CHAPTER - II

THEORETICAL APPROXIMATIONS AND APPROACH

TO THE PRESENT WORK

2.1   Introduction :

Soon after the advent of ''Quantum mechanics'', collision processes between electron and atoms were studied particularly at intermediate and in high energy regions. The theoretical methods employed in the calculation of scattering amplitudes are reviewed by Callaway (1980), Bransden and Mc Dowell (1977-78), Burke and Williams (1977) and Moiseiwitsch (1977). These methods were broadly classified as (1) expansion methods (2) methods based on the construction of optical model potentials (3) the Born approximation and extensions (4) the distorted wave methods (5) semiclassical methods and (6) many - body theory.

Inspite of large amount of work done, still there exist significant differences between theoretical and experimental results. Theoretically the problem was basically attempted from two sides

(1) nature of the interaction (direct or static, exchange and polarization, interactions) (2) validity (angular and energy regions) of the methods for cross section calculations.

The theoretical study of electron collisions with atomic systems gained considerable amount of interest in recent years. This is due to several reasons. Firstly, there is an increasing demand for electron collision cross sections in other fields. Secondly a number of important advances have occured on the experimental side (Dalba , 1979 ; Blaauw et al 1980 ; Shuttle worth, 1979 ; Klewer , 1980 ; Srivastava et al 1980 and Vuskovic and Srivastava, 1980). Many of these provide very stringent tests of the theory and have stimulated the development of new theoretical approaches. Finally the availability of increasingly more powerful computers has made it possible to perform calculations which would have been impossible to carry out a decade ago.

The purpose of the present chapter is to review few of the important theoretical approximations related to the present study. The following sections deal with the theory of electron collisions with atoms.

2.2 Basic formula for the electron collisions with atoms :

2.2.1 Potential scattering : For the better understanding of the problem, consider the non - relativistic scattering of a spinless particle by a potential field V (r). This will allow us to introduce in a simple way some of the basic ideas which are required in the analysis of electron scattering by atoms. The total energy of the system is

equal to the sum of the kinetic energy and potential energy of the incident particle. Then the corresponding time - independent Schrodinger equation in a.u. (atomic units) can be given as

$$\left[- \frac{1}{2} \nabla^2 + V (\underline{r}) \right] \psi (\underline{r}) = E \psi (\underline{r}) \qquad (2.1)$$

where the mass of the particle has been set equal to one, and E is its total energy. $\underline{k}_i$ and $\underline{k}_f$ are the initial and final momenta of the particle, with $k = | \underline{k}_i | = | \underline{k}_f |$ and $E = k^2/2$. The momentum transfer is given by $\underline{q} = \underline{k}_i - \underline{k}_f$, where $q = 2 k \sin \Theta/2$, Θ is the scattering angle and q is the magnitude of the wave vector transfer $\underline{q}$. It is also convenient to introduce the '' reduced potential '' by $U (\underline{r}) = 2 V (\underline{r})$ and the strength of this is $| U_o | = 2 | V_o |$, where $| V_o |$ is a typical strength of the potential $V (\underline{r})$. For a potential vanishing faster than r^{-1} at large distance the stationary scattering wave function $\psi_{\underline{k}_i}^{(+)}$ representing a plane wave incident in the Z - direction (which we choose along $\underline{k}_i$) and an outgoing (+) spherical wave has the asymptotic form given as

$$\psi_{\underline{k}_i}^{(+)} (\underline{r}) \xrightarrow[r \to \infty]{} A (k) \left[e^{i \underline{k}_i \cdot \underline{r}} + f (k, \Theta, \phi) \frac{e^{i k r}}{r} \right]$$

$$\dots (2.2)$$

where f (k, Θ, ϕ) is the scattering amplitude correspon-
ding to scattering in the direction $\Omega = (\Theta , \phi)$, and
the coefficient A is independent of $\underline{r}$. A number of
methods have been used to found the scattering amplitude.
Few of these methods are outlined in the following sections.

2.2.2 The integral equation of potential scattering : For
the potentials which vanish faster than r^{-1} at large r the
stationary scattering wave function $\psi_{\underline{k}_i}^{(+)}$ has been defined
above as a solution of the Schwinger equation (2.1) satis-
fying the boundary condition (2.2) . It can be shown
(Bransden , 1970 ; Joachain, 1979 ; Burke, 1977) that
$\psi_{\underline{k}_i}^{(+)}$ is also a solution of an equivalent integral equa-
tion - the Lippmann - Schwinger equation - which directly
takes in to account the boundary condition (2.2). That is

$$\psi_{\underline{k}_i}^{(+)} (\underline{r}) = \Phi_{\underline{k}_i}^{(+)} (\underline{r}) + \int G_0^{(+)} (\underline{r}, \underline{r}') U (\underline{r}')$$

$$\psi_{\underline{k}_i}^{(+)} (\underline{r}') d \underline{r}' \qquad (2.3)$$

where $\Phi_{\underline{k}_i} (\underline{r}) = \langle \underline{r} | \underline{k}_i \rangle = (2 \pi)^{-3/2} e^{i \underline{k}_i \cdot \underline{r}}$ is

is a plane wave corresponding to the incident momentum $\underline{k}_i$
and the free Green's function $G_0^{(+)} (\underline{r}, \underline{r}')$ is given
by

$$G_o^{(+)} (\underline{r}, \underline{r}') = - (2 \pi)^{-3} \int \frac{e^{i \underline{k}' \cdot (\underline{r} - \underline{r}')}}{k'^2 - k^2 - i \epsilon} d\underline{k}',$$

$$\epsilon \longrightarrow 0^+ \qquad (2.4)$$

or

$$G_o^{(+)} (\underline{r}, \underline{r}') = - \frac{1}{4\pi} \frac{e^{i k | \underline{r} - \underline{r}' |}}{| \underline{r} - \underline{r}' |} \qquad (2.5)$$

By looking at the asymptotic behaviour of (2.3) one can show that the scattering amplitude f is given by the integral representation.

$$f = - 2\pi^2 < \Phi_{\underline{k}_f} | U | \psi_{\underline{k}_i}^{(+)} >$$

$$= - (2 \pi)^2 < \Phi_{\underline{k}_f} | V | \psi_{k_i}^{(+)} >$$

$$= - (2 \pi)^2 T_{fi} \qquad (2.6)$$

where $\Phi_{\underline{k}_f} (\underline{r}) = < \underline{r} | \underline{k}_f > = (2 \pi)^{-3/2} e^{i \underline{k}_f \cdot \underline{r}}$

is a plane wave corresponding to the final momentum $\underline{k}_f$, and T_{fi} is called the transition matrix element given as

$$T_{fi} = < \Phi_{\underline{k}_f} | V | \psi_{\underline{k}i}^{(+)} > \qquad (2.7)$$

The plane waves have been '' normalised '' here in such a way that

$$\langle \Phi_{\underline{k}_f} | \Phi_{\underline{k}_i} \rangle = \langle \underline{k}_f | \underline{k}_i \rangle = \delta (\underline{k}_i - \underline{k}_f) \qquad (2.8)$$

We shall now give briefly a few important approximate methods which have been proposed for the case where the energy of the projectile electron is higher than the first ionization energy of the target atom. Detailed discussions of several of these methods may be found in the review articles of Joachain and Quigg (1974), Bransden and Mc Dowell (1977-78), Byron and Joachain (1977).

