ELASTIC SCATTERING OF ELECTRON BY BARIUM ATOM USING DISTORTED WAVE METHOD

KAGO JAMES NDUNGU (B. Ed (Sc.))

I56/CE/28347/2013

A thesis submitted in partial fulfillment of the requirements for the award of the degree of Master of Science (Physics) in the School of Pure and Applied Sciences of Kenyatta University.

February, 2019
DECLARATION

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

KAGO JAMES NDUNGU  …………………  …………………
(I56/CE/28347/2013)  signature  date

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

PROF. CHANDRA SINGH  …………………  …………………
Signature  date

Department of Physics
Kenyatta University

PROF. JOHN OKUMU  …………………  …………………
Signature  date

Department of Physics
Kenyatta University
DEDICATION

I dedicate this work to my son Lawrance.
ACKNOWLEDGEMENTS

My deepest gratitude and appreciation goes to my supervisor, Prof. C.S. Singh for his unwavering support. Without whose patience and guidance none of this would have happened on schedule, or at all. His experience in the field of atomic collisions was exceedingly beneficial in the success of this work. Thanks to my second supervisor, Prof. J. Okumu for taking an interest in my work. I thank the department of physics, Kenyatta University, for admitting me to the master degree program. I extend my appreciation to my colleague Martin Kimani for his helpful discussions we held and his supportive encouragements. Am highly indebted to my parents Mr. and Mrs. Kago for having given me the education foundation and the desire to aim for the best in life.

Above all, thanks to God without whom this work would not have been successful.
TABLE OF CONTENTS

DECLARATION .................................................................................................................. ii
DEDICATION ...................................................................................................................... iii
ACKNOWLEDGEMENTS ..................................................................................................... iv
TABLE OF CONTENTS ...................................................................................................... v
LIST OF TABLES ................................................................................................................. vii
LIST OF FIGURES ............................................................................................................... viii
ABBREVIATIONS ............................................................................................................. ix
ABSTRACT ........................................................................................................................... x
CHAPTER 1 ......................................................................................................................... 1
INTRODUCTION .................................................................................................................. 1
1.1 Background Of The Study ......................................................................................... 1
1.2 Statement Of The Problem ....................................................................................... 4
1.3 Objectives .................................................................................................................... 4
   1.3.1 General Objective ............................................................................................... 4
   1.3.2 Specific Objectives ............................................................................................. 4
1.4 Rationale For The Study ............................................................................................ 5
CHAPTER 2 ....................................................................................................................... 6
LITERATURE REVIEW ...................................................................................................... 6
2.1 Experimental Studies On Electron-Barium Scattering ................................................. 6
2.2 Theoretical Calculations ............................................................................................ 6
   2.2.1 The Born Approximation .................................................................................. 11
   2.2.2 Coulomb–Projected Born (Cpb) Approximation .............................................. 12
   2.2.3 The R-Matrix Method ...................................................................................... 12
   2.2.4 Convergent Close Coupling (Ccc) Method .................................................... 13
CHAPTER 3 ....................................................................................................................... 10
THEORETICAL BACKGROUND OF APPROXIMATION METHODS .................. 10
3.1 Introduction To Theoretical Methods ........................................................................ 10
3.2 Quantum Mechanical Methods ................................................................................ 11
   3.2.1 The Born Approximation ................................................................................. 11
   3.2.2 Coulomb–Projected Born (Cpb) Approximation ............................................ 12
   3.2.3 The R-Matrix Method ..................................................................................... 12
   3.2.4 Convergent Close Coupling (Ccc) Method .................................................... 13
LIST OF TABLES

Table 4.1: 1s, 2s, 3s, 4s, 5s and 6s radial atomic wave functions for ground state of barium (mclean and mclean, 1981).......................... 33

Table 5.1: Present dwm differential cross section (in $a_0^2/sr$) for elastic scattering of electron by barium atom, at different impact energies. .... 38

Table 5.3: DWM integral cross sections (in $a_0^2$) for elastic scattering of electron by barium atom. ................................................................. 53
LIST OF FIGURES

Figure 1.1: A schematic diagram for atomic scattering ............................................. 2

Figure 5.1: Differential cross section for elastic scattering of electron by barium atom at 10 ev incident energy.)................................................................. 39

Figure 5.2: Differential cross sections for elastic scattering of electron by barium atom at 15 ev incident energy................................................................. 40

Figure 5.3: Differential cross section of elastic scattering of electron by barium atom at 20 ev incident energy................................................................. 41

Figure 5.4: Differential cross sections of elastic scattering of electron by barium atom at 30 ev incident energy................................................................. 42

Figure 5.5: Differential cross sections of elastic scattering of electron by barium atom at 40 ev incident energy................................................................. 43

Figure 5.6: Differential cross sections of elastic scattering of electron by barium atom at 60 ev incident energy................................................................. 44

Figure 5.7: Differential cross sections of elastic scattering of electron by barium atom at 80 ev incident energy................................................................. 45

Figure 5.8: Differential cross section of elastic scattering of electron by barium atom at 100 ev incident energy.............................................................. 46

Figure 5.9: Differential cross sections of elastic scattering of electron by barium atom at 200 ev incident energy.............................................................. 47

Figure 5.10: Integral cross sections for elastic scattering of electron by barium atom................................................................. 54
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CC2</td>
<td>Two-State Close Coupling</td>
</tr>
<tr>
<td>CCC</td>
<td>Convergent Close Coupling</td>
</tr>
<tr>
<td>CCC115</td>
<td>One hundred and fifteen – state Convergent Close Coupling</td>
</tr>
<tr>
<td>CPB</td>
<td>Coulomb Projected Born</td>
</tr>
<tr>
<td>DCS</td>
<td>Differential Cross Section</td>
</tr>
<tr>
<td>DHF</td>
<td>Dirac-Hartree-Fock</td>
</tr>
<tr>
<td>DWM</td>
<td>Distorted Wave Method</td>
</tr>
<tr>
<td>DWBA</td>
<td>Distorted Wave Born Approximation</td>
</tr>
<tr>
<td>DWBA1</td>
<td>e–H inelastic scattering computer program</td>
</tr>
<tr>
<td>eV</td>
<td>electron Volt</td>
</tr>
<tr>
<td>FBA</td>
<td>First Born Approximation</td>
</tr>
<tr>
<td>HFS</td>
<td>Hartree-Fock-Slater</td>
</tr>
<tr>
<td>ICS</td>
<td>Integral Cross Section</td>
</tr>
<tr>
<td>STO</td>
<td>Slater-Type Orbitals</td>
</tr>
</tbody>
</table>
Knowledge of differential and integral cross sections for electron scattering from atoms and molecules is very important for explanation and understanding of electron interaction with matter and for determining dynamics of collision processes. It is also important in the study of astrophysics, plasma physics and laser development. For the past three decades, experimental and theoretical results for electron-barium elastic scattering have been reported however, these results are inconsistent. Theoretical results do not agree with the experimental results and theoretical results do not agree among themselves. In this study the distorted wave method has been applied to calculate the differential and total cross section for elastic scattering of electron by barium atom at electron impact energies of 10-200 eV and a range of scattering angles of (θ) from 0° to 180°. Being an elastic scattering process, both initial and final distortion potentials are taken as static potential of a barium atom in the initial state. The distorted waves are determined by partial wave expansion method by expanding them in terms of spherical harmonics while the radial equation corresponding to distorted waves are evaluated using Numerov method. A computer program DWBA1, for e- H scattering was modified for the process under consideration and used for the above calculation. The results for differential and integral cross section are compared with experimental and theoretical results available. The comparison of the integral cross section results with other theoretical and experimental results shows that the present results are in good qualitative agreement with experimental and most of theoretical results. At lower incident energies 10-20 eV the present DCS are not in satisfactory agreement with the experimental and theoretical results. However at higher incident energies, 30-100 eV the present DCS are in satisfactory agreement with other theoretical and experimental results. So, it can be said the present distorted wave method works well for electron-barium elastic scattering and recommend be extended to metals such as gadolinium and radium.
CHAPTER 1

INTRODUCTION

1.1 Background of the study

Theory of atomic collision is crucial for theoretical as well as experimental studies in atomic physics, in particular cross sections of e\(^{-}\) - Ba scattering are needed for modeling the behavior of Ba vapor lasers, discharge lamps, plasma switches and various ionosphere where Ba has often been used as trace element for diagnostic purpose (Fursa et al., 1999). On the academic side benchmark laboratory cross section are needed for testing various theoretical approximation and calculation methods hoping to predict these cross sections (Fursa et al., 1999).

In the study of atomic collisions a beam of free projectile is made to interact with the target and a detector record the scattered particles in the asymptotic region. A schematic diagram of the experimental arrangement is shown in figure 1.1. After the interaction between the projectile and target, their respective energy configuration may be conserved, this is known as elastic scattering. If exchange of energy between projectile and target occurs, resulting in target excitation, ionization, annihilation or positronium formation, this is an inelastic scattering (Ali and Soding, 1988).

Electron-atom scattering yields differential cross section (DCS) results. The differential cross section is a measure of probability that electrons will be scattered in a given direction specified by the polar and azimuthal angles \(\theta\) and \(\phi\) respectively. Other cross sections such as integral cross section (ICS) may also be calculated from the differential cross section results.
Figure 1.1: A schematic diagram for atomic scattering

In quantum mechanics scattering is described as a probability event. We can only calculate the probability that the particles got scattered into a certain direction, not precise angles of scattering. The aim of electron–atom scattering is to model as accurately as possible the behavior of the electron–atom system in the interaction region, such knowledge is used in the interpretation and prediction of results from electron-atom scattering experiments.

