CHAPTER - I

Introduction to the scattering theory

INTRODUCTION :

The study of interaction of electrons and photons with atoms and ions has attracted considerable interest in the recent years. This is due to several reasons. Firstly due to increasing demand for the electron and photon collision cross sections in the astrophysics, laser physics, plasma physics, atmospheric and intersteller science, isotope separation, MHD (Magneto Hydro Dynamics) generators, electrical discharge, radiation chemistry and radiophysics. Scattering phenomena i.e. elastic/inelastic scattering of electrons by atoms and molecules is an important area of theoretical work in the field of physics. Whereby newer methods and results are being reported continously which has important practical application in numerous scientific and technical fields described below.

Elastic and inelastic cross sections for electron and photon scattering by atoms and molecules are required for the study of the energy spectrum of the secondary electrons ejected during the bombardment of the upper atmosphere by electrons, ions, cosmic particles and electromagnetic radiation in the UV (Ultra -violet) and X -ray region. This information in turn gives an idea of

chemical composition, temperature and density of the constituents of the upper atmosphere. Thus the energy spectrum of electrons is a very important parameter for all atmospheric calculation. The analysis of scattering phenomena plays an important role in theoretical and experimental investigation on the structure of matter on microscopic scale, and also of fundamental importance in Atomic and Molecular physics. It also plays an important role in numerous scientific and technical fields like aeronomy, gas lasers, controlled thermo nuclear fusion, biophysics, aurora, airglow, chemical composition etc.. The ionic layers in the ionosphere of the earth are mainly formed due to the ionization of the neutral constituent of the atmosphere by solar radiation leading to production of energatic electrons further excite the neutral particles and then the particles in the excited state, on decay to lower states, give rise to fluorescence. This is an important component of the day glow. On the earth's magnetic poles, the charged particles are absorbed by constituent particles, these ionised and excited species produce the atmospheric emmision known as aurora. Hence for the proper understanding of different phenomena occuring in upper atmosphere, we need a wide knowledge of atomic and molecular processes. Aurora and airglow emmisions are the visual menifestations of the scattering processes in the atmosphere. Various parameters dependent on collision cross sections like stopping power and the mean energy expended per ion pair etc., are required to estimate

necessary dose and the duration of exposure in the radiation therapy in present day of energy crisis. The magneto hydro dynamic (MHD) generators have their own significance, where some alkali atoms like caesium are used in it. Thus study of collision process is an important parameter designed in such uses. Collisional cross sections are required to monitor the impurity control introduced in fusion plasma due to 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 number of free electrons and their frequencies of collision with molecules. The frequency in turn, depends on momentum transfer cross section.

A number of important technological advancement have occured on experimental side. This includes the availability of electron beams (with milli volt energy resolution), the synchrotron radiation sources, intense tunable lasers and new instruments for absolute measurement of cross sections. Many of the experiments in this field provide very straight tests of theory and have stimulated the development of new theoretical models and methods. Finally the availability of powerful computers recently have made possible the exact and accurate study of complex collision processes theoretically which otherwise were not possible to study before.

Apart from this, the subject is playing a leading part in the establishment of the quantum theory and includes many aspects of

fundamental importance in the theory of atomic structure. Thus the phenomena of electron scattering by atoms and molecules seems to have important bearing on many branches of science and engineering. This manifold applications make atomic and molecular collision physics a very important subject of experimental and theoretical investigations.

A collision is said to have taken place between two particles when they collide with each other, if and only if any physical change occurs, which can be detected. All the scattering processes can be classified mainly in three catagories viz., the elastic, inelastic and super elastic. The scattering process in which the internal states and structure of the colliding particles do not change are characterized as elastic. If the internal states and/or the structure of the colliding particles change, the collision is called inelastic. The super elastic collision is one in which the incident particle gains some energy from the target atom. The probability of observing certain final states out of the infinite set of possible states belonging to the above three catagories is usually expressed in terms of the collision cross -sections which can be determined by means of the quantum theory. Hence we can define the cross section as " The cross section of a certain type of event in a given collision process is the ratio of the number of events of these type per unit time and per unit scatterer, to the relative flux of the incident particles with respect to the target ".