2.2.3 The_Born_approximations : We begin by the Born series, which is obtained if one elects to solve the Lippmann — Schwinger equation (2.3) by perturbation theory. Starting from the '' Unperturbed '' incident plane wave $\Phi_{\underline{k}_i} (\underline{r})$, we then generate for $\Psi_{\underline{k}_i}^{(+)}$ the Born series

$$\Psi_{\underline{k}_i}^{(+)} (\underline{r}) = \sum_{n=0}^{\infty} \phi_n (\underline{r}) \qquad (2.9)$$

with

$$\phi_0(\underline{r}) = \Phi_{\underline{k}_i} (\underline{r})$$

$$\phi_n (\underline{r}) = \int K_n (\underline{r} , \underline{r}') \phi_o (\underline{r}') d\underline{r}' \qquad n \geq 1$$

and

$$K_1(\underline{r}, \underline{r}') = G_o^{(+)} (\underline{r}, \underline{r}') U (\underline{r}'),$$

$$K_n (\underline{r}, \underline{r}') = \int K_1(\underline{r}, \underline{r}'') K_{n-1}(\underline{r}'' , \underline{r}') d\underline{r}''$$

$$n \geq 2 \qquad\qquad (2.10)$$

we see that the Born series (2.9) is a perturbation series in powers of the interaction potential. Substituting the series (2.9) into the expression (2.6) we obtain the Born series for the scattering amplitude, namely.

$$f = \sum_{n=1}^{\infty} \overline{f}_{Bn} \qquad\qquad (2.11)$$

where

$$\overline{f}_{B1} = - 2\pi^2 \langle \Phi_{\underline{k}_f} | U | \Phi_{\underline{k}_i} \rangle$$

$$= - \frac{1}{4\pi} \int e^{i \underline{q} \cdot \underline{r}} U (\underline{r}) d\underline{r} \qquad (2.12)$$

and

$$\overline{f}_{Bn} = -2\pi^2 \langle \Phi_{\underline{k}_f} | U G_o^{(+)} U \ldots G_o^{(+)} U | , \Phi_{\underline{k}_i} \rangle$$

$$n \geq 2 \qquad\qquad (2.13)$$

In this last expression the potential appears n times and

the Green's function (n - 1) time. The Jth order Born approximation to the scattering amplitude can be defined as

$$f_{BJ} = \sum_{n=1}^{J} f_{Bn} \qquad\qquad (2.14)$$

So that $f_{B1} = f_{B1}$; $f_{B2} = f_{B1} + f_{B2}$ etc . It is apparent from the above equations that the Born series (2.11) may be pictured as a multiple scattering series in which the particle interacts repeatedly with the potential and propagates freely between two successive interactions. We should therefore expect that the Born series will converge if the incident particle has a sufficiently large energy and (or) if the potential is weak enough. Very wide application to scattering problems has been made of the first term of the expansion (2.13) since its simplicity is often felt to compensate for all it may lack in accuracy. Unfortunately its error is usually substantial, and further terms of the series, of order higher than the first or second are quite difficult to compute.

2.2.4 The eikonal approximation : More recently, atomic collision processes have been studied by means of the eikonal approximation. Originally introduced in quantum scattering theory by Moliere (1947), this eikonal approximation has been considerebly developed by Glauber (1959) who proposed

à very fruitful many - body generalization of the method.
To construct the eikonal approximation it was assumed that
the incident particle satisfied the ''Short wave length''
condition (ka > > 1) to gether with the ''high-energy''
requirement given as

$$\frac{|V_0|}{E} = \frac{|U_0|}{k^2} \ll 1 \qquad (2.15)$$

With these conditions the eikonal scattering wave function can be
obtained from (2.3) by a linearization of the Green's fun-
ction (2.4). The corresponding eikonal wave function can
be given as

$$\Psi_E (\underline{r}) = (2 \pi)^{-3/2} \exp [i \underline{k_i} \cdot \underline{r} - \frac{i}{2k} \int_{-\infty}^{Z} U (\underline{b} , Z') dZ']$$

$$\cdots \cdots (2.16)$$

Having obtained this we may now substitute this expression
in to the integral representation (2.6) of the scattering
amplitude. This yields

$$f = - \frac{1}{4\pi} \int \exp (i \underline{q} \cdot \underline{r}) U (\underline{r}) \exp [- \frac{i}{2k}$$

$$\int_{-\infty}^{Z} U (\underline{b} , Z') dZ'] d\underline{r} \qquad (2.17)$$

It was shown by Joachain (1979) that the eikonal scattering
amplitude can be given as

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

$$\cdots\cdots \quad (2.18)$$

where the quantity

$$x(k, \underline{b}) = -\frac{1}{2k} \int_{-\infty}^{\infty} U(\underline{b}, Z) \, dZ$$

is called the eikonal phase shift function. The eikonal multiple scattering series can be obtained from (2.18) by the expansion of exp (i x) in powers of x . And define the eikonal multiple scattering expression as

$$f_E = \sum_{n=1}^{\infty} \bar{f}_{En} \qquad (2.19)$$

where,

$$\bar{f}_{En} = \frac{k}{2\pi i} \frac{i^n}{n!} \int d^2 \underline{b} \, \exp(i \, \underline{q} \cdot \underline{b}) [x(k, \underline{b})]^n$$

$$\cdots\cdots \quad (2.20)$$

and from equations (2.18 to 2.20) we get

$$f_{E1} = -\frac{1}{4\pi} \int d^2 \underline{b} \int_{-\infty}^{\infty} dZ \, e^{i \, \underline{q} \cdot \underline{b}} \, U(\underline{b}, Z) \qquad (2.21)$$

it is worth noting that since we have assumed the potential to be real the quantaties $\bar{f}_{En}$ given by (2.20) are alternately purely real and purely imaginary.

Let us now investigate the relationship between the terms of the Born series (2.11) and of the eikonal series (2.19) when $Ka >> 1$ (where ''a'' is range of the potential). First of all it is clear from quations (2.12) and (2.21) that

$$\bar{f}_{B1} = \bar{f}_{E1} \qquad\qquad (2.22)$$

for all interaction potentials, all energies and all momentum transfers. We note that if the z integration in (2.18) had been performed along the direction k_i , using the coordinate system, we would only have approximately $\underline{q} \cdot \underline{b} = \underline{q} \cdot \underline{r}$ for small q's and the relation (2.22) only hold at small angles. Since we know that the Born Series converges at sufficiently high energies for non - relativistic potential scattering it is very desirable to secure the relation (2.22) at all angles. Remarkable relationships between the higher terms of the eikonal and Born series have also been discovered recently (Byron et al 1973 ; Moore , 1970 ; Byron and Joachain , 1973).

