CHAPTER - VI

SUMMARY AND CONCLUSIONS

This chapter is devoted to the summary of the entire thesis and the conclusions drawn. Eventhough the conclusions drawn in the course of the discussions on the previous chapters are pointed out towards the end of the respective chapters, the final recapitulation of the various results obtained/arrived at during the entire study gives us an opportunity to assess the successes/failures in meeting the targets set up at the beginning of the research. Hence, in what follows, a general summary of the thesis, the important conclusions and some suggestions for further work are highlighted.

A basic approach common to all the problems studied in the thesis is the high energy methods of scattering theory. Generally, the energy of the incident electron considered is above 100 eV and in some cases the incident energy is stretched down to lower values due to specific reasons like non-availability of data at higher energies. A variety of atomic targets are considered here and the entire work deals with elastic and inelastic processes excluding ionization, dissociation etc. The computer is made use of extensively, but only to generate the numerical results from the analytical expressions. Most of the final results are given in terms of standard integrals which are given in the appendix. A list of the symbols used has been given seperately and all the results are presented in the form of graphs and tables and adequate comparisons are made. Now, let us go through the various results chapterwise and make some concluding remarks based on these results.

In the first chapter, the choice and approach to the various 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.

The various problems chosen for the present study have to make use of a variety of theoretical formulations which are taken up in the second chapter and the discussions are oriented towards the target problems to be taken up. After a brief introduction on various developments on the theoretical side of the scattering theory and the high energy methods in general, the following approximations are given special attention:

1) The first Born approximation.
2) The Modified Born approximation.
3) The Second Born Approximation.
4) The Glauber Approximation.
5) Glauber Eikonal Series Method.

6) Two-potential Eikonal Approximation.

7) Eikonal Born Series Method.

8) The High Energy Higher Order Born Approximation.

The High Energy Higher Order Born (HHOB) method of Yates (1979), relatively new and challenging, was discussed in full detail with application to e - H elastic scattering in the high energy region. The conclusion is that the method is quite good at small angles of incidence say upto 50°, and thereafter the results are overestimating. The various reasons for this type of behaviour are enumerated and some other related approaches like UEBS method and modified Glauber method are discussed. It was observed that the HHOB method has enough scope for improvement which was tried in a later chapter. The HHOB approximation was formulated using the static potential of the target atoms and the second Born amplitude so obtained was used to find out the differential and total cross sections for the e - H elastic scattering.

Based on the behaviour of the various theoretical approximations, a new method - the modified Glauber Eikonal Series (MGES) method - was formulated in the third chapter. Roughly speaking, a termwise analysis of the wallace-corrected-Glauber-Series (Byron et al, 1982), this method is expected to retain the simplicity of the GES method, remove the shortcomings of the Glauber method and at the same time produce plausible results. The newly formulated MGES method was applied to the following scattering phenomena.

(1) e - H (1S) elastic scattering.

(2) e - H (2S) scattering.

(3) e - He elastic scattering.

(4) e - Li elastic scattering.

(5) e - H inelastic scattering.

It was found that in all the above cases, the results are quite satisfactory. The discussions in this chapter led to further work such as the generalisation for the GES method for the scattering of the electrons from any of the ns or np states of hydrogen atom.

The studies in chapter four are centred around another giant pillar in the field of scattering theory - namely the Born approximation. The modified Born approximation is significant by virtue of its simplicity. The inclusion of polarisation and exchange within the framework of the MBA still retains the simplicity of the method. This method was used to study the scattering of electrons from the metastable state of hydrogen and the ground state of Lithim atom. The results produced had the limitations of the limits of the method used. For Lithim atom, the results were not so good as those for H atom.

During the course of the discussion on HHOB method, it was pointed out that the large angle behaviour of the scattering parameters in this approximation is not satisfactory and hence the need for improving upon the method was stressed.

