastava et al., 1989). Besides the static potential, the distortion potential may also include the exchange potential, polarization potential and absorption potential in order to take care of exchange effects, polarization effects of the incident electron and absorption of particles from the incident channel respectively. In this study, we have used the static potential of the target atom in its initial state as the distortion 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 as the distortion potential for the final state of the projectile electron. That is,

\[
U_i = \langle \psi_i | V | \psi_i \rangle 
\]  
(4.12)

\[
U_f = \frac{1}{2} \langle \psi_i | V | \psi_i \rangle + \frac{1}{2} \langle \psi_f | V | \psi_f \rangle 
\]  
(4.13)

where subscripts \(i\) and \(f\) denote initial and final states respectively and \(V\) is the electron-atom interaction potential given by equation (4.2).

The reason for taking the above choices is that when the projectile electron is in its initial state, it 'sees' the initial-state static potential of the target atom because for all the time it is in the field of the target atom in its initial state (Singh, 2004). However, when the energy of the projectile electron is transferred to the target atom, it takes some time (relaxation time) for the atom to go to its final state. That is, there is a time lag between the time of transfer of energy and the instant when the atom reaches the 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

The mathematical formulation of static potentials is generally expressed as

\[ U_s = \langle \psi_s | V | \psi_s \rangle \]  

(4.14)

where \( \psi_s \) is the target wave function, \( s = i \) or \( f \) for initial or final state respectively and \( V \) is the interaction between the target and the projectile. For the target state, we have used the Hartree-Fock wave functions developed by Clementi and Roetti, (1974). In these wave functions, \( \psi_s \) is summed over Slater type orbitals of the basis set as

\[ | \psi_s \rangle = \sum_n C_n | \phi_n \rangle \]  

(4.15)

and

\[ \langle \psi_s | = \sum_n C^*_n \langle \phi_n | \]  

(4.16)

The values of \( C_n \) represent the expansion coefficients and \( \phi_n \) are the Slater type orbitals of the basis set. Using equations (4.15) and (4.16) in equation (4.14), we can now write the distortion potential as

\[ U_s = \sum_n \sum_n C_n C^*_n \langle \phi_n | V | \phi_n \rangle \]  

(4.17)

where the interaction potential \( V \) in atomic unit is given as

\[ V = \frac{-N}{r_0} + \sum_i \frac{1}{r_{0i}} \]  

(4.18)

\( r_0 \) is the position vector of the projectile from the nucleus of the target and \( r_{0i} \) is the displacement vector of the projectile electron relative to the \( i^{th} \) bound electron of the target.

Since we have treated the target states as hydrogenic orbitals in the above framework, the interaction potential reduces to
\[ V = -\frac{1}{r_0} + \frac{1}{r_{01}} \]  

(4.19)

But \( \frac{1}{r_{01}} \) can be expanded in terms of the spherical harmonics as

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

(4.20)

where \( r_i(r_j) \) is the lesser (greater) between \( r_0 \) and \( r_1 \).

In distorted wave calculations, the spherically symmetric distorting potential normally used consists of the nuclear term given by the first term on the right hand side of equation (4.19) plus the monopole term \((l=0)\) of the summation in equation (4.20), since the effect of non-spherical terms is negligible if one is mainly interested in cross sections but not in angular correlation parameters (Madison and Bartschart, 1991). Thus the static potential can effectively be expressed (in Rydberg units) as

\[
U_s = 2 \sum_n \sum_n C_n C_n^* \langle \phi_n | \frac{1}{r_j} - \frac{1}{r_0} | \phi_n \rangle
\]

(4.21)

since

\[
Y_{0,0}(r) = \frac{1}{\sqrt{4\pi}}
\]

(4.22)

From Clementi and Roetti, (1974) tables, the Slater type orbitals are expressed as a product of radial wave functions and spherical harmonics \( Y_{l,m} \) and are given as

\[
\phi_n = N_n r_\mu n^{-1} \exp(-\xi r) Y_{l,m}(r)
\]

(4.23)

Here \( \mu_n \) is the principal quantum number of the \( n^{th} \) orbital of the basis set, \( \xi \) is a constant and the normalization factor \( N_n \) of the orbital is given as
Substituting the values of the wave function given by equation (4.23) and replacing the Bra and Ket notation with the standard integrals, the static potential can be fully expanded as

\[
U_s = 2 \sum_{nml} C_n C_n^* N_n N_n^* \int_{r_1}^{\infty} \left( \frac{1}{r_1} - \frac{1}{r_0} \right) \exp\left( -\left[ \xi_n + \xi_n^* \right] r_1 \right) d\Omega = \sum_{n \times n'} \mathbf{N}_{nn'}
\]

In this equation, we have made use of partial integration of the radial component such that from the radial distance 0 to \( r_0 \), we consider \( r_0 \) to be greater than \( r_1 \) while from \( r_0 \) to infinity, we consider \( r_1 \) to be greater than \( r_0 \). Since the spherical harmonics are orthonormal, the last integral on the right hand side of this equation vanishes unless \( l=l' \) and \( m=m' \).

Therefore, the distortion potential in effect reduces to

\[
U_s = 2 \sum_{n} C_n C_n^* N_n N_n^* \int_{r_1}^{\infty} \left( \frac{1}{r_1} - \frac{1}{r_0} \right) \exp\left( -\left[ \xi_n + \xi_n^* \right] r_1 \right) d\Omega
\]

In this study, this integral was evaluated analytically to obtain the exact static potentials which have been used as the distortion potentials. It can be easily seen that the total static potential is summation of all the elements of a \( n \times n' \) matrix. The analytical solution of each element of equation (4.26) varies in form depending on the sum of the principal quantum numbers, \( \mu_n \) and \( \mu_{n'} \). This sum varies between 2 and 8 for the problem that was to be solved. The analytical solutions of the various forms were evaluated and were found to be as given in table 1 below.
Table 1 Analytical solutions for distortion potential elements

| $\mu_n + \mu_{n'}$ | Distortion potential elements form, $\langle n' | U_s | n \rangle$. |
|-------------------|--------------------------------------------------------------|
| 2                 | $- \text{const}(n,n') \times (X + 2!)e^{-X}$                |
| 3                 | $- \text{const}(n,n') \times (X^2 + 4X + 3!)e^{-X}$         |
| 4                 | $- \text{const}(n,n') \times (X^3 + 6X^2 + 18X + 4!)e^{-X}$  |
| 5                 | $- \text{const}(n,n') \times (X^4 + 8X^3 + 36X^2 + 96X + 5!)e^{-X}$ |
| 6                 | $- \text{const}(n,n') \times (X^5 + 10X^4 + 60X^3 + 240X^2 + 600X + 6!)e^{-X}$ |
| 7                 | $- \text{const}(n,n') \times (X^6 + 12X^5 + 90X^4 + 480X^3 + 1800X^2 + 4320X + 7!)e^{-X}$ |
| 8                 | $- \text{const}(n,n') \times (X^7 + 14X^6 + 126X^5 + 840X^4 + 4200X^3 + 15120X^2 + 35280X + 5!)e^{-X}$ |

The variables used in table 1 above are defined as

$$X = (\xi_n + \xi_{n'})r_0$$  \hspace{1cm} (4.27)

and

$$\text{const}(n,n') = \frac{C_n C_{n'} N_n N_{n'}}{Xr_0}$$  \hspace{1cm} (4.28)

Since the values of $C_n$, $\mu_n$ and $\xi_n$ are obtainable from the atomic data tables for the atomic wave functions compiled by Clementi and Roetti, (1974), it was possible to write a computer program to sum the various matrix elements accurately to generate the desired static potential.
4.4 Evaluation of Direct and Exchange Matrix Elements

We have treated the excitation processes as follows:

\[ e^- + Li(1s^2 2s)^2 S_{1/2} \rightarrow e^- + Li(1s 2s^2)^2 S_{1/2} \]

\[ e^- + B[np^6 (n+1)s]^2 S_{1/2} \rightarrow e^- + B[np^5 (n+1)s^2]^2 P_{3/2}, \frac{1}{2} \]

where B can be any alkali atom such as Na (n=2) and K (n=3).

In these processes, excitation involves only one atomic electron. We have considered the transitions 1s-2s in Li, 2p-3s in Na, and 3p-4s in K as one electron excitation process as has been considered by Srivastava et al. (1982).

