

Chpater 6

Summary and conclusions

6.1	Towards the end	350
6.2	The summary	350
6.3	Results and conclusions	354

6.1 Towards the End

The last chapter is devoted to summary of the entire thesis and the conclusions drawn, essentially in the spirit of an epilogue. Towards the end of the thesis, the last chapter gives us an opportunity to assess our successes and failures in meeting the targets set up in the approach to the problems. The next two sections belong to summary of the thesis and conclusions respectively.

6.2 The Summary

A basic approach common to all the problems studied in the thesis is the high-energy methods of scattering theory. The energy of incident electron considered is 100-1000 eV with two exceptions; (1) the DWBA theory developed in chapter 5 has been tried at 50 eV also. (2) chapter 2 is entirely concerned with low and thermal energy electrons. A variety of targets is considered here, including atoms as well as molecules. The entire work deals with elastic and inelastic processes, excluding ionization, dissociation etc. In the work presented, the use of computer is limited only to generate the last numbers. At this stage let us mention that, for elastic scattering of electrons by C, N and O atoms, we

had in mind, two plans as follows. (i) to obtain the Wallace-corrected eikonal amplitude using the static potentials and (ii) to obtain the third Born term which reduces to the third eikonal term with the static potentials, by numerical procedures. However, as the thesis goes to submission the outcome in this regard has not been satisfactory. All our results are presented in the form of graphs and tables and adequate comparisons are made. Many of the results presented are inclusive of the zero scattering angle. While, the upper limit of the angle does not exceed 140° .

As far as the text is concerned, due attention is paid to physical aspects and discussion. This is necessary in view of the condensed material usually given in the published works. A list of symbols used, has been given separately. Most of the final results are given in terms of standard integrals, which are given in the appendix.

Now, a summary of the atomic and molecular targets presently investigated, follows.

- * The $e + \text{CsCl}$ (dipole) system was investigated at 4.77 ev, for rotational excitation.
- * The $e + \text{H}_2\text{O}$ (dipole) system was studied for

elastic scattering via temporary capture of thermal electrons.

* The elastic scattering of fast electrons by Hydrogen atoms was studied in details. A simple treatment was also afforded to elastic scattering from C, N and O atoms.

* Among the molecular targets, the elastic scattering of fast electrons from H_2 molecules were studied in detail. Also, a simple treatment was afforded to the elastic electron-scattering by N_2 , O_2 , CN, O_3 and LiH molecules.

* The electron-impact excitation of Hydrogen atoms to 2S state was analysed in chapter 5, in the energy range 50-400 ev. The electronic excitation of molecular hydrogen by fast electrons, leading to final states $B^1 \Sigma_u^+$ and $A^3 \Sigma_g^+$ was studied.

Next, we summarize the different theoretical formulations employed in the present study.

* The first Born and the Glauber approximations have often appeared in the chapters 2, 3, 4 and 5 in various different contexts. These two theories served as guide-lines for further work.

* The second Born approximation is employed in quite

a few different situations. In chapter 2, the second Born amplitude is attempted for electron scattering from a fixed dipole (in the fixed scatter^{er} approximation). Also attempted for this target, is the modified Born approximation of Junker (1975).

* The method of evaluating the second Born term in the high energy higher order Born approximations (HHOB) of Yates (1979) is employed for obtaining the elastic e-H scattering amplitudes. Based on this, a new modified Glauber amplitude has been proposed by us in chapter 3. Corrections to the second Born amplitude in HHOB are also discussed. Further the HHOB calculations are also done for e-H₂ system using a simple wave function of the H₂ molecule.

* Inelastic scattering of electrons by H-atoms is treated in chapter 5, in the framework of DWBA. We have developed a distorted wave first Born approximation by using the Green's function expansion under the high-energy, small-angle assumptions. The exchange and polarization are included.

* The treatment of electron-molecule scattering has remained a more difficult task. An elegant theory making use of atomic scattering amplitudes for molecular problems is the Independent Atom Model, which has been used for

elastic $e\text{-H}_2$ scattering here through the HHOB amplitudes for elastic $e\text{-H}$ scattering. The inclusion of Valance-distortion and exchange has been discussed in details, while, the effects of multiple scattering and nuclear vibrations are discussed in outline. The IAM has been extended to several other molecules and to the inelastic $e\text{-H}_2$ scattering as well. Further, the procedure of including exchange under different types of transitions in H_2 is also laid down.

* Finally the exact second Born amplitude is calculated for Li, C, N and O atoms using the static potentials.

6.3 Results and Conclusions

The purpose of this section is two-fold, viz, to emphasize the specific results obtained in the thesis and to make some concluding remarks based on these results. The points noted below are the conclusions, drawn from the work reported in the chapters 1 to 5.

Experimental aspects

1. As noted in chapter 1, several interesting experiments have been performed by various workers providing a great boost to theoretical workers. It will be surely welcome if a comprehensive review article on experiments in electron-atom-molecule scattering, is published.

2. A general observation pertaining to the literature of the last five years or so, is that there have been more studies on intermediate to high energy electrons, (> 10 ev) as compared to slow electron-collisions.

