Chapter 1

Introduction and experimental aspects

1.1 Resume

Theoretical studies of scattering of particles like electrons from atomic and molecular targets, are now acquiring an important status in the sphere of scientific activities, the world over. Some aspects of this kind of study are attempted in this thesis, in which, not only the boundaries of this bound volume, but also the upper bound of my abilities, form a limitation. The contents of the present thesis are summarized as follows.

The first chapter begins with a resume of various phenomena observed in the scattering of particles by atoms and molecules. Experimental quantities are defined and an outline of applications of the electron atom molecule collision physics in various fields is given. Some experimental aspects are taken up, briefly. The second chapter deals with those aspects of the scattering low-energy electrons, where the high-energy methods are used. This discussion will be mainly pertaining to molecules. The third chapter is concerned with the intermediate and high incident-energy region. It covers the studies on elastic scattering theories, with its applications, ranging from Hydrogen and Helium atoms to complex atoms like Oxygen. The elastic scattering of fast electrons by molecules is also considered in the next chapter, i.e. chapter 4, where a high energy method, called the independent atom model, is utilized. The chapter 5 deals with inelastic scattering of electrons by atoms and molecules, in particular, atomic and molecular hydrogen. In the last chapter, I have given a summary of the whole thesis and have drawn conclusions, so as to point out the new venues opening up as a result of the present work.

1.2 Scattering Processes

Consider the physical processes that would occur when a single particle, say an electron, collides with a single atom or a molecule. If 'e' represents a projectile electron and A is the target, i.e. a free atom or a molecule, (i.e. in gas-phase) then the simplest possibility is given by

$$e + A \longrightarrow e + A \qquad (1.1)$$

Here, the electron interacts with the target in such a way that the total kinetic energy of the reactants (incident electron plus target) is the same as that of the products (outgoing electron plus the same A-particle). If the electron suffers a change in its direction, in the above process, then it suffers an energy-loss due to conservation of linear momentum. For an electron colliding with a heavy particle like an atom or a molecule, this loss of energy is quite small, being dependent on m/M, where 'm' is the electronic mass and M is the mass of the target atom. The process described above is the elastic scattering of the electron by the target. A possibility should not be missed here, and that is the exchange of the incident electron and one of the electrons of the target 'A'. In that case, the process would be called elastic scattering with exchange.

In the inelastic collision, a part of the kinetic energy of the incident electron is transferred as the internal energy of the target and the latter attains one of its excited states. If A and A^* are respectively the initial and the final states of the target, then the inelastic scattering is represented by

$$e + A \longrightarrow e + A^* \qquad (1.2)$$

The energy of the scattered electron correspondingly decreases. If A is an atom, its electronic state can be excited in the above process, while if A is a molecule, then any one or more of its rotational, vibrational or electronic degrees of freedom can be excited. Again here the exchange of electron is also a possibility,

A collision is called superelastic if the electron hits a target already in an excited state, e.g. a metastable atom, and if this results into transfer of energy of the target to the electron. This is given by,

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

As an extension of the inelastic collision, we can think of ionization of the target by the incident electrons,

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

or, attachment of the projectile to the target,

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

etc. One can think of many more phenomena like electron-capture, dissociation, dissociative attachment in molecular targets, etc. In fact, the most general process of this class of phenomena would be,

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

where A, B, C and D are different (or the same) particles, atoms, molecules or one or two of them can be even photons.

Here we have only described the different processes that are possible. It must be borne in mind that they can actually occur in accordance with the well established conservation laws and follow certain fundamental rules like the Pauli exclusion principle etc. The term 'channel' means a possible mode of fragmentation of a system, e.g. (A + B) in eqn. (1.6). Thus, eqn. (1.1) shows the elastic channel eqn. (1.2) shows the inelastic channel etc. A channel is said to be open, if it is allowed by the conservation laws.

1.3 Cross-sections for Collision Processes

From the viewpoint of Physics, the collision processes are quantified and studied in terms of certain parameters or quantities, usually called cross-sections.