There are mainly three experimental method commonly used for the total scattering cross section measurements. They are : the transmission method, the recoil method and the transmission with the time of flight discrimination.

In a typical scattering experiment, a well defined collimated homogeneous beam of mono -energatic pro, ctile 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 detector per unit solid angle per unit time per unit inciden flux is called the differential cross sections over all solid angles yields the total collisional cross -sections.

In the transmission method, the attenuation of an electron beam passing through a gas is measured and is related to the total scattering cross section. This technique has been applied to a large number of atoms and molecules.

The recoil technique is basically also a transmission technique wherein the attenuation of the molecular beam, rather than the electron beam, is measured. This method has been applied extensively to atomic species but applies equally well (in principle) to molecules.

In time -of -flight method, the time distribution of the electron beam signal is converted into an energy distribution with an empty gas cell. When gas is present in the cell, the

attenuation of the electron beam as a function of energy (time distribution) can be determined and related to the total scattering cross section. This method has been applied to many molecular species. It is limited to low impact energy (below few tenth of an eV) by flux and at high impact energies (above 5Ø eV) by time resolution capabilities.

An exact evaluation of Schrodinger equation corresponding to particular scattering process is a formidable task even if the interaction potential is a known quantity, this is because the exact wave function of the target atoms except hydrogen and hydrogenic ions are not known, the Schrodinger equation contains infinite set of coupled integro differential equation to solve. Hence with the limitation of obtaining the exact analytical solution of a many body problem in the quantum mechanical frame work, the approximate methods acquires a great importance. But it rather strange that none of the theoretical approximation explains equally successfully all observed phenomena in the scattering problems or which can give uniformly satisfactory results at all impact energies.

It has been a usual practice to devide the incident energies into three regions i.e. -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 satisfactory results belong to the high energy region. The energy region lying between the two is referred

to as the intermediate energy region. There are different approximation devised to explain the scattering process in these energy regions i.e at low, intermediate and high.

A detail account of the numerous approximate methods used to explain the scattering theory can be available from the review articles, selected papers and from the number of books (Bates, 1962 ; Mott and Massey, 1965 ; Massey et al,1969 ; Moiseiwitsch and Smith, 1968; Rudge,1968; Gerjuoy and Thomas, 1974; Joachain, 1977; Burke and Williams, 1974; Walters, 1976a; Byron and Joachain, 1977a; Bransden and Mc Dowell, 1977,11978; Ishihara, 1978; Jhanwer et al, 1978a; Burke, 1979; Lane, 198Ø; Joachain, 198Ø; Kessler, 1982; Schwenke et al,1983; Staszewska et al, 1984) and so on.

In the present work we have restricted ourself to study the elastic scattering of electrons by atoms in the intermediate and high energy region. The choice for this energy region are, that the effect on the elastic scattering are greatly magnified at low energies and there are plenty of absolute experimental cross sections for these energy region are available, as well as there are various theoretical methods and different models described in these energy region.

Atomic units will be used except where otherwise stated.

First we start here with the basic equations which describes the scattering phenomena.

BASIC EQUATIONS :

Let us consider the elastic scattering of an electron by a neutral atom of atomic number Z. We assume that the collision is nonrelativistic. Since we are interested in the intermediate and high -energy region. We shall first neglect the effects of the Pauli principle between the incident and target electrons, correction due to exchange will be considered separately. The initial and final wave vectors of the electron will be denoted by $\vec{k}_i$ and $\vec{k}_f$ respectively, with $| \vec{k}_i | = | \vec{k}_f | = k_i$. The nucleus of the atom being the origin of our coordinate system, we shall denote the coordinate of the projectile electron by $\vec{r}_\emptyset$, while the positions of the atomic electrons will be labeled by $\vec{r}_i$ (i=1,..,Z).

The free motion of the two colliding particles is described by the Hamiltonian

$$H_\emptyset = K + h \qquad (1),$$

where K is the kinetic -energy operator

$$K = -\frac{1}{2}\nabla^2_{r_0} \qquad (2),$$

and h is the internal Hamiltonian of the target.

