CHAPTER - I

INTRODUCTION

The analysis of scattering phenomena plays an important role in numerous scientific and technical fields like astrophysics, aeronomy, gas lasers, controlled thermonuclear fusion, biophysics, aurora, air glow, chemical composition etc. Elastic and inelastic cross - sections for electron and photon scattering by atoms and molecules are required for the study of the energy spectrum of secondary electrons ejected during the bombardment of the upper atmosphere by electrons, ions, cosmic particles and electromagnetic radiation in the UV and X-ray region. This information in turn gives an idea of the chemical composition, temperature and density of the constituents of the upper atmosphere. Auroral and airglow emissions are visual manifestations of the scattering processes in the atmosphere.

In laser systems, the electron impact excitation of various modes of CO_2 molecule and other species are required to be known. The mechanism for the cooling of interstellar gases can be understood through collisional process. Accurate cross-sections

are also necessary if plasma heating is done by injection of fast neutral particles into the beam.

Various parameters dependent on collision cross sections, like the stopping power and mean energy expended per ion pair etc are required to estimate the necessary radiation dose and duration of exposure in radiation therapy. In the present day energy crisis, the magneto hydro dynamic (MHD) generators have their own significance. Some alkali atoms like caesium are used in it. The study of the collision process is an important design parameter in such uses. Collisional cross-sections are required to monitor the impurity content introduced in fusion plasma due to its striking the container walls on cooling off. Fast electron scattering can be used as a probe to map the charge distribution within the target atoms and molecules. The electrical conductivity of an ionised gas depends on the number of free electrons and their frequency of collision with molecules. The frequency in turn, depends on the momentum transfer cross-section. These manifold applications make atomic and molecular collision physics a very important subject of experimental and theoretical investigations.

In a typical scattering experiment, a well defined collimated homogeneous beam of mono energetic projectile is directed towards a target from a large distance. After the impact, the particles of the incident beam are scattered in all directions and their angular distribution is observed at large distances from the scatterer. The number of particles scattered into the detector per unit solid angle per unit time per unit incident flux is called the differential cross-section for that particular directions. The integration of the differential cross-sections over all solid angles yields the total collisional cross-sections.

All the scattering processes can be classified into 3 broad catagories namely, the elastic, inelastic and super elastic. The scattering process in which the internal states and structures of the colliding particles do not change are characterised as elastic. If the internal states and/or the structurer of the colliding particle change, the collision is called inelastic. The super elastic collision is one in which the incident particle gains some energy from the target. The probability of observing a certain final state out of the infinite set of possible states belonging to the above 3 categories is usually

expressed in terms of the collision cross-sections which can be determined by means of the quantum collision theory.

To calculate collision cross-sections exactly, we need accurate knowledge of relevant interactions. The interaction can be decomposed to a good approximation, into the following parts, static, polarisation, exchange and absorption. The static part of the interaction is the electrostatic interaction between the incident charged particle and the undeformed charge distribution of the target. The polarisation interaction comes from the deformation of the atomic charge cloud by the approach of the point charge of the incident particle. If the incident particle is an electron, then its indistinguishability from the target electron gives rise to exchange interaction. The effect of inelastic processes on the elastic scattering are termed the absorption effects which arise in the energy region where the inelastic channels are open.

An exact evaluation of schrodinger equation corresponding to particular scattering process is a formidable task even if the interaction potential is known . This is because the exact wave functions of

target atoms except hydrogen and hydrogenic ions are not known. However, even if the wave functions of the atoms are known, the schrodinger equation contains infinite set of coupled integro - differential equations which can not be exactly solved even with the fast digital computers. In view of the limitations of obtaining the exact analytical solution of a many body problem in the quantum mechanical frame work, approximate methods acquire paramount importance. To date no single theory is available which can give uniformly satisfactory results at all impact energies. It has been a usual practice to divide the incident impact energies into 3 regions-low, intermediate and high. The energy region lying below the first excitation threshold of the target is taken as the low energy region. The energies at which the first Born approximation gives reliable results belong to the high energy region. The energy region lying between the two is referred to as the intermediate energy region. Different approximations are then devised to explain the scattering process in these energy regions. A detailed account of the numerous approximate methods can be obtained from a no. of books, reviews and selected papers (Bates, 1962 ; Mott and Massey, 1965 ; Massey et al 1969 . Moiseiwitsch and Smith 1968; Rudge 1968 ;

Gerjuoy and Thomas, 1974 ; Walters, 1976a ; Joachain, 1977 ; Burke and Williams, 1977 ; Byron and Joachain, 1977a ; Bransden and McDowell, 1977,1978 ; Ishihara, 1978 ; Jhanwar et al, 1978a ; Burke, 1979 ; Lane, 1980 ; Joachain, 1980 ; Kessler, 1982 ; Schwenke et al, 1983 ; Staszewska et al, 1984). Our area of interest is confined to the elastic scattering of electrons by atoms in the intermediate energy region. All the physical concepts described thus far can be seen to arise from a rigorous mathematical formulation of the scattering problem. We now proceed to formulate the collision problem in a mathematical frame work.

Let us consider the scattering of an electron by a neutral atom of atomic number Z . The spatial co-ordinates of the incident particle and the atomic electrons denoted by $\underline{r}$ and $\underline{r}_i$ (i = 1, 2, 3,...., Z) refer to the atomic nucleus which is taken as the origin of our co-ordinate system. The non-relativistic, time - independent schrodinger equation for the system is

$$(H - E) \Psi (\underline{x}, \underline{x}_i) = 0 \qquad (1.1)$$

where H is the Hamiltonian of the system, E is the total energy of the system and $\Psi (\underline{x}, \underline{x}_i)$ is the wave function of the system.

