Chapter 2

High energy methods used in slow electron scattering

2.1   Introduction

The second chapter deals with some of the high energy methods that find applications in the low-energy work. The reason for taking up this particular aspect here, immediately after the first chapter is two-fold, viz. (i) in the most part of the present work after this chapter, we have dealt with high energy problems only, so that the subject matter of this chapter is independent and self-consistent, (ii) the author himself started his work on the kind of problems described here and then, from the trends in the literature, a switch over to the problems described later on, was though of. We begin, in the next section, after specifying the meaning of 'high' and 'low' energies, with an outline of various theoretical methods in vogue, in various energy domains. The basic idea underlying different methods is very briefly mentioned. The theoretical methods of our interest in this chapter, viz. the Born and the Glauber approximations are treated somewhat at length. The reason why 'high' energy theories are suitable for some of the 'low' energy problems is also discussed.

2.2 ' Various Theoretical Methods

First of all, the study of electron collisions with atoms and molecules 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 domains of the energy of the projectile electron. If the speed of the incident electron $'v_e'$ is less than or nearly equal to the speeds $'v_a'$ of target electrons (of the atom/molecule), then the range of energy is termed as 'low'. Equivalently in the low energy region, only a few channels are open. Thereafter, the 'intermediate' energy is near the excitation threshold of the target and extends upto a few times the ionization threshold. Then, from a few times the ionization threshold, upwards, we are in the 'high' energy region. This last one finally goes over to very high energies where relativistic considerations become demanding. Obviously, this classification depends very much on the target. So, quite generally, 'low' energy is the region below 10 eV incident energy, 'intermediate' range extends from about 10 eV to nearly 100 eV, and above that, is the high energy region. In this connection, let us recall that 'thermal' electrons are the ones having energy of the

order of 'kT', with k as the Boltzmann constant and T
as the absolute temperature. Near room temperatures,
this amounts to nearly 0.025 eV energy.

We now classify different theories. All
the theories of collision Physics, now in practice, are
mainly quantum mechanical, and the whole of quantum
mechanics stems from the famous Schroedinger equation.
Thus all the different methods, that we are going to
mention now, are but different approximate ways to solve
the Schroedinger equation. Basically, various theories of
our study, fall under two categories, as follows.

1.   differential approach : here, attempts are made
       to solve the Schroedinger equation itself, which
       is a differential equation.

2.   integral approach : here, the attempts are made
       to solve an integral equation of scattering,
       i.e. the Lippmann-Schwinger equation, which is
       equivalent to the Schroedinger equation.

We do not attempt to describe how various
approximation methods originate from either of the two
approaches stated above. Rather it will suffice to give
only an introduction of various approximate methods
together with their range of applicability. However, many

of the theories have been stretched beyond their usual
energy domains, often with successes. Given below are
various approximations used in various ranges of energy.
The list is not at all exhaustive.

Approximation method	Broad energy range
1 eigen-function expansion, or close-coupling method	Low
2 L^2-methods	Low
3 R-matrix theory	Low, intermediate
4 Partial wave analysis	Low, intermediate
5 Many body theories	Low, intermediate
6 Optical potential methods	Intermediate
7 distorted wave methods	Intermediate to high
8 Born approximations	Intermediate to high
9 Semiclassical methods, eikonal and Glauber theories	Intermediate to high
10 EBS, modified Glauber approaches, etc.	Intermediate to high

Now, we follow the (non relativistic)
time - independent Schroedinger equation. This is
because, it is assumed that our system has reached a

stationary state, i.e. the incident beam has been acting

for a long time. Consider the time independent Schroedinger

equation for the system of incident electron plus the

target,

$$(H - E) \, \psi \, (\underline{r} \, , \, \underline{X}) \; = \; 0 \qquad (2.1)$$

where, the wave function of the system $\psi(\underline{r} \, , \, \underline{X})$ is a

function of the coordinates of the incident electron $(\underline{r})$

and of the target $(\underline{X})$. The hamiltonian of the system is

(in a.u.)

$$H \; = \; -\frac{1}{2}\nabla_{\underline{r}}^2 \; + \; V \, (\underline{r}, \, \underline{X}) \; + \; H_t \, (\underline{X}) \qquad (2.2)$$

with, $-\frac{1}{2}\nabla_{\underline{r}}^2$ as the kinetic energy operator of the

incident electron, $V(\underline{r} \, , \, \underline{X})$ as its potential energy of

interaction with the target and, $H_t(\underline{X})$ as the hamiltonian

of the target alone. The total energy of the system E is

the sum of energies of the projectile and the target. At

large distances the total wavefunction of the system

appears as a sum of the wave functions in the incident

and the scattered channels. There are certain basic

assumptions or formulations which help us in tackling the

Schroedinger equation with a relative ease. Broadly

speaking, some of them are as follows.

1.   Born-oppenheimer approximation : Since, the
      ratio of the electronic to nuclear masses is
      very small, it is possible to separate out
      the nuclear i.e. rotational and vibrational
      motions from electronic motions in a molecule.

2.   Secondly, we mention two reference frames
      that are used in the theory of electron
      molecule collisions. They are, the space
      fixed or LAB frame and the BODY-frame.

3.   Fixed nuclei formation : By this, we mean an
      adiabatic approximation in which the incident
      particle is fast enough, so that the nuclei of
      the target molecule can be assumed to be
      fixed.

Now the equation (2.1) can be used to
understand the basic idea underlying various approximation
methods. Thus, e.g., in the close coupling formulation,
one seeks a solution of the Schroedinger equation, as an
expansion of $\psi(\underline{r}, \underline{X})$ in terms of the eigen
functions of the target states.

The other approach towards the solution
of equation (2.1) stems from the fact that the potential

$V(\underline{r}, \underline{X})$ and the wave function $\psi(\underline{r}, \underline{X})$ are the functions of the coordinates of the incident electron and of the target as well. Difficulties arise because of many coordinates involved. The 'optical o potential' methods, therefore, are aimed at determining an equivalent, local, central potential, dependent on $\underline{r}$ only, which can be used to extract solutions of the scattering problems.

One must also mention an important formalism in the scattering problems, and that is the partial wave analysis. This is a well established theoretical procedure in which the scattering wave function is expanded in terms of partial waves and the basic quantity to be evaluated is the phase shift that leads to scattering amplitudes and hence the cross-sections.

The high energy methods, to be discussed below, arise from an integral equivalent of the Schroedinger equation.

