POSITRON-IMPACT EXCITATION OF THE LOWEST AUTOIONIZING STATE IN RUBIDIUM ATOM USING DISTORTED WAVE METHOD

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MAY 2014
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

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DEDICATION

This work is dedicated to my entire family, my friends: Sekeyian, Muriithi and my supervisor C.S Singh.
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CCC - Convergent Close Coupling
DCS - Differential Cross Section
DWBA1 - First order Distorted Wave Born Approximation
DWD - Distorted Wave Born method without exchange
DWE - Distorted Wave Born method with exchange
DWM - Distorted Wave Born method
DZ - Double Zeta wave functions
ICS - Integral Cross Sections
MZ - Multi Zeta wave functions
Rb - Rubidium
\[ \frac{+i}{e^{i\phi}} \] - Positron
\[ \frac{-i}{e^{i\phi}} \] - Electron
RHF - Roothan Hatree Fock
RDW - Relativistic Distorted Wave method
WKB - Wentzel Kramers Brillouin
ABSTRACT

Many calculations on atomic collisions and scattering processes have been performed on electron impact excitation of the lowest autoionizing state of rubidium, but not much attempt has been made with positron impact which is of equally fundamental importance and is receiving attention nowadays with the availability of improved positron beam experiments. So, in this study, total cross-sections, differential cross-sections, lambda parameter, R parameter and the alignment parameter for positron impact excitation of the lowest autoionizing state of rubidium have been calculated using Distorted Wave method. The wave functions used are the Roothan Hatree Fock double zeta and multi zeta wave functions due to Clementi and Roetti. Variations in distortion potential have been made such that the static potential of the initial state of rubidium atom is used as the initial channel distortion potential and a linear combination of static potentials of the initial and final states as the final channel distortion potential to check its effect on cross-sections. Numerical calculations have been done using a modified DWBA1 FORTRAN computer program which was originally made for hydrogen atom. The results for positron impact excitation of the lowest autoionizing state of rubidium have been analyzed and compared with experimental and theoretical results for positron and electron impact excitation of the same state available in literature. From the comparison of the results, it is seen that in general the electron impact excitation cross section results are higher than the positron impact excitation cross section especially near excitation threshold energy. This can be attributed to the exchange process which takes place in the case of electron impact and not in the case of positron impact and also due to larger interaction between the projectile and the target in case of electron impact than in case of positron impact. It is also found from the alignment parameter results that the integral cross section results for m=0 level are larger compared to m=1 level for impact energies up to about 500 eV beyond which integral cross-sections for the magnetic sublevel m=1 become greater. The lambda parameter indicates that more particles are scattered towards m=0 for electron impact compared to positron impact excitation near threshold energy. R parameter results have been calculated to account for phases of scattered amplitudes in the collision process.
CHAPTER 1
INTRODUCTION

1.1 Background of the study

Rubidium is the second most electropositive alkali element when involved in atomic collisions and reactions. The positron or anti electron is the antiparticle or the antimatter counterpart of the electron with an electric charge of +1, a spin of \( \frac{1}{2} \), and has the same mass as an electron. A positron projectile beam approaching a target atom such as rubidium will experience an electrostatic field causing it to scatter in different directions or angles. After colliding, the energy of the projectile is transferred to the target leading to excitation.

Collisions can be classified as elastic, where the state of the target is unchanged or inelastic, which lead to excitation, ionization or recombination of target. In the various excitation processes, collisions may lead to excitation of atoms and ions by atomic particles such as electrons, protons, positrons, ions and neutrons to states which in turn spontaneously decay by electron emission. Such a radiationless transition mechanism is called autoionization and these states are called autoionizing states. An autoionizing state can occur due to excitations of one inner-shell electron into a higher orbital, resulting in a missing electron in an inner shell. For instance, rubidium autoionizing states such as \( 4p^55s^2 \) involve the excitation of a 4p core-electron into the 5s orbital. An autoionizing state lies energetically above the lowest ionization threshold (Rai and Srivastava, 1984).

Atomic collisions involve scattering of electrons, positrons, protons, ions or neutrons by target atoms, molecules or ions. Detectors are placed at different angles past the target, to record the scattered particles in the asymptotic region, hence enabling the determination of respective differential cross-sections.
Exact solutions for atomic collision cross sections are theoretically difficult to obtain. This is because the total wave function for the system (projectile + target) cannot be solved exactly. Also, in most cases, the target wave functions are not completely accurate and the approximate wave functions that must be relied on are sometimes not orthogonal. As a result, approximate methods must be employed to solve Lippmann-Schwinger equations. Collision problems can be solved by making approximations classified into quantum mechanical approaches such as close coupling, R-matrix, variation method, perturbation series or semi classical approaches such as Monte Carlo method and Glauber approximations. Some of the perturbation series methods include; Born series, distorted wave series, Eikonal series, many body theory among others (Madison and Bartschat, 1996). Some of the factors that determine the most appropriate approximation method to be used are the masses involved and velocity or energy of the incident beam.

The study of autoionizing states provides information about the atomic structure and the dynamics of a state’s excitation. If the impact energy of a positron projectile is relatively high, it can lead to direct ionization of the target provided that the excitation threshold is exceeded (Madison and Bartschat, 1996). Consequently, when the positron collides with a target electron, they may cancel out to form a photon and emit gamma rays, that is, annihilation or form a positronium which is a combination of a positron and electron. Alternatively, the target can be excited to higher states above the threshold, which are the autoionizing states. If the target is excited to any of these autoionizing states, they can in principle decay through radiative transition to a bound state of the system below the first autoionization limit or by a non-radiative transition to the ground state or to one of the excited states of the corresponding ion (Jobunga, 2009). If autoionization takes place in a negative ion, it may produce a neutral atom.
Autoionizing states are usually short-lived, approximately $10^{-13}$ to $10^{-14}$ seconds and thus can be described as resonances rather than normal bound states (Feldman and Novick, 1963).

To fully describe an atomic collision mechanism, transition probabilities, cross sections, angular correlation and alignment parameters are determined. Only a small amount of the data needed can be determined experimentally. This is due to the difficulties and costs associated with setting up and performing such experiments. As a result, a major goal of theoretical atomic physics, therefore, has been to develop reliable and efficient computational methods to calculate the outcome of the various collision processes of interest (Madison and Bartschat, 1996). The atomic collision results are in turn applied in fields of science like electronics, astrophysics, plasmas, laser spectroscopy, solution chemistry, biophysics amongst others.

1.2 Research problem statement

In this study positron impact excitation of the lowest lying autoionizing level in rubidium has been investigated by use of the Distorted Wave method. Integral cross sections are compared in the energy range of 15 eV to 1500 eV using multi zeta and double zeta wave functions. The results for ICS have been compared to those of Pangantiwar and Srivastava (1987) and Borovik et al. (2012). Angular correlation parameters and alignment parameter for the excited state have also been calculated.
1.3 Objectives of the research

1.3.1 General objective

The general objective of this research was to study the positron impact excitation of the lowest autoionizing state in rubidium.

1.3.2 Specific objectives

The specific objectives were as follows:

(i) To formulate the problem for positron impact excitation of the autoionizing states in rubidium and modify DWBA1 computer code for our calculations.

(ii) To determine differential and total cross-sections for the positron-impact excitation of the lowest autoionizing state of rubidium at energies above the first excitation threshold.

(iii) To determine angular correlation parameters.

(iv) To compare positron impact results obtained with available data.

(v) To compare our results with results for electron impact excitation of the same state.

1.4 Rationale of the study

Due to recent progress in positron beam experiments, the cross section data for positron-alkali atom scattering are also becoming available. Though there are many calculations on electron impact excitation of autoionizing states of alkali atoms, not much attempt has been made with positron impact which is of equally fundamental importance and receiving more attention (Pangantiwar and Srivastava, 1988). It is desirable to extend this study to theoretical calculations for positron impact excitation. It is also important to compare results with those for electron impact excitations to see the variation in results due to the change in projectile charge.
The choice of using the DWM lies in the fact that more of the important physical effects may be included in the leading terms of the perturbation series expansion making it converge faster than the Born series (Madison and Bartschat, 1996). It has also been found to be successful in explaining various features of an excitation process providing results which are in good agreement with experimental data. At the same time the DWBA is less expensive computationally as compared to other reliable theories like R-matrix and close-coupling methods (Katiyar and Srivastava, 1988).

In the problem stated, the theoretical result available for a similar study by Pangantiwar and Srivastava (1987) has no experimental or theoretical result on positron impact to compare with. So it would be interesting to see how the change in the projectile charge, use of different distortion potentials and double zeta wave functions affects the results for both positron and electron impact.
2.1 Studies on electron impact excitation of autoionizing states in alkalis

Feldman and Novick (1963) carried out an experimental study on autoionizing states in alkali atoms with microsecond lifetimes. In this work they reported the existence of atomic energy levels in lithium, potassium, and rubidium which lie between the first and second ionization potentials and which are metastable against both radiation and autoionization with lifetimes in the microsecond region. They presented excitation cross section curves for long lived autoionizing states in neutral lithium, potassium, and rubidium atoms excited by electron bombardment. They observed that the lithium curve exhibits an increase in the cross section starting at $56\pm1$ eV rising sharply to a maximum at $58$ eV, corresponding to a production cross section of $10^{-19}$ cm$^2$. For K, and Rb the maximum was observed at $17.5\pm1$ and $14.2\pm1$ eV respectively both corresponding to cross sections of about $10^{-18}$ cm$^2$.

Roy and Rai (1973) studied electron-impact ionization of alkali metals using classical binary-encounter calculations using a Hartree Fock velocity distribution for the bound electrons in alkali metals. Effects of inner-shell ionization as well as the excitation of some autoionizing levels were included. For rubidium, they presented results for ionization cross section at an energy range of $0$ eV to $50$eV with autoionization peaks revealed at about $18.8$ eV, $24$ eV and $33$ eV. They observed that the removal of an electron from the inner shell, as well as excitation of an inner electron to autoionizing levels, contributes significantly to the cross section.

Nygaard (1975) carried out an experimental study on electron impact autoionization in heavy alkali metals where the autoionizing levels in cesium, rubidium, and potassium were studied by electron impact in a crossed-beam apparatus. They made comparisons with the binary-encounter
calculations of Roy and Rai (1973). They observed that effects of autoionization and inner-shell ionization have been overestimated in the theory. They presented results for ionization cross sections with an aim to check the contribution of autoionization processes, that is, by observing where autoionization peaks occur in the electron-impact ionization cross sections for the heavy alkali metals. For rubidium electron impact ionization cross sections Nygaard and Hahn (1973) observed a maximum at 16.5 eV which is due to excitation of the autoionizing levels at 15.31 and 16.16 eV.