Morever, we have

$$h \mid n > = \omega_n \mid n > \qquad (3),$$

where $\mid n >$ denoted an eigenstates of the target Hamiltonian and ω_n is the corresponding internal energy. We shall denote by $\mid \emptyset >$ the initial state (and final) eigenket of the target.

The full Hamiltonian of the system is such that

$$H = H_{\emptyset} + V \qquad (4),$$

where V, the interaction potentiai between the projectile and the target, is simply

$$V = \sum_{i=1}^{z} \frac{1}{r_{i\emptyset}} - \frac{z}{r_{\emptyset}} \qquad (5),$$

with $r_{i\emptyset} = | \vec{r}_i - \vec{r}_{\emptyset} |$.

The scattering amplitude for elastic scattering is then given by the expressions

$$f = - (2\Pi)^2 < \phi_f | V | \psi_i^+ > \qquad (6a),$$

or

$$f = - (2\Pi)^2 < \psi_f^- | V | \phi_i > \qquad (6b),$$

where ϕ_i and ϕ_f are eigenstates of $H_{\emptyset}$ (i.e., free waves), while ψ_i^+ and ψ_f^- denote the full scattering wave functions satisfying the Lippmann -Schwinger equation

$$\psi_i^+ = \phi_i + G_{\emptyset}^+ V \psi_i^+ \qquad (7a),$$

and

$$\psi_f^- = \phi_f + G_{\emptyset}^- V \psi_f^- \qquad (7b).$$

In this equations, the Green's operator $G_{\emptyset}^{\pm}$ are given by

$$G_{\emptyset}^{\pm} = (E - H_{\emptyset} + i \epsilon)^{-1} \qquad (8).$$

Since we are considering only norrelativistic collisions and we neglect the Pauli principle between the incident and target electrons, we may ignore the spin of the projectile, the indices i and f therefore label the momentum of the projectile together with the internal quantum numbers of the target. In what follows we shall write the asymptotic states $| \phi_i >$ and $| \phi_f >$ more

explicitly as $| \emptyset, \ k_i \rangle$ and $| \emptyset, \ k_f \rangle$, respectively. More generally, an eigenstate $| \phi_c \rangle$ of $H_\emptyset$ will be written as $| n, \vec{q} \rangle$. The normalizaion condition which we adopt is such that

$$\langle n', \vec{q}' \mid n, \vec{q} \rangle = \delta_{nn'} \, \delta (\vec{q} - \vec{q}') \quad (9),$$

Hence, in the coordinate representation

$$\phi_c (\vec{r}_\emptyset , \zeta) = (2\pi)^{-3/2} \, e^{iq \, r_\emptyset} \, \psi_n (\zeta) \quad (10),$$

where ζ denotes the collection of all target coordinates.

Consider the nonrelativistic Schrodinger equation for the system

$$(H - E) \psi (x , x_i) = \emptyset \quad (11),$$

where E is the total energy of the system and $\psi (x, x_i)$ is the wave function of the system.

The initial state of the system is given as

$$\phi_{ki}(r, r_i) = (2\pi)^{-3/2} \ e^{i \, k_i \cdot r} \ \phi_i (r_i) \quad (12),$$

solution of the equation (11) is denoted by $\psi (r , r_i)$

$$\psi(r , r_i) \dashrightarrow (2\pi)^{-3/2} [\ e^{ik_i r} \ \phi_n(r_i) + \sum_n f_{ni}(\theta,\phi) \ e^{ik_i r} \ \phi_n(r_i) \ ] \quad (13),$$

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

The differential cross section (DCS) can be written as

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} \mid f(\theta , \phi) \mid^2 \quad (14),$$

for the elastic scattering we have $| k_i | = | k_f | = k$.

The DCS can be written as

$$\frac{d\sigma}{d\Omega} = | f(\theta , \phi) |^2$$

The total cross section (TCS) are obtained using the optical theorem as

$$\sigma^{tot} = \frac{4\Pi}{k}2 \quad \text{Im } f \ (\theta = \emptyset) \qquad (15).$$

For the study of any collision problems these two quantities i.e. DCS and TCS becomes the key quantities and can be determined by solving equation (11).

