# STUDY OF ATOMIC COLLISIONS IN GLAUBER APPROXIMATION

## Thesis

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**MAY 1977**

*To my brother*

*RADHA KRISHAN GUPTA*

# C E R T I F I C A T E

This is to certify that the thesis entitled 'STUDY OF ATOMIC COLLISIONS IN GLAUBER APPROXIMATION' which is being submitted by Shri Suresh Kumar in fulfilment for the award of the degree of Doctor of Philosophy in Physics of the University of Roorkee, Roorkee is a record of his own work carried out by him under my supervision and guidance. He has worked for a period equivalent to 24 months full time research for preparing his thesis for Ph.D. degree at this university.

The matter embodied in this thesis has not been submitted for the award of any other degree.

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# R E S U M E

The work reported in this thesis is author's attempt to study the collision processes, at high and intermediate energies, in which a beam of charged particles (e.g. electrons) is bombarded onto an atomic or ionic target. Throughout this work, the eikonal or the Glauber approximation (the latter is an special case of the former) has been the main tool of investigation.

In the first chapter, various quantal, classical and semi-classical approaches for the study of these collision processes have been briefly reviewed. The eikonal multiple scattering expansion and its relationship with the Born series have also been discussed. The second chapter is devoted to the details of the Glauber approximation. This chapter basically describes (i) the underlying assumptions and the expected range of validity of the approximation and (ii) its alternative forms for the scattering wavefunction and amplitude. In the third chapter, a method for the Glauber predicted scattering amplitudes in a one-dimensional integral form for e-H(1s) scattering has been proposed to study the excitation of atomic hydrogen to highly excited states from a low lying state. Earlier expressions [B.K. Thomas and E. Gerjuoy, J.Maths. Phys. 12, 1567(1971) ] were a bit cumbersome due to the appearance of an increasing number of hypergeometric functions depending on the principal quantum number of the excited state. In the fourth chapter the Glauber approximation

has been applied to the study of elastic and inelastic scattering of electrons by lithium atom by explicitly treating all the three electrons by suitably adapting Franco's procedure [Phys. Rev. Lett. 26, 1088(1971) ]. The percentage polarization of the resulting resonance line (2p → 2s) emitted from $^{6}Li$ and $^{7}Li$ following electron excitation has also been obtained. The fifth chapter is devoted to the study of elastic scattering of electrons by helium like ions (such as $H^-$ and $Li^+$) using the optical model approach in eikonal approximation. In the sixth chapter an attempt has been made in a very simple way to improve upon the Glauber (straight-line) approximation at large scattering angles. It has been used to study e-H(1s) elastic scattering and the results have been compared with other approaches and the recent experimental data. The seventh chapter summarizes the work reported in earlier chapters and contains some comments, pointing out the drawbacks and the suggestions for their elimination.

A numerical procedure to exactly take into account the wiggles of the Bessel functions in integrals of the type $\int F(x)\, J_\nu(ax)\, dx$ is presented in Appendix A1.

## PUBLICATIONS

1. $e\text{-}H^-$ elastic scattering in eikonal approximation (with A.N. Tripathi and M.K. Srivastava), J.Phys. B8, No.7,1082 (1975).

2. Elastic e-Li scattering in Glauber approximation (with M.K. Srivastava), Phys. Rev.A12, 801(1975).

3. Intermediate energy $e\text{-}Li^+$ elastic scattering in eikonal approximation (with M.K. Srivastava and A.N. Tripathi), J.Phys.B8, No.4, 612(1975).

4. Glauber cross sections for the 2s-2p resonance transition in lithium by electron impact (with M.K. Srivastava), Phys. Rev.A13, 1307(1976).

5. Polarization of the 2p→2s resonance line of lithium (with M.K. Srivastava), J.Phys.B9, 1911(1976).

6. Glauber amplitudes for transitions from low lying states in hydrogen atom by charged particle impact (with M.K. Srivastava), Pramana(1977), to appear .

7. e-H elastic scattering in Glauber-Born approximation (with Archana Gupta and M.K. Srivastava), Phys. Rev.A14 (1977), to appear.

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# CHAPTER 1

# I N T R O D U C T I O N

## 1.1 GENERAL REMARKS

The analysis of collision phenomena plays a central role in almost all investigations into the structure of matter. For example, electrons of high energy are particularly well suited to probe the charge distribution in nuclei. Electrons and heavier projectiles of low energy are scattered from atoms to obtain data which can serve as an input information for calculation of kinetic processes in gases where low energy electrons predominate. In fact, most of our detailed information about the forces and interactions between atoms or between electrons and atoms are learned through scattering experiments in which a well defined beam of charged particles is allowed to interact with the atoms of a target. In such a scattering experiment there are many possibilities through which a reaction can take place. For instance, the target and the projectile may contain respectively the same particles before and after the collision or some particles are transferred between the colliding systems during the reaction. The first is just the scattering and the second a rearrangement collision. Each of these arrangements open further possibilities. For example, in the case of scattering the projectile beam of charged particles may be scattered by the target without the target being excited (elastic scattering) or by leaving the target in some excited state (inelastic scattering or excitation). Each different initial or final

state of the colliding system defines a reaction channel. For example, the reactions

$$e + H(1s) \rightarrow e + H(1s) \qquad (a)$$

$$\rightarrow e + H(2s) \qquad (b)$$

$$\rightarrow e + H(2p) \qquad (c)$$

define three different channels. A particular channel is 'open' if the total energy E of the system is sufficient to inject the system into that channel; otherwise the channel is said to be 'closed' for the reaction. In a rearrangement collision there are, thus, many possible open channels carrying out reactions such as charge exchange, charge transfer etc. However, it should be noted that not all reactions are possible between a given set of particles, even if sufficient energy is available, because the appropriate quantum numbers (angular momentum, parity etc.) must be conserved. Such atomic and molecular collision processes are of common occurrence in many fields such as chemical kinematics, astrophysics, plasma physics, atmospheric physics etc. In most of the atomic and ionic collision processes occurring in the universe, the projectile entities are generally elementary particles (e.g. electrons, protons or photons). For this reason, we have carried out our investigations using electrons as incident particle. These can similarly be carried out for protons as well.

In atomic and ionic collision processes as in all

other collisions the most important thing to study from theoretical as well as experimental point of view is the cross section which correlates the observed intensities to the theoretical probabilities calculated from the assumed or known wavefunctions and interactions.

In an idealized scattering experiment, a single fixed scattering centre is bombarded by particles incident along the chosen z-axis. After scattering, the particles are detected at a large distance from the scattering centre. If $\vec{r}(r,\theta,\phi)$ are the coordinates of the scattered particles relative to the scattering centre, $I_o$ is the incident current density (i.e. number of particles incident per unit area per unit time) and $Id\Omega$ the number of these scattered into the solid angle $d\Omega$ subtended by the detector at the scattering centre, then we define the differential cross section as

$$\frac{d\sigma}{d\Omega} = \frac{I(\theta,\phi)}{I_o} , \qquad \ldots (1.1)$$

i.e. as the number of particles scattered into the detector per unit solid angle per unit time per scattering centre per unit incident current density. The width of the beam is determined by slits, which, although quite narrow from an experimental point of view, are nevertheless very wide compared with the spatial extension of the interaction region. We can, therefore, assume that the particles in the beam, represented by very long and very broad wavepackets at distances far from

the target scattering centre, can be described approximately by plane waves $e^{ikz}$; $\hbar\vec{k}$ is the momentum of the incident beam of particles. During scattering, the incident wave gets distorted by the scatterer. Therefore, at large distance r from the interaction region, the scattering wavefunction $\Psi$ must be represented as a superposition of the incident plane wave and an outgoing spherical wave, with amplitude $f(\vec{k}',\vec{k}) \equiv f_k(\theta,\phi)$, i.e., we must have

$$\Psi(\vec{r}) \xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}} e^{ikz} + f(\vec{k}',\vec{k}) \frac{e^{ikr}}{r}, \quad \ldots (1.2)$$

where $\hbar\vec{k}$ and $\hbar\vec{k}'$ are the centre of mass (CM) momenta of the incident and scattered particles. The differential cross section is then related to the elastic scattering amplitude by the relation

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}',\vec{k})|^2. \quad \ldots (1.3)$$

The description presented above for the elastic scattering can be easily extended to the inelastic case. The Eqs.(1.1) and (1.3) correlate the experimentally measured and theoretically calculated entities.

## 1.2 REVIEW OF THE THEORETICAL METHODS

Theoretically, any physical system at not too high an energy can be described using the principles of quantum mechanics through the application of the non-relativistic Schroedinger equation. An exact quantum mechanical solution is, however,

possible only for a two-body problem. Moreover, the wave functions of the target containing only one electron (such as hydrogen atom or hydrogenic ion) are known exactly. Even, if the wavefunctions of the targets are known exactly, the exact quantum mechanical formulation of the electron-atom scattering is a formidable task because even the simplest e-H atom scattering problem is a many-body (three-body) problem. Obviously, one has to resort to the appropriate approximate methods to solve, quantum mechanically, the problem of electron-atom or electron-ion scattering. The only way to assess the accuracy of the approximate methods is by comparing them with each other and with the experimental data. In the following, in order to define the scope of the present work, we make a brief survey of some approximate methods applicable to the study of elastic and inelastic scattering of electrons by atoms and ions involving a few electrons.

In order to describe a physical system involving a beam of charged particles interacting with an atomic target, we start with the stationary state description of the scattering problem and use the time-independent Schroedinger equation

$$(H - E)\Psi_i = 0, \qquad \ldots (1.4)$$

where E is the total energy of the complete system and is given by

$$E = \frac{\hbar^2 k^2}{2\mu} + w_i = \frac{\hbar^2 k'^2}{2\mu} + w_f , \qquad \ldots (1.5a)$$

where $\mu$ is the reduced mass of the system, $w_i$ and $w_f$ are the target internal energies in the initial and final channels respectively, H is the total Hamiltonian given by

$$H = H_t + \mathcal{T} + V , \qquad \ldots (1.5b)$$

$\mathcal{T}$ is the kinetic energy operator of the incident particle, V is the total interaction potential between the projectile and the atomic nucleus and electrons and $H_t$ is the Hamiltonian of the target. This stationary state description of the scattering situation is, in principle, quite adequate if we assume that the energy of the incident particles, represented by a very long and very broad wave packet or approximately by a plane wave, is well defined for very long but finite times in the remote past and the far future. Obviously the transition probability per unit time can be related to the scattering element defined by

$$S_{fi} = \langle f|S|i\rangle = (2\pi)^3 \left\langle \Phi_f , \Psi_i^{(+)} \right\rangle = (2\pi)^3 \left\langle \Psi_f^{(-)} , \Phi_i \right\rangle ,$$

from which the scattering amplitude and the cross section can be obtained directly. Here $\Psi_i^{(+)}$ and $\Psi_f^{(-)}$ are respectively the outgoing and the ingoing solutions of the Schroedinger Eq.(1.4). Various approximations needed involve the evaluation of the wavefunction $\Psi$ of the complete system.

1.2.1 QUANTAL APPROXIMATIONS

(i) The Atomic Eigenfunction Expansion Method

Here one expands the properly antisymmetrized total wavefunction $\Psi(\vec{r},\vec{x})$ of the complete system, the incident particle plus the target atom, in the complete set of unperturbed atomic eigenfunctions $\phi_j$:

$$\Psi(\vec{r},\vec{x}) = A \sum_j X_j(\vec{r})\phi_j(\vec{x}), \qquad \ldots (1.7)$$

where $X_j$ represents the scattering wavefunction of the projectile particle, A is an antisymmetrizing operator, $\vec{x}$ denotes collectively all the particle coordinates of the target atom and $\vec{r}$ the coordinate of the projectile particle relative to the target centre of mass. This expansion gives the exact wavefunction for the complete system. The symbol $\sum_j$ in Eq.(1.7) involves the summation over all the discrete states and integration over the continuum states of the target. More explicitly, Eq.(1.7) can be written as

$$\Psi^{\pm}(\vec{r},\vec{x}) = \frac{1}{\sqrt{2}} \sum_j \left[ X_j^{\pm}(\vec{r})\phi_j(\vec{x}) \pm X_j^{\pm}(\vec{x})\phi_j(\vec{r}) \right] \ldots (1.8)$$

where the plus and minus sign stands for singlet (antiparallel spin) and triplet (parallel spin) states, respectively.

The eigenfunction expansion method, in principle, requires retention of all the terms in the summation which, in turn, leads to an infinite set of integrodifferential equations as can be easily seen by combining Eqs.(1.4)

and (1.8):

$$(\nabla_r^2 + k_j^2) X_j^{\pm}(\vec{r}) = \sum_{j'} \left[ U_{jj'}(\vec{r}) X_{j'}^{\pm}(\vec{r}) \pm \int \mathcal{J}_{jj'}^{\pm}(\vec{r},\vec{x}) X_{j'}^{\pm}(\vec{x}) d^3x \right], \quad \ldots (1.9)$$

Here

$$k_j = \left[ 2\mu(E-w_j) / \hbar^2 \right]^{1/2}$$

$$\equiv \begin{cases} k' & j = f \\ k & j = i \end{cases}, \quad \ldots (1.10)$$

is the wavenumber of the scattered particle and $w_j$ is the eigen energy of the target in an intermediate channel j and, $U_{jj'}$ and $\mathcal{J}_{jj'}$ are respectively the direct interaction potential and the exchange Kernel defined by

$$U_{jj'}(\vec{r}) = \frac{2\mu}{\hbar^2} V_{jj'}(\vec{r}) = \frac{2\mu}{\hbar^2} \int \phi_j^*(\vec{x}) V(\vec{r},\vec{x}) \phi_{j'}(\vec{x}) d^3x, \quad \ldots (1.11)$$

and

$$\mathcal{J}_{jj'}(\vec{r},\vec{x}) = \pm \frac{2\mu}{\hbar^2} \left( \phi_j^*(\vec{x}) \left[ H(\vec{r},\vec{x}) - E \right] \phi_{j'}(\vec{r}) \right) . \quad \ldots (1.12)$$

If the incoming particle interacts with the target atom in its ground state i, the asymptotic conditions satisfied by $X_j^{\pm}$'s are

$$X_j^{\pm}(\vec{r}) \xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} \delta_{ji} + F_{ji}^{\pm}(\vec{k}_j,\vec{k}) \frac{e^{ik_j r}}{r} . \quad \ldots (1.13)$$

The interaction potential $V(\vec{r},\vec{x})$ for electron-atom scattering is of the form

$$V(\vec{r},\vec{x}) = -\frac{Z e^2}{r} + \sum_{j=1}^{Z} \frac{e^2}{|\vec{r} - \vec{x}_j|} , \quad \ldots (1.14)$$

where e is the electronic charge and Z is the atomic number.

Eq. (1.9) is exact if all the terms in the expansion, Eq.(1.8), are taken into account. In its present form it is not practically solvable. One needs an approximation to simplify the infinite set.

(ii) The Close Coupling Approximation

This approximation[1] retains the first few states in the infinite summation in Eq.(1.8) and neglects the effect of the rest. The order of the approximation depends on the number of atomic states which are retained out of the infinite summation. This method has been successful in predicting resonances but less successful in treating excitation processes showing a lack of convergence with respect to the addition of more atomic states into the trial wavefunction expansion[2,3]. Improvement to this method has been suggested by Smith[2] and Burke[3]. The truncated summation leads to the neglect of the coupling with the higher discrete states and with the continuum; this, in turn, leads to the partial neglect of adiabatic and non-adiabatic polarization[4,5] of the target. These long range polarization effects arise due to the interaction between the electric field of the incident electron and the induced multipole moments in the target. The adiabatic approximation assumes that the incident electron is moving so slowly that its kinetic energy operator can be neglected.

The adiabatic polarization potential[4] ($\sim \frac{1}{r^4}$) effective at large separation r is attractive in nature and using the perturbation theory it comes out to be of second order in the interaction energy. The perturbation induced in the target orbital by a moving charge is reduced as compared to that due to a stationary charge at the same distance because of the decreasing time of interaction. This velocity dependence of the target orbital gives rise to a 'dynamic' or 'non-adiabatic' polarization potential which is constructed by applying the kinetic energy operator of the incoming particle on the static polarized wavefunction of the target. The non-adiabatic potential ($\sim 1/r^6$) being repulsive in nature reduces the effect of the adiabatic part. These long range effects can not be neglected at intermediate (roughly two times the threshold to twenty times the threshold) and low electron impact energies. It is found that about 18.6% of the dipole polarizability (induced dipole moment per unit electric field) of the hydrogen atom and about 54.6% of that of the helium atom comes from the continuum states only[1,7]. Obviously, an adequate description of the scattering process needs proper allowance of these continuum states which in turn, leads to the polarization effects. An alternative approach, the so-called pseudo-state approximation[7] accounts for the higher states and the continuum of the target by replacing them by pseudostates. These pseudostates are chosen to be orthogonal to each other and to the first few atomic eigenstates included in the eigenfunction expansion, such that

they give the exact polarizability of the atom.

The approaches discussed above require knowledge of a number of atomic eigenstates of the target included in the eigenfunction expansion. These eigenfunctions of the target are usually determined by Hartree-Fock self-consistent field (SCF) method[8,9]. It is thus evident that these approaches involve a lot of computational labour even if a few eigenstates in the infinite summation are employed in order to account for the polarization of the target.

(iii) Method of the Polarized Orbitals

This method, developed by Temkin[10] and Temkin and Lamkin[11] takes account of the polarization of the target by just adding a 'perturbing part' representing the polarization of the target to the unperturbed wavefunction. The first order perturbation theory is employed to calculate this part of the wavefunction and the infinite set, Eq.(1.9), is reduced to just one integro-differential equation. The computational labour is thus reduced considerably, but at the cost that all channels other than the initial one are taken to be closed. The method of polarized orbitals is only applicable to very low energy (less than the first excitation threshold of the target)elastic scattering.

(iv) Comments

There are other approximate methods, such as variational approximation[12,13], the second order potential method of Bransden et al[14] and so on, which can also be used to solve

the integro-differential equations. All these methods employ, in one way or the other, the partial-wave analysis. The number of significant partial waves in the partial wave expansion increases with increasing energy. Obviously, at intermediate and high energies this number will become quite large. LaBahn and Callaway[15] have considered in the forward direction as many as 10,051 partial waves for e-He elastic scattering in the 100-500 eV energy range.

All these quantal methods thus seem quite impracticable to study scattering processes at high electron impact energies where large number of channels are open for scattering. In order to tackle the scattering problems in the said energy region we, therefore, seek an alternative approach which does not involve partial wave analysis. Such an approach is obtained by expressing the Schroedinger equation, instead of integro-differential form, in an inhomogeneous integral form:

$$X_j^{\pm}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}.\vec{r}} \delta_{ji} + \sum_{j'} \int \mathcal{G}_{k_{j'}}(\vec{r},\vec{r}') U_{jj'}(\vec{r}') X_{j'}^{\pm}(\vec{r}') d^3r'$$

$$\pm \sum_{j'} \int \mathcal{G}_{k_{j'}}(\vec{r},\vec{r}') \mathcal{F}_{jj'}(\vec{r}',\vec{x}') X_{j'}^{\pm}(\vec{x}') d^3r' d^3x', \qquad \ldots (1.15)$$

where $\mathcal{G}_{k_j}$ is the free Green's function for energy $k_j^2$ and is given by

$$\mathcal{G}_{k_j}(\vec{r},\vec{r}') = -\frac{1}{4\pi} \frac{e^{ik_j|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}. \qquad \ldots (1.16)$$

The solution $X_j^{\pm}$, Eqs.(1.15), when compared with its asymptotic

form, Eq.(1.13), yields expressions for the direct and the exchange scattering amplitudes represented by $F_{fi}(\vec{k}', \vec{k})$ and $g_{fi}(\vec{k}', \vec{k})$ respectively.

$$F_{fi}^{\pm}(\vec{k}', \vec{k}) = F_{fi}(\vec{k}', \vec{k}) \pm g_{fi}(\vec{k}', \vec{k}) \qquad \ldots (1.17)$$

$$F_{fi}(\vec{k}', \vec{k}) = -\frac{1}{4\pi} \sum_j \int e^{-i\vec{k}'.\vec{r}'} U_{fj}(\vec{r}') X_j^{\pm}(\vec{r}') d^3r' \qquad \ldots (1.18)$$

$$g_{fi}(\vec{k}', \vec{k}) = -\frac{1}{4\pi} \sum_j \int e^{-i\vec{k}'.\vec{r}'} \mathcal{F}_{fj}(\vec{r}', \vec{x}') X_j^{\pm}(\vec{x}') d^3r' d^3x'. \qquad \ldots (1.19)$$

The expressions (1.18) and (1.19) are formal in the sense that they involve summation over infinite set of target eigenstates which , in turn, lead to infinite coupled integral equations. Thus, to obtain a practical solution of these equations we seek approximate methods, quantal as well as semi-classical, which ever suit better according to the physical conditions (such as energy).

(V) Born Series Approximations

At high energies the exchange effects can be neglected because of a small interaction time. The inhomogeneous integral Eq.(1.15) then reduces to the standard Lippmann-Schwinger equation

$$X_j(r) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}.\vec{r}} \delta_{ji} + \sum_{j'} \int \mathcal{G}_{k_{j'}}(\vec{r}, \vec{r}') U_{jj'}(\vec{r}') X_{j'}(\vec{r}') d^3r'. \qquad \ldots (1.20)$$

The iterative solution of this equation give rise to an infinite perturbation series for the perturbed wavefunction, $X_j$, of the system and is known as Born series.

First Born approximation is obtained when the unperturbed wavefunction [first term in Eq.(1.20)] is substituted for the perturbed wavefunction $X_j$ yielding the scattering amplitude:

$$F_{fi}^{B1}(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\int e^{-i\vec{k}'.\vec{r}}\,\phi_f^{*}(\vec{x})\;U(\vec{r},\vec{x})\,\phi_i(\vec{x})\;e^{i\vec{k}.\vec{r}}\;d^3r d^3x \qquad \ldots (1.21)$$

$$= -\frac{1}{4\pi}\int e^{i\vec{\Delta}.\vec{r}}\;U_{fi}(\vec{r})\;d^3r \quad . \qquad \ldots (1.22)$$

It clearly implies that FBA ignores the distortion of the incident particle wavefunction as well as the polarization of the target and this explains why FBA, even with the inclusion of exchange, does not provide satisfactory agreement with the experimental differential cross section data.

The distortions of the target are taken into account partially by the second Born approximation (SBA). The SBA scattering amplitude can be easily obtained by substituting the first iterative solution of Eq.(1.20) for $X_j$ and then comparing it with the asymptotic behaviour, Eq.(1.13):

$$F_{fi}^{B2}(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\sum_j \int e^{i(\vec{k}.\vec{r}'-\vec{k}'.\vec{r})}\,\mathcal{G}_{k_j}(\vec{r},\vec{r}')$$

$$\times U_{fj}(\vec{r})\;U_{ji}(\vec{r}')\;d^3r\;d^3r'. \qquad \ldots (1.23)$$

It is clear from Eq.(1.23) that SBA involves an infinite summation over the intermediate discrete and the continuum

states of the target. This makes it very difficult to evaluate it exactly. However, it can be simplified by setting $k_j = k$ for all j[16], where k is independent of j. The summation in Eq.(1.23) can then be performed by using the closure method

$$\sum_j \phi_j^*(\vec{x})\ \phi_j(\vec{x}') = \delta(\vec{x} - \vec{x}'). \qquad \ldots (1.24)$$

Moiseiwitsch[17] has pointed out that this closure approximation corresponds to taking infinite value for the polarizability of the atom and results in a logarithmic divergence in the imaginary part of the forward scattering amplitude. The logarithmic divergence can be removed easily by introducing non-zero average excitation energy of the target. Using closure methods SBA can still be obtained in a relatively simple way[18-25]. The simplified SBA is better, in the intermediate and high energy region, than the partial wave analysis but it still involves considerable labour due to the inclusion of a large number of terms which are to be evaluated exactly[20-23].

(vi) Plane Wave Approximation (PWA)

This approximation takes into account the distortion of the target in the form of local potentials but completely neglects the distortion of the incident particle. The local distortion potential is taken to be the sum of the adiabatic and non-adiabatic polarization potentials[4,5]. This approach deals with the infinite sum of SBA in terms of the well known

properties of the target such as dipole and quadrupole polarizibilities etc. The exchange contribution can also be included directly. This approach has been used by Khare and Shobha[26,27] to study e-He elastic scattering cross sections.

(vii) Distorted Waves Approximation (DWA)

The SBA makes partial allowance for the effect of distortion. A better account of the distortion of the incident and scattered waves can be achieved in a two state approximation involving just the initial state (say, the ground state) and another coupled state f( which is chosen to be the finally excited state in case of excitation). The coupling to all other states except these two states, giving rise to polarization, is neglected. This simplifies the infinite set of coupled integrodifferential equations into a pair of coupled equations which are solved by the distorted waves approximation[28] based upon the assumption that the back coupling of the final state f to the initial state i is small. The solution of the resulting equations requires the partial wave analysis to obtain the cross sections. The method is, therefore, not practicable at high energies.

(viii) Exchange Approximations

In the above description we have not included exchange effects assuming that the impact energies are high enough to neglect them. At intermediate energies they can not be neglected. They can be easily included to the

non-exchange (Born) amplitudes discussed above through the relation (1.17). We discuss below some of the simplest exchange approximations in order to evaluate Eq.(1.19).

(a) Born-Oppenheimer Approximation (BOA)

Since we are interested in electron exchange phenomenon, the projectile particle is an electron. The recoil effects of the target are then negligible as compared with the motion of the projectile electron and the CM system coincides with the laboratory system. The earlier results are true even in the laboratory system with the modifications that the CM wave numbers k and k' are replaced by the corresponding laboratory quantities $\vec{k}_i$ and $\vec{k}_f$, and $\vec{\Delta} = \vec{k}-\vec{k}'$ is replaced by $\vec{q} = \vec{k}_i-\vec{k}_f$. Here $\vec{k}_i$ and $\vec{k}_f$ are now the initial and final momenta of the projectile electron.

The exchange amplitude for e-atom scattering in BOA can be obtained from Eq.(1.19) by substituting, for the perturbed wavefunction $X_j$, the unperturbed wavefunction

$$X_j^{\pm}(\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}_i\cdot\vec{x}} \delta_{ji} , \qquad \ldots (1.25)$$

yielding BOA amplitude in the lab. system as

$$g_{fi}^{BO}(\vec{k}_f,\vec{k}_i) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int e^{-i\vec{k}_f\cdot\vec{r}'}\phi_f^*(\vec{x})\left[H(\vec{r},\vec{x})-E\right]\phi_i(\vec{r}')e^{i\vec{k}_i\vec{x}}d^3r'd^3x . \qquad \ldots (1.26)$$

Eq.(1.26) can further be simplified if we assume that each target electron contributes equally to the exchange scattering.

The situation is then identical to the e-H atom exchange scattering. Eq.(1.26) can now be readily shown to yield

$$g_{fi}^{BO}(\vec{k}_f, \vec{k}_i) = -\frac{1}{4\pi} Z \int e^{-i\vec{k}_f\cdot\vec{r}} \phi_f^x(\vec{x})\, U'(\vec{x},\vec{r})\, \phi_i(\vec{r}) \times e^{i\vec{k}_i\vec{x}}\, d^3r\, d^3x, \qquad \ldots (1.27)$$

where $\vec{x}$ now corresponds to single target-electron coordinate and $U'(\vec{x},\vec{r})$ is the e-H atom interaction potential in prior form:

$$U'(\vec{x},\vec{r}) = \frac{2\mu}{\hbar^2}\left(-\frac{e^2}{x} + \frac{e^2}{|\vec{r}-\vec{x}|}\right), \qquad \ldots (1.28)$$

whereas Eq.(1.14) denotes the post-form of interaction potential. Eq.(1.27) can also be obtained from the direct (Born) scattering amplitude, Eq.(1.21a), simply by interchanging the incident and target electron coordinates in the incident wavefunction as well as in the interaction potential. The BOA scattering amplitude suffers from the undesirable feature that the addition of a constant to the interaction potential U leaves unaltered the exchange scattering amplitude owing to the lack of orthogonality between the approximate initial and final state wavefunctions of the system[20]. This, in turn, leads to very large values for the exchange cross section which, very often, exceed conservation limits especially near threshold. BOA also leads to the post-prior discrepancy in the exchange scattering amplitude.

(b) Ochkur Approximation

Ochkur[29] suggested that better results can be obtained if, instead of using the full BOA expression for the scattering amplitude, one retains only the leading term in the expansion

of BOA amplitude in powers of $k_i^{-1}$. Writing Eq.(1.27) as

$$g_{fi}(\vec{k}_f, \vec{k}_i) \equiv g_{fi}^{(1)} + g_{fi}^{(2)}, \qquad \ldots (1.29)$$

where

$$g_{fi}^{(1)} = \frac{Ze^2}{4\pi} \int d^3r \phi_i(\vec{r}) e^{-i\vec{k}_f \cdot \vec{r}} \int d^3x \frac{\phi_f^*(\vec{x})\, e^{i\vec{k}_i \cdot \vec{x}}}{x}, \qquad \ldots (1.30)$$

and

$$g_{fi}^{(2)} = -\frac{Ze^2}{4\pi} \int d^3r \phi_i(\vec{r}) e^{-i\vec{k}_f \cdot \vec{r}} \int d^3x \frac{\phi_f^*(\vec{x})\, e^{i\vec{k}_i \cdot \vec{x}}}{|\vec{r} - \vec{x}|}, \qquad \ldots (1.31)$$

and using appropriate target eigenfunction, one can easily see that $g_{fi}^{(1)}$, which corresponds to the electron-proton contribution, behaves as $1/k^6$. Using the peaking approximation[30] in the second integral of Eq.(1.31), yields

$$\begin{aligned} g_{fi}^{(2)} &= -\frac{Z}{k_i^2} \int d^3r\, \phi_i(\vec{r}) e^{-i\vec{k}_f \cdot \vec{r}}\, \phi_f^*(\vec{r}) e^{i\vec{k}_i \cdot \vec{r}} \\ &= -\frac{Z}{k_i^2} \int d^3r\, e^{i\vec{q} \cdot \vec{r}}\, \phi_f^*(\vec{r}) \phi_i(\vec{r}) \\ &= -\frac{Z q^2}{k_i^2} F_{fi}^H(\vec{k}_f, \vec{k}_i), \qquad \ldots (1.32) \end{aligned}$$

where $F_{fi}^H$ denotes the direct scattering amplitude for e-H scattering.

Since $g_{fi}^{(1)}$ decays much faster than $g_{fi}^{(2)}$, the first term in Eq.(1.29) is neglected. Thus the exchange scattering amplitude in Ochkur approximation[29] takes the form

$$g_{fi}^{Och} \simeq -\frac{Z}{k_i^2} \int d^3r e^{i\vec{q} \cdot \vec{r}} \phi_f^*(\vec{r}) \phi_i(\vec{r}). \qquad \ldots (1.33a)$$

$$= -\frac{Z q^2}{k_i^2} F_{fi}^H(\vec{k}_f, \vec{k}_i). \qquad \ldots (1.33b)$$

For an unpolarized incident beam the relative probability in the singlet and triplet states is 1:3 so the mean differential cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{k'}{k}\left[ \frac{1}{4} |F_{fi}^{+}(\vec{k}_f,\vec{k}_i)|^2 + \frac{3}{4}|F_{fi}^{-}(\vec{k}_f,\vec{k}_i)|^2 \right]$$

$$= \frac{k'}{k}\left[ \frac{1}{4}|F_{fi}+ g_{fi}|^2 + \frac{3}{4}|F_{fi}-g_{fi}|^2 \right]$$

$$= \frac{k'}{k}\left[ |F_{fi}|^2+|g_{fi}|^2-\mathrm{Re}(F_{fi}g_{fi}^{*}) \right]. \qquad \ldots (1.34)$$

1.2.3 CLASSICAL APPROXIMATIONS

Classical approaches in the study of scattering phenomenon have received attention because of the following reasons. The gain in accuracy by the use of quantum theory is lost to some extent in making the various approximations. Further for a complex atomic or molecular system the task of solving the quantum mechanical scattering equations leads to great many analytical and computational difficulties. On the other hand, the cross-sections obtained from the classical calculations by Gryzinski[31] and Stabler[32] have simple analytic form and may be evaluated conveniently. In all the classical approaches, the collision is treated as a binary electron-electron encounter. The transfer of energy from the incident to the bound electron during a collision is computed as if the two electrons were free. The energy transfer must, therefore, be large compared to the binding energy of the atomic electron. Hence the methods are best suited for ionizing collisions. However, for excitation also, approximate results can be obtained. In a more refined

classical approach, proper allowance for the velocity of atomic electrons is made by averaging over the velocity distributions of the bound electrons in various ways to obtain cross section for the process of interest[31]. The results suggest that these procedures may be reasonable if only order of magnitude estimates are required. Another drawback is that they predict a $E^{-1}$ decay of the cross sections which is a more rapid fall than the predicted $E^{-1}\ln E$ fall by the quantum theory. In order to obtain a correct high energy behaviour Burgess[33] has tried to combine the binary encounter theory with the impact parameter method. He has used classical approach at low energies and semi-classical impact parameter approach at high energies.

(i) Comments

All the methods discussed so far are either mathematically complex because of involving enormous computational labour (quantal case) or unable to provide correct energy dependence of cross sections and are reasonable only if order of magnitude cross sections are required (classical case). We, therefore, seek to attempt some semi-classical approaches to get physically reasonable and mathematically simple and tractable expressions for the scattering amplitudes.

1.2.3 SEMI-CLASSICAL APPROXIMATIONS

From the theory of optics it is well known that when the wavelength of light is small compared with the distance

over which the refractive index changes appreciably, the rays which follow the laws of geometrical optics can be defined. In the same way, if the wavelength ($\lambda = 1/k$) of a particle is sufficiently short compared with the distance over which the potential changes appreciably, it is possible to define particle trajectories which obey the laws of classical mechanics. If the potential V is of range a, the short wavelength condition (classical optics) requires

$$k\,a \gg 1 \,. \qquad \ldots (1.35)$$

When the classical condition holds, the angle of scattering $\theta$ must be well defined, that is, the uncertainty $\delta\theta$ in the angle of scattering must be small compared with $\theta$. The uncertainty $\hbar\delta k$ in the transverse momentum imparted to the scattered particle is, by Heisenberg's uncertainty principle, of order $(\hbar/a)$. The corresponding uncertainty in the angle of scattering is

$$\delta\theta = \frac{\delta k}{k} \sim \left( \frac{1}{ka} \right). \qquad \ldots (1.36)$$

If $|V|$ is the magnitude of the potential within the range $0 < r < a$, the momentum transfer in the transverse direction, $\hbar\vec{\Delta}$, is of order

$$\hbar\Delta = \int F dt \sim \bar{F}t \qquad \ldots (1.37)$$

where the magnitude of the force, $\bar{F}$, is given by

$$\bar{F} \sim \frac{|V|}{a}\,, \qquad \ldots (1.38)$$

and the time taken in crossing the potential is given by

$$t = \int dt \sim a/v \qquad \ldots (1.39)$$

From this, it can be easily seen that the angle of scattering for small angles scattering is approximately given by

$$\theta \sim \frac{\hbar\Delta}{\hbar k}$$

$$\sim \frac{|V|}{\hbar k v} \sim \frac{|V|}{E}, \qquad \ldots (1.40)$$

where v is the speed of the particle in potential scattering. For classical condition to apply, we must have

$$\theta \gg \delta\theta \qquad \ldots (1.41a)$$

i.e. $$\frac{|V|a}{\hbar v} \gg 1 \qquad \ldots (1.41b)$$

Born approximation, as pointed out earlier, is also a high energy approximation but it applies to angles of scattering within the cone $\theta < \frac{|V|}{E}$, whereas the classical scattering condition applies when $\theta > 1/ka$, and the two regions do not overlap.

In order to fill up the gap between the two regions we, therefore, seek a semi-classical approximation which is intermediate in character between a full classical and a full quantal treatment, so that it may be valid for arbitrary values of the parameter $\frac{|V|a}{\hbar v}$ which combines the short wavelength condition ($ka \gg 1$) and high energy approximation ($|V|/E \ll 1$). One such approximation is the eikonal or ray approximation. In order to understand the underlying assumptions let us briefly present the derivation of the eikonal approximation, following Gerjuoy and Thomas[34].

Let us consider potential scattering. The wavefunction $\psi(\vec{r})$ is written as

$$\psi = A\, e^{iS} \quad , \qquad \ldots (1.42)$$

where $A(\vec{r})$ and $S(\vec{r})$ are chosen to be real. Using Eq.(1.42), the real and imaginary parts of the Schroedinger Eq.(1.4) yield respectively

$$\nabla^2 A - A(\vec{\nabla}S)^2 + (k^2 - U)A = 0 \quad , \qquad \ldots (1.43a)$$

$$2\vec{\nabla}A \cdot \vec{\nabla}S + A\nabla^2 S = 0 \quad , \qquad \ldots (1.43b)$$

where

$$k^2 = \frac{2mE}{\hbar^2} \qquad \ldots (1.44a)$$

$$U(\vec{r}) = \frac{2m}{\hbar^2} V(\vec{r}) \quad , \qquad \ldots (1.44b)$$

and m is the mass of the incident particle.

Eq.(1.43b) can be rewritten as

$$\vec{\nabla}\cdot(A^2\vec{\nabla}S) = 0, \qquad \ldots (1.45)$$

and expresses the flux conservation as

$$\frac{1}{2i}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*) = A^2\vec{\nabla}S \quad . \qquad \ldots (1.46)$$

So far no approximation has been made except that $V(\vec{r})$ has been considered to be real. Equation (1.43a) can not be solved, in general, without approximation. The fundamental eikonal approximation is the assumption

$$\frac{\nabla^2 A}{A} \ll k^2 \quad , \qquad \ldots (1.47)$$

in which case (1.43a) simplifies to

$$(\vec{\nabla}S)^2 = k^2 - U. \qquad \ldots (1.48)$$

The solution of this equation is

$$S(\vec{r}) - S(\vec{a}) = \int_{\vec{a}}^{\vec{r}} d\vec{r}' \cdot \hat{\zeta}\left[k^2 - U(\vec{r}')\right]^{1/2}, \qquad \ldots (1.49)$$

where $\vec{a}(\vec{r})$ is some initial point on the ray path through $\vec{r}$, and at each point $\vec{r}' = \vec{r}_o$ on the ray path the unit vector $\hat{\zeta}(\vec{r}_o)$ is perpendicular to the surface of constant S. Eq. (1.48) may be identified as the classical Hamilton-Jacobi equation, if $S(\vec{r})$ is identified with Hamilton's characteristic function. In optics this equation, which determines the rays, is called the eikonal equation and $S(\vec{r})$, the eikonal function. The integral form (1.49) of this equation determines the orbits, which are just those given by the more elementary theory of classical mechanics. Using Eq.(1.49), $A(\vec{r})$ can be evaluated, in principle at least, from (1.45) and hence the wavefunction $\psi$ in (1.42) can be found out.

Equation (1.47) may be regarded as a high energy approximation because $k^2$ is proportional to E. In the context of the wave theory, writing $k = 1/\lambda$, it is better thought of as a short wavelength approximation and may be written as

$$\lambda^2 \nabla^2 A \ll A. \qquad \ldots (1.50)$$

This equation holds only if, in a Taylor series expansion of $A(\vec{r})$ about any point $\vec{r}_o$, the non-linear terms are negligible

for distances $|\vec{r} - \vec{r}_o| \lesssim \lambda$. A more explicit high energy approximation to the eikonal $S(\vec{r})$ is obtained by making the Binomial expansion of the square root in Eq.(1.49) and taking the leading term, giving

$$S(\vec{r}) - S(\vec{a}) = \int_{\vec{a}}^{\vec{r}} d\vec{r}' \cdot \hat{\zeta} \left[ k - \frac{1}{2} \frac{U(\vec{r}')}{k} \right], \qquad \ldots (1.51)$$

which is valid when

$$U(\vec{r}) \ll k^2$$

or $$V(\vec{r}) \ll E \, . \qquad \ldots (1.52)$$

As is obvious, the integration path is still supposed to be along the actual rays perpendicular to the surfaces of constant $S(\vec{r})$. However, if curvature of the ray paths is neglected, using cylindrical coordinates $(\vec{r} \equiv \vec{b}, z)$, one gets

$$S(\vec{b},z) - S(\vec{b},a_z) = k(z-a_z) - \frac{1}{\hbar v} \int_{a_z}^{z} dz' V(\vec{b},z'), \qquad \ldots (1.53)$$

where the z-direction now has been chosen to coincide with the assumed every where constant ray direction $\hat{\zeta}$ in (1.51), so that the point $\vec{a}$ has component $(\vec{b}, a_z)$ when $\vec{r}$ has components $(\vec{b},z)$. In the scattering problem, the most obvious choice of z-direction and straight line (ray) integration path in (1.53) is the incident direction $\hat{k}$, in which case neglect of ray curvature amounts to a small angle approximation. The incident wavefronts, as pointed out earlier, are plane and uniformly spaced particularly at points far from the interaction region

where $a_z \to -\infty$, one can write

$$S(\vec{b}, a_z) = k\, a_z.$$

Thus, with the approximations made and with the plane wave incident along $z \equiv \hat{k}$, Eq.(1.53) takes the form (after letting $a_z \to -\infty$)

$$S(\vec{b},z) = kz - \frac{1}{\hbar v} \int_{-\infty}^{z} dz' V(\vec{b},z'). \qquad \ldots (1.54)$$

Moreover, if all ray paths are supposed to be parallel to $\hat{k}$, the spreading of the rays can be neglected. The conservation of flux now implies that $A^2$ is constant. Therefore, using the approximate form (1.54) with A supposed to be constant and the z-direction along $\hat{k}$, Eq.(1.42) finally yields,

$$\psi(\vec{r}) \to \psi^E(\vec{r}) = \exp(i\vec{k}.\vec{r}) \exp(-\frac{i}{\hbar v} \int_{-\infty}^{z} dz' V(\vec{b},z')). \qquad \ldots (1.55)$$

$\psi^E(\vec{r})$ is known as the eikonal wavefunction in potential scattering. Its use in the expression for the scattering amplitude (Ref.35, p.802)

$$f(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\langle\phi_f|V|\psi_i^{(+)}\rangle$$

$$= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r\, e^{-i\vec{k}'.\vec{r}}\, V(\vec{r})\psi_i^{(+)}(\vec{r}) \qquad \ldots (1.56)$$

forms the basis of the eikonal or ray approximation, yielding in cylindrical coordinates

$$f_E(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^2b\, dz\, e^{i\vec{\Delta}.(\vec{b}+\hat{k}z)} V(\vec{b},z) \exp(-\frac{i}{\hbar v}\int_{-\infty}^{z} dz' V(\vec{b},z')),$$

$$\ldots (1.57)$$

The momentum transfer vector $\vec{\Delta}$ can be assumed nearly perpendicular to the incident direction $\hat{k}$ for small angles of scattering $\theta$,

$$\vec{\Delta}.\hat{k}z = k(1-\cos\theta)z \simeq \tfrac{1}{2}\theta^2 kz. \qquad \ldots (1.58)$$

This is not an additional approximation as the eikonal approximation is only reliable at small angles, because of the assumption of straight-line (ray)trajectories. The maximum value of z of importance in the integration is $\sim a$, where a is the range of the potential, so that the term $\exp(i\vec{\Delta}.\hat{k}z)$ may be replaced by unity for angles such that

$$\theta^2 ka \ll 1. \qquad \ldots (1.59)$$

The z-integration in Eq.(1.57) can now be easily performed to give the eikonal scattering amplitude

$$f_E(\vec{k}',\vec{k}) = -\frac{ik}{2\pi}\int d^2b\; e^{i\vec{\Delta}.\vec{b}}\left[e^{i\chi(\vec{b})} - 1\right], \qquad \ldots (1.60)$$

where the eikonalphase function $\chi$ is

$$\chi(\vec{b}) = -\frac{1}{\hbar v}\int_{-\infty}^{\infty} dz'\, V(\vec{b},\vec{z}'). \qquad \ldots (1.61)$$

For central potentials, the integration in Eq.(1.60) over the azimuthal angle $\phi_b$ can also be performed to yield

$$f_E(\vec{k}',\vec{k}) = -ik\int_0^{\infty} db\; b\, J_0(\Delta b)\left[e^{i\chi(b)} - 1\right]. \qquad \ldots (1.62)$$

Various other forms of the eikonal approximation and its improved versions have been proposed. Their details are given in papers by Moliere[36], Malenka[37], Schiff[38], Saxon and

Schiff[39], Glauber[40], Blankenbecler and Goldberger[41], Feshbach[42], Willets and Wallace[43], Sugar and Blankenbecler[44], Levy and Sucher[45], Abarbanel and Itzykson[46], Moore[47], Wallace[48], Lebedeff[49], Baker[50], Obu[51] and Swift[52]. Glauber's approach[40] deserves special attention because of the fact that it clarifies the underlying assumptions and the ranges of applicability of the approximation in an explicit way. His approach originally applied to problems in nuclear physics has, at present, wide applications in atomic collisions. We shall discuss his approach in detail in the next chapter.