2.3   High Energy Methods

2.3.1   General

Consider the non-relativistic scattering of an electron by a structureless target, generating a potential $V(\underline{r})$. The Schroedinger equation (2.1) can be

rewritten as,

$$(\nabla_r^2 + k^2)\ \psi(k\ ,\ \underline{r}) = U(\underline{r})\ \psi(k,\ \underline{r}) \qquad (2.3)$$

Here, ∇_r^2 is the k. E. operator of the incident electron. $k_i = k = |\underline{k}_i|$ and $\underline{k}_i$ is incident momentum vector (in a.u.). The reduced potential is,

$$U\ (\underline{r}) = 2\ V\ (\underline{r}) \qquad (2.4)$$

The solution of eqn. (2.3), also denoted by $\psi_{k_i}^+ (\underline{r})$, satisfies the boundary condition as follows.

$$\psi_k^+ (\underline{r}) \xrightarrow[\ r \longrightarrow \infty\ ]{} e^{i\underline{k}_i \cdot \underline{r}} + f(\theta,\emptyset))\ \frac{e^{ikr}}{r} \qquad (2.5)$$

with $f(\theta\ ,\ \emptyset)$ as the scattering amplitude. This quantity is of utmost importance, as it is related to the differential cross section through,

$$\frac{d\sigma\ (\theta,\ \emptyset)}{dW} = \frac{k_f}{k_i}\ |f(\theta\ ,\ \emptyset)|^2 \qquad (2.6)$$

The last eqn. is the meeting ground of the theory and experiments. We must mention one more fundamental relation

of scattering theory, called the optical-theorem, given as

$$\sigma^{tot} = \frac{4\pi}{k_i} \cdot \text{Imf} (\Theta = 0) \qquad (2.7)$$

where, σ^{tot} is the total collision cross-section and $\text{Imf} (\Theta = 0)$ is the imaginary part of the scattering amplitude in the forward direction (scattering angle $\Theta = 0$). Although, we have started with a particular case of scattering by a structureless target, the fundamental equations like (2.6) and (2.7) are quite general.

Coming back to the Schroedinger eqn. (2.3) the general solution is written, after some mathematics, as (Joachain, 1975),

$$\psi_{k_i} (r) = \phi_{k_i} (r) + \int G_0^+ (r,r') \qquad (2.8)$$
$$U(r') \psi_{k_i} (r) \, dr'$$

The normalized plane wave is,

$$\phi_{k_i} (r) = (2\pi)^{-3/2} e^{+ik_i \cdot r} \qquad (2.9)$$

Similarly, with k_f as the scattered electron momentum,

$$\phi_{k_f} (r) = (2\pi)^{-3/2} e^{ik_f \cdot r} \qquad (2.10)$$

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

$$G_o^+ (\underline{r} , \underline{r}') = - \frac{1}{4\pi} \frac{\exp ik_i |\underline{r} - \underline{r}'|}{|\underline{r} - \underline{r}'|} \qquad (2.11)$$

The eqn. (2.8) is the Lippmann-Schwinger equation. The general expression of the scattering amplitude is, in a.u.,

$$f(\theta,\emptyset) = -4\pi^2 < \emptyset_{k_f} | V | \psi_{k_i}^+ (\underline{r}) > \qquad (2.12)$$

2.3   High Energy Methods

2.3.1   The Born approximations

The zeroath approximation to the solution of the Lippmann-Schwinger equation is to replace $\psi_{k_i}^+ (\underline{r})$ simply by $\emptyset_{k_i}(\underline{r})$. Substituting this in the right hand side of eqn. (2.8), we obtain the first Born scattering amplitude as,

$$f_{B1} = -4\pi^2 < \emptyset_{k_f} | V | \emptyset_{k_i} > \qquad (2.13)$$

The second Born approximation is then obtained by next iteration. This procedure generates the Born series as a

perturbative expansion in the powers of the potential
U(r). If the potential is weak enough, the expansion
coverages to a limit.

Let us now analyse the first Born approximation,
eqn. (2.13). The first Born amplitude as a function of the
scattering direction (θ, ∅) and the momentum transfer is,
obtained from,

$$f_{B1} = -\frac{1}{2\pi} \int e^{i\underline{q}\cdot\underline{r}} V(\underline{r}) \, d\underline{r} \qquad (2.14)$$

The momentum transfer,

$$q = |\underline{k_i} - \underline{k_f}| \quad \text{in a. u.} \qquad (2.15)$$

For a central potential, the scattering amplitude is
independent of azimuthal angle ∅. Written as above in
eqn. (2.14) f_{B1} is the Fourier transform of potential
V(r). Now, ✗ what are the physical conditions under
which the first Born approximation is valid ? We find that
it is essentially a high energy approximation. At high
energies, it is valid if only,

$$\frac{|U_o|a}{2k} \ll 1 \qquad (2.16)$$

where, $'U_o'$ is the strength and $'a'$ is the range of the potential. For low energies, i.e. $ka \longrightarrow 0$, this becomes

$$\frac{1}{2} \mid U_o \mid a^2 \ll 1 \qquad (2.17)$$

i.e. it is valid only if the potential is very weak.

Further insight into the nature of the first Born approximation is obtained by considering a target with an internal structure. We must then go back to eqn. (2.1) and introduce the wave function of the target through,

$$\mid \underline{k}_i, \, i \rangle \; = \; \phi_{\underline{k}_i} \, (r) \, \psi_i \, (\underline{X}) \qquad (2.18)$$

where, $\psi(\underline{X})$ is the eigen function of the target in its initial state i. A similar expression holds for the final state of the system. Thus, the first Born amplitude for the scattering of electrons by a target, leading to its transition $i \longrightarrow f$, becomes,

$$f_{B1} \; = \; - \frac{1}{2\pi} \int e^{-i\underline{q}.\underline{r}} \, V_{fi} \, d\underline{r} \qquad (2.19)$$

with

$$V_{fi} = \langle f \mid V(\underline{r}, \underline{X}) \mid i \rangle \qquad (2.20)$$

Let us now point out how, the first Born approximation, though a high energy approximation, holds true in a limited class of low energy problems.

We are presently interested in polar molecules as targets of our investigation. These molecules possess a permanent electric dipole moment, so that the interaction between a polar molecule and an incident electron, at large distances, is dominated by the point dipole potential,

$$V_{PD} = - \frac{De}{r^2} \cos \Theta \qquad (2.21)$$

'e' and 'D' are the electronic charge and the dipole moment of the target respectively, wherever the constants 'e', 'h' or 'm' appear explicitly, we are NOT working in a.u. In this chapter, we have frequently switched over to either system of units. In eqn. (2.21), Θ is the angle between $\underline{r}$ and the dipole axis (see fig. 2.1). Further, the following relation is quite often used.

$$\cos \Theta = \cos \Theta' \cos \Theta_m + \sin \Theta' \sin \Theta_m \cos (\phi' - \phi_m) \qquad (2.22)$$

Table 2.1 shows some of the well known polar molecules and their dipole moments. Additionally polar ions are

Table 2.1

Some of the well-known polar molecules and
their dipole-moments (Itikawa, 1978)

Molecule	Dipole Moment (a.u.)
CN	0.570
CO	0.0441
CsCl	4.09
CsF	3.10
HBr	0.325
HCl	0.436
HF	0.719
HI	0.176
KCl	4.04
KF	3.38
KI	4.26
LiH	2.31
NO	0.0624
NaCl	3.54
H_2O	0.728
H_2S	0.38
HCN	1.17
NO_2	0.124
NH_3	0.578
O_3	0.210
H_2CO	0.917

FIG. 2.1

ORIENTATION OF A DIPOLE

also found to be existing.

We see from eqn. (2.21), that the dipole
interaction has a long-range nature and its 'strength'
depends on 'D'. As early as in 1931, Massey pointed out
that the rotational excitation cross-sections for
electron-polar molecule collisions must be quite large and
the Born approximation can be applied to this case. To
understand how the Born approximation can be useful for
such potentials even with slow electrons, we must decompose
the plane wave part in the f_{B1} into partial waves of
different angular momenta 'l'.