One of the ways to proceed beyond first order, perturbation theory i.e. first Born approximation (2.12) is to employ higher order Born approximation. However calculation of the Born series to higher orders requires a considerable amount of work. Another promising and yet still simple way to improve over the first order theory is to apply Glauber

approximation . The Glauber approximation (1959) is
the generalization of the eikonal multiple scattering
expansions to many body scattering problems. It was first
proposed to study high – energy hard on nucleus collisions,
but has also been applied in recent years to analyze atomic
Collision processes. The formulation of the Glauber
scattering amplitudes are given in the following section.

2.3.1 The scattering of fast electrons by atoms :

Let us consider the nonrelativistic scattering of an
electron by a neutral atom of atomic number z . We choose
the nucleus of the atom as the origin of the coordinate
system, and denote respectively by $\underline{r}$ and $\underline{r}_J$ ($J = 1,2,...z$)
the coordinates of the incident particle and of the atomic
electrons. We shall also use the symbol X to represent
all the target coordinates. We shall first consider the
direct scattering . The free motion of the colliding parti-
cle before the collision is described by the direct arrang-
ement channel Hamiltonian $H_d = K_i + h_i$ where K_i is the
kinetic energy operator of the projectile and h_i the
internal target Hamiltonian, such that $h_i \mid n > = W_n \mid n >$.
The full Hamiltonian of the system is

$$H = H_d + V_d \qquad (2.23)$$

where V_d is the interaction between the electron and the

target in the initial (direct) arrangement channel, given as

$$V_d = -\frac{z}{r} + \sum_{J=1}^{z} \frac{1}{|\underline{r} - \underline{r}_J|} \qquad (2.24)$$

And the Green's operator for the direct scattering can be written as

$$G_d^{(+)} = (E - H_d + i\epsilon)^{-1} \qquad (2.25)$$

The S - matrix element corresponding to Transition a ⟶ b (initial to final) is given by (Byron and Joachain , 1977).

$$\langle b \mid S \mid a \rangle = S_{ba} - 2\pi i \delta (E_b - E_a)$$

$$\times \delta (\underline{p}_b - \underline{p}_a) T_{ba} \qquad (2.26)$$

where we have factored out the total energy and momentum conserving delta-functions and the reduced T - matrix element on the energy - momentum shell is given by

$$T_{ba} = \langle \Phi_b \mid V_f \mid \Psi_a^{(+)} \rangle \qquad (2.27)$$

Here $\Psi_a^{(+)}$ is the exact scattering state - vector satisfy the Lippmann - Schwinger equation

$$\Psi_a^{(+)} = \Phi_a + G_i^{(+)} V_i \Psi_a^{(+)} \qquad (2.28)$$

We shall '' Normalize '' the free states in such a way that in a given arrangement channel

$$\langle \Phi_{k''} | \Phi_{k'} \rangle = \langle k'', n'' | k', n' \rangle$$

$$= \delta_{n'n''} \delta(k' - k'') \qquad (2.29)$$

The differential cross section for a binary collision process is given as (in a.u.)

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} | f_{ba} |^2 \qquad (2.30)$$

where we have introduced the scattering amplitude

$$f_{ba} = -(2\pi)^2 T_{ba} \qquad (2.31)$$

Before we analyze how the eikonal methods can be used to evaluate the scattering amplitude, We begin by considering the Born series, which is obtained by solving (2.28) by iterating (2.25) and substituting in (2.27). This yields the T - matrix for direct scattering given as

$$T^d_{ba} = \langle \Phi_b | V_d + V_d G_d^{(+)} V_d + V_d G_d^{(+)} V_d G_d^{(+)} V_d + \ldots | \Phi_a \rangle$$

$$\ldots \ldots \qquad (2.32)$$

The corresponding scattering amplitude can be given as

$$f^d_{ba} = \sum_{n=1}^{\infty} \bar{f}_{Bn} \qquad (2.33)$$

where

$$\bar{f}_{Bn} = - (2\pi)^2 \langle \Phi_b | V_d G_d^{(+)} V_d \ldots$$

$$G_d^{(+)} V_d | \Phi_a \rangle \qquad (2.34)$$

In this last expression the interaction V_d between the projectile and the target appears n times and the Green's operator $G_d^{(+)}$, (n - 1) times.

Similarly if we take into account the spins of the incident and scattered particles, in (2.23 to 2.31) we can define the exchange scattering amplitude.

$$g_{ba} = - (2\pi)^2 T_{ba}^{ex} \qquad (2.35)$$

where

$$T_{ba}^{ex} = \langle \Phi_{pb} | V_p | \psi_a^{(+)} \rangle$$

In the above equations the interaction V_p is tthe potential in the rearranged channel (obtained by permutation of the coordinates of the incident and ejected electrons). Φ_{pb} , $\psi_a^{(+)}$ are the corresponding free wave and full scattering wave functions respectively. By analogy with (2.32 to 2.34) the Born exchange scattering amplitude can be given as

$$g_{ba} = \sum_{n=1}^{\infty} \bar{g}_{Bn} \qquad (2.36)$$

where

$$\overline{g}_{Bn} = - (2\pi)^2 \langle \Phi_{pb} | V_p G_d^{(+)} V_d \cdots G_d^{(+)} V_d | \Phi_a \rangle$$

$$\cdots \quad (2.37)$$

In the above expression $G_d^{(+)}$ appears $(n - 1)$ times. A similar equation using the rearranged Green's operator

$$G_p^{(+)} = (E - H_p + i\epsilon)^{-1}$$ may clearly be written down

by using (2.35).

2.3.2 $\underline{\text{The Glauber approximation}}$: This method is a many -

body generalization of the eikonal approximation, which we described in the previous section. For a direct collision leading from an initial target state $| 0 \rangle$ to a final state $| n \rangle$ the Glauber scattering amplitude is given by Glauber ,(1959).