Tiwary and Rai (1975) studied electron impact excitation of the lowest autoionizing level in alkali metal atoms where the total cross sections were calculated in the first Born approximation, modified first Born approximation and Vainshtein approximation (neglecting exchange). The calculated contributions for autoionization were of the same order of magnitude as those observed for K, Rb and Cs by Nygaard and Hahn results of 1973. They presented results for total cross sections at a range of 20 eV to 70 eV. They observed that agreement between the three results at high energies is better.

Jobunga (2009) calculated integral cross sections, differential cross sections, alignment and lambda parameter for electron impact excitation of the lowest autoionizing states of Li, Na and K using DWM, applying the static potential of the initial state as the initial channel static potential and a linear combination of the initial and final state static potential as the final channel distortion potential. Integral cross sections were compared to those in the study of Pangantiwar and Srivastava of 1987. Results from this study for Na predict near threshold resonance but not for K and Li.
2.2 Studies on electron impact excitation of the lowest autoionizing state in rubidium

Kaur and Srivastava (1999) studied excitation of the lowest autoionizing states of Na, K, Rb and Cs by electron impact using relativistic distorted-wave (RDW) calculations. They obtained detailed results in the range of near threshold to 1.5 keV incident electron energies for total cross sections of the magnetic sub states of the individual \( ^2P_{3/2} \) and \( ^2P_{1/2} \) states. Utilizing this, they presented results for total cross sections, alignment parameter \( A_{20} \) of the \( ^2P_{3/2} \) state and the intensity of the ejected electrons from the \( ^2P_{3/2} \) state. RDW calculations without the exchange effect (RDWD) and relativistic Born approximation calculations were also performed for comparison with earlier results of Pangantiwar and Srivastava (1987) and experimental data from the Freiburg group from Germany. For rubidium, unlike for Na and K, peaks in the RDW and RDWD calculations were very close to the threshold energy. The observed peak becomes dominant towards heavier alkali atoms. No experimental results were available for comparison.

Borovik et al. (2012 a) carried out an experimental study on the \( 4p^6 \) autoionization cross section of rubidium atoms excited by low-energy electron impact. The autoionization cross section of rubidium atoms was obtained by measuring the total normalized intensities of ejected-electron spectra arising from the decay of the \( 4p^5n_1l_1n_2l_2 \) autoionizing levels. The ejected-electron spectra were measured at the observation angle of 57.4° in an impact energy region from 15.3 eV up to 50 eV. The cross section reached the maximum value of \( (2.9\pm0.6) \times 10^{-16} \text{ cm}^2 \) at 21.8 eV impact energy. In this work, the first data on the autoionization cross section of rubidium atoms in an electron impact energy region from the \( 4p^6 \) excitation threshold up to 50 eV which showed quick rise of the autoionization cross section between 15.3 eV and 18.5 eV was reported.

Borovik et al. (2012 b) carried out a study on resonance excitation of the \( 4p^55s^2 \) autoionizing states in Rb by electron impact at an energy range of 15 eV to 20 eV. The near-threshold
excitation dynamics of the $4p^5s^2$ autoionizing states in rubidium atoms was studied experimentally by measuring the ejected-electron excitation functions and theoretically by applying a fully relativistic Dirac B-spline R-matrix (close-coupling) model. The results of this study revealed that strong negative-ion resonances dominate the electron-impact excitation of the lowest autoionizing states in Rb between 15.3 eV and 18.5 eV.

2.3 Studies on positron impact excitation of the lowest autoionizing state in rubidium.

Pangantiwar and Srivastava (1987) studied electron and positron impact excitation of autoionizing levels in alkalis using Distorted Wave Method approach for incident particle energy varying above the threshold energy of about 15.3 eV to 1000 eV. In this study, multi-zeta RHF wave functions and the initial and final state static potentials as the distortion potentials for the initial and final distorted waves respectively were applied. For Rb, results for the polarization parameter, alignment parameter and the integral cross section (ICS) for positron impact excitation of the lowest autoionizing state were presented. Their results for ICS with and without exchange were almost the same at higher energies of about 500 eV up to 1000 eV.

2.4 Summary of the review

Most of the studies on excitation of the autoionizing states of alkalis revolve around electron impact excitation. Not much has been done for the case of positron impact excitation which is equally important. For the positron impact excitation of the lowest autoionizing states in rubidium, there are no other theoretical and experimental results to compare the result of Pangantiwar and Srivastava (1987). It is on this basis that we conducted a study on positron impact excitation of the lowest autoionizing levels of rubidium by using DWM, but with variations in the distortion potential such that the initial state static potential serves as the initial channel distortion potential and an average of initial and final state static potentials is taken as
the final channel distortion potential. The wave functions that we considered are the RHF double zeta and multi zeta atomic wave functions (Clementi and Roetti, 1974). Results obtained for positron impact excitation of the $4p^55s^2$ autoionizing state are compared with theoretical results, while those for electron impact excitation of the same state are compared to both theoretical and experimental results available in literature.
CHAPTER 3
THEORETICAL FRAMEWORK

3.1 Approximation methods

Scattering amplitudes and transition matrices cannot be solved exactly since most target wave functions are not exact solutions and they are not orthogonal. Secondly, the Lippmann-Schwinger equation for the total wave function (projectile + target) cannot be solved exactly. To simplify the calculations it is assumed that the target wave functions are orthogonal and approximations are used to substitute for the total wave function. In this study, variations in distortion potential is considered as a method of improving results for scattering amplitudes and cross sections in order to compare with available experimental results.

While numerous works on calculation of reliable scattering amplitudes have been reported over the years using both classical and quantal approaches, most of the effort for electron and positron scattering has focused on the quantal methods (Madison and Bartschat, 1996). Within these approaches, essentially all the works fall either into the close coupling approach category which includes close coupling, R matrix and variational methods or into the category of perturbation series expansions such as Born series, Eikonal series, distorted-wave series and many-body theory. Some of the approximation methods apply both classical and quantal approaches. They are referred to as semi-classical approaches and these include Monte Carlo method, Eikonal approximation, Glauber approximation, S-matrix method amongst others.

In this study, emphasis was given only to the quantum mechanical approaches because of the nature of the problem in context. The approximation methods were chosen depending on the impact energy. For example, at low impact energies, the close coupling approaches are preferred while at intermediate and higher energies, the perturbation series expansion approaches are
preferable since they give results with good agreement to experimental work. Some of these approximation methods are discussed in this chapter. In this study, the DWM under perturbation series expansion was preferred in order to investigate the problem at higher energies up to 1500 eV.

3.2 Close coupling methods

The close-coupling approximation is a standard method for the treatment of low-energy scattering of positrons and electrons from atoms. It is based upon an expansion of the total wave function of the system in terms of a sum of products of eigen states \( \psi \) of the atomic Hamiltonian and unknown functions describing the motion of the projectile. These unknown functions or expansion coefficients are then determined from the solution of a set of coupled integro-differential equations derived from Schrödinger equations (Madison and Bartschat, 1996).

3.2.1 The R-matrix method

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

This is another method of approximating solutions to Schrödinger equation with potentials which are not easily expanded using simple coefficients as of the perturbation theory. The aim of variational methods is to search for solutions of the variational problem among trial functions which depend on a finite number of variational parameters (Joachain, 1975). This method involves guessing the form of trial wave function, for example

\[ \psi = A e^{-\alpha r} \]  

(3.1)

where \( \alpha \) and \( A \) are to be determined. The next step is to normalize the wave function in order to determine \( A \). The energy is determined by the formulation

\[ E = \langle \psi_i | H | \psi_i \rangle \]  

(3.2) and lastly \( \alpha \) is obtained by minimizing \( E \) such that

\[ \frac{dE}{d\alpha} = 0 \]  

(3.3)

As a result, the wave function (3.1) is determined with improved accuracy which is then used in determining scattering amplitudes and cross sections.

3.2.3 The convergent close coupling method

This method attempts to solve close coupled differential equations with much accuracy by utilizing the fact that the complete set of eigen states of the target atom (discrete plus continuum) forms a basis for expanding the three-body projectile-target wave function in terms of a complete set of target atom states. Expanding the Schrodinger equation by means of these target states converts it to an infinite system of coupled equations, which is formidable to solve directly because of the infinite sum over the discrete states and the integration over the continuum.
method treats both discrete and continuum parts of the target space through close coupling which allows its validity to be independent of the projectile energy or transition of interest (Fursa and Bray, 1995). Convergence is tested by including the increasing set of target states in the close coupling formalism. The target states wave functions \( \Phi_{nl} \) and coefficients \( C_{nl} \) are obtained by diagonalizing the target Hamiltonian in the Laguerre basis \( \xi_{nl}(r) \) by the formulation

\[
\langle \Phi_f | H | \Phi_i \rangle = \varepsilon_f \delta_{fi} \tag{3.4}
\]

In equation (3.4)

\[ \delta_{fi} = 0 \text{ for } i \neq f \text{ and } \delta_{fi} = 1 \text{ for } i = f \]

and \( \varepsilon_f \) represents the state energy while

\[
\Phi_{nl} = \sum_{n'} \xi_{nl}(r) C_{n'l} \tag{3.5}
\]

for a one electron atom. The method is suitable only at low projectile impact energies.

### 3.3 Perturbation series expansion approaches

#### 3.3.1 The Born series approximation

To obtain the total wave function of the system of colliding particles (projectile + target), the Lippmann Schwinger equation is considered in the form

\[
+ \hat{\mathcal{I}} r | d r' G_0^{+\hat{\mathcal{I}}}(r, r') U(r') \psi_i^{\hat{\mathcal{I}}} + \hat{\mathcal{I}} r = \exp[i k_i \cdot r] + \int \hat{\mathcal{I}} \psi_i^{\hat{\mathcal{I}}} \tag{3.6}
\]

Here, \( + \hat{\mathcal{I}} \) is the free particle Green’s function and \( U \) is the interaction potential. By iteration starting with the first term on the right hand side, which is the zero order approximation, a sequence of functions can be obtained up to the \( n^{th} \) order.
\[ \psi_0(r) = \Phi_{k_i} |r| = \exp(ik_i \cdot r) \]  
(3.7)

\[ G_0^{*} |r, r'| U(r') \psi_0(r') \, dr' \]
\[ \psi_1(r) = \Phi_{k_i} |r| + \int \cdot \hat{\omega} \]  
(3.8)

\[ G_0^{*} |r, r'| U(r') \psi_{n-1}(r') \, dr' \]
\[ \psi_n(r) = \Phi_{k_i} |r| + \int \cdot \hat{\omega} \]  
(3.9)

The derived wave function is used in determining the scattering amplitude

\[ + \hat{\omega} U + \ldots + \hat{\omega} U G_0^k \]
\[ + \hat{\omega} U + U G_0^k \Phi_{k_i} \]
\[ U + U G_0^k \]
\[ f = -\frac{1}{4\pi} \langle \Phi_{k_i} \hat{\omega} \]  
(3.10)

Scattering amplitude is a power series consisting of the 1st, 2nd… n-th Born approximations.