The transition matrices in general for the one electron systems excited from an initial state \( i \) to a final state \( f \) by electron impact are expressed, using atomic units, as

\[ T^{\text{dir}} = \langle \chi^+_f (r_0) \psi_f (r_1) | V(r_0, r_1) | \chi^+_i (r_0) \psi_i (r_1) \rangle \] \hspace{1cm} (4.29)

for the direct transition matrix and the exchange transition matrix is

\[ T^{\text{ex}} = \langle \chi^+_f (r_0) \psi_f (r_1) | V(r_0, r_1) - U_f (r_0) | \chi^+_i (r_1) \psi_i (r_0) \rangle \] \hspace{1cm} (4.30)

\( V(r_0, r_1) \) is the projectile electron-target atom interaction potential given by

\[ V(r_0, r_1) = \left( \frac{1}{r_0} - \frac{1}{r_{01}} \right) \] \hspace{1cm} (4.31)

\( r_0 \) is the position vector of the incident electron, \( r_1 \) is the position vector of an atomic electron undergoing a transition relative to the nucleus of the alkali atom taken as the origin of the centre of mass and \( r_{01} \) is the displacement vector between the projectile and the target electron.
To evaluate the direct and exchange scattering amplitudes given by the equations (4.29) and (4.30), the distorted waves \( \chi_i^+ \) and \( \chi_j^- \) were first expanded in terms of the partial waves as

\[
| \chi_i^+ \rangle = \frac{2}{\pi} \frac{1}{k_i r} \sum_{l,m} i^l \chi_i^l (k_i, r) Y_{l,m} (r) Y_{l,m}^* (k_i)
\]

(4.32)

and

\[
| \chi_j^- \rangle = \frac{2}{\pi} \frac{1}{k_f r} \sum_{l',m'} i'^l \chi_j^{l'} (k_f, r) Y_{l',m'} (r) Y_{l',m'}^* (k_f)
\]

(4.33)

where \( Y_{lm} \) is a spherical harmonic. In the expansion of \( \chi_j^- \) in equation 4.33, the complex conjugate of the radial part \( \chi_j^{l'} \) is taken so that it satisfies the incoming wave boundary conditions. Substituting the above partial wave expansions of the distorted waves in the equations (4.7) and (4.10), it can be shown that the radial distorted waves are solutions of the following equation

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

(4.34)

for the initial state and \( s = f \) for the final state distorted waves. In the asymptotic region the radial waves satisfy the boundary condition.

\[
\lim_{r \to \infty} \chi_{ls} (k_s, r) = j_{ls} + \alpha_l (-\nu_l + \delta_i)
\]

(4.35)

where \( j_l \) and \( \nu_l \) are regular and irregular Ricatti-Bessel functions, and \( \alpha_l \) is given as

\[
\alpha_l = \exp(i \delta_l) \sin \delta_l
\]

(4.36)

\( \delta_l \) is the elastic scattering phase shift.
The radial distorted waves in equation 4.34 for initial- and final -states are solved by using Numerov method. The transition matrices were fully expanded making use of vector addition coefficients and the incident electron was considered to be along the z-axis to simplify the problem. The differential cross-sections are the probability of scattering per unit incident flux per unit solid angle. These cross sections have been obtained using the relation:

i. For lithium

\[
\left( \frac{d\sigma}{d\Omega} \right)_{1s\rightarrow 2s} = 4\pi^4 \frac{k_f}{k_i} \left( \frac{1}{4} |T_{1s\rightarrow 2s}^{\text{dir}} + T_{1s\rightarrow 2s}^{\text{ex}}|^2 + \frac{3}{4} |T_{1s\rightarrow 2s}^{\text{dir}} - T_{1s\rightarrow 2s}^{\text{ex}}|^2 \right)
\]

ii. For sodium

\[
\left( \frac{d\sigma}{d\Omega} \right)_{2p\rightarrow 3s} = 4\pi^4 \frac{k_f}{k_i} \sum_{m=-1}^{+1} \left( \frac{1}{4} |T_{2p\rightarrow 3s}^{\text{dir}} + T_{2p\rightarrow 3s}^{\text{ex}}|^2 + \frac{3}{4} |T_{2p\rightarrow 3s}^{\text{dir}} - T_{2p\rightarrow 3s}^{\text{ex}}|^2 \right)
\]

iii. For potassium

\[
\left( \frac{d\sigma}{d\Omega} \right)_{3p\rightarrow 4s} = 4\pi^4 \frac{k_f}{k_i} \sum_{m=-1}^{+1} \left( \frac{1}{4} |T_{3p\rightarrow 4s}^{\text{dir}} + T_{3p\rightarrow 4s}^{\text{ex}}|^2 + \frac{3}{4} |T_{3p\rightarrow 4s}^{\text{dir}} - T_{3p\rightarrow 4s}^{\text{ex}}|^2 \right)
\]

The total cross-sections are the probability of scattering per unit incident flux. These cross sections are obtained by summing all differential cross sections at all solid angles.

This summation is shown in the following relation.

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

4.5 Angular Correlation and Alignment Parameters \( \lambda \) and \( A_{20} \)

As a result of development in experimental techniques over the last several years, it is possible to measure scattered electrons in coincidence with radiation or electron emitted from atoms which have become excited by the scattering process. These coincidence
measurements provide more detailed information, especially regarding the population of magnetic sub states, than can be obtained from differential cross section measurement. Two of the parameters that can be obtained from coincidence measurements for exciting from $np \rightarrow (n+1)s$ state are the lambda ($\lambda$) parameter and the R-parameter. These parameters together with differential cross sections completely define the scattering process, that is, using these it is possible to describe as completely as possible the state of an excited target after collision. In this work we have only reported $\lambda$ parameter results for comparison purposes with the calculated values of Pangantiwar and Srivastava, (1987). The $\lambda$ parameter is calculated using the expression:

$$
\lambda = \frac{\sigma_0(\theta, \phi)}{\sigma_0(\theta, \phi) + 2\sigma_1(\theta, \phi)} \quad 0 \leq \lambda \leq 1
$$

(4.41)

The alignment parameter $A_{20}$, which is the measure of angular anisotropy of the autoionizing electrons from the $^2P$ state, is given by the expression below for unresolved fine structure splitting:

$$
A_{20} = \frac{\sigma_1 - \sigma_0}{\sigma}
$$

(4.42)

Here $\sigma_0(\theta, \phi)$ and $\sigma_1(\theta, \phi)$ are the differential cross sections for $np_m \rightarrow (n+1)s$ transition with $m=0$ and $1$ respectively. They are related to their scattering amplitude $f_m(\theta, \phi)$ by

$$
\sigma_m(\theta, \phi) = \frac{k_f}{k_i} |f_m(\theta, \phi)|^2
$$

(4.43)

where as $\sigma_0$ and $\sigma_1$ give total cross sections for the magnetic sublevels $0$ and $1$ respectively while the scattering amplitude is directly connected to the transition matrix using the relation:
\[ f_m(\theta, \phi) = -2\pi^2 T_{if}(m) \]  \hspace{1cm} (4.44)

\( T_{if}(m) \) is the T matrix for the excitation process expressed by equation (4.4).

### 4.6 Atomic Wave Functions

The atomic wave functions we have used in evaluation of the direct and exchange transition matrices outlined above are the Roothan-Hartee-Fock multi zeta wave functions and the double zeta functions as given in the Clementi and Roetti, (1974) tables. They are based on the Roothan-Hartree-Fock (RHF) expansion technique. The double zeta function is an approximate RHF function in which a given electron orbital is described by two Slater functions. In the above model, the total wave function \( \Psi \) is a Slater determinant and it is given by

\[ \Psi = A(\Phi^{(1)}_1...\Phi^{(n)}_n) \]  \hspace{1cm} (4.45)

\( A \) is the anti-symmetrizing operator, \( n \) is the total number of electrons, and \( \Phi^{(1)}_1, \Phi^{(2)}_2, ..., \Phi^{(n)}_n \) are spin orbitals (one electron functions). The spin orbitals are a product of a spin function and an orbital function. The orbitals are assumed to be orthogonal to each other, thus the same holds for spin orbitals. Since we considered target wave functions as one electron wave functions, it is the specific spin orbital wave functions that we have used in the transition matrix as the bound state target wave functions.

The orbitals are characterised by an index \( \eta \), which indicates the symmetry species and it corresponds to the orbital quantum number \( l \), an index \( \gamma \) which indicates the subspecies. These subspecies label individual members of the degenerate set that transform according to
the representation $\eta$. The index $i$, which refers to the $i^{th}$ orbital of symmetry $\eta$ also characterises the orbitals. The orbital $\Phi_{i\eta}$ is expanded in terms of the basis functions according to

$$\Phi_{i\eta} = \sum_p \phi_{p\eta} C_{ip}$$

(4.46)

where $p$ refers to the $p^{th}$ basis function of symmetry $\eta$. The expansion coefficients depends on $i, \eta$ and $p$ but not on $\gamma$. The basis functions $\phi_{p\eta}$ are slater-type orbitals with integer quantum numbers, namely

$$\phi_{p\eta}(r, \theta, \phi) = R_{p\eta}(r)Y_{\eta}(\theta, \phi)$$

(4.47)

where $R_{p\eta} = [(2\mu_{p\eta})!]^{1/2} (2\xi_{p\eta})^{\mu_{p\eta}+1/2} r^{\mu_{p\eta}-1} e^{-\xi_{p\eta} r}$

and $Y_{\eta}(\theta, \phi)$ are normalized spherical harmonics in complex form. It is noted that $\mu_{p\eta} = \eta + 1$ and that the exponent $\xi_{p\eta}$ is chosen so as to give the best energy found by laborious process of optimization.

