CHAPTER - II

RELEVANT THEORETICAL FORMULATIONS

2.1 Introduction :

The second chapter deals with some of the intermediate/high energy methods such that the subject matter of this chapter is independent and self-consistent and useful in the discussions in the succeeding chapters. Since the study of electron-atom collisions cannot be done through one single theory that universally applies to electrons of any energy impinging on any target, specific quantum mechanical theories have been developed for specific energy domains of the projectile electron. The general classification of energy domains is three fold - low, intermediate and high. If the speed of the projectile electron is less or nearly equal to that of the target atom, it refers to the 'low' energy range, where only a few channels are open. The 'intermediate' energy is near the excitation threshold of the target and extends upto a few times the ionization threshold. Thereafter, one is in the 'high' energy region which finally goes over to 'very high' energies where relativistic considerations become prominent. Obviously, the energy domain depends on the target atom and quite generally, a broad classification of different ranges of energy

can be made as follows: the incident energy less than 10 eV is in the low energy range; the intermediate energy ranges from 10 eV to nearly 100 eV and above that comes the high energy region. The present work is mainly concerned with intermediate / high energy regions and a discussion on the various theoretical methods in this energy regime will be instructive.

In recent years, numerous calculations corresponding to nearly as many theoretical descriptions have been made of amplitudes of high energy collisions of charged particles with atomic targets. Because of the enormous complexity in describing and predicting the results of the associated experiments, most of the cited works have had as their objective the determination of accurate and computationally feasible theoretical procedures. Included among the more successful methods are variations of traditional impact parameter studies (Dewangan, 1975), the simplified second Born approximation (Holt and Moiseiwitch, 1968), Glauber (Gerjuoy and Thomas, 1974) and modified Glauber approaches (Hambro et al, 1973), the Coubmb Projected Born calculations (Geltman and Hidalgo, 1971) and the Eikonal Born Series approach (Byron and Joachain, 1973). Before going into the depths of the theories, let us have a bird's eye view of the development of various theoretical methods from time to time.

Among the several methods that have been proposed in the recent past to study the scattering of electrons from atoms at intermediate and high energies, most of them are based on two basic approximations in the field - the eikonal approximation (Joachain and Quigg 1974) and the Born approximation (Schiff, 1968).

The Glauber approximation (Glauber 1959, Gerjuoy and Thomas 1974) has been extensively used with reasonable success to calculate the elastic and inelastic cross sections for simple target systems. It is well-known that the Glauber approximation suffers from several shortcomings, the most prominent one being the logarithmic divergence of the scattering amplitude in the forward direction. Various attempts have been made to rectify these defects. Chen and Hambro (1972) and Chen et al (1973) have corrected the classical straight line trajectory used in the Glauber approximation. The assumption of the straight line trajectory leads to the disappearance of the real part in the second Born term. This was first identified in the case of potential scattering by Byron et al (1973) and Byron and Joachain (1973a) and then for electron-atom scattering by Byron and Joachain (1973b). To account for the missing real part, Mathur (1974) included the polarisation effect externally in the Glauber amplitude by treating the target wave function perturbed by the incident particle. Joachain and Quigg (1974) used an eikonal optical model which includes the second order

potential in the evaluation of the Glauber - phase. Byron and Joachain (1973 b, c, 1974 a, b, 1977) proposed the Eikonal Born series method which consists in expanding the scattering amplitude in alternate terms of the Born series and the Glauber series. Flannery and Mc Cann (1974) have used a multichannel eikonal treatment. Ishihara and Chen (1975) proposed a two-potential eikonal approximation and have demonstrated that the inadequacy of the Glauber approximation to predict elastic scattering cross-sections at all angles is mainly a result of the inadequate semiclassical treatment of the close-encounter collisions. Birman and Rosendroff (1976) have proposed a modified approach to the Glauber approximation.

Simultaneous with these developments, the second-order potential approach of Bransden and Coleman(1972) has also been successfully used at intermediate energies. In this method, allowances are made for the states omitted in the close-coupling method (Burke and Schey 1962). Later Bransden and Noble (1976) used the four - state coupled - channel second-order - potential method to study the e - H elastic Scattering.

Among the first order theories, the first Born approximation (FBA) is the simplest eventhough it is known to be inadequate in the intermediate energy regime. Attempts to improve the FBA by including the second order effects have

been made by Jhanwar et al (1975). Junker (1975) proposed the modified Born approximation by considering the distortion of the incident wave. A similar procedure was used by Geltman and Hidalgo (1971a, b, 1974), Geltman (1976) and Stauffer and Morgan (1975). An extention of the Born model, the distorted wave polarised orbital approximation has been used in the electron-atom scattering by Mc Dowell et al (1973, 1974, 1975a, b).

Of the many attempts to improve the eikonal approximation, the second order eikonal approximation named as the Wallace correction (Wallace 1973) is the most sophisticated method which was applied with success to e - H scattering by Roy and Sil (1974) and Unnikrishnan and Prasad (1982). The Wallace correction has further been elaborated by Franco (1982) and also by Byron et al (1982). As the name implies, the 'modified Glauber method' (Gien 1976, 1977, Tayal et al 1979, Jhanwar et al 1982) has been another successful modification of the Glauber theory. The work of Dewangan (1980) is also relevant with respect to the Glauber theory. Of the several modifications developed for high energy electron-atom collisions, the work of Rosendroff (1977, 1981) and Rosendroff and Birman (1980) is really worthy of mention.

Coming back to the Born frame work, the Fixed Scatterer approximation of Ghosh (1977, 1978), the Simplified Second Born approximation (Byron and Joachain 1973) and the various

calculations associated with it, the High Energy Higher Order Born approximation (Yates 1979) and the distorted wave second Born approximation (Kingston and Walters 1980) have been the major mile stones in the path of progress in the recent past. The review work of Byron and Joachain (1977) and the unitarised eikonal Born series calculations of Byron et al (1982) are also relevant in the context of electron-atom scattering studies.

Apart from the various methods mentioned above which are originating from the two basic approximations - Born and Glauber - there is an important formalism in the scattering problems and that is the partial wave analysis (Schiff-1968). The optical model calculations which involve the evaluation of a model (optical) potential and further evaluation of the scattering amplitude is still another method followed in the collision physics.

Hence, we have seen that so many theoretical methods have come up to describe the electron-atom scattering. Some of the high energy methods are used in the present work. So it will be useful to elaborate upon those popular and prominent methods such that it will serve the purpose of ready reference for the later chapters of the thesis.

2.2 High Energy Methods :

The different theories of collision physics, now in practice, are mainly quantum mechanical and thus originate from the well known Schroedinger equation. The different collision theories are, in general, different approximate ways to solve the differential Schroedinger equation or its integral counterpart - the Lippmann Schwinger equation.

The non-relativistic, time-independent Schroedinger equation for the system of incident electron plus target atom is

$$(H - E)\ \Psi\ (\underline{r}, \underline{x}) = 0 \qquad (2.1)$$

where H is the Hamiltonian of the system, E is the total energy of the system and $\Psi\ (\underline{r}, \underline{x})$ is the wavefunction which contains the co-ordinates of the incident electron ($\underline{r}$) and of the target ($\underline{x}$). There are certain basic assumptions or formulations like Born - Oppenheimer approximation, fixed nuclei formulation etc. which help us to tackle the Schroedinger equation with relative ease. Various approximations originate from (2.1). For e.g., in close-coupling formulation, one seeks a solution of the equation (2.1), as an expansion of Ψ in terms of the eigen functions of the target states. The high energy methods arise from the integral equivalent of the Schroedinger equation.

For the scattering of an electron by a structureless target generating a potential V ($\underline{r}$), equation (2.1) can be rewritten as

$$(\nabla_{\underline{r}}^2 + k_i^2)\ \Psi\ (k_i, \underline{r}) = U\ (\underline{r})\ \Psi\ (k_i\ \underline{r}) \qquad (2.2)$$

where $\nabla_{\underline{r}}^2$ is the K.E operator, $\underline{k_i}$ is the incident momentum vector and $U\ (\underline{r}) = 2\ V\ (\underline{r})$ is the reduced potential. The solution of (2.2) denoted by $\Psi_{k_i}^{+}\ (\underline{r})$ satisfies the boundary condition

$$\Psi_{k_i}^{+}\ (\underline{r}) \xrightarrow[r \to \infty]{} e^{(i \underline{k_i} \cdot \underline{r})} + f\ (\theta, \phi)\ \frac{e^{ik_i r}}{r} \qquad (2.3)$$

where $f\ (\theta, \phi)$ is the scattering amplitude. The differential cross section can now be written as

$$\frac{d\sigma}{dw} = \frac{k_f}{k_i}\ /\ f\ (\theta, \phi)/^2 \qquad (2.4)$$

The total cross section σ^{tot} is related to the scattering amplitude as $\sigma^{tot} = \frac{4\pi}{k_i}\ \text{Im}\ f(\theta = 0)$ (2.5)

where Im $f\ (\theta = 0)$ means the imaginary part of f for $\theta = 0$.

Coming back to (2.2), the general solution is written as (Joachain, 1975)

$$\Psi_{k_i}\ (r) = \phi_{k_i}\ (r) - \int G_o^{+}\ (\underline{r}, \underline{r}')\ U\ (\underline{r}')\ \Psi_{k_i}\ (r)\ dr' \qquad (2.6)$$

where ϕ_{k_i} is the normalized plane wave given as

$$\phi_{k_i}\ (r) = (2\pi)^{-3/2}\ e^{\,i\,\underline{k_i} \cdot \underline{r}} \qquad (2.7)$$

Similarly with $\underline{k}_f$ as the scattered electron momentum,

$$\phi_{k_f}(r) = (2\pi)^{-3/2} \; e^{i\underline{k}_f \cdot \underline{r}} \qquad (2.8)$$

The Green's function or the free-particle propagator is given by

$$G_o^+(\underline{r}, \underline{r}') = -\frac{1}{4\pi} \frac{\exp(ik_i|\underline{r}-\underline{r}'|)}{|r - r'|} \qquad (2.9)$$

(2.6) is the Lippmann - Schwinger equation. The general expression of the scattering amplitude is

$$f(\theta, \phi) = -4\pi^2 \langle \phi_{k_f} | V | \Psi_{k_i}^+ (\underline{r}) \rangle \qquad (2.10)$$

Now let us see how various high energy methods stem out from the above fundamentals.