There are mainly two approaches in which this equation is solved for any type of collision problem. One is a differential equation appraoch, non iterative in nature and the other is an integral equation approach, which is iterative.

There has been various approximations devised to get the wave function of the target atom to be considered and to solve or to obtain the scattering amplitude for the specific type of collision problem.

POTENTIAL SCATTERING :

Let us consider the nonrelativistic scattering of spinless particle by a potential $V(\underline{r})$, which allows us to introduce in a simple way some of the basic ideas which are required in the analysis of the electron scattering by atoms, where the total energy of the system is equal to the sum of the kinetic energy and potential energy of the incident particle. Introducing the " reduced potential " by $U(\underline{r}) = 2\ V(\underline{r})$ and the strength of this is $| U_{\emptyset} | = 2 | V_{\emptyset} |$, where $| V_{\emptyset} |$ is a typical strength of the potential $V(\underline{r})$. For a potential vanishing faster than $-\frac{1}{r}$ at large distance the stationary scattering wave function $\psi^{+}(k_i)$

representing the plane wave incident in the z -deirection which we choose along k_i, and the outgoing (+) spherical wave has the asymptotic form given by equation

$$\psi^{+}_{ki}(\underline{r}) \underset{r \to \infty}{=\!=\!=} A(K)\left[e^{i\underline{k}_i \cdot \underline{r}} + f(k,\theta,\phi)\frac{e^{ikr}}{r} \right] \qquad (16),$$

where $f(k,\theta,\phi)$ is the scattering amplitude corresponding to scattering in the direction $\Omega = (\theta, \phi)$, and the coefficient A is independent of $\underline{r}$.

THE INTEGRAL EQUATION OF POTENTIAL SCATTERING :

For the potential which vanishes faster than $\frac{1}{r}$ at large r the stationary scattering wave function ψ^{+}_{ki} has been defined above as a solution of the Schwinger equation (7) satisfying the boundary condition (16). Further it is found in the literature (Bransden, 1970 ; Burke , 1977 ; Joachain, 1979 ;) that ψ^{+}_{ki} is also a solution of an equivalent integral equation i.e. Lippmann -Schwinger equation -which directly takes into account the boundary condition (16). Hence

$$\psi^{(+)}_{ki}(\underline{r}) = \phi_{ki}(\underline{r}) + \int G^{(+)}_{\emptyset}(\underline{r}, \underline{r}')\, U(\underline{r}')\, \psi^{(+)}_{ki} d\underline{r}' \qquad (17),$$

where

$$\phi_{ki}(\underline{r}) = \langle \underline{r} \mid \underline{k}_i \rangle = (2\pi)^{-3/2} e^{i\,\underline{k}_i \cdot \underline{r}}$$

is a plane wave corresponding to the incident momentum k_i and the free Green's function $G^{(+)}_{\emptyset}(\underline{r}, \underline{r}')$ is given by

$$G^{(+)}_{\emptyset}(\underline{r}, \underline{r}') = (2\pi)^{-3/2} \int \frac{e^{i\underline{k}'(\underline{r}-\underline{r}')}}{k'^2 - k^2 - i\epsilon}\, d\underline{k}' \qquad (18),$$

$$\epsilon \longrightarrow \emptyset^{+}$$

or

$$G_{\emptyset}^{(+)}(\underline{r}\ ,\ \underline{r}') \ = \ \frac{1}{4\pi}\ \frac{e^{ik(\underline{r}\ -\ \underline{r}')}}{|\ \underline{r}\ -\ \underline{r}'|} \qquad (19).$$

The asymptotic behaviour of (17) gives the integral representation of the scattering amplitude f.