3. The experimental data on Hydrogen, Helium, some of the inert gases and alkali metals are now available. There remains a gap in the range of atomic no. $Z = 4$ to 9 . Perhaps, that is why the progress in the theoretical treatment of these targets is slow. Among the molecules, LiH is one of the simplest, for which one would like to have experimental results.

Electron-polar molecule collisions

1. While the first Born results prove to be a rough estimate for the various cross-sections of the electron-polar molecule collisions at low energies, the Glauber approximation which is nearly as simple, yields reliable results, for elastic and inelastic scattering (rotational transition). The success of the Glauber theory lies in its inclusion of higher order terms.

2. The Glauber theory is presently applied by us to the nuclear excited Feshbach resonance i.e. elastic scattering, via momentary capture and rotational

excitation, in the dipole molecule. Our theory predicts the life-time of the intermediate negative ion to be nearly equal to the rotational period of the molecule. The large momentum-transfer cross-sections in the case of H_2O , D_2O , H_2S etc. are thus understood to be due to capture of the electron followed by decay of the negative ion formed.

3. From our study, we conclude that the Glauber theory is successful in treating the electron-dipole collisions at low energies and further studies on attachment-detachment processes are warranted. In general, the interest in polar molecule targets seems to have waned, now-a-days.

4. Further, the modified Born approximation fails and the second Born approximation has a limited success in the case of slow electron scattering by polar molecules.

Elastic e-H Scattering in HHOB

1. A new modified Glauber amplitude, (chapter 3) should be more plausible than the MG amplitude on Gien (1977). A sample calculation at 200 ev yields a result in accord with the other similar theories. Further

investigations are required.

2. In terms of the results, the DCS of the HHOB calculation are very good upto $40-50^\circ$ scattering angles beyond which it overestimates experimental and other theoretical data.

3. The reason for this overestimation lies in the term, $O(k_1^{-2})$ of real part of the second Born (HHOB) amplitude. Here, we have suggested a remedy, that for $q > k_1$, this term may be replaced by the real part of the second order Wallace-amplitude. The suggestion is shown to be fruitful.

4. The comparison of different higher order theories with experimental measurements shows that all of them tend to be lower than the measured values of the DCS, especially at large angles. Thus, at present, there is definitely a discrepancy between the experiments and the sophisticated theories for elastic e-H scattering.

5. In the medium energy range, it is required to take into account the projectile-distortion also, apart from the polarization, absorption and higher orders of direct and exchange amplitudes.

Elastic Scattering of Electrons from C, N and O atoms

1. The studies in this area are inadequate.

The polarization can be considered through a model potential, but the other effects are not yet successfully taken into account.

2. We have calculated the total elastic cross-sections for C, N and O atoms by employing the static potentials of Cox and Bonham (1967) and compared the results with Inokuti and McDowell (1974). The accord is excellent. The $e + Li$ results agree with those of Ghosh (1979). However, it is required to have the total inelastic cross-sections (σ_{inel}) to obtain total cross-sections (σ_{tot}) for these targets.

3. Calculations on these atoms have not yet been done using the target wave functions. It is noteworthy that Konaka (1982) has developed a method of evaluating the second Born term without an explicit use of the wave functions.

Elastic $e-H_2$ scattering

1. The independent atom model with HHOB amplitude gives a good accord with experiments and other data, for scattering angles upto about 50° . The characteristics of the atomic scattering amplitudes are reflected here. The valance-bond and exchange effects are properly taken into account, while multiple scattering

and vibrational aspect are \$ insignificant for this case.

2. The corrections in the HHOB amplitude, discussed in chapter 3, introduced via IAM lead to satisfactory results for e-H₂ scattering.

3. As in the case of e-H scattering, we can expect that higher order theories (like the MG formulation) would reduce the e-H₂ DCS, at 100 and 200 ev. However, the effect, as seen from the published results, is not as much as in the e-H case. A sample calculation done by us (chapter 4), using the UEBS amplitudes (Byron et al 1982) in the IAM, predicts the lowering of e-H₂ DCS by the higher order theories for large scattering angles. This suggests that accurate atomic scattering amplitudes must be incorporated in the IAM to derive molecular cross-sections.

4. The TCS, TECS and MTCS for e-H₂ scattering calculated by us are in accord with recent data.

Electron Scattering From Molecules other than H₂

1. For molecules other than H₂ the valance-distortion has not yet been taken into account. Presently we have tried to mock this effect for the H-atom of the LiH molecule, as done in the case of H₂. The other important effect, viz. multiple scattering has been

recently analysed by several authors; this effect reduces the cross-sections at medium energies. However, the multiple scattering should be treated by including the valence distortion.

2. The lower limit of validity of the IAM is presently estimated for several molecules. A simple calculation of TECS for LiH, N₂, O₂, ~~#~~ O₃ and CN molecules is given in chapter 4 and adequately discussed. Generally the results are reliable at high energies. The LiH being a light molecule with a large bond-length, our results are expected to be more reliable.