2.3 The first Born approximation (FBA) :

The zeroeth approximation to the solution of the Lippmann-Schwinger equation is to replace $\Psi_{k_i}^+(\underline{r})$ simply by $\phi_{k_i}(\underline{r})$. Hence, the scattering amptitude (2.10) becomes (in the first Born approximation).

$$f_{Bl} = -4\pi^2 \langle \phi_{k_f} | V | \phi_{k_i} \rangle \qquad (2.11)$$

The next iteration gives the second Born approximation and this procedure generates the Born series as a perturbative expansion in powers of U (r). The series converges to a limit if the potential is weak enough.

The analysis of the first Born amplitude is simple giving

$$f_{B_1} = -\frac{1}{2\pi} \int e^{i\underline{q}\cdot\underline{r}} V(\underline{r}) \, dv \qquad (2.12)$$

Where $q = /k_{\underline{i}} - k_{\underline{f}}/$ is the momentum transfer. It can be seen that for central potentials, the scattering amplitude is independent of the azimuthal angle ϕ. f_{B_1} is nothing but the Fourier transform of $V(\underline{r})$. The first Born approximation is essentially a high energy method. For low energies, the potential should be very weak.

For considering a target with internal structure, the wave function of the target should be introduced through

$$/ k_i, i> = \phi_{k_i}(r) \psi_i(\underline{x}) \qquad (2.13)$$

Where $\psi_i(\underline{x})$ is the eigen function of the target in its initial stage i. Hence, the first Born amplitude for the scattering of electrons by a target leading to its transition $i \longrightarrow f$ becomes

$$f_{B_1} = -\frac{1}{2\pi} \int e^{+i\underline{q}\cdot\underline{r}} V_{fi} \, dv \qquad (2.14)$$

with

$$V_{fi} = < f / V(\underline{r}, x) / i > \qquad (2.15)$$

The main attraction of the first Born approximation is its simplicity. It does not take into account the distortion of the incident/scattered plane waves as they approach/recede from the target. The effects like absorption (removal

of electrons from elastic to inelastic channels) and polarisation being recognised to be prominent in electron - atom collisions and since these are not accounted for by the first Born approximation, there is a clear need to go beyond the first Born calculations. The modified Born approximation being one such attempt to improve upon the FBA, let us take it up next.

2.4 The Modified Born Approximation (MBA) :

Junker (1975) has proposed this modification of the Born model for the study of the inelastic scattering, which, while retaining the simplicity of the first Born approach gives much better agreement of the theoretical calculations with the experimental data. The modification of Junker consists in taking the incident wave to be distorted instead of the undistorted incident plane wave in the Born approximation. The distortion of the incident plane wave, which is represented by a coulomb wave is produced by assuming an effective nuclear charge δ at the nucleus.

Let H be the Hamiltonian for the incident electron plus target atom system. Following Junker (1975)

$$H = H_o + V = H_2 + W = H_o + U + W \qquad (2.16)$$

Where H_o is the unperturbed Hamiltonian, V is the interaction potential. $V = U + W$, where for the hydrogen atom

$$U = \frac{-\delta}{r_2} \text{ and } W = -\frac{1-\delta}{r_2} + \frac{1}{/\underline{r}_1 - \underline{r}_2/}$$

with δ as the screening parameter and r_2 and r_1 the incident and target electron co-ordinates. The method for the evaluation of δ for inelastic scattering was prescribed by Junker (1975). Later on Gupta and Mathur (1978) extended this method to the case of elastic scattering also.

The breaking of the Hamiltonian H into H_2 and W contains a certain amount of physical significance and has the advantages that the eigen functions of H_2 are known exactly and closed - form expressions exist for the evaluation of the integrals needed in the calculation of the cross-sections.

Assuming X_i to be the solution of the Schroedinger equation

$$(H_o + U) \; X_i = E_i \, X_i .$$

The differential cross section for a collision in which the target atom is excited from an initial state i to a final state f is given by

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} \quad \frac{1}{4\pi^2} \; / \langle \phi_f \; / \; V \; / \; \Psi_i^+ \rangle /^2 \qquad (2.17)$$

In the modified Born approximation,

$$\Psi_i^+ = X_i^+ (r_1, r_2) = F_o(r_2) \; U_o(r_1) \qquad (2.18)$$

Where $U_o(r_1)$ is the atomic wave function in the initial state and $F_o(r_2)$ is the scattered electron wavefunction

given by

$$F_o(r_2) = \sqrt{(1-ia_i)}\ e\ x\ p\ (i\ \underline{k}_i \cdot \underline{r}_2 + \frac{\pi a_i}{2})_1\ F_1(ia_i, 1, i\ k_i r_2 - i\ \underline{k}_i \cdot \underline{r}_2) \qquad (2.19)$$

Where

$$a_i = \frac{\delta}{k_i}.$$

The above expression used by Junker takes into account the distortion of the incident wave. Later on Gupta and Mathur (1978) included the effects of exchange and polarisation within the framework of the MBA. Introducing exchange, we write the total wavefunction as

$$\Psi_i^{\pm} = X_i^{+}\ (r_1, r_2) \pm X_i^{+}\ (r_2, r_1)$$

The polarisation effect is included through the polarised orbital method of Temkin and Lamkin (1961). Hence, the wave function becomes

$$\Psi_i^{\pm} = F_o(r_2)\ \left(U_o(r_1) + U_{pol}(r_1, r_2) \right) \pm F_o(r_1)\ \left(U_o(r_2) + U_{pol}\ (r_1, r_2) \right) \qquad (2.20)$$

Where U_{pol} is the polarisation term. Substitution of $\Psi_i^{\pm}$ in equation (2.17) will give the DCS. For example, in the case of elastic $\bar{e}$ - H scattering,

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2} \left(\tfrac{1}{4} / T^{+} /^2 + \tfrac{3}{4} / T^{-} /^2 \right) \qquad (2.21)$$

Where $T^{\pm} = \sqrt{(i - ia_i)} \exp(\pi a_i / 2) (I_D + I_P + I_E)$

$$I_D = \int g_2 \langle U_o(r_1) / V / U_o(r_1) \rangle \qquad (2.22)$$

with $g_2 = dr_2 \, e^{i \underline{q} \cdot \underline{r}_2} \, {}_1F_1(ia_i, 1, i k_i r_2 - i \underline{k}_i \cdot \underline{r}_2)$

$$I_P = \int g_2 \langle U_o(r_1) / V / U_{pol}(r_1, r_2) \rangle \qquad (2.23)$$

$$I_E = \int dr_2 \exp\left[i(\underline{k}_i \cdot \underline{r}_1 - \underline{k}_f \cdot \underline{r}_2)\right] {}_1F_1(ia_i, 1, i k_i r_1 - i \underline{k}_i \cdot \underline{r}_1)$$

$$\langle U_o(r_1) / V / U_o(r_2) \rangle \qquad (2.24)$$

The above method was used to study the elastic electron Hydrogen scattering by Gupta and Mathur (1978), and the results were very encouraging. Later on they extended the method to study the scattering from Helium (Gupta and Mathur 1979). Recently Kaushik et al (1982) studied the scattering of electrons from C, O and Ne within the framework of the MBA approximation. They have reported that the results obtained are not at all satisfactory. In the present thesis, the MBA is applied to two different scattering phenomena - the 2S - 2S elastic scattering (in Hydrogen atom) and the alkali scattering with respect to Li target. An assessment of the suitability regarding the application of MBA in the above scattering processes is made.

Let us now switch over to the higher order calculations.

2.5 The Second Born Approximation :

Recalling the origin of the Born series as a perturbative expansion in the powers of the interaction potential, we write it as

$F_B = \sum_{n=1}^{\infty} f_{Bn}$ of which the n = 1 term is the first Born amplitude. In the n^{th} Born amplitude, the potential appears n times and the Green's function (n-1) times. In particular, the direct second Born term is written as

$$f_{B2} = \frac{1}{\pi} \int d\underline{r}\, \exp(i \underline{k}_f \cdot \underline{r}) \sum_n \langle f / V(\underline{r}, \underline{X}) / n \rangle \int d\underline{r}' \, (2\pi)^{-3} \int \frac{d\underline{k}\, e^{i \underline{k} \cdot (\underline{r} - \underline{r}')}}{k^2 - k_n^2 - i\epsilon} \langle n / V(\underline{r}', \underline{x}') / i \rangle e^{i \underline{k}_i \cdot \underline{r}} \qquad (2.25)$$

Here /n> denotes the intermediate state of the target and k_n is the intermediate momentum of the projectile electron. k is the variable coming from the Green's function and the appearance of ϵ implies $\epsilon \longrightarrow 0^+$. The vector $\underline{k}_n$ is related to the internal energy W_n of the target in its n^{th} state through

$$\frac{1}{2} k_i^2 + W_o = \frac{1}{2} k_n^2 + W_n \qquad (2.26)$$

Where W_o is the ground state energy of the target. After some mathematical rearrangements, we get

$$f_{B_2} = 8\pi^2 \int d\underline{k} \sum_n \frac{\langle \underline{k}_f, f \,/v/\, \underline{k}, n \rangle \langle \underline{k}, n /\, v \,/\, \underline{k}_i, i \rangle}{k^2 - k_i^2 + 2(w_n - w_o) - i\epsilon} \qquad (2.27)$$

Where $/\underline{k}_i, i\rangle$ = initial asymptotic state of the system, etc.

The above amplitude represents the fact that the projectile with an incident momentum $\hbar\underline{k}_i$ interacts with the target potential via an intermediate or virtual state from which it scatters with final momentum $\hbar\underline{k}_f$ leaving the target in the final state f. The many times employed approximation to simplify the above expression is

$$w_n - w_o \simeq \bar{w} \qquad (2.28)$$

This turns out to be a good approximation above, say 50 eV incident energy (Walters and Ermolaev, 1980). The simplified second Born approximation obtained using (2.28) is

$$f_{B_2} = \int d\underline{k} \frac{1}{k^2 - k_i^2 + 2\bar{w} - i\epsilon} \langle f / (\langle \underline{k}_f \,/v/\, \underline{k} \rangle \langle \underline{k} \,/\, v \,/\, \underline{k}_i \rangle) / i \rangle \qquad (2.29)$$

Here the closure relation has been used for the target states. The simplified second Born term (2.29) has been evaluated using the Dalitz integrals (Joachain 1975).

Various modes of the second Born amplitude can be obtained from the work of Byron and Joachain (1973, 1977), Ghosh (1977), Tayal et al (1979), Yates (1979) and Kingston and Walters (1980). Special mention should be made about the

Distorted Wave Second Born Approximation of Kingston and Walters (1980) and the high energy higher order Born approximation of Yates (1979) which will be elaborated upon in a later section. Quite generally, it can be stated that the second Born term is complex in nature, containing real and imaginary parts. Further, the imaginary term corresponds to the absorption effects and the real part, to the polarisation effects of scattering. These effects being more significant at small angles, the second Born approximation will take care of these effects neglected in the first Born approximation and will improve upon the first Born results tremendously at small angles of scattering. More about the Born approximation will be discussed in the sections to follow when the context arises.