$$f \ = \ -\ 2\pi^2 \langle \phi_{kf} \mid U \mid \psi_{ki} \rangle$$

$$= -\ (2\pi)^2 \langle \phi_{kf} \mid V \mid \psi_{ki} \rangle$$

$$f \ = -\ (2\pi)^2 \ T_{fi} \qquad (2\emptyset),$$

where

$$\phi_{ki}\ (\underline{r}) \ = \langle\ \underline{r} \mid k_i \rangle \ = (2\pi)^{-3/2} \ e^{ik_f\ \underline{r}}$$

is a plane wave corresponding to the total momentum k_f , and T_{fi} is the transition matrix element. The expression for T_{fi} is given by

$$T_{fi} \ = \langle \phi_{kf} \mid V \mid \psi_{ki} \rangle \qquad (21).$$

The plane wave is " normalized " here in such a manner that

$$\langle \phi_{kf} \mid \phi_{ki} \rangle \ = \langle k_f \mid k_i \rangle \ = \delta\ (\ k_i\ -\ k_f\ ) \qquad (22).$$

Now taking the brief account of some of the approximate methods which are relavant for the present study, where the energy of the projectile electron is taken higher than the first ionization energy of the target atom. Several of these methods are given and described in the literature, review articles of Joachain and Quigg (1974), Byron and Joachain (1977), Bransen and Mc Dowell (1977 -78).

THE BORN APPROXIMATION :

The Born series, which is essentially a perturbative type expansion of the wave function or the scattering amplitude in powers of the interaction potential. At high energies (impact energies at least an oredr of magnitude greater than the kinetic energies of the relavant bounds electrons) electron scattering by atoms or molecules can be described by the first Born approximation.

This assumes the unpolarized bound states for the target and undistorted plane wave states for the scattering electron, which is assumed distinguishable from the bound electrons.

Let us begin with the Born series, which is obtained by solving the Lippmann -Schwinger equation by the perturbation theory. Starting with the "unperturbed " incident plane wave $\phi_{ki}(\underline{r})$, we then generate for $\psi_{ki}^{(+)}$ the Born series

$$\psi_{ki}^{(+)}(\underline{r}) = \sum_{n=1}^{\infty} \phi_n(\underline{r}) \qquad (23),$$

with

$$\phi_{\emptyset}(\underline{r}) = \phi_{ki}(\underline{r})$$

$$\phi_n(\underline{r}) = \int k_n(\underline{r}, \underline{r}')\, \phi_{\emptyset}(\underline{r}')\, d\underline{r}' \qquad n \geq 1$$

and

$$k_1(\underline{r}, \underline{r}') = G_{\emptyset}^{(+)}(\underline{r}, \underline{r}')\, U(\underline{r}')\,,$$

$$k_n(\underline{r}, \underline{r}') = \int k_1(\underline{r}, \underline{r}')\, k_{n-1}(\underline{r}'', \underline{r}')\, d\underline{r}'' \qquad n \geq 2 \qquad (24).$$

From equation (23), one can see that Born series is a

perturbative series in powers of the interaction potential. By the substitution of equation (23) in (2Ø) we can obtain the Born series for the scattering amplitude

$$f = \sum_{n=Ø}^{\infty} \bar{f}_{Bn}$$

where

$$\bar{f}_{B1} = -(2\pi)^2 \langle \phi_{kf} | U | \phi_{ki} \rangle$$

$$= -\frac{1}{4\pi} \int e^{i q \cdot r_Ø} U(r)\, dr \qquad (26),$$

and

$$\bar{f}_{Bn} = -2\pi^2 \langle \phi_{kf} | U G_Ø^+ U \ldots\ldots G_Ø^+ U | \phi_{ki} \rangle \quad n \geq 2 \qquad (27),$$

one can see that in the last expression potential appears n times and the Green's function (n-1) times. The Jth order Born approximation to the scattering amplitude can be written as

$$f_{BJ} = \sum_{n=1}^{J} f_{Bn} \qquad (28),$$

so that

$\bar{f}_{B1} = f_{B1}$, $\bar{f}_{B2} = f_{B1} + f_{B2}$ and so on.

From the equation (25) one can see that Born series as a multiple scattering series in which the particle interacts repeatadly with the potential and propogates freely between two successive interactions. Born series will converge if the incident particle has a sufficiently high energy and (or) if the potential is weak enough.