Total collision cross-section σ_{tot}

Consider eqn. (1.6), in general. A beam of well-collimated, fairly monoenergetic A - particles, with a reasonable beam-intensity is directed towards the target of particles B. Each scatterer acts individually, under the assumption that its number-density is small enough, and further the target material is thin. After the scattering event, the scattered particles C (and D) are registered in a detector at a macroscopic distance. Let N_A denote 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 no. of particles A, crossing per unit time, a unit area, normal to the beam-direction and fixed relative to the target. Under the assumed conditions, N_A is proportional to ϕ_A and n_B. The total (collision) cross-section σ_{tot} for scattering of particles A by target B is defined through,

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

Thus, σ_{tot} is the no. of particles A interacting with the target B per unit time, per scatterer, per unit relative incident flux. The total collision cross-section is related to the probability that an incident particle interacts with a target particle and has therefore been removed from the incident beam. A more detailed insight into the nature of interaction between the incident and target particles can be gained through differential cross-sections.

Differential scattering cross-section (DCS)

Consider elastic scattering. Let, dN denote the no. of particles A, scattered elastically per sec within a solid angle dw about the direction (θ, ϕ) relative to the incident direction as Z axis. Then, as in the case of eqn. (1.7),

$$dN = \phi_A \; n_B \; dw \; I(\theta, \phi) \tag{1.8}$$

Here, I(θ, ϕ), also written as $d\sigma(\theta, \phi)/dw$ is the elastic differential cross-section, to be abbreviated as elastic DCS. The DCS for any other channel may be likewise defined. To define the DCS of collision of any two particles, in general with different (finite) masses, it is required to specify the co-ordinate system i.e. laboratory frame or centre of mass frame, but for electron collisions with atoms or molecules, the two frames are idential. The DCS is related to theoretical 'scattering - amplitudes'.

Total elastic cross-section (TECS)

This is obtained by integrating the DCS over all solid angles, i.e.

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

Already we have defined the total collision cross-section. In the particle-atom collision, several processes (reactions) can occur, so that, we have to define,

$$\sigma_{tot} - \sigma_{el} = \sigma^{r} \qquad (1.10)$$

as the total reaction cross-section, for all non-elastic channels. It is also denoted by σ_{inel}.

Momentum-transfer cross-section: σ_m

Often for low-energy work, the momentum transfer (or diffusion) cross-section is defined as,

$$\sigma_m = \int \frac{d\sigma}{dw} (1 - \cos\theta) \, dw \qquad (1.11)$$

Here, the factor (1 - cos θ) comes from the momentum, transferred by the projectile in the incident direction, during elastic scattering. This factor changes somewhat for inelastic processes, as follows.

$$\sigma_m = \int \frac{d\sigma}{dw}\left(1 - \frac{k_f}{k_i}\cos\theta\right) dw \qquad (1.12)$$

where, k_i and k_f are the magnitudes of the incident and scattered electron wave-vectors. Again here, the factor ($1 - k_f/k_i \cos\theta$) results from the transfer of momentum in the incident direction. Lastly, it may be noted that for some specific purposes, cross-sections averaged over, say magnetic substrates etc. are also defined.

1.4 Experimental Aspects

Now, let us see in an outline, how the cross-sections for the electron scattering are measured. A typical set-up for measurement of cross-sections must consist of the following :

1. a source or an electron-gun, generating an energy-selected beam of electrons,
2. instrumentation for generating target species and measuring its density,
3. detector assembly for detecting and analysing the final products with respect to the

energy etc.

4. peripheral electronic devices.

The measurements are done in a vacuum, where the pressure is of the order of 10^{-8} torr, making sophisticated vacuum techniques, an important part of the whole set up. Various typical parts of the modern set up are summerized on a separate chart titled 'Experimental set-up for electron-atom-molecule-collisions'.