The initial state of the system is given as

$$\phi_{ki}(\underline{r},\underline{r}_i) = (2\pi)^{-3/2} e^{i\underline{k}_i\cdot\underline{r}} \cdot \phi_i(\underline{r}_i) \qquad (1.2)$$

The interaction potential between the incident particle and the target atom is given by

$$V(r,r_i) = Q\left[\frac{Z}{r} - \sum_{i=1}^{Z} \frac{1}{|\underline{r} - \underline{r}_i|}\right]. \qquad (1.3)$$

The solution of (1.1) denoted by $\psi(r,r_i)$ satisfies the boundary condition

$$\psi(\underline{r},\underline{r}_i) \longrightarrow (2\pi)^{-3/2}\left[e^{i\underline{k}_i\cdot\underline{r}}\phi_i(\underline{r}) + \sum_n f_{ni}(\theta,\phi)\, e^{i\underline{k}_i\cdot\underline{r}}\phi_n(\underline{r}_i)\right], \qquad (1.4)$$

where $f(\theta,\phi)$ is the scattering amplitude.

The differential cross section (DCS) can be written as

$$\frac{d\sigma}{d\omega} = \frac{k_f}{k_i} |f(\theta,\phi)|^2 \qquad (1.5)$$

For the elastic scattering $|\underline{k}_f| = |\underline{k}_i| = k$.

The DCS for elastic scattering becomes

$$\frac{d\sigma}{d\omega} = |f(\theta,\phi)|^2. \qquad (1.6)$$

The total collisional cross-sections (TCS) are obtained from the optical thorem

$$\sigma^{tot} = \frac{4\pi}{k_i} \; I_m \; f\,(\,\theta = 0\,). \qquad (1.7)$$

For the study of any collision problem DCS and TCS are the key quantities which can be determined by solving (1.1). The exact solution of it is a formidable task. There are 2 approaches in which this equation is solved for any collision problem. One is a differential equation approach, non-iterative in nature and another is an integral equation approach which is iterative. In the differential equation approach one has to solve infinite no. of coupled integro - differential equations, whereas in the integral equation approach summation over infinite number of terms is required. Various approximations have been devised to obtain the wave function and hence the scattering amplitude. Now a brief account of those various approximate methods which are relevent for the present dissertation is considered.

Born Series Expansion : The differential equation(1.1) can be solved using the Green's function technique to obtain a formal solution for the wave function $\psi(\underline{r},\underline{r}_i)$ in the form, of an integral equation, known as Lippmann Schwinger equation, given as

$$| \psi_{ki}^{+} > = | \phi_{ki} > + G_o^{+} V | \psi_{ki} > , \qquad (1.8)$$

G_o^+ represents the out going Green's function for the unperturbed system and has the form

$$G_o^+ (\underline{r}, r_i, \underline{r}', r_i') = - \frac{1}{2\pi} \sum_n \frac{e^{ik_f|\underline{r} - \underline{r}'|}}{|\underline{r} - \underline{r}'|} \phi_n(\underline{r}_i')\phi_n(\underline{r}_i) \qquad (1.9)$$

in the configuration space. Here $\phi_n(\underline{r})$ is the eigen of the target atom.

$$G_o^+ (\underline{r}, \underline{r}_i, \underline{r}', r_i) = - 2 \times (2\pi)^{-3} \sum_n \int \frac{dq_1 \exp [iq_1.(\underline{r} - \underline{r}')]}{q_1^2 - k_n^2 - i\epsilon} \times \phi_n^*(\underline{r}_i)\phi_n(\underline{r}_i) \qquad (1.10)$$

where q_1 is an intermediate momentum and

$$k_n^2 = k_i^2 - 2 (\epsilon_n - \epsilon_i) \qquad (1.11)$$

substituting (1.9) in (1.8) and compairing the asymptotic expansion of the resultant with(1.4) one obtains a general expression for the scattering amplitude as

$$f_{ni} (\hat{\underline{k}}_i , \hat{\underline{k}}_f) = - (2\pi)^2 < \phi_{kf} | V | \psi_{ki}^+ > \qquad (1.12)$$

The integral equation (1.8) when solved by iteration and substituted in (1.12) gives the Born series expansion for the direct scattering amplitude given as

$$f_{ni}\left(\hat{\underline{k}}_i, \hat{\underline{k}}_f\right) = -(2\pi)^2 \langle \phi_{k_f} | V + V G_o^+ V + V G_o V G_o^+ + | \phi_{k_i} \rangle$$

$$= \sum_{j=1}^{\infty} \bar{f}_{Bj} \qquad (1.13)$$

where $$\bar{f}_{Bj} = -(2\pi)^2 \langle \phi_{k_f} | V \sum_{p=0}^{j} (G_o^+ V)^p | \bar{\phi}_{k_i} \rangle \qquad (1.14)$$

The n^{th} Born approximation to the scattering amplitude is defined as

$$f_{Bn} = \sum_{j=1}^{n} \bar{f}_{Bj} \qquad (1.15)$$

The first Born amplitude for a large no. of charged particle - atom elastic and inelastic scatt-ering processes had calculated by Bell and Kingston (1974). For the elastic scattering the first Born amplitude is given by

$$f_{B1} = -\frac{1}{2\pi} \int e^{i\underline{q}.\underline{r}} \langle \phi_i |V| \phi_i \rangle \, \underline{dr} \qquad (1.16)$$

The first Born approximation (FBA) for elastic scattering is thus just the elastic scattering by the static field of an atom. The FBA is valid for heavier atom for higher energies.