It is found that, in the cross-section of
electron polar molecule collisions, a large contribution
comes from higher partial waves $(1 \gg 1)$, which, in the
classical sense, means that collisions with large impact
parameters (or 'distant encounters' as they are called)
are important. A partial wave analysis to delimit the
lower bound of 'l' has also been performed. (Takayanagi
1966, Clark, 1977). Now, at large distances the potential,
eqn. (2.21), is generally weak enough so that the first
Born approximation is valid. Thus, to summarise, we
emerge with three cases :

1.   For small dipole moments $(D < 1$ a.u.) the
        partial waves, except for the first few are

hardly distorted, so that the first order pertur-
bation theory applies. The lower partial waves
(with small 'l') are surely distorted, and hence
the corresponding large angle scattering is not
truely described by the Born approximation. That
is why, the momentum transfer cross-section obtained
by the Born approximation is not accurate.

2. As the dipole moment 'D' increases, the lower
limit of l for applicability of the Born
approximation, itself goes up and further error
is introduced as the lower partial waves are
strongly distorted.

3. At small distances, the interaction between the
incident electron and the polar molecule is not
represented by eqn. (2.21), and a short range
potential is also required, the inclusion of which
may not be possible within the Born approximation.
The Born approximation also fails when the
dipole moment is too strong to permit a simple
first order perturbation. These conclusions
are confirmed by more elaborate calculations,
such as those by close-coupling method
(Itikawa, 1969).

Thus, in a limited class of low energy

problems, the Born approximation is favourable.

2.3.3   The first-Born calculations for polar molecules

The Born-Oppenheimer approximation allows
us to separate out rotational-vibrational and electronic
motions in a molecule. For the present, we restrict our-
selves to rotational transitions. Further, assuming the
molecule to be a rigid rotator, its eigen functions are
the spherical   harmonics Y_{jm} $(\underline{S})$, with the unit vector
$\underline{S}$ specifying the direction of the rotator (or the dipole
axis). Let (j, m) show the molecular rotational angular
momentum and its   projection respectively. Let us assume
in the fixed nuclei   approach, that the molecular orien-
tation (i.e. unit vector $\underline{S}$) is fixed during the collision.
This assumption holds   true if the incident electron is
relatively faster. The scattering amplitude for rotational
transition (j, m) $\Longrightarrow$ (j', m') which is particularly simple
in the fixed nuclei approach is, (Itikawa, 1978).

$$f_{jm \to j'm'} = \int d\underline{S} \ Y^{*}_{j'm'} (\underline{S})$$

$$f(\underline{S} \ , \ \underline{q}) \ Y_{jm} \ (\underline{S}) \tag{2.23}$$

in which $f(\underline{S} \ , \ \underline{q})$ is the elastic scattering amplitude
from a fixed point dipole. Altsuler (1957) obtained, in

the Born approximation,

$$f_{B1,PD'} \; (\underline{S} \; , \; \underline{q}) = \frac{2i \; Dem}{qh^2} \; \cos \gamma \qquad (2.24)$$

where, γ is the angle between $\underline{q}$ and $\underline{S}$.

This simple expression can be used to evaluate the transition amplitude of eqn. (2.23) and hence the total or integral cross-section and the momentum transfer cross-section can be evaluated. The important outcome of the Born calculations is summarized below.

1. Owing to the cos θ - dependence of the dipole potential (eqn. (2.21)), the rotational transitions $j \longrightarrow j \pm 1$ only are induced in the electron-polar molecule collisions.

2. The elastic scattering amplitude of eqn. (2.24) diverges at $\theta = 0$, or $q = 0$, hence the total cross-section cannot be calculated. However, for the real inelastic collisions, $q \neq 0$ even at $\theta = 0$, and the problem does not arise.

3. Even when the validity of the first Born approximation is not clearly established, it serves as a first and a crude estimate.

Next, we find that the predictions of the

first Born approximation are in general at variance with
experimental results. A Swarm type determination of MTCS
in rotational transitions of polar molecules was done by
Hurst et al (1966), where a rough accord with Born
results was found. Remarkably, for polar molecules like
H_2O, D_2O, H_2S, etc. the experimental observations were
much larger than the Born results. We are going to discuss
this point further towards the end of this chapter. Also
the molecular beam recoil measurements by Slater et al
(1974) on strongly polar molecules like KI are found
to be lower than the Born values of various cross-sections.

It is thus recognised that there is clearly
a need to go beyond the first Born calculations. We have
emphasized in the preceeding that, for electron-polar
molecule collisions, distant encounters dominate, so
that the distortion of the projectile is quite small,
making the weak scattering approximation, i.e. the Born
approximation applicable. However, if that is not so,
ways must be saught to improve upon the first order
calculations. How can this be done ? An effective way
of improving upon the simple Born calculations is the
distorted wave Born approximation. Here, the basic idea
is to calculate the first Born amplitude, eqn. (2.14),
by taking into account the distortion of the incident
(scattered) plane waves as they approach (recede from)

the target. Rudge (1976) has given a distorted wave approximation for the electron polar molecule collisions. Recalling that, in the present chapter, our aim is to study the high energy methods applied to low energy problems, we attempt here the modified (first) Born approximation of Juncker (1975).

2.3.4 The modified Born approximation

As an improvement over the first Born calculations, let us explore the possibility of applying the modified Born approximation as given by Juncker (1975). This is an attempt to take into account the distortion of the incident plane waves approaching the target, by considering partial screening in the nuclear charge. It has been successfully applied to light atoms for elastic and inelastic processes by electrons with energies of 50 - 200 eV (Gupta and Mathur 1978). We employ it here for, the polar molecule targets. The modified Born approximation, with a suitable split up of the hamiltonian, consists in evaluating the T-matrix, (in a.u.) given below.

$$T = \Gamma (1 - ia_i) \exp (\pi a_i /2) I_D \qquad (2.25)$$

With the subscript 'D' meaning direct scattering or

without exchange. Further, in our case for the electron dipole collisions,

$$I_D = \int d\underline{r} \, \exp(i\underline{q}\cdot\underline{r}) \, {}_1F_1(ia_i,1,ik_ir - i\underline{k}_i\cdot\underline{r})$$

$$X < Y_{j'm'}(S)_f | V_{PD} | Y_{jm}(S), \, i > \qquad (2.26)$$

where, $a_i = \delta/k_i$, and the screening parameter δ takes into account the distortion of the incident plane-waves.

Also, $\, {}_1F_1(\, ia_i \,, \, 1, \, ik_ir - i\underline{k}_i\cdot\underline{r} \,)$ is the hypergeometric function, which can be expanded as follows,

$$_1F_1(\alpha, \, \gamma, \, z) = 1 + \frac{\alpha}{\gamma}z + \frac{\alpha(\alpha+1)}{\gamma(\gamma+1)} \frac{z^2}{2!} + \cdots \qquad (2.27)$$