In order to assess the accuracy of the eikonal approximation we briefly analyse, in the next section, the eikonal scattering amplitude, Eq.(1.62), and compare it with the Born series.

## 1.3 THE EIKONAL MULTIPLE SCATTERING EXPANSION AND THE BORN SERIES

The exact scattering amplitude f has an expansion in powers of the interaction potential, namely, the Born series

$$f = \sum_{n=1}^{\infty} \bar{f}_{Bn}, \qquad \ldots (1.63a)$$

where

$$\bar{f}_{Bn} = -2\pi^2 \langle \Phi_f | U(G_o^{(+)} U)^{n-1} | \Phi_i \rangle. \qquad \ldots (1.63b)$$

In the above expression the potential $U( = \frac{2m}{\hbar^2} V)$ appears n times and the free Green's function $G_o^{(+)}$ (n-1) times. In analogy to Eq.(1.63a), we define the eikonal multiple

scattering series expansion:

$$f_E = \sum_{j=1}^{\infty} \bar{f}_{En} \,, \qquad \ldots (1.64a)$$

where

$$\bar{f}_{En} = -ik \frac{i^n}{n!} \int_0^{\infty} db\, b\, J_0(\Delta b) \left[\chi(b)\right]^n. \qquad \ldots (1.64b)$$

We also define $f_{Bn}$ and $f_{En}$, respectively, as the sum of the first n terms of Eqs.(1.63a) and (1.64a). Thus,

$$f_{Bn} = \sum_{j=1}^{n} \bar{f}_{Bj} \qquad \ldots (1.65)$$

and

$$f_{En} = \sum_{j=1}^{n} \bar{f}_{Ej}. \qquad \ldots (1.66)$$

Obviously as $n \to \infty$, $f_{Bn} \to f$ and $f_{En} \to f_E$. We note from Eq.(1.64b) that for real potential the objects $\bar{f}_{Ej}$ are alternately real and imaginary. We now investigate term by term the eikonal and Born series in the semi-classical limit $ka \gg 1$. First of all it is easy to see that

$$f_{E1} = f_{B1} \qquad \ldots (1.67)$$

for all energies and all momentum transfers[40]. We emphasize that the result (1.67) is valid for all angles only when the z-axis used in evaluating the eikonal phase shift function $\chi(b)$ [Eq.(1.61)] is chosen along a direction perpendicular to $\vec{\Delta}$.

Relationships between the higher terms of the eikonal and Borns series have been investigated recently[47,48,52-54]. Byron et al[54] have made a detailed analysis

of this problem for a variety of real central potentials.

For Yukawa-type potentials and for $ka \gg 1$, they have got the Born and eikonal series expansions in the forms:

$$f = \bar{f}_{B1}(\Delta) + \underbrace{\left[\frac{A(\Delta)}{k^2} + \frac{i\,B(\Delta)}{k}\right]}_{\bar{f}_{B2}} + \underbrace{\left[\frac{C(\Delta)}{k^2} + \frac{iD(\Delta)}{k^3}\right]}_{\bar{f}_{B3}} + \ldots . \qquad \ldots (1.68)$$

and

$$f_E = \bar{f}_{B1}(\Delta) + \underbrace{i\,\frac{B(\Delta)}{k}}_{\bar{f}_{E2}} + \underbrace{\frac{C(\Delta)}{k^2}}_{\bar{f}_{E3}} + \ldots . \qquad \ldots (1.69)$$

It is evident, by comparing Eqs.(1.68) and (1.69), that neither $f_{B2}$ nor $f_{E2}$ are correct to order $k^{-2}$. However, since the coefficient $A(\Delta)$ is proportional to $U_o^2$ while $C(\Delta)$ is proportional to $U_o^3$, where $U_o$ is the maximum value of $U$, it is clear that in the weak coupling situation

$$\frac{|V|a}{\hbar v} = \frac{|U_o|a}{2k} \ll 1, \qquad \ldots (1.70)$$

the second Born amplitude should be more accurate than the eikonal amplitude. As the coupling increases in such a way that $|V|a/\hbar v \simeq 1$ but $|V|/E < 1$, the eikonal method should improve steadily. Even for strong coupling situation, for which $|V|a/\hbar v > 1$ and $|V|/E > 1$, Byron et al [54] argue that the eikonal approximation is still accurate at small angles if $k a \gg 1$ is satisfied. This implies that the traditional criteria, Eqs.(1.35) and (1.52), are only sufficient conditions which are often unnecessarily rigid.

A similar comparison of the two series has also been made recently by Byron and Joachain[24,55,56] for collisions involving composite bodies. On the basis of this comparison Byron and Joachain[24] propose that in electron-atom scattering the direct (non-exchange) scattering amplitude (through terms of orders $k^{-2}$) be computed from the relation

$$F = \bar{F}^{B1} + \mathrm{Re}\,\bar{F}^{B2} + \bar{F}^{E3} + i\mathrm{Im}\,\bar{F}^{B2} + \ldots, \quad \ldots (1.71)$$

where $F^N$ denotes the generalized form of the direct scattering amplitude $f_N$ for collisions involving composite bodies (say, electron-atom scattering). This treatment is referred to as the eikonal-Born series (EBS) approximation. Byron and Joachain[24,55-57] have followed this treatment to study the elastic scattering and Byron and Latour[58] have extended it to study excitations of hydrogen and helium atoms by electron and position impact. In order to be consistent through terms $\sim k^{-2}$, they have also included exchange effects through Ochkur approximation[29].

## 1.4 PLAN OF THE THESIS

This thesis contains the work we did to study the scattering of charged particles by atomic and ionic targets at high and intermediate energies. It may be argued on the basis of foregoing discussion that a semi-classical approximation is better suited at these energies. In all the problems investigated here we have used eikonal approximation or Glauber approximation (which is a special case of the former).

We, therefore, completely devote the next chapter to a review of the Glauber approximation in order to understand the underlying assumptions and the ranges of applicability. An explicit expression of the wavefunction, the result (1.55), and hence the expression for the scattering amplitude is given, following Glauber[40] and Gerjuoy and Thomas[34], in both the potential scattering and the collisions involving composite bodies. In the case of collisions involving composite bodies, the importance of a proper choice of the z-(quantization) axis is emphasized.

In Chapter 3, we point out the inefficiency of the closed form expressions of the Glauber scattering amplitude for e-H atom scattering obtained by Thomas and Gerjuoy[59] to study excitation to highly excited states from a low lying state. This arises because of the increasing number of hypergeometric functions depending on the principal quantum number of the excited state. We have overcome this shortcoming by combining the techniques of Franco[60] and Golden and McGuire[61] and treating the Laguerre polynomials appearing in hydrogen atom wavefunctions straightaway rather than breaking them into a series of terms of the form $x^{\mu} e^{-\nu x}$. The usefulness of the one-dimensional Glauber scattering amplitudes thus obtained is commented upon in the study of the excitations of hydrogen atom.

In Chapter 4 we discuss the complications involved in the Glauber scattering amplitude when we study scattering from targets more complicated than the hydrogen atom. These were

usually handled in frozen core Glauber approximation. The calculations of Mathur et al[62] and Walters[63] fall under this class. Franco[60] gave an analytical procedure of converting the (3Z+2)-dimensional integral appearing in the Glauber scattering amplitude for scattering of charged particles from a Z-electron atom into a one-dimensional integral. We have looked at the numerical tractability of Franco's reduction procedure by applying his final expression to the elastic scattering and the 2s - 2p excitation of Li by electron impact. To avoid the encounter with divergent(${}_1F_2$) hypergeometric functions appearing in Franco's final expression, an alternative is suggested. This alternative puts our final expression in a two-dimensional integral form. The results obtained are compared with those of Walters[63] and the experimental data of Leep and Gallagher[64]. This procedure is also used to estimate the percentage polarization of the 2p → 2s resonance line emitted from $^6$Li and $^7$Li by electron impact.

The study of the charged particle scattering from ionic targets presents complications because of the involvement of a pure Coulomb (long-range) interaction between the projectile and the target ion. In Chapter 5, we consider such a problem. The pure Coulomb part is separated out from the total interaction and its contribution is taken into account exactly. The remaining interaction is then treated in eikonal-optical model[65-68]. The total scattering amplitude is then obtained by adding coherently the two parts. We apply this procedure to study scattering from helium like

ions, such as $H^-$ and $Li^+$. There is no experimental data with which these results could be compared. To get some feeling on the procedure adopted here, we have compared our results with those of McDowell[69].

In Chapter 6, we attempt to improve the behaviour of the Glauber approximation at large scattering angles. The poor performance of the Glauber approximation compared to even the first Born approximation is due to the improper semi-classical treatment of the electron-atom interaction[70]. We resolve this shortcoming by proposing a two potential Glauber-distorted Born approximation. We apply it to the elastic e-H(1s) scattering. The exchange effects, significant in the energy range of interest, are included through Ochkur approximation[29]. The results are compared with those obtained by two-potential eikonal approach[70] and the eikonal-Born series analysis[24] and with the recent experimental data of Teubner et al[71], Lloyd et al[72] and Williams[73]. The main feature of this procedure is the simplicity of calculations; it is hardly any more difficult than the ordinary Glauber approximation.[40]

# CHAPTER 2

# THE GLAUBER APPROXIMATION

## 2.1 INTRODUCTION

The Glauber approximation belongs to the class of so called eikonal approximations and is just one example of the many possible quantum mechanical approximations in this class. This point, as pointed out by Gerjuoy and Thomas[34] is not clear from the derivation of Glauber[40], but is apparent from the structure of the Glauber formula for the scattering amplitude. The Glauber version has the distinction of being one of the simplest eikonal approximations. This feature is not too significant in the potential scattering case, but is extremely important in the evaluation of eikonal scattering amplitudes for more complicated collisions. In the next section we derive the Glauber approximation, describe its basic underlying assumptions and discuss its limitations in energy and scattering angle. An alternative derivation of the Glauber approximation, using linearized Green's propagator, will also be outlined in order to understand the underlying assumptions of the approximation. Sec. 2.3 deals with the derivation of the Glauber formula for collisions involving composite bodies.

## 2.2 POTENTIAL SCATTERING

We proceed to derive the Glauber formula[40] for potential scattering. We assume that the interaction potential is short-range i.e. non-Coulombic. Otherwise, as Glauber

pointed out, the eikonal path integral diverges and theoretical development is meaningless. Nevertheless, use of the Glauber approximation even for Coulombic potentials in atomic collisions is not unreasonable; this extension will also be discussed below.

## 2.2.1 GLAUBER'S DERIVATION

For an incident wave $\phi_{\vec{k}} = \frac{1}{(2\pi)^{3/2}} \exp(i\vec{k}.\vec{r})$, the outgoing scattering solution $\psi_i^{(+)}(\vec{r})$ to the Schroedinger equation,

$$(-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r})-E)\psi_i^{(+)}(\vec{r}) = 0, \qquad \ldots (2.1)$$

satisfies the Lippmann-Schwinger integral equation

$$\psi_i^{(+)}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \exp(i\vec{k}.\vec{r}) - \frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}')\psi_i^{(+)}(\vec{r}') \qquad \ldots (2.2)$$

which, via the asymptotic condition

$$\psi_i^{(+)}(\vec{r}) \xrightarrow{r\to\infty} \left[ \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}.\vec{r}} + f(\vec{k}',\vec{k}) \frac{e^{ik'r}}{r} \right] \qquad \ldots (2.3)$$

yields the scattering amplitude

$$f(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2} T_{fi}, \qquad \ldots (2.4a)$$

where

$$T_{fi} = (2\pi)^{3/2} \int d^3r\, e^{-i\vec{k}'.\vec{r}}\, V(\vec{r})\, \psi_i^{(+)}(\vec{r}) \qquad \ldots (2.4b)$$

for scattering from initial direction $\hat{k}$ into final direction $\hat{k}'$. Here $\psi_i^{(+)}$ is an outgoing scattering eigenstate of H corresponding

to an incident plane wave of momentum $\hbar\vec{k}$. Following Glauber[40] we write

$$\psi_i^{(+)}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} \rho(\vec{r}). \qquad \ldots (2.5)$$

where $\rho(\vec{r})$ is a correction or modulating factor to the incident plane wave; its deviation from unity measures the scattering effects of the potential. Making the change of variable $\vec{r}' = \vec{r}-\vec{r}''$, Eq.(2.2) becomes

$$\rho(\vec{r}) = 1 - \frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r'' \frac{e^{ikr''}}{r''} e^{-i\vec{k}'\cdot\vec{r}''} V(\vec{r}-\vec{r}'')\rho(\vec{r}-\vec{r}''). \qquad \ldots (2.6)$$

The integral Eq.(2.6) for $\rho(\vec{r})$ is exact. Glauber now makes the following assumptions

(i) $ka \gg 1$, (classical) ... (2.7a)

(ii) $|V|/E \ll 1$, (quantum). ... (2.7b)

These conditions amount to requiring that V and $\rho$ vary slowly within a particle wavelength ($\lambda = \frac{1}{k}$). The detailed explanation of these conditions has already been given in Chapter 1. Glauber[40] further assumes that the product $V\rho$ also varies slowly within a particle wavelength so that negligibly small contribution to the integral on the right in Eq.(2.6) comes from regions in which the exponential oscillates rapidly. If we consider points $\vec{r}$ which lie within the volume occupied by the potential, the largest contribution to the integral will come from the values of $\vec{r}''$ lying close in direction to $\vec{k}$, since for these the exponential is nearly stationary. The quantitative expression under this approximation

is obtained by carrying out the angular integration over $\vec{r}''$ under the asymptotic approximation $r \to \infty$. Writing the differential element $d^3r''$ as

$$d^3r'' = r''^2 dr'' d\mu d\phi,$$

where

$$\mu = \cos(\hat{k}, \hat{r}'')$$

and $\phi$ is the azimuthal angle, the integration over $\mu$ is carried out by parts. If we suppose that the product $V\rho$ varies appreciably only within a distance d which is taken here to be much larger than $\lambda$, we get for the integral Eq.(2.6), the value

$$\rho(\vec{r}) = 1 + \frac{2m}{4\pi\hbar^2} \int dr'' d\phi \left[ \frac{e^{ikr''(1-\mu)}}{ik} V(\vec{r}-\vec{r}'') \rho(\vec{r}-\vec{r}'') \right]_{\mu=-1}^{\mu=+1}$$

$$+ O\left(\frac{1}{kd}\right). \qquad \ldots (2.8)$$

The terms neglected by the asymptotic approximation, are as indicated, of relative order 1/kd. Now the limit $\mu = -1$ corresponds to $\vec{r}''$ antiparallel to k. Since the exponential varies rapidly in this case, the contribution of the $\mu = -1$ term is of order 1/kd and is, therefore, negligibly small. The Eq.(2.8) corresponding to points of stationary phase $(\vec{r}'' \| \vec{k})$ becomes

$$\rho(\vec{r}) = 1 - \frac{i}{\hbar v} \int_0^\infty V(\vec{r}-\vec{r}'') \rho(\vec{r}-\vec{r}'') \Big|_{\vec{r}'' \| \vec{k}} dr''. \qquad \ldots (2.9)$$

In Cartesian coordinates, with the z-direction along $\hat{k}$, Eq.(2.9) is

$$\rho(x,y,z) = 1 - \frac{i}{\hbar v}\int_{-\infty}^{z} dz' V(x,y,z')\rho(x,y,z'), \qquad \ldots (2.10)$$

after returning to our original coordinates $\vec{r}$ and $\vec{r}'$ in Eq.(2.2) via $z'' = z-z'$. The solution to Eq.(2.10) is immediately seen to be

$$\rho(\vec{r}) \equiv \rho(x,y,z) = \exp\left[-\frac{i}{\hbar v}\int_{-\infty}^{z} dz' V(x,y,z')\right]. \qquad \ldots (2.11)$$

The appropriate wavefunction $\psi_i^{(+)}$ in Glauber approximation is, therefore,

$$\psi_i^{(+)}(\vec{r}) \to \psi_i^{E}(x,y,z) = \frac{1}{(2\pi)^{3/2}} \exp\left[ikz - \frac{i}{\hbar v}\int_{-\infty}^{z} dz' V(x,y,z')\right] \qquad \ldots (2.12)$$

This expression is missing a good many things one looks for in a three-dimensional scattering wavefunction, e.g., a spherical outgoing wave. But we must remember that the arguments from which it is derived are only intended to hold within the volume occupied by the potential. Therefore, expression (2.12) need not represent the wavefunction well elsewhere. This incorrect behaviour of $\psi^{E}(\vec{r})$ for large $\vec{r}$ cannot be argued on the basis of eikonal approximation derivation described in the previous chapter. Moreover, it is worth mentioning that Glauber's derivation of Eq.(2.12) shows that there is no need to assume $V(\vec{r})$ to be purely real as we did in the eikonel approximation of Chapter 1.

2.2.2 DERIVATION USING THE LINEARIZED PROPAGATOR

Let us consider the Fourier integral representation of the three-dimensional free Green's propagator

$$\psi_k^{(+)}(\vec{R}) = -\frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int \frac{d^3\kappa\, e^{i\vec{\kappa}.\vec{R}}}{\kappa^2 - k^2 - i\varepsilon}, \qquad \ldots (2.13)$$

where the limiting process $\varepsilon \to o^+$ is always implied.

Now the situation, we are attempting to describe ($ka \gg 1$, $|V| / E \ll 1$), is one in which the scattering is heavily concentrated at small angles. It is, in fact, very unlikely that at high energies in traversing the potential the particle will be deflected greatly from its initial direction $\hat{k}$. In momentum space we could, therefore, secure an approximation to the wavefunction by expanding its momentum dependence about the initial momentum $\vec{k}$. In an equivalent procedure[74] the momentum space dependence of Green's function can be expanded about $\vec{k}$, where only the values of $\vec{\kappa}$ near $\vec{k}$ in the integrand of Eq.(2.13) will be important. Making the substitution

$$\vec{\kappa} = \vec{k} + \vec{\tau}, \qquad \ldots (2.14)$$

and carrying out the expansion about $\vec{k}$, we have

$$\psi_k^{(+)}(\vec{R}) = \frac{-2m\, e^{i\vec{k}.\vec{R}}}{\hbar^2(2\pi)^3}\int \frac{d^3\tau\, e^{i\vec{\tau}.\vec{R}}}{\tau^2 + 2\vec{\tau}.\vec{k} - i\varepsilon}$$

$$= -\frac{2m\, e^{i\vec{k}.\vec{R}}}{\hbar^2(2\pi)^3}\int \frac{d^3\tau\, e^{i\vec{\tau}.\vec{R}}}{(2\vec{\tau}.\vec{k} - i\varepsilon)}\left[1 + \frac{\tau^2}{2\vec{\tau}.\vec{k} - i\varepsilon}\right]^{-1} \qquad \ldots (2.15)$$

$$\equiv \mathcal{G}_{\gamma_k}^{(1)}(\vec{R}) + \mathcal{G}_{\gamma_k}^{(2)}(\vec{R}) + \mathcal{G}_{\gamma_k}^{(3)}(\vec{R}) + \ldots \quad , \qquad \ldots (2.16)$$

where

$$\mathcal{G}_{\gamma_k}^{(1)}(\vec{R}) = -\frac{2m}{\hbar^2}\frac{e^{i\vec{k}.\vec{R}}}{(2\pi)^3}\int \frac{d^3\tau\, e^{i\vec{\tau}.\vec{R}}}{(2\vec{\tau}.\vec{k}-i\varepsilon)} \quad , \qquad \ldots (2.17)$$

$$\mathcal{G}_{\gamma_k}^{(2)}(\vec{R}) = +\frac{2m}{\hbar^2}\frac{e^{i\vec{k}.\vec{R}}}{(2\pi)^3}\int \frac{d^3\tau\, \tau^2 e^{i\vec{\tau}.\vec{R}}}{(2\vec{\tau}.\vec{k}-i\varepsilon)^2} \qquad \ldots (2.18)$$

and so on. For small scattering angles, we can approximate $\mathcal{G}_{\gamma_k}(\vec{R})$ by $\mathcal{G}_{\gamma_k}^{(1)}(\vec{R})$:

$$\mathcal{G}_{\gamma_k}(\vec{R}) \simeq \mathcal{G}_{\gamma_k}^{(1)}(\vec{R}) = -\frac{2m}{\hbar^2}\frac{e^{i\vec{k}.\vec{R}}}{(2\pi)^3}\int \frac{d^3\tau\, e^{i\vec{\tau}.\vec{R}}}{(2\vec{\tau}.\vec{k}-i\varepsilon)^2}. \qquad \ldots (2.19)$$

$\mathcal{G}_{\gamma_k}(\vec{R})$ represented by expression (2.19) is known as the linearized Green's propagator and can now be solved without further approximation. Using cylindrical coordinates ($\vec{R} = \vec{b}_1 + \hat{k}z_1$) with z-axis for $\vec{\tau}$-integration along $\hat{k}$, the integration over $\tau_{b_1}$ in Eq.(2.19) yields a two-dimensional $\delta$-function. The integration over $\tau_{z_1}$ yields a non-vanishing result only when the contour is closed at infinity in the upper half plane (because the linearization leaves us with a single pole lying always on the positive imaginary axis). Thus (2.19) reduces to

$$\mathcal{G}_{\gamma_k}^{(+)}(\vec{r}-\vec{r}') = -\frac{im}{k\hbar^2} e^{ik(z-z')}\delta(\vec{b}-\vec{b}')\Theta(z-z') \quad , \qquad \ldots (2.20)$$

where $\Theta$ is a Heavyside step function defined by

$$\Theta(z-z') = \begin{cases} 1 & \text{if } z > z' \\ 0 & \text{if } z \leqslant z' \end{cases} \quad , \qquad \ldots (2.21)$$

and the vectors $\vec{b}$ and $\vec{b}'$ are the components, perpendicular to

$\hat{k}$, of $\vec{r}$ and $\vec{r}'$. Using Eq.(2.20), the Lippmann-Schwinger Eq.(2.2) yields

$$\psi_i^{(+)}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{ikz}\left[1 - \frac{i}{\hbar v}\int_{-\infty}^{z} dz' e^{-ikz'} V(\vec{b}, z')\psi_i^{(+)}(\vec{b},z')\right]. \quad \ldots (2.22)$$

With the definition

$$\psi_i^{(+)}(\vec{r}) \equiv \frac{1}{(2\pi)^{3/2}} e^{ikz} \rho(\vec{b},z), \quad \ldots (2.23)$$

the Eq.(2.22) simplifies once more to the form (2.11). Basic content of this approximation is that the significant propagation occurs only in the forward direction at values, of $\kappa$, which are unmodified by the interaction $V(\vec{r})$; in other words the linearization approximation explains in a more elaborate way that the approximate wavefunction, Eq.(2.22), is only adequate for the treatment of small scattering angles and does not contain a correct estimate of the Fourier amplitudes corresponding to large momentum transfer. Quantitatively, the limitation on scattering angle $\theta$ may be given roughly by[40]

$$\theta^2 kd << 1. \quad \ldots (2.24)$$

### 2.2.3 EXPRESSION FOR THE SCATTERING AMPLITUDE

Using cylindrical coordinates with positive z-axis along $\hat{k}$, the vector $\vec{r}$ is

$$\vec{r} = \vec{b} + \hat{k}\, z\ , \quad \ldots (2.25)$$

and the expression (2.12) for the approximate wavefunction

$\psi_i^{(+)}$ is

$$\psi_i^{(+)}(\vec{b},z) \to \psi_i^E(\vec{b},z) = \frac{1}{(2\pi)^{3/2}} \exp\left[ikz - \frac{i}{\hbar v}\int_{-\infty}^{z} V(\vec{b},z')dz'\right]. \quad \ldots (2.26)$$

If the potential V is centred at the origin, the distance $b = |\vec{b}|$ has the interpretation of an impact parameter.

Using Eq.(2.26) for the approximate wavefunction in the expression (2.4) for the scattering amplitude, we have

$$f_E(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^2b\, dz\, e^{i(\vec{k}-\vec{k}')\cdot(\vec{b}+\hat{k}z)} V(\vec{b},z) e^{i\wedge(\vec{b},z)}, \quad \ldots (2.27a)$$

where

$$\wedge(\vec{b},z) = -\frac{1}{\hbar v}\int_{-\infty}^{z} V(\vec{b},z')dz', \quad \ldots (2.27b)$$

and $d^2b \equiv bdbd\phi_b$ denotes integration over the plane of impact parameter vector $\vec{b}$.

Let us consider the case of elastic scattering. Then energy conservation requires $|\vec{k}| = |\vec{k}'| = k$ so that for small scattering angles the momentum transfer $\hbar\vec{\Delta} \equiv \hbar(\vec{k}-\vec{k}')$ is nearly perpendicular to $\vec{k}$. In fact the error of approximating the exponential

$$e^{i(\vec{k}-\vec{k}')\cdot\hat{k}z}$$

by unity is only of order

$$(1-\cos\theta)kd \simeq \tfrac{1}{2}\theta^2 kd. \quad \ldots (2.28)$$

Condition (2.28) along with (2.24) indicates that the neglect

of longitudinal component of momentum transfer imposes no further restriction on the scattering amplitude but leads to simplification of Eq.(2.27a) to a two-dimensional integration over the plane of impact parameter:

$$f_E(\vec{k}',\vec{k}) = -\frac{2m}{4\pi\hbar^2}\int d^2b\, e^{i\vec{\Delta}.\vec{b}}\int dz\left(-\frac{\hbar v}{i}\right)\frac{\partial}{\partial z}\left[e^{-\frac{i}{\hbar v}\int_{-\infty}^{z} V(\vec{b},z')dz'}\right]$$

$$= \frac{k}{2\pi i}\int d^2b\, e^{i\vec{\Delta}.\vec{b}}\left[e^{-\frac{i}{\hbar v}\int_{-\infty}^{\infty} V(\vec{b},z)dz}\right]$$

$$= \frac{ik}{2\pi}\int d^2b\, e^{i\vec{\Delta}.\vec{b}}\left[1-e^{i\chi(\vec{b})}\right], \qquad \ldots (2.29a)$$

where the phase function $\chi(\vec{b})$ is given by

$$\chi(\vec{b}) = -\frac{1}{\hbar v}\int_{-\infty}^{\infty} V(\vec{b},z')dz'. \qquad \ldots (2.29b)$$

Eq.(2.29a) is the final form of the scattering amplitude for elastic scattering in Glauber approximation. The result may be thought of as corresponding to a picture in which each portion of the incident wave passes through the potential along a straight line path and suffers a shift of phase characteristic of that path.

For spherically symmetric potentials, the expression (2.29) is further reduced to a one-dimensional integral over b:

$$f_E(\vec{k}',\vec{k}) = ik\int_0^{\infty} db\, b\, J_0(\Delta b)\left[1 - e^{i\chi(b)}\right], \qquad \ldots (2.30)$$

where we have used the relation (Ref.75, p.620):

$$\int_0^{2\pi} d\phi\, e^{i\lambda\cos\phi} = 2\pi J_0(\lambda). \qquad \ldots (2.31)$$

Here $J_0(\lambda)$ is the cylindrical Bessel function of zeroth order. Following the small angle approximation [Eq.(2.28)], Eq.(2.30) further reduces to

$$f_E(\vec{k}',\vec{k}) = ik\int_0^{\infty} db\, b\, J_0(kb\theta)\left[1 - e^{i\chi(b)}\right]. \qquad \ldots (2.32)$$

2.2.4 SIGNIFICANCE OF THE DISTANCE 'd'

We have assumed that d is the distance over which the product Vρ varies appreciably. The potential V varies over a distance 'a', and according to Eq.(2.11), $\rho(\vec{r})$ varies appreciably over a distance $\sim \hbar v/|V|$. Evidently the distance 'd' is, in order of magnitude, the smaller of these; i.e., for

$$\frac{|V|a}{\hbar v} < 1$$

we have

$$d \sim a$$

and for

$$\frac{|V|a}{\hbar v} > 1$$

we have

$$d \sim \hbar v/|V|.$$

2.2.5 ANGULAR RANGE OF THE APPROXIMATION

Let us recall Eq.(2.24),

$$\theta^2 kd \ll 1,$$

which limits the angular range of the approximation. For the

case.

$$\frac{|V|a}{\hbar v} < 1, \quad d \sim a$$

we have

$$\theta \lesssim \frac{1}{(ka)^{1/2}} \quad \text{for} \quad \frac{|V|a}{\hbar v} < 1. \qquad \ldots (2.33a)$$

Similarly

$$\theta \lesssim \left(\frac{|V|}{E}\right)^{1/2} \quad \text{for} \quad \frac{|V|a}{\hbar v} > 1. \qquad \ldots (2.33b)$$

Both of these, according to the assumptions Eq.(2.7), are small angles. However, it is argued[40] that nearly all of the scattered intensity is concentrated , in both the cases, at angles which are still smaller i.e. in the Born approximation the average angle of scattering is

$$\langle\theta\rangle \sim \frac{1}{ka}, \quad \left(\frac{|V|a}{\hbar v} < 1\right) \qquad \ldots (2.34a)$$

and in the W.K.B. method we have

$$\langle\theta\rangle \sim \frac{|V|}{E}, \quad \left(\frac{|V|a}{\hbar v} > 1\right). \qquad \ldots (2.34b)$$

In both extremes the typical scattering angles are well within the angular range of the approximation.

## 2.26 EXTENSION TO WIDER SCATTERING ANGLES

The expression, Eq.(2.30), could be obtained by the impact parameter method. This method clearly implies that the Fourier-Bessel representation, Eq.(2.30), is exact at all energies and all scattering angles as far as the eikonal phase $\chi(\vec{b})$ is exact[76-79]. The Glauber small angle approximation

restricts $\chi$ to Eq.(2.29b) by choosing the integration path along z' parallel to $\hat{k}$. An important advantage of the Glauber scattering amplitude, Eq.(2.29a), is its comparative simplicity and the resultant ease of calculation. For scattering into winder angles one can modify the form (2.29b) by replacing the integral from $-\infty$ to $+\infty$ along z' by an integral along the actual curved path[80], or by an integral along the two semi-infinite straight lines[38,39], the first parallel to $\vec{k}$ from $-\infty$ to $\vec{r}$ and the second parallel to $\vec{k}'$ from $\vec{r}$ to $\infty$. However, such a procedure would not lead to a convenient form like (2.29b); unless the path integral in the exponent of Eq.(2.27b) is along a single straight line allowing replacement of $e^{i\vec{\Delta}.\vec{r}}$ by $e^{i\vec{\Delta}.\vec{b}}$, it is not strictly possible to reduce (2.27a) to a form like (2.29a). Nevertheless, integration of the exponent in (2.29b) along two semi-infinite straight lines has been used in the Glauber angle approximation[81,82]; these semi-infinite straight lines at each impact parameter b are asymptotic to the classical path.

Glauber[40] has proposed that (2.29a) could be extended to wider scattering angles, without any loss of simplicity or calculational ease, by choosing the path integral over z along a single straight line parallel to the average momentum direction $(\vec{k}+\vec{k}')/|\vec{k}+\vec{k}'|$, from $-\infty$ to $+\infty$ This choice of z (and z') direction in (2.27b) immediately yields (2.29a) from (2.27a) without any need to assume that $\vec{\Delta}$ is perpendicular to the z-direction. This extension of Eq.(2.29a) is known as the wide angle Glauber formula for $f_E(\vec{k}', \vec{k})$ in potential

scattering. For short ranged spherically symmetric potentials it reduces to the form

$$f_L(\vec{k}',\vec{k}) = ik \int_0^\infty db\ b\ J_0(2k\ b\ \sin\theta/2) \left[1 - e^{i\chi(b)}\right]. \quad \ldots (2.35)$$

Here $\vec{\Delta}.\vec{r}$ is replaced by its exact value because, as long as energy is conserved, i.e. $|\vec{k}'| = |\vec{k}|$, $\exp(i\vec{\Delta}.\vec{r})$ is exactly equal to $\exp(i\vec{\Delta}.\vec{b})$ and does not involve any small angle approximation. The above change in angular range, i.e. the replacement of $\theta$ by $2 \sin \theta/2$, is hardly a great one, but it must be remembered that the angular distribution of the scattering with which we are dealing is peaked in the forward direction and consequently decays rapidly with angle. Therefore, even so slight a shift of angular scale at small angles may be of significance in improving the angular range over which the approximation holds. Though the wide angle formula suffers from the defect that it approximates all rays by a single straight line parallel to $\vec{k}+\vec{k}'$, irrespective of their point of origin on the incident wavefront, it has a number of desirable properties for all potentials, including ease of calculation, velocity reversibility and unitarity. Moreover, the wide angle Glauber formula for the Coulomb potential is exact at all angles and all energies except for a phase factor[40] and it is a major reason that the composite collision version of (2.29) has been so successful in atomic collisions.

## 2.3 COLLISION OF COMPOSITE BODIES

### 2.3.1 EXPRESSION FOR THE SCATTERING AMPLITUDE

In atomic collisions between a pair of neutral bodies, or between an ion and a neutral body, the net interaction 'V' between the colliding bodies decreases more rapidly than $\frac{1}{r}$ at large distances. For such collisions, therefore, the path integral for the net interaction converges in Eq.(2.29b), even though the path integral would diverge for the individual pairwise Coulomb potentials comprising the net interaction.

In order to avoid complications associated with the net long range Coulombic interactions in the initial and/or final channels we confine our present considerations to direct collisions of two bodies A and B:

$$A + B \longrightarrow A + B(B^{*}), \qquad \ldots (2.36)$$

in which atleast one of the bodies A, B is neutral. Here $B^{*}$ denotes an excited state. We follow the approach of Gerjuoy and Thomas[34] for the generalization of the potential scattering formula, Eq.(2.24) for collisions of the type (2.36). Let us consider the centre of mass Lippmann-Schwinger equation

$$\psi_i^{(+)}(\vec{r},\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}.\vec{r}}\, \phi_i(\vec{x}) - \frac{2\mu}{4\pi\hbar^2} \int d^3x' d^3r'$$

$$\times \sum_j \frac{\exp(ik_j|\vec{r}-\vec{r}'|)}{|\vec{r}-\vec{r}'|}\, \phi_j(\vec{x})\, \phi_j^{*}(\vec{x}')\, V(\vec{r}',\vec{x}')\, \psi_i^{(+)}(\vec{r}',\vec{x}'). \qquad \ldots (2.37)$$

Here $\vec{r}$ is the displacement of the centre of mass of A relative to B; $\vec{x}$ denotes the collection of internal coordinates specifying the positions of the particles in A and B; $\phi_i(\vec{x})$ is the product of the initial bound states of A and B; the sum over j extends over the complete set of internal states, both discrete and continuous, of A and B; and the total energy of the composite system (A,B) is

$$\frac{\hbar^2 k_j^2}{2\mu} + w_j = \frac{\hbar^2 k^2}{2\mu} + w_i = \frac{\hbar^2 k'^2}{2\mu} + w_f = E, \qquad \ldots (2.38)$$

where $w_j$ is the sum of bound state energies in the intermediate channel j; $k = \mu v/\hbar$ and $k' = \mu v'/\hbar$ are respectively the initial and final wavenumbers, and v and v' the respective speeds in the CM system; $\mu$ is the reduced mass of A,B.

Eq. (2.37), which is exact, is now solved approximately. Gerjuoy and Thomas[34] suggest that the incident particle energies are sufficiently large to assume $k_j = k$ for all j in Eq.(2.37). The sum over j then reduces to the closure relation

$$\sum_j \phi_j(\vec{x})\, \phi_j^*(\vec{x}') = \delta(\vec{x}-\vec{x}'), \qquad \ldots (2.39)$$

thereby immediately simplifying (2.37) to

$$\psi_i^{(+)}(\vec{r},\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}.\vec{r}} \phi_i(\vec{x}) - \frac{2\mu}{4\pi\hbar^2} \int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}',\vec{x}')\, \psi_i^{(+)}(\vec{r}',\vec{x}') \ldots (2.40)$$

The approximate integral Eq.(2.40) for $\psi_i^{(+)}(\vec{r},\vec{x})$

involves the internal coordinates $\vec{x}$ of the incident composites only parametrically; moreover the $\vec{x}$ dependence of $\psi_i^{(+)}(\vec{r},\vec{x})$ is determined only by the initial bound state $\phi_i$ and the interaction potential V. Hence, we may now write, without further approximation,

$$\psi_i^{(+)}(\vec{r},\vec{x}) = \hat{\psi}(\vec{r},\vec{x})\phi_i(\vec{x}), \qquad \ldots (2.41)$$

which yields an even simpler integral equation for $\hat{\psi}(\vec{r},\vec{x})$, namely

$$\hat{\psi}(\vec{r},\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}.\vec{r}} - \frac{2\mu}{4\pi\hbar^2}\int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}',\vec{x})\hat{\psi}(\vec{r}',\vec{x}). \qquad \ldots (2.42)$$

Except for its parametric dependence on $\vec{x}$, Eq.(2.42) for $\hat{\psi}(\vec{r},\vec{x})$ is identical to the potential scattering case, Eq.(2.2). Eq. (2.42) can, therefore, be solved in a similar way by using the method of stationary phase. It yields precisely the approximate solution for $\psi_i^{(+)}(\vec{r},\vec{x})$:

$$\psi_i^{(+)}(\vec{r},\vec{x}) \to \psi_i^{G}(\vec{r},\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}.\vec{r}} \times \exp\left(-\frac{i}{\hbar v}\int_{-\infty}^{z} dz' V(\vec{b},z',\vec{x})\right)\phi_i(\vec{x}). \qquad \ldots (2.43)$$

The centre of mass collision amplitude (Ref.35, p.802 and 866; Ref.83) for the reaction (2.36) is given by

$$F_{fi}(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d^3r d^3x\, e^{-i\vec{k}'.\vec{r}}\, \phi_f^*(\vec{x})\, V(\vec{r},\vec{x})\, \psi_i^{(+)}(\vec{r},\vec{x}), \qquad \ldots (2.44)$$

which, by using, Eq.(2.43) for $\Psi_i^{(+)}$ simplifies, to

$$F_{fi}^{G}(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d^3r\, d^3x\, e^{i\vec{\Delta}\cdot\vec{r}}\phi_f^*(\vec{x})\, V(\vec{r},\vec{x}) \cdot \exp\left(-\frac{i}{\hbar v}\int_{-\infty}^{z} dz'\, V(\vec{b},z';\vec{x})\right)\phi_i(\vec{x}) \qquad \ldots (2.45)$$

and by making the small angle approximation (choosing the z-direction along $\vec{k}$) reduces to

$$F_{fi}^{G}(\vec{k}',\vec{k}) = \frac{ik}{2\pi}\int d^2b\, e^{i\vec{\Delta}\cdot\vec{b}}\int d^3x\, \phi_f^*(\vec{x})\left[1 - e^{i\chi(\vec{b},\vec{x})}\right]\phi_i(\vec{x}), \qquad \ldots (2.46a)$$

where,

$$\chi(\vec{b},\vec{x}) = -\frac{1}{\hbar v}\int_{-\infty}^{\infty} dz'\, V(\vec{b},z';\vec{x}). \qquad \ldots (2.46b)$$

The expression (2.46) is known as the Glauber's formula for composite collisions.

To be more specific, let us consider a direct collision in which a fast, charged, 'elementary' particle A is incident on a composite target B (such as an atom) which contains Z-scatterers. If we assume that the incident particle interacts with the target scatterers via two-body spin-independent interactions, the expression (2.46) is further simplified and can be written, more explicitly, as

$$F_{fi}^{G}(\vec{k}',\vec{k}) = \frac{ik}{2\pi}\int d^2b\, e^{i\vec{\Delta}\cdot\vec{b}}\int d^3x_1 \ldots d^3x_Z \phi_f^*(\vec{x}_1,\ldots,\vec{x}_Z)\cdot \times\Gamma(\vec{b},\vec{s}_1,\ldots,\vec{s}_Z)\phi_i(\vec{x}_1,\ldots,\vec{x}_Z), \qquad \ldots (2.47a)$$

where

$$\Gamma(\vec{b},\vec{s}_1,\ldots,\vec{s}_Z) = 1 - e^{i\chi(\vec{b},\vec{s}_1,\ldots,\vec{s}_Z)}, \qquad \ldots (2.47b)$$

$$\chi(\vec{b},\vec{s}_1,\ldots,\vec{s}_Z) = \sum_{j=1}^{Z} \chi_j(\vec{b}-\vec{s}_j), \qquad \ldots (2.47c)$$

$$\chi_j(\vec{b}-\vec{s}_j) = -\frac{1}{hv}\int_{-\infty}^{\infty} dz' V(\vec{b},z';\vec{x}_j), \qquad \ldots (2.47d)$$

and

$$V(\vec{b},z',\vec{x}_j) = Z_i \frac{e^2}{r} - \frac{Z_i e^2}{|\vec{r}-\vec{x}_j|}. \qquad \ldots (2.47e)$$

Here $Z_i e$ is the total charge on the incident charged particle and $\vec{x}_j$ are the coordinates of the target electrons (relative to the target centre of mass):

$$\vec{x}_j = \vec{s}_j + \hat{k}\, z_j. \qquad \ldots (2.48)$$

The assumption that the internal motion of target particles is slow compared with the relative motion of A and B is implicitly involved in the expression (2.47). The crucial property of the phase-shift additivity, expressed by Eq.(2.47c) is clearly a direct consequence of various approximations, such as, the one-dimensional nature of relative motion and the neglect of three-body forces, target scatterer motions, and the longitudinal component of momentum transfer.

For high energy small angle scattering, the formula (2.47) is valid in the laboratory system as well as in the centre of mass system[84]. If we neglect recoil effects, which are small for scattering near the forward direction, the only modifications are that the centre of mass wave vectors $\vec{k}$ and

$\vec{k}'$ must now be replaced by the corresponding quantities $\vec{K}_i$ and $\vec{K}_f$ while $\vec{\Delta} \equiv \vec{k}-\vec{k}'$ is replaced by $\vec{q} \equiv \vec{k}_i - \vec{k}_f$. Neglecting recoil effects, we may thus write the Glauber scattering amplitude in the laboratory system as

$$F^G_{fi}(\vec{K}_f,\vec{K}_i) = \frac{ik}{2\pi}\int d^2b\ e^{i\vec{q}\cdot\vec{b}}\int d^3x_1,\ldots\ d^3x_Z \phi^*_f(\vec{x}_1,\ldots,\vec{x}_Z)$$
$$\times\Gamma(\vec{b},\vec{s}_1,\ldots,\vec{s}_Z)\phi_i(\vec{x}_1,\ldots,\vec{x}_Z), \qquad \ldots (2.49)$$

where $\hbar\vec{q} \equiv \hbar\vec{k}_i-\hbar\vec{k}_f$ is now the laboratory momentum transfer, and we have denoted the initial and final laboratory wave vectors by $\vec{K}_i$ and $\vec{k}_f$ respectively.