A better way to include the polarisation, absorption and distortion of the incident particle in comparision of FBA, is the second Born approximation ;

$$f_{B_2} = f_{B1} + \bar{f}_{B2} \tag{1.17}$$

with $$\bar{f}_{B2} = -(2\pi)^2 \langle i, \underline{k}_f | V G_o^+ V | i, \underline{k}i \rangle \tag{1.18}$$

where we have denoted $| \phi_{\underline{k}_i} \rangle$ by $|i, \underline{k}_i \rangle$ and $| \phi_{\underline{k}_f} \rangle$ by $|i, \underline{k}_f \rangle$. Substituting G_o^+ from (1.10) we obtain

$$\bar{f}_{B2} = 2(2\pi)^2 \sum_n \int \frac{d\underline{q}_1 \langle i, \underline{k}_f | V | n, q_1 \rangle \langle n, \bar{q}_1 | V | i, \underline{k}_i \rangle}{q_1^2 - k_n^2 - i\epsilon} \tag{1.19}$$

where $$|n, \bar{q}_1 \rangle = \frac{1}{(2\pi)^{3/2}} e^{i \underline{q} \cdot \underline{r}} \phi_n(\underline{r}_i) . \tag{1.20}$$

The integration over the plane wave parts of the matrix elements yields

$$\bar{f}_{B2} = \frac{2Q^2}{\pi^2} \sum_n \int \frac{d\underline{q}_1}{K_i^2 K_f^2} \frac{\langle i | \sum_{i=1}^{z} (e^{i\underline{k}_i \cdot \underline{r}_i} - 1) | n \rangle \langle n |}{q_1^2 - k^2 + 2(\epsilon_n - \epsilon_i) - i\epsilon}$$

$$x \sum_{j=1}^{z} (e^{-i\underline{K}_f \cdot \underline{r}_j} - 1) \, |i> \qquad (1.21)$$

with $\underline{K}_i = \underline{k}_i - q_1$ and $\underline{K}_f = \underline{k}_f - q_1$ (1.22)

The simplest way of solving the above expression is the simplified Second Born approximation (SSB) used by Holt and Moisciwitch (1968). They replaced $(\epsilon_n - \epsilon_i)$ by a mean excitation energy and performed the summation using the closure relation. Thus under SSB approximation we obtain

$$f_{SB2} = \frac{2}{\pi^2} \int \frac{d\underline{q}_1}{K_i^2 K_f^2 (q_1^2 - p^2 - i\epsilon)}$$

$$<i \mid \sum_{i=1}^{z} \sum_{j=1}^{z} (e^{i\underline{K}_i \cdot \underline{r}_i} - 1)$$

$$x \, (e^{-i\underline{K}_f \cdot \underline{r}_j} - 1) \mid i> \qquad (1.23)$$

where $p^2 = k^2 - 2\delta$.

Various modes of the second Born amplitude can be obtained from the work of Byron and Joachain (1973, 1977), Gosh (1977), Tayal et al (1979), Yates (1979) and Kingston and Walters (1980). Special mention should

be made about the High energy higher order Born (HHOB) approximation which will be elaborated upon in a later section.

Glauber Series Expansion

The Glauber approximation belongs to the class of Semiclassical eikonal approximations. The basic assumptions for such approximations are that (a) the energy of the incident particle greatly exceeds the magnitude of the potential and (b) the particle wavelength (proportional to k^{-1}) is much smaller than the range 'a' of the potential. Under these conditions, the Lippmann Schwinger equation can be linearised and this procedure leads to the eikonal scattering wave function.

$$\phi_{(r)} = (2\pi)^{-3/2} \exp\left(i\underline{k}_i \cdot \underline{r} - \frac{1}{2k_i} \int_{-\infty}^{z} U(x,y,z')dz' \right) \qquad (1.24)$$

This shows that a simple modification of the phase of the incident plane wave leads to the eikonal wave function. The eikonal Scattering amplitude is obtained as (Jochain 1975)

scattering amplitude is obtained as (Jochain 1975)

$$f_E = \frac{k_i}{2\pi i} \int d^2 \underline{b} \ \exp (i \ \underline{q}.\underline{b}) \ \exp [i \ X \ (\underline{k}_i.\underline{b})-1 \ ] \qquad (1.25)$$

where b is the impact parameter and

$$X = - \frac{1}{2k_i} \int_{-\infty}^{\infty} U (b, z) \ d_z \qquad (1.26)$$

is called the eikonal phase shift function.

The many-body generalisation of the above treatment was done by Glauber (1959). For the direct collision of an electron with a target containing fixed scatterer, the Glauber scattering amplitude is

$$f_G = \frac{k_i}{2\pi i} \int d^2 \underline{b} \ \exp(i \ \underline{q}.\underline{b}) < f \ | \ \exp (i \ X_G \ ) - 1 | i > \qquad (1.27)$$

where q is assumed to be 2 dimensional and d^2 b is an element of area in the (x, y) plane.

The Glauber phase

$$X_G = X_G \ (\ \underline{b}, \ \underline{r}_i \ ) \qquad (1.28)$$

The Glauber phase has a complicated expression so that the evaluation of (1.27) becomes very difficult except for H and He . Thomas and Gerjuoy (1971) have obtained the closed form expressions for the Glauber amplitude for the collision of charged particles with

hydrogen atom. Of the various attempts made to evaluate the Glauber amplitude Glauber eikonal series (GES) method is significant. In this method (Yates 1974), the Glauber amplitude is written in the form of a series

$$f_G = \sum_{n=1}^{\infty} i^{n-1} f_{Gn} \qquad (1.29)$$

More about the GES method will be discussed in later section devoted for it.

Glauber eikonal series (GES) Method :

The GES , proposed by Yates (1974), is an analytical procedure capable of providing quantitative estimates of the Glauber cross section.