Now, the matrix element of eqn. (2.26) breaks up into two parts, the target part and the incident electron part, of which the former is,

$$< Y_{j'm'}(\underline{S}) | \cos\theta_m | Y_{jm}(\underline{S}) >$$

which gives rise to the transition $j' = j \pm 1$, similar to the case of the usual Born approximation. Now, considering the incident electron part of the T-matrix,

$$I_D' = \int d\underline{r} \; e^{i\underline{q}.\underline{r}} \; {}_1F_1(ia_i, \; 1, \; ik_i r - ik_i.\underline{r})$$

$$X < f \; | \; \frac{-De \cos \theta'}{r^2} \; | \; i > \qquad (2.28)$$

For the case of electron atom scattering, the modified
Born approximation (MBA) has been evaluated using the
integral techniques of Nordsieck (1954) and Mitra and
Sil (1976). In the present case of the dipole potential,
we follow the expansion of the hypergeometric function,
given in eqn. (2.27). With the first term of that expansion
and $\delta = 0$, we end up with f_{B1} . The higher terms of
the MBA are evaluated by us using standard integrals
(Grandshteyn and Ryzhik, 1965). We quote here our final
expression obtained in this way, which is,

$$f_{PD}^{MBA} = f_{B1,PD} \left(1 - \frac{\pi}{2q} - \frac{k_i \; (1 + 5\pi)}{2q^2} \right)$$

$$+ \; .... \qquad (2.29)$$

Let us note here that the plane wave Born approximation
$f_{B1, \; PD}$ is purely imaginary, while the modified Born
amplitude of eqn. (2.29) is complex and contains real
terms also. Unfortunately we recognize, that the above
analysis does not lead to any positive outcome. This is

because of the fact that, in the modified Born amplitude, eqn. (2.29), the corrections over the plane-wave first Born term are of the order of q^{-2} and higher powers. Thus, for $q < 1$, the correction terms are quite large compared to the first Born term. Now in the present case, the first Born prediction itself is larger than the available experimental results, as well as those of the Glauber approximation. Thus, the present treatment of the MBA can lead only to a further disagreement between theory and experiment, and hence it is concluded that the MBA is not suitable for the treatment of low energy electron scattering by polar molecules. There is no computational difficulty, however, It may be recalled that in the electron atom scattering problems, the scattering amplitude always contains a parameter, to be denoted by 'λ' in the later chapters, which comes from the (electronic) wavefunction of the target. In the present case of a rigid rotator dipole, with spherical harmonic eigen functions, this parameter is absent and this fact plays a crucial role. It even makes the amplitude diverge at $q = 0$. We further conclude therefore, that the failure of the MBA can be traced back to the typical nature of the electron molecule interaction considered here. The modified Born approximation may be useful at large momentum transfers and not so low energies together

with modifications in the interaction potential. This has not been tried at present. Lastly, although there is no comparison, it is interesting to note that, according to Kaushik et al (1982 b), the modified Born approximation fails to come up to the experimental and other results for elastic scattering of electrons from complex atoms like C, O and Ne at intermediate energies. Our next task is to study the higher order theories in the present problem.

2.4   The Second Born approximation

Basically to take into account the second order perturbation, the corresponding approximation is made in the Lippmann-Schwinger eqn. (2.8), to obtain the second Born approximation, in a.u., in the form,

$$f_{B2} = 8\pi^2 \int d\underline{K} \sum_n \frac{\langle \underline{k}_f, f|V|\underline{K},n\rangle\langle\underline{K},n|V|\underline{k}_i, i\rangle}{K^2 - k_i^2 + 2(W_n - W_o) - i\varepsilon}$$

$$\varepsilon \longrightarrow 0^+$$

(2.30)

where, $|\underline{K}, n\rangle$ shows an intermediate state of the system with the projectile having momentum hK and the target in its excited state 'n', $'W_o'$ and $'W_n'$ show respectively the energies of the target in its ground (initial) state and the nth state.

.This amplitude represents the fact that, the projectile with an incident momentum hk_i interacts with the target potential via an intermediate or virtual state from which it scatters with final momentum hk_f, leaving the target in the final state 'f'.

In the field of slow-electron scattering by polar molecules, the second (or a higher) Born approximation has not found much headway. The following are the reasons for this.

1. A calculation with f_{B2} involves a fair amount of difficulty.

2. It leads to transitions with $\Delta j = 0, \pm 2$, but does not improve upon the first Born results of the more important transition,

$$\Delta j = \pm 1.$$

3. A higher order perturbation theory, viz. the Glauber approximation has found an ample success in this area of research.

Usually, the literature on electron-scattering by polar molecules does not deal with the second Born approximation, so it is attempted here.

Thus, we wish to evaluate, presently,

$$f_{B2, PD} = 8\pi^2 \int \frac{dK}{K} \frac{\langle \underline{k}_f, f|V_{PD}|\underline{K}, n\rangle\langle\underline{K}, n|V_{PD}|\underline{k}_i i\rangle}{K^2 - k_i^2 + 2(W_n - W_o) - i\epsilon}$$

$$(2.31)$$

Now here it is convenient to adopt the fixed scatterer approximation (FSA) of Ghosh (1977, 1978). In this formulation, the velocity of the projectile is assumed to be high so that, during the collision, the target assumes a fixed configuation. The wave function of the incident particle then has only a parametric dependence on the target coordinates. Thus, in the T-matrix, the coupling of the target and projectile coordinates is removed, and the second Born term is reduced to, (Ghosh 1977),

$$f_2^{FSA} = 8\pi^2 \int d\underline{K} \frac{\langle \underline{k}_f, f|V_{PD}|\underline{K}\rangle\langle\underline{K}|V_{PD}|\underline{k}_i, i\rangle}{K^2 - k_i^2 - i\epsilon}$$

$$(2.32)$$

Some relevent points about the FSA are discussed in the chapter to follow. In the present case of the dipole rigid rotator, we have, from eqn. (2.32),

$$f_2^{FSA} = 8\pi^2 \int Y_{j'm'}^* (\underline{S}) \cos^2 \Theta_m Y_{jm} (\underline{S}) d\underline{S}$$

$$X \int d\underline{K} \frac{\langle \underline{k}_f |V| \underline{K} \rangle \langle \underline{K}|V| \underline{k}_i \rangle}{K^2 - k_i^2 - i\epsilon} \qquad (2.33)$$

where, the plane-wave matrix element,

$$\langle \underline{k}_f | V | \underline{K} \rangle = \frac{1}{(2\pi)^3}$$

$$\int d\underline{r} \frac{D \cos \Theta'}{r^2} e^{i(\underline{K} - \underline{k}_f)\cdot\underline{r}}$$

$$= \frac{D}{(2\pi)^3} \frac{4\pi}{|\underline{K} - \underline{k}_f|} \qquad (2.34)$$

And a similar result is obtained for the other matrix element of eqn. (2.33). Thus,

$$f_2^{FSA} = \int Y_{j'm'}^* (\underline{S}) \cos^2 \Theta_m Y_{jm} (\underline{S}) d\underline{S}$$

$$X \int d\underline{K} \frac{1}{(|\underline{K} - \underline{k}_f|)(| \underline{k}_i - \underline{K} |)(K^2 - k_i^2)} \qquad (2.35)$$

Now, we evaluate the $\underline{K}$-integral of eqn. (2.35). It falls under the general class of Dalitz integrals,

which are discussed by Joachain (1975). The Dalitz integrals are widely used for second Born calculations at intermediate and high energies. It is of interest to note that this evaluation procedure is applicable here also.