The differential and integrated cross sections are obtained from the scattering amplitude, Eq.(2.49), in the usual way. The differential cross section is given by

$$\frac{d\sigma(q)}{d\Omega} = \frac{k_f}{k_i}|F^G_{fi}(\vec{K}_f,\vec{K}_i)|^2, \qquad \ldots (2.50)$$

and the integrated cross section by

$$\sigma(k_i) = \frac{k_f}{k_i}\int d\Omega\ |F^G_{fi}(\vec{k}_f,\vec{K}_i)|^2, \qquad \ldots (2.51)$$

where integration is over all directions $\hat{k}_f$ of the scattered electron. Using the relation

$$q^2 = k_i^2 + k_f^2 - 2k_ik_f\cos\theta\ , \qquad \ldots (2.52a)$$

where

$$\theta = \cos^{-1}(\hat{k}_i.\hat{k}_f), \qquad \ldots (2.52b)$$

Eq. (2.51) becomes

$$\sigma(k_i) = \frac{2\pi}{k_i^2} \int_{k_i-k_f}^{k_i+k_f} dq\, q |F_{fi}^G(\vec{k}_f, \vec{k}_i)|^2 . \qquad \ldots (2.53)$$

For elastic scattering ($k_f = k_i$), we have

$$\sigma(k_i) = \frac{2\pi}{k_i^2} \int_0^{2k_i} dq\, q\, |F_{fi}^G(\vec{k}_f, \vec{k}_i)|^2, \qquad \ldots (2.54a)$$

where

$$q = 2k_i \sin\theta/2. \qquad \ldots (2.54b)$$

The superscript G in $F^G$ will henceforth be dropped for convenience.

2.3.2 CHOICE OF z-AXIX

While making a proper choice of a quantization (z-)axis when (2.45) is used for scattering into wide angles not obeying (2.33), the following points should be noted:

(i) As $k \to \infty$, the z-direction must become perpendicular to $\vec{\Delta}$ if (2.46) is to reduce rigorously to the Born approximation in this limit.

(ii) If $\vec{\Delta}$ is not perpendicular to z, it is not permissible to replace $e^{i\vec{\Delta}.\vec{r}}$ in (2.45) by $e^{i\vec{\Delta}.\vec{b}}$; the integrand in (2.45), including the path integral $\chi$, must be independent of z.

The second point might be defended on the grounds that it is less erroneous to replace $\exp(i\vec{\Delta}.\vec{r})$ by $\exp(i\vec{\Delta}.\vec{b})$ after choosing the path integral along a physically reasonable direction than to perform the eikonal path integral along a physically unreasonable direction strictly perpendicular to $\vec{\Delta}$. Following these arguments, an adequate choice for the

z-direction in (2.46), which always lies in the scattering plane (the plane containing $\vec{k}$ and $\vec{k}'$), is along the direction $(\hat{k}+\hat{k}')$ perpendicular to

$$\vec{\Delta}' = \vec{k}-\vec{k}' = k(\hat{k}-\hat{k}'). \qquad \ldots (2.55)$$

For elastic scattering, $k = k'$ at all energies and $\vec{\Delta}'$ of (2.55) is automatically identical with $\vec{\Delta} \equiv \vec{k} - \vec{k}'$; for elastic scattering, it is, therefore, generally agreed that the z-direction in evaluating the path integral in (2.46b) is to be chosen along a straight line $(\hat{k}+\hat{k}')$ perpendicular to $\vec{\Delta}$. For inelastic scattering choosing z-direction perpendicular to $\vec{\Delta}$ is quite inadequate. However, the direction $(\hat{k}+\hat{k}')$ seems particularly attractive in excitations near threshold, where the direction perpendicular to $\vec{\Delta}$ is always nearly perpendicular to $\hat{k}$, even for small angle scattering. Nevertheless, specially in inelastic scattering at low energies, one cannot rule out the possibility that it would be more accurate, though more arduous, to compute collision amplitudes directly from (2.44) as Byron[85] does, evaluating the path integral along some physically reasonable direction not necessarily perpendicular to $\vec{\Delta}$.

It is important to note that the choice of z-axis does not effect the calculations involving differential cross sections summed over all final magnetic quantum numbers $m_f$, but it may effect whenever such a summation is not involved. Gerjuoy et al[86] have emphasized this point in estimating the percentage polarization (which depends on $m_f$) of Lyman-$\alpha$ radiation emitted

from hydrogen atom following electron excitation to the 2p state. The incorrect prediction, by Tai et al,[87] of the percentage polarization of Lyman-$\alpha$ radiation was due to an incorrect choice of the z-axis[86].

Remembering that the Glauber approximation is an special case of the eikonal approximations and that in the case of potential scattering Glauber's derivation leads to the same expression for the scattering amplitude [Eq.(2.29)] as obtained using the eikonal wavefunction [Eq.(1.55)], we will henceforth call Eq.(2.29) as the eikonal scattering amplitude derived from the eikonal approximation. The composite collision version of Eq.(2.29) which is, according to our present terminology, the many body generalization of the eikonal scattering amplitude will be termed as the Glauber scattering amplitude and will be expressed by Eq.(2.47). Now the Glauber result (2.47) may also be viewed as an eikonal approximation to a model proposed by Chase[88], in which the target particles are frozen in a given configuration[65].

# CHAPTER-3

## $n\ell m - n'\ell' m'$ GLAUBER TRANSITION AMPLITUDES IN CHARGED PARTICLE-HYDROGEN ATOM COLLISIONS

### 3.1 INTRODUCTION

In this chapter we concentrate on inelastic scattering of charged particles by atomic hydrogen in Glauber approximation. The Glauber scattering amplitudes for excitation to $n' = 2$ and 3 levels from the ground state ($n = 1$) of atomic hydrogen have been calculated by Ghosh and Sil[89], Ghosh et al[90], Tai et al[91], Tai et al[87], Bhadra and Ghosh[92], and Franco and Thomas[93]. In these calculations the five-dimensional integral amplitude was reduced without any further approximation into a one-dimensional integral form by methods similar to those employed by Franco[94] for e-H(1s) elastic scattering.

Thomas and Gerjuoy[59] have obtained these amplitudes in a closed form. These expressions, besides being readily calculable are useful in studying the limiting behaviour of the Glauber scattering amplitudes for (say) the high energy or small momentum transfer. For the sake of completeness, we reproduce these expressions from Ref.59:

$$F_{1s-n's}(\vec{k}_f;\vec{k}_i) = ik_i\left(\frac{2}{a_o}\right)^3 \frac{1}{4}(n')^{-3/2} \sum_{j=o}^{n'-1} \alpha_j(n')(-1)^{j+1}$$

$$\times\left(\frac{\partial}{\partial\lambda}\right)^{j+1} I_o(\lambda,q)\Big|_{\lambda=(1/a_o)(1+1/n')}, \qquad \ldots (3.1a)$$

where

$$\alpha_j(n') = \left[(-n'+1)_j/(2)_j\, j!\right]\left(\frac{2}{n'a_o}\right)^j, \qquad \ldots (3.1b)$$

$$I_o(\lambda,q) = -4i\eta\,\Gamma(1+i\eta)\,\Gamma(1-i\eta)\,\lambda^{-2-2i\eta}\,q^{-2+2i\eta} \times {}_2F_1(1-i\eta,\ 1-i\eta;1;-\lambda^2/q^2), \qquad \ldots (3.1c)$$

$$(a)_j = \Gamma(a+j)/\Gamma(a)\ ; \qquad \ldots (3.1d)$$

$$F_{1s\text{-}n'p_o}(\vec{k}_f,\vec{k}_i) = 0, \qquad \ldots (3.2)$$

and

$$F_{1s\text{-}n'p_{\pm1}}(\vec{k}_f,\vec{k}_i) = 2ik_i(3/2)^{1/2}\,\frac{1}{4!}\left(\frac{2}{a_o}\right)^4\frac{1}{n'^3}\left[\frac{(n'+1)!}{(n'-2)!}\right]^{1/2} \times e^{\mp i\phi_q}\sum_{j=o}^{n'-2}\beta_j(n')(-1)^{j+1}\left(\frac{\partial}{\partial\lambda}\right)^{j+1} I_1(\lambda,q)\Big|_{\lambda=(1/a_o)*(1+1/n')} \qquad \ldots (3.3a)$$

where

$$I_1(\lambda,q) = 4i\,\Gamma(1+i\eta)\,\Gamma(2-i\eta)(i\eta)\,\lambda^{-2-2i\eta}\,q^{-3+2i\eta} \times \left\{-{}_2F_1(2-i\eta,\ 1-i\eta;1;-\lambda^2/q^2) + (1+i\eta)\,{}_2F_1(2-i\eta,1-i\eta;2;-\lambda^2/q^2)\right\}, \qquad \ldots (3.3b)$$

$$\beta_j(n') = \left[(-n'+2)_j/j!(4)_j\right](2/n'a_o)^j. \qquad \ldots (3.3c)$$

Here $a_o$ is the Bohr radius and $\eta = e^2/\hbar v$. The quantization direction (i.e. z-axis) has been chosen perpendicular to the momentum transfer vector $\vec{q}$. It is obvious that these expressions [3.1 to 3.3] are quite useful for studying excitation to relatively low lying states from the ground state in e - H atom collisions. The simplicity of these expressions is,

however, lost if $n'$ becomes large because of the increasing number of hypergeometric functions appearing in the expression. Similar is the problem with the Glauber scattering amplitudes obtained recently by Thomas and Franco[95] for the scattering by ionic targets.

We have obtained 'simple' expression in the Glauber approximation for the general transition $n\ell m - n'\ell'm'$ in e-H atom scattering by combining the techniques of Franco[60] and Golden and McGuire[61] and using the Laguerre polynomials appearing in hydrogen atom wavefunctions straight away rather than breaking them into a series of terms of the form $x^{\mu}e^{-\nu x}$. Our final expression involves only a one-dimensional integral over the impact parameter b and is particularly suited to study excitation to highly excited states. It involves only a few hypergeometric functions if n is not too large. There is no restriction on $n'$.

In Sec. 3.2 we present the derivation of these expressions which are commented upon in Sec.3.3. Rydberg atomic units ($\hbar = e = \sqrt{2}$ , $m = 1$) will henceforth be used throughout.

## 3.2 DERIVATION

The Glauber scattering amplitude, in the case of electron-hydrogen atom collisions, for the transition from an initial state i with wavefunction $\phi_i \equiv \phi_{n\ell m}$ to some final state f with wavefunction $\phi_f \equiv \phi_{n'\ell'm'}$ is given by

$$F_{fi}(\vec{k}_f, \vec{k}_i) = \frac{ik_i}{2\pi} \int \phi_f^* \phi_i \left[1 - \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta}\right] e^{i\vec{q}\cdot\vec{b}} d^2b \; d^3x, \ldots \quad (3.4)$$

in which $\vec{q} = (\vec{k}_i - \vec{k}_f)$ is the momentum transfer, in the laboratory system, which the incident electron imparts to the target. The vector $\vec{q}$ is assumed to lie in the plane of $\vec{b}$. The contribution to Eq.(3.4) from the term equal to unity in the square bracket is proportional to the two-dimensional delta function $\delta(\vec{q})$, and therefore vanishes for inelastic transitions.

The normalized wavefunction $\phi_{n\ell m}$ is given by

$$\phi_{n\ell m}(\vec{x}) = N_{n\ell} e^{-x/n} x^{\ell} L_{k_1}^{\alpha_1}\left(\frac{2x}{n}\right) Y_{\ell}^{m}(\theta,\phi), \quad \ldots (3.5a)$$

where $L_{k_1}^{\alpha_1}(\frac{2x}{n})$ is the associated Laguerre polynomial (Ref.96, p.240) and

$$N_{n\ell} = \frac{2^{\ell+1}}{n^{\ell+2}} \left[\frac{(n-\ell-1)!}{(n+\ell)!}\right]^{1/2} \quad \ldots (3.5b)$$

$$\alpha_1 = (2\ell + 1), \quad \ldots (3.5c)$$

and

$$k_1 = (n-\ell-1). \quad \ldots (3.5d)$$

The product $\phi_f^* \phi_i$ in Eq.(3.4) may be written[60] as

$$\phi_f^* \phi_i = A_{nn'}^{\ell\ell'} e^{-\alpha_{nn'} x} x^{\ell+\ell'} L_{k_1'}^{\alpha_1'}\left(\frac{2x}{n'}\right) L_{k_1}^{\alpha_1}\left(\frac{2x}{n}\right)$$

$$\times Y_{\ell}^{m}(\theta,\phi) \; Y_{\ell'}^{m'*}(\theta,\phi)$$

$$= A^{\ell\ell'}_{nn'} e^{-\alpha_{nn'}x} x^{\ell+\ell'} L^{\alpha'_1}_{k'_1}\left(\frac{2x}{n'}\right) L^{\alpha_1}_{k_1}\left(\frac{2x}{n}\right)$$

$$\times \sum_L B_L A_L \exp(im\phi)\, P_L^M(\cos\theta)$$

$$= A^{\ell\ell'}_{nn'} e^{-\alpha_{nn'}x} x^{\ell+\ell'} L^{\alpha'_1}_{k'_1}\left(\frac{2x}{n'}\right) L^{\alpha_1}_{k_1}\left(\frac{2x}{n}\right)$$

$$\times \sum_L B_L A_L \exp(im\phi) \sin^{M+1}\theta \sum_{p=0}^{(L-M)/2} D^p_{LM} \cos^{2p}\theta, \qquad \ldots (3.6)$$

where

$$A^{\ell\ell'}_{nn'} = N_{n\ell'} N_{n\ell},$$

$$\alpha_{nn'} = \frac{n+n'}{nn'},$$

$$m = m-m' \text{ and } M = |m|,$$

$$B_L = (L-M)!/(L+M)!,$$

$$A_L = \frac{1}{4\pi} \xi (-1)^m \left[ (2\ell+1)(2\ell'+1)(L+M)!/(L-M)! \right]^{1/2}$$

$$\times C(\ell,\ell',L;0,0)\; C(\ell,\ell',L;m,-m'),$$

$$\xi = \begin{cases} \exp(i\pi m) & , \quad m \geq 0 \\ 1 & , \quad m < 0 \end{cases}$$

$$D^p_{LM} = \frac{(-1)^{p+(L+M)/2}(L+M+2p-1)!!}{(2p)!\,(L-M-2p)!!} \qquad \ldots (3.7)$$

(L-M) is an even positive integer and C's are the Clebsch-Gordan coefficients. For odd positive integral values of (L-M), the integration over polar angle $\theta$ vanishes. Eq.(3.4) now

reduces to

$$F_{fi}(\vec{k}_f,\vec{k}_i) = -\frac{ik_i}{2\pi} A^{\ell\ell'}_{nn'} \int e^{-\alpha_{nn'}x}\, x^{\ell+\ell'+2} L^{\alpha'_1}_{k'_1}\left(\frac{2x}{n'}\right) L^{\alpha_1}_{k_1}\left(\frac{2x}{n}\right)$$
$$\times\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta} e^{i\vec{q}.\vec{b}}\, e^{im\phi_b}\, \sin^{M+1}\theta\, e^{im(\phi_s-\phi_b)}$$
$$\times\sum_L B_L A_L \sum_{p=0}^{(L-M)/2} D^p_{LM} \cos^{2p}\theta\; b\, db\, d\phi_b dx\, d\theta d\phi_s. \qquad \ldots (3.8)$$

The angular integration over $\phi_s$ and $\phi_b$ can readily be performed (Ref.96,p.55; Ref.97,p.952):

$$\int_0^{2\pi}\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta} e^{im(\phi_s-\phi_b)}\, d\phi_s = \int_0^{2\pi}(1+z^2-2z\cos\phi)^{i\eta}\, e^{im\phi}d\phi$$
$$= \frac{2\pi\Gamma(M-i\eta)}{M!\,\Gamma(-i\eta)}\, G(z), \qquad \ldots (3.9a)$$

where

$$z = \frac{s}{b} = \frac{x\sin\theta}{b}, \qquad \ldots (3.9b)$$

$$G(z) = \begin{cases} z^M\, {}_2F_1(-i\eta, M-i\eta; M+1; z^2), & z<1 \\ z^{-M+2i\eta}\, {}_2F_1(-i\eta, M-i\eta; M+1; z^{-2}), & z>1 \end{cases} \qquad \ldots (3.9c)$$

$$\text{and } \int_0^{2\pi} e^{i\vec{q}.\vec{b}}\, e^{im(\phi_b-\phi_q)}\, d\phi_b = 2\pi\, i^M\, J_M(qb). \qquad \ldots (3.10)$$

Using Eqs.(3.9) and (3.10), Eq.(3.8) reduces to the form

$$F_{fi}(\vec{k}_f,\vec{k}_i) = -2\pi\, i^{M+1}\, k_i \frac{\Gamma(M-i\eta)}{M!\,\Gamma(-i\eta)}\, e^{im\phi_q}\, A^{\ell\ell'}_{nn'}$$

$$\times\sum_L B_L A_L \sum_{p=0}^{(L-M)/2} D^p_{LM} \int e^{-\alpha_{nn'}x}\, x^{\ell+\ell'+2}$$

$$\times L^{\alpha'_1}_{k'_1}(\tfrac{2x}{n'})\, L^{\alpha_1}_{k_1}(\tfrac{2x}{n})\, G(x\sin\theta/b)\, J_M(qb)$$

$$\times b\, \sin^{M+1}\theta\, \cos^{2p}\theta\; db\, dx\, d\theta. \qquad \ldots (3.11)$$

Making the transformation $b \to b\sin\theta$ we have

$$F_{fi}(\vec{k}_f,\vec{k}_i) = -2\pi\, i^{M+1}\, k_i \frac{\Gamma(M-i\eta)}{M!\,\Gamma(-i\eta)}\, e^{im\phi_q}\, A^{\ell\ell'}_{nn'}$$

$$\times\sum_L B_L A_L \sum_{p=0}^{(L-M)/2} D^p_{LM} \int e^{-\alpha_{nn'}x}\, x^{\ell+\ell'+2}$$

$$\times L^{\alpha'_1}_{k'_1}(\tfrac{2x}{n'})\, L^{\alpha_1}_{k_1}(\tfrac{2x}{n})\, G(x/b)\, J_M(qb\sin\theta)$$

$$\times b\, \sin^{M+3}\theta\, \cos^{2p}\theta\; db\, dx\, d\theta\,. \qquad \ldots (3.12)$$

Replacing now a factor of $\sin^2\theta$ by $1-\cos^2\theta$, Eq.(3.12) transforms to

$$F_{fi}(\vec{k}_f,\vec{k}_i) = H^{m}_{nn'\ell\ell'} \sum_L B_L A_L \sum_{p=0}^{(L-M)/2} D^p_{LM}(g^p_{LM} - g^{p+1}_{LM}), \qquad \ldots (3.13)$$

where

$$g^p_{LM} = \int e^{-\alpha_{nn'}x}\, x^{\ell+\ell'+2}\, L^{\alpha'_1}_{k'_1}(\tfrac{2x}{n'})\, L^{\alpha_1}_{k_1}(\tfrac{2x}{n})$$

$$\times G(x/b)\, J_M(qb\sin\theta)\, \sin^{M+1}\theta$$

$$\times \cos^{2p}\theta\; b\, db\, dr\, d\theta\,, \qquad \ldots (3.14)$$

and

$$H^{m}_{nn'\ell\ell'} = -2\pi\, i^{M+1}\, A^{\ell\ell'}_{nn'}\, k_i\, \frac{\Gamma(M-i\eta)}{M!\,\Gamma(-i\eta)}\, e^{im\phi_q} \qquad \ldots (3.15)$$

The integration over $\theta$ may now be performed (Ref.97,p.740):

$$\int_0^{2\pi} J_M(qb\sin\theta)\sin^{M+1}\theta\cos^{2p}\theta\, d\theta = 2(2p-1)!!\,(qb)^{-p} j_{p+M}(qb) \qquad \left[\mathrm{Re}(2p) > -1,\ M > -1\right], \qquad \ldots (3.16)$$

yielding spherical Bessel functions $j_{p+M}$ which can be expanded in inverse powers of qb (Ref.97,p.966):

$$j_{p+M}(qb) = \frac{1}{2qb} \sum_{\lambda=0}^{p+M} \frac{a^{\lambda}_{p+M}}{(qb)^{\lambda}} \left[e^{iqb} + (-1)^{p+M-\lambda-1} e^{-iqb}\right], \qquad \ldots (3.17a)$$

where

$$a^{\lambda}_{p+M} = \frac{i^{-p-M+\lambda-1}(p+M+\lambda)!}{\lambda!(p+M-\lambda)!\ 2^{\lambda}} . \qquad \ldots (3.17b)$$

Finally making the transformation $b \to bx/q$, the integral for $g^{p}_{LM}$ takes the form

$$g^{p}_{LM} = \frac{(2p-1)!!}{q^2} \sum_{\lambda=0}^{p+M} a^{\lambda}_{p+M} \int_0^{\infty} db\, b^{-p-\lambda}\, G(q/b)$$

$$\times \int_0^{\infty} dx\, x^{\ell+\ell'+3-p-\lambda} \left[L^{\alpha'_1}_{k'_1}\left(\frac{2x}{n'}\right)\right] \left[L^{\alpha_1}_{k_1}\left(\frac{2x}{n}\right)\right]$$

$$\times \left[e^{-(\alpha_{nn'}-ib)x} + (-1)^{M+p-\lambda-1} e^{-(\alpha_{nn'}+ib)x}\right]$$

$$\text{or} \quad g^{p}_{LM} = \frac{(2p-1)!!}{q^2} \sum_{\lambda=0}^{p+M} a^{\lambda}_{p+M} \int_0^{\infty} db\, b^{-p-\lambda}\, G(q/b)\, I^{p}_{\lambda}(b), \quad \ldots (3.18)$$

where

$$I^{p}_{\lambda}(b) = \sum_{t=1}^{2} \varepsilon_t \int_0^{\infty} dx\, e^{-\beta_t x}\, x^{d-1}\, L^{\alpha'_1}_{k'_1}\left(\frac{2x}{n'}\right) L^{\alpha_1}_{k_1}\left(\frac{2x}{n}\right), \quad \ldots (3.19)$$

$$\beta_t = \begin{cases} \alpha_{nn'} - ib & , t = 1 \\ \alpha_{nn'} + ib & , t = 2 \end{cases} \quad \ldots (3.20a)$$

$$\varepsilon_t = \begin{cases} 1 & , t = 1 \\ (-1)^{M+p-\lambda-1} & , t = 2 \end{cases} \quad \ldots (3.20b)$$

and

$$d = \ell + \ell' + 4 - p - \lambda\,. \quad \ldots (3.20c)$$

Final reduction of the scattering amplitude to a one-dimensional integral is done by expressing associated Laguerre polynomials in terms of confluent hypergeometric functions and integrating over x (Ref.98, p.54), yielding

$$I^{p}_{\lambda}(b) = B^{\ell\ell'}_{nn'} \sum_{t=1}^{2} \varepsilon_t \int_0^{\infty} dx\, e^{-\beta_t x}\, x^{d-1}$$

$$\times {}_1F_1(-k'_1; \alpha'_1+1; \tfrac{2x}{n'})\, {}_1F_1(-k_1; \alpha_1+1; \tfrac{2x}{n})$$

$$= B^{\ell\ell'}_{nn'} \sum_{t=1}^{2} \varepsilon_t \beta_t^{-d}\, \Gamma(d) \sum_{v=0}^{\infty} \frac{(-k_1)_v (d)_v (2/n)^v}{(\alpha_1+1)_v\, v!\, \beta_t^v}$$

$$\times {}_2F_1(-k'_1, d+v; \alpha'_1+1; 2/\beta_t n'), \quad \ldots (3.21a)$$

where

$$B^{\ell\ell'}_{nn'} = \frac{(n+\ell)!\,(n'+\ell')!}{(2\ell+1)!\,(2\ell'+1)!\,(n-\ell-1)!\,(n'-\ell'-1)!}\,. \quad \ldots (3.21b)$$

## 3.3 COMMENTS

The infinite sum over v in Eq.(3.21a) is really a series terminating at $v = k_1 = (n-\ell-1)$, i.e., the number of terms in the infinite series depends upon the values of n and $\ell$. If $n = 1$, the infinite series, Eq.(3.21a), terminates after the first term. In general, this series will have $(n-\ell)$ hypergeometric functions. It is important to note that the termination of the series does not depend on n'. The number of hypergeometric functions appearing in the expression for scattering amplitude, therefore, does not depend upon the final excited state. Furthermore, the hypergeometric functions in Eq.(3.21a) are terminating in themselves. Thus much computational effort is not needed to evaluate the Glauber scattering amplitudes even for excitations to highly excited states. Our expression is particularly useful for transitions to highly excited states from a low lying state and is simple to compute than the earlier expressions[59]. It may not prove to be of much value when n is large because of the occurrence of large number of hypergeometric functions.

In the following we give explicit expressions for the transitions 1s - n's and 1s - n'p. Eqs. (3.13) and (3.14) together with Eqs.(3.18) and (3.21) reduce to

$$F_{1s\text{-}n'0}(\vec{k}_f,\vec{k}_i) = -2ik_i \frac{1}{(n')^{5/2}}(g^o_{oo} - g^1_{oo})$$

$$= -\frac{2k_i}{q^2(n')^{3/2}} \int db\, G(q/b) \sum_{t=1}^{2} \zeta_t$$

$$\times \left[6(\zeta_t\beta_t)^{-4}\, {}_2F_1(-n'+1,4;2;\frac{2}{\beta_t n'}) \right.$$

$$+2i(\zeta_t\beta_t)^{-3}\, {}_2F_1(-n'+1;3;2;\frac{2}{\beta_t n'})/b$$

$$\left.-(\zeta_t\beta_t)^{-2}\, {}_2F_1(-n'+1;2;2;\frac{2}{\beta_t n'})/b^2\right] \quad \ldots (3.22)$$

and

$$F_{1s\text{-}n'p_{\pm1}}(\vec{k}_f,\vec{k}_i) = \frac{2\sqrt{6}i\eta k_i}{(n')^3} \frac{[(n'-2)!]^{1/2}}{[(n'+1)!]^{1/2}} e^{\mp i\phi_q}[g^o_{11} - g^1_{11}]$$

$$= -\frac{2\sqrt{6}\, i\eta k_i}{(n')^3}\left[\frac{(n'+1)!}{(n'-2)!}\right]^{1/2} \frac{1}{q^2} e^{\mp i\phi_q} \int db\, G(q/b)$$

$$\times \sum_{t=1}^{2} \zeta_t \left[4(\zeta_t\beta_t)^{-5}\, {}_2F_1(-n'+2,5;4;\frac{2}{\beta_t n'}) \right.$$

$$+2i(\zeta_t\beta_t)^{-4}\, {}_2F_1(-n'+2,4;4;\frac{2}{\beta_t n'})/b$$

$$-(\zeta_t\beta_t)^{-3}\, {}_2F_1(-n'+2,3;4;\frac{2}{\beta_t n'})/b^2$$

$$\left.-i(\zeta_t\beta_t)^{-2}\, {}_2F_1(-n'+2,2;4;\frac{2}{\beta_t n'})/(2b^3)\right], \quad \ldots (3.23)$$

where

$$\zeta_t = -(-1)^t. \quad \ldots (3.24)$$

The hypergeometric functions appearing in Eqs.(3.22) and (3.23) can be expressed in simple closed forms. Eq.(3.22), for

example, can be written as

$$F_{1s\text{-}n's}(\vec{K}_f,\vec{K}_i) = \frac{2k_i}{q^2(n')^{3/2}} \int_0^\infty db\ G(q/b) \sum_{t=1}^{2} \zeta_t$$

$$\times \Big[(\zeta_t\beta_t)^{-2}\Big(1-\frac{2}{\beta_t n'}\Big)^{n'-1}/b^2$$

$$-2i(\zeta_t\beta_t)^{-3}\Big(1-\frac{2}{\beta_t n'}\Big)^{n'-2}\Big(\Big(1-\frac{1}{\beta_t}\Big)-\frac{1}{\beta_t n'}\Big)/b$$

$$-2(\zeta_t\beta_t)^{-4}\Big(1-\frac{2}{\beta_t n'}\Big)^{n'-3}\Big(\Big\{\Big(1-\frac{2}{\beta_t}\Big)\Big(1-\frac{1}{\beta_t}\Big)-1\Big\}$$

$$-\frac{6}{\beta_t}\Big(1-\frac{1}{\beta_t}\Big)\frac{1}{n'}+\frac{4}{\beta_t^2 n'^2}\Big)\Big] \qquad \ldots (3.25)$$

$$\xrightarrow{\text{large } n'} \frac{2k_i}{q^2(n')^{3/2}} \int_0^\infty db\ G(q/b) \sum_{t=1}^{2} \zeta_t\, e^{-2/\beta_t}$$

$$\times \Big[b^{-2}(\zeta_t\beta_t)^{-2}-2ib^{-1}(\zeta_t\beta_t)^{-3}\Big(1-\frac{1}{\beta_t}\Big)$$

$$-2(\zeta_t\beta_t)^{-4}\Big(3-\frac{6}{\beta_t}+\frac{2}{\beta_t^2}\Big)\Big]. \qquad \ldots (3.26)$$

# CHAPTER 4

## STUDY OF ELASTIC AND INELASTIC SCATTERING OF ELECTRONS BY LITHIUM

### 4.1.1 INTRODUCTION

In the last chapter we have studied the tractability and usefulness of the one-dimensional integral forms[87,89-94,9] and the closed form expressions[59] of the Glauber transition amplitudes in e-H atom scattering. To obtain closed form expressions for atomic systems containing more than one electron even with the simplest approximate wavefunction is very unlikely[100]. The Glauber amplitude expression (2.49) for the scattering of charged particle by a Z-electron atom involves a (3Z+2)-dimensional [(3Z+2)D] integral. In order to appreciate the difficulties in actual calculation and to be more specific let us consider the next simplest [i.e. next to e-H(1s)] atomic collision, namely, e-He($1s^2$).

### 4.1.2 SCATTERING BY HELIUM

The Glauber scattering amplitude for e-He($1s^2$) requires an 8D integral [2D integration over the impact parameter $\vec{b}$ and 3D integrations over each of the bound electron coordinates $\vec{x}_1$ and $\vec{x}_2$]. For this case, the Glauber phase function $\chi$ of Eq.(2.47c) reduces to

$$\chi(\vec{b},\vec{x}_1,\vec{x}_2) = \chi_1 + \chi_2, \qquad \ldots (4.1a)$$

where

$$\chi_j = -2\eta \ln\left(\frac{|\vec{b}-\vec{s}_j|}{b}\right). \qquad \ldots (4.1b)$$

In Eq.(4.1b), the 2D vector $\vec{s}_j$ is the projection of $\vec{x}_j$ onto the plane (containing impact parameter vector $\vec{b}$) perpendicular to the integration direction $\hat{\zeta}(\perp \vec{q})$ in Eq.(2.47d), and $\eta = 1/k_1$, as in e-H(1s). Inspite of this simple form for $\chi_j$, the profile function

$$\Gamma \equiv 1 - e^{i\chi} = 1 - e^{i(\chi_1+\chi_2)} \qquad \ldots (4.2)$$

is quite complicated than either

$$\Gamma_1 \equiv 1 - e^{i\chi_1} \qquad \ldots (4.3a)$$

or

$$\Gamma_2 \equiv 1 - e^{i\chi_2}, \qquad \ldots (4.3b)$$

and this is why the 8D analogue of e-H(1s) Glauber amplitude expression (3.4) can not be reduced to as simple a form even with factorable helium bound state eigenfunctions. Franco[101] using his Ref.94 procedures could only reduce the e-He($1s^2$) elastic scattering amplitude to a 3D integral which was evaluated numerically. A further reduction to more easily calculable 2D representation for elastic and inelastic scattering has been proposed by Yates and Tenney[100]. Still more recently, Franco[102], Thomas and Chan[103], Chan and Chen[104], and Chan and Chang[105] have shown that Glauber scattering amplitudes both for e-He($1s^2$) elastic and inelastic transitions can be reduced to 1D form without making any further approximation.

These reductions to 1D integrals are readily generalizable to collisions with target atoms involving more than two bound electrons. Franco[102] basically uses the procedures outlined by him earlier [Ref.60]. The method of Thomas and Chan[103] also leads to a 1D form [different that of Franco[102]] involving modified Lommel functions $\mathcal{L}_{\mu,\nu}$; Thomas and Chan[103] break up the profile function $\Gamma$ into single and double scattering terms:

$$\begin{aligned}\Gamma \equiv 1 - e^{i\chi} &= 1 - e^{i(\chi_1+\chi_2)} \\ &= (1 - e^{i\chi_1}) + (1 - e^{i\chi_2}) - (1 - e^{i\chi_1})(1 - e^{i\chi_2}) \\ &\equiv \Gamma_1(\vec{b},\vec{x}_1) + \Gamma_2(\vec{b},\vec{x}_2) - \Gamma_1(\vec{b},\vec{x}_1)\,\Gamma_2(\vec{b},\vec{x}_2), \end{aligned} \qquad \ldots (4.4a)$$

where

$$\Gamma_j = 1 - e^{i\chi(\vec{b},\vec{x}_j)}, \qquad \ldots (4.4b)$$

with $\chi_j$ given by Eq.(4.1b). 'Single scattering' contributions $\Gamma_1$ and $\Gamma_2$ have been evaluated in closed form. It should be noted that the 'single scattering' contribution $\Gamma_1$ is not from a single fundamental particle, but from a hydrogenic atom, composed of electron 1 and a charge $Z = 1$ (at the nucleus, the remaining $Z=1$ charge together with electron 2, forms the another hydrogenic atom whose 'single scattering' contribution is associated with $\Gamma_2$. We now consider the next complicated system i.e. e - Li scattering.

## 4.1.3 SCATTERING BY LITHIUM WITH 'FROZEN CORE' APPROXIMATION

It has been pointed out earlier that the Glauber transition amplitude describing the scattering of a charged

particle by a Z-electron atom involves a (3Z+2)D integral. Thus in order to compute e - Li($1s^2$ $2s^1$) collision amplitudes, an 11D integral has to be performed. Obviously this cannot be handled as it is. Simplifications can be made by either making certain analytic reductions or by introducing some simplifying approximations. One such approximation is to treat the alkali atom 'effectively' as a one-electron (hydrogen-like) system; the core of the atom, consisting of (Z-1) non-valence electrons in the inner orbits and (Z-1) protons at the nucleus, is assumed to be frozen and is ignored. This approximation, the so-called 'frozen core' approximation, thus involves only the active (valence) electron and a nucleus of charge unity and ignores the effects of core electrons. If one looks at the electronic configuration of an alkali atom, one finds that the (Z-1) non-valence electrons forming a closed shell structure are chemically inactive and only the valence electron in the outermost orbit is the active one. One might argue purely on this ground that the 'frozen core' approximation should be quite good. This approximation reduces the full (3Z+2)D Glauber integral (2.49) for a Z-electron target (alkali) atom to a 5D integral, as it is in the case of e-H(1s) scattering. Mathur et al[62] and Tripathi et al[106] have followed this approach.

The effect of core electrons can be taken into account approximately by including a core potential $V_{CR}(r)$ which is obtained by replacing the actual pairwise Coulomb interactions between the incident electron and the (Z-1) non-valence

electrons, together with the balancing $-(Z-1)e^2/r$ interaction between the incident electron and (Z-1) nuclear protons with an effective purely central potential. Such an approach has been followed by Walters[63]. The interaction potential for electron-alkali atom scattering in 'frozen core' approximation is given by

$$V(\vec{r},\vec{x}_1) = P\left[ V_{CR}(\vec{r}) - \frac{2}{r} + \frac{2}{|\vec{r}-\vec{x}_1|} \right] P \qquad \ldots (4.5a)$$

$$\equiv P\left[ V_{CR}(\vec{r}) + V_H(\vec{r},\vec{x}_1) \right] P , \qquad \ldots (4.5b)$$

where $\vec{x}_1$ is the spatial coordinate (relative to the nucleus) of the valence target electron. In Eq.(4.5), the projection operator P is given by

$$P = 1 - \sum_{j=1}^{N} |\phi_j^c(\vec{x}_1)\rangle \langle \phi_j^c(\vec{x}_1)| , \qquad \ldots (4.6)$$

and the core potential $V_{CR}(\vec{r})$ is of the form

$$V_{CR}(\vec{r}) = 2 \sum_{j=1}^{N} \int d^3x_i \phi_j^{c*}(\vec{x}_i) \left( \frac{2}{|\vec{r} - \vec{x}_i|} - \frac{2}{r} \right) \phi_j^c(\vec{x}_i) , \qquad \ldots (4.7)$$

where (2N+1) = Z (atomic number) and $\phi_j^c$(normalized) denotes the spatial wavefunction of the jth core electron of the alkali atom. The core orbitals $\phi_j^c$ are taken to be orthogonal to the valence state $\phi_j^v$. The Glauber scattering amplitude $F_{fi}(\vec{k}_f,\vec{k}_i)$, Eq.(2.49), corresponding to a transition (i→f) in the target from an initial state i with valence wavefunction $\phi_i^v$ to some final state f with valence wavefunction $\phi_f^v$ is given by[63]

$$F_{fi}(\vec{k}_f, \vec{k}_i) = \frac{ik_i}{2\pi} \int d^2b \; e^{i\vec{q}\cdot\vec{b}} \int d^3x_1 \phi_f^{v*}(\vec{x}_1) \Gamma(\vec{b},\vec{x}_1) \phi_i^v(\vec{x}_1), \quad \ldots (4.8)$$

where

$$\Gamma(\vec{b},\vec{x}_1) = 1 - e^{i(\chi_H+\chi_{CR})}$$

$$= (1 - e^{i\chi_H}) + e^{i\chi_H}(1 - e^{i\chi_{CR}}) \quad \ldots (4.9a)$$

$$\equiv \Gamma_H + e^{i\chi_H} \Gamma_{CR}, \quad \ldots (4.9b)$$

$$\chi_H = -\frac{i}{2k_i} \int_{-\infty}^{\infty} V_H(\vec{b},z;\vec{x}_1)dz, \quad \ldots (4.10a)$$

$$\chi_{CR} = -\frac{i}{2k_i} \int_{-\infty}^{\infty} V_{CR}(\vec{b},z)dz. \quad \ldots (4.10b)$$

Walters[63] sets P equal to unity to get

$$F_{fi}(\vec{k}_f,\vec{k}_i) = \frac{ik_i}{2\pi} \int d^2b \; e^{i\vec{q}\cdot\vec{b}} \int d^3x_1 \phi_f^{v*}(\vec{x}_1) \Gamma_H \phi_i^v(\vec{x}_1)$$

$$+ \frac{ik_i}{2\pi} \int d^2b \; e^{i\vec{q}\cdot\vec{b}} \int d^3x_1 \; \phi_f^{v*}(\vec{x}_1) e^{i\chi_H} \Gamma_{CR} \phi_i^v(\vec{x}_1)$$

$$\equiv F_{fi}^{H}(\vec{k}_f,\vec{k}_i) + F_{fi}^{HC}(\vec{k}_f,\vec{k}_i), \quad \ldots (4.11)$$

where

$$\Gamma_H = 1 - \left(\frac{|\vec{b} - \vec{s}_1|}{b}\right)^{2i\eta},$$

$$\vec{x}_1 = \vec{s}_1 + z_1\hat{k}_i,$$

$$\vec{s}_1 \cdot \vec{k}_i = 0 \quad ,$$

$$\eta = 1/k_i \quad . \quad \ldots (4.12)$$

$F^H$ and $F^{HC}$ can now be handled easily by methods used for e-H(1s) scattering.

### 4.1.4 SCATTERING BY LITHIUM WITHOUT 'FROZEN CORE' APPROXIMATION

In the foregoing discussion, the application of the Glauber approximation has been restricted to the scattering by atoms having one or two 'effective' electrons. Obviously these procedures fail if the target atoms have more than two 'effective' electrons or if one wishes to consider all the target electrons explicitly. The difficulties are removed automatically if one follows analytical procedures which first reduce the (3Z+2)D integral sufficiently before attempting any numerical calculation. Such a procedure has been given by Franco[60]. We have adopted this procedure in our e-Li atom scattering calculations. In the following we present its details.

This procedure reduces the (3Z+2)D integral to a 1D integral for the elastic and inelastic scattering of charged particles by arbitrary neutral atoms. It is based (i) on the assumption that the product of the initial $\phi_i$ and the final $\phi_f$ wavefunctions of the target can be written in the form

$$\phi_f^* \phi_i = \sum_{k=1}^{N} \left[ c_k \prod_{j=1}^{Z} \left\{ x_j^{n_{k,j}} e^{-\alpha_{k,j} x_j} Y_{\ell_j m_j}(\theta_j, \phi_j) Y^*_{\ell'_j m'_j}(\theta_j, \phi_j) \right\} \right], \quad \ldots (4.13)$$

where $x_j$, $\theta_j$, $\phi_j$ are the spherical polar coordinates of the jth electron and $Y_{\ell m}$ are the spherical harmonics and (ii) on carrying out the integrations over the coordinates of the target electrons without involving the impact parameter b. This

procedure differs from the one followed in Refs. 100 and 101 for e-He scattering. There the impact parameter is mixed with the coordinates $\vec{x}_1(\vec{s}_1,z_1)$ and $\vec{x}_2(\vec{s}_2,z_2)$ of the target electrons to generate a new set of variables R,ξ and ζ in place of b, $s_1$ and $s_2$. This mixing is not feasible for more than two electrons in the target. The assumption regarding the form, Eq.(4.13), of $\phi_f^*\phi_i$ is really no restriction as the wavefunctions usually employed in describing the atoms can always be put in that form. The result is that the final expression involves just a 1D integral over b. The only problems with this method are the evaluation of the integrand which involves the calculation of the differences between strongly divergent functions and the numerical calculation of the δ-function whenever elastic scattering is considered[103]. Thomas and Chan[103] have modified this procedure to eliminate these difficulties by using the properties of modified Lommel functions and have reported calculations of the elastic and inclastic e-He scattering as pointed out earlier. This has also been used more recently by Chan and Chang[107] to study elastic e-Li scattering. The main attribute of these methods is that the contribution of the inner electrons is explicitly taken into account and can be analysed in contrast to the 'frozen core' approximation.

In the present work we have avoided the encounter with the divergent functions appearing in Franco's final expression[60] by stopping a step earlier (Sec.4.2). The concealed δ-function in the momentum transfer $\vec{q}$ presents no numerical problem. The

price to be paid for this simplification is that our final expression is a 2D integral, irrespective of the atomic number of the target, against Franco's 1D integral. Thomas and Chan[103] have also pointed out this possibility but did not pursue it. We illustrate this procedure by considering the elastic and inelastic scattering of electrons by lithium atoms.

In Sec.4.2 we discuss the case of the elastic e-Li($1s^2 2s^1$) scattering, wherein we outline the method, give the details of the calculation and discuss the results of these calculations. Sec.4.3 is devoted to the inelastic (2s-2p) e-Li scattering. Polarization calculations of 2p→2s resonance line of $^6$Li and $^7$Li following electron impact will be presented in Sec.4.4.