The single electron wave functions shown in equation (4.46) is the constructed using the table of coefficients and the exponents (for radial part of equation (4.47)) provided in the atomic data tables of Clementi and Roetti, (1974). The multi-zeta type wave functions are given as:

(i) For lithium

$$\Phi(1s) = 0.89786\phi_1 + 0.11131\phi_2 - 0.00008\phi_3 + 0.00112\phi_4 - 0.00216\phi_5 + 0.00884\phi_6$$

$$\Phi(2s) = -0.14629\phi_1 - 0.01516\phi_2 + 0.00377\phi_3 + 0.98053\phi_4 + 0.10971\phi_5 - 0.11021\phi_6$$
where

\[ \begin{align*}
\phi_1 &= N_1 r^0 \exp(-2.47673r)Y_{0,0} (\theta, \varphi) \\
\phi_2 &= N_2 r^6 \exp(-4.69873r)Y_{0,0} (\theta, \varphi) \\
\phi_3 &= N_3 r^4 \exp(-0.38350r)Y_{0,0} (\theta, \varphi) \\
\phi_4 &= N_4 r^1 \exp(-0.66055r)Y_{0,0} (\theta, \varphi) \\
\phi_5 &= N_5 r^1 \exp(-1.07000r)Y_{0,0} (\theta, \varphi) \\
\phi_6 &= N_6 r^1 \exp(-1.63200r)Y_{0,0} (\theta, \varphi) \\
\end{align*} \]

and the normalization factors \( N_i \) are given as: \( N_1 = 7.795572, N_2 = 20.370455, N_3 = 0.105168, \)

\( N_4 = 0.409481, N_5 = 1.367505 \) and \( N_6 = 3.928889. \)

(ii) For sodium

\[ \begin{align*}
\Phi(3s) &= 0.03527\phi_1 + 0.00121\phi_2 - 0.01889\phi_3 - 0.06808\phi_4 - 0.09232\phi_5 + 0.00076\phi_6 + 0.40764\phi_7 + 0.64467\phi_8 \\
\Phi(2p) &= 0.48417\phi_9 + 0.03622\phi_{10} + 0.29282\phi_{11} + 0.31635\phi_{12} + 0.07543\phi_{13}
\end{align*} \]

where

\[ \begin{align*}
\phi_1 &= N_1 r^6 \exp(-11.012230r)Y_{0,0} (\theta, \varphi) \\
\phi_2 &= N_2 r^2 \exp(-12.66010r)Y_{0,0} (\theta, \varphi) \\
\phi_3 &= N_3 r^2 \exp(-8.36156r)Y_{0,0} (\theta, \varphi) \\
\phi_4 &= N_4 r^2 \exp(-5.73805r)Y_{0,0} (\theta, \varphi) \\
\phi_5 &= N_5 r^2 \exp(-3.61287r)Y_{0,0} (\theta, \varphi) \\
\phi_6 &= N_6 r^2 \exp(-2.25096r)Y_{0,0} (\theta, \varphi) \\
\phi_7 &= N_7 r^2 \exp(-1.11597r)Y_{0,0} (\theta, \varphi) \\
\phi_8 &= N_8 r^2 \exp(-0.91028r)Y_{0,0} (\theta, \varphi) \\
\phi_9 &= N_9 r^1 \exp(-5.54977r)Y_{1,p} (\theta, \varphi) \\
\phi_{10} &= N_{10} r^3 \exp(-8.66846r)Y_{1,p} (\theta, \varphi) \\
\phi_{11} &= N_{11} r^3 \exp(-5.43460r)Y_{1,p} (\theta, \varphi) \\
\phi_{12} &= N_{12} r^3 \exp(-3.55503r)Y_{1,p} (\theta, \varphi) \\
\phi_{13} &= N_{13} r^3 \exp(-2.31671r)Y_{1,p} (\theta, \varphi)
\end{align*} \]

and the normalization factors are given as: \( N_1 = 73.087466, N_2 = 3044.168677, N_3 = 62.999824, \)

\( N_4 = 190.815660, N_5 = 37.793917, N_6 = 7.214828, N_7 = 0.619045, N_8 = 0.303425, N_9 = 83.783178, \)
\( N_{10} = 1873.326564, N_{11} = 229.154742, N_{12} = 33.936686, N_{13} = 4.940800. \) The subscript \( p = 1, 0 \) or \(-1.\)

(iii) For potassium

\[
\Phi(4s) = -0.01825 \phi_1 + 0.00031 \phi_2 - 0.00899 \phi_3 + 0.06350 \phi_4 + 0.05015 \phi_5 - 0.11346 \phi_6
\]
\[
-0.11474 \phi_7 - 0.03065 \phi_8 + 0.05190 \phi_9 + 0.33431 \phi_{10} + 0.70417 \phi_{11}
\]
\[
\Phi(3p) = -0.20797 \phi_{12} - 0.01176 \phi_{13} - 0.12744 \phi_{14} + 0.56718 \phi_{15} + 0.45273 \phi_{16} + 0.09340 \phi_{17}
\]

where

\[
\phi_1 = N_1 r^0 \exp(-19.13500r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_2 = N_2 r^0 \exp(-31.52500r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_3 = N_3 r^1 \exp(-16.49860r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_4 = N_4 r^1 \exp(-7.67410r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_5 = N_5 r^2 \exp(-6.68508r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_6 = N_6 r^2 \exp(-4.04102r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_7 = N_7 r^2 \exp(-2.66919r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_8 = N_8 r^2 \exp(-2.59794r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_9 = N_9 r^3 \exp(-0.56203r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_{10} = N_{10} r^3 \exp(-1.29017r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_{11} = N_{11} r^3 \exp(-0.76641r)Y_{0,0}(\theta, \varphi)
\]
\[
\phi_{12} = N_{12} r^1 \exp(-8.64187r)Y_{1,p}(\theta, \varphi)
\]
\[
\phi_{13} = N_{13} r^1 \exp(-15.19360r)Y_{1,p}(\theta, \varphi)
\]
\[
\phi_{14} = N_{14} r^2 \exp(-6.91359r)Y_{1,p}(\theta, \varphi)
\]
\[
\phi_{15} = N_{15} r^2 \exp(-3.26163r)Y_{1,p}(\theta, \varphi)
\]
\[
\phi_{16} = N_{16} r^2 \exp(-2.00984r)Y_{1,p}(\theta, \varphi)
\]
\[
\phi_{17} = N_{17} r^2 \exp(-1.68876r)Y_{1,p}(\theta, \varphi)
\]

and the normalization factors are given as: \( N_1 = 167.406646, N_2 = 354.007643, \)
\( N_3 = 1276.694836, N_4 = 188.381393, N_5 = 325.695582, N_6 = 55.931599, N_7 = 13.099869, \)
\( N_8 = 8.273814, N_9 = 8.429318E-3, N_{10} = 0.354639, N_{11} = 0.034037, N_{12} = 253.506261, \)
\( N_{13} = 1039.013259, N_{14} = 366.354398, N_{15} = 26.421664, N_{16} = 4.852929 \) and \( N_{17} = 2.638922. \)
When we use double zeta type Slater orbitals, the wave functions are given as:

(i) For lithium

\[ \Phi(1s) = 0.15502\phi_1 + 0.85766\phi_2 - 0.00309\phi_3 + 0.00191\phi_4 \]
\[ \Phi(2s) = 0.00303\phi_1 - 0.21999\phi_2 + 0.94196\phi_3 + 0.09904\phi_4 \]

where

\[ \phi_1 = N_1 r^0 \exp(-4.61679r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_2 = N_2 r^0 \exp(-2.46167r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_3 = N_3 r^1 \exp(-1.96299r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_4 = N_4 r^1 \exp(-0.67198r)Y_{0,0}(\theta, \varphi) \]

and the normalization factors are given as: \( N_1 = 19.839932 \), \( N_2 = 7.724578 \), \( N_3 = 6.233968 \), and \( N_4 = 0.427282 \).

(ii) For sodium

\[ \Phi(3s) = -0.00483\phi_1 + 0.05111\phi_2 - 0.11828\phi_3 - 0.06624\phi_4 + 0.27943\phi_5 + 0.78135\phi_6 \]
\[ \Phi(2p) = 0.33517\phi_5 + 0.73552\phi_8 \]

where

\[ \phi_1 = N_1 r^0 \exp(-12.58430r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_2 = N_2 r^0 \exp(-9.43884r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_3 = N_3 r^1 \exp(-3.85928r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_4 = N_4 r^1 \exp(-2.39434r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_5 = N_5 r^2 \exp(-1.25277r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_6 = N_6 r^2 \exp(-0.74608r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_7 = N_7 r^1 \exp(-5.47723r)Y_{0,0}(\theta, \varphi) \]
\[ \phi_8 = N_8 r^1 \exp(-2.56267r)Y_{1,p}(\theta, \varphi) \]
and the normalization factors are given as: \( N_f = 89.283990, \ N_r = 57.997321, \)
\( N_s = 33.785869, \ N_e = 10.243159, \ N_5 = 0.927873, \ N_6 = 0.151247, \ N_r = 81.072173, \)
\( N_9 = 12.139508 \) and \( p = 1, 0 \) or -1.

(iii) For potassium

\[
\Phi(4s) = -0.00153\phi_1 - 0.02396\phi_2 - 0.01395\phi_3 + 0.10973\phi_4 - 0.15552\phi_5 - 0.07884\phi_6 \\
+ 0.40578\phi_7 + 0.67568\phi_8
\]

\[
\Phi(3p) = -0.04829\phi_9 - 0.28236\phi_{10} + 0.53002\phi_{11} + 0.57404\phi_{12}
\]

where

\[
\phi_1 = N_1 r^0 \exp(-20.01550r)Y_{0,0} \exp(-20.01550r)Y_{0,0}(\theta, \phi)
\]
\[
\phi_2 = N_2 r^0 \exp(-14.57250r)Y_{0,0}(\theta, \phi)
\]
\[
\phi_3 = N_3 r^1 \exp(-8.50264r)Y_{0,0}(\theta, \phi)
\]
\[
\phi_4 = N_4 r^1 \exp(-6.74543r)Y_{0,0}(\theta, \phi)
\]
\[
\phi_5 = N_5 r^2 \exp(-3.47996r)Y_{0,0}(\theta, \phi)
\]
\[
\phi_6 = N_6 r^2 \exp(-2.32676r)Y_{0,0}(\theta, \phi)
\]
\[
\phi_7 = N_7 r^3 \exp(-1.20531r)Y_{0,0}(\theta, \phi)
\]
\[
\phi_8 = N_8 r^3 \exp(-0.72769r)Y_{0,0}(\theta, \phi)
\]
\[
\phi_9 = N_9 r^1 \exp(-11.89500r)Y_{1,0}(\theta, \phi)
\]
\[
\phi_{10} = N_{10} r^1 \exp(-6.61653r)Y_{1,0}(\theta, \phi)
\]
\[
\phi_{11} = N_{11} r^2 \exp(-3.29528r)Y_{1,0}(\theta, \phi)
\]
\[
\phi_{12} = N_{12} r^2 \exp(-1.99426r)Y_{1,0}(\theta, \phi)
\]

and the normalization factors are given as: \( N_f = 179.093433, \ N_r = 111.257960, \)
\( N_s = 243.418649, \ N_e = 136.456261, \ N_5 = 33.147335, \ N_6 = 8.101572, \ N_r = 0.261107, \)
\( N_9 = 0.026955, \ N_5 = 563.482567, \ N_{10} = 130.030455, \ N_{11} = 27.388097, \ N_{12} = 4.722533 \) and \( p = 1, 0 \) or -1.
4.7 Computer Code and Analysis

In evaluating the various physical parameters, that is, the differential cross sections, integral cross sections, lambda and alignment parameters, we modified an existing computer program (DWBA1) which was originally developed by Madison and Bartschat, (1996) in Fortran Language. This program was tailor made for e-H scattering allowing only transitions from $s$ to higher $l$ values. Relevant sections of the code were modified for our purpose.