3.3.2 The Eikonal approximation

The Eikonal approximation is a useful approximation technique when the de Broglie wavelength of the incident particle is sufficiently short compared with the distance in which the potential varies appreciably (Joachain, 1975). The main advantage that the Eikonal approximation offers is that the equations reduce to a differential equation in a single variable. This reduction into a single variable is the result of the straight line approximation or the Eikonal approximation which allows us to choose the straight line as a special direction. Making use of WKB approximation, the wave function of the scattered system is written in terms of action \( S \), for example

\[ \psi = A e^{iS/\hbar} \]  
(3.11)

The wave function is then inserted in Schrödinger’s equation
\[ H\psi = (E - V)\psi \]

(3.12)

S is then written in a power series

\[ S = S_0 + \frac{\hbar}{i} S_1 + \ldots \]

(3.13)

If only straight trajectories are considered such that \( \nabla^2 \rightarrow \delta_z^2 \) and the zeroth order term

\[ (\nabla S_0)^2 = E - V \]

, the Schrödinger equation reduces to a differential equation in one variable.

3.3.3 The distorted wave formula

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

\[ V = U + W \]

(3.14)

The potential \( U \) fits into the Schrödinger equation

\[ |H_0 + U|\chi^\pm = E \chi^\pm \]

(3.15)

Here, \( H_0 \) is the unperturbed Hamiltonian and \( \chi^\pm \) represents distorted wave which represents the wave functions of the projectile and the target in the collision region \(+\) \((\pm)\) represent the outgoing \((\text{incoming})\) boundary conditions. This equation is solved exactly. The transition matrix elements is given as

\[ T_{ij} = \langle \phi_i | U_i + W_i | \psi_j \rangle \]

(3.16)
\( +\hat{\chi}_f \) is the system initial (final) state total wave function and \( \varphi_i(f) \) is a product of the target wave function and projectile plane wave in the initial (final) channel. The wave function \( \chi_f \) with incoming boundary conditions is given as

\[ -\hat{\chi}_f = \left| \varphi_f \right> + \frac{1}{E_f - H_f + i\epsilon} U_f \left| \varphi_f \right> \]  

(3.17)

Equation (3.17) can also be written as

\[ -\hat{\chi}_f \left| \varphi_f \right> \left< \varphi_f \right| U_f \frac{1}{E_f - H_f + i\epsilon} = \left< \varphi_f \right| \chi_f \]  

(3.18)

Substituting (3.14) and (3.18) into (3.14), it can be shown that

\[ \left.< \varphi_f \right| U_f \frac{1}{E_f - H_f + i\epsilon} W_f \left| \psi_i \right> \]  

Similarly the last term in (3.19) can be solved further by considering the relation below

\[ +\hat{\chi}_f = \left| \varphi_f \right> + \frac{1}{E_f - H_f + i\epsilon} V_f \left| \varphi_f \right> \]  

(3.20)

As a result, the term is simplified further as

\[ \left.< \varphi_f \right| U_f \frac{1}{E_f - H_f + i\epsilon} W_f \left| \psi_i \right> \]  

where \( E_f = E_i \) on the energy shell. Using the operator identity relation (3.22) below, (3.21) can be simplified further
\[
\frac{1}{B}(B - A) = \frac{1}{A} - \frac{1}{B}
\]  
(3.22)

Here, \( A = E_f - H + i\varepsilon \) and \( B = E_f - H_f + i\varepsilon \) with \( H - H_f = W_f \) hence,

\[
\left\langle \varphi_f \left| \frac{1}{E_f - H + i\varepsilon} W_f \frac{1}{E_f - H} V_i \right. \right| \varphi_i \right\rangle = \imath
\]

\[
\left\langle \varphi_f \left| \frac{1}{E_f - H + i\varepsilon} V_i \right. \right| \varphi_i \right\rangle = \left\langle \varphi_f \left| \frac{1}{E_f - H_f + i\varepsilon} V_i \right. \right| \varphi_i \right\rangle
\]  
(3.23)  
Combining (3.17) and (3.20),

(3.23) can be written as

\[
\left\langle \varphi_f \left| \frac{1}{E_f - H_f + i\varepsilon} W_f \frac{1}{E_f - H} V_i \right. \right| \varphi_i \right\rangle = \imath
\]

\[
+\imath \right\rangle - \left( \varphi_f \left| U_f \right. \varphi_i \right) - \left( \varphi_f \left| V_i \right. \varphi_i \right) - \left( \varphi_f \left| V_i \right. \varphi_i \right) + \left( \varphi_f \left| V_i \right. \varphi_i \right)
\]

\[
\left\langle \varphi_f \left| U_f \right. \psi_i \right\rangle
\]  
(3.24)

As a result, (3.19) takes the form

\[
-\imath \right\rangle - \left( \varphi_f \left| V_i \right. \varphi_i \right) + \left( \varphi_f \left| U_f \right. \psi_i \right)
\]

\[
+\imath \right\rangle - \left( \varphi_f \left| V_i \right. \varphi_i \right) + \left( \varphi_f \left| U_f \right. \psi_i \right)
\]

\[
-\imath \right\rangle - \left( \varphi_f \left| W_f \right. \varphi_i \right) + \left( \varphi_f \left| W_f \right. \psi_i \right)
\]

\[
+\imath \right\rangle - \left( \varphi_f \left| U_f \right. \psi_i \right)
\]

\[
T_{if} = \left( \varphi_f \left| U_f \right. \psi_i \right)
\]  
(3.25)

But \( V_i = V_f = V_f \) and \( W_f = V_f - U_f \) and \( U_f = V_f - W_f \). As a result the transition matrix simplifies as

\[
+\imath \right\rangle - \imath \right\rangle \right| V_f - U_f \right. \psi_i
\]

\[
-\imath \right\rangle \left. \right| U_f \right. \varphi_i + \left( \chi^i \right)
\]

\[
T_{if} = \left( \chi_i^i \right)
\]  
(3.26)
The above equation for the scattering of a projectile by and N-electron atom can be written as

(when the total wave function $+\hat{\psi}_i^{\beta}$ is written in its antisymmetrized form and $\chi$ is written as product of the projectile and target wave functions)

$$
-\hat{\psi}_i^0 |\varphi_i|_{1,\ldots,N} U_j |\varphi_i|_{1,\ldots,N} |\beta_i| 0 \rangle + \hat{\chi}_i^0 |\varphi_i|_{0,\ldots,N} + \langle \chi_i^0 \\
-\hat{\psi}_i^0 |\varphi_i|_{1,\ldots,N} V |\psi_i|_{A} |\beta_i| 0 \rangle
$$

$$
T_i = (N + 1) \langle \chi_i^0 
$$

where $A$ is the antisymmetrization operator.

3.3.4 The distorted wave series

To obtain the distorted wave series the total wave function is expressed as a product of the initial state distorted wave $+\hat{\chi}^0_i$ and the initial atomic wave functions $\varphi_i$ as

$$
+\hat{\psi}_i^0 = \varphi_i \chi_i^0 \\
\psi_i^0
$$

A power series expansion is then made for the interaction assumed to be small. The initial state distorted wave is a solution to Schrödinger equation

$$
+\hat{\psi}_i^0 = 0 \\
(T + U_i - E_i) \chi_i^0
$$

$E_i$ is the energy of the projectile (positron), $T$ is the Hamiltonian of the isolated projectile and $U_i$ is an arbitrary distorting potential which vanishes asymptotically. The unsymmetrized Lippmann-Schwinger solution for $+\hat{\psi}_i^0$ is given by
The full Green’s function \( \hat{G} \) is given as

\[
+\hat{i}(E - H + i\eta)^{-1} = +\hat{i} + \hat{i}G^i + \hat{i}(V-U)g^i + \hat{i}(V-U)g^i + \hat{i} + \hat{i}g^i + \hat{i} + \hat{i}g^i
\]

The distorted green’s function given as

\[
+\hat{i}(E - H_0 - U + i\eta)^{-1} \quad \text{(3.32)}
\]

\( H \) is the total Hamiltonian of the projectile-target system and \( H_0 \) is a sum of the Hamiltonian of the isolated atom and the isolated projectile. By substituting (3.30) and (3.31) into (3.27), the distorted wave series for the T-matrix can be written as a series consisting of the 1\(^{st}\), 2\(^{nd}\), …, nth order distorted wave approximations. The DWBA1 refers to the 1\(^{st}\) term of the series.

\[
T = T_1 + T_2 + \ldots
\]

(3.33)

The first and second terms are expressed as shown below

\[
T_1 = N + 1 \langle \chi^i_f \rangle
\]

(3.34)
\[ T_2 = (N+1) \langle \chi_f^i \rangle \]

(Madison and Bartschat, 1996)

The application of distorted wave series is discussed further in chapter 4.
CHAPTER 4

RESEARCH METHODOLOGY

4.1 The distorted wave method

We consider the scattering of a positron by a neutral atom. The total Hamiltonian for the system of collisions is expressed as

\[ H = H_o + V \]  

(4.1)

The operator \( H_o \) is a sum of the Hamiltonian for the isolated atom (target) and the isolated projectile, while \( V \) is the interaction potential between the projectile (positron) and the target which is given by

\[ V = \frac{N}{r_o} - \sum_{i=1}^{N} \frac{N}{r_{0i}} \]  

(4.2)

Here, \( N/r_o \) and \( N/r_{0i} \) are the projectile-target nuclear interaction term and the projectile-target electron interaction term respectively. Furthermore, \( r_o \) and \( r_{0i} \) represent magnitudes of the position vector of the projectile from the target nucleus and the displacement vector of the projectile relative to the \( i^{th} \) target electron respectively. The initial-state full scattering wave function \( \psi_i \) is a solution of the Schrödinger’s equation

\[ +i\dot{\psi_i} = 0 \quad \text{subject to} \quad (H - E)\psi_i \]  

(4.3)

The plus (+) sign indicates the outgoing wave boundary conditions. In this case, the projectile positron experiences either elastic or inelastic collisions with \( N \)-electron atom, the exact transition matrix in the two-potential approach as derived in chapter three is given by
\[-\hat{\mathcal{H}} \psi_i \rangle = \hat{\mathcal{H}} \psi_i \rangle \]

\[+ \hat{\mathcal{H}} \psi_i \rangle = \langle \chi_f^\dagger \]

\[-\hat{\mathcal{H}} \psi_i \rangle = \hat{\mathcal{H}} \psi_i \rangle \]

\[T_{fi} = (N+1) \langle \chi_f^\dagger \]

(4.4)

In equation (4.4), \( \varphi_i \) and \( \varphi_f \) are properly antisymmetrized initial and final atomic wave functions for an isolated atom, which diagonalize the atomic Hamiltonian \( h_a \) according to

\[\langle \varphi_n^\prime \left| h_a \right| \varphi_n \rangle = \varepsilon_n \delta_{nn}^\prime.\]

(4.5)

Furthermore \( \beta_i \) is an initial-state plane wave (Madison and Bartschat, 1996)

For inelastic scattering, the second term of equation (4.4) vanishes for orthogonal wave functions (due to orthogonally of the target states) since \( U_f \) depends only on the single co-ordinate of the projectile when taken as some linear combination of the static potentials of target states. For elastic scattering on the other hand, the second term of equation (4.4) is the dominant term; in fact, it is generally the only contribution term since \( U_f \) is typically chosen such that the matrix elements of \( V-U_f \) vanish.