With so much discussions on the Born approximation, we now take up the Glauber theory.

2.6 Glauber Approximation :

The Glauber theory which stems from the eikonal approximation is one basic formulation in the scattering problems. This is also a high energy approximation wherein the de Broglie wavelength of the incident particle is assumed to be short compared to the distance over which the potential varies appreciably. Thus $k_i a >> 1$ where 'a' is the range of the potential. Under this condition, the Lippmann Schwinger

equation can be linearized and this procedure leads to the eikonal scattering wave function.

$$\psi(r) = (2\pi)^{-3/2} \exp\left(i\,\underline{k}_i \cdot r - \frac{1}{2k_i}\int_{-\infty}^{z} U(b,z')\,dz'\right) \qquad (2.30)$$

This shows that the incident particle suffers a potential-dependent phase change. Thus, the eikonal scattering amplitude is (Joachain 1975)

$$f_E = \frac{k_i}{2\pi i}\int d^2\underline{b}\, \exp(i\underline{q}\cdot\underline{b})\, \exp\left[i\,x\,(k_i,b)-1\right] \qquad (2.31)$$

Where $\underline{b}$ is the impact parameter.

The many-body generalization of the above treatment was done by Glauber (1959). For the direct collision of an electron with a target containing fixed scatterer, the Glauber scattering amplitude is

$$f_G = \frac{k_i}{2\pi i}\int d^2\underline{b}\, \exp(i\,\underline{q}\cdot\underline{b})\, \langle f|\, \exp(i\,X_G) - 1|i\rangle \qquad (2.32)$$

Where $\underline{q}$ is assumed to be two dimensional and $d^2\underline{b}$ is an element of area in the (X, Y) plane.

The Glauber phase

$$X_G = X_G\,(\underline{b}, \underline{b}_1, \ldots \underline{b}_N) \qquad (2.33)$$

Where $\underline{r} = \underline{b} + \underline{z}$, and the target co-ordinates

$$\underline{r}_i = \underline{b}_i + \underline{z}_i$$

The Glauber multiple scattering series can be developed by the expansion of e^{iX} in (2.32) and its connection with the Born terms can be established (Byron and Joachain, 1977).

Because of the exponential phase function, the Glauber amplitude takes into account all orders of perturbation. One major assumption taken in the evaluation of the Glauber amplitude is

$$\underline{q}\cdot\underline{r} \simeq \underline{q}\cdot\underline{b} \qquad (2.34)$$

which is valid for small angle scattering only. The above assumption makes the evaluation of the Glauber amplitude easier and also ensures that the first Glauber term is identical with the first Born term.

The evaluation of the Glauber amplitude depends on the expression of the Glauber phase

$$X = \frac{1}{k_i} \int_{-\infty}^{\infty} dz\ V\ (r,x) \qquad (2.35)$$

where x stands for target co-ordinates. Except for H and He, the Glauber phase has a complicated expression so that the evaluation of (2.32) becomes very difficult. Thomas and Gerjuoy (1971) have obtained the closed form expressions for the Glauber amplitude for the collision of charged particles with hydrogen atom. Because of the difficulty involved in the evaluation of the Glauber amplitude (2.32), the termwise analysis (Glauber eikonal series method) proposed by Yates (1974) becomes very significant. In this method, the Glauber amplitude is written in the form of a series

$$f_G = \sum_{n=1}^{\infty} i^{n-1} f_{Gn} \qquad (2.36)$$

More about the GES method will be discussed in a later section devoted for it. An important point about the second Glauber term should however be mentioned that for elastic scattering it diverges as $\ln q$, as $q \longrightarrow 0$. This can be attributed to the suppression of the off-shell contributions in the evaluation of the Green's function. In the Second Born term also, this behaviour is found if the average excitation energy is replaced by zero (Moiseiwitch and Williams 1959, Yates 1973). Further, the second Glauber term lacks a real part which represents the polarization effects in the target. It is found that at almost all angles, the Glauber cross sections underestimate the experimental data. The importance of the Glauber theory lies in the fact that it contains all orders of a perturbation expansion and hence satisfies the unitarity relation in its own framework. Of the improvements suggested to modify the Glauber amplitude, mention must be made of the Wallace correction (1973). The modified Glauber theory is another attempt of improvement. More about the Glauber approximation is given by Joachain (1975), Byron et al (1977), Gau and Macek (1974, 1975) Dewangan (1978, 1980), Roy and Sil (1978), Unnikrishnan and Prasad (1982), Franco (1982), Byron et al (1982), Gien (1976, 1977) Rosendorff (1981) etc.

Now we will go back to the Glauber Eikonal Series method of Yates (1974) as mentioned in the earlier section.

2.7 Glauber eikonal Series (GES) Method :

The Glauber/Eikonal approximation has been successful in accurately predicting differential and integral cross sections describing the collisions of charged particles with low Z atoms. Its lack of application to complicated systems can be attributed to the rapidly increasing computational complexity involved in evaluating the Glauber amplitude expression. The GES, proposed by Yates (1974), is an analytical procedure capable of providing quantitative estimates of the Glauber cross section.

Glauber's multiparticle amplitude formula is given as

$$f_{i\to f}(q,k_i) = \frac{ik_i}{2\pi} \int d\underline{b}_o \exp(i\,\underline{q}.\underline{b}_o) \langle \Psi_f / 1-\exp(ix) / \Psi_i \rangle \quad (2.37)$$

Thomas and Gerjuoy have evaluated this amplitude in the case of charged particles colliding with H atom. Franco (1971) has reduced the general amplitude expression to a one - dimensional integral representation involving sums and products of hypergeometric functions, by assuming a particular functional form for the atomic wave function. An alternative reduction, also resulting in a one-dimensional integral representation but involving modified Lommel function, has been given by Thomas and Chan (1973). But both the above

procedures still require a good deal of computational analysis before arriving at the final results.

Yates has proposed a third alternative to the evaluation of the Glauber amplitude. His approach involves expanding the amplitude in reciprocal powers of k_i for fixed $q = / \underline{q} /$ and attempting a term wise analysis. It is anticipated that for the energy range of applicability of the Glauber approximation, this Glauber Eikonal series will be rapidly convergent. Other works relevant to the development of this theory include that of Byron and Joachain (1973) and Yates (1973).

Expansion of the phase function e^{iX} in equation (2.37) gives

$$f_{i\longrightarrow f} = \sum_{n=1}^{\infty} i^{n-1} f_{i\longrightarrow f}^{(n)} \qquad (2.38)$$

where

$$f_{i\longrightarrow f}^{(n)} = \frac{k_i}{2\pi n!} \int d\underline{b}_o \, e^{i\underline{q}\cdot\underline{b}_o} \langle \psi_f / X^n / \psi_i \rangle \qquad (2.39)$$

Hence for fixed q, the differential cross section through order $(1/k_i^2)$ is

$$\sigma_{i\longrightarrow f} = \frac{k_f}{k_i} \left(\left[f_{i\longrightarrow f}^{(1)} \right]^2 + \left[f_{i\longrightarrow f}^{(2)} \right]^2 - 2 f_{i\longrightarrow f}^{(1)} f_{i\longrightarrow f}^{(3)} + O\left(\frac{1}{k_i^4}\right) \right) \qquad \ldots(2.40)$$

which suggests that for large k_i, only few terms in equation (2.38) are required to obtain good estimates of the Glauber cross sections. The Glauber phase function is

$$X\ (b_o - - - b_N) = \frac{Z}{k_i}\int_{-\infty}^{\infty} dz_o\left[\frac{N}{r_o} - \sum_{i=1}^{N}\frac{1}{/r_o - r_i/}\right]$$

By using a transformation similar to that used by Tenney and Yates (1972), the X is transformed to obtain a convenient form for $f_{i\longrightarrow f}^{(n)}$. For this, $\frac{1}{r_o}$ and $\frac{1}{/r_o - r_i/}$ are replaced by their 3 - Dimensional Fourier integral representations.

$$\therefore X\ (b_o - - - b_N) = \frac{-z}{2\pi^2 k_i}\sum_{j=1}^{N}\int\frac{dp'}{(P')}\,2\int_{-\infty}^{\infty} dz_o\ e^{-ip'\cdot r_o}\left[1 - e^{i\,P'\cdot r_j}\right]$$

$$= -\frac{z}{\pi k_i}\int\frac{dP}{P^2}\ e^{-iP\cdot b_o}\ B\ (p, b_1 \longrightarrow b_N) \qquad (2.41)$$

Where $P' = P + P_z \hat{k}_i$.

Substitution of (2.41) in (2.39) and further simplification gives

$$f_{i\longrightarrow f}^{(n)} = \frac{2\pi k_i}{n\,!}\left(-\frac{z}{\pi k_i}\right)^n \int\frac{dP_1}{P_1^{\,2}} - - - - \int\frac{dP_{n-1}}{P_{n-1}^{\,2}/q-p/^2}$$

$$< \Psi_f/B(P_1)\ \ldots B\ (P_{n-1})\ B\ (q - P)/\ \Psi_i > \qquad (2.42)$$

Here $B\ (P_i) = B(P_i, b_1 \ldots . b_N)$; $P = \sum_{i=1}^{n-1} P_i$.

For chosen co-ordinate system,

$f_{i\longrightarrow f}^{(1)}$ = first Born approximation,

$f_{i\longrightarrow f}^{(2)} = \frac{z^2}{\pi k_i}\int\frac{dP}{P^2/q-p/^2} < \Psi_f\ /B\ (P)\ B(q-p)/\ \Psi_i >$ and so on.

Hence $f_{i\longrightarrow f}^{(n)}$ becomes much simpler due to the uncoupling of b_o and b_i's as a result of the transformation given by (2.41).

Yates has demonstrated the feasibility and simplicity of the above GES method by the application to electron - hydrogen scattering. All the terms of the scattering amplitude upto n = 3 are derived analytically. It is seen that all infinite integrals cancel exactly with each other. He has compared the DCS values obtained from (2.40) with the exact Glauber result as evaluated by Thomas and Gerjuoy. It is shown that if the inequality $k_i >> 1$ is only marginally satisfied, the first three terms of the GES are sufficient to give a very good representation of the Glauber cross section for all values of q.