The major areas changed in the code are the main program to allow for $p$-$s$ transitions, the wave functions’ and distortion potential’s subroutines and some changes in declarations and other relevant subroutines. The wave functions’ and the distortion potentials’ subroutines were coded in such a way that the it would take in the arguments supplied by Clementi and Roetti, (1974) for any element and from them a wave function is constructed. These wave functions are also used to generate the distortion potentials by summing the matrix elements discussed in chapter 4.

It is also important to note that the code could not work well for all the three elements at lower energies closer to threshold. So we had to include in the program the two bound-continuum state overlap integrals accounting for exchange amplitude that were originally ignored for hydrogen scattering. This inclusion greatly improved our results at lower incident energies for sodium and potassium.
CHAPTER 5
RESULTS AND DISCUSSIONS

5.1 Introduction

We have applied Distorted Wave Method (DWM) to calculate the total cross sections, differential cross sections and where applicable the alignment and angular correlation parameters for the electron impact excitation of the lowest autoionizing states of lithium, sodium and potassium. These calculations have been done for electron impact energies ranging from near threshold to 600 eV for lithium, 1500 eV for sodium and 1000 eV for potassium. We have chosen this range of energy values in order to make suitable comparison with other results available in literature and also the fact that distorted wave models are reliable at intermediate and high impact energies.

Our variation of the distorted wave method is different from the other distorted wave models that have been cited in this work. In this model, we have used the initial state static potential as the distortion potential in the initial channel and a linear combination of the initial state and final state static potentials as the distortion potential in the final channel. We have also evaluated the exchange term completely without making any approximation within this first order Distorted Wave Born Approximation. In fact, we have even included the exchange terms that were neglected in the code we have used (Madison and Bartschart, 1996). In terms of wave functions, we have used the multi-zeta type Hartree-Fock wave functions developed by Clementi and Roetti, (1974). This is similar to the wave functions used by Pangantiwar and Srivastava, (1987). For comparison purposes, we have also evaluated the
total cross sections using the Double zeta Hartree-Fock wave functions (Clementi and Roetti, 1974).

We have presented all our results graphically as illustrated by figures 1-24. We have also compiled samples of our calculated results at various energies for the three elements as shown in the attached tables 2-9.

5.2 Excitation of $1s^2 2s - 1s2s^2 2S$ state of lithium

5.2.1 Integral cross sections

The threshold energy for the excitation of the first autoionizing level $1s2s^2 2S_{1/2}$ of lithium is 56.395 eV (Rassi et al., 1977). Figure 1 shows the excitation cross sections of this state evaluated in the present distorted wave with exchange (DWME) model and without exchange (DWMD) model in comparison with R-matrix and Distorted wave results of Tiwary and Macek, (1985); Glauber approximation (GA), method of Crothers and McCarol (MCM) and First Born approximation (FBA) results of Srivastava et al. (1982); and Distorted wave results with exchange (DWE) and without exchange (DWD) of Pangantiwar and Srivastava, (1987). Present results are in good agreement with other results at higher energies ($\geq 150$ eV). But below that the present distorted wave results with exchange (DWME) rise sharply as the incident energy approaches the excitation threshold and at about 60 eV, the present results (with exchange) are about 10 times higher than other results. But the present distorted wave results without exchange are in good agreement with the other results even at low energies. Tiwary and Macek, (1985) have also reported sharp increase in cross-sections but not so much.
5.2.2 Differential cross sections

We have compared our differential cross section results for DWME with the results of Pangantiwar and Srivastava, (1987) at 75 eV, 100 eV, 200 eV and 300 eV in figures 2-5. Table 1 gives the values of the present DWME differential cross sections at the mentioned incident energies.

In reference to figures 2-5, we see that at higher energies (200 eV and 300 eV) the differential cross section results for the present model and those of Pangantiwar and Srivastava are in excellent agreement at lower scattering angles ($\leq 80^\circ$), however at intermediate and higher scattering angles ($> 80^\circ$) our results are higher. At energies $\leq 100$ eV, present results are much higher than the Pangantiwar and Srivastava's result, as it behaved in case of integral cross-section results.
Table 2. Present integral cross section results for electron impact excitation of \((1s^2 2s - 1s 2s^2)^2S_{1/2}\) state of lithium.

<table>
<thead>
<tr>
<th>ENERGY (eV)</th>
<th>DWME ((\pi a_0^2 \times 10^{-3}))</th>
<th>DWMD ((\pi a_0^2 \times 10^{-3}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>56.99</td>
<td>6.142</td>
</tr>
<tr>
<td>65</td>
<td>37.62</td>
<td>5.128</td>
</tr>
<tr>
<td>70</td>
<td>27.02</td>
<td>4.568</td>
</tr>
<tr>
<td>80</td>
<td>15.51</td>
<td>3.841</td>
</tr>
<tr>
<td>90</td>
<td>9.827</td>
<td>3.351</td>
</tr>
<tr>
<td>100</td>
<td>6.732</td>
<td>2.988</td>
</tr>
<tr>
<td>150</td>
<td>2.230</td>
<td>1.975</td>
</tr>
<tr>
<td>200</td>
<td>1.393</td>
<td>1.488</td>
</tr>
<tr>
<td>300</td>
<td>0.8852</td>
<td>1.000</td>
</tr>
<tr>
<td>400</td>
<td>0.6735</td>
<td>0.7536</td>
</tr>
<tr>
<td>500</td>
<td>0.5483</td>
<td>0.6047</td>
</tr>
<tr>
<td>600</td>
<td>0.4636</td>
<td>0.5050</td>
</tr>
</tbody>
</table>
Table 3. Present DWME differential cross sections results in $a_0^2 sr^{-1}$ for electron impact excitation of $(1s^2 2s - 1s 2s^2)^2 S_1^2$ state of lithium at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>Angle (degrees)</th>
<th>75 eV</th>
<th>100 eV</th>
<th>200 eV</th>
<th>300 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>7.4603E-3</td>
<td>5.8747E-3</td>
<td>7.0500E-3</td>
<td>7.9728E-3</td>
</tr>
<tr>
<td>10</td>
<td>7.3157E-3</td>
<td>5.4682E-3</td>
<td>5.6009E-3</td>
<td>5.5559E-3</td>
</tr>
<tr>
<td>20</td>
<td>6.9317E-3</td>
<td>4.4818E-3</td>
<td>3.0179E-3</td>
<td>2.2146E-3</td>
</tr>
<tr>
<td>30</td>
<td>6.4261E-3</td>
<td>3.3840E-3</td>
<td>1.2857E-3</td>
<td>6.6218E-4</td>
</tr>
<tr>
<td>40</td>
<td>5.9206E-3</td>
<td>2.5035E-3</td>
<td>5.0955E-4</td>
<td>1.9301E-4</td>
</tr>
<tr>
<td>50</td>
<td>5.4931E-3</td>
<td>1.9205E-3</td>
<td>2.2363E-4</td>
<td>6.9132E-5</td>
</tr>
<tr>
<td>60</td>
<td>5.1705E-3</td>
<td>1.5776E-3</td>
<td>1.2315E-4</td>
<td>3.5060E-5</td>
</tr>
<tr>
<td>70</td>
<td>4.9461E-3</td>
<td>1.3922E-3</td>
<td>8.7315E-5</td>
<td>2.4110E-5</td>
</tr>
<tr>
<td>80</td>
<td>4.800E-3</td>
<td>1.3002E-3</td>
<td>7.4477E-5</td>
<td>1.9968E-5</td>
</tr>
<tr>
<td>90</td>
<td>4.7109E-3</td>
<td>1.2610E-3</td>
<td>7.0846E-5</td>
<td>1.8289E-5</td>
</tr>
<tr>
<td>100</td>
<td>4.6612E-3</td>
<td>1.2514E-3</td>
<td>7.1209E-5</td>
<td>1.7666E-5</td>
</tr>
<tr>
<td>110</td>
<td>4.6374E-3</td>
<td>1.2584E-3</td>
<td>7.3385E-5</td>
<td>1.7545E-5</td>
</tr>
<tr>
<td>120</td>
<td>4.6301E-3</td>
<td>1.2741E-3</td>
<td>7.6249E-5</td>
<td>1.7662E-5</td>
</tr>
<tr>
<td>130</td>
<td>4.6325E-3</td>
<td>1.2930E-3</td>
<td>7.9208E-5</td>
<td>1.7877E-5</td>
</tr>
<tr>
<td>140</td>
<td>4.6400E-3</td>
<td>1.3120E-3</td>
<td>8.1910E-5</td>
<td>1.8113E-5</td>
</tr>
<tr>
<td>150</td>
<td>4.6489E-3</td>
<td>1.3288E-3</td>
<td>8.4148E-5</td>
<td>1.8326E-5</td>
</tr>
<tr>
<td>160</td>
<td>4.6569E-3</td>
<td>1.3419E-3</td>
<td>8.5820E-5</td>
<td>1.8489E-5</td>
</tr>
<tr>
<td>170</td>
<td>4.6621E-3</td>
<td>1.3498E-3</td>
<td>8.6829E-5</td>
<td>1.8591E-5</td>
</tr>
<tr>
<td>180</td>
<td>4.6639E-3</td>
<td>1.3524E-3</td>
<td>8.7209E-5</td>
<td>1.8622E-5</td>
</tr>
</tbody>
</table>