Glauber's multiparticle amplitude formula is given as

$$f_{i \to f}(\underline{q}, \underline{k}_i)' = \frac{i\, k_i}{2\pi} \int \underline{db}_o \exp(i\, \underline{q}.\underline{b}_o) \langle \psi_f \mid 1 - \exp(i\, x) \mid \psi_i \rangle \qquad (1.30)$$

Franco (1971) and Thomas and Chan (1973) had reduced the above formula to a one dimensional integral expression and found out the DCS. But their proceedures still requires a good deal of computational analysis before arriving at the final results.

Yates had proposed a method involving the expansion of the amplitude in reciprocal powers of k_i for fixed $q = |\underline{q}|$ and done a term wise analysis of the amplitude expression. Others works relevant to the development of this theory included that of Byron and Joachain (1973) and Yates (1973).

Expansion of the phase function e^{ix} in equation (1.30) gives

$$f_{i\to f} = \sum_{n=1}^{\infty} i^{n-1} f_{i\to f}^{(n)} \qquad (1.31)$$

where $$f_{i\to f}^{(n)} = \frac{k_i}{2\pi n!} \int d\underline{b}_o \; e^{i\underline{q}.\underline{b}_o} \langle \psi_f | x^n | \psi_i \rangle \qquad (1.32)$$

Hence for fixed q, the differential cross section through order $\left(\frac{1}{k_i^2}\right)$ is

$$\sigma_{i\to f} = \frac{k_f}{k_i} \left(f_{i\to f}^{(1)} \right)^2 + \left(f_{i\to f}^{(2)} \right)^2 - 2 f_{i\to f}^{(1)} f_{i\to f}^{(3)} + O\left(\frac{1}{k_i^4}\right) \qquad (1.33)$$

which suggests that for large k_i, only few terms in equation (1.31) are required to obtain good estimates of th e Glauber cross sections. The Glauber phase function is

$$X(b_o \ldots\ldots b_N) = \frac{Z}{k_i}\int_{-\infty}^{\infty} dz_o \left[\frac{N}{r_o} - \sum_{i=1}^{N}\frac{1}{|\underline{r}_o - \underline{r}_1|}\right] \qquad (1.34)$$

By using a transformation similar to that used by Tenney and Yates (1972), the X is transformed to obtain a convenient form of $f^{(n)}_{i->f}$. For this $\frac{1}{r_o}$ and $\frac{1}{|\underline{r}_o - \underline{r}_1|}$ are replaced by their 3 - dimensional Fourier integral representations.

$$\therefore X(b_o - - - - b_N) = \frac{-z}{2\pi^2 k_i}\sum_{j=1}^{N}\int\frac{dp'}{p'} \; 2\int_{-\infty}^{\infty} dz_o\, e^{-i\underline{p}'\cdot\underline{r}_o} \times [1 - e^{i\underline{p}'\cdot\underline{r}_j}]$$

$$= -\frac{z}{\pi k_i}\int\frac{dp}{p^2}\, e^{-i\underline{p}\cdot\underline{b}_o}\, B(\underline{p}, \underline{b}_1 - \underline{b}_N) \qquad (1.35)$$

where $\underline{p}' = \underline{p} + \underline{p}_z k_i$.

Substitution of (1.35) in (1.32) and further simplification gives

$$f^{(n)}_{i->f} = \frac{2\pi k_i}{n!}\left(\frac{-z}{\pi k_i}\right)^n \int\frac{dp_1}{p_1^2} - - - - - \int\frac{dp_{n-1}}{p_{n-1}^2 |\underline{q}-\underline{p}|^2}$$

$$\langle \psi_f \mid B(\underline{p}_i) - - - - B(\underline{p}_{n-1})\, B(\underline{q}-\underline{p}) \mid \psi_i \rangle \qquad (1.36)$$

Here $B(p_i) = B(p_i, b, \text{---} b_N)$; $\underline{p} = \sum_{i=1}^{n-1} \underline{p}_i$

For chosen co-ordinate system,

$f^{(1)}_{i->f}$ = first born amplitude

$$f^{(2)}_{i->f} = \frac{z^2}{\pi k_i} \int \frac{d\underline{p}}{p^2 |\underline{q} - \underline{p}|^2} \langle \psi_f \mid B(\underline{p})\, B(\underline{q}-\underline{p}) \mid \psi_i \rangle \quad \text{and so on} \qquad (1.37)$$

Hence $f^{(n)}_{i->f}$ becomes much simpler due to the uncoupling of b_o and b_i's as a result of the transformation given by (2.41).

Yates had shown the feasibility and simplicity of the above method by applying it to electron - hydrogen scattering. The DCS obtained was compared with the exact glauber result of Thomas and Gerjuoy. It was shown that if the inequality $k_i >> 1$ was only marginally satisfied, the first 3 terms of the GES are sufficient to give good representation of the Glauber cross sections for all values of q.

Later on Singh and Tripathi (1980) used the GES method to analyse the scattering of electrons by He atom. Even though the GES method, represents the Glauber Scattering amplitude satisfactorily it is not free from the short comings associated with the Glauber method - i.e. , logarithmic divergence in forward direction and low cross section values. As mentioned earlier, many efforts were so far made to improve upon the Glauber approximation. One of the prominent effort was Wallace correction (Wallace 1973). The details of this will be given in a later Chapter of the thesis.

The High energy Higher order Born approximation (HHOB) :

This was developed by Yates in 1979 . The primary purpose of this analysis was to develop an alternative high energy expression for differential scattering cross section in terms of reciprocal powers of k_i through $O(\frac{1}{k_i^2})$.

