CHAPTER - VI

DISCUSSIONS AND CONCLUSIONS

Before the conclusion of this work it will be appropriate to review it and to point out the extent of the success in the present deliberations and to suggest further investigations to overcome the limitations.

The entire study was divided into three parts viz electron scattering by (i) hydrogen atom (ii) helium atom and (iii) lithium atom . While scanning through the literature pertaining to the experimental and the theoretical investigations in this field, it was noticed that still there were discrepancies in the experimental results and the theoretical estimates. It was also desirable to have an approximate method which can give better result than the FBA . In view of these and the points mentioned under ''Approach to the present work'' (Chapter - II , Sec. 2.5.1), the present investigations were made by combining the GES and the HEA methods for hydrogen, helium and lithium atoms. Direct, exchange and static potentials were used in these investigations.

It was mentioned earlier that the HHOB approximation employed in this work, combines the small angle, intermediate and high energy, GES (Sec. 2.3.4) and HEA (Sec. 2.3.5) methods of Yates (1974, 1979), and was similar to the EBS (Sec. 2.3.3) up to the term of the order k_i^{-1} in the scattering amplitudes (equations 2.41, 2.66, 3.1). The main difference between EBS and HHOB was the real part $O(k_i^{-2})$ in the second Born approximation and this real part had a leading correction to the third GES in the DCS (equation 3.2) calculations. The main difference between the corresponding terms in the GES and the HEA was the average excitation energy parametr β_i . The comparisons between the corresponding terms in the GES and the HEA were discussed in Sec. (2.3.5). With the formulation of the HHOB , all the scattering contributions (equations 2.12, 2.36, 2.45, 2.57) to the DCS (equation 3.2) are derived (Secs. 3.2.1, 3.3.1 , 3.4.1, 3.5.1 , 4.2.1, 4.3.1, 5.2.1, 5.3.1, 5.4.1)and evaluated at incident energy in the range E = 100 to 800 eV, and these are tabulated only at few incident energies for hydrogen, helium and lithium atoms. Using these scattering contributions, the DCS (equation 3.2), TCS (equation 3.3) and TES are calculated at the incident

energy range E = 100 to 800 eV and are compared with the recent experimental and theoretical results (Secs. 3.2.2, 3.3.2, 3.4.2, 3.5.2, 4.2.2, 4.3.2, 5.2.2, 5.3.2) of hydrogen, helium and lithium atoms. Discussions on these investigations of the atoms can be divided and discussed in the following way.

Numerical technique used in the present work :

All the higher order differentiations in the scattering amplitudes (see for example equation 4.23) were differentiated analytically up to first order (see for example equation 3.11). Using the accurate numerical method (Abramowitz and Stegun, 1964) for this first order, computer programme in FORTRAN was written for the evaluation of first order differentiation. IBM - 360 computer was used in the double precision for the evaluation of these scattering amplitudes. The numerical calculations of the scattering amplitudes, DCS, TCS and TES by the computer are correct up to the 16th decimal point due to the use of double precision. The error committed by the computer than the original value (without any differentiation) was nearly $\pm 10^{-6}$.

Divergent integrals :

No divergent integrals were observed in the present investigations. All the integrals occurring (Appendix) in the scattering amplitudes have finite value in the forward direction. It was also observed that when $\beta_i \longrightarrow 0$ all the present integrals approached the corresponding integrals in GES.

Checking of the present investigations :

At each and every step of the work, the present results are compared with available results of GES and EBS (Figs. 3.1, 3.3, 3.5, 4.2) methods. In absence of real part $O(k_i^{-2})$ in equation (3.2) the corresponding DCS (solid curves b or b') of the investigations approached the EBS results.

Variation of DCS with respect to the choice of excitation energy DE and Re2 in the second Born amplitude :

It was noted from the Tables (3.6, 3.5) and 4.4, 4.3) of ISH (Sec. 3.4.1) and ESGHe (Sec. 4.2.1) processes that the variations of the second Born terms (equations 2.58, 2.59, 2.60) were due to different excitation energies used in these calculations. These

changes are found more in the real parts ($\mathrm{Re}1\int^{(2)}_{HEA}$, $\mathrm{Re}2\int^{(2)}_{HEA}$ than in the imaginary part ($\mathrm{Im}\int^{(2)}_{HEA}$). The dependence of excitation in these imaginary and real parts is as follows.