\( A \) is the antisymmetrizing operator for \( N+1 \) electrons. If \( \psi_i \rangle \) is chosen to be a product of a projectile wave function (electron 0) times an antisymmetrized atomic wave function (electrons 1… N), the antisymmetrization operator may be expressed as:

\[A = \frac{1}{N+1} (1- \sum_{i=1}^{N} P_{io}) (4.6) P_{io} \]

is the operator that exchanges electrons 0 and \( i \). \( P_{io} = 0 \) for positron (projectile) impact since electrons and positrons are not identical, that is, they don’t exchange. The potential \( U_f \) in equation (4.4) is an arbitrary distorting potential for the
projectile, which is used to calculate the distorted wave $\chi_f^-$ by solving the equation (4.7) by Numerov’s method (Hairer and Wanner, 1993).

$$-\dot{\psi} = 0 \quad (4.7)$$

$$-\dot{\psi} = \left( \frac{1}{2} \nabla^2 - U_f + \frac{1}{2} k_f^2 \right) \chi_f^- (-) \text{ denotes the incoming wave boundary conditions, } E_f \text{ is the final state energy of the projectile, } T \text{ is the Hamiltonian of the isolated projectile and } k_f \text{ is the final state wave vector for the projectile in atomic units. In the first order distorted wave method (DWBA1), the }$$

$$\psi_i^+ \text{ in equation (4.4) is replaced by } \varphi_i \chi_i^+ \text{ where } \varphi_i \text{ is the initial state target wave function and the projectile wave function } \chi_i^+ \text{ satisfies the equation}$$

$$+\dot{\chi} = 0 \quad (4.8)$$

$$+\dot{\chi} = \left( \frac{1}{2} \nabla^2 - U_i + \frac{1}{2} k_i^2 \right) \chi_i^+ \text{ where } U_i \text{ is the distortion potential in the initial state and } \vec{K}_i \text{ is the incident wave vector. } \chi_i^+ \text{ satisfies the outgoing wave boundary condition.}$$

### 4.2 Discussion of distorting potentials $U_i$ and $U_f$

In principle, $U_i$ and $U_f$ can be any potential as long as $\chi_i^+$ and $\chi_f^-$ fulfill the appropriate boundary conditions. In this study we choose the static potential of the target atom in its initial state as the distorting potential for the initial state of the projectile positron 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 positron. The reason behind these choices is that, in the initial state of the projectile, it only ‘sees’ the initial-state static potential of the target atom,
but when the energy of the projectile is transferred to the atom, it takes some time before the atom goes to its final state. As a result, the projectile in its final state ‘sees’ an intermediate potential between the initial and final state static potentials of the target (Singh, 2004). That is,

\[ U_i = \langle \Phi_i | V | \Phi_i \rangle \]  
(4.9)

\[ U_f = \frac{1}{2} \langle \Phi_i | V | \Phi_i \rangle + \frac{1}{2} \langle \Phi_f | V | \Phi_f \rangle \]  
(4.10)

\( V \) is the interaction potential between the projectile and the target and \( U \) is the distortion potential for the projectile, where subscript \( i \) (\( f \)) represent the initial (final) state of the target. Apart from static potentials, the distortion potentials may include polarization and absorption potentials in order to take care of polarization effects and absorption of particles from the initial channel.

### 4.3 Atomic wave functions

We have used RHF atomic wave functions, both multi zeta (MZ) and double zeta (DZ) functions as given in the Clementi and Roetti (1974) tables. They are based on the RHF expansion technique. The total wave function for an \( N \)-electron system is a Slater determinant given by

\[ \psi \equiv \Lambda (\Phi_1^{(1)} \cdots \Phi_n^{(n)}) \]  
(4.11)

\( A \) is the antisymmetrizing operator and \( n \) is the total number of electrons, while \( \Phi_i^{(j)} \) are the spin orbital which are assumed orthogonal to each other. The orbitals are characterized by an index \( \lambda \), which indicates the symmetry species (\( \lambda \) corresponds to the quantum number \( l \)), by an index \( \alpha \), which indicates the subspecies (the subspecies label the individual members of the degenerate set that transform according to the representation \( \lambda \)) and by an index \( i \), which
refers to the $i^{th}$ orbital of symmetry $\lambda$ (Clementi and Roetti, 1974). Here, tables are presented for exponents for the basis functions and the coefficients to be used in analytic wave functions expanded in the RHF method to obtain the orbital wave functions. The orbital is expanded in terms of basis functions as

$$\Phi_{i\lambda} = \sum_p \chi_{p\lambda} C_{ip}\ldots(4.12)$$

Subscript $p$ refers to the $p^{th}$ basis function of symmetry $\lambda$. The expansion coefficient depends on $i$, $\lambda$ and $p$ but not on the subspecies $\alpha$. The basis functions $\chi$ are Slater-type orbitals with integer quantum numbers, namely

$$\chi_{p\lambda}(r,\theta,\phi) = R_{p\lambda}(r) Y_{\lambda\alpha}(\theta,\phi)\ldots(4.13)$$

The radial part is expressed as;

$$R_{p\lambda}(r) = N r^{n-1} e^{-\zeta r}\ldots(4.14)$$

The normalization factor $N$ takes the form below

$$N = \left(\frac{1}{(2n)!}\right)^{1/2} e^{\frac{1}{2}(2\zeta)^{n+0.5}}\ldots(4.15)$$

Here, $n$, and $\zeta$ represent the principal quantum number and orbital exponent zeta respectively. $Y_{\lambda\alpha}(\theta,\phi)$ are normalized complex spherical harmonics generally expressed as

$$Y_{lm}(\theta,\phi) = (-1)^m \left[\frac{(2l+1)!}{4\pi (l+m)!}\right]^{1/2} P_{lm}(x) e^{i\phi}\ldots(4.16)$$

In equation (4.16), $P_{lm}(x)$ represents the Legendre functions which depend on quantum numbers $l$ and $m$. For Rubidium, the 4p state (initial state), the double zeta wave functions for the radial part as constructed by summing up all $p^{th}$ basis functions given in the atomic data tables of Clementi and Roetti (1974) such that

$$\Phi_{4p} = \sum_p \chi_i C_i$$
\[ \Phi|4p\rangle = 0.00881 \chi_1 + 0.12882 \chi_2 + (-0.24895) \chi_3 + \chi_4 + 0.61394 \chi_5 + 0.51815 \chi_6 \]

(4.17)

In the initial orbital wave function

\[
\begin{align*}
\chi_1 &= N_1 r^1 \exp(-24.49670r) Y_{1,0} \theta \phi, \text{ for } n = 2 \\
\chi_2 &= N_2 r^1 \exp(-15.27970r) Y_{1,0} \theta \phi, \text{ for } n = 2 \\
\chi_3 &= N_3 r^2 \exp(-8.15357r) Y_{1,0} \theta \phi, \text{ for } n = 3 \\
\chi_4 &= N_4 r^2 \exp(-5.54448r) Y_{1,0} \theta \phi, \text{ for } n = 3 \\
\chi_5 &= N_5 r^3 \exp(-3.41258r) Y_{1,0} \theta \phi, \text{ for } n = 4 \\
\chi_6 &= N_6 r^3 \exp(-2.02457r) Y_{1,0} \theta \phi, \text{ for } n = 4
\end{align*}
\]

Furthermore, the normalization constants are:

\[
\begin{align*}
N_1 &= 3429.55939, \quad N_2 = 1053.79574, \quad N_3 = 652.61350, \quad N_4 = 169.21997, \\
N_5 &= 28.23238 \quad \text{and} \quad N_6 = 2.69384, \quad \text{are calculated from equation (4.15)}.
\end{align*}
\]

For the 5s state (final state),

\[
\Phi|5s\rangle = \sum_p \chi_f C_f
\]

\[ \Phi|5s\rangle = 0.00018 \chi_1 + 0.01441 \chi_2 + 0.02387 \chi_3 + (-0.07354) \chi_4 + 0.02451 \chi_5 + 0.08837 \chi_6 + (-0.16671) \chi_7 + (-0.07389) \chi_8 + 0.44807 \chi_9 + 0.65575 \chi_{10} \]

(4.18)

Similarly, in the final orbital wave function

\[
\begin{align*}
\chi_1 &= N_1 r^0 \exp(-38.08620r) Y_{0,0} \theta \phi, \text{ for } n = 1 \\
\chi_2 &= N_2 r^0 \exp(-26.53380r) Y_{0,0} \theta \phi, \text{ for } n = 1 \\
\chi_3 &= N_3 r^1 \exp(-17.71900r) Y_{0,0} \theta \phi, \text{ for } n = 2 \\
\chi_4 &= N_4 r^1 \exp(-15.24460r) Y_{0,0} \theta \phi, \text{ for } n = 2 \\
\chi_5 &= N_5 r^2 \exp(-9.31323r) Y_{0,0} \theta \phi, \text{ for } n = 3
\end{align*}
\]
\[ \chi_6 = N_6 r^2 \exp(-6.76640r) Y_{0,0}(\theta, \varphi), \text{for } n = 3 \]
\[ \chi_7 = N_7 r^3 \exp(-3.88610r) Y_{0,0}(\theta, \varphi), \text{for } n = 4 \]
\[ \chi_8 = N_8 r^3 \exp(-2.52497r) Y_{0,0}(\theta, \varphi), \text{for } n = 4 \]
\[ \chi_9 = N_9 r^4 \exp(-1.38017r) Y_{0,0}(\theta, \varphi), \text{for } n = 5 \]
\[ \chi_{10} = N_{10} r^4 \exp(-0.80400r) Y_{0,0}(\theta, \varphi), \text{for } n = 5 \]

Furthermore, the normalization constants are:
\[ N_1 = 470.09048, \quad N_2 = 273.35635, \quad N_3 = 1526.04517, \quad N_4 = 1047.75430, \]
\[ N_5 = 1039.41717, \quad N_6 = 339.77434, \quad N_7 = 50.66261, \quad N_8 = 7.27826, \quad N_9 = 0.13977, \]
\[ \text{and } N_{10} = 0.00716, \text{ again determined using equation (4.15).} \]

The procedure explained above is for the construction of double zeta functions, which is an approximate RHF function in which a given electron orbital is described by two Slater functions. The same procedure can be used to derive MZ functions, where an electron orbital is described by two or more Slater functions, by adjusting the C, \( \zeta \) and N parameters from the Clementi and Roetti tables.