In the early days of atomic scattering experiments, only total cross sections were measured and most theoretical approaches gave results in reasonable agreement with the experimental data, at least for higher energies (Madison and Bartschart, 1996). During this time the first Born approximation (FBA) became very popular due to its ease of calculation. In 1960’s experimental techniques were improved and differential cross section measurement started to be reported, thus experiments
revealed that the FBA was valid only for small angles and further that the angular range over which the FBA was valid decreased with energy of incident projectile. The reason that the FBA gave good results for the total cross section was that its major contribution came from very small scattering angles where the FBA was reliable. For application which are sensitive to large angle differential cross section, theoretical approach superior to FBA were required. As a result a number of theoretical methods have been developed for calculation of cross section including the distorted wave Born approximation DWBA (Joachain, 1975), the close-coupling method (McCarthy and Weigold, 1995) and R-matrix method (Burke and Berrington, 1993).

In the First order DWBA the continuum wave function of incident electron and scattered electron are calculated using some distortion potential. In the close-coupling method, the electron-atom wave function is expanded in terms of known target atom states and unknown scattered electron states. In the R-matrix approach, the electron –atom system is treated as a compound system using atomic structure theory. There is also optical model potential method (Joachain, 1975) which formulates suitable potential in which the incident electron moves while in the interaction region. The Schrödinger’s equation is solved for electron moving in the potential and the solution used to calculate differential cross section. One of the most successful approaches is the distorted wave method. As a result, in this study used the distorted wave method to study elastic scattering of electron from barium atom.
1.2 Statement of the problem

Over the last three decades several theoretical DCS and ICS results for elastic scattering of e\(^{-}\) - Ba scattering at intermediate energies have been reported. The first calculated result were obtained using two state close-coupling (CC2) method (Fabrikant, 1980), later Fursa and Bray (1999) used convergent close coupling method (CCC-115). Also there has been result from relativistic polarized orbital method (Szmytkowski and Sienkiewzc, 1994). Miloshevsky et al. (2000) used phase theory to compute these cross sections. However, no known results on elastic scattering of electron by barium have been reported using distorted wave method (DWM), so it was interesting to see how it works.

1.3 Objectives

1.3.1 General objective

The main objective was to study the elastic scattering of electron by barium atom using the distorted wave method.

1.3.2 Specific objectives

i. To formulate the distorted wave method applied to electron - barium scattering.

ii. To modify the computer program DWBA1 for the calculation.

iii. To calculate the differential cross section (DCS) and integral cross section (ICS) for e\(^{-}\) - Ba elastic scattering at impact energies 10-200 eV.
iv. To compare the result with other available theoretical and experimental results and draw conclusions on the suitability of the DWM for this calculation.

1.4 Rationale for the study

Jensen et al. (1978) used beam-beam configuration experiment technique to measure cross sections for elastic scattering of electron by barium at impact energies of 20, 30, 40, 50, 60, 80 and 100 eV in the $3^\circ$ to $130^\circ$ angular range. However, these results are in serious disagreements with the work of Szmytkowski and Sienkiewicz (1994) where relativistic polarized orbital method was used to calculate the cross sections for electron scattering from barium at impact energies of 15, 20, 30, 40, 60, 80 and 100 eV.

Fursa and Bray (1999) have reported DCS and ICS for electron scattering from barium at impact energies of 15, 20, 30, 50, 60, 80 and 100 eV using convergent close-coupling method (CCC-115). However, the ICS are inconsistent with the results of Adibzadeh and Theodosiou (2004) where the DCS and ICS were computed using partial wave expansion at impact energies of 15, 20, 30, 40 and 60 eV. Since there is a disagreement between theoretical and experimental results and also between theoretical results themselves, this shows there is a gap and further work on the problem is inevitable.
LITERATURE REVIEW

2.1 Experimental studies on electron-barium scattering

There are various data available from experimental results data on e−-Ba elastic scattering at intermediate energies. Jensen et al. (1978) used beam-beam configuration experiment to study the elastic scattering of electron from barium at impact energies of 20, 30, 40, 50, 60, 80 and 100 eV in the 3° to 130° angular range. Wang et al. (1994) measured the elastic cross section for impact energies of 5, 10, 15 and 20 eV at angular range of 3° to 130°. Extrapolations to larger angles were performed using theoretical calculations. When the ICS and momentum transfer cross sections were compared with other experimental and theoretical results, good agreement was found at small angles but significant deviation was found at large angles. Trajmar et al. (1999) were interested in measurement of collision and coherence parameters as well as cross sections associated with an atomic ensemble prepared with an arbitrary in–plane laser geometry and linear polarization (with respect to collision frame) or equivalently with any magnetic sublevel superposition which were obtained at 20 eV impact energy at 10° and 20° scattering angles.

2.2 Theoretical calculations

Fabrikant (1980) have reported DCS for elastic scattering of electron from barium for a few intermediate energies using two state close-coupling method (CC2). The results were found by solving the close coupling equation including the ground state and resonance target state. These results are found to be in good agreement with convergent close coupling (CCC -115) results of Fursa and Bray (1999) and
experimental results of Jensen et al. (1978) and Wang et al. (1994) at impact energies of 20 and 30 eV. However, this agreement is only at small angle but not at intermediate scattering angles. Fursa and Bray (1999) used convergent close coupling (CCC-115) to calculate DCS and ICS at impact energies of 15, 20, 30, 50, 60, 80 and 100 eV. The calculation of barium structure was performed in the non-relativistic LS coupling scheme. For the Ba structure the model of two valence structure electrons above an inert Hartree-Fock core was used. Configuration-Interaction (CI) expansion (for valence electrons) was used to calculate target wave function. These theoretical results are in good agreement with experimental data of Jensen et al. (1978) and Wang et al. (1994). However, these results are in poor agreement with calculations of Szymytkowski and Sienkiewicz (1994) up to 60 eV but relatively good agreement is found at 80 and 100 eV.

Szymytkowski and Sienkiewicz (1994) used relativistic polarized orbital approximation to calculate DCS and ICS and momentum transfer cross sections at impact energies of 15, 20, 30, 40, 60, 80 and 100 eV for all angles. A static part of the projectile target interaction was generated by solving the Dirac-Hartree-Fock (DHF) equation for isolated target and a polarization was obtained by solving the coupled DHF equation for the target perturbed by an electric field. When the results are compared with experimental results it is found that at energies up to 60 eV, DCS differs both in magnitude and shapes from experimental data of Jensen et al. (1978) but quite satisfactorily reproduces shapes of curves measured by Wang et al. (1994). At energies above 80 eV the agreement with result of Jensen et al. (1978) is much more satisfactory.
Miolshevsky et al. (2000) used phase theory to calculate DCS and ICS for e⁻-Ba elastic scattering at impact energies of 15, 20, 30, 40, 60 and 100 eV. The calculation were performed with Hartree-Fock-Slater (HFS) approximation taking into account the polarization effect but excluding exchanges and spin interaction between incident and atomic electron. When their results are compared with experimental data of Jensen et al. (1978) and Wang et al. (1994) satisfactory agreement is seen.

Adibzadeh and Theodosiou (2004) have given a comprehensive result for differential, total and momentum transfer cross section and Sherman function for impact energies of 15, 20, 30, 40 and 60 eV. These results were obtained using standard method of partial wave-expansion in potential scattering and the partial wave phase shift which were obtained by solving the time-independent Dirac-equation. When compared with other experimental and theoretical results, DCS are in good agreement with the results of Wang et al. (1994) and CCC (115) results of Fursa and Bray (1999) but differ from results of Jensen et al. (1978). The ICS are in good agreement with experimental results but are found to be higher than those of CCC (115) results of Fursa and Bray (1999) at intermediate energies.

The study by Kelemen et al. (1995) was concerned with elastic scattering in the energy range up to 200 eV. Using phenomenological complex optical potential they calculated DCS for elastic electron–barium scattering at energies below the inelastic threshold and integral elastic cross section in the whole energy region up to 200 eV. Their results were found to be in agreement with experimental results of Jensen et al. (1978)
Kumar et al. (1994) employed semi-relativistic approach to compute the DCS, ICS, spin polarization P and spin polarization parameters T and U for electron scattering from barium atom in the energy range 2-300 eV. The projectile target interaction was represented both by real potential and complex potential in the solution of Dirac equation for scattered electrons. The real optical potential included the static, a parameter free correlation polarization and a modified semi classical exchange potentials. The complex optical potential was constructed by adding a model absorption potential as its imaginary part to the real optical potential.

2.3 Summary of review

From the above it is clear that so far no study can claim to be in perfect agreement with other results at intermediate and high energy region. It is on this basis that a study of electron-barium elastic scattering using distorted wave method has been conducted. This study employs static potential of barium atom at ground state as the distortion potential. The wave functions that have been used are Roothan-Hartree-Fock (RHF) double zeta wave functions (McLean and McLean, 1981). The results obtained have been compared with available experimental and theoretical results.
CHAPTER 3

THEORETICAL BACKGROUND OF APPROXIMATION METHODS

3.1 Introduction to theoretical methods

Due to the demand for the atomic collision data set in various fields of physics, various experimental techniques and theoretical approaches have been developed in order to get reliable data sets for atomic collision processes. Theoretical approaches to scattering are either classified as quantum mechanical approaches or semi-classical approaches. Quantum approaches which use the principle of quantum mechanics exclusively are further classified as perturbative methods and close coupling methods. The latter is based on close coupling techniques that expand trial wave functions. Some of the close coupling methods include convergent close coupling and the R-matrix methods. Perturbative methods are based on Born series expansion and examples include First Born approximation, eikonal Born series, Coulomb Projected Born approximation, many body theory and the Distorted wave series.