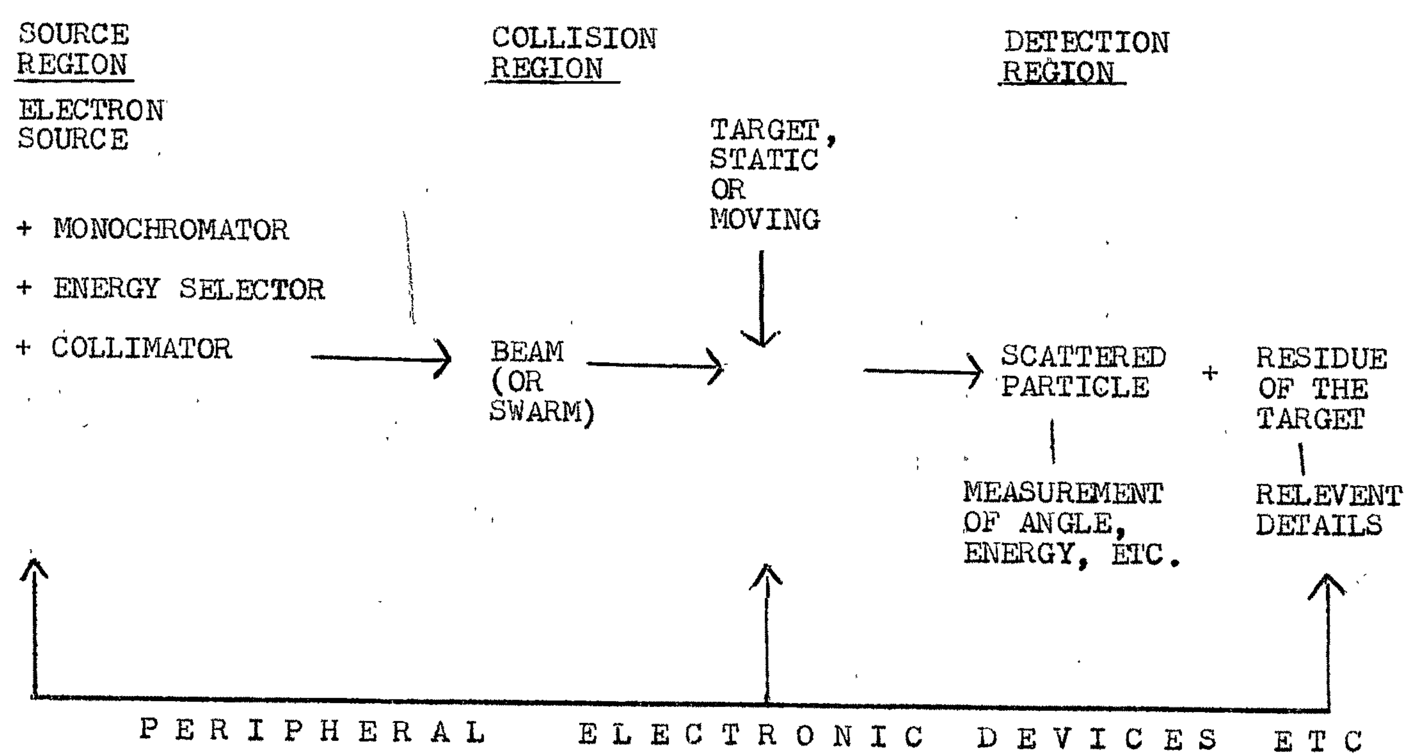
The experimental methods, as well as some of the results, are well discussed in 'Atomic and Molecular Radiation Physics' by Christophorou (1970), and also by Massey, Burhap and Gilbody (1969). This aspect will now be touched here briefly.

Experimental methods for collisions of particles with atoms and molecules, broadly fall into three categories, as under :

1. Electron swarm experiments.
2. Electron beam experiments.
3. A suitable combination of the swarm and beam methods.

Let us understand the basic differences between the swarm and the beam methods. The electron swarm experiment is meant for low electron-energy work,

EXPERIMENTAL SET UP FOR ELECTRON-ATOM-MOLECULE COLLISIONS



nearly or below ≈ 1 eV. At these energies, it is extremely difficult to obtain fairly monoenergetic beam of electrons. Hence, a swarm of electrons, having a wide distribution of energy is utilized. A pulse of such electrons, say from a photocathode, enters a gas under investigation, at a relatively high pressure. These electrons undergo many collisions and diffuse into the gas medium. The electron-swarm drifts through the gas under the effect of an applied electric field. The velocity of the centre of mass of the electron-swarm is called the drift velocity. The problem of a theoretical physicist is then to relate the macroscopic behaviour of the electron-swarm to the quantities defined for a single collision (see e.g. Altshuler 1957, Fabrikant 1976, 1977). Three methods are well-known in the swarm experiments :

1. the drift-velocity method,
2. the diffusion method,
3. the microwave method (from thermal to several eV).