### 4.4 Evaluation of static potentials \( V_i \) and \( V_f \)

The general mathematical formulae for the average (static) potential \( V_s \) felt by the incident positron in the field of the rubidium atom is (Joachain, 1975)
\[ V_s = \langle \Phi_s | V | \Phi_s \rangle \]
(4.19)

Here, \( \Phi_s \) represents either the ground state target atom wave functions for the initial (i) or the excited final (f) states such that
\[ \Phi_i = \Phi_{4p} = \sum_p C_i \chi_i \]

(4.20)

\[ \Phi_f = \Phi_{5s} = \sum_p C_f \chi_f \]  

(4.21)

\( V \) is the interaction potential between the target and projectile as described in equation (4.2).

In the two potential approach, the interaction takes the form

\[ V = -2 Z_p \left( \frac{1}{r_{o1}} - \frac{Z_N}{r_o} \right) \]  

(4.22)

\( Z_p = +1 \) is the charge of the positron and \( Z_N = 1 \) as the charge of the target nucleus (considering rubidium as one electron atom).

The distorting potentials used in the DWBA1 calculations are spherically symmetric and the effect of the non spherical terms being negligible (Madison et al., 1991).

The static potentials for the initial \( V_i \) and final \( V_f \) states take the form of (4.23) and (4.24).

\[ V_i = \langle \Phi_{4p} | V | \Phi_{4p} \rangle \]  

(4.23)

\[ V_f = \langle \Phi_{5s} | V | \Phi_{5s} \rangle \]  

(4.24)

Substituting the wave functions for the initial (final) states i (f) into (4.23) and (4.24), we get

\[ V_{if} = \sum_n \sum_n C_{i,n} C_{f,n} \langle \chi_{i,n} | V | \chi_{f,n} \rangle \]  

(4.25)

Substituting in equation (4.25) the potential \( V \) as given in equation (4.22), expanding \( 1/r_{o1} \) in terms of spherical harmonics as
\[
\frac{1}{r_{01}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} \frac{r_l^j}{r_{0l}^{l+1}} Y_{lm}^{j} \bar{r}_0 \bar{Y}_{lm}^{j} \bar{r}_1 \tag{4.26}
\]
where \( r_{0l} \) and \( r_{1l} \) are respectively the lesser or greater of the \( r_0 \) and \( r_1 \), and substituting the wave function as given in equation (4.14), we get

\[
V_{ij} = 2 \sum_n \sum_{n'} N_k C_k N_k C_k \int_{r_e}^{r_0} r^{2(n-1)} e^{-(\xi_1 + \xi_2)r(\frac{1}{r_0} - \frac{1}{r})} r^2 dr \tag{4.27}
\]
The static potential is further expanded to obtain

\[
\int_{0}^{r_0} r^{2(n-1)} e^{-(\xi_1 + \xi_2)r(\frac{1}{r_0} - \frac{1}{r})} r^2 dr \tag{4.28}
\]
The integral in equation (4.28) vanishes since in the limit \( r_0 \) is greater than \( r \). The problem reduces to analytically calculating the integrals with respect to \( r \). The analytical solutions to the distortion potential elements for initial and final states are listed below according to the powers of \( r \) under the integral starting from \( r^2 \) when the principal quantum number \( n=1 \) for the atomic wave functions constructed in section (4.3).
### Table 4. Analytical solutions for the distortion potential elements.

<table>
<thead>
<tr>
<th>Term with $r^i$</th>
<th>Corresponding distortion potential elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r^2$</td>
<td>$\frac{\text{ANCO}_2}{r_0 \xi}^3 e^{-\beta(\beta + 2)}$</td>
</tr>
<tr>
<td>$r^3$</td>
<td>$\frac{\text{ANCO}_3}{r_0 \xi^4} e^{-\beta(\beta^2 + 4\beta + 6)}$</td>
</tr>
<tr>
<td>$r^4$</td>
<td>$\frac{\text{ANCO}_4}{r_0 \xi^5} e^{-\beta(\beta^3 + 6\beta^2 + 18\beta + 24)}$</td>
</tr>
<tr>
<td>$r^5$</td>
<td>$\frac{\text{ANCO}_5}{r_0 \xi^6} e^{-\beta(\beta^4 + 8\beta^3 + 36\beta^2 + 96\beta + 120)}$</td>
</tr>
<tr>
<td>$r^6$</td>
<td>$\frac{\text{ANCO}_6}{r_0 \xi^7} e^{-\beta(\beta^5 + 10\beta^4 + 60\beta^3 + 240\beta^2 + 600\beta + 720)}$</td>
</tr>
<tr>
<td>$r^7$</td>
<td>$\frac{\text{ANCO}_7}{r_0 \xi^8} e^{-\beta(\beta^6 + 12\beta^5 + 90\beta^4 + 480\beta^3 + 1800\beta^2 + 4320\beta + 5040)}$</td>
</tr>
<tr>
<td>$r^8$</td>
<td>$\frac{\text{ANCO}_8}{r_0 \xi^9} e^{-\beta(\beta^7 + 14\beta^6 + 126\beta^5 + 840\beta^4 + 4200\beta^3 + 15120\beta^2 + 35280\beta + 40320)}$</td>
</tr>
<tr>
<td>$r^9$</td>
<td>$\frac{\text{ANCO}_9}{r_0 \xi^{10}} e^{-\beta(\beta^8 + 16\beta^7 + 168\beta^6 + 1344\beta^5 + 8400\beta^4 + 40320\beta^3 + 141120\beta^2 + 322560\beta + 362880)}$</td>
</tr>
<tr>
<td>$r^{10}$</td>
<td>$\frac{\text{ANCO}_{10}}{r_0 \xi^{11}} e^{-\beta(\beta^9 + 18\beta^8 + 216\beta^7 + 2016\beta^6 + 15120\beta^5 + 90720\beta^4 + 423360\beta^3 + 1451520\beta^2 + 32}$</td>
</tr>
</tbody>
</table>

In the table above

$\beta = r_0 \xi$

The value $\text{ANCO}_i$ consists of the expansion coefficient $C$ and the normalization factor $N$ obtained from Clementi and Roetti (1974) atomic data tables. For every distortion potential element, the $\text{ANCO}_i$ value is given in tables 2 and 3.
Table 4.. 5s state ANCO values for the distortion potential elements

5s state

<table>
<thead>
<tr>
<th>Term with</th>
<th>Corresponding value of ANCO_i</th>
</tr>
</thead>
<tbody>
<tr>
<td>r^2</td>
<td>((N_1C_1 + N_2C_2)^2)</td>
</tr>
<tr>
<td>r^3</td>
<td>(2(N_1C_1 + N_2C_2)(N_3C_3 + N_4C_4))</td>
</tr>
<tr>
<td>r^4</td>
<td>(2(N_1C_1 + N_2C_2)(N_5C_5 + N_6C_6) + (N_3C_3 + N_4C_4)^2)</td>
</tr>
<tr>
<td>r^5</td>
<td>(2(N_1C_1 + N_2C_2)(N_7C_7 + N_8C_8) + 2(N_3C_3 + N_4C_4)(N_5C_5 + N_6C_6))</td>
</tr>
<tr>
<td>r^6</td>
<td>(2(N_3C_3 + N_4C_4)(N_7C_7 + N_8C_8) + (N_5C_5 + N_6C_6)^2 + 2(N_1C_1 + N_2C_2)(N_9C_9 + N_{10}C_{10}))</td>
</tr>
<tr>
<td>r^7</td>
<td>(2(N_9C_9 + N_{10}C_{10})(N_3C_3 + N_4C_4) + 2(N_5C_5 + N_6C_6)(N_7C_7 + N_8C_8))</td>
</tr>
<tr>
<td>r^8</td>
<td>(2(N_9C_9 + N_{10}C_{10})(N_5C_5 + N_6C_6) + (N_7C_7 + N_8C_8)^2)</td>
</tr>
<tr>
<td>r^9</td>
<td>(2(N_9C_9 + N_{10}C_{10})(N_7C_7 + N_8C_8))</td>
</tr>
<tr>
<td>r^{10}</td>
<td>((N_9C_9 + N_{10}C_{10})^2)</td>
</tr>
</tbody>
</table>

Table 4.. 4p state ANCO values for the distortion potential elements.