43
Figure 1. Integral cross sections for electron impact excitation of \((1s^2 2s - 1s 2s^2)^2S_{1/2}\) state of lithium. — Present DWME results, —— Present DWMD results, ——— DWE results (Pangantiwar and Srivastava, 1987), ———— DWD results (Pangantiwar and Srivastava, 1987), —·—— GA results (Srivastava et al., 1982), ·——· MCM results (Srivastava et al., 1982), ——— R-MATRIX results (Tiwary and Macek, 1985) and ——+— DWBE results (Tiwary and Macek, 1985).
Figure 2. Differential cross section results for electron impact excitation of \((1s^2 2s - 1s^2 2s^2)^2S_{\frac{3}{2}}\) state of lithium at 75 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 3. Differential cross section results for electron impact excitation of $(1s^2 2s^2 - 1s 2s^2)^2S_{1/2}$ state of lithium at 100 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987).
Figure 4. Differential cross section results for electron impact excitation of \((1s^2 2s^2 - 1s 2s^2)^2S_{1/2}\) state of lithium at 200 eV. Present DWME results,

- DWE results of Pangantiwar and Srivastava, (1987)
Figure 5. Differential cross section results for electron impact excitation of \((1s^2 2s - 1s 2s^2)^2S_{1/2}\) state of lithium at 300 eV. —— Present DWME results, • DWME results of Pangantiwar and Srivastava, (1987)
5.3 Excitation of $2p^5 3s^2 P$ state of Sodium

5.3.1 Integral Cross sections

In figure 6, integral cross sections of the lowest autoionizing state of sodium evaluated in the present model are compared with other previously reported theoretical results (Pangantiwar and Srivastava, 1987; Kaur and Srivastava, 1998; Srivastava et al., 1982) and the experimental results of Feuerstein et al. (1997) and Borovik et al. (2008). Borovik's experimental results were reported for the incident electron energies ranging from the excitation threshold to 36 eV. The threshold energy for excitation of this state is 30.77 eV (Grum-Grzhimailo et al., 1999). In the present calculations, we considered spin unresolved excitation cross sections.

It is evident that the present distorted wave model with exchange (DWME) results is in qualitative agreement with the experimental results of Feuerstein et al. (1998). This model also predicts the near threshold resonant excitation of this autoionizing state of sodium as predicted by the mentioned experimental results. At energies below 150 eV, our DWME results are higher than the experimental results. For comparison purposes, we normalized these experimental relative excitation cross sections results with our results at 1.5 keV. Our results are also in good agreement with experimental results of Borovik et al.

Our distorted wave results for direct excitations only (DWMD) are lower than the DWME results at lower energies (below 60 eV) and shows that exchange dominates in this energy range. Above 60 eV to about 300 eV, the reverse is true. In this case, the effect of exchange is to reduce the excitation cross sections. Beyond 300 eV, the DWME and DWMD results
are approximately equal. This leads us to a conclusion that in this energy range the effect of exchange is ignorable and that excitation is basically taking place through direct scattering.

When we used the double zeta wave functions, our results are comparable to Glauber approximation (G.A) of Srivastava et al. (1982) at energies above 100 eV. For lower energies, again the near threshold resonant excitation is predicted. Generally, our DWME and DWMD results are in good agreement with DWE and DWD results of Pangantiwar and Srivastava, (1987) especially above 200 eV.

The difference between our results and those of Kaur and Srivastava, (1998) could be as a result of wave functions (since they used Dirac-Fock wave functions in their relativistic distorted wave approximation where as we have used multizeta Hartree-Fock wave functions) and the choice of the distortion potential. Their distortion potential was a linear combination of static potential calculated in the final state and the exchange potential of Furness and McCarthy, (1973) for both the channels.

5.3.2 Differential Cross Sections

Table 5 shows the differential cross sections of our current DWME results. The only results available to us for comparison purposes are those of Pangantiwar and Srivastava, (1987). Figure 7-10 shows the differential cross section results at various impact energies.

At 40 eV, both results (present and Pangantiwar and Srivastava’s) are in qualitative agreement, that is, both show peaking at lower scattering angles. At higher scattering angles
their differential cross sections are slightly higher while at the intermediate angles \((40^\circ < \theta \leq 120^\circ)\), ours are slightly higher. The present DWME results experience a minimum at about 55 eV where as the DWE results of Pangantiwar and Srivastava have their minimum at about 80 eV.

At 70 eV, both the results are in excellent agreement at lower scattering angles. Our results experience a minimum at about 50\(^\circ\) while DWE results have a minimum at about 60\(^\circ\). Both results show some mild peak at intermediate angles. At higher scattering angles the DWE results are higher. Similarly, at 100 eV there is a near perfect quantitative agreement between our results and the DWE results at lower angles (\(\leq 40^\circ\)), and at angles \(> 40^\circ\) our results are slightly lower. At this energy both results portray a dip at about 40\(^\circ\). At 200 eV, there is an exact agreement between the two results from 0\(^\circ\) to 40\(^\circ\) with both results having a dip at 30\(^\circ\). Beyond 40\(^\circ\) the shapes are similar but our results are slightly higher.

### 5.3.3 Alignment parameter \(A_{20}\)

Figure 11 shows present DWME alignment parameter results for the excitation of \(2p^53s^22P\) state of sodium compared with experimental results of Feuerstein et al. (1998) and relativistic distorted wave results of Kaur and Srivastava, (1998). As can be seen from the figure, our results have better qualitative agreement with Feuerstein’s experimental results as compared to those of Kaur and Srivastava, (1998).
5.3.4 Lambda $\lambda$ parameter

Figures 12-15 show the lambda parameters evaluated in our present DWME method in comparison with DWE results of Pangantiwar and Srivastava, (1987). At 40 eV, both results are similar in shape but they disagree quantitatively at intermediate and higher scattering angles. Again at 70 eV, the results agree qualitatively and quantitatively at lower angles (below $60^\circ$) but disagree at higher scattering angles.

At 100 eV, the results are in good agreement both quantitatively and qualitatively up to about $70^\circ$ beyond which they lack agreement. At 200 eV, both results are in close agreement at all scattering angles except between $110^\circ$ and $170^\circ$ where our results are slightly lower.
Table 4. Present integral cross section and alignment parameter results for electron impact excitation of 
\((2p^63s)^2S_{1/2} - (2p^53s)^2P\) state of sodium.