$$f_G = \frac{k}{2\pi i} \int d^2 \underline{b} \, e^{i \underline{q} \cdot \underline{b}} \langle m | \left\{ e^{i x_G(\underline{b}, X)} -1 \right\} | 0 \rangle$$

$$\cdots \quad (2.38)$$

where the Glauber phase shift function is given in terms of the V_d

$$x_G(\underline{b}, X) = - \frac{1}{k} \int_{-\infty}^{\infty} V_d (\underline{b}, Z, X) \, dZ$$

the integration being performed along a Z - axis perpendicular to $\underline{q}$. A few important points concerning the Glauber approach are : firstly, it may be viewed as an eikonal

approximation to a '' frozen target'' model proposed

by Chase (1956) in which closure is used with an

average excitation energy DE = 0 , secondly , consider-

able insight into the properties of the Glauber method

may be gained by expanding (2.37) in powers of V_d ,

namely

$$f_G = \sum_{n=1}^{\infty} \overline{f}_{Gn} \qquad (2.39)$$

where

$$\overline{f}_{Gn} = \frac{k}{2\pi i} \frac{-i^n}{n!} \int d^2 \underline{b} \, e^{i \, \underline{q} \cdot \underline{b}} < m \mid [\, x \, (\, \underline{b} \, , \, X \,) \,]^n \mid 0 >$$

$$\qquad \qquad \qquad \qquad \qquad (2.40)$$

and comparing the terms of $\overline{f}_{Gn}$ with those of the Born

series $\overline{f}_{Bn}$. We note that $\overline{f}_{B1} \mp \overline{f}_{G1}$, and also the

terms $\overline{f}_{Gn}$ are alternatively real or purely imaginary,

while the corresponding Born terms $\overline{f}_{Bn}$ are complex for

n ≥ 2 . This special feature of the Glauber amplitude

leads to several defects such as (i) the absence of the

important real term for elastic scattering and (ii)

identical cross sections for electron - and positron -

atom scattering. Other deficiencies of the Glauber

amplitude (2.40) include a logarithmic divergence for

elastic scattering in the forward direction, and a poor

description of inelastic collisions involving non-spheri-

cally symmetric states. Its major role in atomic collision

theory has been to stimulate interest in eikonal methods

(Byron and Joachain , 1977). Such as the ''eikonal -

Born series '' (EBS) theory (Byron and Joachain ,

1973, 1974, 1975, 1977).

2.3.3 The eikonal Born series method (EBS) : This method

combines the Born and Glauber series to obtain a consistent

expansion of the scattering amplitude in powers of k^{-1}.

The Glauber Term $\overline{f}_{Gn}$ gives in each order perturbation

theory the leading piece of the corresponding Born term

(for large k) for all q's except in second order where

the long range of the coulomb potential is responsible for

the anomalous behaviour of $\overline{f}_{G2}$ all small q. In the EBS

approximation a consistent calculation of the direct scatter-

ing amplitude through order k^{-2} was obtained by the

replacement of real part of $\overline{f}_{B3}$ by $\overline{f}_{G3}$ in the Born

scattering amplitude. In this way the EBS direct scatter-

ing amplitude

$$f^{d}_{EBS} = \overline{f}_{B1} + \overline{f}_{B2} + \overline{f}_{G3} \qquad (2.41)$$

in addition, exchange effects are taken into account by

the use of Ochkur amplitude g_{och} (Ochkur, 1963, 1964).

The EBS method has been applied to various electron

- atom collision processes (Byron and Joachain , 1977) at

intermediate and high energies. And it is an improvement

over the second Born or Glauber approximations. It was also analyzed that the convergence of the Born series for the direct amplitude is slower at large q than in the small q region. Thus an '' all - order '' treatment would be clearly desirable at large q, and it was done by the optical model (Joachain, 1979 ; Mittleman and Waston , 1959, 1960 ; Byron and Joachain, 1974, 1977 ; Joachain and Vanderpoorten et al 1977 ; Vanderpoorten , 1975 ; Furness and Mc Carthy , 1973; Riley and Truhlar , 1976) methods and target expansion (Burkey and Webb, 1973 ; Callaway and Wooten , 1973, 1974, 1975 ; Callaway and Mc Dowell, Morgan, 1976) methods.

After the formulation of Glauber eikonal approximation (Glauber, 1959) very less amount of work was done for the calculation of DCS and integral cross sections. This was due to the computational complexity involved in evaluating the Glauber amplitude (2. 38) for systems more complicated than helium. Even for simple system (hydrogen) also, it was found difficult to get the closed form of the Glaubers scattering amplitude. Very few methods (Franco, 1971 ; Thomas and Chan, 1973) were proposed to evaluate the Glaubers amplitude with some assumptions on the atomic wave functions. These methods also required a good deal

of computational analysis for the calculation of scattering cross sections. Recently Yates (1974) has proposed another way for the evaluation of (2.38) and obtained the closed form of the three Glauber terms for the elastic scattering of electrons by hydrogen atoms. He made the term wise analysis of the ''Glauber eikonal series'' (GES), and derived the expression for DCS through order (k_i^{-2}) for electron - atom collision processes, at intermediate and high energies. The basic assumptions followed in this GES study of Yates (1974) were as follows.

2.3.4 The Glauber Eikonal Series (GES) : Denote $\tilde{\psi}_i$ and $\tilde{\psi}_f$ as the initial and final state wave functions of the target atom, and Q is the charge of the incident particle. And q is assumed perpendicular to the incident direction and k_i is chosen as the polar axis for the integrations. Substituting the Fourier integral representation of the interaction V_d (2.24) in the Glauber phase shift function (2. 38) we will get the corresponding phase shift

$$x (b , \underline{b}_1 \ldots \underline{b}_z) = - \frac{Q}{\pi k_i} \sum_{J=1}^{z} \int \frac{d\underline{p}}{p^2} e^{-i \underline{p} \cdot \underline{b}} [1 - e^{i \underline{p} \cdot \underline{b}_J}]$$

$$= - \frac{Q}{\pi k_i} \int \frac{d\underline{p}}{p^2} e^{-i \underline{p} \cdot \underline{b}} B(\underline{p} , \underline{b}_1 \ldots \underline{b}_z) \quad (2.42)$$

where $\underline{p}$ is a two – dimensional vector. Again substitution of (2.42) into (2.40) gives the corresponding GES given as

$$f^{(n)}_{GES} (q, k_i) = 2\pi k_i \frac{(- Q)^n}{(\pi k_i)^n n!} \int \frac{d\underline{p}_1}{p_1^2} \quad .....$$

$$\int \frac{d\underline{p}_{n-1}}{p_{n-1}^2 | \underline{q} - \underline{p} |^2} < \bar{\psi}_f | B(\underline{p}_1) ...$$

$$B (\underline{p}_{n-1}) B (\underline{q} - \underline{p}) | \bar{\psi}_i > \qquad (2.43)$$

where $B (\underline{p}_i) = B (\underline{p}_i , \underline{b}_1 ... \underline{b}_z)$ and

