CHAPTER - 1

INTRODUCTION

1.1 Resume :

It can be seen from the review of the recent literature that electron scattering from atoms and molecules is being considered as an important area of theoretical work in the field of Physics. Newer methods and results are being reported continuously in this area which has important practical applications in various other fields. In the present thesis, I have undertaken the study of electron scattering by atoms using various significant approximations in the field and trying to understand various aspects of the problem.

In the first chapter, a brief introduction to the problem is given. In the second chapter, various theoretical methods pertaining to the present work are discussed so that they may be useful in the chapters to follow. Special attention is given to the High energy Higher Order Born approximation which is discussed in detail. In the third chapter, a new method - the modified Glauber Eikonal Series (MGES) method - is proposed and is applied to a variety of scattering phenomena. The fourth chapter mainly deals with modifications to the Born approximation and in the course of discussion the two potential Eikonal approximation also appears. The HHOB approximation and its modifications, the modified Born approximation and the partial wave analysis are the relevant theoretical methods of this chapter, with applications to different scattering processes. The fifth chapter is exclusively devoted to electron scattering from alkali atoms with special attention to Na atom as the target. In the last chapter a general discussion of the conclusions drawn in the course of my study is attempted with a view to enumerate further venues of research which are opened through the present work.

As mentioned above, the following chapters are going to be purely theoretical discussions on the scattering of charged particles like electrons from atoms. For comparative purposes, the experimental results arrived at by other workers will be referred to as an when the need arises. Hence, it will be useful to have a brief introduction to the fundamentals of the problem as given in the following sections of this chapter.

1.2 Scattering Processes :

We consider the physical processes that occur when a single particle (projectile) collides with a single atom or molecule (target). Since the present thesis deals mainly with collisions between electron and atom, we consider the projectile electron 'e' colliding with a free atom 'A'. Now the simplest possibility is

$$e + A \longrightarrow e + A \quad \text{----} \quad (1.1)$$

where the total energy of the reactants is the same as that of the products. If the electron is deviated from its original direction, then it suffers a change in energy. For an electron of mass m colliding with a heavy particle like an atom of mass M, this change in energy is quite small, being dependent on m/M. This type of scattering process is known as elastic scattering. Under the same conditions, a possibility may arise in which there is an exchange of the incident electron with one electron of the target 'A'. In this case, the scattering process is termed as elastic scattering with exchange.

In another possibility of the collision of 'e' with 'A', a part of the kinetic energy of the incident electron is transferred as the internal energy of the target such that the latter is excited to a higher energy state. This possibility of collision between 'e' and 'A' can be represented as

$$e + A \longrightarrow e + A^{*} \quad \ldots \quad (1.2)$$

Where A and A^{*} are the initial and final states of the target atom. This type of scattering process is known as inelastic scattering. It should be mentioned that the energy of the scattered electron also decreases correspondingly. In the inelastic scattering also, the exchange of electrons is possible.

In the case of an electron colliding with a target atom already in an excited state, the collision is termed super elastic. This can be represented as

$$e + A^{*} \longrightarrow e + A^{*} \qquad \ldots (1.3)$$

The three scattering processes given above constitute a broad classification of the various scattering processes. All other possible processes can be grouped in one of the above categories. For e.g., as an extension of the inelastic collisions, we can think of ionization of the target given by

$$e + A \longrightarrow e + \overset{+}{A} + e \qquad \ldots (1.4)$$

or, attachment of the projectile to the target given as

$$e + A \longrightarrow A^{-} \qquad \ldots (1.5)$$

Similarly there can be many other phenomena like electron - capture, dissociation etc. which can be generalized as

$$A + B \longrightarrow C + D \qquad \ldots (1.6)$$

where A, B, C and D are different (or even same) particles, atoms, molecules or even photons.

It should be borne in mind that the above mentioned scattering processes can occur in accordance with the well-known conservation laws and follow certain fundamental rules like the Pauli exclusion principle. A possible mode of fragmentation of a system is termed as a 'Channel'. e.g. (A + B) in (1.6). Thus (1.1) shows the elastic channel and (1.2) shows the inelastic channel. A channel allowed by the conservation laws is said to be an open channel.