The general integral is given by

$$I_{m,n} (\alpha, \beta, k_i, k_f) = \int d\underline{K} \frac{1}{(K^2 - k_i^2 - i\epsilon)}$$

$$\frac{1}{(\alpha^2 + |\underline{K}-\underline{k_i}|^2)^m (\beta^2 + |\underline{K}-\underline{k_f}|^2)^n} \quad (2.36)$$

In the present case, we have,

$$m = n = 1/2, \qquad \alpha = \beta = 0 \quad (2.37)$$

As discussed by Joachain (1975), the $\underline{K}$-integral of eqn. (2.35) can be reduced to the following form.

$$I = \frac{1}{\pi} \int_0^1 dt \ t^{-1/2} (1 - t)^{-1/2}$$

$$\frac{\pi^2}{\Delta} \ln \left(\frac{k_i + \Delta + i \ \Gamma}{k_i - \Delta + i \ \Gamma} \right) \quad (2.38)$$

with

$$\underline{\Delta} = t\underline{k}_i + (1 - t) \underline{k}_f \qquad (2.39)$$

and

$$\Gamma^2 = t(1 - t) \mid \underline{k}_i - \underline{k}_f \mid^2 \qquad (2.40)$$

Let us observe here that q= 0, for elastic scattering, so that, because of the log-function in the eqn. (2.38), the amplitude diverges at q = 0. This is similar to the behaviour of the first Born term and it confirms the well known fact that the total cross-section for the dipole potential diverges. Due to this reason, we consider the inelastic scattering i.e. rotational transition, in what follows.

To evaluate eqn. (2.38), we expand the log-function as given below,

$$z = k_i + i \Gamma , \qquad (2.41)$$

$$\ln \left(\frac{z/\Delta + 1}{z/\Delta - 1} \right) = \frac{2\Delta}{z} + \frac{2\Delta^3}{z^3} + \dots \qquad (2.42)$$

This holds provided that $z \neq \pm \Delta$ (see Abramowitz and

Stegun, (1974). The evaluation of the t-integral is
easier if the first term only is retained.

Thus, we get,

$$I \doteq \pi i \int_0^1 dt \; t^{-1/2} (1 - t)^{-1/2} \; \frac{1}{2z} \qquad (2.43)$$

which yields upon substitution, $t = \sin^2 \theta$,

$$I = \frac{4\pi i}{\sqrt{q^2 + 4k_i^2}} \left(\pi - i \ln \left(\frac{\sqrt{(q^2 + 4k_i^2)} + q}{\sqrt{(q^2 + 4k_i^2)} - q} \right) \right) \qquad (2.44)$$

Now, going back to the second Born expression (2.35), we
find that owing to the presence of $\cos^2 \theta_m$ in the
target part of that equation the allowed transitions
obey $\Delta j = 0, \pm 2$. We are presently interested in
the rotational transition, $j = 0 \longrightarrow 2$, for which
we get the following result for the differential cross-
sections (DCS), in a. u.

$$\left(\frac{d\sigma}{dw}\right) = C \left[\frac{64\ D^4}{\pi^2\ (q^2 + 4k_i^2)}\right.$$

$$X \quad \left(\pi^2 + \left(\ln \frac{\sqrt{(q^2 + 4k_i^2)} + q}{\sqrt{(q^2 + 4k_i^2)} - q}\right)^2\right) \left.\right] \qquad (2.45)$$

where, the constant C depends on,

$$j = m = 0,$$

$$j' = 2, \quad m' = 0 \ \text{etc.}$$

Based on the above result, a sample calculation has been made for e + CsCl system, at the incident energy 4.77 eV. Ashihara et al (1975) have investigated the same system at the same energy, employing the Glauber approximation. The table 2.2 represents a comparative statement of our results and those of Ashihara (1975). Given below are the conclusions drawn therefrom.

1.   The Glauber DCS fall off too steeply as the scattering angle increases (see also fig. 2.2). The Glauber theory being a small angle approximation, these results may not be quite reliable at large angles. The experimental cross-sections (Slater et al, 1974) also fall off rapidly. The

Table 2.2

DCS   for   e + CsCl   at 4.77 eV   for

j = 0 → 2   inelastic process   (a_o^2 /sr units)

| Θ_{deg}	Present	Glauber results
0	.1125	1800
30	1048	--
60	890	010
90	795	--
120	700	--

present DCS decrease rather slowly with angles. This behaviour i.e. slow variation with q is also found in the DCS obtained by the first Born approximation. The behaviour can be seen from fig. 2.2 taken from Itikawa (1978).

2. The present results agree with the Glauber results near forward direction. It may be concluded that the true behaviour at large angles might be somewhere in between the Glauber and the present results.

There are also some limitations of the present simple calculations, as pointed out below.

1. It is not possible to include higher orders of perturbation in the Born approximation, and it is this point that makes the Glauber theory superior. The higher orders contain higher powers of $\cos \theta_m$ hence in those cases too, $\Delta j = 0, \pm 1, \pm 2$ etc. transitions are induced, they effectively couple with the first and second order results.

2. Presently also, the second Born term is simplified in order to keep the computations simpler. Actually, eqn. (2.38) must be evaluated exactly.

FIG. 2.2

e + CsCl at 4.77 ev (Ashihara 1975)
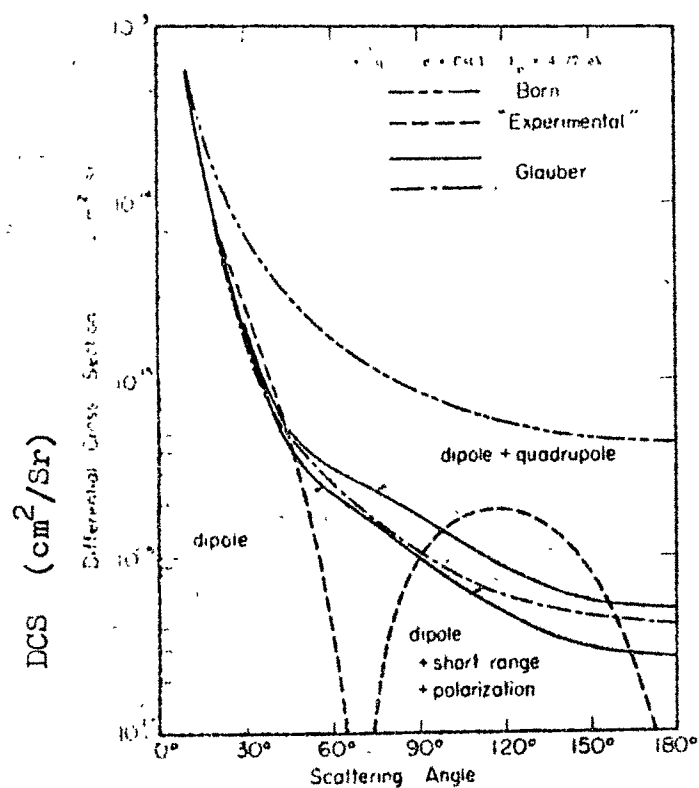
The next section is, therefore devoted to the Glauber approximation.

2.5   The Glauber Approximation

In the previous section, we saw that the first Born approximation predicts the important transition $\Delta j = \pm 1$, while the second Born approximation predicts $\Delta j = 0, \pm 2$. In the higher order terms, higher powers of the potential, and hence of the factor $\cos \Theta_m$ appear, and overlappingly, all transitions $\Delta j = 0, \pm 1, \pm 2$ etc. will be allowed. Thus the higher terms interact with the first Born term, whence they cannot be neglected. This amply speaks of the importance of a higher order perturbation theory.