## 4.2 ELASTIC SCATTERING

### 4.2.1 METHOD

Recalling Eqs.(2.49), the Glauber scattering amplitude $F_{fi}(\vec{k}_f, \vec{k}_i)$ of a charged particle with momentum $\vec{k}_i$ by a Z-electron target atom which undergoes a transition from an initial state i with wavefunction $\phi_i$ to some final state f with wavefunction $\phi_f$ is given by[40,60]

$$F_{fi}(\vec{k}_f,\vec{k}_i) = \frac{ik_i}{2\pi} \int \phi_f^*(\vec{x}_1,\ldots,\vec{x}_Z) \Gamma(\vec{b},\vec{x}_1,\ldots,\vec{x}_Z) \times \phi_i(\vec{x}_1,\ldots,\vec{x}_Z) e^{i\vec{q}.\vec{b}} d^2b\, d^3x_1 \ldots d^3x_Z; \quad \ldots (4.14a)$$

and the profile function $\Gamma$ is given by

$$\Gamma(\vec{b},\vec{x}_1,\ldots,\vec{x}_Z) \equiv \Gamma(\vec{b},\vec{s}_1,\ldots,\vec{s}_Z)$$

$$= 1 - \exp\left[i\chi(\vec{b},\vec{s}_1,\ldots,\vec{s}_Z)\right]$$

$$= 1 - \prod_{j=1}^{Z}\left(\frac{|\vec{b}-\vec{s}_j|}{b}\right)^{2i\eta} \qquad \ldots (4.14b)$$

Combining Eqs.(4.14a) and (4.14b), the scattering amplitude $F_{fi}(\vec{k}_f, \vec{k}_i)$ takes the form

$$F_{fi}(\vec{k}_f,\vec{k}_i) = \frac{ik_i}{2\pi}\int d^2b\, e^{i\vec{q}\cdot\vec{b}}\Big\{1-\int d^3x_1\ldots d^3x_Z \phi_f^*\phi_i$$

$$\times\left[\prod_{j=1}^{Z}\left(\frac{|\vec{b}-\vec{s}_j|}{b}\right)^{2i\eta}\right]\Big\}. \qquad \ldots (4.15)$$

The contribution of the first term in curly brackets in Eq.(4.15), though proportional to the 2D delta function $\delta(\vec{q})$, can not be ignored for otherwise the integrand over $\vec{b}$ would not tend to zero, as it should, for large values of the impact parameter b and would create numerical difficulties.

For the product $\phi_f^*\phi_i$, we prefer the form

$$\phi_f^*\phi_i = \prod_{j=1}^{Z}\left(\sum_{k=1}^{N_j} c_{k,j}x_j^{n_{k,j}}\, e^{-\alpha_{k,j}x_j}\right) Y_{\ell_j m_j}(\theta_j,\phi_j)\, Y^*_{\ell_j' m_j'}(\theta_j,\phi_j), \qquad \ldots (4.16)$$

which can be obtained by regrouping the terms in Eq.(4.13). For elastic scattering by lithium atoms only s states are involved, i.e., $\ell_j = \ell_j' = m_j = m_j' = 0$ for all j. Thus

$$\phi_f^* \phi_i = (4\pi)^{-3} \prod_{j=1}^{3} \left( \sum_{k=1}^{N_j} c_{k,j} x_j^{n_{k,j}} e^{-\alpha_{k,j} x_j} \right) \qquad \ldots (4.17a)$$

$$= (4\pi)^{-3} \prod_{j=1}^{3} \sum_{k=1}^{N_j} c_{k,j} (-1)^{1+n_{k,j}} \left( \frac{\partial}{\partial \alpha_{k,j}} \right)^{1+n_{k,j}} \frac{e^{-\alpha_{k,j} x_j}}{x_j} . \qquad \ldots (4.17b)$$

Using Eq.(4.17b) in Eq.(4.15), and carrying out the integration over $\phi_b$, yields

$$F_{fi}(\vec{k}_f, \vec{k}_i) = ik_i \int_0^\infty db\, J_0(qb)\, b \left[ 1 - (4\pi)^{-3} \prod_{j=1}^{3} \sum_{k=1}^{N_j} c_{k,j} (-1)^{1+n_{k,j}} \right.$$

$$\left. \times \left( \frac{\partial}{\partial \alpha_{k,j}} \right)^{1+n_{k,j}} I(\alpha_{k,j}, b) \right], \qquad \ldots (4.18)$$

where

$$I(\alpha_{k,j}, b) = \int \frac{e^{-\alpha_{k,j} x_j}}{x_j} \left( \frac{|\vec{b} - \vec{s}_j|}{b} \right)^{2i\eta} d^3 x_j . \qquad \ldots (4.19)$$

It is worth mentioning here that the limit $b \to \infty$ of the second term in Eq.(4.18) is unity. The integral in Eq.(4.19) can be performed by introducing cylindrical coordinates $\vec{s}_j, z_j$ for $\vec{x}_j$ and following the methods of Franco[60] and Thomas and Gerjuoy[59] to give

$$I(\alpha_{k,j}, b) = 2 \int_0^\infty ds_j s_j \int_0^\infty dz_j (s_j^2 + z_j^2)^{-1/2}$$

$$\times \exp\left[ -\alpha_{k,j} (s_j^2 + z_j^2)^{1/2} \right] \int_0^{2\pi} d\phi \left( 1 + \frac{s_j^2}{b^2} - \frac{2s_j}{b} \cos\phi \right)^{i\eta}$$

$$= 2b^2 \int_0^\infty ds\, s K_0(\alpha_{k,j} bs) \int_0^{2\pi} d\phi (1 + s^2 - 2s\cos\phi)^{i\eta}$$

$$= 2b^2(-\pi\ 2^{1+2i\eta}\ \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\ )\int_0^\infty ds\ s\ K_o(\alpha_{k,j}bs)$$

$$\times \int_0^\infty dt\ t^{-2i\eta}\ \frac{d}{dt}[J_o(t)J_o(st)]$$

$$= 2b^2E(\eta)\int_0^\infty dt\ t^{-2i\eta}\ \frac{d}{dt}(J_o(t)\int_0^\infty ds\ s\ K_o(\alpha_{k,j}bs)J_o(st))$$

$$= 2b^2E(\eta)\int_0^\infty dt\ t^{-2i\eta}\ \frac{d}{dt}\left(\frac{J_0(t)}{t^2+(\alpha_{k,j}b)^2}\right), \qquad \ldots (4.20a)$$

where

$$E(\eta) = -\pi\ 2^{1+2i\eta}\ \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\ . \qquad \ldots (4.20b)$$

Franco[60] integrates Eq.(4.20) by parts, to get (Ref.108,p.434)

$$I(\alpha_{k,j},b) = 4i\eta b^2E(\eta)\int_0^\infty dt\ \frac{t^{-2i\eta-1}\ J_o(t)}{(t^2+\alpha_{k,j}^2b^2)}$$

$$= 4i\eta b^2E(\eta)[E_1(\eta)(\alpha_{k,j}b)^{-2-2i\eta}\ {}_oF_1(---;1;\alpha_{k,j}^2b^2/4)$$

$$+E_2(\eta)\ {}_1F_2(1;2+i\eta,\ 2+i\eta;\ \alpha_{k,j}^2b^2/4)], \ldots (4.21)$$

where

$$E_1(\eta) = \Gamma(-i\eta)\Gamma(1+i\eta)/2 \qquad \ldots (4.22)$$

and

$$E_2(\eta) = \Gamma(-1-i\eta)\ /\ (2^{3+2i\eta}\Gamma(2+i\eta)). \qquad \ldots (4.23)$$

The hypergeometric functions appearing in Eq.(4.21) are themselves divergent functions of $\alpha_{k,j}b$ although their combination as appearing in Eq.(4.21) is convergent. This can be clearly seen by carrying out the differentiation indicated in Eq.(4.20a):

$$I(\alpha_{k,j}, b) = -2b^2 E(\eta) \int_0^\infty dt\; t^{-2i\eta} \left[ \frac{J_1(t) + 2tJ_0(t)/(t^2 + \alpha_{k,j}^2 b^2)}{(t^2 + \alpha_{k,j}^2 b^2)} \right]. \qquad \ldots (4.24)$$

The integral in Eq.(4.24) can be easily evaluated numerically. We have used this form to avoid the problems associated with the calculation of the differences between strongly divergent functions appearing in Franco's expression [Eq.(4.21)].

The differentiations of I with respect to $\alpha_{k,j}$ in Eq.(4.18) can be done analytically.

4.2.2 CALCULATION

For elastic scattering by lithium atoms we need only $\phi_i$ where the electrons are in $(1s)^2(2s)^1$ configuration. We have taken these orbitals of the form given by Clementi[109], and $\phi_i$ is obtained by taking their antisymmetric combination. This leads to

$$\begin{aligned} \phi_f^* \phi_i &= (1/3!) \left| \det(\phi_{1s}^c, \phi_{1s}^c, \phi_{2s}^v) \right|^2 \\ &= \left| \phi_{1s}^c(1)\; \phi_{1s}^c(2)\; \phi_{2s}^v(3) \right|^2 \\ &\quad - \left| \phi_{1s}^c(1) \right|^2 \phi_{1s}^{c*}(2) \phi_{2s}^v(2) \phi_{1s}^c(3) \phi_{2s}^{v*}(3). \end{aligned} \qquad \ldots (4.25)$$

The orbitals $\phi^{c,v}$ are of the form (Ref.109):

$$\phi^{c,v}(\vec{x}) = R(x) Y_{oo}(\theta, \phi). \qquad \ldots (4.26a)$$

with

$$R(x) = \sum_{j=1}^{2} A_j e^{-\xi_j x} + \sum_{j=3}^{6} A_j x\, e^{-\xi_j x}. \qquad \ldots (4.26b)$$

Both the terms in Eq.(4.25) for $\phi_f^* \phi_i$, with $\phi^{c,v}$'s of the

form (4.26) lead to the expression (4.17a) with

$$N_j = 21$$

$$n_{k,j} = \begin{cases} 0 & k \leq 3 \\ 1 & 3 < k \leq 11 \\ 2 & 11 < k \leq 21 \end{cases} \qquad \ldots (4.27)$$

The values of the constants $c_{k,j}$ and $\alpha_{k,j}$ are obtained from the values of the parameters $A_i$ and $\xi_i$ given by Clementi[109] and are tabulated in Table 4.1.

The integrals in Eqs.(4.18) and (4.24) were done by the Filon's method[110]. The wiggles of the Bessel functions were accurately taken into account by combining the Simpson's rule with the standard Bessel function integrals (Appendix A1).

The differential and integrated cross sections for elastic scattering are obtained from the scattering amplitude expression (4.18) in the usual way. Recalling Eqs.(2.50) and (2.54a), these are given by

$$\frac{d\sigma_{el}(q)}{d\Omega} = |F_{fi}(\vec{k}_f, \vec{k}_i)|^2 \text{ in units of } a_o^2, \qquad \ldots (4.28)$$

and

$$\sigma_{el}(k_i) = \frac{2}{k_i^2} \int_o^{2k_i} dq\, q |F_{fi}(\vec{k}_f, \vec{k}_i)|^2 \qquad \ldots (4.29)$$

in units of $\pi a_o^2$.

## 4.2.3 RESULTS AND DISCUSSION

In Fig.4.2 we have plotted the differential cross-section against the scattering angle $\theta$ upto $80^o$ at electron laboratory

TABLE 4.1

Coefficients $c_{k,j}$ and exponents $\alpha_{k,j}$ for the products of the type $|\phi^{lc}_{ls}|^2$, $|\phi^{v}_{2s}|^2$ and $\phi^{v*}_{2s}\phi^{c}_{ls}$ appearing in e-Li scattering.

| k | $c_{k,j}$ | | | $\alpha_{k,j}$ |
|---|---|---|---|---|
| | 1s×1s | 2s×2s | 1s×2s | |
| 1 | 49.19403076 | 1.27017689 | -7.90478706 | 4.9606 |
| 2 | 5.07708359 | 0.10466754 | -0.72890657 | 9.4142 |
| 3 | 31.60772705 | 0.72923636 | -4.80836201 | 7.1874 |
| 4 | -0.00007043 | -0.00038102 | 0.00119128 | 2.8303 |
| 5 | 0.00624801 | -0.90173423 | 2.80539989 | 3.1403 |
| 6 | -0.02332481 | -0.23625112 | 0.73701036 | 3.4803 |
| 7 | 0.60178995 | 0.92508828 | -2.92692184 | 4.2153 |
| 8 | -0.00002262 | -0.00010938 | 0.00038248 | 5.0571 |
| 9 | 0.00200702 | -0.25885248 | 0.90118235 | 5.3671 |
| 10 | -0.00749251 | -0.06781840 | 0.23668224 | 5.7071 |
| 11 | 0.19331002 | 0.26555651 | 0.93854916 | 6.4421 |
| 12 | 0.00000000 | 0.00000003 | 0.00000000 | 0.6999 |
| 13 | 0.00000020 | 0.16004151 | 0.00017819 | 1.3200 |
| 14 | 0.00000276 | 0.01098560 | -0.00017428 | 2.0000 |
| 15 | 0.00184042 | 0.16843867 | -0.01760677 | 3.4700 |
| 16 | -0.00000000 | 0.00013525 | -0.00000193 | 1.0100 |
| 17 | 0.00000002 | 0.00003544 | -0.00000081 | 1.3500 |
| 18 | -0.00000043 | -0.00013875 | 0.00000931 | 2.0850 |
| 19 | -0.00000148 | 0.08386087 | -0.00061851 | 1.6600 |
| 20 | 0.00003822 | -0.32837284 | 0.01697948 | 2.3950 |
| 21 | -0.00014267 | -0.08603281 | 0.00517890 | 2.7350 |

*See Eq.(4.16)

energy of 54.38 eV ($k=2a_o^{-1}$). The curves a and b correspond to the calculations(---) in the 'frozen core' Glauber approximation without and with core potential, respectively. These are similar to those in Refs.62 and 63. The curve c corresponds to the present calculation (——). Clementi wavefunctions have been used in all the calculations. All the curves show almost identical variation indicating that the inner electrons (those in the 1s state) are not very active. A more quantitative picture is given in Table 4.2. The slight increase in cross section, when the core potential is included, is in agreement with the findings of Walters[63]. The differential cross sections with the present calculation differ little from those in the 'frozen core' approximation. Similar is the case with the total cross section for energies upto 200 eV. [Fig. 4.3].

In order to assess the accuracy of our theoretical differential cross sections we have compared, in Fig.4.1, our results (curve c) at 20 eV with the recent experimental data (Q) of Williams et al[111]. It is evident from the figure and as expected the Glauber approximation underestimates the differential cross sections at such a low energy over the entire angular range. Our total cross sections, plotted in Fig.4.3, are also quite low as compared with the experimental data[111] (Q) even at intermediate energies (upto 60 eV).

To summarize it appears that nothing much is gained by including explicitly the inner electrons and the 'frozen core' Glauber calculation is good enough.

TABLE 4.2

Elastic e-Li differential cross sections in units of $a_o^2$ at $k_i = 2a_o^{-1}$.

| Scattering angle (in degrees) | Frozen-core Glauber approximation | | |
|---|---|---|---|
| | Without core potential | with core potential | Present calculation |
| 10 | 27.11 | 27.06 | 26.90 |
| 20 | 5.59 | 5.52 | 5.01 |
| 30 | 1.58 | 1.57 | 1.37 |
| 40 | 0.61 | 0.63 | 0.54 |
| 50 | 0.29 | 0.31 | 0.27 |
| 60 | 0.16 | 0.18 | 0.16 |
| 70 | 0.10 | 0.12 | 0.10 |
| 80 | 0.06 | 0.08 | 0.06 |

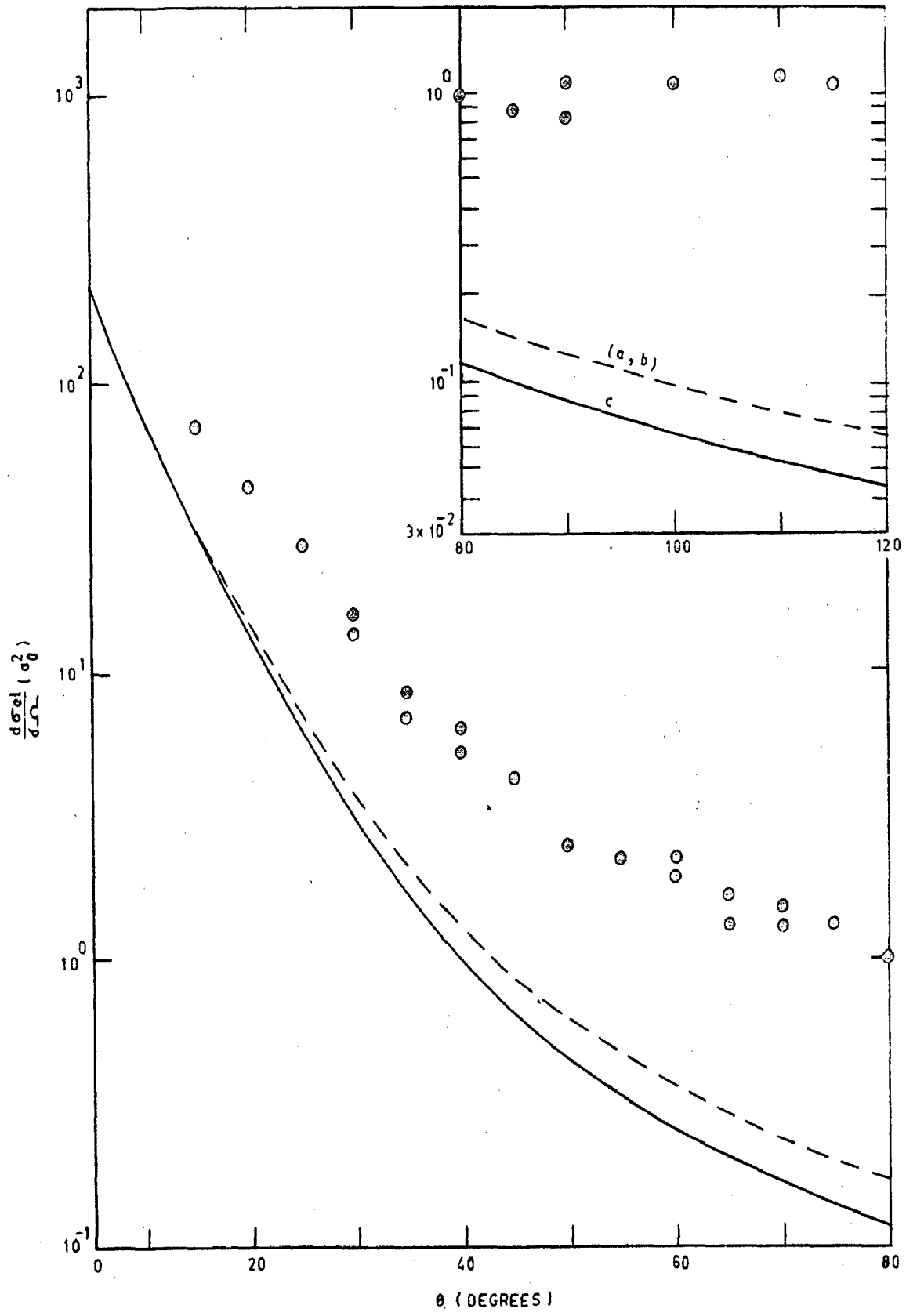


FIG.4.1 – ELASTIC e-Li DIFFERENTIAL CROSS SECTION FOR SCATTERING ANGLE θ UPTO 120° AT $k_i^2$ – 20 eV. ___, PRESENT CALCULATION (c); – – –, FROZEN CORE GLAUBER CALCULATIONS (a, b) WITHOUT AND WITH CORE POTENTIAL INCLUDED; ●, EXPERIMENTAL DATA OF WILLIAMS et al[111].

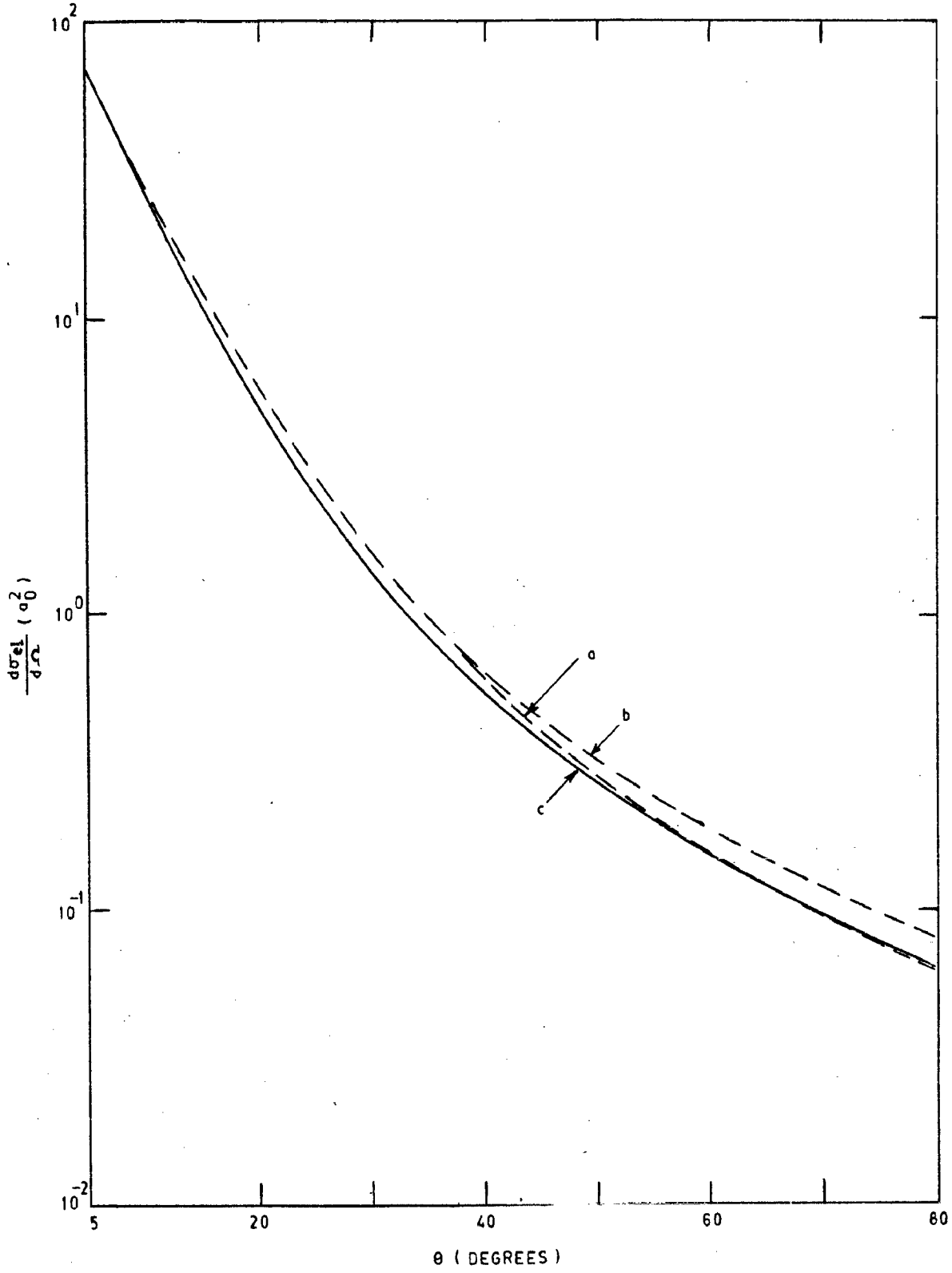


FIG 4.2 — ELASTIC e–Li DIFFERENTIAL CROSS SECTION FOR SCATTERING ANGLE θ UPTO 80° AT $k_i^2$ = 54.38 eV. ——, PRESENT CALCULATION (c); – – –, FROZEN CORE GLAUBER CALCULATIONS (a, b) WITHOUT AND WITH CORE POTENTIAL INCLUDED.

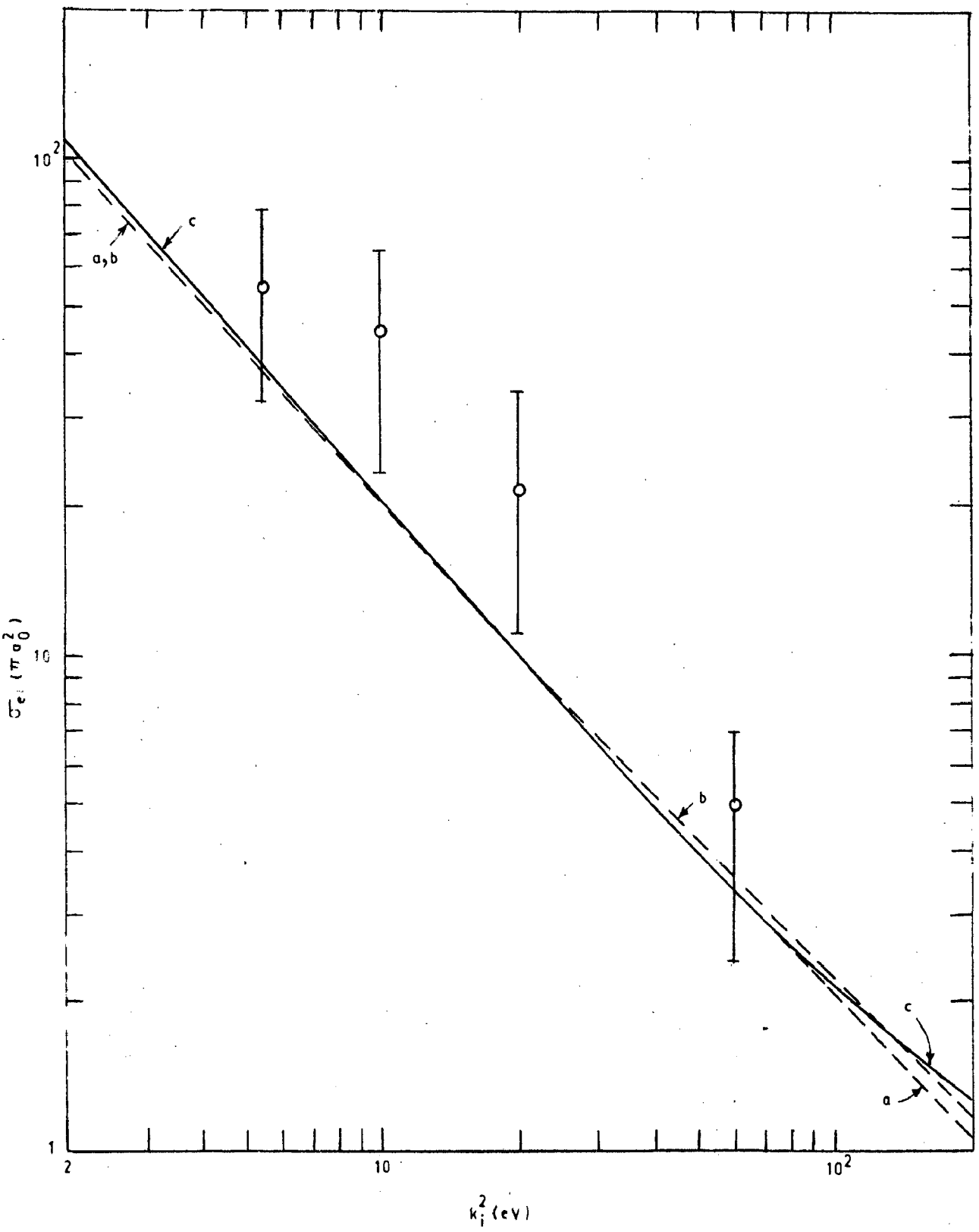


FIG 4.3 – TOTAL e – Li ELASTIC SCATTERING CROSS SECTION FOR ELECTRON IMPACT ENERGIES UPTO 200 eV. ——, PRESENT CALCULATION (c); – – –, FROZEN CORE GLAUBER CALCULATIONS (a, b) WITHOUT AND WITH CORE POTENTIAL INCLUDED; ⊼, EXPERIMENTAL DATA OF WILLIAMS et al[111].

## 4.3 INELASTIC SCATTERING

### 4.3.1 METHOD

Since we are concerned here with the electron impact resonance transition $(1s)^2(2s)^1 \rightarrow (1s)^2(2p)^1$ in lithium atoms, we have

$$\ell_1 = \ell_2 = \ell_3 = m_1 = m_2 = m_3 = 0,$$

$$\ell_1' = \ell_2' = m_1' = m_2' = 0$$

and $$\ell_3' = 1,\ m_3' = 0, \pm 1. \qquad \ldots (4.30)$$

In the present case Eq.(4.16) simplifies to

$$\phi_f^* \phi_i = \prod_{j=1}^{3} a_j \Big( \sum_{k=1}^{N_j} c_{k,j}\, x_j^{n_{k,j}}\, e^{-\alpha_{k,j} x_j} \Big) \qquad \ldots (4.31a)$$

$$= \prod_{j=1}^{3} P_j , \qquad \ldots (4.31b)$$

where

$$a_1 = a_2 = 1/(4\pi) , \qquad \ldots (4.31c)$$

and

$$a_3 = Y^*_{1m_3'}(\theta_3, \phi_3) \,/\, \sqrt{4\pi} . \qquad \ldots (4.31d)$$

Using Eqs.(4.31) in Eq.(4.14a) gives

$$F_{fi}(\vec{k}_f, \vec{k}_i) = - \frac{ik_i}{2\pi} \int d^2b\, e^{i\vec{q}.\vec{b}} \prod_{j=1}^{3} \int P_j \Big( \frac{|\vec{b}-\vec{s}_j|}{b} \Big)^{2i\eta} d^3x_j \ldots (4.32)$$

The terms $P_1$ and $P_2$ also appear in the case of elastic scattering and have been evaluated in Eqs.(4.20a) and (4.24):

$$\int P_j \Big( \frac{|\vec{b}-\vec{s}_j|}{b} \Big)^{2i\eta} d^3x_j = \frac{1}{4\pi} \sum_{k=1}^{N_j} c_{k,j} (-1)^{1+n_{k,j}} \Big( \frac{\partial}{\partial \alpha_{k,j}} \Big)^{1+n_{k,j}} I(\alpha_{k,j}, b)$$

$$\equiv \frac{1}{4\pi} T_j(b) , \qquad j = 1,2 \qquad \ldots (4.33)$$

where

$$I(\alpha_{k,j},b) = -2b^2E(\eta)\int_0^\infty dt\,\frac{t^{-2i\eta}\left[J_1(t)+2tJ_0(t)/(t^2+\alpha_{k,j}^2b^2)\right]}{(t^2+\alpha_{k,j}^2b^2)}, \qquad \ldots (4.34)$$

and $E(\eta)$ is given by Eq.(4.20b). We now calculate the contribution to Eq.(4.32) from the factor $P_3$:

$$\int P_3\left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta} d^3x_3 = \frac{1}{\sqrt{4\pi}}\int\sum_{k=1}^{N_3} c_{k,3}x_3^{n_{k,3}}e^{-\alpha_{k,3}x_3}\left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta}$$

$$\times Y^*_{1m_3'}(\theta_3,\phi_3)d^3x_3$$

$$= \frac{1}{4\pi}\left[\frac{3(1-m_3')!}{(1+m_3')!}\right]^{1/2}(-1)^{m_3'}\sum_{k=1}^{N_3}c_{k,3}\int(s_3^2+z_3^2)^{n_{k,3}/2}$$

$$\times e^{-\alpha_{k,3}(s_3^2+z_3^2)^{1/2}}\left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta}P_{1m_3'}\left(\frac{z_3}{(s_3^2+z_3^2)^{1/2}}\right)$$

$$\times e^{-im_3'\phi_3}\,s_3ds_3d\phi_3dz_3. \qquad \ldots (4.35)$$

For $m_3' = 0$, the associated Laguerre polynomial $P_{1m_3'}$ is an odd function of $z_3$ and therefore, the integral over $z_3$ vanishes. For $m_3' = \pm 1$, Eq.(4.35) can be written as

$$\int P_3\left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta} d^3x_3 = \mp\frac{\sqrt{6}}{2(4\pi)}\sum_{k=1}^{N_3}c_{k,3}\left[2\int_0^\infty ds_3s_3^2\int_0^{2\pi}d\phi_3\right.$$

$$\times e^{\mp i\phi_3}\left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta}(-1)^{n_{k,3}}\left(\frac{\partial}{\partial\alpha_{k,3}}\right)^{n_{k,3}}\int_0^\infty dz_3$$

$$\left.\times\frac{\exp\left[-\alpha_{k,3}(s_3^2+z_3^2)^{1/2}\right]}{(s_3^2+z_3^2)^{1/2}}\right].$$

$$= \mp \frac{\sqrt{6}}{2(4\pi)} \sum_{k=1}^{N_3} c_{k,3}(-1)^{n_{k,3}} \left(\frac{\partial}{\partial \alpha_{k,3}}\right)^{n_{k,3}} I(\alpha_{k,3},b), \quad \ldots (4.36)$$

where

$$I(\alpha_{k,3},b) = 2\int_0^\infty ds_3\, s_3^2 K_o(\alpha_{k,3}s_3) \int_0^{2\pi} d\phi_3\, e^{\mp i\phi_3} \left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta}. \quad \ldots (4.37)$$

Eq.(4.37) can now be solved by procedures [Ref.60, Eqs.(11)-(21); Ref.112, Eqs.(9) and (12)] used in Eq.(4.19), to yield

$$I(\alpha_{k,3},b) = e^{\mp i\phi_b}\left[2b^3E(\eta)\int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}\left(J_1(t)\int_0^\infty ds\, s^2K_o(\alpha_{k,3}bs)J_1(st)\right)\right]$$

$$= e^{\mp i\phi_b}\left[2b^3E(\eta)\int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}\left(\frac{2t\,J_1(t)}{(t^2+\alpha_{k,3}^2b^2)}\right)\right]$$

$$= e^{\mp i\phi_b}\left[8i\eta E(\eta)b^3\int_0^\infty dt\, t^{-2i\eta}\frac{J_1(t)}{(t^2+\alpha_{k,3}^2b^2)^2}\right]. \quad \ldots (4.38)$$

Using Eq.(4.38) in Eq.(4.36) gives

$$\int P_3\left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta} d^3x_3 = \mp \frac{\sqrt{6}}{2(4\pi)} e^{\mp i\phi_b}\left[8i\eta E(\eta)b^3 \times \sum_{k=1}^{N_3} c_{k,3}(-1)^{n_{k,3}}\left(\frac{\partial}{\partial\alpha_{k,3}}\right)^{n_{k,3}} H(\alpha_{k,3},b)\right]$$

$$= \mp \frac{\sqrt{6}}{2(4\pi)} e^{\mp i\phi_b} T_3(b), \quad \ldots (4.39a)$$

where

$$H(\alpha_{k,3},b) = \int_0^\infty \frac{J_1(t)\, t^{-2i\eta}}{(t^2+\alpha_{k,3}^2b^2)^2}dt. \quad \ldots (4.39b)$$

We have evaluated the integrals in Eqs.(4.34) and (4.39b) numerically rather than expressing them as a difference of two diverging

hypergeometric functions (Eq.(22) of Ref.60) as we do in the case of the elastic scattering[112]. The integrands in these integrals [Eqs.(4.34) and (4.39b)], except for the factor $t^{-2i\eta}$, need be evaluated only once at mesh points and can be stored.

The scattering amplitude can now be obtained by putting together the contributions $P_1$, $P_2$ and $P_3$ [Eqs. (4.33) and (4.39)] in Eq.(4.32). Integrating it with respect to $\phi_b$ gives

$$F_{fi}(\vec{k}_f, \vec{k}_i; m_3' = \pm 1) = \frac{\sqrt{6}\, k_i}{2(4\pi)^3} e^{\mp i\phi_q} \int_0^\infty db\, bJ_1(qb) \prod_{j=1}^{3} T_j(b). \quad \ldots (4.40)$$

4.3.2 CALCULATION

The ground-state wavefunction $\phi_i$ of a lithium atom with electronic configuration $1s^2 2s^1$ has been obtained by taking the antisymmetric combination of the 1s, 1s and 2s orbitals, of the form given by Clementi[109]. Similarly the final-state wavefunction $\phi_f$ is the antisymmetric combination of the 1s, 1s and 2p orbitals. This leads to

$$\begin{aligned}\phi_f^* \phi_i &= (1/3!)\left[\det(\phi_{1s\uparrow}^c, \phi_{1s\downarrow}^c, \phi_{2p}^v)\right]^* \\ &\quad \times \left[\det(\phi_{1s\uparrow}^c, \phi_{1s\downarrow}^c, \phi_{2s}^v)\right] \\ &= |\phi_{1s}^c(1)|^2 \left[|\phi_{1s}^c(2)|^2 \phi_{2p}^{v*}(3)\phi_{2s}^v(3) \right. \\ &\quad \left. - \phi_{2p}^{v*}(2)\phi_{1s}^c(2)\phi_{1s}^{c*}(3)\phi_{2s}^v(3)\right]. \end{aligned} \quad \ldots (4.41)$$

The 1s and 2s orbitals of Clementi[109] are of the form

$$\phi^{c,v}_{ns}(\vec{x}) = R_{ns}(x) Y_{oo}(\theta,\phi), \quad n = 1,2, \qquad \ldots (4.42a)$$

with

$$R_{ns}(\vec{x}) = \sum_{i=1}^{2} A_{in}\, e^{-\xi_{in} x} + \sum_{i=3}^{6} A_{in} x\, e^{-\xi_{in} x} \qquad \ldots (4.42b)$$

The 2p orbital has been taken to be of the form given by Stone[113],

$$\phi^{v}_{2p}(\vec{x}) = R_{2p}(x)\, Y_{1m}(\theta,\phi), \qquad \ldots (4.43a)$$

with

$$R_{2p}(x) = A\, x\, e^{-\xi x}, \qquad \ldots (4.43b)$$

where

$$A = 0.228205, \qquad \ldots (4.43c)$$

$$\xi = 0.5227. \qquad \ldots (4.43d)$$

Both the terms in Eq.(4.41) for $\phi^{*}_{f}\,\phi_{i}$ with $\phi^{c,v}$'s of the form (4.42) and (4.43) lead to the expression (4.31a), with $N_j$ and $n_{k,j}$ given by Eq.(4.27) for the products of the type $|\phi^{c}_{1s}|^2$ and $\phi^{v*}_{2s}\phi^{c}_{1s}$, and

$$N_j = 6,\ n_{k,j} = \begin{cases} 1, & 1 < k \leq 2 \\ 2, & 2 < k \leq 6 \end{cases} \qquad \ldots (4.44)$$

for $\phi^{c*}_{2p}\phi^{v}_{1s}$ and $\phi^{v*}_{2p}\phi^{v}_{2s}$. The values of the constants $c_{k,j}$ and $\alpha_{k,j}$ appearing in Eq.(4.31a) are obtained from the value of the parameters $A_{in}$ and $\xi_{in}$ given by Clementi[109] and the values of A and $\xi$ given in Eqs.(4.43c) and (4.43d). They have

been tabulated in Table 4.1 for the products of the type $|\phi_{1s}^{c}|^2$ and $\phi_{2s}^{v*}\phi_{1s}^{c}$ and in Table 4.3 for the products of the type $\phi_{2p}^{v*}\phi_{1s}^{c}$ and $\phi_{2p}^{v*}\phi_{2s}^{v}$.

The differential and the integrated total cross sections are given by

$$\frac{d\sigma_{2s-2p}(q)}{d\Omega} = \frac{k_f}{k_i}\left[|F_{fi}(\vec{k}_f, \vec{k}_i; m_3' = 1)|^2 + |F_{fi}(\vec{k}_f, \vec{k}_i; m_3' = -1|^2\right]$$

$$= \frac{2k_f}{k_i}|F_{fi}(\vec{k}_f, \vec{k}_i)|^2 \text{ in units of } a_o^2, \qquad \ldots (4.45)$$

and

$$\sigma_{2s-2p}(k_i) = \frac{4}{k_i^2}\int_{k_i-k_f}^{k_i+k_f} |F_{fi}(\vec{k}_f, \vec{k}_i)|^2 q\, dq \qquad \ldots (4.46)$$

in units of $\pi a_o^2$.

### 4.3.3 RESULTS AND DISCUSSION

In Fig.4.4 we have plotted the differential cross section against the momentum transfer q upto $1.6a_o^{-1}$ at an electron laboratory energy of 54.38 eV ($k = 2a_o^{-1}$). The curve a corresponds to the calculation (---) in 'frozen core' Glauber approximation. This is similar to the one by Walters[63]. The curve c corresponds to the present calculation (—). Same wavefunctions have been used in both the calculations. Both the curves show almost identical variation indicating that the inner electrons (those in the 1s state) are rather inert in agreement with our earlier findings in the case of e-Li elastic scattering[112]. In the forward direction, $q \lesssim 0.4\ a_o^{-1}$, the two curves overlap as expected. This region is dominated by the contributions for large b and the incoming particle

TABLE 4.3

Coefficients $c_{k,j}$ and exponents $\alpha_{k,j}$ [see Eq. (4.16)] for the products of the type $\phi^{v*}_{2p}\phi^{c}_{1s}$ and $\phi^{v*}_{2p}\phi^{v}_{2s}$ appearing in inelastic (2s-2p)e-Li scattering.

| k | $c_{k,j}$ | | $\alpha_{k,j}$ |
|---|---|---|---|
| | 1s×2s | 2s×2p | |
| 1 | -1.59950750 | 0.25701719 | 3.0031 |
| 2 | -0.51385103 | 0.07377956 | 5.2298 |
| 3 | 0.00000228 | -0.00003950 | 0.8727 |
| 4 | -0.00010198 | -0.09123183 | 1.1827 |
| 5 | 0.00037886 | -0.02390242 | 1.5227 |
| 6 | -0.00968662 | 0.09359463 | 2.2577 |

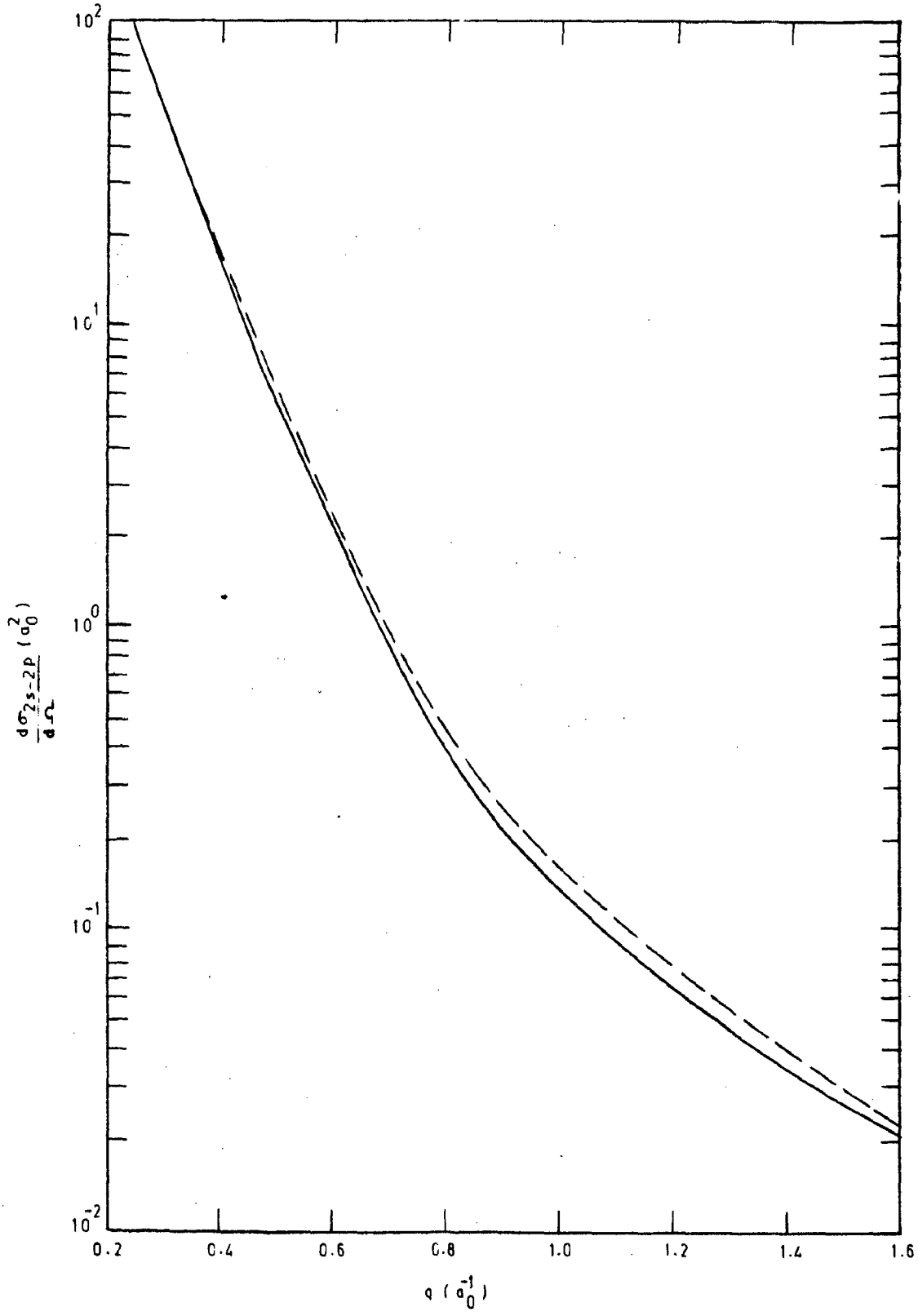


FIG. 4.4 — DIFFERENTIAL CROSS SECTION FOR THE 2s – 2p EXCITATION OF Li FOR MOMENTUM TRANSFER q UPTO 1.6 $a_0^{-1}$ AT $k_i^2 = 54.38$ eV. ——, PRESENT CALCULATION (c); — — — —, FROZEN CORE GLAUBER CALCULATIONS (a, b) WITHOUT AND WITH CORE POTENTIAL INCLUDED.

does not see much of inner electrons. Fig.4.5 shows the total 2s-2p cross sections in units of $\pi a_o^2$ for electron energies upto 250 eV. The results for both the 'frozen core' Glauber and the present calculations again show similar variations. Our results are always smaller than the 'frozen core' Glauber results and approach to them as the energy increases. This is because the inner electrons are more tightly bound and their involvement decreases the calculated cross section. This difference in binding energies is naturally reflected more at lower energies. The results for both the 'frozen core' Glauber and the present calculations are in very good agreement above 15 eV with the recent experimental data (——·——·——) of Leep and Gallagher[64]. However, at lower energies, they appear to fail badly and give a cross section peak at too high an energy. We have also plotted in the figure the recent experimental data (ϕ) of William etal[111]. A more quantitative picture is provided by Table 4.4. It appears that, for any further improvement in the Glauber scattering amplitudes, one should look for corrections for including the exchange effect, polarization of the target and the next term in the eikonal expansion.