1.3 Cross - Sections :

From the view point of physics, the collision processes are quantified and studied in terms of certain parameters or quantities, known as the cross-sections. These are the important design parameters in the practical applications of the scattering processes. The cross-sections derived using theoretical calculations may be compared with their experimental counterparts, thus enabling us to assess the accuracy of the theoretical methods used. The four important parameters used to study the scattering processes are: the total collision cross-section, the differential scattering cross-section, the total elastic cross-section and the momentum transfer cross-section.

Total Collision Cross-section (TCS) :

Consider the general equation of scattering (1.6). A well-collimated, fairly mono-energetic beam of particles 'A' with a reasonable beam - intensity is directed towards the particles of target 'B'. Each scatterer acts individually, under the assumption that its number density is small enough. After the scattering from the thin target material, the scattered particles are registered in a detector at a macroscopic distance.

Let N_A be the number of particles A interacting per unit time with target scatterers B, numbering n_B. The relative flux ϕ_A of incident particles is the number of particles A crossing a unit area normal to the beam direction and fixed relative to the target in unit time. Hence N_A is proportional to ϕ_A and n_B. Thus, for the scattering of particles A by target B,

$$N_A = \phi_A \; n_B \; \sigma_{tot} \qquad \ldots (1.7)$$

where σ_{tot} is the total collision cross section (TCS). Hence σ_{tot} is the number of incident particles A interacting with the target B per unit time, per scatterer, per unit relative incident flux. The TCS is related to the probability that an incident particle interacts with a target particle and has therefore been removed from the incident beam.

<u>Differential Scattering Cross Section (DCS)</u> :

A detailed account of the scattering process can be obtained through the DCS. Consider an elastic scattering process in which dN number of particles A are scattered per unit time within a solid angle dw about the direction (θ, ϕ) relative to the incident direction along the z-axis. Then, as in the case of (1.7).

$$dN = \phi_A n_B \, dw \, I(\theta, \phi) \qquad \ldots(1.8)$$

Here $I(\theta, \phi)$ is the elastic differential cross section which may also be written as $d\sigma(\theta, \phi) / dw$. For other channels also, the DCS may be defined likewise. The DCS is related to the scattering amplitude. To define the DCS of the collision between any two particles, the co-ordinate system - i.e. laboratory frame or centre of mass frame - should be specified. However, for electron scattering from atoms and molecules, the two frames are identical.

Total elastic cross-section (TEC) :

The total elastic cross-section σ_{el} is obtained by integrating the DCS over all solid angles. Hence

$$\sigma_{el} = \int \frac{d\sigma(\theta,\phi)}{dw} \, dw \qquad \ldots(1.9)$$

For the non-elastic channels, the total reaction cross section denoted by σ_r or σ_{inel} can be defined as

$$\sigma_r = \sigma_{tot} - \sigma_{el} \qquad \ldots(1.10)$$

where σ_{tot} is the TCS defined earlier.

Momentum-transfer Cross Section (MTC) :

Because of the momentum transferred by the projectile in the incident direction during the scattering, for low energy work, the momentum transfer (or diffusion) cross section is defined as

$$\sigma_m = \int \frac{d\sigma}{dw} \left(1 - \frac{k_f}{k_i} \cos \theta \right) dw \qquad \ldots(1.11)$$

where k_i and k_f are the magnitudes of the incident and scattered electron wave vectors. For elastic scattering,

$$k_f = k_i \quad \text{such that}$$

$$\sigma_m = \int \frac{d\sigma}{dw} (1 - \cos \theta) \; dw \qquad \ldots(1.12)$$

Here also the factor $(1- \cos \theta)$ comes from the transfer of momentum.

The above discussed cross-sections can be directly measured experimentally or calculated analytically using theoretical methods. Now let us take up the experimental measurements in brief.