3. Finally the use of IAM can also be extended to elastic scattering of other projectiles like positrons, protons etc. Not many attempts are made in this direction. For protons, we can show that the IAM holds down to 1 ev. The IAM will continue to play an important role in electron-molecule scattering studies.

The Inelastic e-H Scattering

1. The HHOB is not fruitful for H(2S) excitation beyond 20-30° scattering angle.
2. There have been several attempts to analyse the 1S → 2S process in atomic hydrogen by incident

electrons, using the DWPO methods. In many of them the use of numerical procedures is resorted to. Various relevant aspects are discussed in chapter 5. In essence, there is considerable variance in different theories upto, say 54.4 ev, at which energy, measured values for $1S \rightarrow 2S$ DCS are now available. At 100 ev and above, the DCS become insignificantly small beyond $30-40^\circ$.

3. Our new DWBA results agree with those of Calboun (1976) except at 54.4 ev. Thus, we conclude that the present DWBA method, which makes no use of numerical methods, is quite satisfactory at and above 100 ev, below which, a high energy method such as this, is not expected to be good. Our method can be extended to any system for which distorting static potentials are available.

4. The inclusion of polarization improves the results at small angles. These results are somewhat higher than those of second order eikonal calculations (Unnikrishnan and Prasad, 1982) and DWSBA (Kingston and Walters, 1980). The present work can be extended also by analysing the second order term in our DWBA.

5. The $1S \rightarrow 2p$ cross-sections are not obtained in the present DWBA. These cross-sections are

dominated by the plane-wave first Born approximation, for small angles upto about 15° .

6. The higher order theories such as the Glauber approximation, are in general unsatisfactory for inelastic scattering. These problems together with ionization, offer great challenges to experimental as well as theoretical physicists.

7. From the theoretical point of view, an important restriction on Glauber, HHOB and similar formulations is the two dimensional nature of the momentum-transfer q . At present the unrestricted Glauber theory rests on numerical evaluation of the amplitudes and has not gained a remarkable success.

8. The study of inelastic collisions of charged particles by atoms other than H, He and Li is very much scopeful.

The Inelastic e-H₂ Scattering

1. Compared to rotational and vibrational excitations, the electronic excitations of molecules by incident electrons is much less studied. Quite recently, there have been several attempts. The experimental work is just isolated.

2. Perhaps for the first time, the IAM finds application in our work for $e\text{-H}_2$ inelastic scattering. For the final state $B^1 \Sigma_u^+$ the theoretical and experimental data are known only upto 60 ev. We find that the IAM does not hold at that low energy. No studies are known at and above 100 ev. Hence, we have obtained the DCS of excitation to two states of H_2 by employing our DWBA amplitudes. The valance-bond correction is retained for the ground state.

3. Two results of these calculations are noteworthy. Firstly, if the final state has a 'u'-symmetry, the diffraction pattern is 'inverted'. This reduces the DCS in the forward direction and hence the sharp peak otherwise observed, is missing. Secondly, although $B^1 \Sigma_u^+$ and $a^3 \Sigma_g^+$ states lie close together, the DCS for the former are lower than that of the latter, again because of their different symmetries. The only confirmation about this particular point comes from the experiments of Swick and Karle (1961) on Br_2 molecules. Thus, we conclude that measurements on inelastic $e\text{-H}_2$ scattering are very much required. It will be also interesting, to calculate these DCS theoretically by employing the wave functions.

4. The $1S \longrightarrow 2S$ excitation of one of the atoms

in the H_2 molecule can give rise to four different states, varying in spin and symmetry; there are two symmetries 'g' and 'u', and with each, there can be a triplet and a singlet state. All these must be analysed along the lines of our present approach. Further, $1S \rightarrow 2p$ excitation can give rise to π states of the H_2 molecule. Within the first Born approximation, the $e-H_2$ excitation to these states can be investigated employing the IAM, for small angles upto about 15° . The DCS of these states, will widely differ, these of 'g'-state being very high, as observed presently.

5. The electronic excitation of other molecules will continue to be difficult. ∇ Even with IAM, one needs the atomic excitation cross-sections to begin with. There have been a few very recent attempts to study the electronic excitation and dissociation of N_2 , CO, CO_2 , etc.

6. It will be interesting to initiate IAM studies on the electronic excitation of molecules by other charged particles like protons.

Apart from these conclusions I would like to mention a few points of general nature :

* The study of particle-atom-molecule collisions now covers a variety of processes, targets,

and energies. But the mathematical tools have been more or less traditional. One should incorporate this aspect also in research. As an example, we mention the catastrophe theory of mathematics, which has been employed by Connor (1976) to study the molecular collisions (see also Poston and Stewart, 1979).

* Theoretical results published on any system must be supported by numerical tables. Many times, it becomes difficult to read off values from the graphs published.

* It is my impression that, though the study of electron-atom-molecule collisions is useful in the fields of science and technology, it has not been directly linked with specific projects of practical interest. This sort of connection will lead to more meaningful and channelized, rather than scattered research work. Points like this, should be adequately discussed in the national and international conferences on the subject.

I happily wind up the thesis with an humble remark that the present work will prove to be a modest beginning for me in the direction of continued efforts.