$\underline{p} = \sum\limits_{i=1}^{n-1} \underline{p}_i$. Now the DCS can be given as

$$\sigma_{GES} = \frac{k_f}{k_i} [| f^{(1)}_{GES} |^2 + | f^{(2)}_{GES} |^2 - 2 f^{(1)}_{GES} f^{(3)}_{GES}]$$

$$\qquad\qquad .... \quad (2.44)$$

where all the terms in the last expression can be obtained from (2.43) for n = 1 , 2 , and 3. It is obvious from equations (2.43) and (2.34) that

$$f^{(1)}_{GES} = \bar{f}_{B1} , \text{ and } f^{(2)}_{GES} = \bar{f}_{B2}$$

(Massey - Mohr approximation , 1934). Using the equation (2.43) Yates (1974) has obtained the closed forms of the three GES terms for elastic scattering of electrons by hydrogen atoms. He found some divergent integrals in the scattering amplitude for $n \geq 2$, and these were cancelled exactly for particular combinations in the scattering amplitudes. The corresponding third term of scattering amplitude for elastic scattering of electrons by hydrogen atom can be given as

$$f_{GES}^{(3)} = \frac{1}{8k_i^2 T^3} \left(-\frac{\partial}{\partial T} \right) \frac{T^4}{1 + T^2} \left[4 \mid \log \left(\frac{1 + T^2}{T} \right) \mid^2 \right.$$

$$\left. + \frac{\pi^2}{3} - A(T) \right] \quad (2.45)$$

where

$$A(T) = 2 (\log T)^2 + \frac{\pi^2}{6} + \sum_{n=1}^{\infty} \frac{(-T^2)^n}{n^2} , \qquad T \leq 1$$

$$= - \sum_{n=1}^{\infty} \frac{(-1/T^2)^n}{n^2} , \qquad T > 1$$

($T = \frac{q}{2}$, dimensionless vector)

This expression Was obtained after the cancellation of the divergent integrals.

A number of comments can be made regarding (2.43). For example in the forward direction ($T \longrightarrow 0$),

$f_{GES}^{(1)}$ and $f_{GES}^{(3)}$ approaches finite values, whereas $f_{GES}^{(2)}$ diverges as log T. And in the high energy limit ($k_i > > 1$) the imaginary part of second Born term (Moiseiwitsch and Williams , 1959 ; Massey - Mohr , 1934) reduces to $f_{GES}^{(2)}$ given as

$$\text{Im} (\overline{f}_{B2}) = \frac{1}{2k_i(1 + T^2)^2} [2(2 + T^2) \log (\frac{1 + T^2}{T}) + T^2 - 1]$$

$$= f_{GES}^{(2)} \qquad\qquad (2.46)$$

The main advantages in this GES approach are i) The principal difficulty (Coupling of $\underline{b}$ and $\underline{b}_J$'s) in the Glauber phase function (2.38) is evaluated by considering the fourier form of V_d , ii) All the scattering terms are obtained in the closed form, iii) The calculation of the scattering cross sections are easier than the Glauber's calculations iv) Equation (2.44) gives good estimation of the Glauber cross section. The discouraging point in this approach is the underestimation of DCS when compared with other data (Singh and Tripathi, 1980) due to, the rapid convergence of the series (2.43).

After the formulation of GES, Yates (1979) has proposed another theoretical development for the high –

energy — higher order Born approximations (HEA) for electron — atom collision processes. The assumptions made in HEA were similar to those of Glauber theory. The computation procedure in HEA was similar to that of GES. A number of advantages were observed over GES and some related approximations. This new theoretical study of Yates (1979) was an extension of his earlier work (Yates, 1973,1974). This is one of the powerful approximations(Dewangan , 1975 ; Gerjuoy and Thomas , 1974 ; Glen ·, 1976 ; Gau and Macek , 1975 ; Chan and Chang, 1976 ; Golden and McGuire , 1976 ; Hambo et al 1973 ; Flannery and McChan , 1974 ; Joachain and Vanderpoorten , 1973 ; Geltman, 1971 ; Stauffer and Morgan , 1975 ; Byron and Joachain , 1973 ; Byron and Latour , 1976 ; Byron and Joachain , 1977 ; Joachain et al 1977 ; Yates, 1973 ; Yates, 1974 ; Joachain et al 1982), for the description of small angle scattering of electrons by atoms at intermediate and high energies. The theoretical development proposed by Yates (1979) was to obtain consistent approximation for the DCS through order k_i^{-2} , and to obtain closed form of second and third Born Terms. The computation procedure in HEA will be described now.

2.3.5   High — energy higher order Born approximations(HEA):

Consider the three terms of the Born series from (2.34), and interaction V or V_d from (2.24) and the

Greens function from (2.4) for the evaluation of the second and third terms of Born series. A more convenient form for $f_{i \to f}^{(2)}$ and $f_{i \to f}^{(3)}$ can be obtained by transforming the integration variables ($\underline{r}_0$, $\underline{r}_0'$) to the set ($\underline{r}_0$, $\underline{y}$) ; $\underline{y} = \underline{r}_0 - \underline{r}_0'$; in the matrix elements of second and third Born terms, and replacing $\underline{y}$ by $\underline{r}_0'$, then the two terms reduce in the following form

$$f_{i \to f}^{(2)} = \frac{1}{\pi} \sum_n \int d\underline{r}_0 \, e^{i \, \underline{q} \cdot \underline{r}_0} \, V_{fn} (\underline{r}_0) \, I_n \quad (2.47)$$

$$f_{i \to f}^{(3)} = \frac{2}{\pi} \sum_{n,n'} \int d\underline{r}_0 \, e^{i \, \underline{q} \cdot \underline{r}_0} \, V_{fn}(\underline{r}_0) \, I_{n \, n'} \quad (2.48)$$

where

$$I_n = \int d\underline{r}_0' \, e^{i \, \underline{k}_i \cdot \underline{r}_0'} \, V_{ni} (\underline{r}_0 - \underline{r}_0') \, G_n (\underline{r}_0')$$

$$I_{nn'} = \int d\underline{r}_0' \, e^{i \, \underline{k}_i \cdot \underline{r}_0'} \, V_{nn'} (\underline{r}_0 - \underline{r}_0') \, G_n (\underline{r}_0') \int d\underline{r}_0''$$

$$e^{i \, \underline{k}_i \cdot \underline{r}_0''} \, V_{n'i} (\underline{r}_0 - \underline{r}_0' - \underline{r}_0'') \, G_{n'}(\underline{r}_0'')$$

The basic approximations are introduced by the transformation of variable $\underline{S} = \underline{K}' - \underline{k}_n$, in I_n ,

$$I_n = \frac{1}{(2\pi)^3} \int d\underline{r}_0' \, e^{i \, (\underline{k}_i - \underline{k}_n) \cdot \underline{r}_0'} \, V_{ni} (\underline{r}_0 - \underline{r}_0')$$

$$\int \frac{dS\ e^{i\ \underline{S}\cdot\underline{r}_o'}}{S^2 + 2\underline{S}\cdot\underline{k}_n - i\epsilon} \tag{2.49}$$

and assuming $k_n a >> 1$, $\underline{k}_n = \underline{k}_i$, then expanding $(\ S^2 + 2\underline{S}\cdot\underline{k}_n - i\epsilon\ )^{-1}$ in powers of S^2, the $d\underline{S}$ integral of equation (2.49) can be obtained as

$$\int \frac{dS\ e^{i\ \underline{S}\cdot\underline{r}_o'}}{S^2 + 2\underline{S}\cdot\underline{k}_n - i\epsilon} = \int \frac{d\underline{S}}{2\underline{S}\cdot\underline{k}_n - i\epsilon} [\ 1 + \frac{D^2_{r_o'}}{2\underline{S}\cdot\underline{k}_n - i\epsilon}\ ]$$

$$e^{i\ \underline{S}\cdot\underline{r}_o'}$$

where D is differential operator w.r.t. $\underline{r}_o'$, and $d\underline{S} = dS_x\ dS_y\ dS_z$. In the above $d\underline{S}$ integral, $dS_x\ dS_y$ integrals can be evaluated by the use of definitions of delta functions and the dS_z integral can be evaluated using the contour integral techniques for first and second order poles (Boas, 1966). Then the closed form of the $d\underline{S}$ integral can be obtained. With this, equation (2.49) can be written as