The success of the two-potential eikonal (TPE) approximation (Ishihara and Chen 1975) served as an eye-opener for a similar modification of the HHOB method. First of all, with an intention to study the TPE approximation in full detail, this approximation was applied to the particular case of e - H (2S) scattering with generalisation to e - H (nlm) elastic scattering. The reasons for the improvement of the TPE method over the conventional eikonal method were enumerated. Thereafter a two-potential method within the frame-work of the HHOB method was formulated. This two potential HHOB (TPHB) method was applied to the elastic scattering of electrons from the ground states of hydrogen and helium atoms. The improvement over the basic HHOB method was studied by way of comparisons.

Another attempt towards the modification of the HHOB method was made by employing a Wallace-type of tragectory correction. The scattering amplitude was derived accordingly and as a test-case e - H (1S) elastic scattering was studied. It was noted that the theoretical DCS curve shifts slightly towards the experimental curve on the application of the Wallace type correction, but the improvement isnot remarkable.

The fifth chapter is devoted entirely to the scattering from alkali atoms, with Na atom in the focus. Various types of approximations are applied to e - Na elastic scattering process and the results are compared with one another. This includes studies in the first Born approximation, GES approximation, second Born approximation, two-potential approximation, Partial Wave analysis etc.

It will be interesting and useful to enumerate comprehensively some of the points brought to light during the work reported in the previous chapters.

(A) <u>Experimental Aspects</u> :

[1] Since theory and experiment go hand in hand, new interesting experiments provide a great boost to theoretical works. The publications of comprehensive review articles on experiments in this field will be really useful.

[2] Many a time, it is observed that the experimental data available for a particular scattering process is limited to certain incident energies only. For e.g. the availability of experimental data on e - Li scattering at 20 eV and 60 eV only persuades theoretical workers to stretch down their high energy limits to lower energy regions. Hence, more rigorous and extensive experimental work has to be done.

[3] Perhaps the progress in the theoretical treatment of some of the target atoms like Na is very slow

due to the shortage or non-availability of their experimental counterparts. Of late, a tendency on the part of experimentalists to embark upon heavier atoms other than the usual hydrogen and helium atoms is evident which is a healthy symptom.

(B) The HHOB Approximation :

[1] The results of the HHOB approximation when applied to e - H elastic scattering are quite good upto the scattering angle 50^{o} or so, whereafter the results are found to be high.

[2] If one puts the average excitation energy parameter $\beta=0$ in the HHOB expressions, the corresponding GES terms will be obtained.

[3] From an analysis of the various terms of the HHOB scattering amplitude, it is evident that the $0(k_i^{-2})$ term of the real part of the second Born term is responsible for the inflated results at large angles.

[4] In the present study, the third Born term is replaced by the third GES term for various reasons. Perhaps the third Born term may take care of the $0(k_i^{-2})$ term mentioned above. The attack on the calculationally hazardous third HHOB term may turn out to be rewarding.

[5] The MGES method proposed in the Chapter III compares very much with the HHOB amplitude, a major change being the replacement of the $O(k_i^{-2})$ real term by the second order Wallace term. The encouraging results of the MEGS method further strengthens the point (3) cited above.

[6] Even though the HHOB amplitude takes care of polarization and absorption effects, apart from them it is required to take into account the projectile-distortion also, especially in the medium energy range. The modified Born approximation (MBA) is one way of taking into account the projectile distortion. The replacement of the first Born term in HHOB by the corresponding MBA term may take care of the projectile-distortion partly, and this is worth-trying.

[7] In spite of e - H (1S) elastic scattering being the simplest scattering problem, at the large angles of scattering the different higher order sophisticated theories as well as experimental measurements deviate from each other thus giving sufficient ground for suspicion of some sort of discrepancy which remains to be investigated.

[8] The HHOB scattering amplitude is derived for static potentials of the target atom and is used to obtain the total cross sections for e-H elastic

scattering. The results are found to be good at high energies because the static potential chosen for this study holds good at higher energies.

[9] The differential cross sections obtained using the static potential for e - H elastic scattering are quite encouraging in the large angle region and compare nicely with experimental data.

(c) Modified Glauber Eikonal Series (MGES) Approximation :

[1] In all the scattering processes studied here using the newly formulated MGES approximation the results are found to be quite encouraging.

[2] The method retains the calculational simplicity of the GES method, but the incorporation of the Wallace term improves the results.