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>DWME ( (\pi a_0^2 \times 10^{-3}) )</th>
<th>DWMD ( (\pi a_0^2 \times 10^{-3}) )</th>
<th>Alignment par. ( A_{20} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>31</td>
<td>5.409</td>
<td>1.424</td>
<td>-0.9582</td>
</tr>
<tr>
<td>35</td>
<td>11.41</td>
<td>3.763</td>
<td>-0.1916</td>
</tr>
<tr>
<td>40</td>
<td>11.67</td>
<td>5.940</td>
<td>-0.1206</td>
</tr>
<tr>
<td>50</td>
<td>8.948</td>
<td>8.033</td>
<td>-0.3113</td>
</tr>
<tr>
<td>60</td>
<td>7.873</td>
<td>8.945</td>
<td>-0.4653</td>
</tr>
<tr>
<td>70</td>
<td>7.776</td>
<td>9.343</td>
<td>-0.5017</td>
</tr>
<tr>
<td>80</td>
<td>7.949</td>
<td>9.470</td>
<td>-0.4800</td>
</tr>
<tr>
<td>90</td>
<td>8.143</td>
<td>9.466</td>
<td>-0.4433</td>
</tr>
<tr>
<td>100</td>
<td>8.277</td>
<td>9.384</td>
<td>-0.4065</td>
</tr>
<tr>
<td>150</td>
<td>8.132</td>
<td>8.586</td>
<td>-0.2812</td>
</tr>
<tr>
<td>200</td>
<td>7.505</td>
<td>7.737</td>
<td>-0.2121</td>
</tr>
<tr>
<td>300</td>
<td>6.344</td>
<td>6.439</td>
<td>-0.1323</td>
</tr>
<tr>
<td>400</td>
<td>5.487</td>
<td>5.542</td>
<td>-0.0851</td>
</tr>
<tr>
<td>500</td>
<td>4.858</td>
<td>4.900</td>
<td>-0.0559</td>
</tr>
<tr>
<td>600</td>
<td>4.357</td>
<td>4.388</td>
<td>-0.0285</td>
</tr>
<tr>
<td>800</td>
<td>3.647</td>
<td>3.715</td>
<td>0.0062</td>
</tr>
<tr>
<td>1000</td>
<td>3.102</td>
<td>3.156</td>
<td>0.0670</td>
</tr>
<tr>
<td>1500</td>
<td>2.232</td>
<td>2.224</td>
<td>0.2317</td>
</tr>
<tr>
<td>Angle (degrees)</td>
<td>40 eV</td>
<td>70 eV</td>
<td>100 eV</td>
</tr>
<tr>
<td>----------------</td>
<td>-----------</td>
<td>-----------</td>
<td>-----------</td>
</tr>
<tr>
<td>0</td>
<td>1.1738E-2</td>
<td>9.4926E-2</td>
<td>2.0112E-1</td>
</tr>
<tr>
<td>10</td>
<td>1.0329E-2</td>
<td>5.6068E-2</td>
<td>7.8489E-2</td>
</tr>
<tr>
<td>20</td>
<td>7.3029E-3</td>
<td>1.6963E-2</td>
<td>1.2698E-2</td>
</tr>
<tr>
<td>30</td>
<td>4.5807E-3</td>
<td>3.5826E-3</td>
<td>1.2960E-3</td>
</tr>
<tr>
<td>40</td>
<td>2.9836E-3</td>
<td>6.5905E-4</td>
<td>1.8953E-4</td>
</tr>
<tr>
<td>50</td>
<td>2.3695E-3</td>
<td>2.8145E-4</td>
<td>2.1970E-4</td>
</tr>
<tr>
<td>60</td>
<td>2.2940E-3</td>
<td>3.0922E-4</td>
<td>2.4500E-4</td>
</tr>
<tr>
<td>70</td>
<td>2.4170E-3</td>
<td>3.5624E-4</td>
<td>2.3445E-4</td>
</tr>
<tr>
<td>80</td>
<td>2.5632E-3</td>
<td>3.8174E-4</td>
<td>2.0883E-4</td>
</tr>
<tr>
<td>90</td>
<td>2.6652E-3</td>
<td>3.8460E-4</td>
<td>1.7594E-4</td>
</tr>
<tr>
<td>100</td>
<td>2.7079E-3</td>
<td>3.6720E-4</td>
<td>1.4200E-4</td>
</tr>
<tr>
<td>110</td>
<td>2.6973E-3</td>
<td>3.3521E-4</td>
<td>1.1247E-4</td>
</tr>
<tr>
<td>120</td>
<td>2.6475E-3</td>
<td>2.9607E-4</td>
<td>9.0435E-5</td>
</tr>
<tr>
<td>130</td>
<td>2.5719E-3</td>
<td>2.5658E-4</td>
<td>7.6559E-5</td>
</tr>
<tr>
<td>140</td>
<td>2.4870E-3</td>
<td>2.2151E-4</td>
<td>6.9732E-5</td>
</tr>
<tr>
<td>150</td>
<td>2.4052E-3</td>
<td>1.9350E-4</td>
<td>6.7798E-5</td>
</tr>
<tr>
<td>160</td>
<td>2.3371E-3</td>
<td>1.7357E-4</td>
<td>6.8363E-5</td>
</tr>
<tr>
<td>170</td>
<td>2.2940E-3</td>
<td>1.6128E-4</td>
<td>6.9397E-5</td>
</tr>
<tr>
<td>180</td>
<td>2.2798E-3</td>
<td>1.5887E-4</td>
<td>7.0986E-5</td>
</tr>
</tbody>
</table>
Table 6. Present DWME $\lambda$ parameter results for electron impact excitation of $(2p^5 3s)^2 S_{\text{J}} \rightarrow (2p^5 3s^2) 2p$ state of sodium atom at various incident energies.

<table>
<thead>
<tr>
<th>Angle (degrees)</th>
<th>40 eV</th>
<th>70 eV</th>
<th>100 eV</th>
<th>200 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>10</td>
<td>9.7569E-1</td>
<td>7.9196E-1</td>
<td>5.8545E-1</td>
<td>2.3621E-1</td>
</tr>
<tr>
<td>20</td>
<td>9.0506E-1</td>
<td>5.4456E-1</td>
<td>3.1842E-1</td>
<td>1.3100E-1</td>
</tr>
<tr>
<td>30</td>
<td>7.7534E-1</td>
<td>4.3829E-1</td>
<td>2.9797E-1</td>
<td>7.5869E-1</td>
</tr>
<tr>
<td>40</td>
<td>5.5209E-1</td>
<td>4.9413E-1</td>
<td>8.2636E-1</td>
<td>4.0382E-1</td>
</tr>
<tr>
<td>50</td>
<td>2.8677E-1</td>
<td>6.1607E-1</td>
<td>6.2918E-1</td>
<td>3.0925E-1</td>
</tr>
<tr>
<td>60</td>
<td>1.1090E-1</td>
<td>5.6077E-1</td>
<td>5.1480E-1</td>
<td>2.6888E-1</td>
</tr>
<tr>
<td>70</td>
<td>4.5211E-2</td>
<td>5.4171E-1</td>
<td>5.5976E-1</td>
<td>2.9096E-1</td>
</tr>
<tr>
<td>80</td>
<td>4.4245E-2</td>
<td>5.4494E-1</td>
<td>6.7001E-1</td>
<td>3.6342E-1</td>
</tr>
<tr>
<td>90</td>
<td>7.9133E-2</td>
<td>5.2881E-1</td>
<td>7.6818E-1</td>
<td>4.5580E-1</td>
</tr>
<tr>
<td>100</td>
<td>1.4016E-1</td>
<td>4.7568E-1</td>
<td>7.9679E-1</td>
<td>5.3449E-1</td>
</tr>
<tr>
<td>110</td>
<td>2.2570E-1</td>
<td>3.9189E-1</td>
<td>7.2567E-1</td>
<td>5.7150E-1</td>
</tr>
<tr>
<td>120</td>
<td>3.3558E-1</td>
<td>3.0558E-1</td>
<td>5.7668E-1</td>
<td>5.7183E-1</td>
</tr>
<tr>
<td>130</td>
<td>4.6666E-1</td>
<td>2.6198E-1</td>
<td>4.4318E-1</td>
<td>5.9214E-1</td>
</tr>
<tr>
<td>140</td>
<td>6.1168E-1</td>
<td>3.0852E-1</td>
<td>4.3491E-1</td>
<td>6.7446E-1</td>
</tr>
<tr>
<td>150</td>
<td>7.5661E-1</td>
<td>4.6620E-1</td>
<td>5.7227E-1</td>
<td>7.9279E-1</td>
</tr>
<tr>
<td>160</td>
<td>8.8254E-1</td>
<td>6.9934E-1</td>
<td>7.7378E-1</td>
<td>9.0185E-1</td>
</tr>
<tr>
<td>180</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
Figure 6. Integral cross sections for electron impact excitation of $(2p^6 3s^1)^2S_{1/2} - (2p^5 3s^2)^2P$ state of sodium. — present DWME results, —— present DWMD results, ——— DWE results of Pangantiwar and Srivastava, (1987), —— DWD results of Pangantiwar and Srivastava, (1987), —— RDW results of Kaur and Srivastava, (1998), —— GA results of Srivastava et al. (1982), • experimental results of Borovik et al. (2008), ● experimental results of Feuerstein et al. (1998) and present — — — — DWME-DZ results.
Figure 7. Differential cross section results for the excitation of \((2p^63s^1)^2S_{1/2} - (2p^53s^2)^2P\) state of sodium at 40 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 8. Differential cross section results for the excitation of \((2p^63s^1)^2S_{1/2} - (2p^53s^2)^2P\) state of sodium at 70 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 9. Differential cross section results for the excitation of \((2p^63s)^2S_{1/2} - (2p^53s^2)^2P\) state of sodium at 100 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 10. Differential cross section results for the excitation of $(2p^6 3s)^2S_{1/2} - (2p^5 3s^2)^2P$ state of sodium at 200 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 11. Alignment Parameter $A_{20}$ for the excitation of $(2p^6 3s)^2S_{1/2} - (2p^5 3s^2)^2P$ state of sodium. ----- present DWME results, • experimental results of Feuerstein et al. (1998), ……RDW results of Kaur and Srivastava, (1998).
Figure 12. $\lambda$ parameter results for electron impact excitation of $(2p^63s)^2S_{1/2} - (2p^53s^2)^2P$ state sodium at 40 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 13. $\lambda$ parameter results for electron impact excitation of $(2p^63s)^2S_{1/2} - (2p^53s^2)^2P$ state sodium at 70 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 14. $\lambda$ parameter results for electron impact excitation of $\left(2p^6 3s\right)^2S_{1/2} - \left(2p^5 3s^2\right)^2P$ state sodium at 100 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 15. \( \lambda \) parameter results for electron impact excitation of \((2p^6 3s)^2S_{1/2} - (2p^5 3s^2)^2P\) state sodium at 200 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
5.4 Excitation of $3p^54s^2 2P$ state of Potassium

5.4.1 Integral Cross sections

Figure 16 shows the integral cross sections evaluated in the present DWME, DWMD and DWME-DZ methods are compared with DWE and DWD results of Pangantiwar and Srivastava, (1987), RDW results of Kaur and Srivastava, (1998), DWBA and experimental results of Feuerstein et al. (1999). The threshold energy for excitation of this lowest autoionizing state of potassium is 18.722 eV (Borovik et al., 1999). Just like in sodium, we considered spin unresolved excitation cross sections in our present results.

As can be seen from our results, the distorted wave model that we have used does not predict the resonant structure observed in potassium experimental results at near threshold energies, despite its success in sodium excitation. But the Feuerstein’s DWBA result gives the resonant structure near threshold. The difference between the present and Feuerstein’s distorted wave approaches, besides the wave functions used, is in the distortion potential where they used the exchange potential in addition to the static potential when evaluating the distortion potential. This may explain their success in predicting the resonant structure, that is, potassium being a heavy metal experiences a significant effect of the exchange potential as compared to sodium.