On the procedural side our calculations have further confirmed that Franco's procedure presents no numerical problems even when spherically asymmetric states (2p state in lithium) are involved.

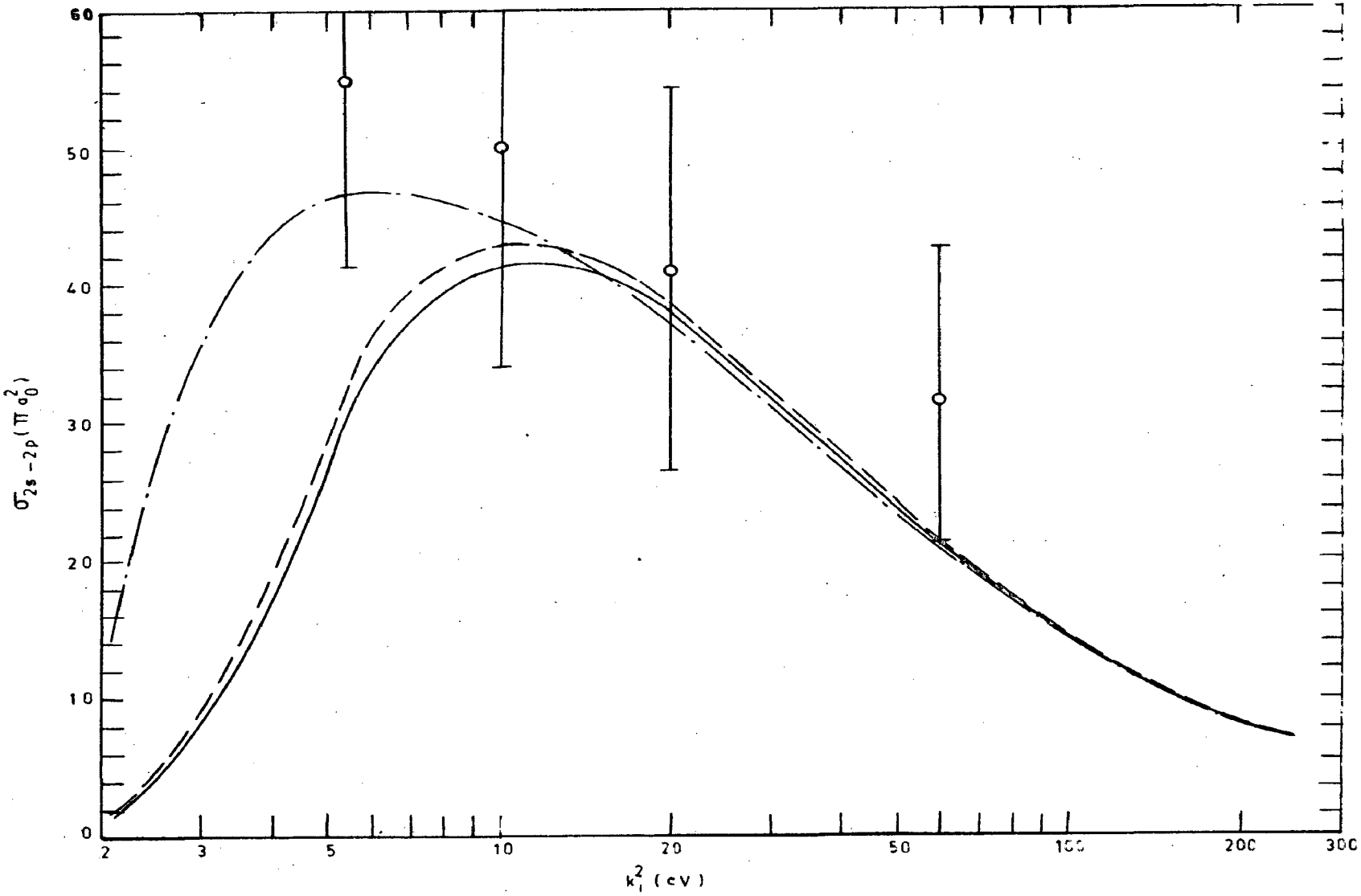


FIG. 4.5 — TOTAL CROSS SECTIONS FOR THE 2s–2p EXCITATION OF Li FOR ELECTRON IMPACT ENERGIES UPTO 250 eV. ———, PRESENT CALCULATION; – – –, CALCULATION IN FROZEN CORE GLAUBER APPROXIMATION; —.—, EXPERIMENTAL RESULTS OF LEEP AND GALLAGHER[64]; ○, EXPERIMENTAL DATA OF WILLIAMS et al[111].

TABLE 4.4

Comparison of the 2s-2p total cross sections at different energies. $\bar{\sigma}_{FC}$ and $\bar{\sigma}$ are the total cross sections in units of $\pi a_0^2$ in the frozen core Glauber approximation and present calculation, respectively, and $\bar{\sigma}_E$ are the experimental results of Leep and Gallagher[64] corrected for cascade. The number in parentheses gives the uncertainty in the last place (s) of the preceding number.

| Energy (eV) | $\bar{\sigma}_E$ | $\bar{\sigma}_{FC}$ | $\bar{\sigma}$ |
|---|---|---|---|
| 2.10(1) | 14.8 | 1.77 | 1.41 |
| 3.10(2) | 37.1 | 10.57 | 9.15 |
| 5.00(3) | 46.7 | 28.93 | 26.85 |
| 10.81(12) | 44.3 | 43.12 | 41.67 |
| 15.64(12) | 40.2 | 41.43 | 40.41 |
| 23.78(12) | 34.5 | 35.99 | 35.40 |
| 38.60(12) | 26.93 | 28.15 | 27.83 |
| 63.56(12) | 19.79 | 20.55 | 20.40 |
| 99.15(15) | 14.51 | 15.00 | 14.94 |
| 149.4 (2) | 10.67 | 10.99 | 10.98 |
| 249.9(2) | 7.089 | 7.31 | 7.30 |

## 4.4 POLARISATION OF THE RESONANCE RADIATION FOLLOWING ELECTRON EXCITATION

### 4.4.1 INTRODUCTION

If an electron beam passes through a gas with energy sufficient to produce excitation of the gas (or vapour), the polarization of the light emitted in a particular direction due to transitions from states so excited will depend on the relative probability of excitation of the magnetic sublevels of the upper states concerned. It is usual, in measuring the percentage polarization of impact radiation following transition, to observe light emitted at $90^{\circ}$ to the beam. Taking reference axes with Oz along the beam and $O_x$ as the direction of observation, let $I_{\parallel}$ and $I_{\perp}$ be the respective intensities of emitted light with electric vector along $O_z$, $O_y$ respectively. The polarization fraction is then defined as

$$P = \frac{I_{\parallel} - I_{\perp}}{I_{\parallel} + I_{\perp}} \qquad \ldots (4.47a)$$

and the percentage polarization as

$$\tilde{P} = 100\,P = 100\,\frac{I_{\parallel} - I_{\perp}}{I_{\parallel} + I_{\perp}} \qquad \ldots (4.47b)$$

The study of the polarization fraction, $P$, of the electron-impact induced lines emitted from hydrogen and alkalies have been of considerable interest both for experimentalists and theoreticians. Gerjuoy et al[86] have recently applied Glauber approximation[40] for the study of the polarization of Lyman-$\alpha$ line resulting from e-H(1s) collision and found a good agreement

with the experimental results of Ott et al[114] even at low energies (above ~18 eV). They remark that close agreement at low energies where the total and differential cross sections are not so close comes about because the polarization fraction depends on the ratio of certain integrals involving differential cross sections. The success of these Glauber predicted values of $P$ particularly at moderate energies between 30 eV and 200 eV has tempted as to extend them to e-Li system.

We now proceed to calculate the polarization fraction of the 2p→2s resonance lines of $^6$Li and $^7$Li following electron excitation to the 2p state in Glauber approximation[40]. We compare our values of the polarization fraction $P$ with (i) those obtained from the 'frozen core' Glauber approximation without core potential and (ii) the experimental data of Leep and Gallagher[64] for energies upto 250 eV. Tripathi et al[115] have done similar polarization calculations for the 2p → 2s resorance line of lithium and 3p → 3s resonance line of sodium following electron excitation in'frozen core' Glauber calculation.Their calculations are, however, in error[63].

The details of the method and the results of the calculation are discussed in the following sections.

4.4.2 METHOD

The percentage polarization of the 2p → 2s resonance line of lithium in a direction of right angles to the collision

axis is given by the following expression[116]

$$\tilde{P} = \frac{300(9\alpha-2)(Q_o-Q_1)}{12Q_o+24Q_1+(9\alpha-2)(Q_o-Q_1)}, \qquad \ldots (4.48)$$

where $Q_o$ and $Q_1$ are the total 2s-2p excitation cross sections with the component $m_\ell$ of the orbital angular momentum equal to 0 and 1 respectively. The value of $\alpha$ depends upon the hyperfine structure and natural lifetime of the 2p level and is 0.413 for $^6$Li and 0.326 for $^7$Li (Ref.116).

The total cross sections $Q_o$ and $Q_1$ appearing in Eq.(4.48) for $\tilde{P}$ are evaluated from the scattering amplitudes $F^{(i)}_{2p,2s}(\vec{k}_f,\vec{k}_i;m_\ell)$ quantized along the incident electron momentum $k_i$. However, the correct 2s-2p Glauber amplitudes are conveniently calculated, for a given initial and final momenta $\vec{k}_i$ and $\vec{k}_f$, by quantizing along a direction $\hat{\zeta}$ perpendicular to $\vec{q}$. The transformation required to obtain the desired amplitudes $F^{(i)}$ in terms of $F^{(\zeta)}$ quantized along $\hat{\zeta}$ have been discussed by Gerjuoy et al[86] and are given by

$$F^{(i)}_{2p,2s}(\vec{k}_f,\vec{k}_i;m_\ell = 0) = -i\sqrt{2}\cos\theta_q F^{(\zeta)}_{2p,2s}(\vec{k}_f,\vec{k}_i) \qquad \ldots (4.49a)$$

$$F^{(i)}_{2p,2s}(\vec{k}_f,\vec{k}_f;m_\ell=\pm1) = \pm i\exp(\mp i\phi_q)\sin\theta_q F^{(\zeta)}_{2p,2s}(\vec{k}_f,\vec{k}_i). \qquad \ldots (4.49b)$$

Finally the total cross sections $Q_o$ and $Q_1$ are obtained from Eqs.(4.44) in the usual way

$$Q_m = \frac{1}{k_i^2}\int_{k_i-k_f}^{k_i+k_f} dq\, q\int_o^{2\pi} d\phi_q \left|F^{(i)}_{2p,2s}(\vec{k}_f,\vec{k}_i;m_\ell)\right|^2. \qquad \ldots (4.50)$$

The amplitudes $F^{(\zeta)}$ are obtained from our calculations[117] reported in Sec.4.3.

4.4.3 RESULTS AND DISCUSSION

Fig.4.6 shows the general trend of how $\tilde{\rho}$ varies with energy for $^6$Li. The full curve represents the present calculations. Also indicated in the figure are the experimental data (—·—) of Leep and Gallagher[64], data points (Ω) of Hafner and Kleinpoppen[118], the results of the close coupling calculations (—Δ—) of Burke and Taylor[119], the modified close-coupling calculations (---) of Feautrier[120] incorporating the dipole polarizability of atomic states, the results of the variational calculations (— o —) of McCavert and Rudge[121] and the 'frozen core' Glauber calculations (— — —) of Tripathi et al[115]. The 'close-coupling' results in the energy range 2-5 eV are certainly better, as one would expect. In Fig.4.7 we have shown the variation of $\tilde{\rho}$ for $^7$Li. An experimental curve for $^7$Li has been obtained from the values of $\rho$ for $^6$Li using the relation given by Leep and Gallagher[64]:

$$\frac{\rho(^7\text{Li})}{\rho(^6\text{Li})} = \left(\frac{9\alpha(^7\text{Li})-2}{9\alpha(^6\text{Li})-2}\right)\left(\frac{3-\rho(^7\text{Li})}{3-\rho(^6\text{Li})}\right). \quad \ldots (4.51)$$

We find that our calculated values of $\tilde{\rho}$ are always higher than the experimental values of Leep and Gallagher[64] and converge towards them as the energy increases. For energies above 60 ev, agreement is within 2%. Even in the

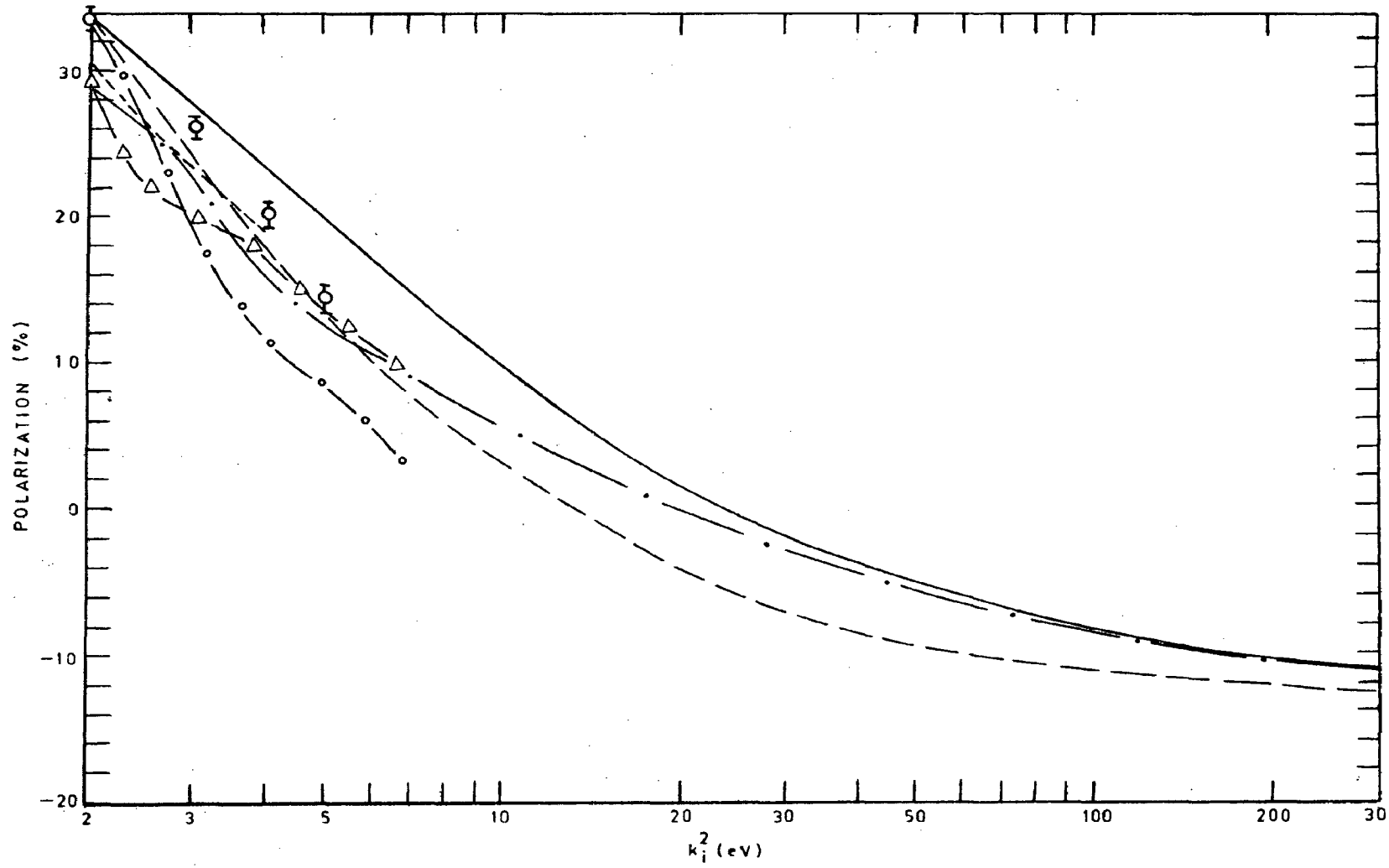


FIG. 4.6 – PERCENTAGE POLARIZATION OF THE 2p→2s RESONANCE LINE EMITTED FROM $^6Li$ BY ELECTRON IMPACT; ——, PRESENT CALCULATION; —△—, CLOSE COUPLING CALCULATION OF BURKE AND TAYLOR[119]; – – – –, MODIFIED CLOSE COUPLING CALCULATION OF FEAUTRIER[120]; —c—, VARIATIONAL CALCULATION OF McCAVERT AND RUDGE[121]; —·—, EXPERIMENTAL RESULTS OF LEEP AND GULLAGHER[64], ⊖, EXPERIMENTAL DATA OF HAFNER AND KLEINPOPPEN[116]. THE FROZEN CORE GLAUBER CALCULATION (— — —) OF TRIPATHI et al[115] IS ALSO INDICATED.

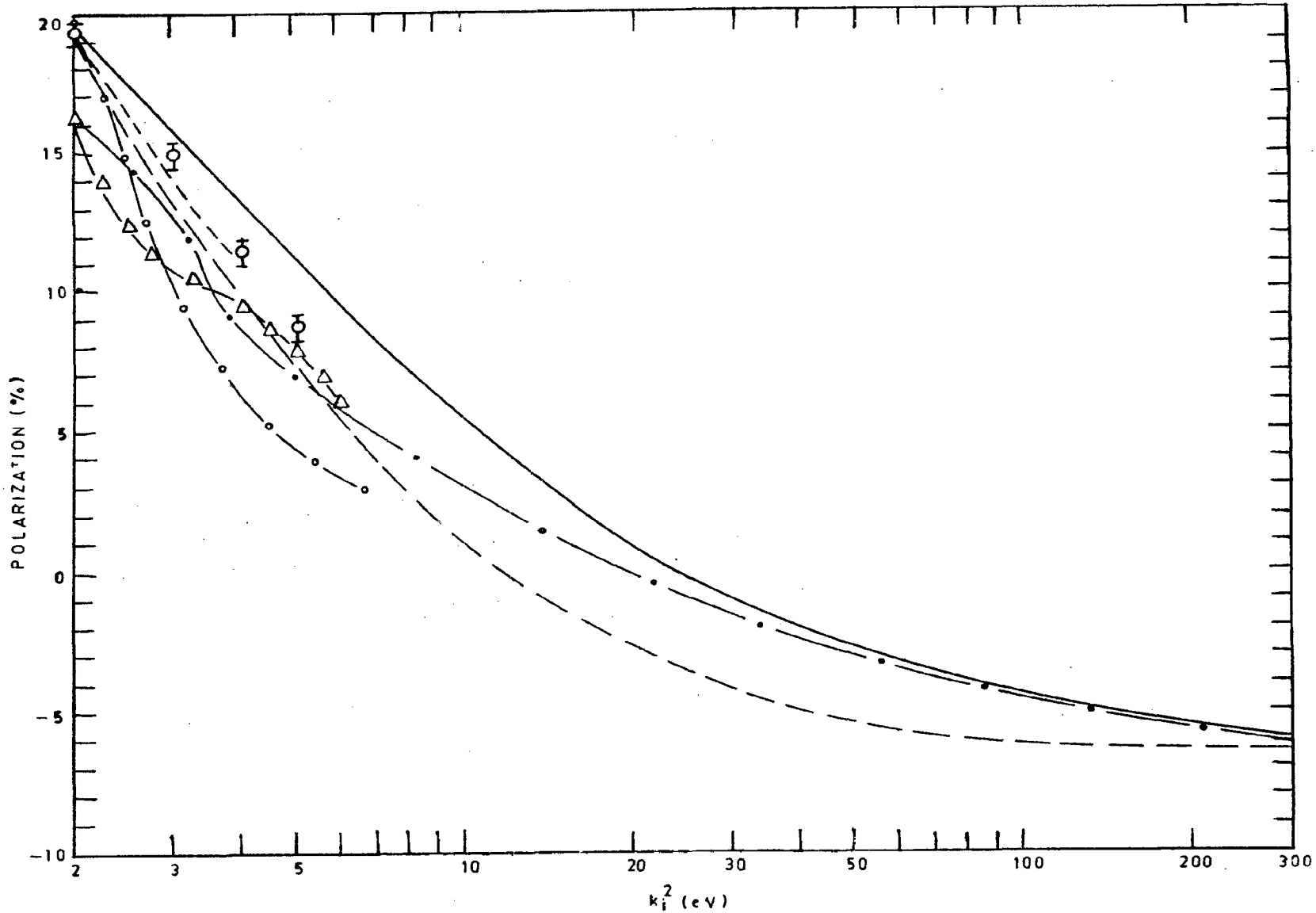


FIG 4.7 – PERCENTAGE POLARIZATION OF THE $2p \rightarrow 2s$ RESONANCE LINE EMITTED FROM $^7Li$ BY ELECTRON IMPACT. NOTATIONS ARE SAME AS IN FIG. 4.6.

low-energy region (2-10 eV) where the total cross sections for the 2s-2p transition in the Glauber approximation differ quite noticeably from the experimental data, the differences in $\tilde{\rho}$ are not as pronounced. We have also calculated $\tilde{\rho}$ in the 'frozen core' approximation and find little difference from our results. This is in agreement with the observation made by Walters[63] that the core electrons have little effect on the 2s-2p transition. Table 4.5 gives a quantitative picture.

TABLE 4.5

Percentage polarization of the 2p→2s resonance line emitted from $^6$Li following electron impact.

| Energy(eV)* | Experimental values* | Present calculation | Frozen core Glauber calculation |
|---|---|---|---|
| 2.10(1) | 28.2(6) | 33.00 | 33.10 |
| 3.10(2) | 22.1(4) | 27.62 | 27.29 |
| 5.00(3) | 12.7(3) | 19.91 | 19.57 |
| 10.81(12) | 4.8(2) | 8.57 | 8.31 |
| 15.64(12) | 1.85(20) | 4.20 | 3.98 |
| 23.78(12) | -1.19(16) | 0.13 | -0.02 |
| 38.60(12) | -4.02(14) | -3.51 | -3.60 |
| 63.56(12) | -6.46(14) | -6.27 | -6.33 |
| 99.15(15) | -8.22(14) | -8.09 | -8.17 |
| 149.4(2) | -9.56(21) | -9.42 | -9.51 |
| 249.9(2) | -10.93(25) | -10.77 | -10.84 |

*Number in parenthesis gives the uncertainty in the last places of the preceding number.

# CHAPTER 5

# INTERMEDIATE ENERGY CHARGED PARTICLE-ION ELASTIC SCATTERING IN THE EIKONAL OPTICAL MODEL-THE CASES OF $e-H^-$ AND $e-Li^+$ COLLISIONS.

## 5.1 INTRODUCTION

The problem of charged particle-ion collision has recently received considerable attention because of its importance in astrophysics and plasma physics. The excitation of positive ions by electron impact is responsible for most of the line spectra emitted by laboratory and astrophysical plasma.

In this chapter we shall study the scattering of electrons by ionic targets at intermediate energies. An eikonal optical model of intermediate energy electron-atom scattering, proposed by Mittleman[65] and Joachain and Mittleman[66] has been found to be quite useful for the study of the scattering of electrons by helium, particularly, in the region where the energy is large enough for the close-coupling method to be prohibitively difficult due to large number of open channels, and yet small enough for the Born approximation to be inaccurate. The basic ingradient of the model is the calculation of an 'optical' potential. In Sec.5.2 we sketch out the basic features of the 'optical potential'. Sec.5.3 briefly outlines the underlying assumptions and the main features of the eikonal optical model. Its applications to $e-H^-$ and $e-Li^+$ elastic scattering will be described in Sec.5.4.

## 5.2 THE OPTICAL POTENTIAL

The optical potential[67,68,122] attempts to convert the elastic scattering problem involving a many-body target to a one-body problem. We thus seek a one-body potential operator $\mathcal{V}$, which may be non local, such that the scattering given by the solution of the equivalent one-body Schroedinger equation

$$(k_i^2 - \mathcal{T} - \mathcal{V})\psi_i = 0. \qquad \ldots (5.1)$$

is the same as the actual elastic scattering for the same initial wavevector $\vec{k}_i$ in the many-body case. Here $k_i^2$ is the energy of the incident electron, $\mathcal{T}$ is its kinetic energy operator and $\psi_i$ is the scattering wavefunction corresponding to an incident electron with wavevector $\vec{k}_i$. The equivalent one-body potential operator $\mathcal{V}$ is usually referred to as a 'pseudo' potential or an 'optical' potential. It, thus, replaces the actual interaction potential between the incident particle and the many-body target atom by an effective one-body potential in which the incident particle moves.

The determination of an optical potential is a formidable task. It is only in some special circumstances that it can be derived from first principles. Various attempts made in this context have been recently reviewed by Joachain and Quigg[123]. Following Refs.67 and 68, an explicit expression for the optical potential is given by

$$\mathcal{V} = V_{ii} + \langle \phi_i | VG'QV | \phi_i \rangle, \qquad \ldots (5.2)$$

where Q is a projection operator which projects onto the target states ($\phi_j$) other than the ground state ($\phi_i$)., V is the actual interaction and, for electron-atom scattering, has the form

$$V(\vec{r},\vec{x}) = -\frac{2Z}{r} + 2\sum_{j=1}^{Z}\frac{1}{|\vec{r}-\vec{x}_j|}\,, \qquad \ldots (5.3)$$

G' is the Green's function for the partial potential QV:

$$G' = \frac{1}{E - H_o - QV + i\varepsilon} \qquad \ldots (5.4a)$$

$$= G_o + G_o Q V G' \,, \qquad \ldots (5.4b)$$

and

$$V_{ii} = \langle \phi_i | V | \phi_i \rangle \,. \qquad \ldots (5.5)$$

The second term in Eq.(5.2) is the contribution due to virtual transitions which occur during the collision. In general, it will be complex. The physical interpretation of the imaginary part of $\sqrt{}$ is given as follows. Not all the particles colliding with the actual target atom undergo elastic scattering. Those which undergo inelastic collisions must be absent from the purely elastic scattering described by the optical potential. The optical potential describes their removal in terms of an effective absorption. Obviously, below the inelastic threshold it will be real. Apart from being complex above the excitation threshold it is, in general, non-local as pointed out above.

Various orders to optical potential can be obtained by substituting the explicit form of $G^+$ in Eq.(5.2). We can write

$$\mathcal{V} = \mathcal{V}^{(1)} + \mathcal{V}^{(2)} + \mathcal{V}^{(3)} + \ldots, \qquad \ldots (5.6)$$

where,

$$\mathcal{V}^{(1)} = \langle \phi_i | V | \phi_i \rangle , \qquad \ldots (5.7)$$

$$\mathcal{V}^{(2)} = \langle \phi_i | V G_o Q V | \phi_i \rangle , \qquad \ldots (5.8)$$

and so on. We can further simplify the second and higher order terms in $\mathcal{V}$. Eq.(5.8), for example, can be written as

$$\begin{aligned} \mathcal{V}^{(2)} &= \sum_j \langle \phi_i | V G_o | \phi_j \rangle \langle \phi_j | Q V | \phi_i \rangle \\ &= \sum_{j \neq i} \left\langle \phi_i \middle| V \frac{1}{E - H_o + i\varepsilon} \middle| \phi_j \right\rangle \langle \phi_j | V | \phi_i \rangle \\ &= \sum_{j \neq i} \frac{\langle \phi_i | V | \phi_j \rangle \langle \phi_j | V | \phi_i \rangle}{k_i^2 + w_i - \mathcal{J} - w_j + i\varepsilon} , \end{aligned} \qquad \ldots (5.9)$$

where

$$H_o \equiv \mathcal{J} + H_t . \qquad \ldots (5.10)$$

The target Hamiltonian $H_t$ satisfies the eigenvalue equation

$$H_t | \phi_j \rangle = w_j | \phi_j \rangle . \qquad \ldots (5.11)$$

Here $w_i$ and $w_j$ represent the internal target energies respectively in the initial state i and the intermediate state j.

The optical potential approach has been successfully developed in the last few years, by using the eikonal approximation to obtain the scattering amplitude[65,66,124]. More recently, methods[56,125-128] have also been proposed to obtain an approximate local second-order optical potential. The non-local exchange kernel in electron-atom scattering can also be represented by an equivalent local potential. A comparative numerical study of such equivalent exchange potentials[126, 129-134] has been made very recently by Bransden et al[135]. In our present work, described in next sections, we follow the approach proposed in Refs.65, 66 and 124.

## 5.3 THE EIKONAL OPTICAL MODEL

Joachain and Mittleman[66] solve the equivalent one-body Schroedinger Eq.(5.1) for e-atom scattering under the approximations of (i) neglecting the Pauli-principle between the incident and target electrons and (ii) evaluating the optical potential $\sqrt{}$ upto second order. The first order optical potential, Eq.(5.7), referred to as the static potential of the target atom, can be written in configuration space as

$$\sqrt{}^{(1)}(\vec{r}) = \langle \phi_i | V | \phi_i \rangle = \int |\phi_i(\vec{x})|^2 V(\vec{r},\vec{x})\, d^3x \quad \ldots (5.12)$$

The second-order part $\sqrt{}^{(2)}$ can be simplified by making a further approximation, viz., by replacing the difference $'w_j - w_i'$ by an average $'\bar{w}'$ of the excitation energies of the

targets. The expression (5.8) for $V^{(2)}$ then simplifies to

$$V^{(2)} = \sum_{j\neq i} \frac{\langle \phi_i | V | \phi_j \rangle \langle \phi_j | V | \phi_i \rangle}{k_i^2 - \bar{w} - \mathcal{J} + i\varepsilon}$$

$$= \sum_{j\neq i} \frac{\langle \phi_i | V^2 | \phi_i \rangle - |\langle \phi_i | V | \phi_i \rangle|^2}{k_i'^2 - \mathcal{J} + i\varepsilon}, \quad \ldots (5.13)$$

where
$$k_i'^2 = k_i^2 - \bar{w}. \quad \ldots (5.14)$$

In configuration space it can be represented in the form [cf. Appendix A2]:

$$\langle \vec{r} | V^{(2)} | \vec{r}' \rangle = \mathcal{G}_{k_i'}(\vec{r},\vec{r}')\ A(\vec{r},\vec{r}'), \quad \ldots (5.15)$$

where $\mathcal{G}_{k_i'}$ is the free Green's function describing the free propagation of the incident particle in some average intermediate state with energy $k_i'^2$ and is given by

$$\mathcal{G}_{k_i'}(\vec{r},\vec{r}') = \frac{1}{(2\pi)^3} \int \frac{d^3\kappa\ e^{i\vec{\kappa}\cdot(\vec{r}-\vec{r}')}}{k_i'^2 - \kappa^2 + i\varepsilon}, \quad \ldots (5.16)$$

and the function $A(\vec{r},\vec{r}')$ is given by

$$A(\vec{r},\vec{r}') = \int \phi_i^*(\vec{x})\, V(\vec{r},\vec{x})\, (\delta(\vec{x}-\vec{x}') - \phi_i(\vec{x})\phi_i^*(\vec{x}'))$$

$$\times V(\vec{r}',\vec{x}')\phi_i(\vec{x}')\, d^3x d^3x'. \quad \ldots (5.17)$$

The equivalent one-body Schroedinger Eq.(5.1), using Eqs.(5.12) and (5.15), takes the form

$$\left[k_i^2 - J - V^{(1)}(\vec{r})\right] \psi_i(\vec{r})$$
$$- \int G_{k_i'}(\vec{r},\vec{r}') \; A(\vec{r},\vec{r}') \psi_i(\vec{r}) d^3r' = 0. \qquad \ldots (5.18)$$

Eq.(5.18) in its present form is still very complicated because of the structure of $A(\vec{r},\vec{r}')$. Joachain and Mittleman[66] solve it in the eikonal approximation. By changing the variable of integration $\vec{\kappa} = \vec{k}_i' + \vec{\tau}$ and neglecting the term $\tau^2$ in the denominator of Eq.(5.16), the free Green's propagator $G_{k_i'}$ transforms to the linearized form [Eqs.(2.13)-(2.20)] :

$$G_{k_i'}(\vec{r},\vec{r}') = - \frac{i}{2k_i'} e^{i\vec{k}_i'\cdot(\vec{r}-\vec{r}')} \delta(\vec{b}-\vec{b}') \Theta(z-z') \; , \qquad \ldots (5.19)$$

where $\Theta$ is a step function defined in the usual way. The wave vector $\vec{k}_i'$ is taken in the direction of the incident momentum $\vec{k}_i$, $z(z')$ is the component of $\vec{r}(\vec{r}')$ along $\hat{k}_i$ and the vector $\vec{b}(\vec{b}')$ is perpendicular to it. The vector $\vec{\tau}$ can be interpreted as the momentum transfer during the intermediate state. The neglect of $\tau^2$ term in (5.16), therefore, restricts the validity of expression (5.18) to small momentum transfers. Now , using the eikonal form of the wavefunction

$$\psi_i = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}_i\cdot\vec{r} + i\Lambda(\vec{b},z)} \; , \qquad \ldots (5.20)$$

and substituting Eq.(5.19) for $G_{k_i'}$ into Eq.(5.18), we obtain

$$\left[ k_i^2+\nabla^2 - \sqrt{}^{(1)}(\vec{r}) \right] \exp(i\vec{k}_i\cdot\vec{r}+i\Lambda(\vec{b},z)) + \frac{i}{2k_i'} \int \exp(i\vec{k}_i'\cdot(\vec{r}-\vec{r}'))$$
$$\times \delta(\vec{b}-\vec{b}')\ \Theta(z-z')A(\vec{b},z;\vec{b}',z')\ \exp(i\vec{k}_i\cdot\vec{r}'+i\Lambda(\vec{b}',z'))$$
$$\times d^2b'\ dz' \quad = 0,$$

which, by simple manipulation, yields

$$-2\vec{k}_i\cdot\vec{\nabla}\Lambda - \sqrt{}^{(1)}(\vec{r}) - (\vec{\nabla}\Lambda)^2+i\nabla^2\Lambda$$
$$+\frac{i}{2k_i'}\int_{-\infty}^{z} \exp\big(i(\vec{k}'-\vec{k})(z-z')\big)A(\vec{b},z;\vec{b},z')$$
$$\times \exp\left(i\left[\Lambda(\vec{b},z')-\Lambda(\vec{b},z)\right]\right)dz' = 0. \qquad \ldots (5.21)$$

The eikonal approximation in the above expression takes the function $\Lambda$ to be slowly varying on the scale of the de Broglie wavelength $\lambda\!\!\!^{-}(= 1/k_i)$ of the incident particle. Therefore, the higher order terms $(\vec{\nabla}\Lambda)^2$ and $(\nabla^2\Lambda)$ may be neglected and we are left with the following expression for $\Lambda$:

$$-2k_i e^{i\Lambda(\vec{b},z)}\ \frac{d\Lambda}{dz} = \sqrt{}^{(1)}(\vec{b},z)\ e^{i\Lambda(\vec{b},z)}$$
$$-\frac{i}{2k_i'}\int_{-\infty}^{z} dz'\ e^{i(\vec{k}_i'-\vec{k}_i)(z-z')}\ A(\vec{b},z;\vec{b},z')\ e^{i\Lambda(\vec{b},z')}$$

or
$$\frac{d\Lambda}{dz} = -\frac{1}{2k_i}\sqrt{}^{(1)}(\vec{b},z)+\frac{i}{4k_ik_i'}\int_{-\infty}^{z} dz'\ e^{i(\vec{k}_i'-\vec{k}_i)(z-z')} \qquad \ldots (5.22)$$
$$\times A(\vec{b},z;\vec{b},z')\ e^{i\left[\Lambda(\vec{b},z')-\Lambda(\vec{b},z)\right]} \qquad \ldots (5.23)$$

Since $\Lambda$ is a slowly varying function, we may also take the difference $\left[\Lambda(\vec{b},z')-\Lambda(\vec{b},z)\right]$ to be equal to zero. The

expression retained in first order for $\Lambda$ is then readily integrable to yield

$$\Lambda(\vec{b},z) = -\frac{1}{2k_i}\int_{-\infty}^{z} dz' \sqrt{}^{(1)}(\vec{b},z)$$

$$+\frac{i}{4k_i k_i'}\int_{-\infty}^{z} dz' \int_{-\infty}^{z'} dz'' \, e^{-i\xi(z'-z'')} A(\vec{b},z';\vec{b},z''), \qquad \ldots (5.24)$$

where

$$\xi = k_i - k_i' \simeq \vec{w}/2k_i. \qquad \ldots (5.25)$$

The scattering amplitude for elastic scattering is now given by

$$F_{fi}(\vec{k}_f,\vec{k}_i) = -\frac{1}{4\pi}(2\pi)^3 \langle \vec{k}_f | \sqrt{} | \psi_i \rangle \qquad \ldots (5.26)$$

$$\simeq -\frac{1}{4\pi}\int e^{-i\vec{k}_f\cdot\vec{r}} \Big[ \sqrt{}^{(1)}(\vec{r})\,\delta(\vec{r}-\vec{r}') + \mathcal{G}_{k_i'}(\vec{r},\vec{r}')\,A(\vec{r},\vec{r}') \Big] e^{i\vec{k}_i\cdot\vec{r}'+i\Lambda(\vec{b}',z')} \, d^3r\, d^3r'.$$

This expression, by substituting the explicit form for $\mathcal{G}_{k_i'}$ from Eq.(5.19), can be further simplified to the form:

$$F_{fi}(\vec{k}_f,\vec{k}_i) = -\frac{1}{4\pi}\int d^2b\, dz \Big[ e^{i\vec{q}\cdot(\vec{b}+\hat{k}_i z)} \sqrt{}^{(1)}(\vec{b},z) e^{i\Lambda(\vec{b},z)}$$

$$-\frac{i}{2k_i'}\int_{-\infty}^{z} dz' \, e^{ik_i'(z-z')} e^{i\vec{q}\cdot\vec{b}} e^{ik_i(z'-z\cos\theta)}$$

$$\times e^{i\Lambda(\vec{b},z')} A(\vec{b},z;\vec{b},z') \Big], \qquad \ldots (5.27)$$

where $\theta$ is the scattering angle.

Finally, making the Glauber approximation of neglecting the

longitudinal component of momentum transfer in the exponent, the above expression for the scattering amplitude becomes

$$F_{fi}(\vec{k}_f,\vec{k}_i) = -\frac{1}{4\pi}\int d^2b\, e^{i\vec{q}\cdot\vec{b}}\int_{-\infty}^{\infty} dz \Big[\sqrt{}^{(1)}(\vec{b},z)e^{i\Lambda(\vec{b},z)} - \frac{i}{2k_i'}\int_{-\infty}^{z} dz\; e^{i(k_i'-k_i)(z-z')}e^{i\Lambda(\vec{b},z)}A(\vec{b},z;\vec{b},z')\Big]$$

$$= -\frac{1}{4\pi}\int d^2b e^{i\vec{q}\cdot\vec{b}}\int_{-\infty}^{\infty} dz \Big[-2k_i e^{i\Lambda(\vec{b},z)}\frac{d\Lambda}{dz}\Big]$$

$$= -\frac{ik_i}{2\pi}\int d^2b\; e^{i\vec{q}\cdot\vec{b}}\int_{-\infty}^{\infty} dz\,\frac{d}{dz}\Big[e^{i\Lambda(\vec{b},z)}\Big]$$

$$= -\frac{ik}{2\pi}\int d^2b\; e^{i\vec{q}\cdot\vec{b}}\Big[e^{i\chi_{opt}(\vec{b})} - 1\Big], \qquad \ldots (5.28)$$

where the eikonal optical phase function $\chi_{opt}$ is given by

$$\chi_{opt}(\vec{b}) = -\frac{1}{2k_i}\int_{-\infty}^{\infty}\sqrt{}^{(1)}(\vec{b},z)dz + \frac{i}{4k_ik_i'}\int_{-\infty}^{\infty}dz\int_{-\infty}^{z}dz'\, e^{-i\xi(z-z')}A(\vec{b},z;\vec{b},z'). \qquad \ldots (5.29)$$

The first term in Eq.(5.46) is simply the result one would expect from the static charge-cloud and can be written as

$$\chi_{st}(\vec{b}) = -\frac{1}{2k_i}\int_{-\infty}^{\infty}\sqrt{}^{(1)}(\vec{b},z)dz \quad . \qquad \ldots (5.30)$$

The second term is more interesting; it is of order $1/k_i$ relative to the first term and has both a real and an imaginary part. The imaginary part represents the leading contribution from the open channels. Joachain and Mittleman[66] write this term as

$$\chi_{abs}(\vec{b}) = \frac{i}{4k_i k_i'} \int_{-\infty}^{\infty} dz \int_{-\infty}^{z} dz' \cos\xi(z-z') \; A(\vec{b},z;\vec{b},z')$$

$$= \frac{i}{8k_i k_i'} \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \; e^{-i\xi(z-z')} \; A(\vec{b},z;\vec{b},z'), \quad \ldots \quad (5.31)$$

where the fact that A is symmetric has been used (cf. Appendix A3). This multiple integral (recall that a multi-dimensional integration is concealed in A) can be reduced to a one-dimensional integral for any case in which the wavefunction of the target ground state can be represented as a sum of the products of single particle orbitals [124].