4p state

<table>
<thead>
<tr>
<th>Term with</th>
<th>Corresponding value of ANCO_i</th>
</tr>
</thead>
<tbody>
<tr>
<td>r^4</td>
<td>((N_1C_1 + N_2C_2)^2)</td>
</tr>
<tr>
<td>r^5</td>
<td>(2(N_1C_1 + N_2C_2)(N_3C_3 + N_4C_4))</td>
</tr>
<tr>
<td>r^6</td>
<td>(2(N_1C_1 + N_2C_2)(N_5C_5 + N_6C_6) + (N_3C_3 + N_4C_4)^2)</td>
</tr>
<tr>
<td>r^7</td>
<td>(2(N_3C_3 + N_4C_4)(N_5C_5 + N_6C_6))</td>
</tr>
<tr>
<td>r^8</td>
<td>((N_5C_5 + N_6C_6)^2)</td>
</tr>
</tbody>
</table>

All the static potential elements are summed up to get \(V_s\) (the static potential for initial, \(s=i\) and final, \(s=f\) states). The distortion potential elements are fed into the DWBA1 computer code by making adjustments on the relevant subroutine.
4.5 Evaluation of transition matrix elements and cross sections

Generally, the matrices involved are; direct matrix elements and exchange matrix elements, but for positron (\( +\dot{e} \)) projectile, exchange between projectile and target electron does not occur since the particles are not identical. The excitation process for any alkali metal atom \( A \) is expressed as follows (Pangantiwar and Srivastava, 1987):

\[
\begin{align*}
& \begin{pmatrix}
    s \\
    n \ p^6(n+1) \ i \\
    n \ p^5(n+1) \ s^2 \ \ i \\
    e^\pi + A \ i
\end{pmatrix} \\
& n \ p^6 P_{1/2}^{1/2} \ (4.29)
\end{align*}
\]

For rubidium atom whose electronic configuration is \( 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 5s^1 \), \( n=4 \) and we consider the transition \( 4p \to 5s \) and the excitation process for the positron impact excitation of rubidium takes the form

\[
\begin{align*}
& \begin{pmatrix}
    s \\
    4 \ p^6 5 \ i \\
    4 \ p^5 5s^2 \ i \\
    e^\pi + A \ i
\end{pmatrix} \\
& + \dot{\ i} + A \ i
\end{align*}
\]

with the general expression for the transition matrix in the absence of exchange given as

\[
T = \chi^i_f \langle \chi_f\vert \phi_i\rangle \langle r_o\vert V\vert r_o, r_1\rangle \langle \vert r_1\vert \phi_i\rangle \chi^i_i \tag{4.31}
\]

where the projectile positron-target atom interaction is given as:

\[
V\vert r_o, r_1\rangle = \frac{2}{r_o} - \frac{2}{r_{01}}(4.32) r_o \quad \text{and} \quad r_1 \quad \text{are the position vectors of the incident positron and atomic electron undergoing a transition relative to the target nucleus taken as the origin of the center of mass respectively, while} \quad r_{01} \quad \text{is the column vector between the positron and the target}
\]
The wave functions $\varphi_i$ and $\varphi_f$ represents atomic orbitals for the initial and final states.

To evaluate the scattering amplitude given by equation (4.30), the distorted waves $\chi_i$ and $\chi_f$ are first expanded in terms of partial waves as follows:

$$
\chi_i = \sum_l Y_{lm} r^l j_l (k_s r) \left( r^l Y_{lm} k_s r \right)
$$

Here, $Y_{lm}$ is a spherical harmonic. In the expansion of $\chi_f$, the radial distorted wave is taken as complex conjugate so that it satisfies the incoming wave boundary conditions. Substituting (4.33) and (4.34) in equation (4.8) and (4.7) respectively, it can be shown that the radial distorted waves are solutions of the differential equation

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

The radial distorted wave equations are solved by using Numerov’s method (Madison and Bartschat, 1996). Here $s=i$ for the initial state and $s=f$ for the final state distorted waves. In the asymptotic region, they satisfy the boundary condition

$$
\lim_{r \to \infty} \chi_{is} | k_s, r \rangle = j_{ls} + \alpha_l (-\eta_{ls} + ij_{ls})
$$

(4.36)

Here, $j_l$ and $\eta_l$ are regular and irregular Ricatti-Bessel functions (Joachain, 1975), while $\alpha_l = \exp (i \delta_l) \sin \delta_l$ where $\delta_l$ is the elastic scattering phase shift. The differential cross-sections summed over the magnetic sub levels are obtained using the relation
and the DCS for excitation of specific magnetic sublevel $m$ can be obtained as

$$\dot{i} T_{m \rightarrow n} \propto \dot{i}^2 (4.37)$$

$$\left( \frac{d\sigma}{d\Omega} \right)_{m \rightarrow n} = \frac{1}{4\pi^2} \frac{k_f}{k_i} \sum_{m=-1}^{1} \dot{i}$$

The scattering amplitude is given by:

$$f_m(\theta, \phi) = -\frac{1}{2\pi} T_m (4.39)$$

Here, $T_m$ is the transition matrix for the excitation of magnetic sublevel $m$. By summing up the differential cross sections, we obtain the total or integral cross section given by:

$$\sigma = \int_0^{2\pi} \int_0^\pi d\theta d\Omega \sin \theta d\theta d\Phi (4.40)$$

### 4.6 Angular correlation parameters

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

$$\lambda = \frac{\sigma_0(\theta, \phi)}{\sigma_0(\theta, \phi) + 2\sigma_1(\theta, \phi)} (4.41)$$

The R parameter unlike the differential cross sections depends on the phases. This parameter is useful in the prediction of the phases of the amplitude at different scattering angles (Madison, 1991). The R parameter is given by

$$R = \frac{\Re \left( f_0^* f_1 \right)}{\sigma_0(\theta, \phi) + 2\sigma_1(\theta, \phi)} (4.42)$$

The differential cross section $\sigma_m$ for exciting a particular magnetic sublevel $m$ is expressed in terms of a spin average $\langle \rangle$ as
\[ \sigma_m = |f_m^i f_m| = \frac{1}{4} |f_m^S f_m^S + 3 f_m^T f_m^T| \] (4.43) Here, \( \sigma_0(\theta, \phi) + 2 \sigma_1(\theta, \phi) \) is the total differential cross section summed over all magnetic sublevels \( m=0 \) and \( m=1 \). Furthermore, in case of electron impact excitation \( f_m^S \) represents singlet amplitude and \( f_m^T \) represents triplet amplitude for exciting the magnetic sublevel. The total scattering amplitude can be expressed as

\[
f_m = f_m^{direct} + (-1)^S f_m^{exchange} \] (4.44)

In the equation (4.44), \( S \) represents the total spin of incident and atomic electron.

The anisotropy parameter \( \beta \) or the alignment parameter \( A_2 \) of the autoionizing excited state

\[
np^5|n+1\rangle s^2 \cdot \vec{P}_3 \] is such that \( \beta = A_2 = -A_{20} \) (Kaur and Srivastava, 1999)

\[
A_{20} = \frac{\sigma(np_1) - \sigma(np_0)}{\sigma(np_0) + 2\sigma(np_1)} \] (4.45) Here, \( \sigma(np_m) \) is the total cross section of an \( np_m \) electron excited to a \((n+1)s\) state

4.7 Data analysis

The transition matrix elements, target wave functions, cross sections and angular correlation parameters described in chapter 4 have been evaluated using a DWBA1 FORTRAN computer code developed by Madison and Bartschat (1996) for electron-hydrogen scattering. The following modifications have been done to enable us generate data for positron-rubidium scattering:

a) In the main program the 1s-2p transition implying \( s-p \) target electron transition was changed to cater for \( p-s \) transition, that is, \( 4p-5s \). This involved changing angular momentum parameters such as spin, orbital and magnetic quantum numbers for the final state into initial state and initial state parameters into final state.
b) The subroutine FHYD for hydrogen wave functions was modified to generate rubidium wave functions for 4p and 5s states as given in equations (4.17) and (4.18).

c) The subroutine POTENT for hydrogen static potentials was modified to generate static potentials and distortion potentials for rubidium atom as given in tables 4.1, 4.2 and 4.3.

d) The main program has been modified to generate cross sections for energies above 200 eV and to calculate $\lambda$, $R$ and $A_{20}$ (alignment) parameters which take the form of equations (4.41), (4.42) and (4.45).

The version 8 Origin Lab computer software was used for analysis of data which includes generation of graphs of cross sections and angular correlation parameters.
Both DZ and MZ wave functions have been used in this work. The distortion potential is such that the initial state static potential is the initial channel distortion potential while a linear combination of initial and final state static potentials is taken as the final channel distortion potential. We have compared our results with those of Pangantiwar and Srivastava (1987) and Borovik et al. (2012) for electron and positron impact excitation of the lowest autoionizing state of rubidium. The result for Borovik et al. (2012) was obtained through experiment, while the results for Pangantiwar and Srivastava (1987) is a calculation using the distorted wave method where the initial state static potential is the initial channel distortion potential while the final state static potential is the final channel distortion potential.

5.1 Integral cross sections

Integral cross sections for positron and electron impact excitation of the $4p^55s^2$ state of Rb are compared to those in the work of Srivastava and Pangantiwar (1987) and Borovik et al. (2012 a) results with both double zeta (DZ) and multi zeta (MZ) wave functions above threshold energy of 15.73 eV up to 1500 eV. In table 4.4 the present integral cross section results for electron $-e^-$ and positron $+e^+$ impact excitation of the lowest autoionizing state in rubidium atom at various incident energies are given. In the table, DWE means distorted wave calculations with exchange and DWD gives results without exchange.

The present integral cross section results (figure 5.1) results indicate that multi zeta wave functions generate larger cross sections compared to those of double zeta wave functions at all energies. This study also reveals larger cross sections compared multi zeta results in the work of
Srivastava and Pangantiwar (1987) mainly at intermediate energies. This can be attributed to the choice of distortion potential used in this study as described in section 4.2.

At low impact energies up to around 40 eV, all the three integral cross section results for positron impact excitation are in good qualitative agreement, but not at intermediate energies. At higher energies approaching 1000 eV, the cross sections tend towards each other. The disagreement is therefore at intermediate energies.

It is clear (figure 5.2) that the near threshold resonance (sharp increase in cross sections near the threshold excitation energy) for electron impact does not appear for positron impact. This is due to exchange effects between projectile electron and atomic electron during impact. This is not the case for positron impact which do not exchange with electrons during collision. Another reason for the resonance behavior is due to attraction of the electron projectile by the positive nucleus which results in more interaction with target electrons. Unlike electrons, positrons experience a repulsive force from the nucleus once they penetrate the electron cloud, hence less interaction in the atom. Because of this, the near threshold resonance is not observed. The trend for both electron and positron impact total cross sections becomes similar on removing exchange effects (figure 5.3).
Table 5. Present integral cross sections results for electron $\text{e}^-\text{e}^-\text{e}^-$ and positron $\text{e}^+\text{e}^+\text{e}^+$ impact excitation of the lowest autoionizing state in rubidium atom at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>ENERGY(eV)</th>
<th>$\text{e}^-\text{e}^-\text{e}^-$ DWE</th>
<th>$\text{e}^-\text{e}^-\text{e}^-$ DWE-</th>
<th>$\text{e}^+\text{e}^+\text{e}^-$ DWD-</th>
<th>$\text{e}^+\text{e}^+\text{e}^+$ DWD-</th>
<th>$\text{e}^-\text{e}^-\text{e}^-$ DWD-</th>
<th>$\text{e}^+\text{e}^+\text{e}^+$ DWD-</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.8</td>
<td>0.00600</td>
<td>0.00603</td>
<td>0.0001417</td>
<td>0.001343</td>
<td>0.0001343</td>
<td>0.0001343</td>
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<tr>
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<td>0.04200</td>
<td>0.04211</td>
<td>0.0010300</td>
<td>0.0021600</td>
<td>0.0009916</td>
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<td>16.2</td>
<td>0.09302</td>
<td>0.09258</td>
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</tr>
<tr>
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<td>0.17630</td>
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</tr>
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<tr>
<td>18.0</td>
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<td>0.0484900</td>
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<tr>
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<td>0.20050</td>
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<td>0.1122000</td>
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</tr>
<tr>
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<td>0.19500</td>
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<td>0.2570000</td>
<td>0.26820</td>
</tr>
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</tr>
<tr>
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<td>0.2706000</td>
<td>0.26850</td>
</tr>
<tr>
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<td>0.2641000</td>
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</tr>
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</tr>
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</tr>
<tr>
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<tr>
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<tr>
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<td>0.0419000</td>
<td>0.0419000</td>
<td>0.03858</td>
</tr>
</tbody>
</table>
Pangantiwar and Srivastava (1987) Present DZ Present MZ

Figure 5. Integral cross sections results for positron impact excitation of the lowest autoionizing state in rubidium; Pangantiwar and Srivastava (1987) results; present DZ results; present MZ results.
Borovik et al (2012), $e^{i\theta}$

Pangantiwar and Srivastava (1987), $e^{i\theta}$

$-i$ $+i$
Figure 2. Integral cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium; , Borovik et al. (2012 a) electron impact results; , present electron impact DWE-MZ results; , Pangantiwar and Srivastava (1987) electron impact results; , Pangantiwar and Srivastava (1987) positron impact results; , present positron impact MZ results.

