A summary of the thesis

The field of electron scattering by atoms and molecules is now regarded as an important area of theoretical and experimental endeavour. It finds applications in diverse fields of practical interest, such as, atmospheric physics and gas - discharges, plasma physics and magnetohydrodynamics, lasers, molecular structure investigations etc. Hence, there is enough motivation in this active field for one to work. Also, quite a few recent experiments on electron-atom-molecule collisions, give an additional boost to a theoretical worker in this field.

This thesis reports some theoretical investigations on the scattering of electrons by atoms and molecules. This branch of physics now encompasses a wide variety of phenomena and one of the aims of the present work has been to cover a study of some of them. Thus, the thesis may be divided into study of electron scattering by atoms and by molecules, or further, into polar and non-polar molecules as the targets. The thesis can also be classified into work on slow electrons as well as on fast electrons. Similarly, it also divides into the study of elastic and inelastic

processes. Each of these aspects is covered through at least one theoretical investigation.

The first chapter is a resume of various scattering phenomena, their cross-sections and experimental aspects. An informative account of recent experiments of cross-section measurement, done after 1975, is given briefly, with some general remarks on results.

In the second chapter, we first explain how slow electron scattering can be treated in high-energy methods. The interest is centred here around polar-molecule targets. The modified Born approximation of Junker has been applied to scattering of slow electrons by polar molecules. Corrections introduced by this theory over the first Born approximation lead to a further disagreement with experiments, hence numerical estimates are not made. Also evaluated is the second Born approximation for the dipole targets. The method of Dalitz integrals is found to be suitable. This calculation leads to transitions $\Delta j = 0, 2$. For $0 \longrightarrow 2$ case for e + CsCl, the results are close to the Glauber results only near the forward direction. Further, the nuclear excited Feshbach resonance is studied for the polar-molecule targets like H_2O, D_2O, H_2S etc. Though the process studied is elastic scattering, it is known

to occur through the capture of the incident electron followed by the decay of the temporary negative ion, in such targets. This well-known Turner's mechanism, is studied here in the Glauber approximation. The transition probability and the life-time of the temporary binding of electrons are calculated and comparisons are made. After the second chapter, the focus is on scattering of intermediate to high energy electrons, say, in the range of 100 to 1000 ev. We first deal with atomic targets. Though the Glauber approximation has enjoyed immense popularity in this field, it is known to have certain deficiencies. Of the attempts to overcome them, the high energy higher order Born approximations (HHOB) of A.C. Yates, is a recent one. An EBS approach is taken up, with the direct scattering amplitude consisting of the first Born term, the second Born term of the HHOB and the third Glauber term. The differential cross-sections (DCS) for e-H elastic scattering are calculated over different angles and incident energies. Corrections to the present second Born amplitude, viz. that of the trajectory of the incident particle and also for the term $O(k_i^{-2})$ in its real part, are discussed. Presently we have proposed a modified Glauber approach, in which the second Glauber term is to be evaluated with a non-zero

mean excitation energy and the other terms of the usual Glauber approximation are retained. The second term evaluated in this way is in fact the second HHOB term $O(k_i^{-1})$. The consequences of this new amplitude are fully discussed. The present knowledge about the elastic electron-scattering from complex atoms like C, N and O-atoms is inadequate. A simple treatment is given for these targets.

The elastic scattering of electrons by molecules, is studied in the independent atom model (IAM). The elastic e-H scattering amplitudes evaluated in the HHOB are applied along with the exchange, to the molecular hydrogen target. The e-H_2 problem is taken up directly also, by taking a one - centre wave function of the target. The DCS, total elastic cross-sections and momentum transfer cross-sections are calculated and compared. Modifications and extension of IAM to other molecules are briefly treated. Simple calculations for the total cross sections of electron scattering from molecules like N_2, O_2, O_3, CN, LiH etc. are given.