The Glauber theory stems from the eikonal approximation in 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. This is equivalent to the requirement,

$$k_i \, a \gg 1 \qquad\qquad (2.46)$$

Here, 'a' is the range of the potential. Under this

condition, the Green's function in the Lippmann-Schwinger equation can be linearized, i.e. its dependence on $'K^2'$ is removed by a suitable expansion. We are going to discuss this procedure in connection with the high energy higher order Born approximation in the next chapter. This procedure leads here to the eikonal scattering wave function,

$$\psi \ (r) \ = \ (2\pi)^{-3/2} \quad exp \ (i\underline{k}_i \cdot \underline{r} - \frac{i}{2k_i}$$

$$\int_{-\infty}^{z} U(b, z') dz' \ ) \tag{2.47}$$

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

$$f_E \ = \ \frac{k_i}{2\pi i} \int d^2\underline{b} \ exp \ (i\underline{q} \cdot \underline{b}) \ exp \ (iX(k_i, \ b) - 1)$$

$$\tag{2.48}$$

Here, $\underline{b}$ is the impact parameter.

This treatment is for a structureless target. The many body generalization of the eikonal

approximation was done by R. J. Glauber (1959). The Glauber amplitude for a 'direct' collision of an electron with a target containing fixed scatters is expressed as,

$$f^G = \frac{k_i}{2\pi i} \int d^2\underline{b} \exp(i\underline{q} \cdot \underline{b})$$

$$\langle f \mid \exp(iX^G) - 1 \mid i \rangle \qquad (2.49)$$

The momentum transfer $\underline{q}$ is here assumed to be two dimensional. Further, $d^2\underline{b}$ is an element of area in the (X, Y) plane. The Glauber phase is

$$X^G = X^G(\underline{b}, \underline{b}_1 \cdots \underline{b}_N) \qquad (2.50)$$

where $\underline{r} = \underline{b} + \underline{z}$ $\qquad (2.51)$

And the target coordinates look like,

$$\underline{r}_1 = \underline{b}_1 + \underline{z}_1 \qquad (2.52)$$

etc.

Let us note here that the Glauber multiple scattering series can be developed by expanding the exponentiated phase X^G in eqn. (2.49) and its connection with the terms of the Born series can be

established. (Byron and Joachain, 1977). In the last fifteen years or so, the Glauber approximation has acquired an important status in the electron-atom-molecule problems. Some of the special features of this theory are pointed out below. Some pertinent remarks are also made in the later chapters.

1. Because of the exponential phase X^G, the Glauber amplitude takes into account all orders of perturbation, albeit approximately.

2. The longitudinal component of the momentum transfer i.e. that along the incident direction, is neglected. Thus,

$$\underline{q}.\underline{r} \triangleq \underline{q}.\underline{b} \tag{2.53}$$

Hence this approximation is valid for small angle scattering only. However, the assumption eqn. (2.53) makes the evaluation of the Glauber amplitude easier. It also ensures that the first Glauber term is identical with the first Born term.

Let us evaluate the Glauber amplitude of eqn. (2.49) in the case of a dipole potential, assuming a fixed orientation of the vector $\underline{S}$. We need,

$$\chi^G = -\frac{1}{hv_i} \int_{-\infty}^{z} V_{PD}(b, z') \, dz' \qquad (2.54)$$

$'v_i'$ shows the speed of the incident electron.

Upon integration, one gets,

$$\chi^G(\underline{b}, \underline{S}) = \frac{2eD}{hv_i b} (\underline{S} \cdot \underline{b}) \qquad (2.55)$$

The z-axis is chosen here along the direction $(\underline{k}_i + \underline{k}_f)$. Ashihara et al (1975) have applied the Glauber approximation for treating the scattering of slow electrons by strongly polar molecules like KI and CsCl. According to them, the amplitude for a rotational transition from a state (j, m) to ' (j', m'), obtained by expanding $\exp(i\chi^G)$ is given as,

$$f^G(\underline{S}, \underline{q}) = 2ik_i \sum_{l,n} i^l \int (\delta_{lo}\delta_{no} - J_i(\frac{2eD}{hv_i b}))$$

$$Y_{ln}(\underline{b}) \, e^{i\underline{q}\cdot\underline{b}} \, d^2\underline{b} \int Y^*_{j'm'}(\hat{\underline{S}}) \, Y_{ln}(\hat{\underline{S}}) \, Y_{jm}(\underline{S}) \, d\underline{S}$$

$$(2.56)$$

where we have used eqn. (2.55) and also the fact that,

$$1 \ = \ \sum_{1,n} \ \delta_{1o} \ \delta_{mo} \qquad\qquad (2.57)$$

In the eqn. (2.56) j_1 is the spherical Bessel function of order '1'. With this Glauber amplitude, the results obtained for electron scattering from strongly polar molecules like CsCl (D = 4.09 a.u.) are much lower than the Born values and thus agreement with experiments is reached. (Ashihara et al 1975). However, it has been noted that these results do not guarantee that the Glauber approximation would succeed ∨ in any low energy problem. Thus, it is required to be tested in different cases of interest.

Now we turn our attention to a specific low-energy process, to be investigated in the Glauber theory.

2.6   Elastic Scattering via Temporary Capture

As noted earlier, it is   observed that the elastic scattering of slow electrons by polar molecules like H_2O, H_2S, D_2O, etc.   showed a typical behaviour. The experimental momentum transfer (or diffusion) cross-sections were found to be much larger than those obtained by the first Born amplitudes. These molecules have relatively low polarizabilities, so the reason for this

behaviour must be something else. Hurst et al (1963)
suggested that the enhancement of the momentum transfer
cross-section could be due to a temporal attachment of
an electron to the polar molecule. J. E. Turner (1966)
investigated the possibility of 'nuclear excited Feshbach
resonance' i.e. resonant scattering of electron through an
intermediate negative ion formation. The term 'nuclear'
stands for the excitation of nuclear motions i.e. rotation
and/or vibration. Turner observed that stable bound states
of an electron can exist in the field of a stationary
dipole, if its dipole moment exceeds a certain critical
value of 0.64 a.u. Garrett (1970, 1971) studied the same
problem for a rotating dipole. In Turner's mechanism
(1966) this is a two step-process. The electron of the
incident Swarm is first captured by the dipole field of
the target molecule and a rotational state of the target
is excited. Then, the natural decay of the negative ion
thus formed, returns the electron back to the Swarm, thus
contributing to the momentum transfer cross-section. In a
simple Born approximation treatment of Altsuler (1957)
this contribution from quasibound states is absent, hence
a simple treatment underestimates the cross-sections.
The life-time of the negative ion is estimated to be
of the order of the rotational period of the target molecule.

This process differs from the dissociative attachment, given below,

$$MN + e^- \longrightarrow M + N^- \qquad (2.58)$$

Here M and N represent the atoms of the molecule. The present case is that of non-dissociative attachment, either temporary, and autoionizing,

$$MN + e^- \rightleftharpoons MN^- \qquad (2.59)$$

or permanent, i.e.

$$MN + e^- \longrightarrow MN^- \qquad (2.60)$$

We confine ourselves to the process of eqn. (2.59) above, i.e. to the temporary and loose binding of the projectile electron. In the initial state of the system, a free electron in a Swarm is incident on the target polar molecule in a rotational state (j m) and we consider the final state 'f' of the system as that of the bound electron and the molecule in the excited state, (j' m'). (The latter eventually decays back to the initial state). Our problem is to determine the probability of transition from the state 'i' to 'f'. For this, we need the initial and the final state wave

functions. Following Turner (1966), we take the initial state of the electron of the Swarm, represented by a plane wave plus a scattered spherical wave i.e. as

$$e^{ik_i z} + f(\theta, \emptyset) e^{ik_i r} / r \qquad (2.61)$$

Here, $f(\theta, \emptyset)$ is the amplitude of elastic scattering from the fixed dipole. Here lies the point. With our knowledge of an improved scattering amplitude $f(\theta, \emptyset)$ the calculations can be modified.