The desired cross-sections defined for a single collision process, and derived through indirect and sometimes elaborate procedures. From swarm experiments, the following quantities are obtained :

1. the momentum transfer cross-sections,
2. the total inelastic cross-sections,
3. the attachment cross-sections.

It must be emphasized that these results are obtained as a function of mean energy of the electron-swarm. It becomes essential, therefore, to have a knowledge of the energy distribution of swarm-electrons. A simple assumption would be the Maxwellian distribution. Other distributions have also been developed but the question has still venues open. In swarm experiments, the finer details to be gained upon a slight variation of the incident energy, will remain obscured. The importance of swarm experiments is appreciated a lot in view of the fact that slow electrons colliding with molecular targets, can still excite rotational and vibrational modes of motion. On the other hand, below the electronic excitation levels, the slow electron scattering from atoms would be only elastic.

We now mention about the electron-beam experiments which are more direct, and performed with an almost monoenergetic beam of electrons. These are essentially single collision-type experiments, and here the sample gas is free from any external fields. In many cases, of course, with recent exceptions, the beam experiments, provide relative values of measured quantities.

The beam experiments are hardly possible, on the other hand, below 1 eV. The following are the well-known methods in the beam experiments.

1. Single beam method for total cross-sections.
2. Single beam method for differential cross-sections.
3. Crossed beam methods.

The history of beam experiments, dates back to Ramsauer and Kollath's experiments during 1921 (Massey et al. 1969). However, changes in the beam methods are always being made looking to the need of particular cases under study. Viewed in that way, one must mention two more classes of beam experiments, viz. the threshold-electron excitation method and the electron-energy loss method. In a simple form, the well-known Ramsauer's experiment (see e.g. Massey et al 1969) consists in allowing an electron-beam to be absorbed in a gas or vapour. However, if we are interested in studying electron scattering from species of atoms not available in atomic form, then beam of pure atoms is also required, and further the two beams must cross each other generally at 90°, to ensure collisions. In recent years the crossed-beam methods have been quite extensively used for cases like atomic hydrogen, oxygen etc. Let us note at this stage that experiments with molecules like H_2, O_2 etc. are in a way easier to perform as compared to those with atomic hydrogen or oxygen targets, because H_2 or O_2 molecules are easily available and stable compared with their respective atomic forms. Further we note that the atomic beam methods are also found to be useful for studying electron-scattering from monoatomic gases for which the above mentioned problem does not arise.

Now, if we are interested in the measurement of total cross-sections, then we perform a crossed-beam experiment and obtain the attenuation (i.e. loss of intensity) suffered by the electron-beam due to collisions with the atomic beam. Alternatively, the attenuation of the atomic beam by the electron beam can also be measured. In an early experiment, the measurement of total cross-sections for the electron-hydrogen atom case was made by Brackmann, Fite and Neynaber (1958), by measuring the current of scattered electrons. The other alternative, that of measuring the attenuation of the atomic beam, was used up by Perel, Englander and Bederson (1962) for alkali atoms. Here detection of the atoms is made possible by ionizing them and mass-analysing the positive ions. (Sunshine et al 1967). We also make a passing remark here about total cross-sections, and that is the 'fine structure' or sensitive variations of total cross-sections relative to small changes of energies, in a certain energy range. The study of this kind has been made by designing sensitive energy-analysers or monochromators. We do not mention here any aspect of measurement of total cross-sections for inelastic processes i.e. excitation and ionization of targets.