The semi-classical methods use the principles borrowed from both classical and quantum mechanics. Some methods in this category include Glauber approximation, the method of Crother and McCarrol, the impact parameters method, eikonal approximation, classical trajectory and Monte Carlo method. In this chapter some of the quantum approaches have been briefly discussed in section 3.2.
3.2 Quantum mechanical methods

3.2.1 The Born approximation

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

\[
f = -\frac{1}{4\pi} \left( \psi_{k_f} \left| U + U G_0^+ U + U G_0^+ U G_0^+ U + \ldots \right| \psi_{k_i} \right)
\]  

(3.1)

Here \( \psi_{k_f} \) is the product final plane wave \( e^{i k_f r} \) of the projectile and the final target wave function \( \phi_f \).

\( \psi_{k_i} \) is the product of the initial plane wave \( e^{i k_i r} \) of the incident particle and the initial atomic wave function \( \phi_i \). U is the interaction potential and the function \( G_0^+ \) is outgoing Green’s function given as

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

(3.2)

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

\[
f_{B1} = -\frac{1}{4\pi} \left( \psi_{k_f} \left| U \psi_{k_i} \right| \right)
\]  

(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 short duration and the projectiles waves (incident and scattered) can be approximated as plane waves (Joachain, 1975).
3.2.2 Coulomb –Projected Born (CPB) approximation

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

3.2.3 The R-Matrix method

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

3.2.4 Convergent close coupling (CCC) method

This method is suitable for elastic and inelastic scattering at lower impact energies of the projectile. The CCC method relies on close coupling formalism for solving the coupled equation without approximations. The convergence is tested by including the 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 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 transition of interest (Fursa and Bray, 1999).

3.2.5 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 target particles by an optical potential or pseudo potential in which the incident particles moves. Once the optical potential is determined, the original many-body problem reduces to one body problem. However, this reduction is in general a difficult task and approximations are necessary (Joachain, 1975).
3.2.6 The Distorted wave methods (DWM)

Distorted wave methods were introduced because the Born approximation failed to give accurate account of differential cross section for low impact energies and large scattering angles. In the distorted wave approximation, the incident electron is taken to be elastically scattered by the initial state atomic potential. If the scattering is through direct process, the incident electron makes a transition to a state in which it is being elastically scattered by the final state atomic potential. If the scattering of electron is through the exchange process, the incident electron is captured into a bound state of the atom, while one of the initially bound electrons is ejected. In this case, the transition between the initial and final state is calculated by perturbation method. It is suitable for calculation of differential cross section for electron scattering by atoms at intermediate and high incident energies (Itikawa, 1986).

Distorted wave methods have been one of the most successful perturbative methods used. Their advantage lies in the leading term of the perturbation series expansion such that the distorted wave series converges faster than Born series. Distorted wave methods can not only be applied to electron-atom elastic and inelastic scattering but they can also 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 they are quite successful in explaining various features of collision process (Katiyar and Srivastava, 1989). However, their limitation is that they give poor results at lower energies. Distorted wave methods are more conveniently discussed within the framework of the two-potential formalism discussed in the following section.
3.2.6.1 Distorted wave formula using two-potential scattering model

In this section, the distorted wave method is discussed within the framework of a two potential formalism. The total Hamiltonian for the projectile is written as

\[ H = H_0 + V \]  \hspace{1cm} (3.4)

where \( V \) is the interaction potential between the projectile and the target. \( H_0 \) is the unperturbed Hamiltonian of the target atom and the non-interacting projectile. In the two potential formalism the interaction potential is broken in a physically meaningful way in two parts: one which is treated exactly \( (U_s) \), and the other which is handled in an approximate way \( (W_s) \) (Joachain, 1975). That is,

\[ V_s = W_s + U_s \]  \hspace{1cm} (3.5)

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

\[ (H_0 + U)\chi^\pm = E\chi^\pm \]  \hspace{1cm} (3.6)

can be solved exactly. \( \chi \) is the product of target wave function and 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,

\[ T_{if} = \langle \phi_f | V_f | \Psi_i^+ \rangle \]  \hspace{1cm} (3.7)

where \( \phi_f \) is the product of final target wave function and final plane wave of the projectile in the asymptotic region and \( \Psi_i^+ \) is the total wave function of the system satisfying this Schrödinger equation.
Making use of equation (3.2.5), equation (3.2.7) can be written as

\[ T_{if} = \langle \phi_f | U_s + W_s | \Psi_i^+ \rangle \]  

(3.9)

Since

\[ |\chi_f^-\rangle = |\phi_f\rangle + \frac{1}{E_f-H_f-i\varepsilon} U_f |\phi_f\rangle \]  

(3.10)

where \( H_f = H_0 + U_f \) and this Hamiltonian, it can be written as

\[ \langle \phi_f | = \langle \chi_f^- | - \langle \phi_f | U_f \frac{1}{E_f-H_f+i\varepsilon} \]  

(3.11)

Expanding equation (3.9) and making use of equation (3.11), the transition matrix elements can be written as,

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

(3.12)

The third term of (3.12) can be transformed using the relation

\[ |\Psi_i^+\rangle = |\phi_i\rangle + \frac{1}{E_i-H_f+i\varepsilon} V_i |\phi_i\rangle \]  

(3.13)

where \( \phi_i \) is the product of the initial atomic wave function and the initial plane wave for the projectile, as (on the energy shell \( E=E_i = E_f \))

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

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

(3.14)
And further making use of equation (3.11), equation (3.14) can be written as,

\[
\langle \phi_f | U_f \frac{1}{E-H_f+i\epsilon} W_f | \Psi_i^+ \rangle = (\chi_f^- | W_f | \phi_i) - \langle \phi_f | W_f | \phi_i \rangle + \langle \phi_f | U_f \frac{1}{E-H_f+i\epsilon} W_f \frac{1}{E-H+i\epsilon} V_i | \phi_i \rangle
\]  \quad (3.15)

Making use of operator identity

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

where A=E − H + iε and B=E − H_f + iε and recalling that H − H_f = W_f, then

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

\[
-\langle \phi_f | U_f \frac{1}{E-H_f+i\epsilon} V_i | \phi_i \rangle
\]  \quad (3.16)

Using equations (3.11) and (3.13), equation (3.16) can be written as

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

\[
-\langle \chi_f^- | V_i | \phi_i \rangle + \langle \phi_f | V_i | \phi_i \rangle
\]  \quad (3.17)

Substituting equations (3.15) and (3.17) in equation (3.12), we get

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

Using the fact that on the energy shell

\[
\langle \phi_f | U_f + W_f | \phi_i \rangle = \langle \phi_f | V_i | \phi_i \rangle = \langle \phi_f | V_i | \phi_i \rangle
\]
Equation (3.18) can be written as

\[ T_{if} = \langle \chi_f^- | V_i - W_f | \phi_i \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle \]  

(3.19)

This is the two potential formula of Gellmann and Goldberger (Joachain, 1975).

When \( V_i = V_f = V \) and \( W_f = V - U_f \) are taken, the T-matrix can be written as

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

(3.20)
CHAPTER 4

MATERIALS AND METHODS

4.1 Application of distorted wave formula to electron–barium scattering

Total Hamiltonian, $H$, for electron–barium scattering is given as,

$$H = H_a + T + V$$  \hspace{1cm} (4.1)

where $H_a$ is the Hamiltonian of the isolated atom, $T$ the Hamiltonian for the projectile electron (kinetic energy operator) and $V$ is the interaction between the projectile and atom, given as (in atomic units)

$$V = \frac{-z}{r_0} + \sum_{i=1}^{z} \frac{1}{r_{0i}}$$  \hspace{1cm} (4.2)

where $z$ is the atomic number of the atom, $r_0$ is the position coordinate of the projectile electron from the nucleus of the target and $r_{0i}$ is the position coordinate of the projectile relative to $i$th atomic electron.

The initial state full scattering wave function $\Psi_i^+$, representing the projectile-atom is a solution of Schrödinger equation.

$$(H - E)\Psi_i^+ = 0$$  \hspace{1cm} (4.3)

where the (+) superscript indicates the outgoing wave boundary conditions.

The T-matrix for electron-target (N-electron atom) collision in two potential approach is given as (Madison and Bartschat, 1996).
(when the total wave function $\Psi_i^+$ is written in the antisymmetrized form and $\chi$ is written as the product of the projectile and target wave functions, equation (3.20) obtained in the previous chapter takes this form)

$$T_{if} = (N + 1)\langle \chi_f^-(0)\psi_f(1, \ldots, N) | V - U_f | A\Psi_i^+(0, \ldots, N) \rangle$$

$$+ \langle \chi_f^-(0)\psi_f(1, \ldots, N) | U_f | \psi_i(1, \ldots, N) \beta_i(0) \rangle$$  \hspace{1cm} (4.4)

where $\beta_i$ is the initial plane wave given as,

$$\beta_i = exp(ik.r_o)$$  \hspace{1cm} (4.5)

$\psi_i$ and $\psi_f$ are the initial and final wave functions of the barium atom respectively. $A$ is the antisymmetrization operator for the electron-atom system which may be expressed as,

$$A = \frac{1}{N+1}(1 - \sum_{i=1}^{N} P_{i0})$$  \hspace{1cm} (4.6)

where $P_{i0}$ is the operator that exchanges the $i^{th}$ atomic electron with incident electron (denoted by 0).