The closed form of the imaginary part (see for example equation 3.11) is included in I_1 (- - - -) and I_1' (- - - -) (Appendix A-1). The numerical value of β_i (= DE/k_i) is small . I_1 (- - - -) is a function of q^2 the exponential parameter y^2 of the wave function (equation 3.6) and β_i^2 . β_i^2 is an additive quantity to q^2, y^2. In comparison with q^2, y^2 the value of β_i^2 is almost negligible, and for other values of β_i the function I_1 (- - - -) does not change much. This is the reason why small changes are observed in the imaginary part.

Now the real part $\mathrm{Re}1\int^{(2)}_{HEA}$ (equation 3.13) contained I_2 (- - - -) and I_2' (- - - -) associated with the signam function (Appendix A-2), and I_2 (- - - -) is also a function of q^2, y^2, β_i^2 signam and $\sin^{-1} A_1$. A_1 is a function of q^2, y^2 multiplied by β_i^2 . So for a small change of β_i , considerable change can be observed in A_1 and correspondingly in $\sin^{-1} A_1$. Now the signam function changes the sign depending upon whether $y < q$ or $y > q$, correspondingly the complete value of I_2 (- - - -) will be changed. I_2' (- - - -)

is a function similar to I_2 (- - - -) with opposite sign. So the changes due to sigbam and β_i will be nulified by the I_2' (- - - -). These are the reasons for the fluctuations and variations in $\mathrm{Re1}\int^{(2)}_{HEA}$.

Similar to Re1, real part $\mathrm{Re2}\int^{(2)}_{HEA}$ (equation 3.15) contained I_2 (- - - -), I_3 (- - - -) and I_3' (- - - -) (Appendix A-3). I_3 (- - - -) is a function of $\tan^{-1}$ (y/β_i) . So for a small change in β_i , good amount of variation can be observed in this I_3 (- - - -). Since I_3 (- - - -) , I_3' (- - - -) and I_2 (- - - -) are with opposite signs in $\mathrm{Re2}\int^{(2)}_{HEA}$, so comparatively more fluctuations, and variations can be observed in $\mathrm{Re2}\int^{(2)}_{HEA}$ than $\mathrm{Re1}\int^{(2)}_{HEA}$.

From these discussions, the dependence of β_i , y, q on the imaginary and real parts of second Born approximation can be written as

$$\mathrm{Im}\int^{(2)}_{HEA} \ll \mathrm{Re1}\int^{(2)}_{HEA} \ll \mathrm{Re2}\int^{(2)}_{HEA}$$

This is the reason for the fluctuations observed in the real parts of second Born approximation in the present investigations.

It was also noticed that these variations in the second Born terms due to two different excitation

energies, were more in the inelastic process (ISH , Sec. 3.4.1) than in elastic process (ESGHe , Sec. 4.2.1). The corresponding variations in DCS are observed in Tables (3.6, 3.5) and 4.4, 4.3) for hydrogen and helium respectively.

In all the elastic (ESGH, ESEH , ESGHe,ESGLi) and inelastic (ISH, ISHe) processes, the DCS corresponding to with and without $Re2f^{(2)}_{HEA}$ were shown in the form of graphs (solid curves a, a' , b, b') and Tables (3.9, 5.1) and compared with the recent experimental and theoretical results. At small angles, the present elastic process results are found to be in good agreement with the experimental results, good amount of correction due to the third GES was observed due to $Re2f^{(2)}_{HEA}$ At large angles ($q \geq k_i$) these present elastic results are found to be a good amount of over estimation with the compared data. In the case of present inelastic process, these results are comparable at $\theta \leq 20^{\circ}$ with the other theoretical results and over estimation was observed at $\theta > 20^{\circ}$. The over estimation of the present elastic and inelastic results was due to few of the following reasons ;i)the convergence of the series with real part $Re2f^{(2)}_{HEA}(0)$ (k_i^{-2}) was slower at large angles (large momentum transfer)

than at small angles, ii) the choice of the excitation energy was more important in the inelastic process than in the elastic process.

It was also noted from the Tables (3.8, 3.9) and Figs. (3.4, 4.4) for elastic and inelastic processes, that the DCS variation due to $Re2f^{(2)}_{HEA}$ for fixed k_i was more at large angles ($q > k_i$) than at small angles, and for fixed Θ this variation was negligible in the high energy incident region than in low energy region.