It has been recognized that more Physics is contained in differential, cross-sections rather than total cross-sections, hence experiments are designed for measuring angular distributions of electrons scattered from a target. Thus, the electron detector is generally required to be capable of analysing the electrons with respect to energy and scattering angle. A particular care must be taken to investigate the scattering near the forward direction as well as in the backward direction. Earlier on a very small angle scattering was investigated in the experiments of Geiger (1963). One might wonder how at all the scattering in the backward direction i.e. at 180° could be observed, expecting the interference with the incident beam, but that was studied by e.g. Gagge (1933). Further, crossed-beam methods are also successfully applied in the case of differential cross-sections. Some of them are mentioned later in this chapter.

At least two comments are worthy of note, both of them in an identical spirit. Firstly, 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, otherwise in the phenomena of fine structure, the true nature of the quantities will not be revealed. Secondly, the resolving power of the electron-detector as regards energy is required to be high, or else, in cases like rotational or vibrational excitations, the electrons suffering minute energy-losses may not be distinguished, or in other words, the cross-sections determined in that case would not be truely elastic. They are sometimes referred to as energy unresolved cross-sections. Lastly, the total cross-section is derived from the area under the curve of DCS x $2\pi \sin \theta$ against 'θ'. The momentum transfer cross-section is also obtained similarly from its definition. One can be mathematically more accurate in determining the area under the curve.

In the above discussion on experimental aspects, we have avoided describing experiments by particular groups of workers. It must be admitted however, that in science, the real test of all knowledge is an experiment. Hence, it will be instructive to have a bird's eye view of some recent experiments, also since they find references in our work to be described, in the chapters to follow.

1.5 Some of the Recent Measurements

Quite arbitrarily here 'recent' means the year 1975 onwards, although, a significant progress has been made in the last 15 years or so. In what follows, no attempt has been made to describe the apparatus etc. One finds an interesting pattern that, just as new theoretical work seeks to get an agreement with experimental data, so too, a new measurement is saught to be confirmed through the theoretical results. We now take up some of the recent experiments, in electron-atom-molecule collisions.

Experiments of Williams (1975)

In these experiments, measurements were done for electron scattering from atomic hydrogen in two ranges of incident energy,

1. below $n = 2$ level of hydrogen atom, thus not allowing the inelastic and 'resonance' effects,
2. in the upper energy region, from 20 eV to 680 eV. Interestingly, the theoretical description of electron-hydrogen atom collisions is simpler, but the experimental study of the system is not so simple. Here, absolute elastic differential cross-sections were measured in the angular range from 10 to 140 degrees. A cross electron and the

modulated-atom beam were employed and momentum analysis of the incident and scattered electrons was carried out. Atomic hydrogen was obtained by dissociation of H_2 molecules at a high temperature and 90-96 % purity was secured. These were the first absolute measurements for the e-H case, at high energies. The experiments were later extended to 2S and 2p state excitation of H-atoms.

Experiments of Srivastava et al (1975)

These were one of the first experiments in the intermediate energy range for electron-molecule interactions. A well-defined crossed-beam geometry was used for measurements of elastic DCS relative to those of He, and then absolute DCS of He were used to derive absolute elastic DCS for e-H_2 system in the energy range 3-75 eV and angle 20° - 135°. Integral and momentum transfer cross-sections were also reported. Rotational transitions were not resolved. Various experimental errors were summarized, making the whole presentation quite a reliable one, within its errors. Later the experiments were extended to electron scattering from N_2, (Srivastava et al 1976), where one also finds a summary of experiments on N_2 upto that date. All the cross-sections are given upto ranges similar to e-H_2 data. In passing we note that elastic e-N_2 cross-sections were also measured by Hermann et al (1976) with additional results of total collision cross-sections.

Experiments of Van Wingerden et al (1977)

The absolute elastic differential cross-sections were obtained for molecular hydrogen, by allowing the electron beam to scatter in a collision chamber containing the hydrogen gas. The energy range was between 100 eV and 2000 eV. and angular range between 5 and 50 degrees. These results, together with previous measurements were used to obtain a new set of data for atomic hydrogen, through the independent atom model. For the first time, absolute data for e-H_2 elastic scattering were obtained above 100 eV and its importance was recognised to derive elastic e-H scattering cross-sections. Total elastic cross-sections were considered as well, and extensive comparisions were made, both with theory and experiment. Also plotted was the graph of (σ_{el} x E) against energy E. Discrepancies between theories and the reported experiments were pointed out in terms of certain physical effects not covered in the then existing theories.