1.4 Experimental Aspects :

As mentioned elsewhere, the present work is purely theoretical and only comparisons are made with experimental data. Because of this, and also with an aim to reduce the bulkness of this thesis, the experimental aspects of the scattering processes are not discussed in detail. But since a knowledge of the experimental methods will be helpful in understanding the physics behind the processes in a better way, an outline of different experimental aspects of collision processes is given here with sufficient references.

A typical set up for the measurement of cross sections must consist of: a source or an electron gun generating an energy selected beam of electrons, the instrumentation for generating target species and measuring its density, the detector assembly for detecting and analysing the final products and the peripheral electronic devices.

The experimental methods as well as some of the results are well discussed by Christophorou (1970) and also by Massey, Burhop and Gilbody (1969). The basic methods remain the same even now, only the level of sophistication of the methods being increased from time to time. The basic experimental methods for the study of collisions of particles with atoms and molecules can be broadly categorised as the electron swarm experiments, the electron beam experiments and a suitable combination of the two methods.

The electron swarm experiments is meant for low energy work say around 1 eV, at which it is very difficult to obtain fairly monoenergetic beam of electrons. Hence, a swarm of electrons having a wide distribution of energy is utilized. More about this method has been discussed by Altshuler (1957) and Fabrikant (1976, 77). From Swarm experiments, the momentum-transfer cross-sections, the total inelastic cross-sections and the attachment cross-sections can be obtained. Since these results are obtained as a function of the mean energy of the electron-swarm, one should have a good knowledge of the energy distribution of Swarm-electrons. In Swarm experiments, the finer details to be gained upon a slight variation of the incident energy will remain obscure. Eventhough, below the electronic excitation the slow electron scattering from atoms would be only elastic, the slow electrons colliding with molecular targets can still excite rotational and vibrational modes of motion. In view of this, the importance of Swarm experiments is appreciated.

The electron-beam experiments which are more direct are performed with an almost mono-energetic beam of electrons. These are single collision type experiments and are hardly possible below 1 eV. The single beam method and the crossed beam method are well known in the beam experiments. The history as well as the details of the beam experiments is discussed by Massey et.al. (1969). In recent years, the crossed-beam methods have been extensively used for cases like atomic hydrogen, oxygen etc. The experiments with molecular targets are easier to perform as compared to those with atomic hydrogen or oxygen targets because the molecules are easily available and stable compared with their respective atomic forms. In the case of monoatomic gases the above mentioned problem does not arise.

The analysis of the total collision cross section for various target atoms has been performed by Brackmann et al (1958), Perel et al (1962) and Sunshine et al (1967). The study of the 'fine structure' or sensitive variations of total cross-sections relative to small changes of energies in a certain energy range has been made by designing sensitive energy-analyzers or monochromators.

It is a popular fact that more physics is contained in the DCS than the TCS, hence experiments are designed for measuring angular distributions of electrons scattered from a target. Thus the electron detector should be capable of analysing the electrons with respect to energy and scattering angle. Scattering near the forward direction was investigated in the experiments of Geiger (1963) and the backward scattering with the expected complication of interference with the incident beam - was studied by Gagge (1933). Crossed beam methods have been successfully applied to measure the DCS over the full angular range.

In the measurement of total as well as differential cross-sections, the spread in the energy of the projectile beam must be very small and accurately known so that in the phenomena of fine structure, the true nature of the quantities may be revealed. Similarly, the resolving power of the electron-detector should be high enough to distinguish even minute energy-losses. Otherwise, the cross-sections determined in such cases will not be true. They are referred to as energy unresolved cross-sections.

The total elastic cross section (TEC) and the momentum transfer cross section can be derived knowing the DCS. The TEC is given by the area under the curve of DCS x $2\pi \times \sin\theta$ against θ. Similarly MTC can be also obtained using the definition (1.12).

So far, we have been discussing certain general aspects of the experimental methods in the field of scattering processes. There is a belief that the real test of knowledge is in the experiment. Hence, new theoretical work seeks a comparison with experimental data. Thus new theoretical methods can lead to more experiments which may be confirmed through the agreement between the two. Because of this correlation between theory and experiments, a theoretical worker has to be fully aware of the experimental developments. Hence, in what follows, I have tried to scan through the very recent experiments pertaining to our area of interest. These experiments are later on referred to for comparative purposes.