Figure 5. Integral cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium; , Borovik et al. (2012 a) electron impact results; , present electron impact DWE-MZ results; , Pangantiwar and Srivastava (1987) electron impact results; , Pangantiwar and Srivastava (1987) positron impact results; , present positron impact MZ results.
Present DWD, $e^{-i\theta}$
Figure 3.  —— present electron dwe-dz results  — present positron-dz results  
—— present electron dwd-dz results

Figure 5. Present Integral cross sections DZ results for electron and positron impact excitation 
of the lowest autoionizing state in rubidium; , DWE electron impact results; , DWD positron 
impact results; , DWD electron impact results.
5.2 Differential cross sections

Present results for positron impact are compared to those of electron impact in this study and that of Pangantiwar and Srivastava (1987) from 20 eV to 600 eV. In tables 5.5 and 5.6, the present ICS results for electron and positron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies are given.

Generally (figures 5.4-5.9), differential cross sections have maximum value at small scattering angles and they reduce as the angles increase. It is also observed that the differential cross sections for positron impact are smaller at larger scattering angles compared to those of electron impact at all energies. More particles are scattered at small scattering angles and less at large angles. A projectile at high incident energy encounters less interaction with the target atom electrons, hence it is scattered at a small angle.

Differential cross sections for electron impact are larger at all angles compared to those of positron impact. This observation is more visible at 20 eV. This is because at energies near excitation threshold, there is more interaction of the projectile electron with the target electrons due to attraction by the positive nucleus compared to larger energies unlike for positrons which experience repulsion in the electron cloud; hence interact less with the target electrons.

Although the differential cross sections at all energies are large at small scattering angles, fewer particles are scattered at high projectile energies compared to those at lower energies. This can be justified by comparing the total area (which actually gives the integral cross section) enclosed by any two curves, at different energies. DCS in this study and the study of Pangantiwar and Srivastava (1987) have a similar trend at different angles even with increase in energy, but slight variations are due to the different type of distortion potential chosen.
Table 5. Present differential cross sections results for electron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>PRESENT ELECTRON IMPACT DIFFERENTIAL CROSS SECTIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>impact energy scattering angle(degrees)</td>
</tr>
<tr>
<td>0</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>20</td>
</tr>
<tr>
<td>30</td>
</tr>
<tr>
<td>40</td>
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<td>80</td>
</tr>
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<td>100</td>
</tr>
<tr>
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<tr>
<td>140</td>
</tr>
<tr>
<td>160</td>
</tr>
<tr>
<td>180</td>
</tr>
</tbody>
</table>

Table 5. Present differential cross sections results for positron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>PRESENT POSITRON IMPACT DIFFERENTIAL CROSS SECTIONS</th>
</tr>
</thead>
<tbody>
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<td>impact energy scattering angle(degrees)</td>
</tr>
<tr>
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</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td></td>
</tr>
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<td>-----</td>
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</tr>
<tr>
<td>30</td>
</tr>
<tr>
<td>40</td>
</tr>
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<td>60</td>
</tr>
<tr>
<td>80</td>
</tr>
<tr>
<td>100</td>
</tr>
<tr>
<td>120</td>
</tr>
<tr>
<td>140</td>
</tr>
</tbody>
</table>

Pangantiwar and Srivastava (1987), $-\frac{1}{\alpha^i}$
Figure 5. Differential cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 20 eV; Pangantiwar and Srivastava (1987) results for electron impact; present electron impact DZ results; present positron impact DZ results.
Figure 5. Differential cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 25 eV; , present electron impact DZ results; , present positron impact DZ results.

Pangantiwar and Srivastava (1987),
Figure 5. Differential cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 30 eV; , Pangantiwar and Srivastava (1987) results for electron impact; , present electron impact DZ results; , present positron impact DZ results.
Figure 5. Differential cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 50 eV; , Pangantiwar and Srivastava (1987) results for electron impact; , present electron impact DZ results; , present positron impact DZ results

Pangantiwar and Srivastava (1987),
Figure 5. Differential cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 100 eV; , Pangantiwar and Srivastava (1987) results for electron impact; , present electron impact DZ results; , present positron impact DZ results
Figure 5. Differential cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 200 eV; , present electron impact results; , present positron impact results.
5.3 Alignment parameter $A_{20}$

The present alignment parameter result is compared with the work of Pangantiwar and Srivastava (1987) for positron impact excitation at an energy range of 0 eV to 1000 eV. Table 5.7 gives present alignment parameter results for electron and positron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies.

The present alignment parameter results for positron impact (figure 5.10) are in good qualitative agreement with the results of Pangantiwar and Srivastava (1987) at almost throughout the energy range of 20-1000 eV. The small difference between the two results can be attributed to the choice of distortion potential.

The present results for positron and electron impact (figure 5.11) disagree at energies near excitation threshold due to high electron interaction and exchange effects. The two results tend to converge at higher energies similar to the results for integral cross sections for electron and positron impact. From the formula for the alignment parameter, if $A_{20}$ is negative, then

$\sigma_0 \gg \sigma_1$ implying that the excited states are aligned more to the magnetic sub-state $m=0$ or this sub-state is largely populated compared to the magnetic sub-state $m=1$. Otherwise $m=1$ is largely populated (see equation 4.45).
Table 5. Present alignment parameter results for electron $-\hat{L}_e$ and positron $+\hat{L}_e$ impact excitation of the lowest autoionizing state in rubidium atom at various incident energies.

<table>
<thead>
<tr>
<th>Energy(eV)</th>
<th>POSITRON DZ</th>
<th>POSITRON MZ</th>
<th>ELECTRON DZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>-0.68982</td>
<td>-0.69533</td>
<td>-0.92910</td>
</tr>
<tr>
<td>30</td>
<td>-0.60179</td>
<td>-0.60639</td>
<td>-0.56000</td>
</tr>
<tr>
<td>40</td>
<td>-0.51960</td>
<td>-0.52451</td>
<td>-0.46890</td>
</tr>
<tr>
<td>50</td>
<td>-0.45655</td>
<td>-0.46189</td>
<td>-0.42280</td>
</tr>
<tr>
<td>60</td>
<td>-0.40578</td>
<td>-0.41142</td>
<td>-0.37840</td>
</tr>
<tr>
<td>69</td>
<td>-0.36687</td>
<td>-0.37265</td>
<td>-0.34110</td>
</tr>
<tr>
<td>90</td>
<td>-0.30011</td>
<td>-0.30612</td>
<td>-0.27520</td>
</tr>
<tr>
<td>100</td>
<td>-0.27613</td>
<td>-0.28220</td>
<td>-0.25178</td>
</tr>
<tr>
<td>200</td>
<td>-0.13505</td>
<td>-0.14103</td>
<td>-0.11670</td>
</tr>
<tr>
<td>300</td>
<td>-0.07244</td>
<td>-0.07799</td>
<td>-0.05742</td>
</tr>
<tr>
<td>400</td>
<td>-0.00715</td>
<td>-0.01213</td>
<td>0.056950</td>
</tr>
<tr>
<td>500</td>
<td>0.04541</td>
<td>0.04118</td>
<td>0.056770</td>
</tr>
<tr>
<td>600</td>
<td>0.09717</td>
<td>0.09343</td>
<td>0.107500</td>
</tr>
<tr>
<td>999</td>
<td>0.25928</td>
<td>0.25708</td>
<td>0.267400</td>
</tr>
</tbody>
</table>

Pangantiwar and Srivastava (1987), 
Alignment parameter results for positron impact excitation of the lowest autoionizing state in rubidium; , present MZ results; , Pangantiwar and Srivastava (1987) results.

Figure 5. Alignment parameter results for positron impact excitation of the lowest autoionizing state in rubidium; , present MZ results; , Pangantiwar and Srivastava (1987) results.
Figure 5. Present alignment parameter results for positron and electron impact excitation of the lowest autoionizing state in rubidium; electron impact DZ results; positron impact DZ results.

5.4 Lambda parameter $\lambda$

Results for lambda parameter are presented at 20 eV, 30 eV, 50 eV and 100 eV projectile energies. Tables 5.8 and 5.9 give present lambda parameter results for electron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies.

Figures 5.12-5.14 show that, apart from the result at 20 eV which is closer to the excitation energy, all other results give a similar trend for positron and electron impact results. The disparity at 20 eV is due to the behavior of electrons to interact more with the target electrons at energies near excitation threshold. At the small and large angles, that is close to $0^\circ$ and $180^\circ$, particles are scattered more to the magnetic sub-state $m=0$ since from the formula (4.41) it is clear that for $\lambda=1$, $\sigma_0 \gg \sigma_1$. At intermediate angles $\sigma_0$ decreases and $\sigma_1$ increases, but still in most cases $\sigma_0 > \sigma_1$ except for 100 eV where $\sigma_0 < \sigma_1$ for $80^\circ$-$160^\circ$ for positron impact (figure 5.15). If $\sigma_0 = \sigma_1$, the value of lambda is approximately 0.3. This happens when the magnetic sub-states are equally populated after excitation. For $\sigma_0 < \sigma_1$, $\lambda < 0.3$. From the
electron impact results at 20 eV, it is clear that scattering is mainly towards the magnetic sub-state $m=0$, but at higher energies, this is not the case.