In the HHOB analysis the well known generalised Born Series description of the collision process was transformed into a more convenient form. Thereafter, the approximate formulae were developed through a partial expansion of the free particle Green's function. The second Born term can be written as

$$f^{(2)}_{i->f} = \frac{1}{\pi} \sum_n \int d\underline{r}_o \; e^{i\underline{q}\cdot\underline{r}_o} \; V_{fn}(\underline{r}_o) \int d\underline{r}_o' \; G_n(\underline{r}_o') \; V_{n_i}(\underline{r}_o - \underline{r}_o') \; e^{-ik_i\cdot r_o'} \quad (1.38)$$

where

$$V_{nm}(\underline{r}_o) = \langle \psi_n(\underline{r}_1 - - -, \underline{r}_N) \mid V(r_o, r_1, - - -, r_N) \mid \psi_m(\underline{r}_1, - - - - - -, \underline{r}_N) \mid \rangle,$$

and

$$G_m(\underline{r}_o - \underline{r}_o') = \frac{1}{(2\pi)^3} \int \frac{d\underline{k}' \; e^{i\,\underline{k}'\cdot(\underline{r}_o - \underline{r}_o')}}{k'^2 - k_m^2 - i\epsilon},$$

$$\epsilon \longrightarrow 0^+ \quad (1.39)$$

Now the second Born term is partially expanded parallel to the method of Glauber which is most akin to the high energy small angle potential scattering analysis of schiff. The basic approximations were introduced in the integral.

$$I_n = \int d\,\underline{r}_o' \; G_n(\underline{r}_o') \; V_{n_i}(\underline{r}_o - \underline{r}_o') \; e^{-i\underline{k}_i\cdot\underline{r}_o'} \quad (1.40)$$

Here, the variable transformation

$\underline{S} = \underline{k}' - \underline{k}_n$ was made. If it is assumed that $V_{\underline{r}_i}$ is

slowly varying over the distance of a wavelength of the scattering electrons and that $\underline{k}_n$ does not differ greatly from k_i in either magnitude or direction, then the principal contribution to the $\underline{r}_o'$ integral occurs for small S. Hence, after performing the the $\underline{S}$ integration in cylindrical polar co-ordinates by choosing $\underline{k}_n$ as the pola r axis,

$$I_n = \frac{i}{2k_n} \int d\underline{r}_o' \; e^{-i(\underline{k}_i - \underline{k}_n).r_o'} \; V_{n_i}(\underline{r}_o - \underline{r}_o') \left[\delta(\underline{b}_o') \; H(z_o') + \frac{i}{2k_n} \nabla^2_{r_o'} \left\{ \delta(\underline{b}_o') \; z_o' \; H(z_o') + O(k_n^{-2}) \right\} \right] \qquad (1.41)$$

where $H(z)$ is the Heaviside function. Again integrating the second term of the above equation by parts twice and simplifying further,

$$I_n = \frac{i}{2k_i} \int_{-\infty}^{\infty} dz_o' \; e^{-i \beta_{in} z_o'} \; H(z_o') \left[1 + \frac{i z_o}{2k_i} \nabla^2_{\underline{r}_o'} \right] V_{n_i}(\underline{r}_o - \underline{r}_o') \mid \underline{b}' = 0, \qquad (1.42)$$

where $\beta_{in} = k_i - k_n \simeq \Delta E \; / \; k_i$, ΔE is the average excitation energy.

In simplifying the present approximations, it is better to express the interaction potential in Fourier form as

$$V(\underline{r}_o , \underline{r}_1, - - - - - , \underline{r}_N) = \int d\underline{p}\ e^{-i\underline{p}\cdot\underline{b}_o} \times \int_{-\infty}^{\infty} dp_z\ e^{-ip_z z_o}\ \bar{V}\ (\underline{p}+p_z\hat{y}, \underline{r}_1 - - - -,\underline{r}_N) \qquad (1.43)$$

where

$$\bar{V}\ (\underline{p} + p_z\hat{y},\underline{r}_1- - - -\underline{r}_N) = \frac{1}{2\pi^2(p^2 + p_z^2)} \sum_{j=1}^{N} (e^{i\underline{p}\cdot\underline{b}_j} e^{ip_z z_j} - 1) \qquad (1.44)$$

Substitution of (1.42) in (1.41), we get

$$f^{(2)}_{HEA} = \frac{i}{2\pi k_i} \int d\underline{r}_o\ e^{i\underline{q}\cdot\underline{r}_o} \langle \psi_f \mid V(\underline{r}_o,- - -\underline{r}_N) \int_{-\infty}^{\infty} d z_o'\ H(z_o')\ e^{-i\beta_i z_o'} \times [V(\underline{r}_o - z_o'\hat{y} , \underline{r}_1 - - - - \underline{r}_N) + \frac{i z_o'}{2k_i} \nabla^2_{r_o'}\ V(\underline{r}_o - \underline{r}_o' , \underline{r}_1---\underline{r}_N)|_{b'=0} \mid \psi_i \rangle \qquad (1.45)$$