A simplest choice for $f(\theta, \emptyset)$ would be the amplitude of eqn. (2.24) given in the first Born approximation. Desai and Maru (1972) calculated the amplitude variationally and later Desai et al (1974) obtained the amplitude in the finite dipole Born model. Both of these afford a small change in Turner's calculations. We (Joshipura and Desai, 1980) have applied the Glauber amplitude in this problem.

We thus go back to the main track of our discussion. The Glauber amplitude eqn. (2.56) for elastic scattering of electrons by polar molecules, to be used here, requires the evaluation of the integral,

$$I_{ln} (t) = \int_0^\infty (j_1(t/x) - \delta_{lo}) J_n(x) \, x \, dx \qquad (2.62)$$

with $\not{J}_m(x)$ as the ordinary Bessel function. This is evaluable in the form of a rapidly convergent infinite series (Ashihara et al, 1975). The expression for the Glauber amplitude is now,

$$f^G(\underline{S}, \underline{q}) = \frac{ik_i}{2\pi} \left(\frac{2\beta}{q}\right)^2 \left[2 \sin \Theta_S \cos(\emptyset_S - \emptyset_q)\right.$$

$$X \left(\frac{1}{4\beta} - \frac{\beta}{40}\right) - 2 \ln\left(\frac{\beta}{2}\right).$$

$$\left. + \frac{1}{4} \Psi(5/2) + \frac{1}{4} \Psi(2) + \frac{1}{2} \Psi(1) \right] \quad (2.63)$$

where, we define,

$$\beta = \left(\frac{meD}{h^2 k_i}\right) q \qquad (2.64)$$

Also $(\Theta_S, \emptyset_S)$ show the orientation of the molecule relative to a fixed frame, as shown in fig. 2.1. '$\emptyset_q$' is the angle made by $\underline{q}$ vector in the (x, y) plane. $\Psi(a)$ is a digamma function.

We used the amplitude of eqn. (2.63), to calculate the transition probability T_{fi}, for the decay of the negative ion, discussed in the preceeding. The following derivation rests heavily on Turner (1966).

Writing for the matrix element of the decay, we have,

$$T_{fi} = \frac{-h^2}{I\sqrt{a_o}} \left(\frac{Z}{a_o}\right)^{3/2} (I_1 + I_2 + I_3) \qquad (2.65)$$

Here $Z^2 = .04$, Z is the scaling factor, a_o is the Bohr radius. Further, the integrals I_1, I_2 and I_3 are as follows (see also Maru, 1975),

$$I_1 = \left(\frac{5}{4\pi}\right)^{1/2} \iint d\underline{v} \, d\underline{S} \, e^{-Zr/a_o} \, Y^*_{j'm'}(\underline{S})$$

$$\bigoplus \, ^2 f^G(\underline{S}, \underline{q}) \frac{e^{ik_i r}}{r} Y_{jm}(\underline{S}) \qquad (2.66)$$

where,

$$d\underline{v} = r^2 \, dr \, \sin\Theta \, d\Theta \, d\emptyset, \qquad \text{for the}$$

scattered electron.

$$d\underline{S} = \sin\Theta_S \, d\Theta_S \, d\emptyset_S$$

Further, if $j' \neq j$, $I_1 = 0$.

The next is, I_2, which is the same as f in Turner (1966).

Finally,

$$I_3 = \left(\tfrac{4\pi}{3}\right)^{1/2} \iint d\underline{v}\ d\underline{S}\ e^{-Zr/a_0}\ (Y_{1,-1}(\underline{r})\ Y_{1,-1}(\underline{S})$$

$$+ Y_{1,0}^*(\underline{r})\ Y_{1,0}(\underline{S}) + Y_{1,1}^*(\underline{r})\ Y_{1,1}(\underline{S}))$$

$$Y_{j',m'}(\underline{S})\ \textcircled{B}^2\ f^G(\underline{S},\underline{q})\ \frac{e^{ik_i r}}{r}\ Y_{jm}(\underline{S}) \tag{2.67}$$

Specifically, this I_3 is evaluated here, with the Glauber amplitude, and found to be,

$$I_3 = \frac{2iP}{k_i}(3\pi)^{1/2}\ Q(1-R)\ S_{fi}^3$$

$$+ \frac{4i}{5}\left(\tfrac{2\pi}{3}\right)^{1/2}\frac{P^3 h^3}{k_i}\ Q(1-R)\ S_{fi}^3$$

$$+ \frac{14i}{k_i}\left(\tfrac{3\pi}{4}\right)^{1/2} P^2\ j(j+1)\ Q(1-R)\ S_{fi}^3$$

$$\times\left(\left(\frac{(j'+1+m')(j'+1-m')}{(2j'+1)(2j+3)}\right)^{1/2}\delta_{j'+1,j}\ \delta_{m',m}\right.$$

$$\left. + \left(\frac{(j'+m')(j'-m')}{(2j'+1)(2j'-1)}\right)^{1/2}\delta_{j'-1,j}\ \delta_{m',m}\right) \tag{2.68}$$

where,

$$P = \frac{meD}{h^2} \quad , \quad Q = \left(\frac{Za_o}{z^2 + k_i^2 a_o^2} \right)^2$$

$$\text{and} \quad R = \left(\frac{k_i a_o}{Z} \right)^2 + 2i \left(\frac{k_i a_o}{Z} \right) \tag{2.69}$$

The quantities S_{fi}^3 are defined by Maru (1975).

For a sample calculation we consider, for water molecule the initial rotator state $j = 2$, $m = 0$, the final state being $j' = 3$, $m = 0$. This case is frequently studied in the literature. The mean energy of the incident electron Swarm is 0.025 eV, corresponding to the room temperature. From the transition probability, T_{fi}, eqn. (2.65) the lifetime of the intermediate negative ion is obtained by the following equation,

$$T = \frac{\pi h^4}{m(2mE)^{1/2}} \times \frac{1}{|T_{fi}|^2} \tag{2.70}$$

And finally, the capture cross-section can also be calculated from the transition probability
A comparison of the present result with those of other workers is given in the table 2.3. We have already mentioned the other calculations referred to in the table 2.3.

Table 2.3

Results of $|T_{fi}|^2$ and the life time T of the $(H_2O)^-$ temporary negative ion, obtained by different theoretical methods

Quantity	a	b	c	d
$|T_{fi}|^2 \times 10^{-47}$	1.183	1.182	1.248	0.27
$T \times 10^{-14}$ Sec	3.488	3.49	3.307	15.0 (38.2)[*]

a, Turner (1966)

b, Variational method (Desai et al 1972)

c, Finite dipole (Maru and Desai 1978)

d, Glauber results (Joshipura and Desai, 1980)

* Rotational period of the target

Our results indicate that, the lifetime of the negative ion is longer than that predicted by any other theory, but it is shorter than the period of rotation of the molecule, which means that a stable negative ion is not formed. Further, in our results, the transition probability is small, so that the capture cross-section is reduced and the momentum transfer cross-section (MTCS) should increase. This last point was the beginning of the present article no. (2.6). The MTCS are not calculated here, but we refer to a recent comparison of results by Desai and Chhaya (1979). The present results can bring a closer agreement with the experimental results of this quantity.