It was observed that the agreements of elastic results with the compared data were more than the inelastic results through out the present investigations on hydrogen, helium and lithium atoms. This was due to some draw backs in the inelastic process formulation.

Exchange effects :

Through out the work, first order Ochkur exchange term (equation 2.36) was included in the DCS (equation 3.2) calculations of elastic process (Secs. 3.2.1, 3.3.1, 4.2.1). This exchange correction was observed more in the small angle region than in the large

angle region, and negligible correction was observed at higher incident energies than at lower incident energies. Another interesting point in the present investigations was that exchange correction in ESEH process (Sec. 3.3.1, Table 3.8) was almost negligible in comparison with ESGH process (Sec. 3.2.1 , Table 3.1). It was noted from the Figs. (3.1 , 3.2) and Tables (3.1, 3.2) of ESGH process (Secs. 3.2.1, 3.5.1) that at small angles considerable exchange corrections were obtained by the inclusion of second Born exchange amplitude to the direct scattering amplitude, in the DCS (equation 3.2) calculations, corresponding improvements were also observed in TCS (Table 3.4) and TES (Table 3.4) calculations. For a small change in the DCS due to first order Ochkur (Table 3.1) and second order Ochkur (Table 3.2) exchange corrections, considerable variation in the area enclosed by these DCS curves (Fig. 3.7) was observed in the TES calculations . Since maximum contribution to the TES was obtained from the small angle region, for a small change in DCS causes considerable change in TES calculation due to those two type of exchange corrections in the small angle region. The DCS, TCS, and TES obtained by means of the higher order exchange correction were in good agreement

with the compared data. In the inelastic process we have not included the exchange corrections in DCS calculations. This was one of the reasons for the disagreement of our inelastic results with the compared data.

Based on these discussions of our results on hydrogen ; helium and lithium atoms, the following conclusions and future plans can be made for the improvements and the extensions of our investigations.

All the elastic (ESGH, ESEH, ESGHe and ESGLi) and inelastic (ISH, ISHe) processes can be further improved by considering the third Born term (equation 2.62) in the scattering amplitude for the DCS calculations. With this modification the results at large momentum transfer ($q > k_i$) can be found to be in good agreement with other data . It can be concluded from our above discussions that the selection of excitation energy was more important in the inelastic elastic process than in elastic process, so better it is to use proper excitation energy in the calculation of higher order Born terms. One can include some intermediate p - states and exchange corrections in ISH and ISHe process derivations for the exact comparison of results with experimental data.

The higher order exchange derivations (Sec. 3.5.1) of our investigations can be easily extended to ESGHe (Sec. 4.2.1) and ESGLi (Sec. 5.2.1) processes. Considerable exchange correction was observed by the inclusion of the higher order exchange terms in the ESGH process. Similar improvements can be observed in ESGHe and ESGLi process if one includes these types of exchange corrections. Our ESGLi process (Sec. 5.2.1) derivations can be easily extended to the other alkali atoms. More accurate results than the present ESGLi (Sec. 5.2.1) results can be obtained by including core - potential (equation 5.12) in the second Born derivations, similar type of results can be expected in the case of other alkali atoms. In order to show the simplicity of our employed HHOB approximation an analytical study was made for elastic and inelastic scattering of electrons by lithium atoms (Sec. 5.4.1), and first order exchange amplitude was derived using Lewis (1956) integral technique. Using the derived amplitudes (equations 5.39 to 5.42) one can calculate DCS, TCS and TES very easily.

Finally all the HEA scattering amplitudes (Sec. 2.3.5) were reformulated by considering the interaction potential (equation 2.24) as a static

potential (equations 5.22, 5.23). These derived static amplitudes are given in (Sec. 5.3.1). Only to see the validity of these amplitudes, we made rough calculations for lithium atom, using first and second Born amplitudes. And few guide lines were given to obtain the closed form of third Born term. Using these derived expressions one can study the cross sections for a variety of atoms. Reasonable results can be expected from these static field calculations.

According to the knowledge of the author perhaps the present DCS results (shown in Tables and Figs.) are the only the results with the real part $O (k_i^{-2})$ in the second Born approximation.

To sum up I believe that without ignoring the simplicity and the beauty of the FBA, mathematicians Physicists and the Chemists should see that there is a real challange for the approximate method to be applied to atoms with many electrons. We ought to learn how to develop a consistent better approximation realizing the limitations of the computers.