Now, on using equation (1.43) and carrying out the ∇^2 operation, the preceeding result can be written as

$$f^{(2)}_{HEA} = \frac{i}{2\pi k_i} \int d\underline{p} \int_{-\infty}^{\infty} dp_z \int d\underline{p}' \int_{-\infty}^{\infty} dp_z' \, \langle \psi_f \, | \, \bar{V}(\underline{p} + p_z \hat{y}, \ldots, \underline{r}_N) \, \bar{V}(\underline{p}' + p_z' \hat{y}, \ldots \ldots, \underline{r}_N) \, | \, \psi_i \rangle \times \int d\underline{b}_o \, e^{i(\underline{q} - \underline{p} - \underline{p}') \cdot \underline{b}_o} \int_{-\infty}^{\infty} d_{zo} \, e^{-i(p_z + p_z')_{zo}} \left(1 + \frac{p'^2 + p_z'^2}{2k_i}\right) \frac{\partial}{\partial \beta_i}) \int_{-\infty}^{\infty} d_{zo}' \, e^{-i(p_z' - \beta_i)_{zo}'} H(zo')$$

$$= \frac{4\pi^3}{k_i} \left[i \int d\underline{p} \left(1 + \frac{1}{2k_i} \frac{\partial}{\partial \beta_i}(p^2 + \beta_i^2)\right) U^{(2)}_{fi}(\underline{q} - \underline{p} - \beta_i \hat{y}, \underline{p} + \beta_i \hat{y}) - \frac{1}{\pi} \mathcal{P} \int d\underline{p} \int dp_z \left(1 + \frac{p^2 + p_z^2}{2k_i} \frac{\partial}{\partial p_z}\right) \frac{1}{p_z - \beta_i} U^{(2)}_{fi}(\underline{q} - \underline{p} - p_z \hat{y}, \underline{p} + p_z \hat{y}) \right]$$

where $\mathcal{P}$ means the principal value and

$$U^{(2)}_{fi}(\underline{p} + p_z \hat{y}, \underline{p}' + p_z' \hat{y}) = \langle \psi_f \, | \, \underline{V}(\underline{p} + p_z \hat{y}, \underline{r}_1 \ldots\ldots\ldots \underline{r}_N)$$

$$\bar{V}\left(\underline{p}' + p_z' \hat{y}\,,\ \underline{r}_1 \cdots\cdots \underline{r}_N\right) |\psi_i\rangle$$

(1.46)

In arriving at the final form of equation (1.46) it has been necessary to use the usual integral representations of the one and two dimensional δ functions and the additional result

$$\int_{-\infty}^{\infty} dx\ e^{-i\alpha x} H(x) = \pi \delta(\alpha) - i \mathcal{P}\left(\frac{i}{\alpha}\right)$$

The real and imaginary parts of $f^{(2)}_{HEA}$ are

$$\mathrm{Re}\, f^{(2)}_{HEA} = -\frac{4\pi^2}{k_i} \mathcal{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{p_z - \beta_i} U^{(2)}_{fi}\left(\underline{q} - \underline{p} - p_z \hat{y}\,,\ \underline{p} + p_z \hat{y}\right) - \frac{2\pi^2}{k_i^2} \frac{\partial}{\partial \beta_2} \mathcal{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z\,(p^2 + p_z^2)}{p_z - \beta_i} U^{(2)}_{f_i}\left(\underline{q} - \underline{p} - p_z \hat{y}\,,\ \underline{p} + p_z \hat{y}\right)$$

(1.47)

and

$$I_m f^{(2)}_{HEA} = \frac{4\pi^3}{k_i} \int d\underline{p}\, U^{(2)}_{f_i}\left(\underline{q} - \underline{p} - \beta_i \hat{y}\,,\ \underline{p} + \beta_i \hat{y}\right)$$

(1.48)

If β_i is set equal to zero in real part of $f^{(2)}_{HEA}$ the first term becomes zero and the leading

term is proportional to $\frac{1}{k_i^2}$. Similarly, the imaginary part of $f^{(2)}_{HEA}$ identically becomes Glauber's estimate of the second Born term.

Das Method

Das (1978) has suggested a method for computing scattering amplitudes and total cross sections. In this method he started from the Fredholm integral equation for the scattering amplitude. The Fredholm integral equation is the another way of representation of the Born series. The amplitude for scattering from intial state O to final state f can be written as

$$f_{f_o}(\hat{\underline{k}}_f, \hat{\underline{k}}_o) = -(2\pi)^2 \langle \Phi_{k_f}(\underline{r}, \underline{r}_j) \mid V_{int}(\underline{r}, \underline{r}_j) \mid \Phi_{k_o}(\underline{r}, \underline{r}_j) \rangle - (2\pi^2) \langle \Phi_{k_f}(\underline{r}, \underline{r}_j) \mid V_{int}(\underline{r}, \underline{r}_j) G_o^{+} V_{int}(\underline{r}', \underline{r}'_j) \mid \psi_o^{+}(\underline{r}', \underline{r}'_j) \qquad (1.49)$$

The substitution of G_o^{+} from (1.10) yields

$$f_{fo}(\hat{\underline{k}}_f, \hat{\underline{k}}_o) = f^{Bl}_{fo}(\hat{\underline{k}}_f, \hat{\underline{k}}_o) + (2\pi)^2 \frac{2}{(2\pi)^3} \sum_n \int$$

$$\phi^{*}_{kf}(\underline{r},\underline{r}_j)\times V_{int}(\underline{r},\underline{r}_j)\exp[i\underline{q}(\underline{r},\underline{r}')]\phi_n(\underline{r}_j')\phi(\underline{r}_j)$$

$$\times V_{int}(\underline{r}',\underline{r}_j')\psi_o(\underline{r}',\underline{r}_j')d\underline{r}\int^{\pi} dr_j \int^{\pi} dr_j' \, d\underline{q}\, d\underline{r}'$$

$$\frac{}{q^2 - k_n^2 - i\epsilon}$$

$$= f^{Bl}_{fo}(\hat{\underline{k}}_f, \hat{\underline{k}}_o) + \frac{1}{\pi}\sum_n \phi^{*}_{kf}(\underline{r},\underline{r}_j)V_{int}(\underline{r},\underline{r}_j)e^{i\underline{q}\cdot\underline{r}}\times\phi_n(\underline{r}_j)d\underline{r}\, d\underline{r}_j$$