It is expected[124] that $\chi_{abs}(\vec{b})$ should contribute significantly at small angles where the amplitudes for transitions into optically allowed channels are very large. At wide angles, the amplitudes for these transitions diminish rapidly, as do all other amplitudes except the elastic amplitude; thus $\chi_{st}$ which represents the effect of the ground state (or the elastic channel), is expected to dominate in all orders of perturbation theory at large angles.

Now let us consider the real part of the second term in Eq.(5.29);

$$\chi_{pol}(\vec{b}) = \frac{1}{4k_i k_i'} \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \sin\xi(z-z') \; A(\vec{b},z;\vec{b},z'). \quad \ldots \quad (5.32)$$

It corresponds to the polarization of the target[124]. This effect can easily be included phenomenologically by adding directly to

$\chi_{opt}(\vec{b})$ a term corresponding to a polarization potential (say) of the Buckingham form[136]:

$$V_p(r) = -\frac{\bar{\alpha}}{(r^2+d^2)^2}, \qquad \ldots (5.33a)$$

where

$$d^4 = (\tfrac{1}{2}\bar{\alpha})Z^{-1/3}. \qquad \ldots (5.33b)$$

Here $\bar{\alpha}$ is the polarizability of the target of atomic number Z and d is a phenomenological parameter. The complete eikonal optical phase can thus be written as

$$\chi_{opt} = \chi_{st} + \chi_{abs} + \chi_{pol}. \qquad \ldots (5.34)$$

## 5.4 APPLICATIONS OF THE EIKONAL OPTICAL MODEL TO ELECTRON-ION SCATTERING

The problem of the elastic scattering of charged particles by ionic targets requires special attention because of the fact that the overall interaction between the target and the charged particle now involves a long-range Coulomb interaction. A simple procedure to deal with such a problem is to separate out the Coulomb term from the overall interaction and consider its contribution exactly. The total elastic scattering amplitude can then be obtained by adding the contribution from the remaining part of the optical potential to that from the Coulomb potential of a point target, i.e., we write

$$F^T_{fi}(\vec{k}_f,\vec{k}_i) = F^C_{fi}(\vec{k}_f,\vec{k}_i) + F_{fi}(\vec{k}_f,\vec{k}_i). \qquad \ldots (5.3$$

Here the superscript C denotes the Coulomb part and T the total scattering amplitude. We use this procedure to apply the eikonal optical theory to the elastic scattering of electrons by helium like ionic targets ($H^-$ and $Li^+$). This problem is simple in the serse that both the target electrons can be easily treated explicitly and no correction need be made for any core. The elastic scattering of electrons by $H^-$ and $Li^+$ ions was earlier treated by McDowell[69] in variational approximation using two-parameter trial wavefunctions and accounting for the exchange, and diple and quadrupole polarization potentials.

### 5.4.1 e-$H^-$ ELASTIC SCATTERING

In the present work we proceed to calculate the e-$H^-$ elastic scattering cross sections at 0.5 and 1.0 Rydbergs. We have selected these energies just to compare our results with the variational calculations of McDowell[69]. To our knowledge there is no other theoretical calculation. Experimental results are still unavailable on e-$H^-$ elastic scattering. Although the eikonal optical model can only be successfully applicable to intermediate energies (from two times of the threshold to twenty times of the threshold), our main aim is (i) to know how far one can use this method, which is comparatively very simple, to study collisions such as e-$H^-$ elastic scattering even at low energies, and (ii) to analyse the contributions of the second order terms of the optical potential. In the case of e-He elastic scattering these have

been found to make substantial contributions at small momentum transfers. In the next subsections we outline the procedure giving details of the calculation and discuss the results.

(i) Procedure

In the case of e-$H^-$ elastic scattering, the interaction potential V is of the form

$$V = 2\left(-\frac{1}{r} + \frac{1}{|\vec{r} - \vec{x}_1|} + \frac{1}{|\vec{r} - \vec{x}_2|}\right). \qquad \ldots (5.36)$$

We have used hydrogen-like form (Ref.137, p.240) for the ground state target wavefunction.

$$\phi_i(\vec{x}) \equiv \phi_i(\vec{x}_1, \vec{x}_2) = \left(\frac{\alpha^3}{\pi}\right) e^{-\alpha(x_1+x_2)}, \quad \alpha = 0.688\ a_o^{-1} \qquad \ldots (5.37)$$

This wavefunction is similar to the one considered by Ref.66. The first order interaction potential $\sqrt{}^{(1)}(r)$ given by Eq.(5.12) now simplifies to

$$\begin{aligned}\sqrt{}^{(1)}(r) \equiv \sqrt{}^{(1)}(b,z) &= 2(\alpha^3/\pi)^2 \int e^{-2\alpha(x_1+x_2)} \\ &\quad \times \left(\frac{1}{|\vec{r}-\vec{x}_1|} + \frac{1}{|\vec{r}-\vec{x}_2|} - \frac{1}{r}\right) d^3x_1 d^3x_2 \\ &= -(4/r)(1+\alpha r)\ \exp(-2\alpha r) + \frac{2}{r}. \qquad \ldots (5.38)\end{aligned}$$

The last factor in Eq.(5.38) is a pure Coulomb interaction due to the net (point) charge on the target. It is dropped in the main calculation and is treated separately. The Coulomb scattering amplitude corresponding to this factor can easily

be obtained exactly and is of the form

$$F^{C}_{fi}(\vec{k}_f,\vec{k}_i) = (2/q^2)\ \exp\{i[\pi + 2\delta_o - (1/k_i)\ln(\sin^2\theta/2)]\}, \quad \ldots (5.39a)$$

where

$$\delta_o = \arg\Gamma(1+i/k). \quad \ldots (5.39b)$$

The scattering angle $\theta$, is related to the momentum transfer $\vec{q}$ via the relation

$$|\vec{q}| \equiv |\vec{k}_i - \vec{k}_f| = 2k_i\sin(\theta/2). \quad \ldots (5.40)$$

We evaluate the second part $F_{fi}(\vec{k}_f, \vec{k}_i)$ in Eq.(5.35) by using the eikonal optical model of Joachain and Mittleman[66]. We use their results directly to simplify the eikonal optical phase $\chi_{opt}$, Eq.(5.29):

$$\chi_{opt}(\vec{b}) = -(1/k_i)[u_1(\vec{b}) + u_p(\vec{b})] + \frac{i}{2k_i k_i'} W(\vec{b}), \quad \ldots (5.41)$$

where

$$u_1(\vec{b}) = \frac{1}{2}\int_{-\infty}^{\infty} V^{(1)}(\vec{b},z)\,dz$$

$$= -2\int_{-\infty}^{\infty} \left(\frac{1}{(b^2+z^2)^{1/2}} + \alpha\right) e^{-2\alpha(b^2+z^2)^{1/2}}\,dz$$

$$= -4[K_o(2\alpha b) + \alpha b K_1(2\alpha b)], \quad \ldots (5.42)$$

$$u_p(\vec{b}) = \frac{1}{2}\int_{-\infty}^{\infty} V_p(\vec{b},z)\,dz = -\pi\left(\frac{1}{4}\bar{\alpha}\right)(b^2+d^2)^{3/2}, \quad \ldots (5.43)$$

$$\bar{\alpha} = 203.0 \text{ for } H^-, \quad \ldots (5.43a)$$

and

$$W(\vec{b}) = \frac{1}{4}\int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \; e^{-i\xi(z-z')} A(\vec{b},z;\vec{b},z') , \qquad \ldots (5.44)$$

which, by using the definition of A, Eq.(5.34), is written as

$$W(b) = W_1(b) - W_2(b) , \qquad \ldots (5.45)$$

where

$$W_1(b) = 2\int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \; e^{-i\xi(z-z')} \int d^3x \, \frac{|\phi_i(\vec{x})|^2}{|\vec{r}-\vec{x}|\,|\vec{r}'-\vec{x}|}$$

$$= 16\int_0^{\infty} dv \, \frac{v\, J_0(\xi b \sinh v)}{\left[1 + (\xi \sinh v/\alpha)^2\right]^2} , \ldots (5.46)$$

and

$$W_2(b) = 2\left|\int_{-\infty}^{\infty} dz \; e^{i\xi z} \int d^3x \, \frac{|\phi_i(\vec{x})|^2}{|\vec{r}-\vec{x}|}\right|^2$$

$$= 8\left|K_0(\xi b) - K_0(ab) - (2\alpha^2 b/a)K_1(ab)\right|^2 . \qquad \ldots (5.47)$$

$$a = (\xi^2 + 4\alpha^2)^{1/2} , \qquad \ldots (5.48)$$

$J_0$ is an ordinary Bessel function, and $K_0$ and $K_1$ are modified Bessel functions. We have taken the average excitation energy $\bar{w}$ of the target in Eq.(5.42) to be 0.05 Ryd following the crude estimate procedure of Joachain and Mittleman[66] that it is of the order of the ionization energy. The results, however, are not very sensitive to its value. The reason is that the values of W(b) for different values of $\bar{w}$ differ only for large b, which contribute little to the scattering amplitude[138] .

It is evident from the Eqs.(5.42) to (5.47) that the

eikonal optical phase $\chi_{opt}$ no longer depends on the directions of $\vec{b}$. The $\phi_b$-integration in Eq.(5.38) can thus be easily performed to yield

$$F_{fi}(\vec{k}_f, \vec{k}_i) = ik_i \int_0^\infty db\, b\, J_0(qb)(1-e^{i\chi_{opt}(b)}). \quad \ldots (5.49)$$

The differential cross section is now obtained in the usual way and is given by

$$\frac{d\sigma(\vec{q})}{d\Omega} \equiv I(\theta, k_i^2) = |F_{fi}^C(\vec{k}_f, \vec{k}_i) + F_{fi}(\vec{k}_f, \vec{k}_i)|^2 . \quad \ldots (5.50)$$

We compare it with that due to the pure Coulomb field

$$I^C(\theta, k_i^2) = |F_{fi}^C(\vec{k}_f, \vec{k}_i)|^2 . \quad \ldots (5.51)$$

Another convenient quantity to be examined is the ratio $R(\theta, k_i^2)$ of the calculated differential cross section $I(\theta, k_i^2)$ to $I^C(\theta, k_i^2)$.

(ii) Results and Discussion

Figs.5.1 and 5.2 show the calculated values of the differential cross section at 0.5 Ryd and 1.0 Ryd respectively. These values are quite large at small angles due to the associated Coulomb contribution. The deviations from the Coulomb cross section are of interest. Our calculations without the polarization potential and absorption effects (— · — · —) show a suppression over the Coulomb cross section upto $\theta \sim 80^\circ$, in agreement with the results of

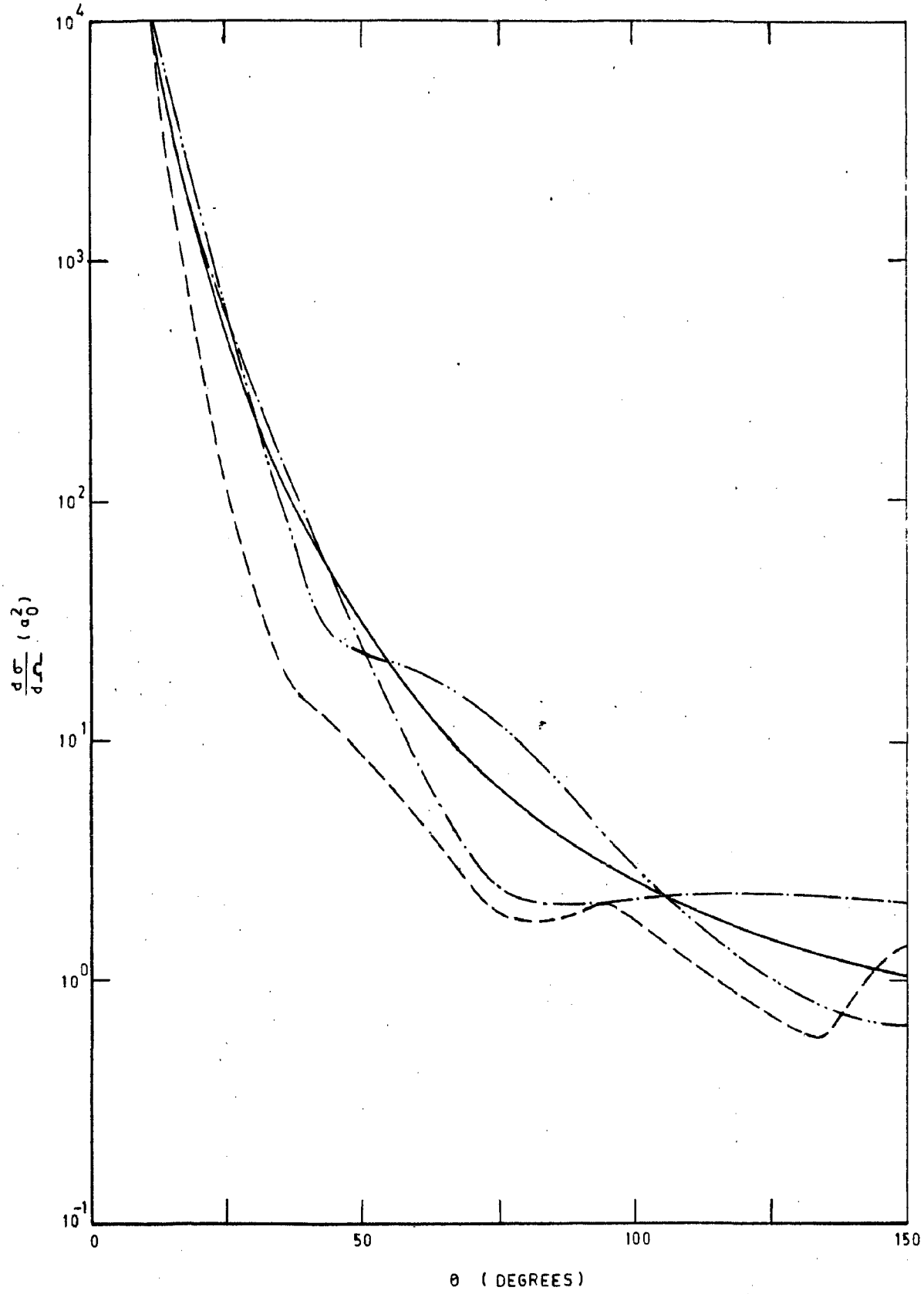


FIG. 5.1 – CALCULATED DIFFERENTIAL CROSS SECTION $I(\theta, k_i^2)$ COMPARED TO THE COULOMB CROSS SECTION $I^c(\theta, k_i^2)$ (———) AND THE RESULTS OF Mc DOWELL[69] (– – – –) FOR SCATTERING ANGLE θ UPTO 150° FOR $e-H^-$ ELASTIC SCATTERING AT $k_i^2 = 0.5$ RYD. —·—·→PRESENT CALCULATION WITH POLARIZATION AND ABSORPTION EFFECTS NEGLECTED; —··—,PRESENT CALCULATION WITH THESE FEATURES INCLUDED.

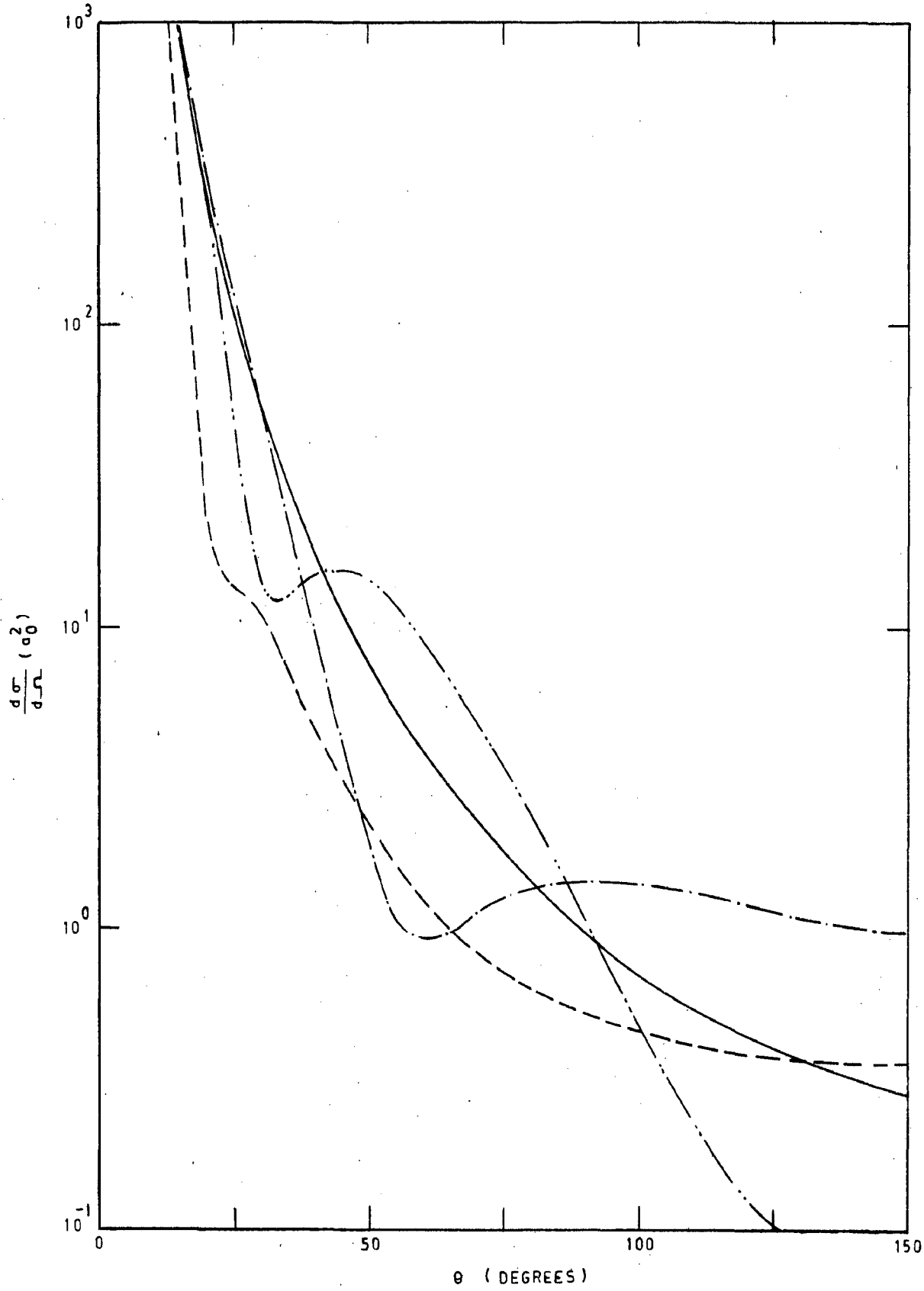


FIG. 5.2 – SAME AS FIG. 5.1 BUT AT $k_i^2 = 1.0$ RYD.

McDowell (— — —). The overall shape of these curves is, however, different although this improves considerably when the polarization potential and the absorption effects are taken into account (—·—·—·—). This change is mainly brought about by the absorption effects; the inclusion of the polarization potential makes only a small change. For large $\theta$, our results are very different from those of McDowell.

In Figs.(5.3) and (5.4) we have shown the ratio $R(\theta,k_i^2)$ of $I(\theta,k_i^2)$ to $I^C(\theta,k_i^2)$ for $k_i^2 = 0.5$ and 1.0 Ryd respectively. These figures display the main features of the calculated cross sections more prominently. The calculated $R(\theta,k_i^2)$ (——··——··——) curve shows oscillations in fair agreement with the results of McDowell[69] (– – –) except for large $\theta$. The position of the first minimum moves towards smaller angles as the energy increases just as in McDowell's case. The main difference is the enhancement ($R(\theta,k_i^2) > 1$) in the backward direction. Our calculations without the absorption effects do indicate the enhancement, but they can not be relied upon at large angles.

In conclusion, we have shown that the main features of the results of McDowell[69] can be reproduced, at least qualitatively, by this method, which is comparatively very simple.

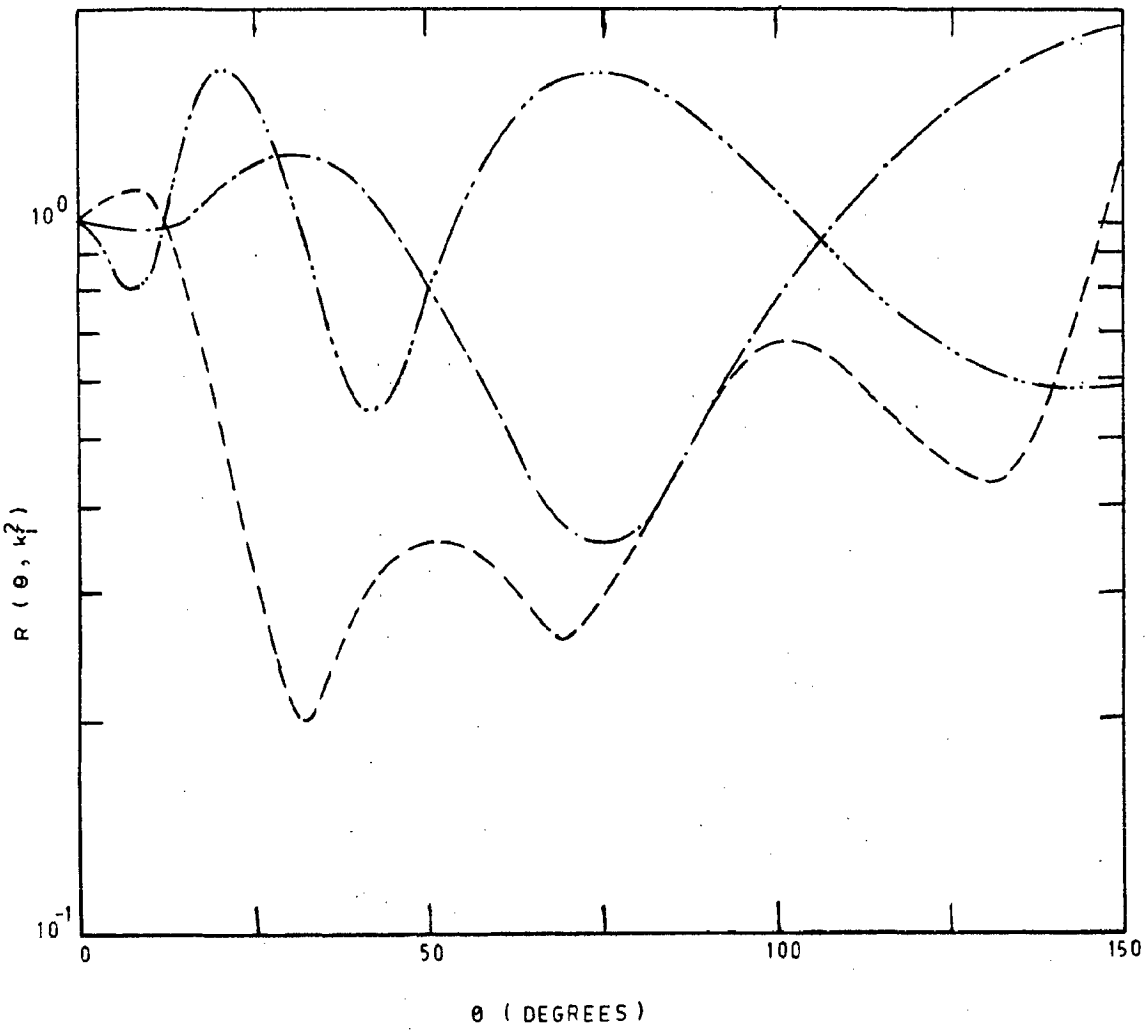


FIG 5.3 – CALCULATED VALUES OF $R(\theta, k_i^2)$ COMPARED TO THOSE OF McDOWELL[69] (– – –) FOR $e-H^-$ ELASTIC SCATTERING AT $k_i^2 = 0.5$ RYD. —·—·—, PRESENT CALCULATION WITH POLARIZATION AND ABSORPTION EFFECTS NEGLECTED; —··—··—, PRESENT CALCULATION WITH THESE FEATURES INCLUDED.

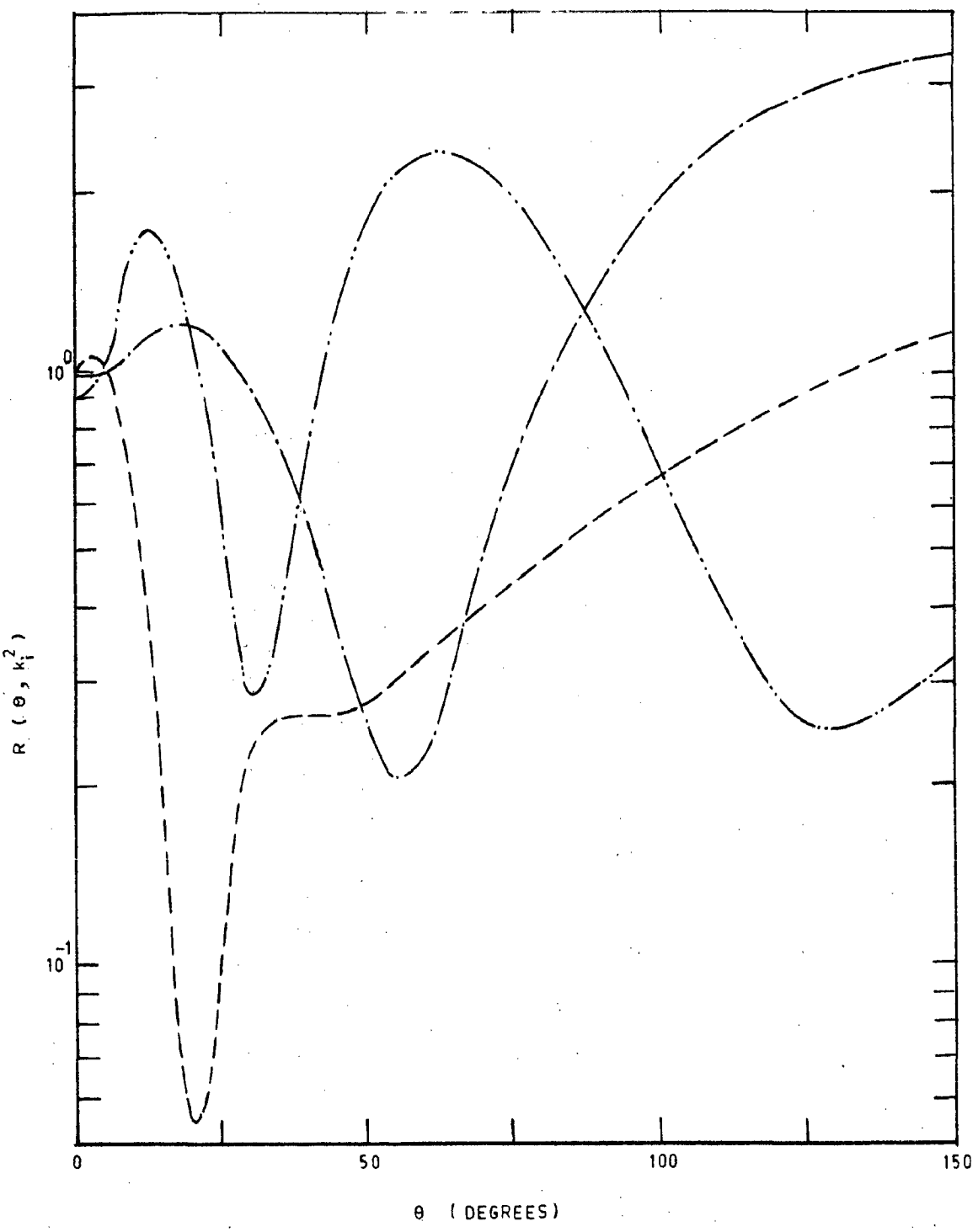


FIG. 5.4 — SAME AS FIG. 5.3 BUT AT $k_i^2 = 1.0$ RYD.

## 5.4.2 INTERMEDIATE ENERGY e-$Li^+$ ELASTIC SCATTERING

We have calculated e-$Li^+$ elastic scattering cross sections in the energy range ~300 eV. At low energies (less than 3 Ryd), it has been treated earlier by McDowell[69]. The eikonal optical model has the flexibility of accurately taking into account the contribution of any particular inelastic channel to the optical potential. In the present calculation we have exploited this feature to include accurately the contribution from the first excited state. The effect of the polarization of the target has also been taken into account. In the next subsections we outline the procedure giving details of calculations and then discuss the results.

### (i) Procedure

If the contribution of any particular excited state (say, the first one) in the summation of Eq.(5.13) is to be taken accurately, the approximation made in respect to it in Eq.(5.13) can be easily corrected for, to get

$$f^{(2)} = \frac{\langle \phi_i | V^2 | \phi_i \rangle - |\langle \phi_i | V | \phi_i \rangle|^2}{k_i'^2 - J} + |\langle \phi_i | V | \phi_1 \rangle|^2 \left( \frac{1}{k_1^2 - J} - \frac{1}{k_i'^2 - J} \right), \quad \ldots (5.52)$$

where

$$k_1^2 = k_i^2 - (w_1 - w_i) \quad \ldots (5.53)$$

In configuration space, Eq.(5.52) takes the form .

$$\langle \vec{r}|V^{(2)}|\vec{r}'\rangle = \mathcal{G}_{\vec{k}_i}(\vec{r},\vec{r}')A(\vec{r},\vec{r}') + \left(\mathcal{G}_{\vec{k}_1}(\vec{r},\vec{r}') - \mathcal{G}_{\vec{k}_i}(\vec{r},\vec{r}')\right)B(\vec{r},\vec{r}'), \quad \ldots (5.54)$$

where $A(\vec{r},\vec{r}')$ is defined by Eq.(5.17) and

$$B(\vec{r},\vec{r}') = \int \phi_i^*(\vec{x})\, V(\vec{r},\vec{x})\, \phi_1(\vec{x})\, d^3x \int \phi_1^*(\vec{x}')\, V(\vec{r}',\vec{x}')\, \phi_i(\vec{x}')\, d^3x'. \quad \ldots (5.55)$$

Here $\phi_1(\vec{x})$ is the wavefunction for the first excited state of the target and $\mathcal{G}_{\vec{k}_1}$ is the free Green's function corresponding to a wave vector $\vec{k}_1$.

This form of the optical potential leads, in eikonal approximation, to the expression (5.28) for the elastic scattering amplitude, where the eikonal optical phase $\chi_{opt}$ is now given by

$$\chi_{opt}(b) = -(1/k_i)\left[\bar{u}_1(b) + u_p(b)\right] + (i/2k_ik_i')\,W(b) + (i/2k_i)\,y(b). \quad \ldots (5.56)$$

Here

$$y(b) = \frac{1}{4}\int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \left[(1/k_1)\exp(-i\xi_1(z-z')) - (1/k_i')\exp(-i\xi(z-z'))\right] B(b,z;b,z'), \quad \ldots (5.57)$$

where

$$\xi_1 = k_i - k_1 \simeq (w_1 - w_i)/2k_i. \quad \ldots (5.58)$$

The other parameters are defined in the usual way. The target polarizibility $\bar{\alpha}$ for $Li^+$ in Eq.(5.60) is equal to 0.19 [Ref.69].

The interaction potential V for e-$Li^+$ elastic scattering is given by

$$V = 2\left( \frac{1}{|\vec{r} - \vec{x}_1|} + \frac{1}{|\vec{r} - \vec{x}_2|} - \frac{3}{r} \right). \qquad \ldots (5.59)$$

We have used the following hydrogenlike wavefunctions[139] for the ground state and the first excited state (excitation energy $w_1 - w_i = 4.47$ Ryd) of $Li^+$

$$\phi_i(\vec{x}) \equiv \phi_i(\vec{x}_1, \vec{x}_2) = (\mu^3\alpha^3/\pi) \exp(-\mu\alpha(x_1+x_2)) \ldots (5.60)$$

$$\begin{aligned}\phi_1(\vec{x}) \equiv \phi_1(\vec{x}_1, \vec{x}_2) = {} & 2^{-1/2}(\mu'^3\alpha'^3/\pi)^{1/2}(\mu'^5/3\pi N)^{1/2}\{\exp(-\mu'\alpha' x_1) \\ & \times [x_2\exp(-\mu' x_2) - (3M/\mu')\exp(-\mu'\beta' x_2)] \\ & + \exp(-\mu'\alpha' x_2)[x_1\exp(-\mu' x_1) - (3M/\mu') \\ & \times \exp(-\mu'\beta' x_1)]\}, \qquad \ldots (5.61a)\end{aligned}$$

where

$$\mu\alpha = 2.69$$

$$\mu'\alpha' = 3.00$$

$$\mu'\beta' = 2.17$$

$$2\mu' = 2.19$$

$$M = (\alpha'+\beta')^3/(1+\alpha')^4$$

and

$$N = 1+(3M^2/\beta'^3) - 48M/(1+\beta')^4. \qquad \ldots (5.61b)$$

The first order interaction potential $\sqrt{}^{(1)}(r)$ in Eq.(5.12) with $\phi_i(\vec{x}_1, \vec{x}_2)$ of the form (5.60) and V of the form (5.59) simplifies to the form

$$\sqrt{}^{(1)}(r) \equiv \sqrt{}^{(1)}(b,z) = -(4/r)(1+\mu\alpha r)\exp(-2\mu\alpha r) - \frac{2}{r} \quad \ldots (5.62)$$

The last factor in (5.62) is due to the net charge on ionic target $Li^+$. We drop it in the main calculation as pointed out earlier. As is evident that the form (5.61) of $\phi_i(\vec{x}_1, \vec{x}_2)$ is similar to the one considered by Joachain and Mittleman[66] and Kumar et al[140], we directly use Eqs.(5.45) to (5.47) for W(b) with

$$a = (\xi^2 + 4\mu^2\alpha^2)^{1/2} \quad \ldots (5.63)$$

We have taken $\bar{w}$ = 5.5 Ryd. As pointed out earlier in the case of e-$H^-$ elastic scattering, the results for e-$Li^+$ are also not very sensitive to its value (see Fig.5.5).

The calculation of y(b), though lengthy, is simple. The matrix element

$$\langle \phi_i | V | \phi_1 \rangle = \int \phi_i^*(\vec{x}_1,\vec{x}_2)\left(\frac{1}{|\vec{r} - \vec{x}_1|} + \frac{1}{|\vec{r} - \vec{x}_2|}\right)\phi_1(\vec{x}_1,\vec{x}_2)\, d^3x_1 d^3x_2$$

$$= 2^{1/2}\Big(C_2\Big[\frac{1}{r} - (\alpha_1 + \frac{1}{r})\exp(-2\alpha_1 r)\Big]$$

$$+C_1\Big\{\frac{1}{2\beta_1^4}\Big[\frac{3}{r} - (2\beta_1^2 r + 4\beta_1 + \frac{3}{r})\exp(-2\beta_1 r)\Big]$$

$$-\frac{3M}{\mu^3\gamma_1^3}\Big[\frac{1}{r} - (\gamma_1 + \frac{1}{r})\exp(-2\gamma_1 r)\Big]\Big\}\Big) \quad \ldots (5.64)$$

in Eq.(5.55) and the integrations indicated in Eq.(5.57) give

$$y(b) = y_1(b) - y_2(b), \quad \ldots (5.65)$$

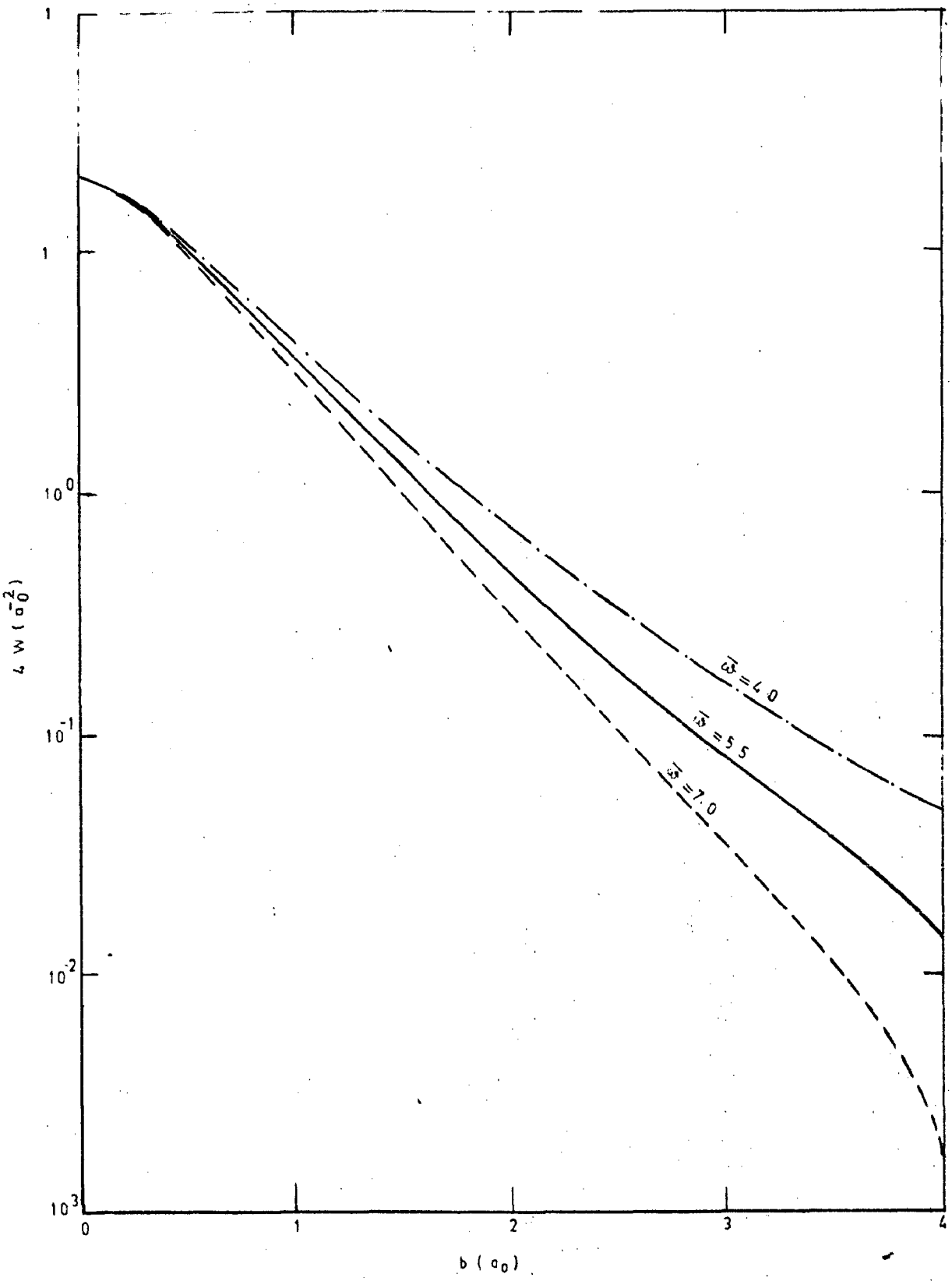


FIG. 5.5 – THE FUNCTION W, SEE (5.45), FOR DIFFERENT VALUES OF THE AVERAGE EXCITATION ENERGY $\bar{\omega}$ FOR e-$Li^+$ ELASTIC SCATTERING AT 300 eV.

$$y_1(b) = \frac{2}{k_1}\Big|C_2\Big[K_o(\xi_1 b) - K_o(\eta_1 b) - \frac{2\alpha_1^2 b}{\eta_1} K_1(\eta_1 b)\Big]$$

$$+ C_1\Big(\frac{1}{2\beta_1^4}\Big\{3K_o(\xi_1 b) - 3K_o(\eta_2 b) - \frac{8\beta_1^2 b}{\eta_2} K_1(\eta_2 b)$$

$$- \frac{4\beta_1^4 b^2}{\eta_2^2}\Big[K_o(\eta_2 b) + K_2(\eta_2 b)\Big] + \frac{2\beta_1^2 b}{\eta_2} K_1(\eta_2 b)\Big\}$$

$$- \frac{3M}{\mu'\gamma_1^3}\Big[K_o(\xi_1 b) - K_o(\eta_3 b) - \frac{2\gamma_1^2 b}{\eta_3} K_1(\eta_3 b)\Big]\Big)\Big|^2 \qquad \ldots (5.66)$$

$$\eta_1 = (\xi_1^2 + 4\alpha_1^2)^{1/2} = \Big[\xi_1^2 + (\mu\alpha + \mu'\alpha')^2\Big]^{1/2}, \qquad \ldots (5.67)$$

$$\eta_2 = (\xi_1^2 + 4\beta_1^2)^{1/2} = \Big[\xi_1^2 + (\mu\alpha + \mu')^2\Big]^{1/2}, \qquad \ldots (5.68)$$

$$\eta_3 = (\xi_1^2 + 4\gamma_1^2) = \Big[\xi_1^2 + (\mu\alpha + \mu'\beta')^2\Big]^{1/2}, \qquad \ldots (5.69)$$

$$C_1 = \frac{\mu^3\alpha^3\mu'^4}{\alpha_1^3}\Big(\frac{\alpha'^3}{3N}\Big)^{1/2} \qquad \ldots (5.70)$$

and

$$C_2 = \frac{3}{2} C_1\Big(\frac{1}{\beta_1^4} - \frac{2M}{\mu'\gamma_1^3}\Big). \qquad \ldots (5.71)$$

$y_2(b)$ is given by an expression similar to (5.66) with $k_1'$ for $k_1$ and $\xi$ for $\xi_1$.

The total scattering amplitude for e-$Li^+$ elastic scattering is now given by expression (5.35) where $F_{fi}^C$ is the Coulomb contribution corresponding to the second factor in Eq.(5.62) and is given by

$$F^{C}_{fi}(\vec{k}_f,\vec{k}_i) = (2/q^2)\ \exp\{i[\pi+2\delta_o+(2/k_i)\ln(\sin\theta/2)]\}\ , \quad \ldots\ (5.72)$$

$$\delta_o = \arg\ \Gamma(1-i/k_i);$$

and $F_{fi}(\vec{k}_f,\vec{k}_i)$ is obtained from (5.49) using $\chi_{opt}(b)$ given by Eq.(5.56). The differential cross section $I(\theta,k_i^2)$ and $I^C(\theta,k_i^2)$, and the ratio $R(\theta,k_i^2)$ of $I(\theta,k_i^2)$ to $I^C(\theta,k_i^2)$ are now obtained from (5.50) and (5.51) with the new values of $F^C_{fi}$ and $F_{fi}$.

(ii) Results and Discussion

Figs.(5.6) and (5.7) show the calculated values of the differential cross section along with the corresponding Coulomb cross section for the point target at 200 eV and 500 eV respectively. The values are, as expected, quite large at small angles due to the associated Coulomb contribution. Our calculations without the absorption effects (i.e. without the second-order term in the optical potential) and the polarization potential (—— — ——) show a suppression over the Coulomb cross section (————) but this is off-set when the absorption effects (—·—·—·—) and the absorption effects and the polarization potential together (—·· ——··) are included.