The first absolute measurements forthe DCS in the electron hydrogen scattering at high energies was done by Williams (1975). It should be remembered that eventhough the theoretical description of e^{-}-H collision is simple, the experimental study of the system is not simple. Williams made the experimental measurements below n = 2 level of H atom, thus not allowing the inelastic and resonance effects. He has reported the results in the upper energy region from 20 eV to 680 eV. Since the 2S and 2p states of hydrogen appear essentially identical in the energy loss spectra, it is difficult to measure the cross sections corresponding to these states separately. Williams (1981) later on extended his experiments to 2S and 2p state excitation of H-atom. Williams and Willis (1975) have measured the DCS for the n = 2 excitation (2S + 2p) in atomic hydrogen.

Van Wingerden et al (1977) reported the absolute data for e - H_2 elastic scattering above 100 eV for the first time and recognised its importance to derive elastic e - H scattering cross sections. He has reported the total elastic cross sections as well and could point out the discrepancies between theoretical and experimental results in terms of certain physical effects not covered in the then existing theories. The authors have reported the results for e - H scattering DCS at the energies 100 eV and 200 eV alongwith the corresponding TEC values.

The measurement of DCS for the super elastic scattering in H-atom is in itself difficult practically. As such no reliable experimental results are available so far.

As mentioned earlier, He being monoatomic, the experimental study of $\bar{e}$ - He scattering is simpler than that for Hydrogen target. As such, a wealth of experimental data is at our disposal. To mention a few, the works reported by Bromberg (1974), Mc Conkey and Preston (1975), Kurepa and Vuskovic (1975), Dalba et al (1979), Blaauw et al (1980), Jansen et al (1976), Register et al (1980) etc. are the latest results in the high energy region. Going from He to Li target, experimental study becomes much more difficult as is evident from the scarcity of experimental data for Li target. Williams et al (1976) have reported the absolute measurements for $\bar{e}$ - Li elastic scattering at 20 eV and 60 eV. Hence high energy workers are confronted with the problem of non-availability of experimental data for comparative purposes.

Electron - Sodium atom scattering is another process taken up in the present thesis work. For this process, fortunately enough, there has been a very recent revival of interest in the field of experiments. Teubner et al (1978) and Sirvastava and Vuskovik (1980) have reported the experimental data measured at 54.4 eV and 100 eV. Again there is lack of data at high energies which are of major importance in the present work.

Certain general remarks are worthy of metnion at this juncture. Many of the theories show up discrepancies in their predictions of the forward DCS and it is exactly in the forward direction that no experimental data exist for any collision process. There are practical problems involved in this type of measurement. As such measurements generally go down to a minimum of 5° angle of scattering, a remarkable exception being the work of Bromberg (1974) who secured a minimum of 2°. Similarly, the general maximum of scattering angles in the experiments is 130°.

The total cross sections are generally expressed in units of a_o^2 or πa_o^2 where a_o is the Bohr radius. This is in accordance with the atomic units where 1 a.U of energy is equal to 27.2 eV. Similarly DCS values are in units of a_o^2 per steradian (a_o^2 Sr^{-1}).

At a fixed energy for a particular target atom, the DCS shows a strong peak in the forward direction and fall off rapidly with increasing angles. The backward scattering is sometimes 3 to 4 orders of magnitude smaller compared to forward scattering. However, the cross-sections depend greatly on the atomic number of target and on the incident energy. For example, in the case of Na target at 54.4 eV, the DCS curve shows a dip around 100°, and the DCS increases with still higher scattering angles, instead of falling off smoothly. These types of variations themselves provide further motivation for the search of the physics governing them.

Eventhough, the DCS values only can exhibit the real nature of the scattering process, the TCS measurements are also significant. For example, because of the relation between the TCS and the imaginary part of the forward elastic scattering amplitude, the imaginary part can be checked making use of the experimental values for TCS. Surveying through the experimental work done on electron-atom collisions, it can be easily felt that much remains to be investigated especially with respect to complex atomic targets. The recent rate of progress in the field is a healthy symptom. For theoretical workers, the absence or scarcity of experimental data on a desired system is always a discouraging factor. However, maiden attempts by theoretical workers can boost up corresponding experimental work also. The option for comparison of a theoretical work with another theoretical method is also there.