Later on Singh and Tripathi (1980) used the GES method to analyze the scattering of electrons by He atom. They have made a detailed assessment of the suitability of the GES method in comparison with the conventional Glauber calculations. It should be mentioned here that the GES expressions can be used in analyzing the higher order correction within the frame work of EBS and modified Glauber method of Byron and Joachain, thus avoiding the numerical evaluation adoptedby them. Eventhough the GES method represents the Glauber scattering amplitude satisfactorily, it is not free from the shortcomings associated with the Glauber method - i.e. logarithmic divergence in forward direction (for elastic scattering) and low cross section values. As mentioned earlier, many efforts were so far made to improve

upon the Glauber approximation, one such prominent effort being the Wallace correction (Wallace 1973). We are not discussing this here in detail because the details will appear in a later chapter of the thesis. We will now take up another approach towards the modification of the Glauber framework i.e. the two potential eikonal approximation of Ishihara and Chen (1975).

2.8 Two Potential Eikonal Approximation (TPE) :

The Glauber approximation is known to be in appreciable error at all angles when applied to the elastic electron-atom scattering at medium and lower energies. Ishihara and Chen (1975) have shown that this discrepancy is not due to the frozen-target approximation, but mainly due to the inadequate semiclassical treatment of close-encounter collisions in the Glauber approximation. They have proposed a simple method - the TPE approximation to correct this inadequacy by separating out a central - force potential for which the semiclassical approximation is no longer valid at these energies, and treating it quantum mechanically. The basic formula is derived for potential scattering and is generalized to the case of a composite target in a straight forward manner.

Consider the scattering by a central field $V(r)$ which may be singular at $r = 0$. An arbitrary potential V_1 is so chosen that $V_o = V - V_1$ satisfies the semiclassical conditions; V_o being a slowly varying function and

$\frac{|V_o|}{E} \ll 1$ for all values of r, E being the energy of the system. In the two potential form of Rodberg and Thaler (1967), the scattering amplitude can be written as

$$F(\theta) = \frac{1}{k_i} \sum_l (2l+1)\, T_l\, P_l(\cos\theta) \qquad .. \quad (2.43)$$

with

$$T_l = e^{i\delta_l^{(o)}} \sin\delta_l^{(o)} + e^{2i\delta_l^{(o)}}\, e^{i\delta_l^{(1)}} \sin\delta_l^{(1)} \qquad (2.44)$$

and $\delta_l^{(o)} = \delta_l - \delta_l^{(1)}$ where δ_l and $\delta_l^{(1)}$ are the phase shifts for the potentials V and V_1, θ is the scattering angle. With our choice of V_1, $\delta_l^{(o)}$ may be evaluated by the Jeffreys Wenzer - Kramers - Brillouin (JWKB) approximation to the first order in V_o.

Since most of the effect of V_1 is included in the second term of equation (2.44), the contribution of the first term to equation (2.43) is concentrated in the forward direction and may be evaluated by using the asymptotic formula

$$P_l(\cos\theta) \simeq J_o\left((2l+1)\sin\frac{\theta}{2}\right)$$

and $\sum_{l=0}^{\infty} \simeq \int_0^{\infty} dl$.

Thus

$$f(\theta) = \frac{k_i}{i}\int_0^{\infty} b\, db\, (e^{i\chi(b)} - 1)\, J_o(2kb\sin\frac{\theta}{2})$$

$$+ \frac{1}{k_i}\sum_l (2l+1)\, P_l(\cos\theta)\, e^{i\chi(b_l)}\, e^{i^2\delta_l^{(1)}} \sin\delta_l^{(o)};$$

where we have introduced the impact parameter by

$$b_l = (l + \tfrac{1}{2})/k_i \text{ and } \chi(b_l) = 2\delta_l^{(o)}.$$

Generalizing the above formula to the case of electron atom

scattering in the frozen target approximation, the interaction $V(r, \xi)$ depends on the target electron co-ordinates also.

Hence $$X(b,\xi) = X_o(b,\xi) + \Delta X(b,\xi), \qquad (2.45)$$

Where

$$X_o(b,\xi) = -\frac{1}{k_i}\int_{-\infty}^{\infty} V_o(r,\xi)\, dz,$$

$$\Delta X(b,\xi) = \frac{2}{k_i} V_o(z=0) \int_0^{\infty} \left(1 - \frac{z}{(z^2 - \frac{V_1}{E} r^2)^{1/2}}\right) dz.$$

Now the transition amplitude from the target state $/i\rangle$ to the state $/f\rangle$ may be given as

$$F_{fi}(\theta) = \frac{k_i}{2\pi i} \int d^2b\, e^{i\underline{q}\cdot\underline{b}} \left(\overline{\Gamma(b)} - 1\right) + \frac{1}{k_i} \sum_{l} (2l+1)$$

$$P_l(\cos\theta)\, e^{i\delta_l^{(1)}} \sin\delta_l^{(1)} \int \frac{d\phi}{2\pi} \overline{\Gamma}_{fi}(\underline{b}_l), \qquad (2.46)$$

Where q is the momentum transfer and

$$\overline{\Gamma}_{fi}(\underline{b}) = \langle f / e^{i\chi(b,\xi)} / i\rangle \qquad (2.47)$$

The two - potential scattering amplitude given by (2.46) does not add much practical difficulties to the usual Glauber approximation calculations. If we choose 'd', the range of V_1 small enough, we need take only a few terms in the second term of (2.46).

Ishihara and Chen (1975) have studied the $\bar{e}$ - H scattering in the TPE approximation and have shown that this method provides an effective way to treat the close-encounter collisions properly. Later on Tayal et al (1980)

used the TPE approximation to study the elastic scattering of electrons from He and Li targets. Even though their results are much better than their Glauber counterparts, the improvement obtained is much less than that which is observed in the case of e - H elastic scattering. They have reached the conclusion that it is perhaps a reflection of the limitations of this method rather than the choice of the target wavefunction.

Having discussed the various aspects of the Born and Glauber/Eikonal approximations, let us now turn to another major development in the field of scattering theory - the Eikonal Born Series method which, as the name suggests, is a blend of the two approximations.

2.9 Eikonal Born Series (EBS) Method :

Byron and Joachain (1973, 1974) proposed a new approach - the Eikonal Born Series method - to the analysis of electron/positron - atom collisons at intermediate and high energies. This method combines the Born and Glauber Series to get a consistent picture of the scattering amplitude through $O\left(\frac{1}{k_i^2}\right)$.

The Born series for the direct scattering amplitude is

$$f_B = \sum_{n=1}^{\infty} f_{Bn} = f_{B1} + \text{Im}\, f_{B2} + \text{Re} f_{B2} + f_{B3} + - - - \quad (2.48)$$

The Glauber approximation to the scattering amplitude is

$$f_G = \sum_{n=1}^{\infty} f_{Gn} = f_{G1} + \text{Im}\, f_{G2} + f_{G3} + - - - \qquad (2.49)$$

With the choice of the z - axis perpendicular to q ,

$$f_{G1} = f_{B1}$$

The EBS amplitude is written as

$$f = f_{B1} + \text{Im}\, f_{B2} + \text{Re}\, f_{B2} + f_{G3} \qquad (2.50)$$

Here the third Born term is approximated as the third Glauber term since the direct evaluation of f_{B3} is extremely difficult and in the light of the relation between the different terms of the Born and Glauber Series (for e.g.both f_{B3} and f_{G3} are zero for elastic scattering in the forward direction (Dewangan 1980). Knowing different terms of the above scattering amplitude, the DCS can be obtained as

$$\frac{d\sigma}{d\Omega} = / f /^2 \qquad (2.51)$$

A comparison of the amplitudes (2.48), (2.49) and (2.50) instantaneously reveals that the replacement of the second Glauber term Im f_{G2} by the second Born terms (Im f_{B2} and Re f_{B2}) will result in the EBS amplitude (2.50). Hence one imaginary term is replaced by another imaginary term and a new real part has been included. The Glauber imaginary term is divergent in the forward direction whereas the corresponding Born term is free from this defect because of the average excitation energy parameter. Further, the new

real part in the second Born term i.e. Re f_{B2} will take care of the polarisation effect which is neglected in the Glauber amplitude (2.49). These are the two main achievements attained through the construction of the EBS amplitude (2.50) from the Born and Glauber amplitudes. The application of the EBS method to Scattering problems makes it explicit that the EBS amplitude is superior to the usual Born or Glauber amplitudes.

The EBS has already been applied successfully in the analysis of the elastic scattering of electrons and positrons by atomic hydrogen and helium (Byron & Joachain 1973a, b, 1974 a, b). Later on detailed analysis of the above problem was carried out by the same authors (Byron & Joachain 1977). In the recent past the EBS has been used to study the scattering of electrons from excited 2S state of H atom (Joachain et al 1977) and the Li atom (Byron and Joachain 1977). Within the basic frame work of the EBS method itself, various alternatives are possible depending on the various modes of evaluation of the different terms appearing in the series. One such alternative approach is the recently proposed High Energy Higher Order Born approximation of Yates (1979) which was extensively explored by our group.

2.10 The High Energy Higher Order Born Approximation (HHOB):

This method, which is aimed at suggesting yet another description of high energy collisions, is motivated by two

factors. The first is prompted by the work and success of Byron and Joachain in their Eikonal Born Series approach to medium to high energy electron atom collisions and constitutes an extension of earlier work of Yates (1974). The primary purpose of the HHOB analysis was to develop an alternative high energy expansion of differential scattering cross section in terms of reciprocal powers of k_i through $O\left(\frac{1}{k_i^2}\right)$ which is computationally tractable yet derived from analogously treated second and third Born terms. A second consideration has been the suggestion of anomalous behaviour of the small angle high energy differential cross section in electron atom collisions.