Experiments of Shyn and Sharp (1981)

Angular distributions of electrons by H_2 molecules were measured by a crossed-beam method, in the energy range 2 eV - 200 eV and angular range -96° to $+156^{\circ}$. The energy resolution of scattered electron measurement reported is quite high, so as to enable the detection of rotational or vibrational transitions. The results, especially at low energies, are at variance with previous results. Momentum transfer cross-sections are also obtained upto 200 eV. Later on, (Shyn et al 1982) the experiments have been extended to O_2 molecules.

Experiments of Daimon et al (1982)

$e-O_2$ elastic differential cross-sections are measured between 200 eV and 500 eV and between 4° and 150° scattering angles by the crossed-beam method. These relative DCS are normalized with respect to the absolute ones given by Bromberg (1974). A special care is taken here to measure small angle scattering, as it is needed in connection with the analysis of 'intra-molecular' or multiple scattering. The above outline is sufficient to indicate a surge of activities on the experimental side in the recent past.

1.6 Some General Remarks

We thus see that, a wealth of experimental data is now at our disposal. Some general remarks about various cross-sections are made below.

1. A word about units. The total cross-section and the momentum transfer cross-section are generally expressed in terms of a_o^2 or πa_o^2 where 'a_o' is the Bohr radius. The differential cross sections are expressed in a_o^2 per steradian (a_o^2 /Sr). These are in accordance with the atomic units (a. u.), in which m = e = h = 1, and 1 a.u. of energy is equal to 27.2 eV. In a.u. the momentum h<u>k</u> of an electron becomes <u>k</u> itself and its kinetic energy becomes 1/2 k^2. The 'rydberg' unit of energy equals 13.6 eV.

2. All the cross-sections depend on the atomic number of the target and on the incident energy. Depending on the target, the total cross-sections show typical resonant structure around the excitation thresholds. At high energies they tend to fall off more or less smoothly. An explanation of such a behaviour in terms of a quantum mechanical theory, is in itself a triumph.

3. At a fixed energy and for any particular target (both atomic and molecular), the DCS show a strong peak in the forward direction and fall off rapidly with increasing angles. Compared to forward scattering, the backward scattering may be 3 to 4 orders of magnitude smaller.

4. At least in molecular targets like N_2 and O_2 it is observed that the fall of DCS with angles, at a fixed incident energy, is exponential near small angles (θ) and it can be represented by $e^{-a\theta}$, with the parameter 'a' depending on energy (see Daimon et al 1982, Herrman et al 1976).

5. Later on we will show that 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. Admittedly, there are practical problems involved in this type of measurement, say, regarding finite angular resolution and the like. All the same, the 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°.

Furthermore, scattering data are also rare at very large angles, say beyond 130°.

6. Further in continuation with (5) above, we note that the total collision cross-section is related to the imaginary part of the forward elastic scattering amplitude, through the famous optical theorem. Hence, if the total cross section is determined experimentally, we can test at least the imaginary part of any theoretical elastic scattering amplitude, in the forward direction. Thus the total cross-section measurements are important.

7. Most of the measurements are done on systems like H-atom (first three states), or atoms like He, Li, Ne and molecules like H_2, N_2, O_2, etc. Besides these, low energy experiments are done on molecules possessing permanent dipole moments, like alkali halides, or on molecules with permanent quadrupole moments like H_2. Thus it follows that much remains to be investigated in complex atomic and molecular targets, for both elastic as well as inelastic scattering of electrons. In this connection let us also note that, looking to the recent progress in this field, a need for an extensive review - article

on collision-experiments is being incresingly felt.