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

$$[\ 1 + i\ D^2_{r_o'}\ Z_o'\ /2k_n\ ]\ \delta\ (\underline{b}_o')\ H\ (Z_o')$$

$$= \frac{i}{2k_n} [\ I_{n1} + I_{n2}\ ] \tag{2.50}$$

where $H(Z)$ is the Heaviside function, and $\underline{S}$ integration has been performed in cylindrical polar coordinates by choosing $\underline{k}_n$ as the polar axis and writing

$$\underline{r}'_o = \underline{b}'_o + Z'_o \, \hat{k}_n \quad .$$

The above integral can be further simplified by using the delta function properties, σ one obtains

$$I_{n1} = \int_{-\infty}^{\infty} e^{-i(\underline{k}_i - \underline{k}_n) \cdot \hat{k}_n Z'_o} H(Z'_o) V_{ni}(\underline{r}_o - \underline{r}'_o)$$

$$dZ'_o \; \Big|_{\underline{b}'_o = 0}$$

Now consider the integral I_{n2}

$$I_{n2} = \frac{i}{2k_n} \int d\underline{r}'_o \, e^{i(\underline{k}_i - \underline{k}_n) \cdot \underline{r}'_o} V_{ni}(\underline{r}_o - \underline{r}'_o)$$

$$D^2_{\underline{r}'_o} \, \mathcal{S}(\underline{b}'_o) Z'_o \, H(Z'_o)$$

integrating by parts

$$= \frac{i}{2k_n} \left\{ \int d\underline{r}'_o \, D_{\underline{r}'_o} [\, \mathcal{S}(\underline{b}'_o) Z'_o H(Z'_o)\,] \right.$$

$$e^{i(\underline{k}_i - \underline{k}_n) \cdot \underline{r}'_o} V_{ni}(\underline{r}_o - \underline{r}'_o) -$$

$$\int d\underline{r}_o{}' \, D_{r_o}{}' \, [\, \delta(\underline{b}_o{}') \, Z_o{}' \, H(Z_o{}') \,]$$

$$[\, e^{i\,(\underline{k}_i - \underline{k}_n)\cdot \underline{r}_o{}'} \, V_{ni}(\underline{r}_o - \underline{r}_o{}') \,] \,\}$$

again performing integration by parts in the second term of the above expression

$$= \frac{i}{2k_n} \{\, \int d\underline{r}_o{}' \, D_{r_o}{}' \, [\, \delta(\underline{b}_o{}') \, H(Z_o{}') \, Z_o{}' \,]$$

$$e^{i\,(\underline{k}_i - \underline{k}_m)\cdot \underline{r}_o{}'} \, V_{ni}(\underline{r}_o - \underline{r}_o{}') \,-$$

$$[\, \int d\underline{r}_o{}' \, \delta(\underline{b}_o{}') \, Z_o{}' \, H(Z_o{}') \, D_{r_o}{}'$$

$$e^{i\,(\underline{k}_1 - \underline{k}_n)\cdot \underline{r}_o{}'} \, V_{ni}(\underline{r}_o - \underline{r}_o{}')$$

$$\int d\underline{r}_o{}' \, \delta(\underline{b}_o{}') \, Z_o{}' \, H(Z_o{}') \, D^2{}_{r_o}{}'$$

$$e^{i\,(\underline{k}_1 - \underline{k}_n)\cdot \underline{r}_o{}'} \, V_{ni}(\underline{r}_o - \underline{r}_o{}') \,] \,\}$$

$$= \frac{i}{2k_n} \int d\underline{r}_o{}' \, \delta(\underline{b}_o{}') \, Z_o{}' \, H(Z_o{}') \, D^2{}_{r_o}{}'$$

$$e^{i\,(\underline{k}_i - \underline{k}_n)\cdot \underline{r}_o{}'} \, V_{ni}(\underline{r}_o - \underline{r}_o{}')$$

After the $D^2{}_{r_o}{}'$ operation, the corresponding I_{n2} and I_{n1} gives I_n

$$I_n = -\frac{i}{2k_n} \int_{-\infty}^{\infty} d Z_o' \; e^{i (\underline{k}_i - \underline{k}_n) \cdot \hat{\underline{k}}_n Z_o'} H (Z_o')$$

$$[(1 + \frac{i Z_o'}{2k_n} O) V_{ni} (\underline{r}_o - \underline{r}_o')]_{\underline{b}_o' = 0}$$

Further simplification of I_n , consistent with the original assumptions, is possible on noting that

$$(\underline{k}_i - \underline{k}_n) \cdot \hat{\underline{k}}_n = k_i \cos \Theta_{in} - k_n$$

$$= \underline{k}_i - \underline{k}_n + O (\underline{k}_i \Theta_{in}^2)$$

$$\simeq \underline{k}_i - \underline{k}_n$$

$$\therefore \; I_n \simeq \frac{i}{2k_n} \int_{-\infty}^{\infty} d Z_o' \; e^{i \beta_i Z_o'} H (Z_o')$$

$$(1 + \frac{i Z_o'}{2k_n} D_{r_o'}^2) V_{ni} (\underline{r}_o - \underline{r}_o') \Big|_{\underline{b}_o' = 0}$$

$$\dots\; (2.51)$$

where $\beta_i = k_i - k_n \simeq DE_{in} / k_i$, on using the energy conservation condition, the above expression embodies the central approximation.

The evaluation of the scattering amplitude can be performed in cylindrical polar coordinates. The

orientation of the coordinate system is chosen such that the Z - axis is always perpendicular to $\underline{q}$. Thus $\underline{q}$ is two dimensional, and the position coordinates of the $z + 1$ electrons will be written as $\underline{r}_i = \underline{b}_i + Z_i \hat{y}$, $i = 0 , 1 \ldots\ldots z$, where y is a unit vector in the Z - direction. Denote X for target coordinates.