In the HHOB analysis the well-known generalized Born Series description of the collision process is transformed into a more convenient form. Thereafter, the approximate formulae are developed through a partial expansion of the free particle Green's function. We will take up the important second Born term.

$$f^{(2)}_{i\longrightarrow f} = \frac{1}{\pi} \sum_n \int d\underline{r}_o \, e^{i\underline{q}\cdot\underline{r}_0} \, V_{fn}(r_o) \int d\underline{r}_o' \, G_n(\underline{r}_o') \, V_{ni}(\underline{r}_o - \underline{r}_o') \, e^{-i\underline{k}_i\cdot\underline{r}_o'} \qquad (2.52)$$

Where

$$V_{nm}(\underline{r}_o) = \langle \psi_n(T_1 - - - -, T_N) / V(\underline{r}_o, \underline{r}_1, - - -, \underline{r}_N) / \psi_m(T_1, - - - T_N) \rangle,$$

and $$G_m(\underline{r}_o - \underline{r}_o') = \frac{1}{(2\pi)^3} \int \frac{d\underline{k}' \; e^{i\underline{k}'\cdot(\underline{r}_o - \underline{r}_o')}}{k'^2 - k_m^2 - i\epsilon}, \; \epsilon \longrightarrow 0^+$$

Now the second Born term is partially expanded parallel to the method of Glauber which is most akin to the high energy small angle potential scattering analysis of Schiff. The basic approximations are introduced in the integral:

$$I_n = \int d\underline{r}'_o \; G_n(\underline{r}_o') \, V_{ni}(\underline{r}_o - \underline{r}'_o) \, e^{-i \underline{k}_i \cdot \underline{r}'_o} \qquad (2.53)$$

Here, the variable transformation

$\underline{S} = \underline{k}' - \underline{k}_n$ is made. If it is assumed that V_{ni} is slowly varying over the distance of a wavelength of the scattering electron and that k_n does not differ much from k_i in either magnitude or direction, then the integrated expansion of $(S^2 + 2S.k_n - i\epsilon)^{-1}$ in powers of S^2 should be rapidly covergent. Hence, after performing the $\underline{S}$ integration in cylindrical polar co-ordinates by choosing $\underline{k}_n$ as the polar axis,

$$I_n = \frac{i}{2k_n} \int d\underline{r}'_o \; e^{-i(\underline{k}_i - \underline{k}_n).\underline{r}'_o} \, V_{ni}(\underline{r}_o - \underline{r}_o')$$

$$\left[\delta(\underline{b}_o') \, H(\underline{z}_o') + \frac{i}{2k_n} \nabla^2_{r'_o} \left(\delta(\underline{b}_o') \, z_o' \, H(\underline{z}_o') + O(k_n^{-2}) \right) \right]$$

Where $H(z)$ is the Heaviside function. Again integrating the second term of the above equation by parts twice and simplifying further,

$$I_n \simeq \frac{i}{2k_i} \int_{-\infty}^{\infty} dz'_o \; e^{i\beta_{in} z'_o} \; H(z'_o) \left[1 + \frac{i z'_o}{2k_i} \nabla^2_{r'_o} \right]$$

$$v_{ni}(\underline{r}_o - r'_o) \Big/ \underline{b}_o = 0 \qquad (2.54)$$

where $\beta_{in} = k_i - k_n \simeq \beta_i = \Delta E / k_i$ where ΔE is the average energy transferred to intermediate atomic states during the course of the collision.

In simplifying the present approximations, it is useful to express the interaction potential in Fourier form as

$$V(\underline{r}_o, - - -, \underline{r}_N) = \int d\underline{p}\ e^{-i\,\underline{P}\underline{b}_o} \int_{-\infty}^{\infty} dP_z\, e^{-iP_z z_o}$$

$$\bar{V}(\underline{P} + P_z\hat{\underline{\chi}}, \underline{r}_1, - - - -, \underline{r}_N) \qquad (2.55)$$

Where

$$\bar{V}(\underline{P} + P_z\hat{\underline{\chi}}, ----\underline{r}_N) = \frac{1}{2\pi^2(P^2+P_z^2)} \sum_{j=1}^{N} (e^{i\,\underline{P}\cdot\underline{b}_j}\ e^{i\,P_z z_j} - 1)$$

Now substituting (2.54) and (2.55) in (2.52), we get

$$f^{(2)}_{HEA} = \frac{i}{2\pi k_i} \int d\underline{P} \int_{-\infty}^{\infty} dP_z \int d\underline{P}' \int_{-\infty}^{\infty} dP'_z$$

$$< \psi_f / \bar{V}(\underline{P} + P_z\hat{\underline{\chi}}, ---\underline{r}_N)\, \bar{V}(\underline{P}' + P'_z\hat{\underline{\chi}}, ---\underline{r}_N) / \psi_i >$$

$$\int d\underline{b}_o\ e^{i(\underline{q}-\underline{P}-\underline{P}')\cdot\underline{b}_o} \int_{-\infty}^{\infty} dz_o\, e^{-i(P_z+P'_z)z_o}$$

$$\left[1 + \frac{P'^2_z+P'^2_z}{2k_i} \frac{d}{d\beta_i}\right] \int_{-\infty}^{\infty} dz'_o\, e^{-i(P'_z-\beta_i)z'_o} H(z'_o) \qquad (2.56)$$

$$= \frac{4\pi^3}{k_i}\Big[i\int d\underline{P}\,(1+\frac{1}{2k_i}\frac{d}{d\beta_i}(P^2+\beta_i^2))\, U^{(2)}_{fi}(\underline{q}-\underline{P}-\beta_i\hat{\underline{\chi}}, \underline{P}+\beta_i\hat{\underline{\chi}})$$

$$- \frac{1}{\pi} \fint \int d\underline{P} \int_{-\infty}^{\infty} dP_z\, (1+\frac{P^2+P_z^2}{2k_i}\frac{d}{d\beta_i}) \frac{1}{P_z-\beta_i}$$

$$U^{(2)}_{fi}(\underline{q}-\underline{P}-P_z\hat{\underline{\chi}}, \underline{P}+P_z\hat{\underline{\chi}})\Big] \qquad (2.57)$$

Where $\fint$ stands for the principal value of integral and

$$U^{(2)}_{fi}(\underline{P}+P_z\hat{\chi}\,,\underline{P}'+P'_z\hat{\chi}) = \langle \Psi_f \,/\, \bar{V}\,(\underline{P}+P_z\hat{\chi}\,,---\underline{r}_N)$$

$$\bar{V}\,(\underline{P}'+P'_z\hat{\chi}\,,---\underline{r}_N)/\,\Psi_i\rangle \qquad (2.58)$$

Application to $\bar{e}$ - H elastic Scattering :

The real analysis of any theoretical formulation should be with respect to the application to practical problems. Now we evaluate the second term in HHOB approximation for the $\bar{e}$ - H scattering. For this process, the interaction potential is

$$V = -\frac{1}{r_o} + \frac{1}{/\underline{r}_o-\underline{r}_1/}$$

The groundstate wave function for H atom is $\Psi = \frac{1}{\sqrt{\pi}}\, e^{-r_1}$

The evaluation of expression (2.58) gives

$$U^{(2)}_{fi}\,(\underline{q}-\underline{P}-P_z\hat{\chi}\,,\underline{P}+P_z\hat{\chi}) = \frac{1}{\pi^4(/\underline{q}-\underline{P}/^2+P_z^2)(P^2+P_z^2)}\left(-\frac{d}{d\lambda}\right)$$

$$\left(\frac{q^2+2\lambda^2}{\lambda^2(q^2+\lambda^2)} - \frac{1}{/\underline{q}-\underline{P}/^2+P^2{}_z+\lambda^2} - \frac{1}{P^2+P_z^2+\lambda^2}\right) \qquad (2.59)$$

Here $\lambda=2$ and is obtained from the product of the initial and final wave functions written as

$$\Psi_f^*\,\Psi_i = \frac{1}{\pi}\left(-\frac{d}{d\lambda}\right)\frac{\bar{e}^{\lambda r_1}}{r_1}\,\Big|_{\lambda=2}\,.$$

Now substitution of (2.59) in (2.57) and further simplifications

using the method of partial fractions will give the real and imaginary parts of $f^{(2)}_{HEA}$ for the $\bar{e}$-H elastic scattering.

$$\text{Thus} \quad \text{Im } f^{(2)}_{HEA} = \frac{-4}{\pi k_i} \frac{d}{d\lambda} \frac{1}{\lambda^2} \left[2\, I_1(\beta_i^2, \lambda^2) - \frac{q^2}{q^2+\lambda^2} I_1(\beta_i^2, 0) \right] \quad (2.60)$$

and

$$\text{Re } f^{(2)}_{HEA} = \frac{4}{\pi^2 k_i} \frac{d}{d\lambda} \left\{ \frac{1}{\lambda^2} \left[2\, I_2(\beta_i^2, \lambda^2) - \frac{q^2}{q^2+\lambda^2} I_2(\beta_i^2, 0) \right] \right.$$

$$\left. + \frac{1}{2k_i} \frac{d}{d\beta_i} \left[\frac{1}{\lambda^2+q^2} I_3(\beta_i, 0) + \frac{1}{\lambda^2} I_3(\beta_i, \lambda^2) - I_2(\beta_i, \lambda^2) \right] \right\} \quad (2.61)$$

The integrals I_1, I_2, I_3 are defined and evaluated in the appendix. It should be noted that only the $O(\frac{1}{k_i})$ term of imaginary part is taken since we are interested in the DCS $O(\frac{1}{k_i^2})$. If we take k_i is large and $q \longrightarrow 0$ in the imaginary part, equation (2.60) reduces to exact agreement with the large k_i limit of the imaginary part of the SSB approximation as given by Byron and Joachain (1973) and behaves as $\frac{\ln k_i}{k_i}$ for q approaching zero. Further, if β_i is set equal to zero in (2.60), the corresponding term in the GES is obtained and diverges as lnq as q goes to zero. Similar analysis can be made with the real part also, for the $O(\frac{1}{k_i})$ term. Differences between the SSB and HHOB methods begin to manifest themselves in their predictions of terms proportional to $\frac{1}{k_i^2}$. However, for decreasing q, similarities between the two descriptions should be enhanced. More comparisons

can be made in respect of the cross-sections. To evaluate the DCS, we should have the first and third terms of the HHOB approximation also. The first Born term is simple and straight forward giving $f^{(1)}_{HEA} = -\frac{1}{2\pi}\int dv\, e^{ig\cdot r} \lesssim \Psi_f/V_{in}/\Psi_i>$

where V_{in} is the interaction potential ..(2.62)

Turning to the third Born term, the treatment parallels that of the second Born term except that only the first term of I_n is required. Further analysis gives

$$f^{(3)}_{HEA} = f_1^{(3)} + f_2^{(3)} + f_3^{(3)} + f_4^{(3)}$$

where the first two terms are real and 0 $\left(\frac{1}{k_i^2}\right)$ and the last two are imaginary and 0 $\left(\frac{1}{k_i^2}\right)$. For the present purpose only the real part of $f^{(3)}_{HEA}$ is needed which is given as

$$\text{Re}\ f^{(3)}_{HEA} = f_1^{(3)} + f_2^{(3)} \qquad ..(2.63)$$

Coming to the evaluation of $f_1^{(3)}$ and $f_2^{(3)}$, they are found to be algebraically very tedious. Further, if β_i is set equal to zero, it is found that $f^{(3)}_{HEA}(\beta_i=0) = f_1^{(3)}(\beta_i=0)$ which is the third GES term, which has been evaluated in closed form (Yates, 1974). Hence, in the present study we take the third GES term as an approximate of third Born term. Now the direct scattering amplitude can be written as

$$f_{HEA} = f^{(1)}_{HEA} + \text{Im}\, f^{(2)}_{HEA} + \text{Re}\, f^{(2)}_{HEA} + f^{(3)}_{GES} \qquad (2.64)$$

Knowing the scattering amplitudes, the DCS can be calculated

$$\text{as} \quad \frac{d\sigma}{d\Omega} = / f_{HEA} /^2$$

Having obtained the expressions for the various terms of the scattering amplitude in HHOB, it will be interesting to have an analysis of the characteristics of the various terms. We note the following important points:

(1) Unlike the case of the Second Born term f_{B2} of EBS, here the momentum transfer q is two - dimensional.