Feuerstein’s results are generally high as compared to other results. This is because, in the evaluation of DWBA cross sections and normalization of experimental relative cross section results, they used multizeta Hartree-Fock ground state wave functions for the initial state while for the final state they used multi-configuration intermediate-coupling wave functions.
of the autoionizing states $2p^5 3s^2 2p^J$ and $2p^J$. This, as outlined by Kaur and Srivastava, (1998), raises serious issues on orthogonality of states that need to be addressed. Similarly, our results differ with RDW results because of the difference in the choice of wave functions and distortion potential where as for DWE and DWD, the difference is in the distortion potential and the method of evaluation of the exchange amplitude.

From the same figure we can also see that exchange lowers cross sections at energies below 200 eV. Beyond this energy range, exchange effects can be considered as insignificant. Also, just as in sodium transitions, when double zeta wave functions are used the cross sections are slightly lower for all energies.

5.4.2 Differential Cross sections

Figures 17-20 show our DWME differential cross section results in comparison with DWE results of Pangantiwar and Srivastava, (1987). At 24.3 eV, both results show peaking at lower angles, though our results are lower. At intermediate angles, again both results have a minimum with DWME results at about $50^\circ$ while theirs is at about $80^\circ$. At large angles, the differential cross sections increase gently as shown.

At 40 eV, the two results are in very good agreement at angles below $60^\circ$, though our results are slightly lower. Beyond $60^\circ$, the agreement is only qualitative but in this range our results are slightly higher. When the incident energy is 70 eV, the match is almost perfect at angles below $40^\circ$. Above this angle, the qualitative agreement holds but the DWME results are slightly higher. Again at 100 eV, the shapes of both curves are exactly the same, all showing
some dip at about $30^\circ$. Below $40^\circ$, the both DWME and DWE results are in exact agreement quantitatively. Beyond this angle, the DWME results are slightly higher with both showing a minimum at about $110^\circ$.

### 5.4.3 Alignment Parameter $A_{20}$

Figure 21 shows the alignment parameter results evaluated using the present DWME results and compared with the experimental and DWBA results of Matterstock et al. (1995) and RDW results of Kaur and Srivastava, (1998).

At higher energies (above 100 eV), all the results are in agreement in shape. Our results also show some resonance at about 20 eV. This behaviour in the alignment parameter is also predicted by the distorted wave approach of Matterstock et al. (1995). In this paper they have used the same set of wave functions and distortion potential as Feuerstein et al. (1999) discussed earlier. Though the experimental results show a minimum at around 80 eV, these experimental results are not available below 30 eV which could have predicted the resonant structure. The resonant structure predicted by the present method is similar is to the one predicted in the case of sodium, though in this case it is not so pronounced. This structure can be attributed to exchange effect.

### 5.4.4 Lambda $\lambda$ Parameter

Figures 22-25 show $\lambda$ parameter results evaluated using the present DWME method and are compared with DWE results of Pangantiwar and Srivastava, (1987). At 24.3 eV, the two results are in good qualitative agreement with both showing a minimum at about $63^\circ$ and
approximately equal values at angles below 60° and above 140°. When the incident energy rises to 40 eV, the $\lambda$ parameter results are more structured. At angles below 40°, there is exact agreement between the two results. Above this angle, the agreement is only qualitative with DWME method reporting lower values. Another notable feature in the DWME results is the slight peaking at about 100° which coincides with some minimum in the DWE results.

At 70 eV, the two results agree qualitatively at all angles. Below 40°, the quantitative agreement between the results is exact. At about 113°, DWME reports a sharp dip where as in the DWE results it is shallow and is at 100°. But at 100 eV, the agreement, both qualitative and quantitative, is almost exact for all angles below 80°. Above this angle, DWE results are slightly higher. The dip observed at 70 eV is comparatively more prominent for both results at 100 eV, though in this case it occurs at around 103°.
Table 7. Present integral cross section and alignment parameter results for electron impact excitation of \((3p^64s)^2S_{1/2} - (3p^54s^2)^2P\) state of potassium.