The first Born (approximation) amplitude for a lrge number of charged particle -atom, elastic and inelastic scattering

processes had been calculated by Bell and Kingston (1974). Equation (27) is widely used or applied to scattering problems. Because of its simplicity it fails to compensate for all it may lack in accuracy. Above all the error is usually substaintial which seeks the further terms of the series, of higher order than the first or second are quite difficult to evaluate.

But a better way is to include the polarization, absorption and distortion of the incident particle in comparison of first Born approximation (FBA) i.e., second Born approximation.

In this approximation the distortion of the incident particle as well as that of the target atom due to the presence of each other are completely ignored. Thus it is a weak interaction and its validity increases with the increase in energy. But in any case the energy at which it becomes accurate, varies from target to target and from process to process. At intermediate energies the incident particle stays in vicinity of target for sufficiently longer time to make the interaction quite appreciable. Thus at intermediate energies polarization, absorption and distortion of incident particle effects (due to the presence of each other i.e. target as well as incident particle) becomes important.

THE EIKONAL APPROXIMATION :

Originally introduced in quantum theory by Moliere (1947), this eikonal approximation has been considerably developed by Glauber (1959) who proposed a very fruitful many body

generalization of the method. In this recent time, most atomic collision processes have been studied by means of the eikonal approximation. To construct this approximation it was assumed that the incident particle satisfied the " short wave length " condition (ka >> 1) to gether with the "high energy" requirement given as

$$\frac{|V_{\emptyset}|}{E} = \frac{|U_{\emptyset}|}{k^2} << 1 \qquad (29),$$

with these conditions the eikonal wave function in eikonal approximation can be obtained from (17) by a linearization of the Green's function (19). Hence, corresponding eikonal wave functions can be given as

$$\psi_E(\underline{r}) = (2\pi)^{-3/2} \exp\left[i \underline{k}_i \cdot \underline{r} - \frac{i}{2k} \int_{-\infty}^{z} U(\underline{b}, z')\, dz' \right] \qquad (30).$$

Substitution of this expression into the integral form (20) of the scattering amplitude yields into

$$f = -\frac{1}{4\pi} \int e^{i\underline{q}\cdot\underline{r}_{\emptyset}} U(\underline{r}) \exp\left[-\frac{i}{2k} \int_{-\infty}^{z} U(\underline{b}, z')dz' \right] d\underline{r} \qquad (31).$$

Further, Joachain (1970) showed that the eikonal scattering amplitude can be given as

$$f_E = \frac{k}{2\pi i} \int e^{i\,\underline{q}\cdot\underline{b}}\, d^2\underline{b} \left[e^{i\,\chi(\underline{k},\underline{b})} - 1 \right] \qquad (32),$$

where the quantity

$$\chi(\underline{k},\underline{b}) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} U(\underline{b}, z)\, dz$$

is the eikonal phase shift function. Further, to have the eikonal multiple scattering series can be obtained from (32) by the

expansion of exp $(i\chi)$ in powers of χ. The eikonal multiple scattering expression can written as

$$f = \sum_{n=1}^{\infty} \bar{f}_{En} \qquad (33),$$

where

$$\bar{f}_{En} = \frac{k}{2\pi i} \frac{i^n}{n!} \int e^{i\, q\cdot b}\, d^2\underline{b}\, [\, \chi(\underline{k}, \underline{b})\,]^n \qquad (34),$$

from the set of equations (32 to 34), we get

$$f_{E1} = -\frac{1}{4}\frac{1}{\pi} \int d^2\underline{b} \int_{-\infty}^{+\infty} e^{i\, q\cdot b}\, U(\underline{b}, \underline{z})\, dz \qquad (35),$$

it is worth noting that the assimed potential to be real, the quantities f_{En} given in equation (34) are alternatively purely real and imaginary. When $ka >> 1$ (where "a" is the range of the potential) and comparing the relation between the terms of Born series (25) and of the eikonal series (33). It is clear from the equation (26) and (35) that

$$\bar{f}_{B1} = \bar{f}_{E1} \qquad (36),$$

for all interaction potentials, all energies and all momentum transfer. Now if the z -integration in (32) is performed along the direction k_i, using the coordinate system, we would only have approximately $q\cdot b = q\cdot r$ for small q's and the relation (35) only hold at small angles. Since the Born series converges at sufficiently high energies for nonrelativistic potential scattering, it is desirable to secure the relation (35) at all angles. Remarkable relationships between the higher terms of the eikonal and Born series have also been discovered by Moore, 1970;

Byron and Joachain, 1973; Byron et al, 1973.