(2) The assumptions of HHOB (especially in the evaluation of the integral I_n (2.53) make the theory valid for only small angles of scattering.

(3) The final integrals (in second and third Born terms) over the variable $\underline{P}$ are two-dimensional, making the evaluation comparatively easier.

(4) Unlike the second and third Glauber terms where the individual integrals are singular, in HHOB, all the integrals are absolutely convergent.

(5) If we put the average excitation energy parameter $\beta = 0$ in HHOB, we get the corresponding terms in GES.

(6) Because of the β parameter, the imaginary part of the second HHOB term does not diverge for forward elastic scattering.

(7) At $q = 0$, the imaginary part of the present second Born amplitude agrees with the imaginary part of the simplified second Born result of Byron and Joachain (1973). Hence, the TCS obtained from both the approximations will be identical.

(8) Similarly in the HHOB as well as in the EBS of Byron and Joachain (1973) the real parts of second Born amplitude are identical at $q = 0$.

$$\mathrm{Re}f^{(2)}_{HEA} = \frac{\bar{\Lambda}}{k_i} + \frac{3}{2k_i^2} - \frac{5\bar{W}}{4k_i^2} \quad , q=0$$

This shows that the series expansion of the Green's function in (2.53) is rapidly convergent in the forward direction.

(9) In the above case, the contribution of k_i^{-2} order term (Re_2) is quite small compared to that of k_i^{-1} term (Re_1). But at large angles, as can be seen from the later tables, Re_2 contribution is very high which makes the DCS values also high. It should be again stressed that HHOB is a small angle approximation.

(10) For $q = 0$ and $\beta = 0$, $Re_2 = (3/2)k_i^2$, which is exactly the real part of the second term of the Wallace amplitude at $q = 0$ obtained recently by Byron et al (1982). This correlation is made use of in the later part of my work.

(11) Making use of the relations (Dewangan 1980) $f_G(2n+1) = 0$ at $q = 0$; $n = 1, 2 - - -$ and $f_{B(2n+1)}=0$ at $q=0$, $n = 1, 2 - - -$, one can see that $f_{G3} \simeq f_{B3}$ at very small angles. Thus, our replacement of the difficult third Born term with the computationally feasible third glauber term is justified for small angles of scattering.

2.11 Results and Discussion :

Calculations have been made for the DCS for the $\bar{e}$ - H elastic scattering for energies 100 eV to 600 eV using the scattering amplitude (2.64) given above. In fig. (2.1) and (2.2) the results at 100 eV and 200 eV are displayed along with the data of other workers for comparison. It can be found that at $\theta \leq 50^{\circ}$, the present results are very good and they overestimate for large angles of scattering. It should be remembered that the HHOB analysis has been concerned with the elucidation of the character of the second and third Born terms for short wave length collisions and for small momentum transfers. Specifically, the integral I_n has been expanded using small angle approximations. In order to understand more about the behaviour of the HHOB scattering amplitude, we study the individual terms as given in tables (2.1) and (2.2). It can be seen that the real term of $0\left(\frac{1}{k_i^2}\right)$ has a peculiar behaviour. This term gives spurious values at large angles which, when coupled with

the first Born term to form part of the scattering cross section, results in high values of cross section. It should be noted that Yates (1979) has commented that a detailed analysis of $\frac{1}{k_i^2}$ terms in second Born term should include a discussion of the pertinent third Born terms. It should also be remembered that in the third Born term (2.63), apart from the Glauber-like term $f_1^{(3)}$ there is a second term of $0\left(\frac{1}{k_i^2}\right)$ which contributes to the real part of the third Born term. In the present analysis where the third Born term is approximated as $f_{GES}^{(3)}$, it is totally ignored. The relation which $f_2^{(3)}$ bears with Re $f_{HEA}^{(2)}$ $0\left(\frac{1}{k_i^2}\right)$ has to be and remains to be explored and studied in detail. Perhaps this may give a clue regarding the presently observed overestimating DCS values at large angles. The DCS values at different energies are tabulated in table (2.3).

Eventhough the EBS results (Byron and Joachain 1977) are arrived at through a similar procedure as the HHOB, the EBS results are found to be much better than the HHOB results at large angles of scattering. This is because, a more accurate second Born amplitude is obtained by treating exactly the first term of the sum over states in equation (2.27) and employing closure to the rest of them. This procedure exactly treats the static potential of the atom and hence improves the large angle scattering. The UEBS results are also much superior to the present results since the UEBS takes into account all orders of perturbation.

Similar is the modified Glauber approach. Here, the Glauber term is replaced by the second Born term to remove the divergence of the Glauber amplitude and to account for the absorption and polarization effects through fB_2. The UEBS approach goes a step further to take into account the Wallace correction to the Glauber amplitude. Hence, the UEBS result should give very satisfactory results.

In the ordinary EBS methods to remove the drawbacks of the second Glauber term, there has been an arbitrary diggression from the basic framework of the Glauber theory and use has been made of an altogether different apparatus i.e. that of the Born theory, which has been criticised by Rosendorff (1980). But in the HHOB method, the new Born term has been evaluated using Glauber methods, but retaining average excitation energy parameter. Hence, the basic procedure stands valid in the HHOB method. Only the basic assumptions in HHOB make it good for small angles of scattering; thus the overestimation at large angles.

From the foregoing discussion, it is clear that the HHOB approximation is reasonably good at small angles of scattering as is evident from the results displayed earlier. However, there is much scope for improvement which is attempted in a later part of the present study.

It will be interesting to formulate the HHOB approximation with respect to the static potentials of the

target atom. The static potential $V_{st}(r)$ contains only the incident electron co-ordinate and the absence of the target electron co-ordinates r_1, r_2 etc. reduces the complications in the formulation. In the following section, the HHOB formulation for the static potentials of target atoms is given. This type of analysis is employed in the later chapters of this thesis.

2.12 HHOB approximation for the static potentials of the target atoms :

Consider the static potential $V_{st}(r)$. In the present study, the static potential given by Bonham and Strand (1963) is chosen because it is of the form

$$V_{st}(r) = \sum_j - \gamma_j \frac{e^{-\lambda_j r}}{r} \qquad (2.65)$$

which is simple in view of analytical purposes and the same formulation can be extended to different atoms with changes only in γ_j and λ_j.

Now the scattering amplitude in the HHOB approximation is given by (2.64). We have to evaluate the various terms using the static potential of the form (2.65).

The evaluation of the first Born term is simple and straightforward, which gives,

$$fB_1 = 2 \sum_j \frac{\gamma_j}{q^2 + \lambda_j^2} \qquad (2.66)$$

Imaginary part of the second Born term is given by (2.57).

$$f \quad Im = \frac{4\pi^3}{k_i} \int d\underline{P} \quad U_{fi}^{(2)}$$

Here, we are interested in the 0 $\left(\frac{1}{k_i}\right)$ term of the imaginary part only because we are considering the DCS through 0 $\left(\frac{1}{k_i^2}\right)$.

For the case of static potentials,

$$U_{fi}^{(2)} = \bar{V}_1\left(\underline{P} + P_z\hat{\mathcal{K}}\right)\bar{V}_2\left(/\,q-p\,/-P_z\hat{\mathcal{K}}\right)$$

For the potential (2.65)

$$U_{fi}^{(2)} = \frac{1}{4\pi^4}\sum_i\sum_j \frac{\gamma_i\,\gamma_j}{(P^2+P_z^2+\lambda_i^2)\,(/q-P/^2+P_z^2+\lambda_j^2)} \qquad (2.67)$$

so that $f \quad Im = \frac{4\pi^3}{k_i}\int d\underline{P}\ \bar{V}_1\,\bar{V}_2$

$$= \frac{1}{\pi k_i}\sum_i\sum_j \gamma_i\,\gamma_j\,\frac{\pi}{\xi}\ \ln\frac{2\xi^2+b(\beta^2+\lambda_i^2)+2\xi Y}{(\beta^2+\lambda_i^2)\,(b+2\xi)} \qquad (2.68)$$

where

$$\xi^2 = (q^2-\lambda_i^2+\lambda_j^2)^2 + 4q^2(\beta^2+\lambda_i^2)$$

$$b = -2q^2-\lambda_i^2+\lambda_j^2$$

and $Y = \left[(\beta^2+\lambda_i^2)^2 + (\beta^2+\lambda_i^2)b + \xi^2\right]^{\frac{1}{2}}$.

Now, the 0 $\left(\frac{1}{k_i}\right)$ real part of the second Born term

$$f\ Re_1 = -\frac{4\pi^2}{k_i}\,\mathcal{P}\int d\underline{P}\int_{-\infty}^{\infty} dP_z\,\frac{1}{P_z-\beta}\ \bar{V}_1\,\bar{V}_2$$

where $\bar{V}_1\,\bar{V}_2$ is given by (2.67) and $\mathcal{P}$ stands for the principal value of the integral.

$$\text{Hence } f\,Re_1 = -\frac{1}{\pi^2 k_i}\sum_i\sum_j \gamma_i\,\gamma_j \quad I_{St} \qquad (2.69)$$

$$\text{Where } I_{St} = \fint d\underline{P}\int_{-\infty}^{\infty}\frac{dP_z}{P_z-\beta}\quad\frac{1}{(P^2+P_z^2+\lambda_i^2)\ (/q-p/^2+P_z^2+\lambda_j^2)}$$

the derivation of which is given in the appendix.