<table>
<thead>
<tr>
<th>ENERGY (eV)</th>
<th>DWME ((\pi a_o^2 \times 10^{-2}))</th>
<th>DWMD ((\pi a_o^2 \times 10^{-2}))</th>
<th>A_{20}</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.4635</td>
<td>0.8922</td>
<td>-0.4342</td>
</tr>
<tr>
<td>30</td>
<td>2.926</td>
<td>3.945</td>
<td>-0.5165</td>
</tr>
<tr>
<td>40</td>
<td>4.199</td>
<td>4.712</td>
<td>-0.4383</td>
</tr>
<tr>
<td>50</td>
<td>4.581</td>
<td>4.956</td>
<td>-0.3993</td>
</tr>
<tr>
<td>60</td>
<td>4.632</td>
<td>4.979</td>
<td>-0.3710</td>
</tr>
<tr>
<td>70</td>
<td>4.582</td>
<td>4.9100</td>
<td>-0.3459</td>
</tr>
<tr>
<td>80</td>
<td>4.474</td>
<td>4.793</td>
<td>-0.3217</td>
</tr>
<tr>
<td>90</td>
<td>4.395</td>
<td>4.656</td>
<td>-0.2985</td>
</tr>
<tr>
<td>100</td>
<td>4.298</td>
<td>4.523</td>
<td>-0.2785</td>
</tr>
<tr>
<td>150</td>
<td>3.801</td>
<td>3.888</td>
<td>-0.1941</td>
</tr>
<tr>
<td>200</td>
<td>3.375</td>
<td>3.412</td>
<td>-0.1404</td>
</tr>
<tr>
<td>300</td>
<td>2.750</td>
<td>2.759</td>
<td>-0.0747</td>
</tr>
<tr>
<td>400</td>
<td>2.346</td>
<td>2.338</td>
<td>-0.0336</td>
</tr>
<tr>
<td>500</td>
<td>2.035</td>
<td>2.032</td>
<td>0.0072</td>
</tr>
<tr>
<td>600</td>
<td>1.790</td>
<td>1.777</td>
<td>0.0464</td>
</tr>
<tr>
<td>800</td>
<td>1.443</td>
<td>1.422</td>
<td>0.1075</td>
</tr>
<tr>
<td>1000</td>
<td>1.179</td>
<td>1.148</td>
<td>0.1674</td>
</tr>
</tbody>
</table>
Table 8. Present DWME Differential cross sections results in $a_0^2sr^{-1}$ for electron impact excitation of $(3p^6 4s)^2S_{1/2} - (3p^5 4s^2)^2P$ state of potassium at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>Angle (degrees)</th>
<th>24.3 eV</th>
<th>40 eV</th>
<th>70 eV</th>
<th>100 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3.9311E-2</td>
<td>4.0240E-1</td>
<td>1.4318E0</td>
<td>3.4003E0</td>
</tr>
<tr>
<td>10</td>
<td>3.6098E-2</td>
<td>2.4809E-1</td>
<td>4.3323E-1</td>
<td>3.8387E-1</td>
</tr>
<tr>
<td>20</td>
<td>2.8743E-2</td>
<td>8.0325E-2</td>
<td>4.6386E-2</td>
<td>1.5719E-2</td>
</tr>
<tr>
<td>30</td>
<td>2.1765E-2</td>
<td>1.9928E-2</td>
<td>4.0146E-3</td>
<td>1.4059E-3</td>
</tr>
<tr>
<td>40</td>
<td>1.7827E-2</td>
<td>6.6471E-3</td>
<td>3.1356E-3</td>
<td>2.1436E-3</td>
</tr>
<tr>
<td>50</td>
<td>1.6875E-2</td>
<td>4.5866E-3</td>
<td>3.0614E-3</td>
<td>1.4303E-3</td>
</tr>
<tr>
<td>60</td>
<td>1.7823E-2</td>
<td>4.1968E-3</td>
<td>2.3966E-3</td>
<td>8.0257E-4</td>
</tr>
<tr>
<td>70</td>
<td>1.9640E-2</td>
<td>3.9410E-3</td>
<td>1.7008E-3</td>
<td>4.2465E-4</td>
</tr>
<tr>
<td>80</td>
<td>2.1628E-2</td>
<td>3.6256E-3</td>
<td>1.1138E-3</td>
<td>2.1354E-4</td>
</tr>
<tr>
<td>90</td>
<td>2.3426E-2</td>
<td>3.2157E-3</td>
<td>6.8182E-4</td>
<td>1.0965E-4</td>
</tr>
<tr>
<td>100</td>
<td>2.4894E-2</td>
<td>2.7610E-3</td>
<td>4.1515E-4</td>
<td>6.8557E-5</td>
</tr>
<tr>
<td>110</td>
<td>2.6021E-2</td>
<td>2.3532E-3</td>
<td>2.9069E-4</td>
<td>6.0551E-5</td>
</tr>
<tr>
<td>120</td>
<td>2.6848E-2</td>
<td>2.0664E-3</td>
<td>2.6817E-4</td>
<td>6.5454E-5</td>
</tr>
<tr>
<td>130</td>
<td>2.7425E-2</td>
<td>1.9284E-3</td>
<td>3.0628E-4</td>
<td>7.3474E-5</td>
</tr>
<tr>
<td>140</td>
<td>2.7815E-2</td>
<td>1.9212E-3</td>
<td>3.7136E-4</td>
<td>8.0101E-5</td>
</tr>
<tr>
<td>150</td>
<td>2.8073E-2</td>
<td>1.9991E-3</td>
<td>4.3957E-4</td>
<td>8.4304E-5</td>
</tr>
<tr>
<td>160</td>
<td>2.8222E-2</td>
<td>2.1069E-3</td>
<td>4.9566E-4</td>
<td>8.6547E-5</td>
</tr>
<tr>
<td>170</td>
<td>2.8287E-2</td>
<td>2.1963E-3</td>
<td>5.2999E-4</td>
<td>8.7666E-5</td>
</tr>
<tr>
<td>180</td>
<td>2.8301E-2</td>
<td>2.2209E-3</td>
<td>5.2912E-4</td>
<td>8.7605E-5</td>
</tr>
</tbody>
</table>
Table 9. Table Present DWME λ parameter results for electron impact excitation of
\((3p^6\ 4s)^2S_{1/2} - (3p^5\ 4s^2)\ 3P\) state of potassium at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>Angle (degree)</th>
<th>24.3 eV</th>
<th>40 eV</th>
<th>70 eV</th>
<th>100 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>10</td>
<td>9.6949E-1</td>
<td>7.9547E-1</td>
<td>4.8220E-1</td>
<td>3.1289E-1</td>
</tr>
<tr>
<td>20</td>
<td>8.9347E-1</td>
<td>5.2123E-1</td>
<td>2.2921E-1</td>
<td>1.5348E-1</td>
</tr>
<tr>
<td>30</td>
<td>7.9864E-1</td>
<td>4.2306E-1</td>
<td>5.3498E-1</td>
<td>7.6996E-1</td>
</tr>
<tr>
<td>40</td>
<td>6.9963E-1</td>
<td>5.6105E-1</td>
<td>6.4929E-1</td>
<td>4.7473E-1</td>
</tr>
<tr>
<td>50</td>
<td>6.0172E-1</td>
<td>5.7186E-1</td>
<td>4.5965E-1</td>
<td>4.1849E-1</td>
</tr>
<tr>
<td>60</td>
<td>5.3663E-1</td>
<td>4.4029E-1</td>
<td>3.6732E-1</td>
<td>4.0665E-1</td>
</tr>
<tr>
<td>70</td>
<td>5.9191E-1</td>
<td>3.6890E-1</td>
<td>3.4825E-1</td>
<td>4.1191E-1</td>
</tr>
<tr>
<td>80</td>
<td>7.2435E-1</td>
<td>3.7703E-1</td>
<td>3.6206E-1</td>
<td>3.8795E-1</td>
</tr>
<tr>
<td>90</td>
<td>8.1426E-1</td>
<td>4.4101E-1</td>
<td>3.5063E-1</td>
<td>2.6870E-1</td>
</tr>
<tr>
<td>100</td>
<td>8.5912E-1</td>
<td>4.3287E-1</td>
<td>2.5898E-1</td>
<td>1.0644E-1</td>
</tr>
<tr>
<td>110</td>
<td>8.8586E-1</td>
<td>4.1819E-1</td>
<td>1.2832E-1</td>
<td>1.4074E-1</td>
</tr>
<tr>
<td>120</td>
<td>9.0757E-1</td>
<td>3.9786E-1</td>
<td>1.5469E-1</td>
<td>3.4417E-1</td>
</tr>
<tr>
<td>130</td>
<td>9.2850E-1</td>
<td>4.2795E-1</td>
<td>3.6133E-1</td>
<td>5.5959E-1</td>
</tr>
<tr>
<td>140</td>
<td>9.4976E-1</td>
<td>5.3785E-1</td>
<td>5.9385E-1</td>
<td>7.2797E-1</td>
</tr>
<tr>
<td>150</td>
<td>9.6956E-1</td>
<td>6.9838E-1</td>
<td>7.7762E-1</td>
<td>8.5210E-1</td>
</tr>
<tr>
<td>180</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
Figure 16. Integrated cross section results for electron impact excitation of \((3p^6 4s)^2S_{1/2} - (3p^5 4s^2)^2P\) state of potassium. —— present DWME results; —— present DWMD results; —— DWM results of Pangantiwar and Srivastava, (1987); —— DWD results of Pangantiwar and Srivastava, (1987); —— RDW results of Kaur and Srivastava, (1998); —— present DWME-DZ results; • experimental results of Feuerstein et al. (1999) and —— DWBA results of Feuerstein et al. (1999).
Figure 17. Differential cross section results for the electron impact excitation of 
$(3p^64s)^2S_{1/2} - (3p^54s^2)^2P$ state of potassium 24.3 eV. — Present DWME results,
• DWE results of Pangantiwar and Srivastava, (1987)
Figure 18. Differential cross section results for the electron impact excitation of 
\((3p^6\,4s)^2S_{1/2} - (3p^7\,4s^2)^2P\) state of potassium 40 eV. Present DWME results,
• DWE results of Pangantiwar and Srivastava, (1987)
Figure 19. Differential cross section results for the electron impact excitation of 
\((3p^64s)^2S_{1/2} - (3p^54s^2)^2P\) state of potassium 70 eV. — Present DWME results,
• DWE results of Pangantiwar and Srivastava, (1987)
Figure 20. Differential cross section results for the electron impact excitation of $(3p^64s)^2S_{1/2} - (3p^54s^2)^2P$ state of potassium 100 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 21. Alignment Parameter $A_{20}$ for electron impact excitation of $(3p^6 4s)^2S_{1/2}$ - $(3p^5 4s^2)^2P$ state of potassium. ___ present DWME results, • experimental results of Matterstock et al. (1995), - - - RDW results of Kaur and Srivastava, (1998), ... DWBA of Matterstock et al. (1995).
Figure 22. \( \lambda \) parameter results for electron impact excitation of \((3p^64s)^2S_{1/2} - (3p^54s^2)^2P\) state of potassium at 24.3 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 23. $\lambda$ parameter results for electron impact excitation of $(3p^6 4s)^2 S_{1/2} - (3p^5 4s^2)^2 P$ state of potassium at 40 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 24. λ parameter results for electron impact excitation of \((3p^6 4s)^2 S_{1/2} - (3p^5 4s^2)^2 P\) state of potassium at 70 eV. — Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
Figure 25. $\lambda$ parameter results for electron impact excitation of $(3p^54s)^2S_{1/2} - (3p^54s^2)^2P$ state of potassium at 100 eV. —— Present DWME results, • DWE results of Pangantiwar and Srivastava, (1987)
5.5 Summary of Results and Discussions

From the present results that we have presented for electron impact excitation of the lowest autoionizing states of lithium, sodium and potassium, one is able to see that the present variation of the distorted wave method gives reliable results at all energies especially for sodium. In this excitation, we have been able to predict the near threshold resonance structures that have been reported in the previous experimental results of Feuerstein et al. (1998). Our differential cross sections and $\lambda$ parameter results are in very good agreement with the previous theoretical results of Pangantiwar and Srivastava, (1987) at intermediate and high energy range, with the differences arising due to the different choice of the distortion potentials used and the method of evaluation of the exchange scattering amplitudes.

We can also make an inference that the exchange process enhances the excitation cross sections for lithium and sodium at lower energies while for potassium; it reduces the excitation cross sections. When double zeta wave functions of Clementi and Roetti, (1974) are used in place of the multi zeta wave functions, the excitation cross sections for sodium and potassium are lowered at all energies.
CHAPTER 6
CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

We have evaluated integral cross sections, differential cross sections and where applicable, the alignment and lambda parameters for electron impact excitation of the lowest autoionizing levels of lithium, sodium and potassium from threshold to high incident energies of the projectile using Distorted Wave Method (DWM). Our present DWM involved the use of a linear combination of initial and final state static potentials as the final state distortion potential and initial state static potential as the initial state distortion potential. In our calculations, we used the multi zeta ground state single electron wave functions compiled by Clementi and Roetti, (1974) as wave functions both for the ground and the excited states of the target. In the code that we modified, we included the exchange terms that were previously neglected.

The results obtained are in good agreement with previously reported results at intermediate and high energy range. It is important to note that our results predict the near threshold resonance structures observed in the experimental results of sodium reported by Feuerstein et al. (1998), Grum-Grzhimailo et al. (1999). In lithium and sodium, the results show that exchange process enhances excitation cross sections at lower energies while for potassium, exchange process lowers the excitation cross sections at lower energies. Except for lithium at lower energies, our differential cross section and λ parameter results are in very good agreement with the DWE results of Pangantiwar and Srivastava, (1987). Our Distorted wave
results with exchange included for lithium at near threshold energies is too high (about 10
times high at 60 eV), and this needs further investigation.

In conclusion, the present distorted wave method with multi zeta and double zeta wave
functions for atomic states gives results which are in good agreement with experimental and
theoretical results. In case of sodium atom, it predicts the near threshold resonance structure
which is observed in the experimental results.

6.2 Recommendations

Considering the performance of this method for $1s^2 2s - 1s^2 s^2$ transition in lithium,
$2p^6 3s - 2p^5 3s^2$ transition in sodium, and $3p^6 4s - 3p^5 4s^2$ transition in potassium by
electron impact, the following recommendations are made:

(i) Further studies should be done by including the exchange and the polarization
potential in the distortion potentials successively to see the effect of these potentials
in the excitation cross sections.

(ii) The present method to be extended to higher autoionizing states of lithium, sodium
and potassium and also to other alkalis like cesium and rubidium.

(iii) More experimental and theoretical studies on differential cross sections, angular
correlation parameters and alignment parameters for the excitations considered
should be conducted for comparison purposes with the present results.

(iv) The present method should also be extended to electron impact excitations of alkali
earth metals amongst others.
REFERENCES