8. We just mentioned about certain resonant structures in total cross-section with respect to energy. In the case of differential cross-section, however, at a certain energy E_c and a certain angle θ_c, for a heavy target, the elastic DCS show a 'dip'. These parameters (E_c, θ_c) are called the critical points of the elastic DCS and they are interpreted in terms of spin-polarization of scattered electrons by the target, (see e.g. Kaushik, 1982b and references therein).

9. In the absence of data on a desired system, one is discouraged to calculate them theoretically. However, as it is being practised, the calculations are done with two different theoretical methods and then compared.

10. In the last decade, experiments have been done on several important molecular targets, but in general the theory e-molecule collisions is lagging behind the experiments.

With these general remarks, let us turn now to the next part of discussion on applications of the physics of collision processes.

1.7 Applications of the Study of Electron Atom-Molecule Collisions

This is one more introductory aspect of general nature that we now take up. In the early part of this century, experiments were performed to study the passage of electrons through gases. It was found that, the assertion, 'faster the electron, more its transmission', was not wholly true. Since those early researches, advances have taken strides in many spheres of scientific activities and needs are felt to study the collision processes. Like every branch of science, this study, too is gaining an "applied flavour" now-a-days. Experiments on electron diffraction have been used to understand the structural properties of complicated molecules. (see e.g. Massey, Burhop and Gilbody 1969 also, Manas Chandra 1979).

fast e^- for ele-microscopy.

Let us focus on the question ; why do we study collision problems ?

Now, quite basically, the cumulative effects of electron-atom-molecule collisions in a gas would be to change certain macroscopic properties of the macro-system i.e. the gas. So quite a few macroscopic phenomena can be interpreted in terms of collision processes. As an example, the properties of a weakly ionized polar gas are governed by low energy electron-polar molecule collisions. The electrical conductivity of an ionised gas depends on the number of free electrons and also on their frequency of collisions with molecules. The frequency in turn depends on the momentum transfer cross-section.

Further, in the present day energy crisis magnetohydrodynamics (MHD) generators have been one of the energy sources. In an MHD plasma, many polar molecules are present and they play a role to determine the properties of the plasma.

In an ionized gas, the electron temperature exceeds the temperature of neutral particles and the thermal balance occurs via rotational excitations in molecules. These molecules, in turn, lose energy via radiation. This is recognized as a possible mechanism for the cooling of interstellar gases. This is also supported by the fact that rotational cross-sections being large, electrons are 10^4 times more effective in exciting molecular rotations, than neutral particles. The effect of electron-molecule collisions on spectral intensity of molecular clouds is recently studied by Bhattacharya and Barua (1982). This can be useful in estimating the electron concentration and kinetic temperature of these objects.

An interesting phenomenon that happens with dipole molecules is that the field of these molecules can bind an electron if the dipole moment is sufficiently large. This fact plays a special role in electron attachment and detachment processes (Crowford and Koch 1974). A good discussion on polar molecules may be found in a review by Itikawa (1978). The slow electron capture has also been found to be useful in understanding certain biological phenomena. Among the other applications of collision studies, we mention the one in laser systems, where the electron-impact excitations of various modes of CO_2 molecule and other species are required to be known.

H_2, O_2, N_2 etc are prominent atmospheric gases, not only on the earth but also of the other planets like Jupiter and Saturn, as well as of interstellar space, and the spectral characteristics of their radiations tell us of physical conditions therein. Now, the radiation emitted depends on transitions ø to various atomic or molecular levels and, these, in turn, are also caused by various electrons (e.g. photoelectrons, secondary cosmic-ray electrons), colliding with them. Closer to home, the phenomena of Aurora Borealis and different properties of different parts of our earth's atmosphere are the results of complicated interactions of charged particles with atoms and molecules, of our atmosphere.

In the phenomena described above, of the interaction of electrons with gaseous matter, in various situations, not only molecules but atoms also are involved, hence electron-atom problems are also important and relevant. They are more fundamental. The electron scattering cross-sections by C, N, O atoms 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.