All these features are very prominently displayed by Figs.(5.8) and (5.9) where we have plotted the ratio $R(\theta,k_i^2)$ of $I(\theta,k_i^2)$ to $I^C(\theta,k_i^2)$ for 200 and 500 eV respectively. It is found that the inclusion of the absorption

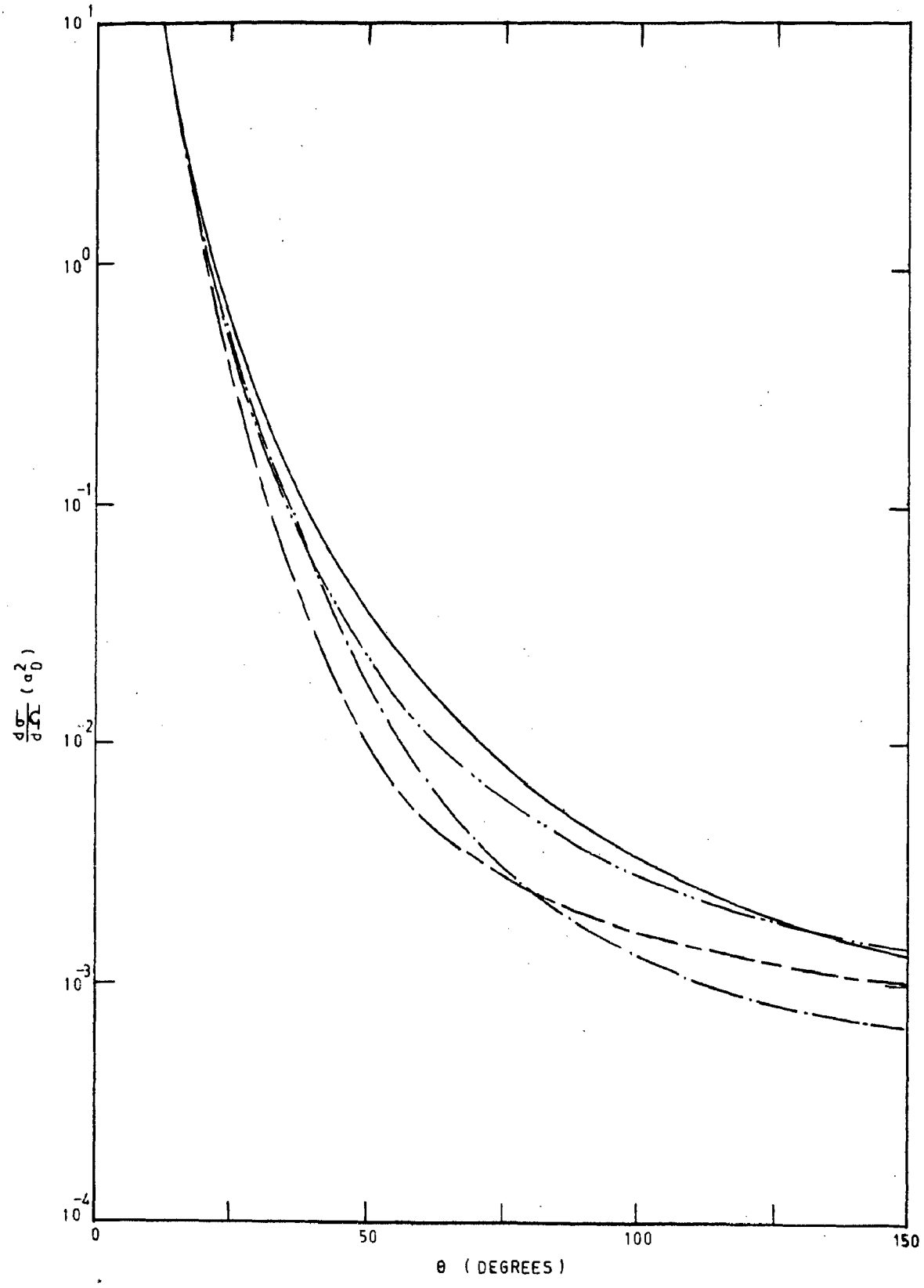


FIG. 5.6 – CALCULATED DIFFERENTIAL CROSS SECTION $I(\theta, k_i^2)$ COMPARED TO THE COULOMB CROSS SECTION $I^C(\theta, k_i^2)$ (——) FOR $e-Li^+$ ELASTIC SCATTERING AT $k_i^2 = 200$ eV. – – –, PRESENT CALCULATION NEGLECTING POLARIZATION AND ABSORPTION (i.e. WITH STATIC POTENTIAL ONLY); —·—, NEGLECTING POLARIZATION BUT INCLUDING ABSORPTION; —··—, INCLUDING BOTH POLARIZATION AND ABSORPTION.

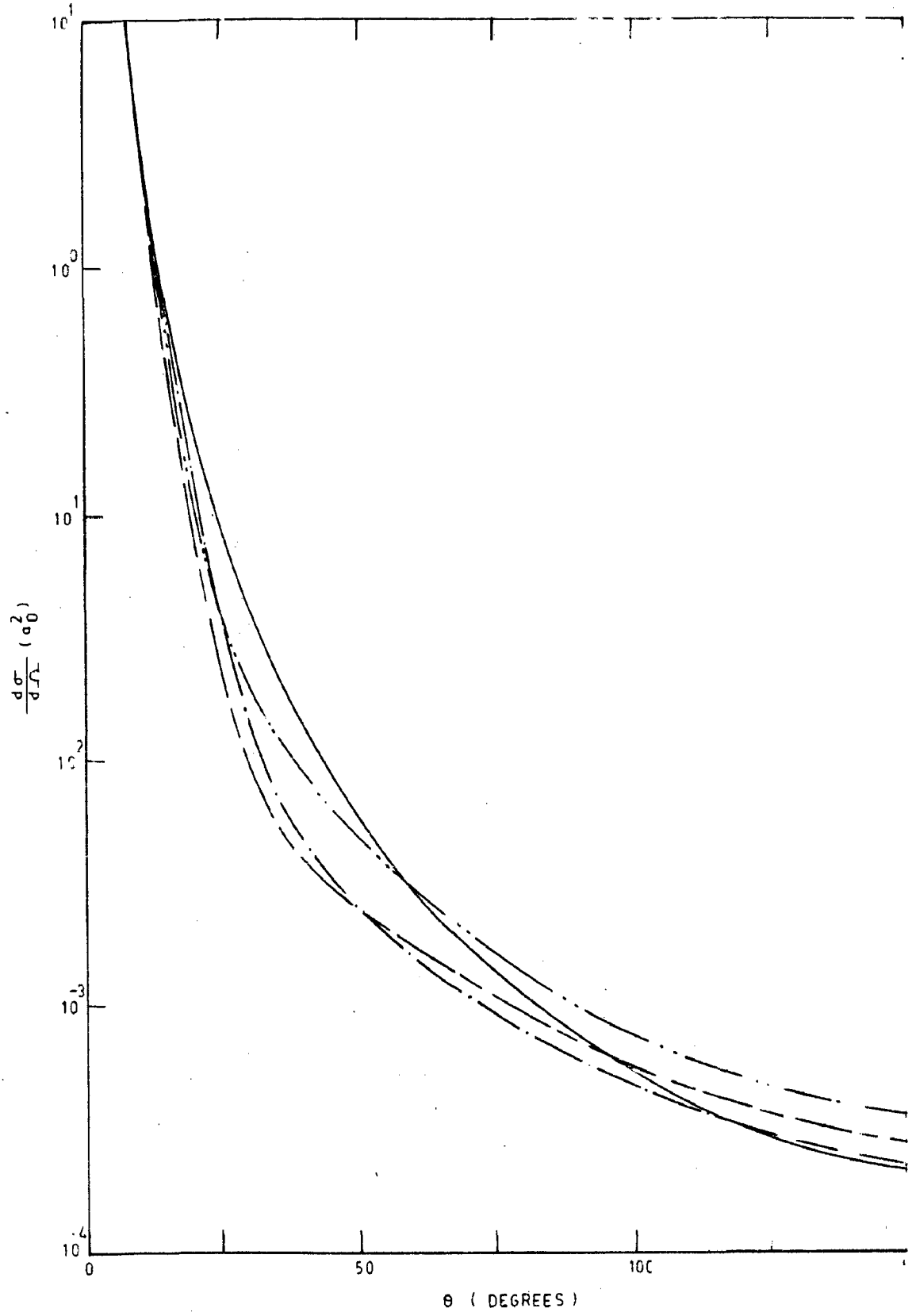


FIG. 5.7— SAME AS FIG. 5.6 BUT FOR 500 eV

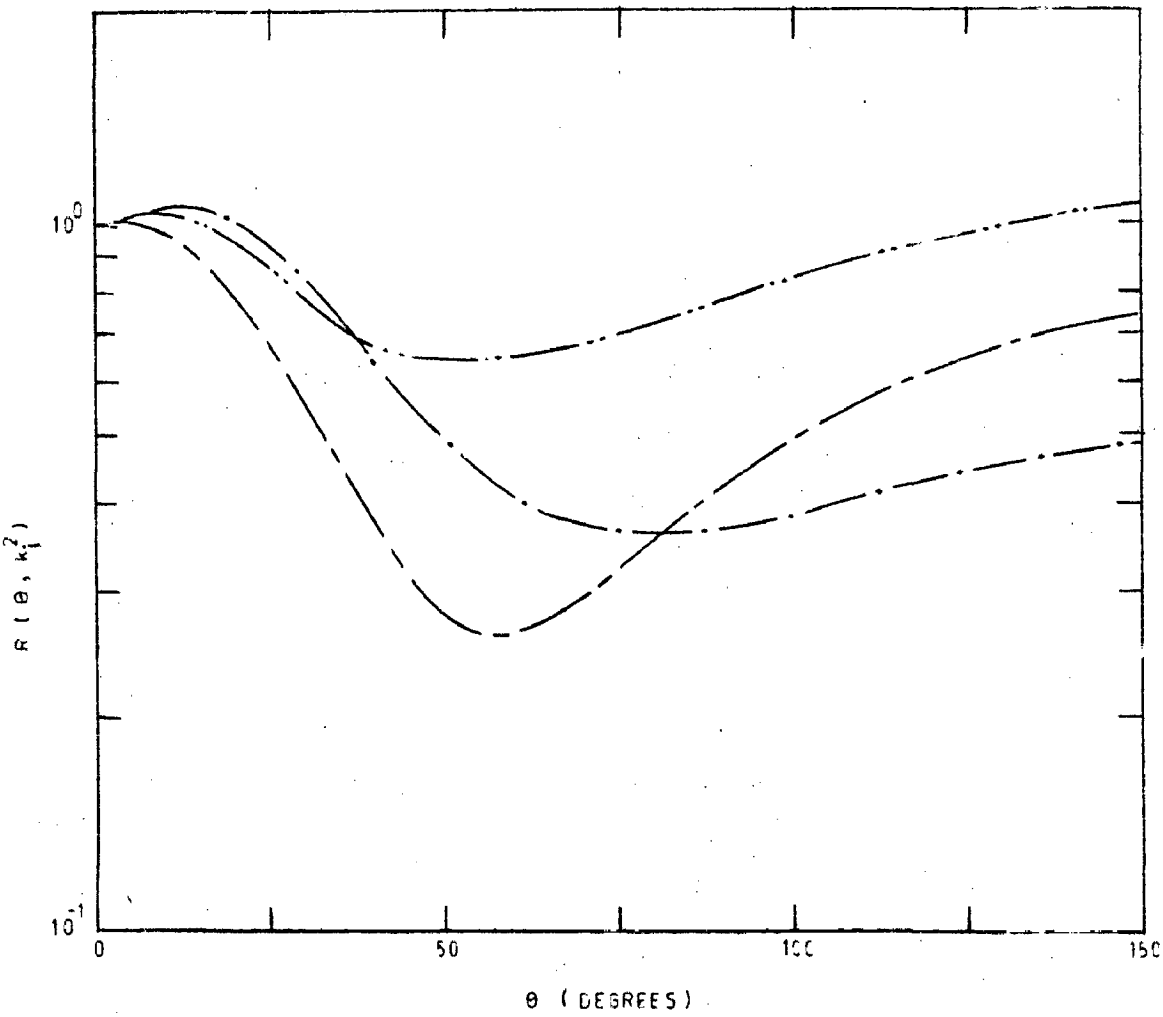


FIG. 5.8 - CALCULATED VALUES OF $R(\theta, k_i^2)$ FOR $e^- - Li^+$ ELASTIC SCATTERING AT $k_i^2 = 200$ eV. — — —, PRESENT CALCULATION NEGLECTING POLARIZATION AND ABSORPTION; —— . ——, NEGLECTING POLARIZATION BUT INCLUDING ABSORPTION; —— .. ——, INCLUDING BOTH POLARIZATION AND ABSORPTION.

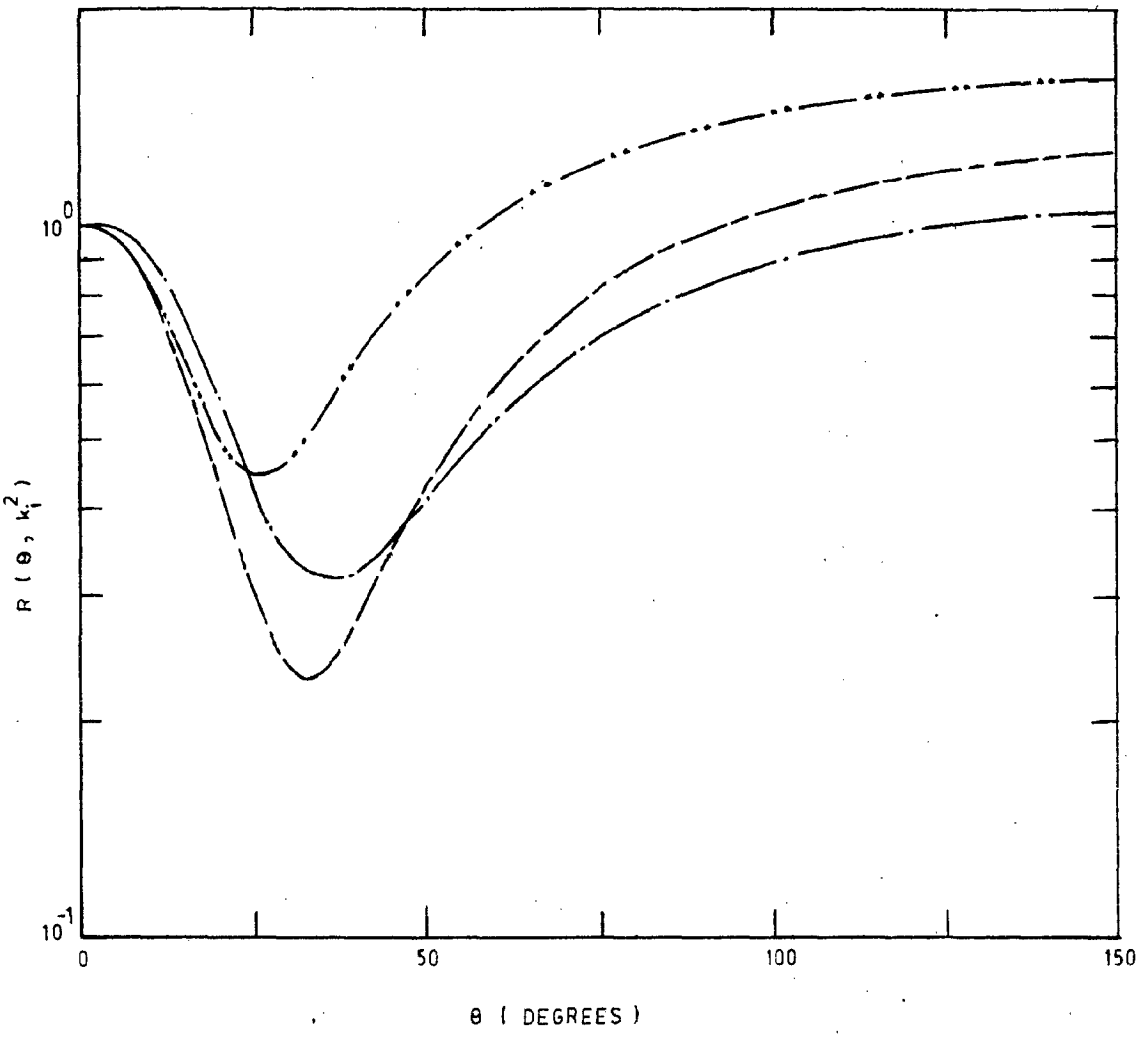


FIG. 5.9 - SAME AS FIG. 5.8 BUT FOR 500 eV.

effects reduces the suppression over Coulomb cross section for $\theta$ upto about $80^{\circ}$. This range decreases as the energy increases. When the polarization potential is also included the suppression is reduced further over almost the whole range except for small angles. Actually the cross section in this case shows enhancement ($R(\theta,k_i^2) > 1$) over Coulomb cross section for large angles ($\theta > 130^{\circ}$ at 200 eV, $\theta > 55^{\circ}$ at 500 eV).

Another feature, in agreement with the findings of McDowell[69], exhibited by these curves is the occurrence of a minimum in $R(\theta,k_i^2)$. This minimum becomes sharper and moves to smaller angles for all curves as the energy increases. The inclusion of the absorption and polarization effects shifts the position of this minimum (absorption effects towards larger angles and polarization towards smaller) and makes the curve shallower.

y(b) in Eq.(5.56) is found to be of almost no consequence. Its values are much too small compared to W(b) indicating thereby that the coupling to the first excited state (2s) in this case is very weak.

# CHAPTER 6

## e-H ELASTIC SCATTERING IN GLAUBER-BORN APPROXIMATION

### 6.1 INTRODUCTION

In the preceding chapters we have discussed the Glaube. approximation and its applications to study the elastic and inelastic scattering of charged particles from atoms and ions at intermediate and high energies. The range of validity of the Glauber 'straight-line' approximation (GSA) with angle and energy have been discussed in Chapter 2. It is well known that in the limit of high energies the Glauber amplitude approaches the first Born amplitude. At intermediate and low energies it is expected to contain more information than the first Born approximation (FBA). But the recent measurements of the differential cross section for e-H elastic scattering[71-73] have indicated that GSA underestimates the cross section and gives a value lower than even FBA at large scattering angles in the intermediate and the low energy region. For small scattering angles anyway the Glauber amplitude diverges as $\ln q$ in the limit $q \to 0$, $q$ being the momentum transfer. Various attempts have been made to improve upon GSA and to extend the range of its applicability to lower energies. In the angle Glauber approximation[81,82] a correction to the straight-line classical trajectory has been made by replacing it by two semi-infinite straight lines. The eikonal optical

model[65-68, 124-128] includes the second order optical potential in the evaluation of eikonal phase and also removes the logarithmic divergence in the forward direction by introducing an average excitation energy of the target. The eikonal-Born series[24,55-58] approach combines, in the spirit of exact scattering amplitude expansion, the Born series and the Glauber series. We have already touched upon these procedures in our earlier discussion. Birman and Rosendorff[141] have recently proposed a procedure to eliminate the small angle divergence, within the framework of the Glauber approximation, by incorporating a non-zero average excitation energy of the target. All these procedures make a distinct improvement over GSA but are quite a bit tedious to apply in actual calculations. Ishihara and Chen[70] have recently pointed out that the poor performance of GSA (even relative to FBA) is primarily due to the improper semiclassical treatment of the electron-atom interaction $V(\vec{r},\vec{x})$. This interaction behaves like $-Z/r$ as the incident electron coordinate $r \to o$. Ishihara and Chen have attempted to eliminate this shortcoming of GSA by separating out, from V, a central-force potential $V_1(r)$ for which semiclassical approximation is not valid. They treat it quantum mechanically taking few partial waves and the rest of the interaction $V_o(\vec{r},\vec{x}) = V(\vec{r},\vec{x}) - V_1(r)$, which satisfies the semi-classical conditions, in the Glauber approximation.

In the present work our motivation is to obtain a simple

expression giving results considerably better than GSA yet with no additional effort. In order to achieve it, we use the standard two potential approach and treat $V_o$ in GSA and $V_1$ in the Glauber-distorted Born approximation. We have applied this procedure to elastic e-H scattering. The exchange effects have been taken into account in the well known Ochkur approximation[29]. A similar approach treating the primary interaction responsible for the transition to first order and the initial- and final-state interactions in eikonal approximation has been followed by Chen, Joachain and Watson[142] for the study of 1s-2s and 1s-2p excitations of hydrogen atom.

In the next section we give an explicit expression for the two-potential form of the scattering amplitude in distorted wave Born approximation (DWBA). Sec. 6.3 outlines our procedure. The details of the calculation are presented in Sec.6.4 and the results are discussed in Sec.6.5.

## 6.2 TWO POTENTIAL FORM OF THE SCATTERING AMPLITUDE- THE DISTORTED WAVE BORN APPROXIMATION (DWBA)

Let us consider the scattering of an electron by a Z-electron target atom. The complete Hamiltonian of the system is given by

$$H = H_o + V , \qquad \ldots (6.1)$$

where the unperturbed Hamiltonian $H_o$ is given by

$$H_o = T + H_t , \qquad \ldots (6.2a)$$

and the interaction potential, V, has the form

$$V = -\frac{2Z}{r} + 2\sum_{j=1}^{Z} \frac{1}{|\vec{r} - \vec{x}_j|}. \qquad \ldots (6.2b)$$

In Eqs.(6.1) and (6.2) $\mathcal{T}$ is, as usual, the kinetic energy operator of the incident electron, $\vec{x}$'s are the coordinates of the target electrons and $H_t$ is the target (neutral atom) Hamiltonian

$$H_t = -\sum_{j=1}^{Z} \nabla_j^2 + V_t, \qquad \ldots (6.3)$$

where

$$V_t = 2\sum_{j=1}^{Z} \left(-\frac{Z}{x_j}\right) + 2\sum_{j>i=1}^{Z} \frac{1}{|\vec{r}-\vec{x}_j|}. \qquad \ldots (6.4)$$

All the positions coordinates have been taken, as usual, relative to the target nucleus. In Eq.(6.4), i denotes the ground state of the target.

The transition matrix element corresponding to a transition of the target atom from an initial state i to some final state f is given by

$$T_{fi} = (2\pi)^3 \langle \Phi_f | V | \Psi_i^{(+)} \rangle = (2\pi)^3 \langle \Psi_f^{(-)} | V | \Phi_i \rangle, \qquad \ldots (6.5)$$

where $\Psi_i^{(+)}$ and $\Psi_f^{(-)}$ denote the scattering wave functionsof the whole system described by the Hamiltonian H and satisfy respectively the following Lippmann-Schwinger equation

$$\Psi_i^{(+)} = \Phi_i + \frac{1}{E - H_o + i\varepsilon} V\Psi_i^{(+)}, \qquad \ldots (6.6)$$

$$\Psi_f^{(-)} = \Phi_f + \frac{1}{E - H_o - i\varepsilon} V^*\Psi_f^{(-)}. \qquad \ldots (6.7)$$

Here $\Phi_j$ is the unperturbed wavefunction and satisfies the Schroedinger equation

$$H_o \Phi_j = E \Phi_j, \qquad . \quad (6.8)$$

where

$$E = \frac{k_i^2}{2} + w_i = \frac{k_f^2}{2} + w_f. \qquad \ldots \quad (6.9)$$

and is given by

$$\Phi_j = \frac{1}{(2\pi)^{3/2}} e^{i \vec{k}_j \cdot \vec{r}} \phi_j(\vec{x}), \qquad \ldots (6.10)$$

ignoring the (spin) exchange effects. $w_j$ is the internal target energy of the target in the state j with wavefunction $\phi_j(\vec{x})$.

We now write the interaction potential V as the sum of two parts

$$V = V_o + V_1. \qquad \ldots (6.11)$$

If $h_j$ is scattering wavefunction of the system in the presence of the potential $V_o$ alone, it satisfies the Lippman-Schwinger equation:

$$h_i^{(+)} = \Phi_i + \frac{1}{E - H_o + i\varepsilon} V_o h_i^{(+)} \qquad \ldots (6.12)$$

$$h_f^{(-)} = \Phi_f + \frac{1}{E - H_o - i\varepsilon} V_o h_f^{(-)} . \qquad \ldots (6.13)$$

Substituting for $\Phi_i$ from Eq.(6.13), the transition matrix

element $T_{fi}$, Eq.(6.6), takes the form

$$(2\pi)^{-3}T_{fi} = \langle \psi_f^{(-)} | V_o+V_1 | (h_i^{(+)} - \frac{1}{E-H_o+i\varepsilon} V_o h_i^{(+)} \rangle$$

$$= \langle \psi_f^{(-)} | V_o | h_i^{(+)} \rangle + \langle \psi_f^{(-)} | V_1 | h_i^{(+)} \rangle$$

$$- \langle \psi_f^{(-)} | V_o + V_1 | \frac{1}{E-H_o+i\varepsilon} V_o h_i^{(+)} \rangle$$

$$= \langle \psi_f^{(-)} | V_o | h_i^{(+)} \rangle - \langle \psi_f^{(-)} | V \frac{1}{E-H_o+i\varepsilon} V_o | h_i^{(+)} \rangle$$

$$+ \langle \psi_f^{(-)} | V_1 | h_i^{(+)} \rangle , \qquad \ldots (6.14)$$

Using the operator identity $(AB)^* = B^*A^*$, it becomes

$$(2\pi)^{-3}T_{fi} = \langle \psi_f^{(-)} - \psi_f^{(-)} \frac{1}{E-H_o-i\varepsilon} V^* | V_o | h_i^{(+)} \rangle + \langle \psi_f^{(-)} | V_1 | h_i^{(+)} \rangle$$

$$= \langle \phi_f | V_o | h_i^{(+)} \rangle + \langle \psi_f^{(-)} | V_1 | h_i^{(+)} \rangle . \qquad \ldots (6.15a)$$

Similarly, proceeding with the alternate form of $T_{fi}$ in Eq.(6.5), it can be readily shown that

$$(2\pi)^{-3} T_{fi} = \langle \phi_f | V_o | h_i^{(+)} \rangle + \langle h_f^{(-)} | V_1 | \psi_i^{(+)} \rangle . \qquad \ldots (6.15b)$$

The distorted wave Born approximation (DWBA) corresponds to approximating $\psi_j^{(\pm)}$ in the second term in Eqs.(6.15) by $h_j^{(\pm)}$:

$$T_{fi}^{DWBA} = (2\pi)^3 \left[ \langle \phi_f | V_o | h_i^{(+)} \rangle + \langle h_f^{(-)} | V_1 | h_i^{(+)} \rangle \right] \qquad \ldots (6.16a)$$

$$\equiv T_{fi}^{(1)} + T_{fi}^{(2)} \qquad \ldots (6.16b)$$

6.3 PROCEDURE

If the potential $V_o$ is smooth enough and $|V_o|/E \ll 1$ for all values of $\vec{r}$, the distorted wave $h_j^{(\pm)}$ described by the Hamiltonian $H_o+V_o$ can be obtained in the Glauber approximation:

$$h_i^{(+)} \to h_i^{(+)G} = \frac{1}{(2\pi)^{3/2}} \exp\{i\vec{k}_i.\vec{r} + i\Lambda_i(\vec{b},z;\vec{x})\}\phi_i(\vec{x}) \quad \ldots (6.17a)$$

$$h_f^{(-)} \to h_f^{(-)G} = \frac{1}{(2\pi)^{3/2}} \exp\{i\vec{k}_f.\vec{r} - i\Lambda_f(\vec{b},z;\vec{x})\}\phi_f(\vec{x}), \quad \ldots (6.17b)$$

where

$$\Lambda_i(\vec{b},z;\vec{x}) = -\frac{1}{2k_i}\int_{-\infty}^{z} V_o(\vec{b},z';\vec{x})\,dz' \quad \ldots (6.18a)$$

$$\Lambda_f(\vec{b},z;\vec{x}) = -\frac{1}{2k_f}\int_{z}^{\infty} V_o(\vec{b},z',\vec{x})\,dz' \quad \ldots (6.18b)$$

$$\vec{r} = \vec{b} + \hat{\zeta}z\,; \quad \ldots (6.19)$$

the unit vector $\hat{\zeta}$ is taken along the incident direction, $\vec{k}_i$ and $\vec{k}_f$ are, as usual, the initial and final momenta and $\vec{b}$ is the impact parameter. Using these distorted waves in Eqs.(6.16), the first term can be written as

$$T_{fi}^{(1)} = \int e^{i\vec{q}.\vec{r}}\, e^{i\Lambda_i(\vec{b},z;\vec{x})}\, \phi_f^*(\vec{x})\, V_o(\vec{r},\vec{x})\, \phi_i(\vec{x})\, d^2b\,dz\, d^3x$$

$$= -2ik_i \int d^2b\, e^{i\vec{q}.\vec{b}} \int d^3x\, \phi_f^*(\vec{x})\Gamma(\vec{b},\vec{x})\phi_i(\vec{x}), \quad \ldots (6.20)$$

where

$$\Gamma(\vec{b},\vec{x}) = 1 - e^{i\chi(\vec{b},\vec{x})}, \quad \ldots (6.21)$$

$$\chi(\vec{b},\vec{x}) = -\frac{1}{2k_i}\int_{-\infty}^{\infty} V_o(\vec{b},z;\vec{x})\,dz. \quad \ldots (6.22)$$

In the above, we have made the usual Glauber approximation of neglecting the longitudinal component of momentum transfer.

Let us now consider the second term, $T_{fi}^{(2)}$, of Eqs.(6.16). With the present choice of $h_j^{(\pm)}$, it is given by

$$T_{fi}^{(2)} = \int d^3r\, d^3x\, e^{i\vec{q}\cdot\vec{r}}\, V_1(r)\phi_f^*(\vec{x}) \times\exp\{i[\Lambda_i(\vec{b},z;\vec{x}) + \Lambda_f(\vec{b},z;\vec{x})]\}\,\phi_i(\vec{x})$$

$$= \int d^3r\, e^{i\vec{q}\cdot\vec{r}}\, V_1(r) \int d^3x\, \phi_f^*(\vec{x})\, e^{i\chi(\vec{b},\vec{x})}\, \phi_i(\vec{x}) \qquad \ldots (6.23)$$

for elastic scattering.

## 6.4 CALCULATION

In this section we apply the expressions obtained above to elastic e-H scattering. For hydrogen (Z = 1), the interaction potential V is given by

$$V(\vec{r},\vec{x}) = -\frac{2}{r} + \frac{2}{|\vec{r}-\vec{x}|}\,. \qquad \ldots (6.24)$$

The arbitrary potential $V_1$ is chosen to be equal to the static potential of the hydrogen atom in the ground state. We thus have

$$V_1(r) \equiv V_{st} = -2\left(1+\frac{1}{r}\right) e^{-2r} \qquad \ldots (6.25)$$

and

$$V_o(\vec{r},\vec{x}) = V - V_1 = -\frac{2}{r} + \frac{2}{|\vec{r}-\vec{x}|} + 2\left(1+\frac{1}{r}\right)e^{-2r} \ldots . \quad (6.26)$$

This choice of $V_1$ makes $V_o$ quite smooth.

Writing $\vec{x} = \vec{s} + \hat{\zeta}\, z_1$, Eq.(6.22) gives

$$\chi(\vec{b},\vec{x}) \equiv \chi(\vec{b},\vec{s}) = \chi_o(\vec{b},\vec{s}) + f(b), \qquad \ldots (6.27)$$

where

$$\chi_o(\vec{b},\vec{s}) = -\frac{1}{2k_i}\int_{-\infty}^{\infty}\left(-\frac{2}{r}+\frac{2}{|\vec{r}-\vec{x}|}\right)dz$$

$$= 2\eta \ln\left(\frac{|\vec{b}-\vec{s}|}{b}\right), \quad \eta = 1/k_i \qquad \ldots (6.28)$$

is the usual Glauber phase function for e-H scattering and

$$f(b) = -\frac{1}{2k_i}\int_{-\infty}^{\infty} 2\left(1+\frac{1}{r}\right) e^{-2r}\, dz$$

$$= -\frac{2}{k_i}\int_{o}^{\infty}\left(e^{-2\sqrt{b^2+z^2}} + e^{-2\sqrt{b^2+z^2}}\Big/\sqrt{b^2+z^2}\right)dz$$

$$= -2\eta\left[K_o(2b) + bK_1(2b)\right], \qquad \ldots (6.29)$$

$K_o$ and $K_1$ are the modified Bessel functions of zeroth and first order respectively. Using Eqs.(6.27) to (6.29) and the ground state (normalized) wavefunction of the hydrogen atom, Eq.(6.20) reduces, for elastic scattering, to the form

$$T^{(1)}_{1s-1s} = -2ik_i \int d^2b\, e^{i\vec{q}.\vec{b}}\left[1 - \frac{1}{\pi}\int d^2s \int_{-\infty}^{\infty} dz_1 e^{-2\sqrt{s^2+z_1^2}} \times \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta} e^{if(b)}\right]$$

$$= -2ik_i \int_o^{\infty} db\, b \int_o^{2\pi} d\phi_b\, e^{i\vec{q}.\vec{b}}\left[1 - \frac{2}{\pi} e^{if(b)} \int_o^{\infty} ds\, s^2 K_1(2s) \times \int_o^{2\pi} d\phi_s \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta}\right]. \qquad \ldots (6.30)$$

Following Franco[94] and Tai et al[91] $\phi_s$- and $\phi_b$ - integration

can be easily performed:

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi_s \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta} = \frac{1}{2\pi}\left(\frac{2s}{by}\right)^{i\eta}\int_0^{2\pi} d\phi(1-y\cos\phi)^{i\eta}$$

$$= \left(\frac{2s}{by}\right)^{i\eta}\left|\frac{b^2-s^2}{b^2+s^2}\right|^{2i\eta+1} {}_2F_1\left(\tfrac{1}{2}+\tfrac{1}{2}i\eta, 1+\tfrac{1}{2}i\eta; 1; y^2\right)$$

$$\equiv I_o(b,s;\eta), \qquad \ldots (6.31a)$$

$$y = \frac{2bs}{(b^2+s^2)}, \qquad \ldots (6.31b)$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi_b \; e^{i\vec{q}.\vec{b}} = J_o(qb). \qquad \ldots (6.32)$$

Using Eqs.(6.31) and (6.32), the transition matrix element, Eq.(6.30), simplifies to a two-dimensional integral form

$$T^{(1)}_{1s-1s} = -16ik_i\pi \int_0^\infty db\; b\; J_o(qb)$$

$$\times\left[\frac{1}{4} - e^{if(b)}\int_0^\infty ds\; s^2 K_1(2s) I_o(b,s;\eta\right]. \qquad \ldots (6.33)$$

Let us now consider Eq.(6.23) for the contribution from $V_1$. Writing

$$\vec{q}.\vec{r} = \vec{q}_b.\vec{b} + q_z\, z, \qquad \ldots (6.34)$$

where $|\vec{q}_b| = q\cos(\theta/2)$ and $q_z = -q\sin(\theta/2)$ are respectively the components of $\vec{q}$ in the plane of $\vec{b}$ and along the z-axis, and using the explicit form of $V_1$ from Eq.(6.25), Eq.(6.23) simplifies to

$$T^{(2)}_{1s-1s} = -\frac{2}{\pi}\int d^2b\, e^{i\vec{q}_b\cdot\vec{b}}\, e^{i\bar{E}(b)} \int d^2s \int_{-\infty}^{\infty} dz_1\, e^{-2\sqrt{s^2+z_1^2}} \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta}$$

$$\times \int_{-\infty}^{\infty} dz\, e^{iq_z z} \left(1 + \frac{1}{\sqrt{b^2+z^2}}\right) e^{-2\sqrt{b^2+z^2}}$$

$$= -\frac{8}{\pi}\int d^2b\, e^{i\vec{q}_b\cdot\vec{b}}\, e^{if(b)} \left[K_o\left(b\sqrt{q_z^2+4}\right) + \frac{2b}{\sqrt{q_z^2+4}} K_1\left(b\sqrt{q_z^2+4}\right)\right]$$

$$\times \int d^2s\; s\, K_1(2s) \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta}.$$

The longitudinal component $q_z$ of the momentum transfer has been retained here as $T^{(2)}$ is expected to contribute significantly for large scattering angles. The integrations over the azimuthal angles $\phi_s$ and $\phi_b$ can be performed as before to yield

$$T^{(2)}_{1s-1s} = -32\pi \int_0^{\infty} db\; b\, J_o(q_b b) \left[K_o\left(b\sqrt{q_z^2+4}\right) + \frac{2b}{\sqrt{q_z^2+4}} K_1\left(b\sqrt{q_z^2+4}\right)\right]$$

$$\times e^{if(b)} \int ds\; s^2 K_1(2s) I_o(b,s;\eta). \qquad \ldots (6.35)$$

The s-integration in Eq.(6.35) is identical to that in Eq.(6.33). The direct contribution to the scattering amplitude for the elastic scattering of electrons by hydrogen atom in Glauber-distorted Born approximation is now given by

$$F_{1s-1s}(\vec{k}_f,\vec{k}_i) = -\frac{1}{4\pi}\left(T^{(1)}_{1s-1s} + T^{(2)}_{1s-1s}\right). \qquad \ldots (6.36)$$

So far the exchange effects, which are important at intermediate and low energies, have been ignored. We have included them in Ochkur approximation rather than following the procedure of

Ishihara and Chen[70] in order to keep the calculations simple which is the prime motivation behind the present work. The Glauber approximation for the exchange contribution cannot be used because of the indeterminate phase factor appearing therein[143].

The differential and total cross sections are obtained in the usual way:

$$\frac{d\bar{\sigma}_{el}(\vec{q})}{d\Omega} = |F|^2 + |g|^2 - \mathrm{Re}(F\, g^*) \qquad \ldots (6.37)$$

and

$$\bar{\sigma}_{el}(k_i) = \frac{2\pi}{k_i^2}\int_0^{2k_i} dq\; q\; \frac{d\bar{\sigma}(q)}{d\Omega}\ , \qquad \ldots (6.38)$$

where g is the Ochkur exchange amplitude.

## 6.5 RESULTS AND DISCUSSION

We have shown our calculated differential cross sections at low energies (20 eV and 30 eV) in Figs.6.1 and 6.2, and at intermediate energies (50 eV and 100 eV) in Figs.6.3 and 6.4. They are compared with (i) the usual Glauber (GSA) results including exchange in Ochkur approximation[29], (ii) the two-potential eikonal calculations of Ishihara and Chen[70], (iii) the eikonal-Born series calculations of Byron and Joachain[24] (Figs.6.3 and 6.4) and (iv) the recent experimental measurements of Tenbner et al[71], Lloyd et al[72] and Williams[73]. Also plotted are the cross sections in FBA. In the low energy region our results exhibit considerable improvement over the

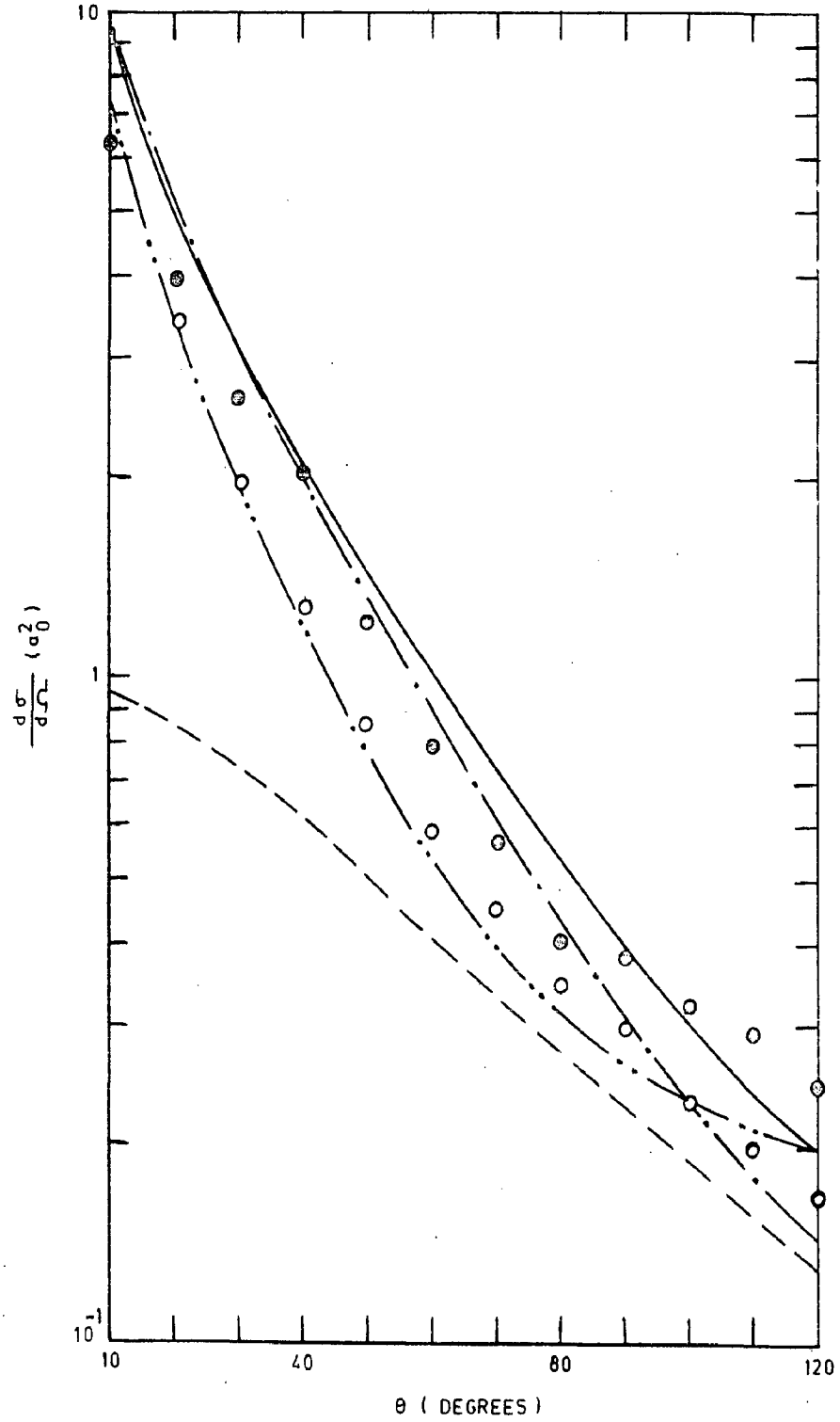


FIG 6.1 — DIFFERENTIAL CROSS SECTION FOR e–H ELASTIC SCATTERING AT $k_i^2 = 20$ eV. ——— , PRESENT CALCULATION; – – – , BORN CALCULATION; —·—·— , GLAUBER CALCULATION INCLUDING EXCHANGE IN OCHKUR APPROXIMATION[29] ——··—— , TWO-POTENTIAL EIKONAL CALCULATION OF ISHIHARA AND CHEN[70]; ⊙, EXPERIMENTAL DATA OF WILLIAMS[73]; O , RELATIVE ANGULAR DISTRIBUTION DATA OF TEUBNER et al[71].