$\chi_f^-$ is the distorted wave (distorted by distortion potential $U_f$) satisfying incoming wave boundary condition and is a solution of the wave equation

$$\left(\nabla_0^2 + U_f - k_f^2\right)\chi_f^- = 0$$  \hspace{1cm} (4.7)

$k_f$ is the final state wave vector of projectile electron ($k_f^2$ gives kinetic energy (in Rydberg) of projectile in final state).
$U_f$ is an arbitrary potential (which is generally chosen as a static potential of the target) for distortion of the final projectile electron wavefunction.

The value of $\Psi_i^+$ in (4.3) cannot be evaluated exactly and hence need for more approximation. Its value is expressed in terms of product of initial state distorted wave $\chi_i^+$ times an initial atomic wave function $\psi_i$. That is,

$$\Psi_i^+(0, 1, \ldots N) = \psi_i(1, 2, \ldots N)\chi_i^+(0)$$ (4.8)

where $\chi_i^+$ is the distorted wave function representing the projectile electron in the initial state and is solution to wave equation

$$(\nabla_0^2 + U_i - k_i^2)\chi_i^+ = 0$$ (4.9)

The Lippmann-Schwinger solution for $\Psi_i^+$ in terms of $\chi_i^+$ is given by

$$\Psi_i^+ = [1 + G^+ (V - U)]\psi_i\chi_i^+$$ (4.10)

where $G^+$ is the Green’s function having the form

$$G^+ = (E - H + i\varepsilon)^{-1}$$ (4.11)

Introducing a third arbitrary potential $U$ and hence the Green’s function in the form

$$g^+ = (E - H_a - T - U + i\eta)^{-1}$$ (4.12)

associated with potential, the full Green’s function $G^+$ may be expressed in terms of the distorted Green’s function as

$$G^+ = g^+ + G^+ (V - U) g^+$$ (4.13)

Equation (4.13) can be iterated to obtain the series expansion for full Green’s function as
If the Lippmann-Schwinger solution (4.10) is substituted in (4.3) along with Green’s function expansion (4.1.14) we get

\[ T_{if} = T_1 + T_2 + T_3 + \ldots \] \hspace{1cm} (4.15)

where

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

\[ + \langle \chi_f^- (0) | \psi_f (1, \ldots N) | U_f | \psi_i (1, \ldots N) \beta_i (0) \rangle \] \hspace{1cm} (4.16)

\[ T_2 = (N + 1) \langle \chi_f^- (0) | \psi_f (1, \ldots N) | A g^+ (V - U_i) | \psi_i (1, \ldots N) \chi_i^+ (0) \rangle \] \hspace{1cm} (4.17)

and

\[ T_3 = (N + 1) \langle \chi_f^- (0) | \psi_f (1, \ldots N) | V - U_f \rangle \]

\[ A g^+ (V - U_i) g^+ (V - U_i) | \psi_i (1, \ldots N) \chi_i^+ (0) \rangle \] \hspace{1cm} (4.18)

Equation (4.15) is the distorted wave series for the T-matrix while (4.16) is the first order distorted wave approximation (DWBA1).

Within the above frame work (DWBA1) one is able to calculate the expressions for direct and exchange- matrices.

For a case of the elastic scattering for two electron atom (when considering the two valence electrons of atom in the collision process) we get
\[ T_{if} = T^d - T^{ex} \tag{4.19} \]

where direct matrix

\[ T^d = \langle \chi_f^- (0) \psi_i (1, 2) | U_f | \psi_i (1, 2) \beta_i (0) \rangle \tag{4.20} \]

and exchange matrix

\[ T^{ex} = -\langle \chi_f^- (0) \psi_i (1, 2) | V - U_f | \psi_i (0, 2) \chi_i^+ (1) + \psi_i (1, 0) \chi_i^+ (2) \rangle \tag{4.21} \]

Since \( \psi_i = \psi_f \) the first term in equation (4.6) vanishes for direct scattering. When making calculations we are going to neglect the term associated with \( U_f \) in \( T^{ex} \), assuming that the overlap integral between the bound state and distorted wave will be negligible because of oscillatory nature of distorted wave. The \( T^{ex} \) then takes the form

\[ T^{ex} = -\langle \chi_f^- (0) \psi_f (1, 2) | V | \psi_i (0, 2) \chi_i^+ (1) + \psi_i (1, 0) \chi_i^+ (2) \rangle \tag{4.22} \]

### 4.2 The distorted wave

The distorted wave \( \chi_i^+ \) and \( \chi_f^- \) for projectile in the initial and final states are expanded in terms of partial waves (Singh, 2005), as

\[ | \chi_i^+ \rangle = \frac{2}{\pi k_i r} \sum_{l_i m_i} i^{l_i} \chi_{l_i} (k_i, r) Y_{l_i m_i} (\hat{r}) Y_{l_i m_i}^* (\hat{k}_i) \tag{4.23} \]

and

\[ | \chi_f^- \rangle = \frac{2}{\pi k_f r} \sum_{l_f m_f} i^{l_f} \chi_{l_f}^* (k_f, r) Y_{l_f m_f} (\hat{r}) Y_{l_f m_f}^* (\hat{k}_f) \tag{4.24} \]
where \( Y_{lm} \) are spherical harmonics and \( \hat{r} \) and \( \hat{k} \) are unit vectors denoting the direction of \( r \) and \( k \). In the expansion of \( \chi_f^r \) the complex conjugate of radial part is taken so that it satisfies the incoming wave boundary condition.

Substituting (4.23) and (4.24) into equations (4.7) and (4.9) respectively we find that the radial distorted waves are solutions of the following equation,

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

(4.25)

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

\[
\lim_{r \to \infty} \chi_l(s,k_s,r) = j_l - \eta_l j_l + B_l \eta_l i j_l
\]  

(4.26)

where \( j_l \) and \( \eta_l \) are regular and irregular Riccati-Bessel functions and \( B_l \) is given as,

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

(4.27)

where \( \delta_l \) is elastic scattering phase shift.

4.3 Differential cross section (DCS) and integral cross section (ICS)

The radial distorted wave equations (4.23) for initial and final states was solved using Numerov method (Madison and Bartschart, 1996) and differential cross section was obtained using the relation,

\[
\frac{d\sigma}{d\Omega} = 4\pi^4 \frac{k_f}{k_l} \left| T^d - T^{ex} \right|^2
\]  

(4.28)

The integral cross section, \( \sigma \) was obtained by using the formula
\[ \sigma = \int \frac{d\sigma}{d\Omega} d\Omega = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin \theta d\theta \] (4.29)

4.4 Distortion potential

4.4.1 Introduction

Since elastic scattering is being considered, both the initial and final distortion potential were taken as static potential of a barium atom in the initial state, that is,

\[ U_i = U_f = \langle \psi_i | V | \psi_i \rangle \] (4.30)

where \( U_i \) and \( U_f \) are initial and final distortion potentials respectively.

4.4.2 Evaluation of static potential

The mathematical formulation of static potential is generally expressed as

\[ U_s = \langle \psi_s | V | \psi_s \rangle \] (4.31)

where \( \psi_s \) is target wave function, \( s=i \) or \( f \) for initial or final state respectively and \( V \) is the interaction between the projectile and the target. For the target state we have used the Roothan–Hartree-fock wave functions compiled by McLean and McLean (1981).

Since we are considering a target with two electrons,

\[ \psi_s = \psi_0(r_1)\psi_0(r_2) \] (4.32)

and

\[ V = \frac{2}{r_{01}} + \frac{2}{r_{02}} - \frac{4}{r_0} \text{ (in Rydberg units) } \] (4.33)

Using (4.32) and (4.33) in (4.31) we can now write the distortion potential as,
\[ U_s = \left( \psi_0(r_1)\psi_0(r_2) \right) \frac{2}{r_{01}} + \frac{2}{r_{02}} - \frac{4}{r_0} \left[ \psi_0(r_1)\psi_0(r_2) \right] \]  

\text{(4.34)}

Equation (4.34) simplifies to

\[ U_s = 2 \left( \psi_0(r_1) \left| \frac{2}{r_{01}} \right| \psi_0(r_1) \right) - \left( \psi_0(r_1) \left| \frac{4}{r_{01}} \right| \psi_0(r_1) \right) \]  

\text{(4.35)}

Equation (4.35) can now be written as,

\[ U_s = 4 \left( \psi_0 \left| \frac{1}{r_{01}} - \frac{1}{r_0} \right| \psi_0 \right) \]  

\text{(4.36)}

The wave function \( \psi_s \) is summed up over slater type orbitals of the basis set as,

\[ |\psi_0\rangle = \sum_n C_n |\phi_n\rangle \]  

\text{(4.37)}

and

\[ \langle \psi_0 | = \sum_{n'} C_{n'}^* \langle \phi_{n'} | \]  