We have noted earlier that, the most general processes occurring in collision physics are those of eqn. (1.6), and its variants e.g. electron-ion collisions, ion-atom molecule collisions etc. However, the progress in the theoretical understanding of electron atom collisions has been much more, so that these theories serve as guidelines for a general class of phenomena, of eqn. (1.6). The study of atom molecule or molecule-molecule collisions can lead to a better understanding of chemical reactions, because a chemical reaction is a macro-version of a collision process of the type of eqn. (1.6).

Lastly, let us emphasize that electron-atom scattering theories are more basic and progress is continuously being reported in them. Electron atom theories have paved ways for electron molecule theories, in many cases. Methods also exist for reducing electron molecule problems to appropriate electron atom problems. This line of approach has also been successful in treating solids and complicated surfaces (Siegel, Dill and Dehmer, 1978).

The outline of the applications in the above paragraphs is sufficient to motivate a beginner to do work on electron-atom-molecule collisions. However, when one starts peeping into the current literature on the subject, certain specific motivations and aims begin to take a shape in one's mind. In the following passage, I give my reflections on how I approached the problems I selected for my work.

1.8 An Approach to the Problems

Generally in a research work of this kind the following alternatives are open for pursuit.

1. There is already a well established theory before you, and it has been tried in many cases under similar situations, but you find that the theory can still be stretched to some new situation.

2. A relatively new theory has come up, but it requires to be tested for simple cases of atomic and/or molecular targets.

3. You feel that modifications are possible in a basic framework or a new theory can be built up, for a specific purpose.

4. You find that certain simple calculations e.g. evaluation of total collision cross-sections, would be meaningful in some of the 'vacant' or untouched area.

The reason for specifying the above alternatives is that, quite humbly, one or more of them at a time have been tried in the present work. Let us illustrate; it is well known that the Glauber theory is extensively used for high energy collision problems. There are reasons to show that it can work in certain low-energy problems also. In the present work, this theory is successfully used in a low energy problem, viz. that of elastic scattering of thermal electrons by polar molecules via temporary capture.

It is to be noted that in the last five years or so, the interest has been towards the development of medium and high-energy methods and a good amount of literature appears on intermediate and high energy problems. In this connection, the high energy higher order Born approximations of Yates (1979) is a recent attempt to evaluate second and third order terms of the Born series, along the lines of the Glauber theory. This new theory has been applied to simple atoms and the e-H_2 system here. Also in recent years, the independent atom model has been applied to several simple molecules. This is also tried in the present work. Further since simple wave functions are available for ground state H_2 molecule, explicit calculations on the molecular level are done and comparisons are made with the results obtained in the independent atom-model.

The attention of workers these days is devoted to higher order theories, such as the modified Glauber (MG) approximation. In the thesis, we have proposed an MG approach different from that of Gien (1977).

Coming back to the atomic targets it is observed that, the present knowledge of cross-sections for the electron-collisions with atoms like carbon, nitrogen, oxygen etc. is inadequate. Theories put forward in this connection disagree with each other. Also, simple calculations such as those of total collision cross-sections are not performed. It is instructive to carry out these calculations and to try to use them to estimate the electron-molecule cross-sections through the independent atom-model. The experimental results on N_2, O_2, etc. molecules are now available.

Now, in order of simplicity, the problem next to e-H elastic scattering is, the inelastic e-H scattering, leading to 1S —— 2S transition. For the study of this problem, presently a method is devised to calculate the distorted wave first Born approximation. The important consideration here has been to avoid any numerical procedure in the calculations. Further, the exchange and polarization are also included.

Finally, we ~~also~~ have observed one thing that the independent atom model is fairly used for elastic scattering, but not for inelastic electron scattering, leading to (electronic) excitation in molecules. A simple test case would be H_2 molecule, which has been attempted here, but only a few results are found in recent literature for a comparison. Excitations to two of the low-lying electronic states of H_2 by fast electrons are attempted. No data is available for comparison.

We hope that the above discussion elucidates where we stand as we approach the problems attempted in the thesis.

Thus, to summarise, in the first chapter the introductory and experimental aspects were covered, some of the recent experiments were outlined and lastly the approach to the problems considered is discussed. In the next chapter, we go over to the high energy methods in slow electron scattering.