Now the $0\left(\frac{1}{k_i^2}\right)$ real part of the second Born term

$$f\,Re_2 = -\frac{2\pi^2}{k_i^2}\fint\int d\underline{P}\int_{-\infty}^{\infty} dP_z\ (P^2+P_z^2)\frac{d}{d\beta_i}\frac{1}{P_z-\beta_i}\ \bar{V}_1\,\bar{V}_2$$

$$= -\frac{1}{2\pi^2 k_i^2}\sum_i\sum_j \gamma_i\gamma_j \fint\int d\underline{P}\int_{-\infty}^{\infty} dp_z\frac{d}{d\beta}$$

$$\frac{(P^2+P_z^2+\lambda_i^2-\lambda_i^2)}{(P_z-\beta)\ (P^2+P_z^2+\lambda_i^2)\quad(/q-p^2/+P_z^2+\lambda_j^2)}$$

$$= -\frac{1}{2\pi^2 k_i^2}\sum_i\sum_j \gamma_i\,\gamma_j\frac{d}{d\beta}\left\{\fint\int d\underline{P}\int_{-\infty}^{\infty}\frac{dP_z}{(P_z-\beta)}\quad\frac{1}{/q-P/^2+P_z^2+\lambda_j^2}\right.$$

$$\left. -\lambda_i^2\fint\int d\underline{P}\int_{-\infty}^{\infty}\frac{dP_z}{(P_z-\beta)}\quad\frac{1}{(P^2+P_z^2+\lambda_i^2)\ (/q-p^2/+P_z^2+\lambda_j^2)}\right\}$$

$$= \frac{-1}{2\pi^2 k_i^2}\sum_i\sum_j \gamma_i\gamma_j\frac{d}{d\beta}\left[I_3\ (\beta,\lambda_j^2) - \lambda_i^2\ I_{St}\right] \qquad \ldots(2.70)$$

where $I_3\ (\beta,\lambda_j^2)$ is the same as the I_3 integral appearing in (2.61) and I_{St} is defined above.

Now the scattering amplitude for the static potential is given as

$$f = f\,B_1 + f\,Im + f\,R_{e_1} + f\,Re_2 \qquad (2.71)$$

In order to have a check of the above formulation, the TCS values for the e-H elastic scattering is evaluated. For this purpose, the famous optical theorem is used. Hence,

$$TCS = \frac{4\pi}{k_i}\, f\,Im\,(q=0)$$

$$= \frac{4\pi}{k_i}\,\frac{1}{\pi k_i}\sum_i\sum_j \gamma_i\gamma_j \int \frac{d\underline{P}}{(P^2+P_z^2+\lambda_i^2)\,(P^2+P_z^2+\lambda_j^2)}$$

$$= \frac{4\pi}{k_i^2}\sum_i\sum_j \gamma_i\gamma_j \begin{cases} \dfrac{1}{\lambda_j^2-\lambda_i^2}\ln\dfrac{\beta^2+\lambda_j^2}{\beta^2+\lambda_i^2} & \Big/\ \lambda_i \neq \lambda_j \\ \dfrac{1}{\beta^2+\lambda_i^2} & \Big/\ \lambda_i = \lambda_j \end{cases} \qquad (2.72)$$

Using the above formula, the total cross section for e-H collision was calculated. For this, the static potential for hydrogen atom given by Cox and Bonham (1967) as follows was made use of:

$$V_{ST} = \sum_{i=1}^{3} \gamma_i \frac{e^{-\lambda_i r}}{r}$$

Where

$\gamma_1 = 0.0524$	$\lambda_1 = 1.9986$
$\gamma_2 = 5.0360$	$\lambda_2 = 1.8954$
$\gamma_3 = -4.0876$	$\lambda_3 = 2.1161$

It should be remembered that the cross sections so obtained using the static potentials will be the total elastic cross sections only. The results are displayed in table (2.4). It can be seen that with the increase in incident energy, the

agreement of the present results with the compared data becomes closer.

In order to have a rough estimate of the differential cross sections using the static potentials, the DCS values are calculated using the scattering amplitude (2.71), and the static potential given by Bonham and Strand (1963). In the present calculation, only the 0 $(\frac{1}{k_i})$ terms of the second Born approximation were used because this calculation was done in a casual way as a rough approximate. The results obtained for the incident energy of 100 eV are displayed in fig.2.3. It can be seen that in the large angle region, the results are quite reasonable whereas in the low angle region the present values are very low. This is precisely the expected behaviour because the static potentials are supposed to hold good only in the large angle region due to the absence of the absorption and polarisation effects which are all-important in the small angle region.

From the above analysis the following conclusions can be made.

(1) that the formulation of the HHOB approximation using static potentials is a success in view of the above mentioned results.

(2) that the validity of the static potentials used here at the intermediate energy region is indirectly checked.

The above formulation using the static potentials will be used in a later chapter of the thesis.

In the foregoing sections of this chapter various theoretical formulations were discussed. After a brief scan through the recent developments, some of the popular approximations were taken up in detail, with more attention to the recently proposed HHOB method which was discussed with respect to the e-H elastic scattering. This method was formulated using the static potentials of the target atoms and applications were made in the case of e-H elastic scattering. With a clear understanding of the shortcomings of this method attempts were made to improve upon it, which will be discussed in a following chapter. In the next chapter, a modification of the GES method discussed in this chapter is studied.

Table 2.1 - Behaviour of the different terms in the HHOB scattering amplitude (2.64) for the ESGH process at 100 eV.

θ	$f^{(1)}_{i\to f}$	$\mathrm{Im}\, f^{(2)}_{HEA}$	$\mathrm{Re}_1 f^{(2)}_{HEA}$	$\mathrm{Re}_2 f^{(2)}_{HEA}$	$f^{(3)}_{GES}$	$f_{exch.}$
10	0.9220	0.9331	0.1398	0.1810	-0.0634	-0.2439
20	0.7442	0.4642	0.0182	0.1405	-0.1178	-0.1822
30	0.5594	0.2831	0.0085	0.1091	-0.1283	-0.1221
40	0.4132	0.2092	0.0108	0.0934	-0.1176	-0.0786
50	0.3095	0.1772	0.0121	0.0880	-0.1053	-0.0508
60	0.2382	0.1488	0.0119	0.0873	-0.0938	-0.0338
80	0.1545	0.1181	0.0099	0.0897	-0.0768	-0.0167
120	0.0885	0.0857	0.0068	0.0938	-0.0593	-0.0064

Table 2.2 - Behaviour of the different terms of the HHOB scattering amplitude for the ESGH process at 400 eV.

θ	$f^{(1)}_{i\longrightarrow f}$	$\mathrm{Im}\, f^{(2)}_{HEA}$	$\mathrm{Re}_1 f^{(2)}_{HEA}$	$\mathrm{Re}_2 f^{(2)}_{HEA}$	$f^{(3)}_{GES}$	f_{exch}
10	0.7427	0.2204	0.0011	0.0342	-0.0295	-0.0454
20	0.4054	0.1018	0.0022	0.0225	-0.0291	-0.0191
30	0.2249	0.0723	0.0029	0.0217	-0.0229	-0.0077
40	0.1375	0.0557	0.0023	0.0227	-0.0182	-0.0035
50	0.0927	0.0443	0.0018	0.0235	-0.0152	-0.0017
60	0.0670	0.0361	0.0014	0.0241	-0.0129	-0.0009
80	0.0409	0.0259	0.0009	0.0246	-0.0101	-0.0004
120	0.0226	0.0169	0.0005	0.0249	-0.0073	-0.0001

Table 2.3 - DCS for the e - H elastic scattering in the HHOB approximation (without exchange).

θ / E	100 eV	200 eV	400 eV	600 eV
5	4.09615	2.00516	1.14114	0.91077
10	2.21504	1.04366	0.60546	0.44541
20	0.83061	0.37904	0.17104	0.09803
30	0.38125	0.15783	0.05661	0.02863
40	0.20364	0.07553	0.02401	0.01149
50	0.12241	0.04213	0.01244	0.00580
60	0.08158	0.02644	0.00747	0.00343

Table 2.4 - Total cross sections for e - H elastic scattering using the static potential of Hydrogen atom within the framework of the HHOB approximation.

E eV	Present results	a UEBS	b MGES	c OM	d DWSBA
100	10.20	7.19	7.56	7.68	7.40
200	5.10	4.27	4.37	4.38	4.34
300	3.40	3.10	3.14	3.14	3.11
400	2.55	2.45	2.48	2.48	2.46
500	2.04	-	2.06	-	-
600	1.70	-	1.77	-	-
700	1.46	-	1.55	-	-

(a) Byron et al (1982)
(b) Chapter III of the present work
(c) Byron and Joachain (1981)
(d) Kingston and Walters (1980)

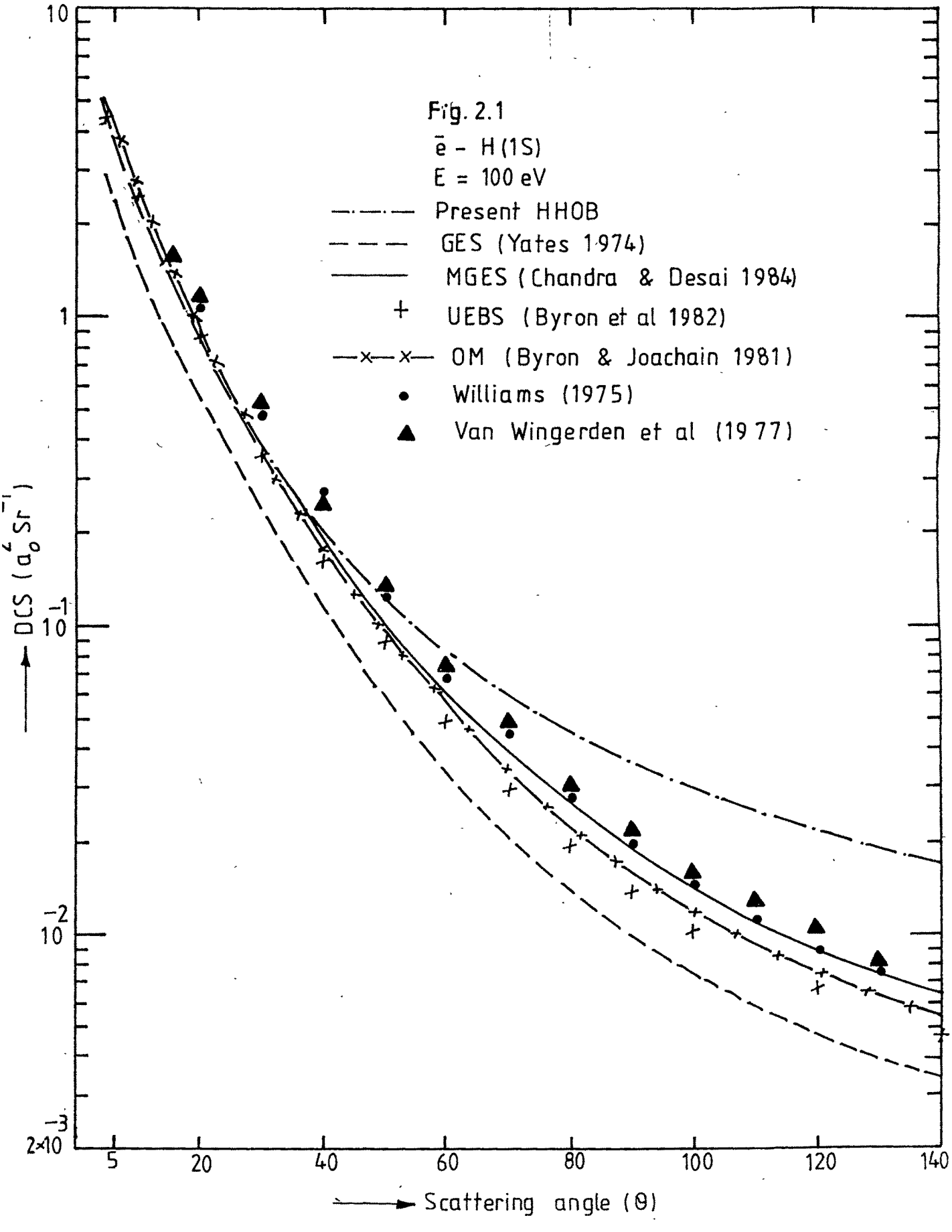
Fig. 2.1
ē - H(1S)
E = 100 eV
Present HHOB
GES (Yates 1974)
MGES (Chandra & Desai 1984)
UEBS (Byron et al 1982)
OM (Byron & Joachain 1981)
Williams (1975)
Van Wingerden et al (1977)
DCS ($a_0^2 Sr^{-1}$)
10
1
10^{-1}
10^{-2}
2×10^{-3}
5
20
40
60
80
100
120
140
Scattering angle (θ)