After the fundamental discussions of the foregoing sections, we will now turn to the applications of the study of the electron-atom/molecule collisions.

1.5 Applications of the Study of Electron Scattering by atoms and molecules :

Electron-atom/molecule collision is directly or indirectly involved in many spheres of Science. Electron-atom collision is more fundamental than electron-molecule collision, but there exists a strong binding or inter-relation between the two. Hence, the fields of application of electron-atom collisions and electron-molecule collisions are almost identical in a general spirit.

The cumulative effects of electron-atom/molecule collisions in a gas would be to change the macroscopic properties of the gas. Hence, quite a few of these macroscopic phenomena can be interpreted in terms of the collision processes. For example, the electrical conductivity of an ionized gas depends on the number of free electrons and their frequency of collisions with molecules. The frequency, in turn, depends on the momentum transfer cross-section.

In the present day energy crisis, the magnetohydrodynamic (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.

The mechanism for the cooling of interstellar gases can be understood through this branch of physics. The rotational exictation in molecules and the resulting loss of energy via radiations occur due to the thermal balance in an ionized gas when the electron temperature exceeds the neutral particles' temperature. This is being recognized as a possible mechanism for the cooling of interstellar gases. The effect of electron-molecule collisions on spectral intensity of molecular clouds was recently studied by Bhattacharya and Barua (1982). This is useful in the estimation of the electron concentration and kinetic temperature of these objects.

In laser systems, the electron-impact excitation of various modes of CO_2 molecule and other species are required to be known. The low electron capture has been found useful in understanding certain biological phenomena. In electron attachment and detachment processes, the fact that the field of dipole molecules can bind an electron if the dipole moment is sufficiently large, plays the key role (Crowford and Koch 1974).

The atmospheric gases like H_2, O_2 and N_2 are also prominent in other planets as well as inter-stellar space. The spectral characteristics of their radiations tell us of physical conditions therein. The emitted radiations depend on transitions to various atomic or molecular levels and these, in turn, are caused by various electrons like photoelectrons and secondary cosmic ray electrons colliding with them. Similarly various phenomena like Aurora Borealis observed in different parts of our earth's atmosphere are the results of complicated interactions of charged particles with atoms and molecules of the atmosphere.

The electron scattering cross sections by atoms like C and N as well as alkali atoms are useful for fusion research and plasma physics work. Energy degradation of electrons passing through a medium is an important aspect in radiation physics and dosimetry. Experiments on electron diffraction have been used to understand the structural properties of complicated molecules (Massey et al 1969, Chandra 1979).

The most general process occurring in collision physics are those of equation (1.6) and its variations. The electron - atom collision is a particular case of the class of collisions described by (1.6). Hence, more knowledge in the case of $\bar{e}$ - atom collisions will serve as guidelines for the general class of phenomena (1.6). The chemical reaction is a macro version of the collision process of the type (1.6). Hence, the study of atom-molecule and molecule-molecule collisions can lead to a better understanding of chemical reactions.

On most ofthe occasions, electron - atom collision theories pave the way for electron - molecule collision theories. On the contrary, methods also exist for the reduction of $\bar{e}$ - molecule problems to appropriate $\bar{e}$ - atom problems. This line of approach has been useful in treating solids and complicated surfaces (Siegel et al 1978).

From the foregoing discussion the applications of the study of electron-atom (molecule) collisions in divergent fields are brought out in brief. The prominence of this branch of physics is in itself sufficient motivation for one to enter into the branch. Within my own limitations, I have picked up a small area in the huge branch of collision physics - i.e. "electron - scattering by atoms". How I came across with the particular problems in this area studied by me - that will be mentioned in the section to follow.