\text{(4.38)}

The values of \( C_n \) represent the expansion coefficient and \( \phi_n \) are the slater type orbitals of the basis set. Using equations (4.37) and (4.38) in equation (4.36) we can now write the distortion potential as,

\[ U_s = 4 \sum_n \sum_{n'} C_n C_{n'}^* \left( \phi_{n'} \right| \frac{1}{r_{01}} - \frac{1}{r_0} | \phi_n \rangle \]  

\text{(4.39)}

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

\[ \frac{1}{r_{01}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{\sqrt{2l+1} r_0^l}{2l+1 r_0^{l+1}} Y_{l,m}(\hat{r}_0) Y_{l,m}^*(\hat{r}_1) \]  

\text{(4.40)}
where \( r < (r >) \) is lesser (greater) between \( r_0 \) and \( r_1 \). Since in our elastic scattering calculation the state involved is the s state, using equation (4.39) and (4.40) the static potential can be written as,

\[
U_s = 4 \sum_n \sum_{n'} C_n C_{n'} \left( \frac{\phi_{n'}}{r} - \frac{1}{r_0} \right) \phi_n \tag{4.41}
\]

From McLean and McLean (1981) tables, the Slater type orbitals are expressed as product of radial function and spherical harmonics \( Y_{l,m} \) and are given as,

\[
\phi_n = N_n r^{\mu_n - 1} \exp(-\xi r) Y_{l,m}(r) \tag{4.42}
\]

where \( \mu_n \) is the principle quantum number of the \( n^{th} \) orbital of the basis set, \( \xi \) is orbital exponent and the normalization factor \( N_n \) of the orbital is given as,

\[
N_n = ((2\mu_n)!)^{-\frac{1}{2}} \left( 2\xi \right)^{\mu_n + \frac{3}{2}} \tag{4.43}
\]

Substituting the value of the wave function given by equation (4.42) and replacing the bra and the ket notation with standard integrals, the static potential can be fully expanded as,

\[
U_s = 4 \sum_{nlm} \sum_{n'l'm'} C_n C_{n'}^* N_n N_{n'}^* \int_{r_0}^{\infty} r_1^{\mu_n + \mu_{n'}} \left( \frac{1}{r_1} - \frac{1}{r_0} \right) \exp(-[\xi_n + \xi_{n'}]r_1) dr_1 Y_{lm}(r_0)Y_{l'm'}^*(r_1) \tag{4.44}
\]

In getting equation (4.44) from (4.41), partial integration of radial component is used such that from the radial distance 0 to \( r_0 \), \( r_0 \) considered to be greater than \( r_1 \) while from \( r_0 \) to infinity, \( r_1 \) is considered to be greater than \( r_0 \). Since the spherical harmonics are orthonormal, the last integral on the right hand side of equation (4.44) vanishes unless \( l = l' \) and \( m = m' \).
Therefore, the distortion potential in effect reduces to,

\[
U_s = 4 \sum_n \sum'_{n'} C_n C_n' N_n N_n' \sum_{r_1} \sum_{r_2} C_n C_n' N_n N_n' \int_{r_0}^{\infty} \mu_n + \mu_n' \left( \frac{1}{r_1} - \frac{1}{r_0} \right) \exp \left( -[\xi_n + \xi_n'] r_1 \right) d r_1
\] (4.45)

In this study the integral was evaluated analytically to obtain the exact static potential which has been used as the distortion potentials. It can be easily seen that the static potential is summation of all the elements of a nxn matrix. The analytical solution of each element of equation (4.45) varies in form depending on the sum of principle quantum numbers, \(\mu_n\) and \(\mu_n'\). This sum varies between 2 and 12 for the problem that was solved as follows

For \(r^2\)

\[
\int_{r_0}^{\infty} e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^2 dr
= -e^{-kr_0} \left[ \frac{1}{k^2} + \frac{2}{k^3 r_0} \right]
\] (4.46)

For \(r^3\)

\[
\int_{r_0}^{\infty} e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^3 dr
= -e^{-kr_0} \left[ \frac{r_0}{k^2} + \frac{4}{k^3} + \frac{6}{k^4 r_0} \right]
\] (4.47)

For \(r^4\)
\[ \int_{r_0}^\infty e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^4 \, dr \]

\[ = -e^{-kr_0} \left[ \frac{r_0^2}{k^2} + \frac{6r_0}{k^3} + \frac{18}{k^4} + \frac{24}{k^5 r_0} \right] \quad (4.48) \]

For \( r^5 \)

\[ \int_{r_0}^\infty e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^5 \, dr \]

\[ = -e^{-kr_0} \left[ \frac{r_0^3}{k^2} + \frac{8r_0^2}{k^3} + \frac{36r_0}{k^4} + \frac{96}{k^5} + \frac{120}{k^6 r_0} \right] \quad (4.49) \]

For \( r^6 \)

\[ \int_{r_0}^\infty e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^6 \, dr \]

\[ = -e^{-kr_0} \left[ \frac{r_0^4}{k^2} + \frac{10r_0^3}{k^3} + \frac{60r_0^2}{k^4} + \frac{120r_0}{k^5} + \frac{600}{k^6} + \frac{720}{k^7 r_0} \right] \quad (4.50) \]

For \( r^7 \)

\[ \int_{r_0}^\infty e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^7 \, dr \]

\[ = -e^{-kr_0} \left[ \frac{r_0^5}{k^2} + \frac{12r_0^4}{k^3} + \frac{90r_0^3}{k^4} + \frac{480r_0^2}{k^5} + \frac{1800r_0}{k^6} + \frac{4320}{k^7} + \frac{5040}{k^8 r_0} \right] \quad (4.51) \]

For \( r^8 \)

\[ \int_{r_0}^\infty e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^8 \, dr \]
\[ -e^{-kr_0} \left[ \frac{r_0^6}{k^2} + \frac{14r_0^5}{k^3} + \frac{126r_0^4}{k^4} + \frac{840r_0^3}{k^5} + \frac{4200r_0^2}{k^6} + \frac{1512r_0}{k^7} + \frac{35280}{k^8} + \frac{40320}{k^9r_0} \right] \quad (4.52) \]

For \( r^9 \)

\[
\int_{r_0}^{\infty} e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^9 dr
\]

\[ -e^{-kr_0} \left[ \frac{r_0^7}{k^2} + \frac{16r_0^6}{k^3} + \frac{168r_0^5}{k^4} + \frac{1344r_0^4}{k^5} + \frac{8400r_0^3}{k^6} + \frac{40320r_0^2}{k^7} + \frac{141120r_0}{k^8} + \frac{322560}{k^9} + \frac{362880}{k^{10}r_0} \right] \quad (4.53) \]

For \( r^{10} \)

\[
\int_{r_0}^{\infty} e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^{10} dr
\]

\[ -e^{-kr_0} \left[ \frac{r_0^8}{k^2} + \frac{18r_0^7}{k^3} + \frac{216r_0^6}{k^4} + \frac{2016r_0^5}{k^5} + \frac{15120r_0^4}{k^6} + \frac{90720r_0^3}{k^7} + \frac{423360r_0^2}{k^8} + \frac{1451520r_0}{k^9} + \frac{3265920}{k^{10}} + \frac{3628800}{k^{11}} \right] \quad (4.54) \]

For \( r^{11} \)

\[
\int_{r_0}^{\infty} e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^{11} dr
\]

\[ -e^{-kr_0} \left[ \frac{r_0^9}{k^2} + \frac{20r_0^8}{k^3} + \frac{270r_0^7}{k^4} + \frac{2880r_0^6}{k^5} + \frac{25200r_0^5}{k^6} + \frac{181440r_0^4}{k^7} + \frac{1058400r_0^3}{k^8} + \frac{4838400r_0^2}{k^9} + \frac{16329600r_0}{k^{10}} + \frac{36288000}{k^{11}} + \frac{39916800}{k^{12}r_0} \right] \quad (4.55) \]
For $r^{12}$

$$\int_{r_0}^{\infty} e^{-kr} \left( \frac{1}{r} - \frac{1}{r_0} \right) r^{12} = -e^{-kr_0} \left[ \frac{r_0^3}{k^2} + \frac{22r_0^3}{k^3} + \frac{330r_0^3}{k^4} + \frac{3960r_0^3}{k^5} + \frac{39600r_0^3}{k^6} + \frac{332640r_0^3}{k^7} + \frac{2328480r_0^3}{k^8} + \frac{13305600r_0^3}{k^9} + \frac{59875200r_0^3}{k^{10}} + \frac{199584000r_0^3}{k^{11}} + \frac{439084800}{k^{12}} + \frac{479001600}{k^{13}r_0} \right]$$  \hspace{1cm} (4.56)

4.5 Atomic wave function

The atomic wave functions used in evaluation of the direct and exchange transition matrices outlined above are the Roothan-Hatree-Fock double zeta functions given in the McLean and McLean (1981) 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 is given by,

$$\Psi = A(\Phi^{(1)}_1 \ldots \ldots \Phi^{(n)}_n)$$  \hspace{1cm} (4.57)

$A$ is the anti-symmetrizing operator, $n$ is the total number of electrons, and $\Phi^{(1)}_1 \ldots \ldots \Phi^{(n)}_n$ are spin orbitals. The spin orbitals are a product of spin function and an orbital function. The orbitals are assumed to be orthogonal to each other, thus the same hold for spin orbitals. The orbitals are characterized by an index $\eta$, which indicates the symmetry species and it corresponds to quantum number $I$, 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 characterizes the orbitals. The orbitals \( \Phi_{i \eta \gamma} \) is expanded in terms of the basis functions according to,

\[
\Phi_{i \eta \gamma} = \sum_p \phi_{p \eta \gamma} C_{i p}
\]  

(4.58)

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

\[
\phi_{p \eta \gamma}(r, \theta, \phi) = R_{\eta p}(r) Y_{\eta \gamma}(\theta, \phi)
\]  

(4.59)

where

\[
R_{\eta p} = \left[ (2\mu_{\eta p}) \right]^{1/2} \left( 2\xi_{\eta p} \right)^{\mu_{\eta p} + 1/2} e^{\xi_{\eta p} r}
\]  

(4.60)

And \( Y_{\eta \gamma}(\theta, \phi) \) are normalized spherical harmonics in complex form. It is noted that \( \mu_{\eta p} \geq \eta + 1 \) and that the exponent \( \xi_{\eta p} \) is chosen so as to give the best energy.