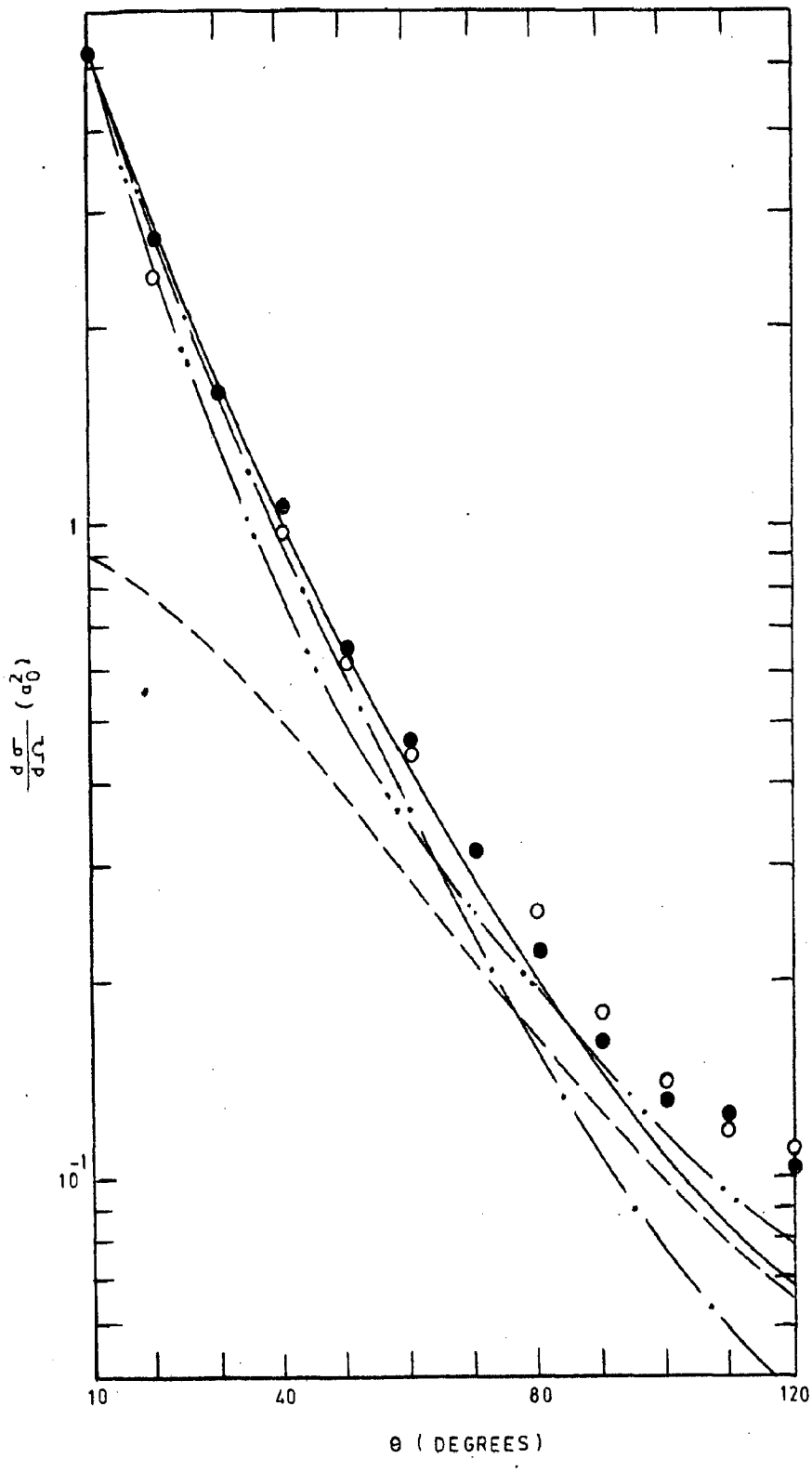


FIG. 6.2 — SAME AS FIG. 6.1 BUT AT 30 eV. OPEN CIRCLES (o) CORRESPOND TO THE EXPERIMENTAL DATA OF LLOYD et al[72].

usual Glauber results at large scattering angles ($\theta \geqslant 50^{o}$). At 20 eV present results compare very favourably with those of Ishihara and Chen[70] and are in very good agreement with the experimental data. At 30 eV, though we are better than FBA, the agreement with experimental data is not so good. As the energy increases (Figs.6.3 and 6.4) our results begin to underestimate the cross sections even with respect to FBA. They continue to remain better, though not very significantly, than GSA.

The overall conclusion is that though the present calculations do not have as good a fit to the experimental data as obtained by Ishihara and Chen[70], they provide a simple and reasonably accurate alternative for elastic scattering studies at low and intermediate energies. The loss of accuracy is compensated by considerable saving in computational labour.

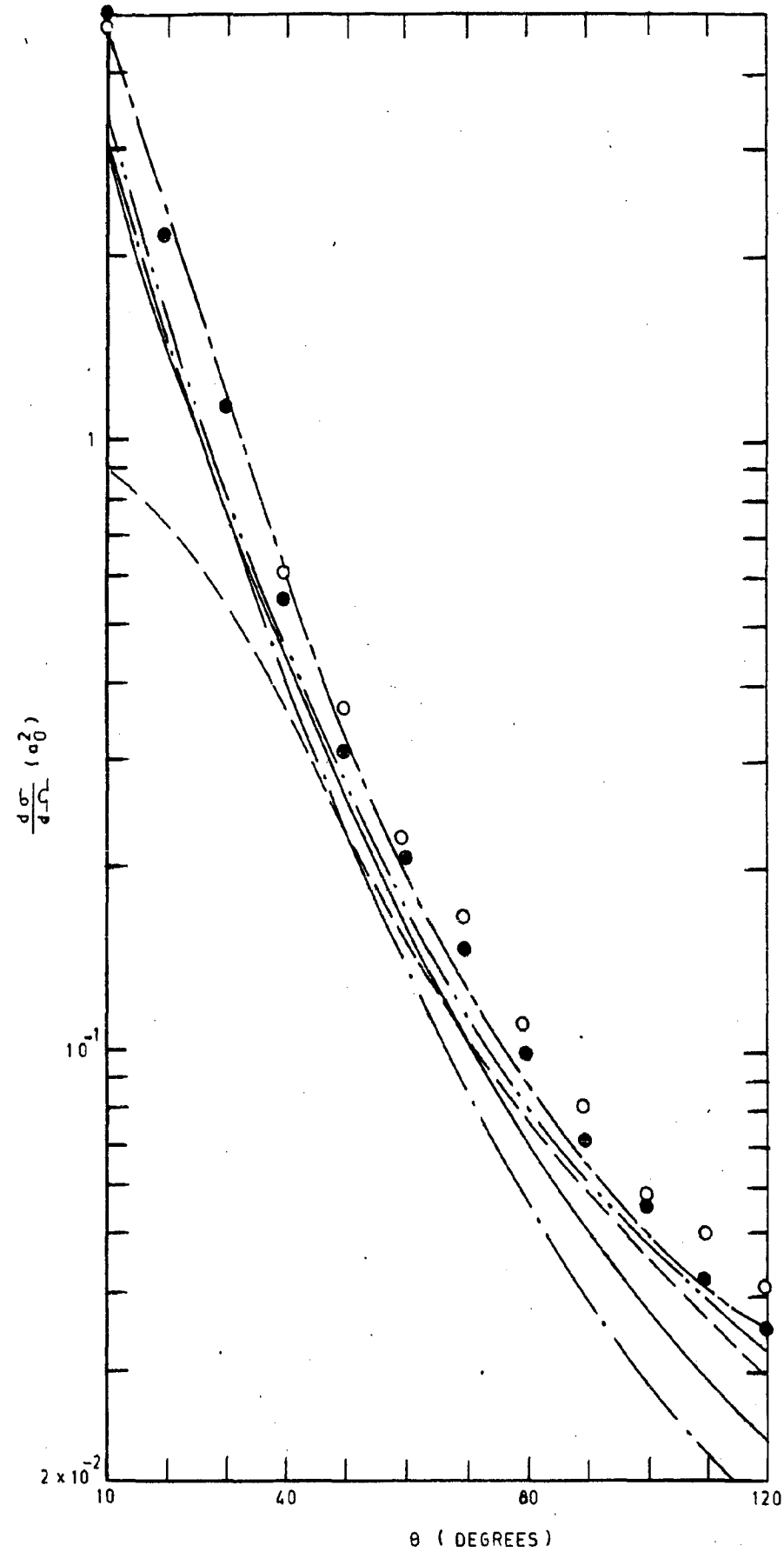


FIG. 6.3 – SAME AS FIG 6.2 BUT AT 50 eV. THE EIKONAL BORN SERIES CALCULATIONS (– – –) OF BYRON AND JOACHAIN[24] ARE ALSO INDICATED.

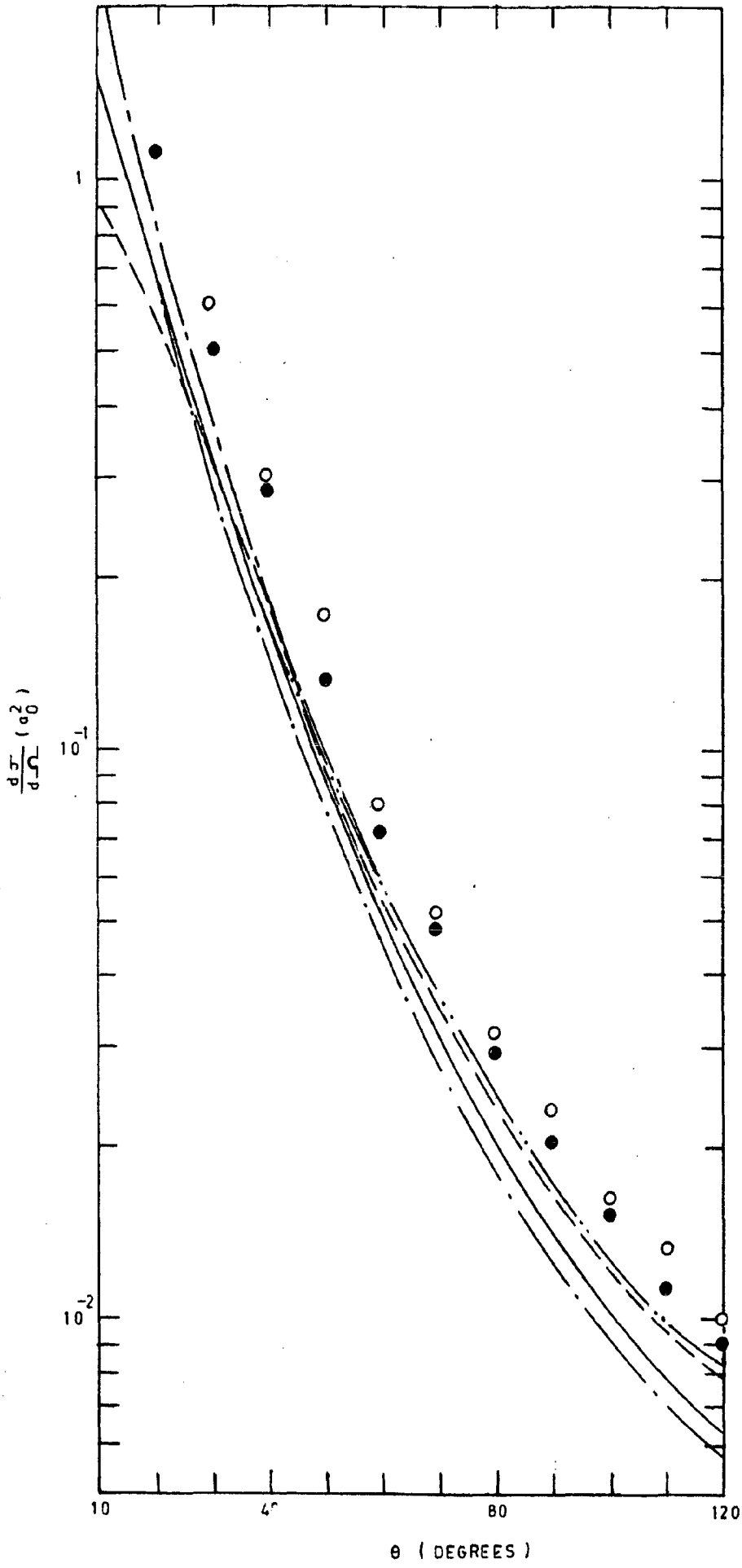


FIG. 6.4—SAME AS FIG. 6.3 BUT AT 100 eV.

# CHAPTER 7

## SUMMARY, CONCLUSIONS AND COMMENTS

Throughout the work reported, the Glauber approximation has been used as the basic tool to study the problems of atomic collisions. The underlying assumptions, the limitations and the range of applicability of this approximation with respect to the scattering angle and the incident energy, and its relationship with the Born approximation have been reviewed.

In the present work following problems were investigated:

(i) We have obtained a 'simple' expression for the Glauber scattering amplitude in a one-dimensional integral form for the general transition $n\ell m - n'\ell'm'$ in e-H(1s) scattering by combining the techniques of Franco[60] and Golden and McGuire[61] and using the Laguerre polynomials appearing in hydrogen atom wavefunctions straightaway rather than breaking them into the form $x^{\mu}e^{-\nu x}$. Our expression is particularly suited to study excitations to highly excited states from a low lying state. Earlier expressions[59], although in closed forms, become a bit complicated because of the increasing number of hypergeometric functions depending on the value of $n'$ [Chapter 3, Publication No.6].

(ii) We have studied the elastic scattering and the 2s-2p excitation of lithium following electron impact by modifying Franco's procedure[60] of explicitly involving all

the three electrons of lithium atom. Earlier Glauber calculations of e-Li elastic and inelastic scattering were made in 'frozen core' approximation without[62,63] and with[63] the core potential. Our main conclusion is that the involvement of inner electrons (those in the 1s state) in lithium causes very little change over the 'frozen core' Glauber results and the latter are good enough for studying e-Li scattering. As a side excercise we have also obtained the percentage polarization of the 2p→2s resonance line emitted from $^{6}$Li and $^{7}$Li following electron excitation.[144] The agreement with the experimental data of Leep and Gallagher[64] is excellent for energies above 60 eV. Even for lower energies the differences are not as pronounced as in the case of total cross sections [Chapter 4, Publication Nos.2,4 and 5].

(iii) We have considered e-$H^-$ and e-$Li^+$ elastic scattering by extending the eikonal optical model of Mittleman[65] and Joachain and Mittleman[66] for e-atom scattering. We have treated separately the pure Coulomb interaction between the projectile electron and the ionic target and taken its contribution into account exactly. The total scattering amplitude has been obtained by adding coherently the contribution due to the pure Coulomb interaction to that due to the remaining interaction treated in eikonal optical model[65,66]. The main aim of the present work was (a) to investigate how far one can use the eikonal optical method, which is comparatively very simple, to study e-ion elastic

scattering at intermediate and low energies and (b) to analyse the contributions of second order terms of the optical potential in the evaluation of the eikonal phase. The main drawback of the method is the neglect of the interference of the Coulomb interaction with the remaining interaction. Recently Narumi and Tsuji[145], Ishihara and Chen[146], and Thomas and Franco[95] have suggested a procedure to study charged particle-ion scattering in Glauber approximation. No results have yet been reported, to our knowledge, using this procedure for charged particle-ion elastic scattering [Chapter 5, Publication Nos.1 and 3].

(iv) A simple procedure based on two potential Glauber-distorted Born approximation has been proposed to improve the behaviour of the Glauber approximation for large scattering angles and used to study e-H(1s) elastic scattering. The main feature of the present method is the simplicity of calculations; it is hardly any more difficult than the ordinary Glauber-approximation. Electron-hydrogen atom scattering has always been an attractive testing ground for investigating various approximations and calculational procedures. Recently good experimental data on e-H(1s) scattering has become available[71-73]. It is found that the Glauber approximation underestimates the cross section even with respect to FBA at large scattering angles. Various attempts have been made to improve the results. These are the 'unrestricted' (without the approximation of neglecting the longitudinal component of momentum transfer) Glauber

approximation[147-150], the eikonal optical model[65-68,122-128], the eikonal-Born series[24,55-58] and the two-potential eikonal approach[70]. Our work[151] is a step in the same direction. [Chapter 6, Publication No. 7].

(v) A numerical technique has been developed in the spirit of Filon's method in order to take into account accurately the wiggles of the cylindrical Bessel functions in the integrals of the type

$$\int F(x) J_{\nu}(ax)\, dx.$$

Such integrals are of common appearance in Glauber calculations. [Appendix A1, Publication No. 1].

Inspite of all the developments, present use of the Glauber approximation still has many weak points. These are:

(i) For elastic scattering, the Glauber amplitude diverges logarithmically in the forward direction. This divergence, in turn, leads to the violation of optical theorem and is, therefore, worth special mention. It is found to occur in the imaginary part of the second-order scattering amplitude.[16,152,153] It has been shown by Moisewitsch and Williams[152], Birman and Rosendorff[153] and Joachain and Mittleman[66] within the framework of the eikonal approximation and by Birman and Rosendorff[141] in the case of Glauber approximation that the logarithmic divergence can be easily removed by introducing

an average target excitation energy in the intermediate states.

(ii) It is difficult to handle the exchange contribution to the scattering amplitude in Glauber approximation. Although Ochkur like reduction of the Glauber exchange amplitude has recently been proposed[154,143], the method suffers from an undesirable feature in the form of an indeterminate phase factor which restricts its application to only optically forbidden exchange allowed transitions.

(iii) The leading contribution from the polarization of the target is missing from the Glauber scattering amplitudes.The need for introducing polarization effect has long been recognised. In the present day Glauber calculations,this has to be added from outside. For example, Mathur[155] has considered, in e-H elastic scattering, the perturbation of the target eigenfunction (by the static field of the incoming charged particle) by including a polarization part as given by Temkin[10].

On the problem of charged particle-ion scattering, we feel that looking at the success of the two potential [illegible] approach of Ishihara and Chen[70], best results within the framework of the Glauber approximation could be obtained by combining the approach of Ishihara and Chen[70] with that of Narumi and Tsuji[145], Ishihara and Chen[146] and Thomas and Franco[95]. The total interaction potential should be broken

up into three parts; the pure Coulomb potential, the static potential due to the remaining neutral target and the remaining potential. For example, in e-$He^+$ scattering

$$V(\vec{r},\vec{x}) = -\frac{4}{r} + \frac{2}{|\vec{r}-\vec{x}|}$$

$$= -\frac{2}{r} + \left(-\frac{2}{r} + \frac{2}{|\vec{r}-\vec{x}|} - V_{st}\right) + V_{st}$$

$$\equiv V_C + V_o + V_{st}, \qquad \ldots (7.1)$$

where

$$V_{st}(r) = \int \phi_i^*(\vec{x}) \left(-\frac{2}{r} + \frac{2}{|\vec{r}-\vec{x}|}\right) \phi_i(\vec{x})\, d^3x; \qquad \ldots (7.2)$$

$\phi_i(\vec{x})$ is the ground state wavefunction of $He^+$. If

$$\delta \equiv \delta_C + \delta_o + \delta_{st} \qquad \ldots (7.3)$$

is the phase shift in any partial wave, its contribution to the scattering amplitude can be written as

$$(e^{2i\delta}-1) \equiv (e^{2i\delta_C} - 1) + e^{2i\delta_C}(e^{2i\delta_o} - 1) + e^{2i(\delta_C+\delta_o)}(e^{2i\delta_{st}}-1). \qquad \ldots (7.4)$$

Now the three terms can be handled , the first two by following the procedures of Refs. 95, 145 and 146 and third by the procedure of Ref. 70. This method will have the merit of treating the singular part of the interaction in a way better than the Glauber approximation.

The problem of electron impact ionization has not been undertaken in this study. The main difficulty comes about

due to the appearance of the Coulomb continuum wavefunction. Expressions in the form of an infinite series[156,157] or a 1D integral[158-160] have been obtained. But the procedure is still quite involved and is restricted to include the contributions of only a few partial waves. A suggestion has been made that by working in hyperbolic coordinates may avoid the expansion in partial waves and save computation time[160]. To our knowledge this suggestion has not yet been followed.

## APPENDIX A1

### EVALUATION OF AN INTEGRAL INVOLVING ORDINARY BESSEL FUNCTIONS

The integrals involving ordinary Bessel function $J_\nu$ of order $\nu$ frequently occur in our calculations. The difficulty in their evaluation arises because of $J_\nu$ whose oscillations must be properly taken into account. We give below a numerical technique to evaluate them. We divide the total range into a suitable number of subintervals and approximate, in each subinterval, the remaining part of the integrand by a parabola

$$\int_{x_{n-1}}^{x_{n+1}} F(x)\, J_\nu(ax)\,dx \simeq \int_{x_{n-1}}^{x_{n+1}} \left(C_{n-1}^{(o)} + C_{n-1}^{(1)}x + C_{n-1}^{(2)}x^2\right) \times J_\nu(ax)\,dx \quad \ldots (A1.1)$$

The constants $C_{n-1}^{(i)}$ are obtained from the values of the function $F(x)$ at $x_{n-1}$, $x_n$ and $x_{n+1}$. The right-hand side can now be exactly evaluated using the equation (Ref.161,p.480).

$$\int_o^x x^\mu J_\nu(x)\,dx = \frac{z^\mu \Gamma\left[\frac{1}{2}(\nu+\mu+1)\right]}{\Gamma\left[\frac{1}{2}(\nu-\mu+1)\right]} \times \sum_{p=o}^{\infty} \frac{(\nu+2p+1)\,\Gamma\left[\frac{1}{2}(\nu-\mu+1)+p\right]}{\Gamma\left[\frac{1}{2}(\nu+\mu+3)+p\right]} J_{\nu+2p+1}(z)$$

$$= z^\mu \beta(\mu,\nu) \sum_{p=o}^{\infty} \gamma(\mu,\nu,p) J_{\nu+2p+1}(z) \quad \ldots (A1.2)$$

to give

$$\int_{x_{n-1}}^{x_{n+1}} F(x) J_\nu(ax)\,dx \simeq \frac{1}{a} \sum_{\mu=o}^{2} C_{n-1}^{(\mu)}\, \beta(\mu,\nu) \sum_{p=o}^{\infty} \gamma(\mu,\nu,p)$$

$$\times \left[ x_n^\mu \, J_{\nu+2p+1}(a\, x_{n+1}) - x_{n-1}^\mu J_{\nu+2p+1}(a\, x_{n-1}) \right] \quad \ldots \text{(A1.3)}$$

The summation over p is, in practice, finite because the Bessel function $J_p(x) \to 0$ as $p \to \infty$. This method is reasonably fast because the constants in Eq.(A1.2) need be calculated only once and the Bessel functions are needed only at half the number of mesh points. No special effort is needed to calculate the Bessel functions of different orders as they are all generated in the standard 'Bessel subroutine' based on recurrence relations.

## APPENDIX A2

### CONFIGURATION REPRESENTATION OF THE SECOND ORDER NON-LOCAL OPTICAL POTENTIAL

The second order term $\sqrt{}^{(2)}$ of the optical potential in Eq.(5.13) is written in the form

$$\sqrt{}^{(2)} = \sum_{j\neq i} \frac{\langle \phi_i | V | \phi_j \rangle \langle \phi_j | V | \phi_i \rangle}{k_i'^2 - \mathcal{T}_j + i\varepsilon}$$

$$= \sum_{j\neq i} V_{ij} \frac{1}{k_i'^2 - \mathcal{T}_j + i\varepsilon} V_{ji}, \qquad \ldots (A2.1)$$

where

$$V_{\beta\alpha} = \langle \phi_\beta | V | \phi_\alpha \rangle . \qquad \ldots (A2.2)$$

If the interaction potential V is local, it can be written in the form:

$$\langle \vec{r} | V_{\beta\alpha} | \vec{r}' \rangle = V_{\beta\alpha}(\vec{r})\,\delta(\vec{r} - \vec{r}')$$

$$= \int \phi_\beta(\vec{x})\, V(\vec{r},\vec{x})\, \phi_\alpha(\vec{x})\, d^3x. \qquad \ldots (A2.3)$$

Let us write $\sqrt{}^{(2)}$ in configuration space of the incident particle coordinates $\vec{r},\vec{r}'$.

$$\langle \vec{r} | \sqrt{}^{(2)} | \vec{r}' \rangle = \sum_{j\neq i} \langle \vec{r} | V_{ij} \frac{1}{k_i'^2 - \mathcal{T}_j + i\varepsilon} V_{ji} | \vec{r}' \rangle \qquad \ldots (A2.4)$$

$$= \sum_{j\neq i} \int \langle \vec{r}| V_{ij} |\vec{r}_1\rangle \langle \vec{r}_1|\vec{\kappa}\rangle \langle \vec{\kappa}| \frac{1}{k_i'^2 - J + i\varepsilon} |\vec{\kappa}'\rangle$$

$$\times \langle \vec{\kappa}'|\vec{r}_2\rangle \langle \vec{r}_2| V_{ji} |\vec{r}'\rangle \, d^3r_1 d^3r_2 d^3\kappa \, d^3\kappa' , \qquad \ldots (A2.5)$$

where the kinetic energy operator $J$ satisfies the Schroedinger equation

$$J|\vec{\kappa}'\rangle = \kappa'^2 |\vec{\kappa}'\rangle . \qquad \ldots (A2.6)$$

Using the relations

$$\langle \vec{r}|\vec{\kappa}\rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{\kappa}.\vec{r}} \qquad \ldots (A2.7)$$

$$\langle \vec{\kappa}|\vec{\kappa}'\rangle = \delta(\vec{\kappa}-\vec{\kappa}') \qquad \ldots (A2.8)$$

and Eq.(A2.3), Eq.(A2.5) simplifies to

$$\langle \vec{r}|V^{(2)}|\vec{r}'\rangle = \sum_{j\neq i} \int V_{ij}(\vec{r}) \frac{e^{i\vec{\kappa}.\vec{r}}}{(2\pi)^{3/2}} \frac{1}{k_i'^2 - \kappa^2 + i\varepsilon} \frac{e^{-i\vec{\kappa}.\vec{r}'}}{(2\pi)^{3/2}}$$

$$\times V_{ji}(\vec{r}') d^3\kappa$$

$$= \sum_{j\neq i} V_{ij}(\vec{r}) V_{ji}(\vec{r}') \frac{1}{(2\pi)^3} \int d^3\kappa \frac{e^{i\vec{\kappa}.(\vec{r}-\vec{r}')}}{k_i'^2 - \kappa^2 + i\varepsilon}$$

$$\equiv \mathcal{G}_{k_i'}(\vec{r},\vec{r}') \; A(\vec{r},\vec{r}') , \qquad \ldots (A2.9)$$

where

$$\mathcal{G}_{k_i'}(\vec{r},\vec{r}') = \frac{1}{(2\pi)^3} \int d^3\kappa \frac{e^{i\vec{\kappa}.(\vec{r}-\vec{r}')}}{k_i'^2 - \kappa^2 + i\varepsilon} \qquad \ldots (A2.10)$$

and

$$A(\vec{r},\vec{r}') = \sum_{j\neq i} V_{ij}(\vec{r})\, V_{ji}(\vec{r}')$$

$$= -\sum_{j\neq i} \langle \phi_i(\vec{x}) \,|\, V(\vec{r},\vec{x}) \,|\, \phi_j(\vec{x}) \rangle \langle \phi_j(\vec{x}') \,|\, V(\vec{r}',\vec{x}') \,|\, \phi_i(\vec{x}') \rangle$$

$$= \langle \phi_i(\vec{x}) \,|\, V(\vec{r},\vec{x})\, V(\vec{r}',\vec{x}) \,|\, \phi_i(\vec{x}) \rangle$$

$$- \langle \phi_i(\vec{x}) \,|\, V(\vec{r},\vec{x}) \,|\, \phi_i(\vec{x}) \rangle \langle \phi_i(\vec{x}') \,|\, V(\vec{r}',\vec{x}') \,|\, \phi_i(\vec{x}') \rangle$$

$$= \int \phi_i^*(\vec{x})\, V(\vec{r},\vec{x})\, V(\vec{r}',\vec{x})\, \phi_i(\vec{x})\, d^3x$$

$$- \int \phi_i^*(\vec{x})\, V(\vec{r},\vec{x})\, \phi_i(\vec{x})\, \phi_i^*(\vec{x}')\, V(\vec{r}',\vec{x}')\, \phi_i(\vec{x}')\, d^3x\, d^3x' \qquad \ldots \text{(A2.11a)}$$

$$= \int \phi_i^*(\vec{x})\, V(\vec{r},\vec{x}) \left[ \delta(\vec{x}-\vec{x}') - \phi_i(\vec{x})\, \phi_i^*(\vec{x}') \right]$$

$$\times\, V(\vec{r}',\vec{x}')\, \phi_i(\vec{x}')\, d^3x\, d^3x' \,. \qquad \ldots \text{(A2.11b)}$$

the shaded area of the square figure. The same area can also be spanned if we first vary $z'$ from a to b and then vary z from $z'$ to b (horizontal arrows) for every value of $z'$. Thus, we should have

$$\int_a^b dz \int_a^z dz' \, f(z,z') = \int_a^b dz' \int_{z'}^b dz \; f(z,z') \; . \qquad \ldots \text{(A3.3)}$$

Interchanging the variables on the right hand side and using (A3.2), it becomes

$$\int_a^b dz \int_a^z dz' \, f(z,z') = \int_a^b dz \int_z^b dz' \, f(z,z') \; . \qquad \ldots \text{(A3.4)}$$

Combining Eqs.(A3.1) and (A3.4) we can now write

$$\begin{aligned} I &= \tfrac{1}{2}\left[ \int_a^b dz \int_a^z dz' \, f(z,z') + \int_a^b dz \int_z^b dz' \, f(z,z') \right] \\ &= \tfrac{1}{2}\left[ \int_a^b dz \left( \int_a^z dz' + \int_z^b dz' \right) f(z,z') \right] \\ &= \tfrac{1}{2} \int_a^b dz \int_a^b dz' \, f(z,z') . \end{aligned} \qquad \ldots \text{(A3.5)}$$

This is the required expression in which the variable upper limit of the integral is transformed to the fixed value b. The integral gets further simplified if the function $f(z,z')$ is separable.

## REFERENCES


1. P.G. Burke and K.Smith, Rev. Mod.Phys.34,458(1962).

2. K.Smith, Rep.Prog. .Phys. 29(2), 373(1966).

3. P.G. Burke, in Adv.At.Mol.Phys.4, 173(1968).

4. N.R.Kestner, J.Jortner, M.H.Cohen and S.A.Rice, Phys. Rev. 140, A56(1965).

5. J.Callaway, R.W.LaBahn, R.T.Pu and W.M. Duxler, Phys. Rev.168,12(1968).

6. L.Castillejo, I.C.Percival and M.J.Seaton, Proc. Phys.Soc. (London) A254, 259(1960).

7. P.G.Burke, S.Ormonde and W.Whitteker, Proc.Phys.Soc.(London) 92, 319(1969).

8. D.R.Hartree, Proc. Camb.Phil.Soc.28, 89,111 and 426(1928).

9. V.Fock, Proc. Phil.Soc.61, 126(1930); 62, 795(1930).

10. A.Temkin, Phys. Rev.107, 1004(1957); Phys.Rev.Lett.4, 566 (1960).

11. A.Temkin and J.C.Lamkin, Phys.Rev.121, 788(1961).

12. B.L.Moiseiwitsch,Phys. Rev.82, 753(1951).

13. M.R.H.Rudge, Proc. Phys. Soc. (London)85, 607(1965).

14. B.H.Bransden, J.P. Coleman and J.Sullivan, J.Phys.B5, 546(1972).

15. R.W.LaBahn and J.Callaway, Phys. Rev.180, 91(1969).

16. H.S.W. Massey and C.B.O. Mohr, Proc. Roy.Soc.(London) 146, 880(1934).

34. E.Gerjuoy and B.K. Thomas, Rep. Prog. Phys.37, 1345(1974).

35. A.Messiah, Quantum Mechanics (Amsterdam: North-Holland, 1962), Vol.2.

36. G.Moliere, Z.Naturf.2a,133(1947).

37. B.J.Malenka, Phys. Rev.95, 522(1954).

38. L.I. Schiff, Phys. Rev.103, 443(1956).

39. D.S.Saxon and L.I. Schiff, Nuovo Cimento 6, 614(1957).

40. R.J. Glauber, in Lectures in Theoretical Physics, ed.W.E. Brittin and L.G.Dunham (New York: Interscience, 1959), Vol.I, p.315.

41. R.Blankenbecler and M.L. Goldberger, Phys. Rev.126, 766(1962).

42. H.Feshbach, Proc. Int. School of Physics Course ed.T.E.O. Erickson (New York: Academic Press, 1967), 38, p.183.

43. L.Willets and S.J. Wallace, Phys. Rev. 169,84,(1968).

44. R.L. Sugar and R.Blankenbecler, Phys. Rev.183, 1387(1969).

45. M.Levy and J.Sucher, Phys. Rev.186, 1656(1969).

46. H.D.I. Abarbanel and C.Itzykson, Phys. Rev. Lett.23, 53(1969).

47. R.J. Moore, Phys. Rev. D2, 313(1970).

48. S.J. Wallace, Phys. Rev. Lett.27, 622(1971); Phys.Rev.D8, 1846(1973a); Ann. Phys. 78, 190(1973b); Phys. Rev.C8, 2043(1973c).

49. S.A.Lebedeff, J.Phys. B4, 819(1971).

50. A.Baker, Phys. Rev.B134, 240(1964); Phys. Rev.D6, 3446(1972); D8, 1937(1973).

51. M.Obu, Prog. Theor. Phys. 46, 1934(1972).

52. A.R.Swift, Phys. Rev.D9, 1740(1974).

53. F.W.Byron, Jr. and C.J. Joachain, Physica 66, 33(1973c).

54. F.W.Byron, Jr., C.J. Joachain and E.Mund, Phys. Rev.D8, 2622(1973).

55. F.W.Byron, Jr.and C.J. Joachain, Phys. Rev.A9, 3266(1973b).

56. F.W.Byron, Jr. and C.J. Joachain, Phys. Lett. 49A, 306(1974b).

57. F.W.Byron, Jr. and C.J. Joachain, J.Phys. B10, 207(1977).

58. F.W. Byron, Jr. and L.J. Latour, Jr., Phys. Rev A13, 649(1976).

59. B.K. Thomas and E.Gerjuoy, J.Math. Phys.12, 1567(1971).

60. V.Franco, Phys. Rev. Lett. 26, 1088(1971).

61. J.E.Golden and J.H. McGuire, Phys. Rev.A12, 80(1975).

62. K.C.Mathur, A.N. Tripathi and S.K. Joshi, J.Phys. B4, L39(1971); Phys. Rev.A5, 746(1972).

63. H.R.J. Walters, J.Phys. B6, 1003(1973).

64. D.Leep and A.Gallagher, Phys. Rev.A10, 1082(1974).

65. M.H.Mittleman, Phys. Rev.A2, 1846(1970).

66. C.J. Joachain and M.H. Mittleman, Phys. Rev. A4, 1492(1971a); Phys. Lett. A36, 209(1971b).

67. M.L. Goldberger and K.M. Watson, Collision Theory (New York: Wiley, 1964), Chap.11.

68. A.L. Fetter and K.M. Watson, in Advances in Theoretical Physics, ed. K.A. Brueckner (New York: Academic Press, 1965), Vol.1, p.115.

69. M.R.C. McDowell, Phys. Rev.175, 189(1968).

70. T.Ishihara and J.C.Y.Chen, Phys. Rev. A12, 370(1975a).

71. P.J.O. Teubner, C.R.Lloyd and E.Weigold, J.Phys.B6, L134 (1973); Phys. Rev.A9, 2552(1974).

72. C.R.Lloyd, P.J.O. Teubner, E.Weigold and B.R.Lewis, Phys. Rev.A10, 175(1974).

73. J.F.Williams, J.Phys. B8, 2191(1975).

74. R.J. Glauber, Phys. Rev.91, 459(1953).

75. P.M. Morse and H.Feshbach, Methods of Theoretical Physics (New York: McGraw-Hill, 1953).

76. T.Adachi and T.Kotani, Prog. Theor.Phys., Supp.Extra, no.316(1965).

77. T.Adachi, Prog. Theor. Phys. 35, 463, 483(1966).

78. E.Predazzi, Ann. Phys. 36, 228, 250(1966).

79. K.Chadan, Nuovo Cimento B53, 12(1968).

80. J.C.Y.Chen and K.M. Watson, Phys. Rev.188, 236(1969).

81. J.C.Y.Chen and L.Hambro, J.Phys. B5, L199(1972).

82. J.C.Y. Chen, L.Hambro, A.L. Sinfailam and K.T.Chung, Phys. Rev.A7, 2003(1973).

83. E.Gerjuoy, Ann.Phys. 5, 586(1958b).

84. V.Franco and R.J.Glauber, Phys. Rev.142, 1195(1966).

85. F.W.Byron, Phys. Rev. A4, 1907(1971).

86. E.Gerjuoy, B.K. Thomas and V.B. Sheorey, J.Phys.B5, 321(1972).

87. H. Tai, R.H. Bassel, E.Gerjuoy and V.Franco, Phys.Rev.A1, 1819(1970).

88. D.M. Chase, Phys. Rev.104, 838(1956).

89. A.S.Ghosh and N.C.Sil, Indian J.Phys. 43, 490(1969); 44, 153(1970).

90. A.S.Ghosh, S.P.Sinha and N.C.Sil, J.Phys. B3, L58(1970).

91. H.Tai, P.J.Teubner and R.H.Bassel, Phys. Rev. Lett.22, 1415(1969); 23E,453(1969).

92. K.Bhadra and A.S.Ghosh, Phys. Rev. Lett.26, 737(1971).

93. V.Franco and B.K.Thomas, Phys. Rev.A4,945(1971).

94. V.Franco, Phys. Rev.Lett.20, 709(1968).

95. B.K.Thomas and V.Franco, Phys. Rev.A13, 2004(1976).

96. W.Magnus, F.Oberhettinger and R.P.Soni, Formulas and Theorems for the Special Functions of Mathematical Physics (New York: Springer-Verlag, 1966).

97. I.S.Gradshteyn and I.M. Ryzhtik, Table of Integrals, Series and Products (New York: Academic Press, 1965), 4th ed.

98. L.J.Slater, Confluent Hypergeometric Functions (Cambridge: University Press, 1960).

99. S.Kumar and M.K. Srivastava, Pramana (1977), to appear.

100. A.C.Yates and A.Tenney, Phys. Rev.A6, 1451(1972).

101. V.Franco, Phys. Rev.A1, 1705(1970).

102. V.Franco, Phys. Rev.A8, 2927(1973).

103. B.K. Thomas and F.T.Chan, Phys. Rev. A8, 252(1973).

104. F.T.Chan and S.T.Chen, Phys. Rev.A8, 2191(1973); A9, 2393(1974a); A10,1151(1974b).

105. F.T.Chan and C.H.Chang, Phys. Rev.A11, 1097(1975).

106. A.N. Tripathi, K.C.Mathur and S.K. Joshi, J.Chem.Phys. 58, 1384(1973a).

107. F.T.Chan and C.H.Chang, Phys.Rev.A14, 189(1976).

108. G.N. Watson, A.Treatise on the Theory of Bessel Functions (Cambridge: University Press, 1944).

109. E.Clementi, IBM J.Res. Dev.9, 2(1965).

110. L.N. G.Filon, Proc. Roy. Soc. Edinb.A49, 38(1928).

111. W.Williams, S.Trajmer and D.Bozinis, J.Phys.B9,1529(1976).

112. S.Kumar and M.K. Srivastava, Phys. Rev.A12, 801(1975).

113. P.M.Stone, Phys. Rev.141, 137(1966).

114. W.R.Ott, W.E.Kauppila and W.L. Fite, Phys. Rev.A1, 1089 (1970).

115. A.N. Tripathi, K.C.Mathur and S.K. Joshi, J.Phys.B6, 1431(1973b).

116. D.R.Flower and M.J.Seaton, Proc. Phys. Soc. (London), 91, 59(1967).

117. S.Kumar and M.K.Srivastava, Phys. Rev.A13, 1307(1976).

118. E.Hafner and H.Kleinpoppen, Z.Phys.198, 315(1967).

119. P.G.Burke and A.J.Taylor, J.Phys.B2, 869(1969).

120. N. Feautrier, J.Phys. B3, L152(1970).

121. P.McCavert and M.R.H. Rudge, J.Phys. B3, 1286(1970).

122. C.J. Joachain, Quantum Collision Theory (Amsterdam: North Holland, 1975), Chap.19-21.

123. C.J. Joachain and C.Quigg, Rev.Mod. Phys.46, 279(1974).

124. F.W.Byron, Jr. and C.J. Joachain, Phys. Rev.A9, 2559 (1974a).

125. F.W.Byron, Jr. and C.J.Joachain, Proc. Int. Symp.on Electron and Photon Interactions with Atoms, Stirling, p.19(1974c).

126. R.Vanderpoorten, J.Phys.B8, 926(1975).

127. F.W.Byron and C.J.Joachain, Phys. Rev. A15, 128(1977b).

128. C.J.Joachain, R. Vanderpoorten, K.H. Winters and F.W. Byron, Jr., J.Phys.B10, 227(1977).

129. J.C.Slater, Phys. Rev.81, 385(1951).

130. E.Bauer and H.N. Browne, Atomic Collision Processes ed M.R.C. McDowell (Amsterdam: North Holland, 1964),p.16.

131. M.H. Mittleman and K.M. Watson, Ann.Phys., N.Y.10,268 (1960).

132. M.E.Riley and D.G.Truhlar, Phys. Rev.(1976), to appear.

133. J.B.Furness and I.E.McCarthy, J.Phys. B6, 2280(1973).

134. B.H.Bransden and C.J.Noble, J.Phys.B9, 1507(1976).

135. B.H. Bransden, M.R.C. McDowell, C.J. Noble and T.Scott, J.Phys.B9, 1301(1976).

136. R.A.Buckingham, Proc. Roy. Soc.A160, 94(1937).

137. H.A.Bethe and E.E.Salpeter, Handb.Phys. ed S.Flugge (Berlin: Springer-Verlag, 1957).

138. S.Kumar, M.K.Srivastava and A.N. Tripathi, J.Phys.B8 , 612(1975a).

139. D.P.Sural and N.C.Sil, Proc. Phys. Soc. (London), 87, 201(1966).

140. S.Kumar, A.N. Triatphi and M.K. Srivastava, J.Phys.B8, 1082(1975b).

141. A.Birman and S.Rosendorff, J.Phys. B9, L189(1976).

142. J.C.Y.Chen, C.J. Joachain and K.M. Watson, Phys.Rev.A5, 2460(1972).

143. R.N. Madan, Phys. Rev. A11, 1968(1975).

144. S.Kumar and M.K.Srivastava, J.Phys.B9, 1911(1976).

145. H.Narumi and A.Tsuji, Prog. Theor. Phys.53, p.671(1975).

146. T.Ishihara and J.C.Y. Chen, J.Phys. B8, L417(1975b).

147. J.Gau and J.Macek, Phys. Rev.A10, 522(1974); A12, 1760(1975)

148. G.Foster and W.Williamson, Jr., Phys. Rev.A13, 936, 1265, 2023(1976).

149. W.Williamson, Jr. and G.Foster, Phys. Rev.A11, 1472(1975).

150. E.J.Kelsey and J.Macek, Phys.Rev.A12, 1127(1975).

151. S.Kumar, Archana Gupta and M.K.Srivastava, Phys.Rev.A14 (1977), to appear.

152. B.L.Moiseiwitsch and A.Williams, Proc. Roy. Soc.(London) A250, 337(1959).

153. A.Birman and S.Rosendorff, Nuovo Cim.B63, 89(1969).

154. A. Tenney and A.C. Yates, Chem. Phys. Lett.17, 324(1972).

155. K.C.Mathur, Phys. Rev.A9, 1220(1974).

156. J.H.McGuire, M.B.Hidalgo, G.D.Doolen and J.Nuttall, Phys. Rev.A7, 973(1973).

157. A.Tsuji, A.Miyamoto and H.Narumi, Prog. Theor. Phys.50, 338(1973).

158. H.Narumi, A.Tsuji and A.Miyamoto, Prog.Theor. Phys.54, 740(1975).

159. A.K.Jain and M.K. Srivastava, J.Phys.B9, 1103(1976).

160. J.Macek (private communication).

161. Y.L. Luke, Handbook of Mathematical Functions eds. M. Abramovitz and I.A.Stegun (New York:Dover).