To describe the inelastic scattering of fast electrons by atoms, a new method, based on the

Green's function expansion, is developed, in the frame work of distorted wave Born approximation. This method is applied to 1S $\longrightarrow$ 2S excitation of Hydrogen atoms by incident fast electrons, in the range 50 - 400 ev by calculating the distorted wave first Born approximation including exchange. This treatment is extended by considering the polarization effects by the method of Temkin and Lamkin. Extensive comparisons with other distorted wave methods are made. An independent atom model is described to treat the electron impact excitation of electronic states of molecules. The IAM is used to describe inelastic e-H_2 collisions, employing our amplitudes for inelastic e-H scattering. We have obtained the DCS for the electronic excitation of H_2 molecule to the states $B^1\Sigma_u^+$ and $a^3\Sigma_g^+$ by the incident electrons in the range 100 - 400 ev. There are hardly any calculations for inelastic scattering ~~of~~ by molecules in this range of energy.

Each chapter ends up with a summary and an outline of further prospects. Finally in the last chapter, after a summary, conclusions are drawn and some new venues opening up for further work are pointed out. It is worthwhile reporting below, some of the specific results achieved in the present study.

1. The Glauber method is successfully applied to

a low energy problem. The best agreement so far, with experimental predictions for the life - time of the temporary negative ion formed in the elastic scattering of slow electrons by certain polar molecules (e.g. H_2O) is obtained.

2. The second Born calculation for the point-dipole potential is attempted and interesting consequences are derived.

3. The HHOB is found to give a good accord of elastic e-H and e-H_2 scattering DCS with experimental and other theoretical data, for small scattering angles, upto nearly 50°, beyond which, our calculated DCS are overestimating. The reasons and remedies for this behaviour are discussed. A sample calculation for e-H scattering using the new modified Glauber amplitude proposed, shows a good accord with other higher order theories. Generally all the higher order theories yield DCS falling below the experimental results.

4. In the elastic e-H_2 scattering treatment in the IAM, the effect of varying the nuclear charge Z are noted. The DCS of e-H_2 elastic scattering calculated with a one centre wave function are found to be satisfactory above 200 ev.

5. The total collision cross-sections for Carbon, Nitrogen and Oxygen atoms are calculated in the exact second Born approximation, using the static potentials of (i) Strand and Bonham and (ii) Cox and Bonham. The results in the second case are comparatively lower. The total elastic cross-sections for C, N and O atoms are found to compare favourably with the only available data of Inokuti and McDowell. The total elastic cross-sections of e-Li scattering compare favourably with available data. These results are converted via IAM, into the total elastic cross-sections for molecules like LiH, N_2, CN, O_2, O_3, etc. These cross-sections are overestimating at lower energies (100-200 ev) and are expected to be reliable at high energies. One of the main reasons for this, i.e. the multiple scattering effect, is calculated in a simple way and found to be insignificant for e-H_2 scattering.

6. The results of inelastic e-H scattering, obtained from our DWBA method are comparable to those of other similar calculations. It underestimates the DCS in the forward direction, so a correction is applied, by the method of polarized orbitals. As expected, the polarization-effect enhances the DCS

near forward direction. The experimental data for H(2S) excitation are available only at 54.4 ev. At this energy none of the theories considered, agrees with the data. The agreement of the present $1S \longrightarrow 2S$ DCS with other theories improves at and above 100 ev. There is also a variance in the forward DCS and its energy dependence, in different theories.

7. Perhaps for the first time, an independent atom model is attempted for electronic excitation of H_2 molecules by fast electrons in the range 100-400 ev.

The IAM predicts a lowering of the DCS near the forward direction, whenever the final state of the target molecule, has a nuclear symmetry different from that of the initial state. The IAM fails to produce an accord with available data at 60 ev. We have obtained the DCS of inelastic e-H_2 scattering leading to the final states $B^1\ \Sigma_u^+$ and $a^3\ \Sigma_g^+$ and have compared them with each other. Though the vertical energy difference of these two states is quite small, there is a large difference in the DCS. The main reason for this lies in the different nuclear symmetries of these two states.

All the results presented are furnished with graphs and tables. Extensive comparisons are made with available experimental and theoretical data and the results of other workers are duly acknowledged under 'references'. All the standard mathematical results used are summarized as an appendix.