The single electron wave function given in equation (4.32) is constructed using the table of coefficient and exponent provided in the atomic data tables of McLean and McLean (1981).

The table 4.1 below shows \( l_n \), \( \xi_n \) and \( C_n \) denoting the orbitals, zetas and coefficient respectively for the \( 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6 6s^2 \) ground state of barium atom.
Table 4.1: 1s, 2s, 3s, 4s, 5s and 6s radial atomic wave functions for ground state of barium (McLean and McLean, 1981).

<table>
<thead>
<tr>
<th>$I_n$</th>
<th>$\xi_n$</th>
<th>$C_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>57.23372</td>
<td>-0.000128</td>
</tr>
<tr>
<td>1</td>
<td>38.044430</td>
<td>-0.012751</td>
</tr>
<tr>
<td>2</td>
<td>27.987527</td>
<td>-0.020361</td>
</tr>
<tr>
<td>2</td>
<td>24.645535</td>
<td>0.058667</td>
</tr>
<tr>
<td>3</td>
<td>19.152848</td>
<td>0.018841</td>
</tr>
<tr>
<td>3</td>
<td>12.964381</td>
<td>-0.109416</td>
</tr>
<tr>
<td>4</td>
<td>7.498241</td>
<td>0.147337</td>
</tr>
<tr>
<td>4</td>
<td>5.270719</td>
<td>0.027911</td>
</tr>
<tr>
<td>5</td>
<td>3.857420</td>
<td>-0.272884</td>
</tr>
<tr>
<td>5</td>
<td>2.597580</td>
<td>-0.030707</td>
</tr>
<tr>
<td>6</td>
<td>1.588608</td>
<td>0.582415</td>
</tr>
<tr>
<td>6</td>
<td>0.952513</td>
<td>0.529369</td>
</tr>
</tbody>
</table>

The atomic wave function is given by

$$
\Phi_{6s} = -0.000128\Phi_1 - 0.012751\Phi_2 - 0.020361\Phi_3 + 0.058667\Phi_4 + 0.018841\Phi_5 - 0.109416\Phi_6 + 0.147337\Phi_7 + 0.027911\Phi_8 - 0.272884\Phi_9 - 0.030707\Phi_{10} + 0.582415\Phi_{11} + 0.529369\Phi_{12} \tag{4.61}
$$

where

$$
\Phi_1 = N_1 r^0 \exp(-57.233372r)Y_{00}(\theta, \phi) \tag{4.62}
$$
\[ \Phi_2 = N_2 r^0 \exp(-38.044430r) Y_{00}(\theta, \phi) \] (4.63)

\[ \Phi_3 = N_3 r^1 \exp(-27.987527r) Y_{00}(\theta, \phi) \] (4.64)

\[ \Phi_4 = N_4 r^1 \exp(-24.645535r) Y_{00}(\theta, \phi) \] (4.65)

\[ \Phi_5 = N_5 r^2 \exp(-19.152848r) Y_{00}(\theta, \phi) \] (4.66)

\[ \Phi_6 = N_6 r^2 \exp(-12.964381r) Y_{00}(\theta, \phi) \] (4.67)

\[ \Phi_7 = N_7 r^3 \exp(-7.498241r) Y_{00}(\theta, \phi) \] (4.68)

\[ \Phi_8 = N_8 r^3 \exp(-5.270719r) Y_{00}(\theta, \phi) \] (4.69)

\[ \Phi_9 = N_9 r^4 \exp(-3.857420r) Y_{00}(\theta, \phi) \] (4.70)

\[ \Phi_{10} = N_{10} \exp(-2.597580r) Y_{00}(\theta, \phi) \] (4.71)

\[ \Phi_{11} = N_{11} \exp(-1.588608r) Y_{00}(\theta, \phi) \] (4.72)

\[ \Phi_{12} = N_{12} \exp(-0.952513r) Y_{00}(\theta, \phi) \] (4.73)

where \( N_1 \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots N_{12} \) are normalization factors given by,

\[ N_i = \left( (2n)! \right)^{-\frac{1}{2}} (2\xi_n)^{n+\frac{1}{2}} \] (4.74)

where \( n \) and \( \xi_n \) are orbital and zeta respectively, given in table 4.1 above.

\[ N_1 = \left( (2*1)! \right)^{-\frac{1}{2}} (2 * 57.233372)^{1+\frac{1}{2}} \] (4.75)

\[ N_2 = \left( (2*1)! \right)^{-\frac{1}{2}} (2 * 38.04430)^{1+\frac{1}{2}} \] (4.76)
\[ N_3 = \left( (2 \times 2)! \right)^{-\frac{1}{2}} (2 \times 27.987527)^{2 + \frac{1}{2}} \]  \hspace{1cm} (4.77)

\[ N_4 = \left( (2 \times 2)! \right)^{-\frac{1}{2}} (2 \times 24.645535)^{2 + \frac{1}{2}} \]  \hspace{1cm} (4.78)

\[ N_5 = \left( (2 \times 3)! \right)^{-\frac{1}{2}} (2 \times 19.152848)^{3 + \frac{1}{2}} \]  \hspace{1cm} (4.79)

\[ N_6 = \left( (2 \times 3)! \right)^{-\frac{1}{2}} (2 \times 12.964381)^{3 + \frac{1}{2}} \]  \hspace{1cm} (4.80)

\[ N_7 = \left( (2 \times 4)! \right)^{-\frac{1}{2}} (2 \times 7.498241)^{4 + \frac{1}{2}} \]  \hspace{1cm} (4.81)

\[ N_8 = \left( (2 \times 4)! \right)^{-\frac{1}{2}} (2 \times 5.270719)^{4 + \frac{1}{2}} \]  \hspace{1cm} (4.82)

\[ N_9 = \left( (2 \times 5)! \right)^{-\frac{1}{2}} (2 \times 3.857420)^{5 + \frac{1}{2}} \]  \hspace{1cm} (4.83)

\[ N_{10} = \left( (2 \times 5)! \right)^{-\frac{1}{2}} (2 \times 2.597580)^{5 + \frac{1}{2}} \]  \hspace{1cm} (4.84)

\[ N_{11} = \left( (2 \times 6)! \right)^{-\frac{1}{2}} (2 \times 1.588608)^{6 + \frac{1}{2}} \]  \hspace{1cm} (4.85)

\[ N_{12} = \left( (2 \times 6)! \right)^{-\frac{1}{2}} (2 \times 0.952513)^{6 + \frac{1}{2}} \]  \hspace{1cm} (4.86)
4.6 Computer code

Due to the complex numerical computation, there was need of a computer program. A computer program DWBA1 (Madison and Bartschat, 1996) designed for electron-hydrogen scattering was modified to perform numerical computation for the present problem of electron–barium collision. The wave function appearing in equation (4.61) replaced the hydrogen wave functions in subroutine FHYD. The calculated static potentials from section 4.4 are different from the hydrogen static potentials in the program. Appropriate replacement for these static potentials were made in subroutine POTENT. The two subroutines were coded in such a way that it would take in the arguments supplied by McLean and McLean (1981) for barium atom and using these a wave function was constructed. These wave functions were also used to generate the distortion potentials. Other minor modifications were also done in subroutine EXCHGE and also on the input file. Computer program origin7 was utilized for data analysis and presenting the data graphically.
CHAPTER 5

RESULTS AND DISCUSSION

5.1 Introduction

In section 5.2 the DWM differential cross section results for elastic scattering of electron by barium atom obtained in this study are presented. The results are compared with available experimental and theoretical results. In section 5.3 the DWM integral cross sections are presented and compared with earlier results. The DCS which has dimensions of area per unit solid angle are in $a_0^2/\text{sr}$ units and ICS are in $a_0^2$ units ($a_0$ and sr are Bohr radius and steradian respectively).

5.2 Differential cross sections

In this study the differential cross section (DCS) for elastic scattering of electron by barium atom have been calculated at 10, 15, 20, 30, 40, 60, 80, 100 and 200 eV for scattering angles from $\theta = 0^\circ$ to $\theta = 180^\circ$ using distorted wave method. To test the reliability of the present model, the present results have been compared with experimental and theoretical data. Results of such comparisons for elastic scattering of electron from barium atom are presented in figures 5.1-5.9. The present results are listed in table 5.1.