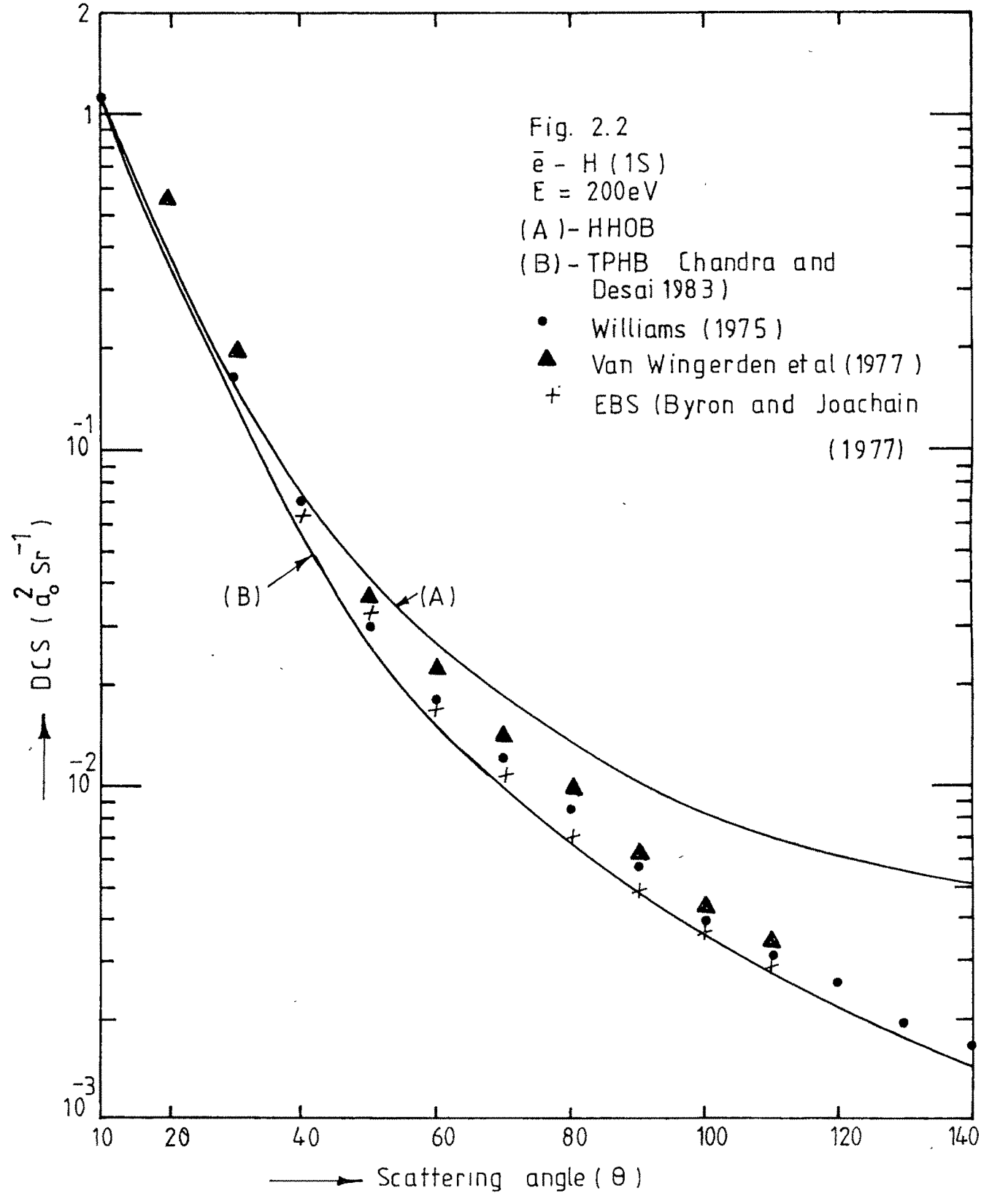
Fig. 2.2
ē - H (1S)
E = 200eV
(A)- HHOB
(B)- TPHB Chandra and Desai 1983)
Williams (1975)
Van Wingerden et al (1977)
EBS (Byron and Joachain (1977)
(A)
(B)
DCS (a_o^2 Sr^{-1})
2
1
10^{-1}
10^{-2}
10^{-3}
10
20
40
60
80
100
120
140
Scattering angle (θ)

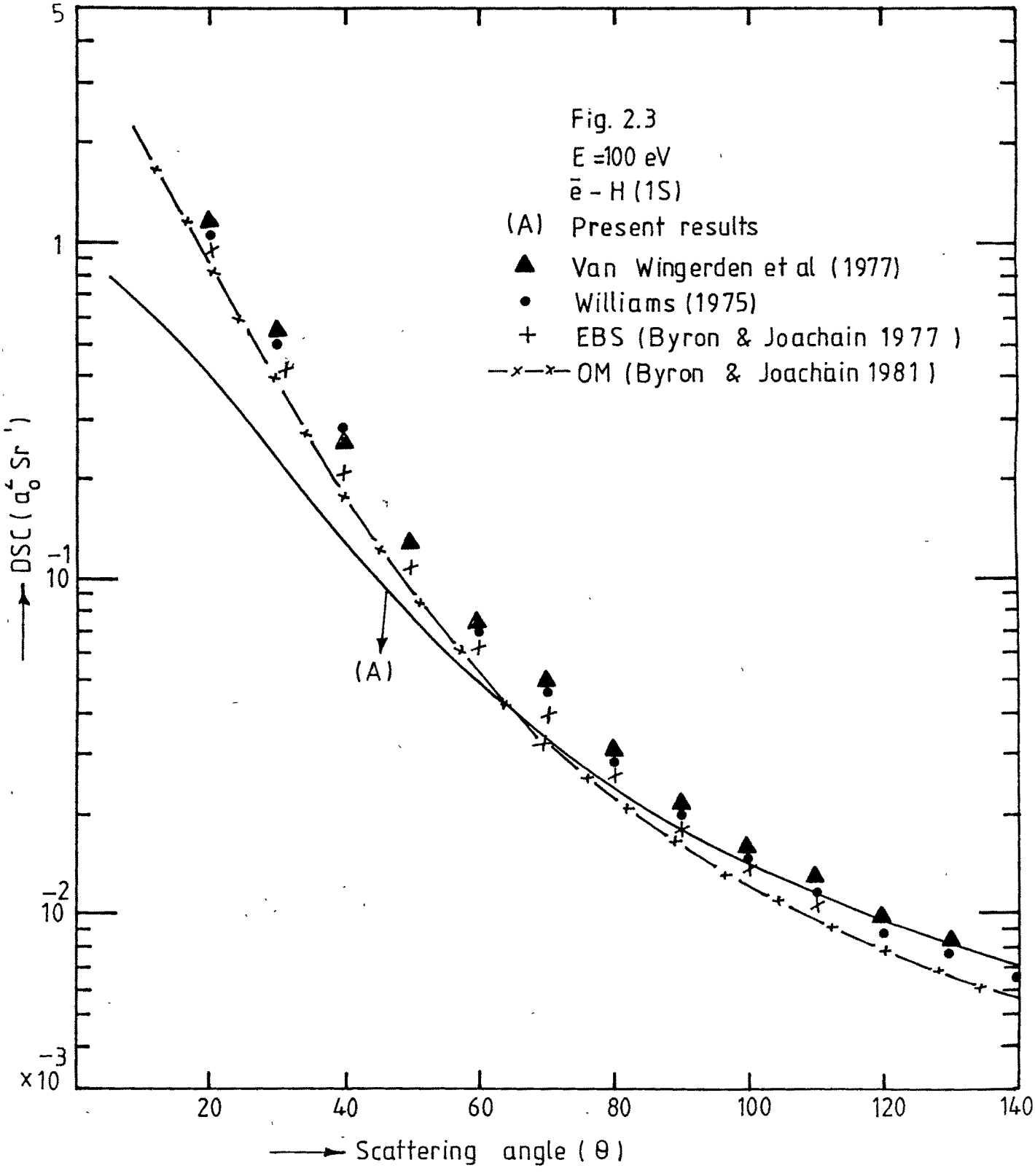
Fig. 2.3
E =100 eV
ē - H (1S)
(A) Present results
Van Wingerden et al (1977)
Williams (1975)
EBS (Byron & Joachain 1977)
OM (Byron & Joachain 1981)
(A)
DSC (a_o^2 Sr^{-1})
x 10^{-3}
10^{-2}
10^{-1}
1
5
20
40
60
80
100
120
140
Scattering angle (θ)