One of the ways to proceed beyond first order, perturbation theory i.e. first Born approximation (26) is to employ higher order Born approximation. However calculation of the Born series of higher orders requires a considerable amount of work. Another promising yet still simple way to improve over the first order theory is to apply Glauber approximation (1959). The Glauber approximation is the generalization of the eikonal multiple scattering expansions to many body scattering problem. The formulation of the Glauber scattering amplitude is given following.

GLAUBER APPROXIMATION :

This is a many body generalization of the eikonal approximation described earlier. For the direct collision from an initial state $| \emptyset >$ to a final state $| n >$, the Glauber scattering amplitude is given by (Glauber, 1959)

$$f_G = \frac{k}{2\pi i} \int e^{i \underline{q}\cdot\underline{b}} \, d^2\underline{b} \, < m | \{ e^{i\chi_G(\underline{b}, \underline{x})} - 1 \} | \emptyset > \quad (37),$$

where, Glauber phase shift function in terms of V_d is given as

$$\chi_G (\underline{b}, \underline{x}) = - \frac{1}{k} \int_{-\infty}^{+\infty} V_d(\underline{b}, z, \underline{x}) \, dz \quad (38),$$

the integration is performed along the z -axis but perpendicular to $\underline{q}$. A few points concerning the Glauber approach are : firstly, it may be viewed as an eikonal approximation to a " frozen target" model proposed by Chase (1956) in which closure is used with an

average excitation energy DE = Ø, secondly, considerable insight into the properties of the Glauber method may be gained by expanding (37) in powers of V_d , viz.

$$f_G = \sum_{n=1}^{\infty} \bar{f}_{Gn} \qquad (39),$$

where

$$\bar{f}_{Gn} = \frac{k}{2\pi i} \frac{i^n}{n!} \int e^{iq\cdot b} \, d^2b \, \langle m \mid [\, \chi(b,x) \,]^n \mid Ø \rangle \qquad (4Ø),$$

comparing the terms of $\bar{f}_{Gn}$ with the Born series $\bar{f}_{Bn}$. We can say that $\bar{f}_{B1} = \bar{f}_{G1}$, also the terms $\bar{f}_{Gn}$ are alternatively real or purely imaginary, while the corresponding Born terms $\bar{f}_{Bn}$ are complex for $n \geq 2$. This features of the Glauber amplitude leads to several defects such as (a) the absence of the important real term for elastic scattering and (b) identical cross sections for electron -and -positron -atom scattering. Other deficiencies of the Glauber amplitude (4Ø) include a logarithmic divergence for elastic scattering in the forward direction, and a poor description of inelastic collisions involving non -spherically symmetric states. Its major role in atomic collision theory has been to stimulate interest in eikonal methods (Byron and Joachain, 1977). Such as the " eikonal Born series " (EBS) theory (Byron and Joachain, 1973,1974,1975,1977).

EIKONAL BORN SERIES METHOD (EBS) :

This method combines the Born and Glauber series to obtain a consistent expansion of the scattering amplitude in power of

$O(k_i^{-1})$. The Glauber term $\bar{f}_{Gn}$ gives in each order perturbation theory to the leading piece of the corresponding Born term (for large k) for all q's except in second order where the long range of the coulomb potential is responsible for anamalous behaviour of $\bar{f}_{G2}$ for all small $\underline{q}$. In the EBS approximation a consistent calculation of the direct scattering amplitude through $O(k_i^{-2})$ was obtained by the replacement of real part of $\bar{f}_{B3}$ by $\bar{f}_{G3}$ in the Born scattering amplitude. In this way the EBS direct scattering amplitude is written as

$$f^{d}_{EBS} = \bar{f}_{B1} + \bar{f}_{B2} + \bar{f}_{G3}$$

in addition, exchange effects are taken into account by using the Ochkur amplitude g_{och} (Ochkur, 1963, 1964).