From figure 5.1 it can be seen that the present differential cross section at 10 eV are in qualitative agreement with the convergent close coupling (CCC) results of Fursa and Bray (1999) but not with the potential scattering results of Adibzadeh and Theodosiou (2004). The present results have two minima at $50^\circ$ and $130^\circ$ as
Table 5.1: Present DWM differential cross section (in $a_0^2/\text{sr}$) for elastic scattering of electron by barium atom, at different impact energies.

<table>
<thead>
<tr>
<th>Energy</th>
<th>10 eV</th>
<th>15 eV</th>
<th>20 eV</th>
<th>30 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>23.78</td>
<td>91.3</td>
<td>72.9</td>
<td>65.11</td>
<td>69.49</td>
<td>84.2</td>
<td>98.27</td>
<td>110.3</td>
<td>148.12</td>
</tr>
<tr>
<td>10</td>
<td>103.29</td>
<td>72.82</td>
<td>55.27</td>
<td>44.14</td>
<td>42.77</td>
<td>44.38</td>
<td>45.58</td>
<td>45.64</td>
<td>38.82</td>
</tr>
<tr>
<td>20</td>
<td>60.69</td>
<td>39.41</td>
<td>27.78</td>
<td>18.42</td>
<td>14.96</td>
<td>12.0</td>
<td>10.44</td>
<td>9.35</td>
<td>6.1</td>
</tr>
<tr>
<td>30</td>
<td>25.98</td>
<td>17.76</td>
<td>13.9</td>
<td>10.16</td>
<td>8.32</td>
<td>6.34</td>
<td>5.17</td>
<td>4.35</td>
<td>2.22</td>
</tr>
<tr>
<td>40</td>
<td>8.72</td>
<td>8.32</td>
<td>8.15</td>
<td>7.04</td>
<td>5.95</td>
<td>4.36</td>
<td>3.34</td>
<td>2.66</td>
<td>1.12</td>
</tr>
<tr>
<td>50</td>
<td>3.22</td>
<td>4.20</td>
<td>4.37</td>
<td>3.81</td>
<td>3.13</td>
<td>2.15</td>
<td>1.57</td>
<td>1.22</td>
<td>0.5</td>
</tr>
<tr>
<td>60</td>
<td>3.1</td>
<td>2.58</td>
<td>1.95</td>
<td>1.28</td>
<td>0.90</td>
<td>0.53</td>
<td>0.39</td>
<td>0.32</td>
<td>0.18</td>
</tr>
<tr>
<td>70</td>
<td>4.85</td>
<td>2.5</td>
<td>1.11</td>
<td>0.27</td>
<td>0.14</td>
<td>0.14</td>
<td>0.17</td>
<td>0.18</td>
<td>0.13</td>
</tr>
<tr>
<td>80</td>
<td>6.42</td>
<td>2.82</td>
<td>1.22</td>
<td>0.61</td>
<td>0.68</td>
<td>0.77</td>
<td>0.69</td>
<td>0.58</td>
<td>0.23</td>
</tr>
<tr>
<td>90</td>
<td>6.53</td>
<td>2.54</td>
<td>1.33</td>
<td>1.42</td>
<td>1.74</td>
<td>1.74</td>
<td>1.40</td>
<td>1.07</td>
<td>0.31</td>
</tr>
<tr>
<td>100</td>
<td>4.94</td>
<td>1.44</td>
<td>0.99</td>
<td>1.94</td>
<td>2.50</td>
<td>2.36</td>
<td>1.78</td>
<td>1.27</td>
<td>0.26</td>
</tr>
<tr>
<td>110</td>
<td>2.56</td>
<td>0.24</td>
<td>0.51</td>
<td>1.93</td>
<td>2.53</td>
<td>2.27</td>
<td>1.61</td>
<td>1.07</td>
<td>0.13</td>
</tr>
<tr>
<td>120</td>
<td>1.02</td>
<td>0.27</td>
<td>0.74</td>
<td>1.72</td>
<td>2.00</td>
<td>1.59</td>
<td>1.03</td>
<td>0.63</td>
<td>0.02</td>
</tr>
<tr>
<td>130</td>
<td>1.80</td>
<td>2.67</td>
<td>2.61</td>
<td>1.94</td>
<td>1.41</td>
<td>0.74</td>
<td>0.41</td>
<td>0.25</td>
<td>0.10</td>
</tr>
<tr>
<td>140</td>
<td>5.55</td>
<td>7.80</td>
<td>6.50</td>
<td>3.07</td>
<td>1.26</td>
<td>0.16</td>
<td>0.084</td>
<td>0.20</td>
<td>0.46</td>
</tr>
<tr>
<td>150</td>
<td>11.64</td>
<td>14.9</td>
<td>11.94</td>
<td>5.12</td>
<td>1.77</td>
<td>0.066</td>
<td>0.21</td>
<td>0.56</td>
<td>1.05</td>
</tr>
<tr>
<td>160</td>
<td>18.38</td>
<td>22.25</td>
<td>17.62</td>
<td>7.56</td>
<td>2.72</td>
<td>0.38</td>
<td>0.65</td>
<td>1.16</td>
<td>1.73</td>
</tr>
<tr>
<td>170</td>
<td>23.61</td>
<td>27.79</td>
<td>21.95</td>
<td>9.55</td>
<td>3.62</td>
<td>0.79</td>
<td>1.12</td>
<td>1.72</td>
<td>2.25</td>
</tr>
<tr>
<td>179</td>
<td>25.54</td>
<td>29.82</td>
<td>23.56</td>
<td>10.29</td>
<td>3.98</td>
<td>0.97</td>
<td>1.31</td>
<td>1.94</td>
<td>2.44</td>
</tr>
</tbody>
</table>
Figure 5.1: Differential cross section for elastic scattering of electron by barium atom at 10 eV incident energy. The present results are compared with results of Fursa and Bray (1999) and Adibzadeh and Theodosiou (2004).
Figure 5.2: Differential cross sections for elastic scattering of electron by barium atom at 15 eV incident energy. The present results are compared with results of Wang et al. (1994), Fursa and Bray (1999) and Adibzadeh and Theodosiou (2004).
Figure 5.3: Differential cross section of elastic scattering of electron by barium atom at 20 eV incident energy. The present results are compared with results of Jensen et al. (1978), Wang et al. (1994), Szmytkowski and Sienkiewicz (1994), Fursa and Bray (1999) and Adibzadeh and Theodosiou (2004)
Figure 5.4: Differential cross sections of elastic scattering of electron by barium atom at 30 eV incident energy. The present results are compared with results of Jensen et al. (1978), Fabrikant (1980), Szmytkowski and Sienkiewicz (1994), Trajmar et al. (1999) and Adibzadeh and Theodosiou (2004).
Figure 5.5: Differential cross sections of elastic scattering of electron by barium atom at 40 eV incident energy. The present results are compared with results of Jensen et al. (1978), Szymkowiski and Sienkiewicz (1994), Adibzadeh and Theososiou (2004) and Fursa and Bray (1999)
Figure 5.6: Differential cross sections of elastic scattering of electron by barium atom at 60 eV incident energy. The present results are compared with results of Jensen et al. (1978), Szmytkowski and Sienkiewicz (1994), Adibzadeh and Theodosiou (2004), Fursa and Bray (1999) and Miloshevsky et al. (2000).
Figure 5.7: Differential cross sections of elastic scattering of electron by barium atom at 80 eV incident energy. The present results are compared with results of Jensen et al. (1978), Szmytkowski and Sienkiewicz (1994), Adibzadeh and Theodosiou (2004) and Fursa and Bray (1999).
Figure 5.8: Differential cross section of elastic scattering of electron by barium atom at 100 eV incident energy. The present results are compared with results of Jensen et al. (1978), Szmytkowski and Sienkiewicz (1994), Adibzadeh and Theodosiou (2004), Fursa and Bray (1999) and Miloshevsky et al. (2000).
Figure 5.9: Differential cross sections of elastic scattering of electron by barium atom at 200 eV incident energy. The present results are compared with results of Adibzadeh and Theodosiou (2004).
those of Fursa and Bray (1999) appearing at $60^\circ$ and $110^\circ$ but deeper than the present ones. Adibzadeh and Theodosiou (2004) have three minima.

At 15 eV, figure 5.2 shows that the present results for the differential cross sections are in some qualitative agreement with experimental results of Wang et al. (1994). Both results have two minima. However, the present calculated result first minimum is shallow and the second one has been shifted towards the left as compared with measured results of Wang et al. (1994). This may be attributed to the approximation method used. The present results are also seen to be in qualitative agreement with calculated convergent close coupling results of Fursa and Bray (1999) and potential scattering results of Adibzadeh and Theodosiou (2004). Quantitatively the present results are higher for angles greater than $120^\circ$ compared to measured results of Wang et al. (1994) as well as the calculated results Fursa and Bray (1999) and Adibzadeh and Theodosiou (2004). This is due to the fact that 15 eV is considered to be low impact energy and DWM is not expected to give good results at low energy. The good qualitative agreement indicates that the distortion potentials in this study are appropriate.