$$\times \int e^{-i\underline{q}\cdot\underline{r}'}\phi^{*}_n(\underline{r}_j') \, V_{int}\frac{(\underline{r}',\underline{r}_j')\psi_o^{+}(\underline{r},\underline{r}_j)d\underline{r}\, d\underline{r}_j'\, d\underline{q}}{q^2 - k_n^2 - i\epsilon}$$

$$= f^{Bl}_{fo}(\hat{\underline{k}}_f,\hat{\underline{k}}_o) + \frac{1}{\pi}\frac{(2\pi)^3}{(4\pi^2)^2}\sum_n \int \frac{d\underline{q}}{q^2 - k_n^2 - i\epsilon}$$

$$\times [-(4\pi^2)\int \phi_{k_f}(\underline{r},\underline{r}_j)\, V_{int}(\underline{r},\underline{r}_j)\,\phi_{k_n}(\underline{r},\underline{r}_j)d\underline{r}\, d\underline{r}_j]$$

$$\times [-(4\pi^2)\int \phi^{*}_{k_n}(\underline{r}',\underline{r}_j')\, V_{int}(\underline{r}',\underline{r}_j')\psi_o^{+}(\underline{r}', r_j')d\underline{r}'\, dr_j']$$

$$= f^{Bl}_{fo}(\hat{\underline{k}}_f,\hat{\underline{k}}_o) + \frac{1}{2\pi^2}\sum_n \int f^{Bl}_{fn}\frac{(\hat{\underline{k}}_f,\hat{\underline{q}})f_{ro}(\hat{\underline{q}},\hat{\underline{k}}_o)\, d\underline{q}}{q^2 - k_n^2 - i\epsilon} \qquad (1.50)$$

where $f^{Bl}_{fo}(\hat{\underline{k}}_f,\hat{\underline{k}}_o)$ is the first Born scattering amplitude. Above equation is the Fredholm integral equation which gives the scattering amplitude . Theevaluation of this equation by iteration method gives the scattering amplitude in Born series. For elastic scattering the equation (1.50) becomes

$$f_{oo}(\hat{\underline{k}}_f, \hat{\underline{k}}_o) = f^{Bl}_{oo}(\hat{\underline{k}}_f, \hat{\underline{k}}_o) + \frac{1}{2\pi^2}\sum_n \int$$

$$\frac{f_{on}^{B_1}\ (\hat{k}_f \cdot \hat{q})\ f_{no}(\hat{q},\hat{k}_o)\ dq}{q^2 - k_n^2 - i\epsilon} \qquad (1.51)$$

To solve this equation Das replaced $f_{no}(\hat{q}, \hat{k}_o)$ by a trial input scattering amplitude $f_{no}^{(in)}(\hat{q}, \hat{k}_o)$ and $f_{oo}(\hat{k}_f, \hat{k}_o)$ so obtained, denoted as output scattering amplitude $f_{oo}^{(out)}(\hat{k}_f, \hat{k}_o)$ was utilised to obtain differential and total cross sections. The scattering amplitude $f_{oo}(\hat{k}_f, \hat{k}_o)$ for the finite values of k_o satisfies the limiting conditions

$$f_{oo}(\hat{k}_f, \hat{k}_o) \underset{k_1 \to o}{\sim} C(k_o)\ f^{B_1}(\underline{k}_o)$$

and $$\underset{k_1 \to o}{\sim} d(k_o)\ f^{B_1}(\underline{k}_o) \qquad (1.52)$$

where C and d are complex quatities which depend on k_o. Therefore Das had chosen the input trial scattering function $f_{no}^{(in)}(\hat{k}_f, \hat{k}_o)$ as

$$f_{no}^{(in)}(\hat{q}, \hat{k}_o) = (a^D + ib^D)\ f_{no}^{B_1}(\hat{q}, \hat{k}_o) \qquad (1.53)$$

where a^D and b^D are energy dependent parameters and he obtained them by minimising the integral of $|f_{oo}^{out} - f_{oo}^{in}|^2$ over the direction of k_o with respect to a^D and b^D. Using the input trial function given in (1.53), Das

obtained the output scattering amplitude

$$f^{D}_{out} = f^{out}_{oo}(\hat{k}_f, \hat{k}_o) + (a^D + i\, b^D)\, \bar{f}^{B_2}_{oo}(\hat{k}_f, \hat{k}_o)$$

$$= f_{B1} + (a^D + i\, b^D)\, \bar{f}_{B_2}$$

$$= f_{B1} + \bar{f}_{B_2} + (a^D + i\, b^D - 1)\, \bar{f}_{B_2} \qquad (1.54)$$

The minimisation of $| f^{D}_{out} - f^{(in)}_{oo} |^2$ gives the values of a^D and b^D as

$$a^D = \frac{\int d\Theta \, \mathrm{Sin}\Theta \; f_{B1}\,(f_{B1} - \bar{f}_{B2R})}{\int d\Theta \, \mathrm{Sin}\Theta \,[(f_{B1} - \bar{f}_{B2R})^2 + \bar{f}^{2}_{B2I}]}$$

$$b^D = \frac{\int d\Theta \; \mathrm{Sin}\Theta \; f_{B1} \; \bar{f}_{B2I}}{\int d\Theta \, \mathrm{Sin}\Theta \,[(f_{B1} - \bar{f}_{B2R})^2 + f^{2}_{B2I}]} \qquad (1.55)$$

Byron and Joachain (1977 a) showed that at large energy range a^D will increase energy and will go to its asymptotic value of unity. On the other hand at large energy region b^D will decrease with energy. Thus in this method the contribution of higher Born terms are taken into account by multiplying Second order Born term by energy dependent complex parameter. A no. of investigati ons were done by D as and his associates using this method (D as, 1979, D as et al, 1981 ;