1.6 Approach to the Problems taken up in this Thesis :

During the course of literature work with the general title of "electron - atom scattering" in mind, it was observed that the recent trend is towards the development of medium and high-energy methods. Interestingly enough, almost all of the work constituting the present study has been carried out in this energy region. While going through the extensive literature available on the topic, it was felt that modifications are possible in the basic frame work of some of the existing theories or even a new theory could be built up. Sometimes, the confrontation with a successful theory reveals that a parallel approach within the frame work of another basic approximation may be equally or even more successful. In certain cases, I felt the need to explore certain known theories fully by application to a variety of scattering phenomena with a view to either solve some puzzles associated with the theory or to develop a parallel approach opening up to a new theory. In yet another circumstance, I found that a relatively new and interesting theory has come up which looked promising enough, thus creating the temptation to apply the theory as a test-case to simple cases of atomic targets. These were some of the approaches by which I took up specific problems in the area. The problems undertaken are briefly introduced in what follows.

The Unitarised Eikonal Born Series (UEBS) approach (Byron et al 1982) was proposed as a successful theory. Its major drawback is the computational complexity. Keeping in mind the simplicity of the Glauber Eikonal Series Method of Yates (1974), I tried a parallel term-wise analysis of the UEBS Series, thus proposing a Modified Glauber Eikonal Series (MGES) method. This method retains the very simplicity of the GES method, incorporates the Wallace Correction - which is the major attraction of the UEBS method - and includes exchange effects. To asses the suitability and success of the newly proposed MGES method, I have applied it to a variety of scattering phenomena - electron scattering (elastic) from H (1S), H (2S), He and Li targets and inelastic scattering in hydrogen atom. All this constistutes chapter III of the thesis.

The High Energy Higher Order Born (HHOB) approximation was another relatively new and promising theory put forward in the recent past. It was an attempt to evaluate the higher order Born terms in the lines of the Glauber theory. I have taken up this newly proposed theory as one of the venues of exploration. Detailed analysis of the method was done with respect to application to $\bar{e}$ - H scattering with a view to understand the theory fully. The advantages and disadvantages were enumerated. Thereafter, my attention was naturally drawn towards the remedies for the disadvantages. The success of the Wallace correction (Wallace 1973) in improving the Eikonal theory tempted me to explore the feasibility of a similar trajectory correction in the HHOB approximation also. The Wallace corrected HHOB method was applied to the case of e - H elastic scattering as a practical test.

Yet another method for improving the HHOB method was attempted along the lines of the two potential Eikonal (TPE) approximation. First of all, to study the TPE approximation itself in a better way, the particular problem of e - H (2S) elastic scattering was studied using this approximation and reasons for the improvement of the TPE method over the basic Glauber approximation were studied. Thereafter, a parallel two - potential formulation in the framework of the HHOB method was developed. The new formulation was applied to the case of elastic scattering of electrons from H and He as test cases.

The modified Born approximation proposed by Junker (1975) has become popular because of the simplicity of the method. Later on, the effects of polarisation and exchange were also incorporated and the method was used to study the elastic and inelastic scattering of electrons by light atoms successfully. A recent development in this approximation was the work of Kaushik et al. (1982) who reported that the MBA is a complete failure for heavier atoms like C, O and Ne. Hence more studies in this regard were necessary to draw a definite conclusion. With this idea, the MBA was applied to the alkali scattering and the scattering in hydrogen H (2S-2S) as a bid to understand the missing link between the successful results obtained for the lighter atoms and the discouraging results arrived at for heavier atoms.

The various studies performed as above based on the Born approximation constitute the fourth chapter of the thesis. So far, the studies were conducted on light atoms only and the need was felt for further studies with heavier atomic targets. The alkali atoms were chosen because of their challenging nature, practical significance as well as the scarcity of data available on them. The sixth chapter is completely devoted to the study of electron-atom scattering with more attention to the Na atom. Interesting consequences were also drawn.

In the foregoing discussion, the choice and approach to the problems studied in the thesis are briefly introduced. To summarise the first chapter, a brief introduction on the background of the study, the experimental aspects, the significance and motivation for the present work and an approach to the problems considered are covered. In the next chapter, some high energy theoretical methods are discussed.