In figure 5.3 we have presented the present DCS results along with experimental and theoretical results at 20 eV. The experimental measurement of Wang et al. (1994) shows two minima in contrast to the observation of Jensen et al. (1978), which shows three minima. The present results are in better qualitative agreement up to $120^\circ$ with measured results of Wang et al. (1994) than those of Jensen et al. (1978). Since Wang et al. (1994) values seem to be more reliable (since it is the latest result) shows the accuracy of the present approximation method. The present
results have two minima at 70° and 110° compared to those of Wang et al. (1994) appearing at 30°, 80° and 140°. The one appearing at 30° is very shallow but those at 80° and 140° are deeper. The calculated results of Fursa and Bray (1999), Adibzadeh and Theodosiou (2004) and Szmytkowski and Sienkiewicz (1994) have also two minima but minima in the results of Szmytkowski and Sienkiewicz (1994) and Adibzadeh and Theodosiou (2004) are deeper compared with the present results. This is because of the potentials used and wave functions employed which are different from the one used in the present study.

Figure 5.4 for impact energy at 30 eV shows, for angle between 10° to 120° the present results are in satisfactory agreement with the measured results of Jensen et al. (1978) and Trajmar et al. (1999) and two state close coupling (CC2) results of Fabrikant (1980), relativistic polarized orbital results of Szmytkowski and Sienkiewicz (1994) and potential scattering results of Adibzadeh and Theodosiou (2004). The minima at 70° almost coincide in position and depth with the measured results. According to Miloshevsky et al. (2000) both the depth and positions of minimum in DCS have significant physical importance since they reflect the structural information of the targets. This agreement signifies the accuracy of the present approximation method. For angle greater than 120° the present DCS values are slightly higher than those of Jensen et al. (1978). This is because within this range (130° – 180°) their results were obtained by, probably incorrect extrapolation (Szmytkowski and Sienkiewicz, 1994).

In figure 5.5 at 40 eV the present results are in satisfactory agreement with measured results of Jensen et al. (1994) and calculated results by Fursa and Bray (1999) and
Adibzadeh and Theodosiou (2004) for angle between $20^\circ$ to $80^\circ$. The minima at $70^\circ$ coincide in position and depth with the measured results of Jensen et al. (1978). For angles greater than $80^\circ$ the present DCS values are higher than those of measured results of Jensen et al. (1978) and theoretical results of Fursa and Bray (1999) and Adibzadeh and Theodosiou (2004). The present results are in poor agreement with calculated results of Szmytkowski and Sienkiewicz (1994) having the oscillatory behavior which is not seen in any of the calculated and experimental results. The minima at $140^\circ$ is shallow compared to the other theoretical results. This might be attributed to static potentials used which are different from the one used in the present study.

At impact energy 60 eV, figure 5.6, the present results have two minima, a shallow first minima at $70^\circ$ and a slightly deeper at $150^\circ$. The present results are in good quantitative agreement with measured results of Jensen et al. (1978) and all the available theoretical results except that of Szmytkowski and Sienkiewicz (1994) which is too oscillatory. All the experimental and theoretical results including the present one show two minima except the one due to Szmytkowski and Sienkiewicz (1994).

In figure 5.7 at 80 eV the present results are in good both quantitative and qualitative agreement with measured results of Jensen et al. (1978). The present results have two minima as the measured results. The first minimum at about $70^\circ$ coincide in position and depth with the measured one. The present results predict deeper second minimum at $140^\circ$ compared to the minimum at $110^\circ$ that is predicted by the measured results. The present results are in poor qualitative agreement with
calculated results of Fursa and Bray (1999), Adibzadeh and Theodosiou (2004) and Szmytkowski and Sienkiewicz (1994) since they predict more than two minima. But the differential cross section values of the present results are in the same range as other calculations.

From figure 5.8 at 100 eV, it is seen that the present results from 20° are in better agreement with measured results of Jensen et al. (1978) compared to the calculated results of Fursa and Bray (1999), Adibzadeh and Theodosiou (2004), Szmytkowski and Sienkiewicz (1994) and Miloshevsky et al. (2000). The present results have two minima as the measured results by Jensen et al. (1978). The position and depth of the first minima almost coincide with the measured results of Jensen et al. (1978) while the second minima have same depth as the experimental results but the position is shifted. The present results have good quantitative agreement (results are in same range) but poor qualitative agreement with the available theoretical results. This is because while the present results have two minima the other calculated results have more than two minima. It is encouraging to note that the present model is capable of reproducing DCS that are in good accord with the measured results.

At 200 eV figure 5.9, there are no experimental results available. The present results are compared with the only available calculated results of Adibzadeh and Theodosiou (2004). Both results fall in the same range but there is no qualitative agreement.

At all impact energies, for small scattering angle the present DCS values are lower than the available results. This is due to the exclusion of polarization potential in this
study which has a great influence on the cross sections at small scattering angles (Kariuki et al., 2015).

### 5.3 Integral cross section

In this study integral cross sections (ICS) for elastic scattering of electron by barium atom has been calculated at 10-200 eV. Table 5.3 gives the present ICS results obtained using DWM method, together with experimental results of Jensen et al. (1978) and calculated results of Szmytkowski and Sienkiewicz (1994), Fursa and Bray (1999), and Adibzadeh and Theodosiou (2004). The results are compared in figure 5.10.

From figure 5.10 it is seen that except for the results of Szmytkowski and Sienkiewicz (1994), the present integral cross sections together with the measured results of Jensen et al. (1978), and calculated results of Fursa and Bray (1999), and Adibzadeh and Theodosiou (2004) show the same trend. In that as the energy increases the cross section decreases because the interaction time between the incident electron and target atom decreases and hence probability of scattering decreases. One may notice that the present ICS values are lower than the available results. This is because the integral cross section is just an integral of the DCS over the angles and since the present DCS values, as portrayed in figures 5.1-5.9 are generally lower at small scattering angles. This is due to the form of distortion potential used in the present study in which the polarization potential has not been included which has great influence at small scattering angles where the DCS values seem to be very large.
Table 5.3: DWM integral cross sections (in $a_0^2$) for elastic scattering of electron by barium atom.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>122.1</td>
<td>105.72</td>
<td>-</td>
<td>160.59</td>
<td>-</td>
</tr>
<tr>
<td>15</td>
<td>92.22</td>
<td>-</td>
<td>311.5</td>
<td>160</td>
<td>-</td>
</tr>
<tr>
<td>20</td>
<td>71.75</td>
<td>93.31</td>
<td>206.9</td>
<td>-</td>
<td>216.3±108.15</td>
</tr>
<tr>
<td>30</td>
<td>51.05</td>
<td>89.35</td>
<td>175.1</td>
<td>130.3</td>
<td>129.8±64.5</td>
</tr>
<tr>
<td>40</td>
<td>41.99</td>
<td>78.85</td>
<td>105.1</td>
<td>-</td>
<td>99.2±49.6</td>
</tr>
<tr>
<td>60</td>
<td>33.62</td>
<td>58.82</td>
<td>95.3</td>
<td>115</td>
<td>112.0±56</td>
</tr>
<tr>
<td>80</td>
<td>29.24</td>
<td>-</td>
<td>127.9</td>
<td>101.5</td>
<td>98.1±49.05</td>
</tr>
<tr>
<td>100</td>
<td>26.31</td>
<td>45.70</td>
<td>82.1</td>
<td>85.78</td>
<td>90.6±45.3</td>
</tr>
<tr>
<td>200</td>
<td>18.56</td>
<td>37</td>
<td>-</td>
<td>51.77</td>
<td>-</td>
</tr>
</tbody>
</table>
Figure 5.10: Integral cross sections for elastic scattering of electron by barium atom. The present results are compared with experimental results of Jensen et al. (1978) and theoretical results of Szmytkowski and Sienkiewicz (1994), Fursa and Bray (1999), and Adibzadeh and Theodosiou (2004).
CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Introduction

Differential and integral cross sections for elastic scattering of electron by barium atom have been calculated at energies 10-200 eV using distorted wave method. Since elastic scattering was being considered, the present DWM took both initial and final distortion potential as the static potential of barium atom in the ground state. In calculations, double Zeta Roothan-Hartree-Fock wave functions compiled by McLean and McLean (1981) were used as wave function of barium atom. This chapter presents important conclusions and recommendations based on the results of study.

6.2 Conclusions

The following conclusions are made

i. The distorted wave method was successfully formulated as applied to electron-barium scattering.

ii. The computer program DWBA1 was successfully modified for the numerical calculation.

iii. For impact energies between 30-100 eV the present DCS results are in satisfactory agreement with experimental results of Jensen et al. (1978) and available theoretical results. This shows that the present results are reliable at intermediate and higher energies.
iv. The present ICS results are in good qualitative agreement with experimental results of Jensen et al. (1978) and calculated results of Fursa and Bray (1999) and Adibzadeh and Theodosiou (2004). However, the present results are lower than the available results, this is due to the exclusion of polarization potential in the distortion potential used in this study which has great influence on DCS at small scattering angles.

6.3 Recommendations

Looking at the performance of this method on elastic scattering of electron by barium atom using DWM, recommend the following:

i. A distortion potential that incorporates exchange, absorption and polarization potentials be used in the DWM.

ii. The method should be extended to energies above 200 eV up to 1000 eV and the results compared with the available results.

iii. The present method should be extended to include metals such as gadolinium and radium.
REFERENCES


Katiyar, A. K. and Srivastava, R. (1988). Distorted-wave calculation of the cross sections and correlation parameters for $e^\pm - He$ $(1^1s, 2^1s \rightarrow 2^1p, 3^1s$ and $3^1)$ collision. *Physical Review A* **38**: 2767-2781.