Thus, the application of the Glauber approximation succeeds in explaining the high momentum transfer cross-sections as resulting out of a temporary attachment process. A similar behaviour can be predicted for molecules like NH_3, HCl, H_2O_2, etc.

2.7   Nonpolar Molecules

Our interest in the previous sections was mainly confined to polar molecules. Now, the prominent gases like H_2, O_2, N_2, etc. are nonpolar. In general the potential of interaction between a molecule and an

incident electron can be expressed as an expansion in
multipole electric moments and in many of the non-polar
molecules, the quadrupole moment dominates,at least at
large distances. The point quadrupole potential
reads as,

$$V_{PQ} (\underline{r}) = - \frac{Q}{r^3} P_2 (\underline{r} \cdot \underline{S}) \qquad (2.71)$$

Here, Q is the electric quadrupole moment of the
molecule and $P_2(\underline{r} \cdot \underline{S})$ is the 2nd order Legendre poly-
nomial in $(\underline{r} \cdot \underline{S})$. The possibility of applying high
energy methods to slow electron scattering by nonpolar
targets also follows from arguments made previously
(Chang, 1970, also Chhaya, 1980), for polar targets. Here
also the first Born results turn out to be first estimates.
The Glauber theory has been applied to slow electron
scattering from quadrupolar molecules by Ashihara (1975)
and also by Rahman (1978). Further, the inclusion of
short range and polarization forces, along with other
methods of calculation, change the picture considerably.
One must mention that an improvement over 'point' dipole
or quadrupole model has been to consider a 'finite' or a
'cut off' dipole or quadrupole potential. Also, in the
case of specific molecules, the linear rigid rotator
model is replaced by a more realistic, symmetric or

asymmetric top model. All these are mentioned only briefly here as the purpose of the present study is not to cover the details of this aspect. With this, we come to the last section of this chapter.

2.8   Chapter Summary, Further Prospects

In the second chapter, we considered some of the theories of high energy electron scattering that find applications in the treatment of scattering of slow electrons from molecules. Our starting point was the Schroedinger equation from which all quantum mechanical theories arise. An integral equivalent of the Schroedinger equation, is the Lippmann-Schwinger equation, which, when attempted to solve approximately, gives rise to the Born, eikonal and Glauber approximations. These high energy approximations have found applications in the calculations of various cross-sections of low-energy electrons by polar and non-polar molecules and we have discussed here the arguments to justify their applicability. The modified Born approximation, for taking into account the distortion of the projectile is attempted, but without success. This method might prove to be useful with some modifications e.g. a cut off procedure. The second Born approximation for dipole targets is attempted here and some interesting consequences are derived. It predicts the transitions with

Δj = 0, $\pm$ 2. The order of magnitude of the DCS for

0 $\longrightarrow$ 2 transition for CsCl molecule, at 4.77 eV

agrees with the Glauber result only near the forward

direction. Our DCS vary very slowly with q. The

limitations of the present treatment are noted.

Glauber's high-energy, small angle approxi-

mation is known to be better than the first Born approxi-

mation, even in the low-energy work. Presently, the

Glauber amplitude for elastic scattering of slow

electrons from polar molecules is employed to obtain

the lifetime of temporary negative ion formed in Turner's

mechanism (1966). A comparative statement is made for a

sample case of j = 2 $\longrightarrow$ 3 transition in the H_2O

polar molecule, showing the present results and those

of others. The present results predict a higher value of

the MTCS, in accord with Swarm experiments. (Christo-

phorou and Christodoulides, 1969). Thus we have a better

understanding now about a peak observed in the MTCS at

the dipole moment around 1 a.u. Turner's theory applies

to only certain molecules with a suitable ratio of the

dipole moment to moment of inertia. An important motivation

for employing the Glauber theory is the simplicity of

the Glauber amplitude of eqn. (2.56) for the dipole

potential. However, if all the dominent a terms of the

interaction potential are taken into account, the sophistication takes tall of simplicity. Reference must be made here of the work of Gianturco et al (1978), who considered the dipole quardupole and polarization terms of interaction in their Glauber formulation for low to intermediate energies upto 50 eV, with a considerable success. As we come to the end of this chapter it will be worthwhile pointing out future prospects for the kind of work shown here. The following points are noteworthy.

1. Now-a-days, in high energy problems, the Wallace correction (1973) to the Glauber and eikonal formulations is gaining more and more attention. This author has not ø seen the Wallace-corrected, Glauber amplitudes for low energy problems and so it will be interesting to do the same. In essence, the Wallace amplitude is given by (see also eqn.2.49),

$$f_W = \frac{k_i}{2\pi i} \int d^2\underline{b} \; e^{i\underline{q}.\underline{b}}$$

$$< f \mid \exp \left(i \left(\frac{X^G}{k_i} + \frac{X_1}{k_1^3} \right) - 1 \mid i \right> \qquad (2.72)$$

The correction over the Glauber phase X^G being,

$$X_1 (\underline{b}, \underline{x}) = \frac{1}{2} \int_{-\infty}^{\infty} (\underline{V} X_+) \cdot (\underline{V} X_-) \; dz \qquad (2.73)$$

with,

$$X_+ \ (\underline{b}, \ z, \ \underline{x}) \ = \ - \int_{-\infty}^{z} V(\underline{b}, \ z', \ \underline{x}) \ dz' \qquad (2.74)$$

And,

$$X_- \ (\underline{b}, \ z, \ \underline{x}) \ = \ - \int_{z}^{\infty} V(\underline{b}, \ z', \ \underline{x}) \ dz' \qquad (2.75)$$

Here, the evaluation of X_1 is easier for central potentials. But for the cases like the dipole potential, it is vastly difficult. Our attempts in this direction have not been successful as yet, but it means that challenges are in store.

2.   However, even the Wallace amplitude is not free from some of the drawbacks of the Glauber amplitude. For high energy electron atom collisions several modifications of the Glauber approximations are developed mention must be made of the work of Rosendorff (1977, 1980, 1981) which is a basic modification. This is also worth trying for electron polar molecule or electron quadrupole collisions, at low energies.

3.   If a high energy method works with a limited success in the realm of electron polar molecule collisions, it may be suitably combined with more successful

theories. Chhaya (1980) has coupled the close-coupling approach for the first few target states with the Born approximation for all the higher states, in his study of electron scattering from alkali halides. Dewangan (1978) has suggested a more general method using the Glauber theory.

4. As an application of electron polar molecule collision studies, we can consider collision of a highly excited long-lived (Rydberg') atom with a polar molecule. In this case, the radius of the rydberg orbit being very large, the problem divides into two parts (i) the excited-electron polar - molecule interaction and (ii) the ionic-core polar-molecule interaction. Thus the studies of electron-dipole and and ion-dipole systems find relevence in this new context.

5. In the previous paragraph, the term 'ion-dipole' stands for, a neutral, polar molecule considered as the target and an ion as a projectile. It is also of interest to consider ions, exhibiting dipole character, as targets.

6. The phase 'nuclear excited Feshback resonance' used in this chapter applies to rotational and/or vibrational excitations. In this chapter, we considered

only rotational excitations. Recently Gauyacq and
Herzenberg (1982) have studied e + HCl scattering
under the nuclear excited Feshback resonance including
the vibrational aspect. Thus there is a renewed
interest in the subject.

With this, we go over to the next
chapter devoted to elastic scattering of fast electrons
by atoms.