[3] The method can in general be considered as a term-wise analysis of the recent and sophisticated UEBS method (Byron et al 1982). The comparison of the MGES and UEBS results for e-H elastic scattering proves this. The enormous difficulty associated with the analysis of the UEBS scattering amplitude for atoms beyond hydrogen and the relative ease in the case of MGES scattering amplitude are two factors to be considered in the choice of the basic approximation. In this connection, the MGES method becomes much more important.

[4] The UEBS method involves numerical analysis using the computer whereas in the case of the MGES method, all the final expressions can be analytically arrived at.

[5] Incidentally, it was noticed that the MGES and HHOB scattering amplitudes compare with each other except for the $0\left(\frac{1}{k_i^2}\right)$ real term and the third Born/GES term. There is enough reason to attribute the vast difference in the HHOB and MGES results (DCS) to the inclusion of the Wallace term. This point was discussed earlier.

[6] The present MGES method can still further be improved by the inclusion of higher order terms of the Glauber Series. For this purpose, instead of taking the first three terms of the Glauber series, the complete Glauber series should be taken and the second term should be replaced by the corresponding terms in the MGES method. i.e. this amplitude will be $f_G - f_{G_2} + \left\{ 0\left(\frac{1}{k_i}\right)\right.$ terms of HHOB + second Wallace term $\left. f_{W_2} \right\}$

Where $f_G = \sum_{n=1}^{\infty} f_{G_n}$.

This method should be even better than the present MGES method and more plausible than the MG amplitude of Gien (1977). However, it should be mentioned that this type of evaluation for higher atoms cannot retain the simplicity of the GES method-because it involves the evaluation of the complete Glauber amplitude.

[7] In the various scattering processes studied, the second GES term is also analysed to compare it with the imaginary part of the second Born (HHOB) term. Similarly the effects of absorption and polarisation in different scattering processes are evident from the tabular forms displaying the invidivual terms of the MGES amplitude.

[8] In the present method, the second order Wallace term is evaluated in an approximate way for the sake of computational simplicity. The same term may be evaluated without the approximation used here and it has to be tested whether it will make any further improvement in the results.

[9] During the study using MGES method, the DCS using the GES method are also calculated and compared with their Glauber counterparts in such scattering processes where this type of work has not been reported so far.

[10] Finally the generalisations for the H (1S) to H(nS) and H(1S) → H (nP) transitions in hydrogen due to electron impact are also studied in the GES method and the final results are used to obtain the results for 1S - 2S and 1S - 2P transitions in hydrogen.

(D) <u>The MBA Approximation</u> :

[1] In the e - H (2S) scattering and e - Li scattering studied here, the results are comparable with their experimental as well as theoretical counterparts. It was noted that the results are not so good as those obtained by Gupta and Mathur (1978) when they applied this approximation to e - H elastic scattering. This type of cumulative effect may be responsible for the discouraging results reported by Kaushik et al (1982) when they studied the scattering of electrons from complex atomic targets. However, more work has to be carried out to ascertain this conclusion.

[2] The MBA retains the simplicity of the first Born approximation even when polarisation and exchange effects are included as done in this thesis. But the lack of a full treatment for the important absorption as well as polarisation effects is a definite drawback. It should be remembered that the method of polarised orbitals as used in this study cannot be successfully applied in the case of all target atoms.

[3] As such the MBA cannot be used as an independent approximation which can be used to describe a scattering process completely. Considering the fact

that the MBA method takes into account the projectile-distortion also, a fruitful suggestion will be the replacement of the first Born term by the corresponding modified Born term in some sophisticated method such as the HHOB series.

[4] In the present work on e - Li scattering using the MBA approximation, the Li atom is given the core-approximation of Walters (1973) and the various aspects of this type of representation of the atom are also studied.

(E) The two Potential Eikonal Approximation :

[1] The generalisation for the e-H (nlm) elastic scattering in the two-potential eikonal approximation is discussed and the results for e - H (2S) scattering are derived and compared with other data.