Das and Biswas 1980, 81 ; Das and Saha 1981,82)

Optical Model potential formalism

The elastic scattering of a given particle by a composite target containing several scatters are conveniently analysed by replacing the complicated interactions between the projectile and the target particles by an optical potential (or pseudopotential) in which the incident partile moves (Joachain, 1975). Once the optical potential is determined, the original many - body elastic scattering problem reduces to a one body situation. However this reduction is impossible at present and approximated methods are necessary. For elastic scattering, the equivalent one body equation is given as

$$[\ \nabla^2 + k^2 - 2\, V_{opt}(\underline{r})\ ]\ F(\underline{r}) = 0 \qquad (1.56)$$

with

$$V_{opt}(\underline{r}) = V_{st}(\underline{r}) + V_{pol}(\underline{r}) + i\,V_{abs}(\underline{r}) + V_{ex}(\underline{r}) \qquad (1.57)$$

where $V_{st}(\underline{r})$, $V_{pol}(\underline{r})$, $V_{abs}(\underline{r})$ and $V_{ex}(\underline{r})$ stand for the static, polarisation, absorption and exchange interactions respectively.

In general $V_{opt}(r)$ is a complex, non local, non spherical and energy dependent potential and its use as such in (1.56) gives rise to coupled differential equations.. For solving these equations we require a considerable computer time. The three most standard approaches used so far to account for polarisation and absorption processes are (i) the inclusion of a sufficient number of excited electronics states or pseudostates of the target. (ii) Calculation of a nonlocal optical potential by greens's function technique, perturbation theory or Freshbach projection operator formalism (iii) use of local, spherically symmetric, energy dependent, effective potentials obtained by high energy, low energy or semiclassical approximations. Approaches (i) and (ii) are more rigorous than (iii) but they need considerable computer time and was not easy to interpret as (iii). Following approach (iii), we can solve (1.56) using partial wave analysis.

$$F(r) = \sum_l A_l \frac{f_l(r)}{r} P_l(\cos\Theta) \qquad (1.58)$$

Where $P_l(\cos\Theta)$ are the Legendre polynomials.

Substituting (1.58) in (1.56) we obtain a one dimensional differential equation for the l^{th} partial wave $f_l(r)$ as

$$\left[\frac{d^2}{dr^2} + k^2 - 2 V_{opt}(r) - \frac{l(l+1)}{r^2} \right] f_l(r) = 0 \qquad (1.59)$$

$f_l(r)$ satisfies the boundary conditions $f_l(r) \underset{r \to 0}{\sim} r^{l+1}$

and $f_l(r) \underset{r \to \infty}{\sim} k_r \left[j_l(kr) - i\, \eta_l(kr) + S_l \; j_l(kr) + i\eta_l(kr) \right]$ (1.61)

where j_l and η_l are the spherical Bessel and Neumann functions and S_l is the scattering matrix given as

$$S_l = e^{2i\delta_l} \qquad (1.61)$$

δ_l is the phase shift for the l^{th} partial wave due to the potential V_{opt}.

We now present a brief account of the work carried out in this dissertation. To study the elastic scattering of electrons by hydrogen and helium a large no. of approximations based on perturbative expansion of scattering amplitude have been devised. To test the suitability and success of such methods it is desirable to apply these to other atoms. Lithium, being the next atom in the periodic table was choosen. Much theoretical interest has been aroused in this problem ever since William et al (1976) measured the DCS and total elastic cross sections (TECS) for $\bar{e}$ scattering by Li. In the intermediate energy region a large no. of investigations were carried out recently (Gregory and

Fink 1974 ; Walters 1976 b ; Chan and Chang 1976 ; Vander poorten, 1976 ; Guha and Ghosh 1979 a, b ; Tayal etal 1980, 81 ; Gien 1981 ; Rao and Desai 1983 a, b ; Tayal 1983, 84). Except Vanderpoorten none of the above methods give a reasonable agreement with the experimental results. In most of these works Li is represented as a one electron system. In view of the success of the HHOB approximation in the investigations on H and He (Rao and Desai 1981, 82, 83 ; Chandraprabha 1983 a, b), we thought of applying this to $\bar{e}$ - Li scattering. We present the details of the theory and the differential cross sections and total cross sections for the same in chapter 2.

Das (1978) has suggested a new method for finding out differential scattering cross section and total cross section. Eventhough it is a simple method, no more difficult than a second Born computation it had some discrepancies. In order to remove these discrepancies we have modified this method using HHOB and Glauber approximations. The presently modified method was then applied to $\bar{e}$ - H, $\bar{e}$ - He and $\bar{e}$ - Li elastic scattering at intermediate energies. The details of this new method and the results of the above cases are furnished in Chapter 3.

An attempt to modify the HHOB approximation was discussed in Chapter 4. The chief motivation behind such an attempt is the success of the Wallace correction (Wallace 1973) in improving the eikonal theory. This new Wallace corrected HHOB was applied to the cases of $\bar{e}$ - H, $\bar{e}$ - He and $\bar{e}$ - Li elastic scattering as test cases.

In Chapter 5 we have investigated the elastic $\bar{e}$ - H scattering in the optical potential model formalism. In this model many body problem is reduced to one body. problem. Optical potential ingeneral is a complex, non-spherical, non local and energy depednent potential consisting of static, exchange polarisation and absorption potentials. The absorption and polarisation were determined using HHOB approximation. The results obtained are compared with other theoretical and experimental data.

Lastly, in the Sixth Chapter we have summerised our conclusions about the present study. Some new venues opening up for further work also pointed out.