For the simplification of the second and third Born Terms (2.47, 2.48), it is useful to take the Fourier form of the interaction (2.24).

$$V (\underline{r}_0 , \ldots\ldots \underline{r}_z) = \int d\underline{p} \; e^{i \, \underline{p} \cdot \underline{b}_0} \int_{-\infty}^{\infty} d p_z$$

$$e^{- i \, p_z \, Z_0} \; \bar{V} (\underline{p} + p_z\hat{y} , \underline{r}_1 \cdots \underline{r}_n)$$

$$\ldots\ldots (2.52)$$

where

$$\bar{V} (\underline{p} + p_z\hat{y}, \underline{r}_1 \ldots\ldots\underline{r}_z) = \frac{1}{2\pi^2 (p^2 + p_z^2)} \sum_{J=1}^{z}$$

$$(e^{i \, \underline{p} \cdot \underline{b}_J + i \, p_z \, Z_J} - 1) \quad (2.53)$$

The general form of the $V_{ni} (\underline{r}_0)$ in the above expressions has been defined as

$$V_{nm} (\underline{r}_0) = < \bar{\psi}_n(X) | V (X) | \bar{\psi}_m (X) > \qquad (2.54)$$

Now substituting (2.52, 2.51) in the second and third Born terms (2.47, 2.48), the corresponding second Born term can be written as

$$f^{(2)}_{HEA} = \frac{i}{2\pi\, k_i} \sum_n \int d\, \underline{r}_o\; e^{i\, \underline{q}\cdot\underline{r}_o}\; V_{fn}(\underline{r}_o) \int_{-\infty}^{\infty}$$

$$d\, Z'_o\; H(Z'_o)\; e^{i\,\beta_{in}\, Z'_o}\; [\; V_{ni}(\underline{r}_o - Z'_o\hat{y})$$

$$+\; \frac{i\, Z'_o}{2k_i}\; D^2_{r'_o}\; V_{ni}(\underline{r}_o - \underline{r}'_o)|_{b'_o = 0}\;] \qquad (2.55)$$

The infinite summation over the atomic states can be treated in a simple way (Woolings and Mc Dowell , 1972 ; Byron and Joachain , 1977).

$$\sum_n V_{fn}(\underline{r}_o)\, V_{ni}(\underline{r}_o - \underline{r}'_o) = V_f(\underline{r}_o)\, V_i(\underline{r}_o - \underline{r}'_o)$$

$$\dots\dots (2.56)$$

It is assumed that $\beta_{in} \simeq \beta_i = DE/k_i$, where DE is the average energy transfered to intermediate atomic states during the course of the collision. Now (2.55) can be written as

$$f^{(2)}_{HEA} = \frac{i}{2\pi k_i} \int d\, \underline{r}_o\; e^{i\, \underline{q}\cdot\underline{r}_o}\; <\Psi_f\; |\; V(\underline{r}_o \dots\dots, \underline{r}_z)$$

$$\int_{-\infty}^{\infty} d Z_o' \, H(Z_o') \, e^{-i\beta_i Z_o'} \, [\, V(\underline{r}_o - Z_o' \hat{y}, \, \underline{r}_1 \cdots, \, \underline{r}_z)$$

$$+ \frac{i Z_o'}{2k_i} \, D^2_{\underline{r}_o'} \, V(\underline{r}_o - \underline{r}_o', \, \underline{r}_1 \cdots \underline{r}_z) \, \Big| \,] \, | \, \hat{\Psi}_i > $$

$$\underline{b}_o' = 0$$

$$\cdots \cdots \quad (2.57)$$

Real and imaginary parts of the above expression can be obtained by using (2.53) and carrying out $D^2_{\underline{r}_o}$ operation in (2.57). Then the corresponding terms through $O(k_i^{-2})$ for DCS can be written as

$$Re1 \, f^{(2)}_{HEA} = -\frac{4\pi^2}{k_i} \, \mathcal{P}\!\int d\underline{p} \int_{-\infty}^{\infty} \frac{d \, p_Z}{p_Z - \beta_i}$$

$$U^{(2)}_{fi} \, (\underline{q} - \underline{p} - p_Z \hat{y}, \, \underline{p} + p_Z \hat{y}) \qquad (2.58)$$

$$Re2 \, f^{(2)}_{HEA} = -\frac{2\pi^2}{k_i^2} \, \frac{\partial}{\partial \beta_i} \, \mathcal{P}\!\int d\underline{p} \int_{-\infty}^{\infty} \frac{d \, p_Z}{p_Z - \beta_i} (p^2 + p_Z^2)$$

$$U^{(2)}_{fi} \, (\underline{q} - \underline{p} - p_Z \hat{y}, \, \underline{p} + p_Z \hat{y}) \qquad (2.59)$$

$$Im \, f^{(2)}_{HEA} = \frac{4\pi^3}{k_i} \int d\underline{p} \, U^{(2)}_{fi} \, (\underline{q} - \underline{p} - \beta_i \hat{y} \, ; \, \underline{p} + \beta_i \hat{y})$$

$$\cdots \quad (2.60)$$

where $\mathcal{P}$ is the principal value. The general form of

$U_{fi}^{(2)}$ (.....; ......) can be given as

$$U_{fi}^{(2)} (x , X ; y, Y) = < \bar{\Psi}_f | \bar{V} (x, X)$$

$$\bar{V} (y, Y) | \bar{\Psi}_i >$$

Now the evaluation of the third Born term is similar to that of second Born term. Substitution of the first term of (2.51) in (2.48) the corresponding third Born term can be given as

$$f_{HEA}^{(3)} = \frac{1}{2\pi k_i^2} \sum_{nn'} \int d\underline{r}_o \; e^{i \underline{q} \cdot \underline{r}_o} V_{fn} (\underline{r}_o) \int_{-\infty}^{\infty} d Z_o'$$

$$e^{i \beta_{in} Z_o'} H (Z_o') V_{nn'} (\underline{r}_o - Z_o' \hat{y}) \int_{-\infty}^{\infty} d Z_o''$$

$$e^{i \beta_{in} Z_o''} H (Z_o'') V_{n'i} (\underline{r}_o - Z_o' \hat{y} - Z_o'' \hat{y})$$

$$..... \quad (2.61)$$

The real parts of this expression can be obtained by using the equations (2.52, 2.56) and integral representation of the δ functions (2.48). Now the real part contribution of the third Born term (2.48) can be given as

$$Re \; f_{HEA}^{(3)} = f_1^{(3)} + f_2^{(3)} \quad\quad (2.62)$$

where

$$f_1^{(3)} = \frac{4\pi^4}{k_i^2} \int d\underline{p} \int d\underline{p}' \; U_{fi}^{(3)})(\underline{p} - \beta_i \hat{y} \; ; \; \underline{p}' \; ;$$

$$\underline{q} - \underline{p} - \underline{p}' + \beta_i \hat{y}) \qquad (2.63)$$

$$f_2^{(3)} = \frac{4\pi^2}{k_i^2} \; \mathcal{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{d\, p_z}{p_z - \beta_i} \int d\underline{p}' \mathcal{P} \int_{-\infty}^{\infty} \frac{d\, p_z'}{p_z' - \beta_i}$$

$$U_{fi}^{(3)} \; (\underline{p} - p_z \hat{y} \; ; \; \underline{q} - \underline{p} - \underline{p}' + p_z \hat{y} - p_z' \hat{y} \; ;$$

$$\underline{p}' + p_z' \hat{y}) \qquad (2.64)$$

The general form of the $U_{fi}^{(3)}$ (....; ......; ......) can

be given as

$$U_{fi}^{(3)} (X' ; Y' ; Z') = \langle \Psi_f \mid \bar{V} (X', \underline{r}_1 \ldots\ldots \underline{r}_z)$$

$$\bar{V} (Y', \underline{r}_1 \ldots\ldots\ldots \underline{r}_z)$$

$$\bar{V} (Z', \underline{r}_1 \ldots \underline{r}_z) \mid \alpha \Psi_i \rangle \qquad (2.65)$$