[2] The reasons for the improvement of this method over the conventional Glauber method are enumerated. The graph showing the variations of the phase function in the eikonal as well as the two-potential method is self-explanatory.

[3] Considering the results obtained in the present study and the results obtained by other workers for scattering from He and Li targets, it can be seen that the results are far less satisfactory when

compared to similar results for H target reported by Ishihara and Chen (1975). Perhaps this reflects upon the limitation of the method itself.

(F) Two-Potential HHOB approximation :

[1] This method which was formulated in this thesis work, was an attempt to check the feasibility of a two-potential Born approximation within the framework of the recent HHOB approximation. In other words, this formulation was aimed at the improvement of the HHOB approximation, particularly in the large angle region.

[2] This formulation was applied here to study the electron scattering from hydrogen and helium atoms and in both cases the DCS results obtained were better than their HHOB counterparts.

[3] The TCS, DCS and TEC values were calculated for the above scattering processes with a conclusion that this method definitely improves upon the basic HHOB method.

[4] In the present analysis of the specific scattering processes, the third Born terms were neglected for reasons listed therein. However, it can be incorporated to see whether this affects the results to any appreciable extent.

[5] The partial wave summation was taken with a view to account for the infinite number of partial waves. For this purpose, the method suggested by Jhanwar et al (1978) was used, which involves the exact and Born phase shifts, their comparison etc. The phase shifts were generated with the aid of computer.

[6] The present method can be extended to other atoms also without much difficulty when compared to the application to hydrogen and helium targets.

(G) Wallace type Correction to HHOB Approximation :

[1] This correction is basically dependent on the expansion of the Green's function giving a trajectory correction.

[2] The HHOB scattering amplitude is derived using the correction and the new amplitude differs from the original. HHOB terms by a multiplication factor $y = 1 + \cos \theta/2$.

[3] The Wallace corrected HHOB amplitude is applied to study the scattering of electrons from H atom. It is learnt that in the small angle region, the DCS curve shifts towards the experimental curve slightly, but the extent of improvement is not that significant.

[4] This formulation is also not free from the small angle requirements and hence holds good for only small angles of scattering.

[5] At $\theta = 0$, $y=1$ i.e. the results are not different from their HHOB counterparts.

[6] Further study by our group of workers has shown that parallel to the Wallace correction in eikonal approximation, further analysis in HHOB approximation will be more fruitful. More work in this direction is in progress.

(H) Electron - Na Elastic Scattering :

[1] The first Born results using the Coulson wave function are in very good agreement with similar results reported by Walters (1973) using the sophisticated Szasz Mc Ginn (1967) wave function.

[2] In the case of alkali scattering where absorption effects are all-important, the first Born results cannot be expected to compare nicely with the experimental data and this fact is made evident here. Hence, the GES approximation is taken up to analyse the e - Na scattering. The results are better than first Born results but they fail in the large angle region.

[3] Another major effect viz. polarisation is incorporated by the replacement of the second GES term by the Born term where the real part corresponds to polarisation. As expected, polarisation effects are negligible in the case of e - Na scattering. Further, it is proved that the imaginary parts of the Second Glauber and Born terms are approximately equal.

[4] Next, the two-potential Born approximation discussed earlier is applied to this scattering process. Only first Born term is retained in the Born amplitude and the results are compared with other data as well as first Born results. The improvement is marked. The DCS curve shows qualitative agreement with the experimental curve with a dip.

[5] Further attempt to obtain quantitative agreement with experimental curve is made by incorporating higher order Born terms in the above method. It is observed that the DCS curve deviates from the experimental data and the anticipated reasons are enumerated.

[6] Electron-Na scattering is now studied using an altogether different method - Partial wave analysis. The results using the static potential given by

Cox and Bonham (1967) are good at intermediate and large angles and poor at low angles for reasons well-known.

[7] The results of the present study are compared with the recent reports and interesting consequences are discussed.

In the foregoing, a gist of the different aspects of the present study is pictured from which it is evident that there is lot of scope for further investigations. I wind up the thesis with the hopeful feeling that the little work presented in this thesis, eventhough only a drop in the ocean of knowledge, will lead to further investigations for myself and for others.