Table 5.. Present lambda parameter results for electron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>Impact energy (degrees)</th>
<th>20eV</th>
<th>30eV</th>
<th>50eV</th>
<th>100eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>10</td>
<td>0.98387</td>
<td>0.84086</td>
<td>0.58008</td>
<td>0.24819</td>
</tr>
<tr>
<td>20</td>
<td>0.95117</td>
<td>0.58322</td>
<td>0.27976</td>
<td>0.15814</td>
</tr>
<tr>
<td>30</td>
<td>0.92882</td>
<td>0.43995</td>
<td>0.34338</td>
<td>0.58295</td>
</tr>
<tr>
<td>40</td>
<td>0.92506</td>
<td>0.55522</td>
<td>0.75735</td>
<td>0.47172</td>
</tr>
<tr>
<td>60</td>
<td>0.92995</td>
<td>0.84551</td>
<td>0.60480</td>
<td>0.76080</td>
</tr>
<tr>
<td>80</td>
<td>0.82489</td>
<td>0.93797</td>
<td>0.8047</td>
<td>0.41345</td>
</tr>
<tr>
<td>100</td>
<td>0.86239</td>
<td>0.86679</td>
<td>0.61507</td>
<td>0.33729</td>
</tr>
<tr>
<td>120</td>
<td>0.95772</td>
<td>0.27190</td>
<td>0.53717</td>
<td>0.53725</td>
</tr>
<tr>
<td>140</td>
<td>0.98282</td>
<td>0.32344</td>
<td>0.80721</td>
<td>0.71471</td>
</tr>
<tr>
<td>160</td>
<td>0.99562</td>
<td>0.79928</td>
<td>0.95495</td>
<td>0.89591</td>
</tr>
<tr>
<td>180</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 5.. Present lambda parameter results for positron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>Impact energy (degrees)</th>
<th>20eV</th>
<th>30eV</th>
<th>50eV</th>
<th>100eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>10</td>
<td>0.9629</td>
<td>1</td>
<td>0.85145</td>
<td>0.60162</td>
</tr>
<tr>
<td>20</td>
<td>0.8651</td>
<td>2</td>
<td>0.61155</td>
<td>0.34969</td>
</tr>
<tr>
<td>30</td>
<td>0.7296</td>
<td>9</td>
<td>0.43929</td>
<td>0.44468</td>
</tr>
<tr>
<td>40</td>
<td>0.5562</td>
<td>7</td>
<td>0.39723</td>
<td>0.96354</td>
</tr>
<tr>
<td>60</td>
<td>0.2490</td>
<td>1</td>
<td>0.96228</td>
<td>0.88518</td>
</tr>
<tr>
<td>80</td>
<td>0.7739</td>
<td>3</td>
<td>0.96569</td>
<td>0.96352</td>
</tr>
<tr>
<td>100</td>
<td>0.8678</td>
<td>8</td>
<td>0.85708</td>
<td>0.54768</td>
</tr>
</tbody>
</table>
Present lambda parameter results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 20 eV; electron impact results, positron impact results.
Figure 5. Present lambda parameter results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 30eV; electron impact results; positron impact results.
present: electron results

present: positron results

\lambda \text{ at } 50 \text{ eV}
Figure 5. Present lambda parameter results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 50 eV; electron impact results; positron impact results.
5.5 R parameter

Results are presented for R parameter (figures 5.16-5.20) for positron and electron impact excitation of the 4p^55s^2 state of Rb at 20 eV, 40 eV, 80 eV, 100 eV and 200 eV.

Since the R parameter depends on the phases of the amplitudes, it is useful in predicting whether the method is giving correct phases or not if provided with experimental and some accurate theoretical results are available to compare with. Since there are no experimental or theoretical results to compare with, we have presented our results for R parameter for electron and positron impact in the tables 5.10 and 5.11 and in the form of figures 5.16-5.20. Results given in this study for positron and electron impact excitation are not compared, but rather useful for any future experimental or theoretical calculation of R parameter for electron or positron impact excitation of the lowest autoionizing state of rubidium.

<table>
<thead>
<tr>
<th>PRESENT ELECTRON IMPACT DZ RESULTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>impact energy scattering angle(degrees)</td>
</tr>
<tr>
<td>0</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>20</td>
</tr>
<tr>
<td>30</td>
</tr>
<tr>
<td>40</td>
</tr>
<tr>
<td>60</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td>80</td>
</tr>
<tr>
<td>100</td>
</tr>
<tr>
<td>140</td>
</tr>
<tr>
<td>160</td>
</tr>
<tr>
<td>179</td>
</tr>
</tbody>
</table>
Table 5.. Present R parameter results for positron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies of the projectile.

<table>
<thead>
<tr>
<th>impact energy scattering angle(degrees)</th>
<th>20 eV</th>
<th>40 eV</th>
<th>60 eV</th>
<th>80 eV</th>
<th>100 eV</th>
<th>200 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>0.1319</td>
<td>0.3129</td>
<td>-</td>
<td>0.3481</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>20</td>
<td>0.2372</td>
<td>0.3307</td>
<td>0.2777</td>
<td>-</td>
<td>0.2279</td>
<td>0.1865</td>
</tr>
<tr>
<td>30</td>
<td>0.3042</td>
<td>0.2285</td>
<td>0.0476</td>
<td>0.1542</td>
<td>0.2566</td>
<td>0.2557</td>
</tr>
<tr>
<td>40</td>
<td>0.3266</td>
<td>0.0098</td>
<td>0.2408</td>
<td>0.2958</td>
<td>0.2988</td>
<td>0.2141</td>
</tr>
<tr>
<td>60</td>
<td>0.0403</td>
<td>0.1792</td>
<td>0.2296</td>
<td>0.1849</td>
<td>0.0578</td>
<td>0.2627</td>
</tr>
<tr>
<td>80</td>
<td>0.2509</td>
<td>0.0568</td>
<td>0.2128</td>
<td>0.3459</td>
<td>0.1631</td>
<td>0.0438</td>
</tr>
<tr>
<td>100</td>
<td>0.2290</td>
<td>0.3122</td>
<td>0.3316</td>
<td>0.2367</td>
<td>0.1094</td>
<td>-</td>
</tr>
<tr>
<td>140</td>
<td>0.1913</td>
<td>0.2634</td>
<td>0.2207</td>
<td>0.1449</td>
<td>0.0849</td>
<td>0.0193</td>
</tr>
<tr>
<td>160</td>
<td>0.1093</td>
<td>0.1847</td>
<td>0.2100</td>
<td>0.1715</td>
<td>0.0000</td>
<td>0.0731</td>
</tr>
<tr>
<td>179</td>
<td>0.0058</td>
<td>0.0114</td>
<td>0.0183</td>
<td>0.0364</td>
<td>0.2248</td>
<td>0.3021</td>
</tr>
</tbody>
</table>
Figure 5. Present R parameter results for positron and electron impact excitation of the lowest autoionizing state in rubidium at 20 eV; , positron impact results; , electron impact results
Figure 5. Present R parameter results for positron and electron impact excitation of the lowest autoionizing state in rubidium at 40 eV; positron impact results; electron impact results.
Figure 5. Present R parameter results for positron and electron impact excitation of the lowest autoionizing state in rubidium at 80 eV; positron impact results, electron impact results.
Figure 5. Present R parameter results for positron and electron impact excitation of the lowest autoionizing state in rubidium at 100 eV; positron impact results; electron impact results
Figure 5. Present R parameter results for positron and electron impact excitation of the lowest autoionizing state in rubidium at 200 eV; , positron impact results; , electron impact results.
5.6 Summary on results and discussions

For the differential cross sections, lambda parameter and R parameter for positron impact excitation of the $4p^5s^2$ state of Rb, there are no other experimental or theoretical results to compare with; therefore results in this study provide a platform for other workers researching on the same problem to compare their findings. This study also shows the difference in integral cross sections for electron and positron impact excitation results at near threshold and also explains the reason for this difference. The same is done for differential cross sections. The agreement between some of the results in this study and those of Pangantiwar and Srivastava (1987) is due to the use of the distorted wave method in both studies. Different methods of calculating cross sections give different trends in results obtained at different projectile energies.
CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

From this study, the following conclusions have been arrived at:

(i). The DWM integral cross section results for positron impact excitation of the lowest autoionizing state of rubidium obtained in the present study and those of Pangantiwar Srivastava (1987) are in good agreement at near threshold and higher energies, but there is disagreement at intermediate energies; this is not the case for the results of electron impact excitation where at low impact energies these two results are in disagreement.

(ii). The near threshold strong negative ion resonances (due to the existence of an extra electron in the vicinity of the target atom electron cloud which makes the target behave like a negative ion) that appear for electron impact excitation results do not appear in positron impact excitation results due to lack of exchange between target electrons and the projectile positron.

(iii). Low interaction between a positron and the target electrons (due to repulsion by the positive nucleus) is also a reason for the low cross sections in case of positron impact. The charge of the projectile determines the level of interaction in the target atom.

(iv). The choice of distortion potential and wave function, for example MZ and DZ in this study may be regarded as the main cause of disagreement between the present result and result due to Pangantiwar and Srivastava (1987). Theoretical cross sections due to MZ wave functions in this study are generally larger at all energies compared to those of DZ wave functions.
(v). The lambda parameter indicates that more particles are scattered towards the magnetic
sublevel m=0 for electron impact excitation compared to positron impact excitation at
energies close to excitation threshold, for example at 20 eV.

(vi). The alignment parameter results indicate that integral cross sections for m=0 are larger
compared to m=1 up to about 500 eV beyond which \( \sigma_1 > \sigma_0 \)

6.2 Recommendations

The following recommendations may be considered for the purpose of improving results
obtained from this study:

(i). There is need to extend experimental research from electron impact excitation of the
lowest autoionizing state in rubidium to positron impact excitation of the same state in
order to verify the results of this theoretical study.

(ii). There is need for more theoretical calculations on integral cross sections, alignment
parameter, lambda and R parameter on positron impact excitation of the lowest
autoionizing state of rubidium using other quantum mechanical approaches such as the R-
matrix and close coupling convergent methods so as to check which method is giving
good results for the individual magnetic sublevels and predicting correct phase of the
amplitude.

(iii). There is need to include more potential such as the polarization and absorption potential
in the target’s distortion potential in order to check its effect on the cross sections.
(iv). There is need to conduct more research aimed at solving Lippmann Schwinger equation for the projectile and target exactly or with more accuracy in order to improve on the results of this study which is based on approximation.

(v). There is need to include the second term of the distorted wave series DWBA2 to the first term DWBA1 in order to improve results of the distorted wave approximation for the problem of positron impact excitation of the lowest autoionizing state of rubidium.
REFERENCES