The EBS method has been applied to various electron -atom collision processes (Byron and Joachain, 1977) at intermediate and high energies. And it is an improvement over the 2nd Born or Glauber approximations. It was also analyzed that the convergence of the Born series for the direct scattering amplitude is slower at large $\underline{q}$, than in the small $\underline{q}$ region. Thus an "all order" treatment would be desirable at large $\underline{q}$, and it was done by the optical model (Joachain, 1979 ; Mittleman and Watson, 1959,1960 ; Byron and Joachain, 1974,1977 ; Joachain and Vanderpoorten et al, 1977 ; Vanderpoorten, 1975 ; Furness and Mc Carthy, 1973 ; Riley and Truhlar, 1976) methods and target expansion (Burkey and Webb, 1973 ; Callaway and Wooten, 1973,1974,1975 ; Callaway and Mc Dowell Morgan, 1976) methods.

After the formulation of the Glauber eikonal approximation (Glauber, 1959) very less amount of work was done for the calculation of DCS and integral cross sections. This was due to the computational complexity involved in evaluating the Glauber amplitude (38) for systems more complicated than helium. It was also found difficult to get the closed form of the Glauber scattering amplitude.

The approximations methods described above have some common problems which are in general described below.

(i) Very few theoretical methods were able to reproduce the various scattering cross section which can be compared satisfactorily with the experimental results.

(ii) Some approximation required complicated numerical techniques for the evaluation of the scattering cross sections.

(iii) Few approximate methods has the divergent integral problems.

(iv) Very few methods have used the higher order exchange correction.

(v) There has been a considerable amount of discrepancy in the results of cross sections measured even for the system like hydrogen.

(vi) There are few approximate methods described are found to be difficult to extend for the higher number of electron system.

(vii) Even though there exists an ample amount of data in this field of atomic and molecular scattering both theoretically

as well as experimentally, but still there are discrepancies observed amongs the methods both theoretically as well as experimentally.

(viii) The evaluation of the exact wave function and the negligance of the cross product terms for a heavy atom also lead to the inaccuracies in the results.

Keeping all these problems in mind and with a aim to reduce the dicrepancies in the scattering cross sections measured for different system, we applied certain refinement to the approximate methods. We get the more accurate wave function of the target atom considered. We also made an attempt to extend the calculation in a different method so that the particular approximate method applies equally well for a variety of energies and for wide angular range.

We now present a brief account of work reported in this thesis. To study the elastic scattering of electrons by hydrogen, helium. lithium and neon a large number of approximations based on perturbative expansion of scattering amplitude have been devised. In view of the HHOB approximation in the investigations on hydrogen, helium (Rao and Desai, 1981,1982,1983 ; Chandraprabha and Desai, 1983a, 1983b) and for lithium (Suja and Desai, 1986,1987,1988), we thought of applying certain refinement to the approximation to study the elastic scattering of electrons by a target like hydrogen, helium and lithium atom. We present the details of the theory and the calculation of the differential cross section and total cross sections for the same in the

chapter II. We have made an adequate comparison of our results with the other theory and experiments results in the graphs and in the tabular form.

In the chapter III, we extend the calculation of differential cross sections and total cross section for the elastic scattering of electrons by a neutral neon atom. Where we employ the method of Roothan -Hartree -Fock wave method and we made use of the Clementii -Roetii tables for the orbital calculations for the neon atom to get the more accurate wave function. Here we have made an adequate comparison both in graphs and in the tables.

In the chapter IV we have made an attempt of increasing the cross sections for the elastic scattering of electrons by a neon atom using the two -potential method in the HHOB theory. We also aimed that this method gives accurate cross sections for the wide angular range and for a variety of energies. We apply theexact treatment is given for the calculation of the phase shift for the neon atom. We compare our results with experiments and theoretical results available.

In the last chapter V we try to summarised our conclusions about the present method of evaluation of the various cross sections for the different target atoms.