The DCS through order ($1/k_i^2$) for direct scattering can

be obtained from the scattering amplitude given as

$$F_{HEA}^d = f_{i \longrightarrow f}^{(1)} + Re1\, f_{HEA}^{(2)} + Re2\, f_{HEA}^{(2)} + Re\, f_{HEA}^{(3)} + i\, Im\, f_{HEA}^{(2)}$$

$$\ldots \quad (2.66)$$

Where $f_{i \longrightarrow f}^{(1)}$ is the first Born approximation.Yates (1979) has made an analytical study of equations (2.58, 2.59 , 2.60, 2.63 and 2.64) for elastic scattering of electrons by hydrogen atoms. And the following behaviour of these axpressions are worth noting.

2.3.6 Behaviour of second and third Born terms in HEA :

The assumptions in HEA were made along with the small angle approximation of Glauber (1959). HEA concerned with the elucidation of character of second and third Born terms for short wave length (ka > > 1) and for small momentum transfers (small angles). The partial expansion of equation (2.49) was necessitated by a desire to include a plausible and reasonably accurate description of virtual excitations (target polarization).

In the second Born term (2.57) if $\beta_i \longrightarrow 0$ the real part of order k_i^{-1} (2.58) vanishes, and of order k_i^{-2} (2.59) remains, similarly the imaginary part (2.60) reduces to the second term of GES. It was also shown for elastic scattering of electrons by hydrogen atoms, that when $q \rightarrow 0$ for large k_i the real and imaginary parts of the second Born term approaches to the corresponding terms of the simplified Born approximation (Byron and Joachain. 1977). The difference between HEA and simplifed Born

approximation is the term of order k_i^{-2} when $q = 0$ in HEA .

In the third Born term (2.61) if $\beta_i \longrightarrow 0$, both the terms (2.63, 2.64) remains. One of them (2.63) approaches to the Glauber's estimation of the third Born term like, the second term (2.64) is an additional contribution to the third Born term apart from the Glauber like term. It was also shown for hydrogen problem that when $q = 0$ equation (2.62) reduces to zero.

Finally it was concluded that the HEA provide an accurate description of these terms for small q.

2.4 <u>Recent theoretical developments in electron - atom scattering calculations</u> :

Recently the developments in theoretical side are not similar to that of experimental side for the calculation of collision cross sections at intermediate and high energies. The intermediate energy electron-atom scattering is most difficult to treat theoretically , because the interaction of an electron with an atom in this energy range can involve all the three processes, viz, elastic scattering, excitation and ionization in a manner that their effects on one another cannot be ignored. Because of these difficulties very limited number of theoretical methods are employed in

this energy range for the study of collision cross sections.

Considerable amount of work has been reported by Byron and Joachain (1977) for the calculation of scattering cross sections for different atoms. Yates (1973, 1974, 1979) has proposed two theoretical methods for the electron – atom scattering processes. Recently Ermolaev and Walters (1979, 1980) have developed procedure to carry out an exact calculation of second Born approximation for the $\bar{e}$ – H (hydrogen) elastic scattering and 1s – 2s transition . Kingston and Walters (1980) have carried out DWSBA calculations for $\bar{e}$ – H elastic scattering and 1s – 2s and 1s – 2p transition in the energy range 30 – 680 eV. Very recently Rao and Desai (1982) have reported $\bar{e}$ – H collision cross sections using higher order exchange amplitudes. Walters (1980) has also calculated the exact plane wave second Born exchange amplitudes. The generalized coulomb projected Born (GCPB) approximation (Morgan, 1975) has been recently modified by Schaub – Shaver and Stauffer, (1980) , and used to calculate collision cross section for $\bar{e}$ – H scattering processes. Mathur et al (1980), have used similar type of GCPB approximation to study the inelastic scattering from the ground state of helium atom and also to study the excitation of atomic hydrogen and helium from the metastable excited s states by electron impact. Similar type of collision cross sections are reported

by Rao and Desai (1983α). Roy and Sil (1978) have used Wallace's second order eikonal approximation to calculate the cross sections for $\bar{e}$ - helium elastic scattering including long - range polarization and non local dynamic effects. Fon et al (1980) have extended their earlier R - matrix method calculation methods for electron impact excitation of helium. Joachain and Winters (1980) have developed an optical model approach to the elastic scattering of electrons from the hydrogen atom in the metastable (2s) state. Elastic scattering of electrons and positrons by lithium atoms are reported by Tayal et al (1981) at incident energies 10 to 200 eV. Recently Rao and Desai (1983C) have reported the elastic collision cross section for Lithium atoms.

2.5 Approach to the present investigations

During an intensive study of the results of various approximations for the description of electron - atom scattering processes , at intermediate and high energies, I found following problems, which are enlisted below.

1) Very few theoretical methods were able to reproduce the scattering cross section which can be compared satisfactorily with the results of the experiments .

2) Some approximations required complicated numerical techniques for the evaluation of the scattering cross sections.

3) Divergent integral problems were comman in some approximations.

4) Very few of the theoretical techniques were used to study the higher order exchange amplitudes.

5) Large variations in scattering cross sections were observed between the experimental and theoretical results, even for the simple systems like hydrogen .

6) Few approximations were found to be difficult in

order to extend them for the study of many electron
system (Z > 1).

7)   Though a large amount of work is done in this field,
        still there exist new results both in the theoretical
        and experimental approaches, which are   in disagree-
        ment with the   results produced in these corelated
        techniques.

During the study of the   GES and   HEA it is noted
that   the combination of these approximations can avoid the
above   raised unavoideable   problems. After the formulation
of HEA , except us (Rao and Desai,   1981, 82, 83 a, b, c)
no one has reported the collision cross sections data.

Keeping all the above raised problems in mind I
have selected the GES and the HEA approaches for the
present investigations. The   HEA is extended to study
different atoms for different interactions . The extended
work of HEA is presented in this thesis.