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CHAPTER – I

INTRODUCTION AND THEORETICAL BACKGROUND

1.1 INTRODUCTION :

The collision phenomenon plays an important role in investigation on the structure of matter on microscopic scale. It is well known that the knowledge of reliable atomic and molecular collision cross sections are in demand in the development of various scientific and technical fields like astrophysics, aeronomy, gas lasers, plasma physics, controlled thermonuclear fusion, chemical reactions, biophysics etc.

The energetic particles and electromagnetic radiation constantly bombard the upper atmosphere. Particularly during solar flare sun emits greatly enhanced electromagnetic radiation in X-ray and UV region, cosmic particles, ions and electrons. These produce further photoelectrons and secondary electrons. These electrons then lose their energy through various elastic and inelastic processes. Thus the energy spectrum of the electrons is a very important parameter for all atmospheric calculations. From the energy spectrum induced by collision process one gets idea of chemical composition, density and temperature of constituent elements of atmosphere. The ionic layers in the ionosphere of earth are mainly formed due to the ionization of the neutral constituent of atmosphere by solar radiation leading to production of energetic free electrons and ions. These energetic electrons further excite the neutral particles and ions then the particles in excited state decay to lower states give rise to fluorescence. Thus we need the knowledge of atomic and molecular collisional process for atmospheric process. For the study of molecular structure in molecular chemistry, a large number of parameters can be evaluated with the help of electron-molecule elastic differential cross sections. These cross sections are also useful in high-energy molecular gas lasers. In radiation therapy when radiation on defective cells are incident, secondary charged particles are produced which starts ionization of other constituent atoms in the tissue. Because of over exposition living tissues are also damaged. Controlling the radiation dose and time of exposition can minimize these damages. For this various parameters like stopping power, energy expanded per ion pair are required which can be evaluated by knowing collisional cross sections. Fusion is one of the promising processes for the generation of energy. Hence it is required to know collisional cross sections for various processes occurring in

fusion. Due to these manifold applications, atomic and collisions have been very important subjects of experimental and theoretical investigations.

In the collision process a free particle with known characteristic is incident upon an atomic, molecular or ionic target and after the interaction it is scattered in to a modified free state. During this scattering process different changes including angular deflection, change in kinetic and internal energies, chemical changes, gain or loss of electrons can be detected. Because of these changes three types of scattering can happen. One is the elastic scattering in which the internal structure of the system remains same. Second is the inelastic scattering (excitation, ionization etc.) in which incident particle transfer its kinetic energy to internal energy of target to excite or ionize it to some higher energy states. Third is known as supper elastic scattering in which incident particle gain some energy from the target. All these collision processes are analyzed quantum collision theory. The probability that a given type of collision will occur under given condition is usually expressed in terms of collision cross sections. An exact quantum mechanical formation of the atomic and molecular collision process can be easily developed. However an exact calculation is very difficult. Therefore numbers of approximate methods have been developed depending on the energy region of interest. The entire energy region is usually divided in to three regions low, intermediate and high. The region below the first excitation energy is taken as low energy region. The region where first Born approximation gives reliable results is taken as high-energy region. The region in between these two regions is intermediate region. In present investigation we have studied the elastic scattering of electrons by atoms and ions within the high-energy region.

In a scattering experiment, a well-defined collimated homogeneous beam of monoenergetic particles is directed towards a scattering target from a large distance. After impact the particles of incident beam are scattered in all directions and their distribution is detected at large distance. The number of particles scattered in to detector per unit solid angle per unit time per unit incident flux is called the differential cross section for that particular direction. An integration of differential cross section over all solid angles yields the total cross section. Thus the total cross section is the cross sectional area which the target present to the direction of the beam and the differential cross section is the effective area which the target present to the beam for the deflection of the incident particle in to a particular solid angle.

Theoretically the scattering of charged particles like electrons or positron by atoms, molecules or ions is considered as follows. The incident particle is represented by a plane wave for a short range potential. When the electric field of charged particle interacts with the electron charge cloud of target, multiple moments are induced. Thus both the incident particle and target atom are distorted. This distortion due to induced multiple moment is attractive in nature and give rise to polarization potential. Besides this other effect also take place in scattering process. The effect of inelastic scattering on elastic scattering can be describe by absorption potential. If the incident particle is an electron then we can not distinguish incident and atomic electrons. Thus exchange between incident and atomic electrons may occur, this effect is taken in terms of exchange potential. At sufficiently high energies the polarization and exchange interaction will become unimportant leaving only the static interaction effective.

An exact evaluation of Schrodinger equation corresponding to particular scattering process is a difficult task even if the interaction potential is known. This is because the exact wave function of target atom except hydrogen and hydrogen like ions are not known. However even if the wave functions of the atom are known, the schrodinger contains infinite set of coupled integro-differential equations which can not be exactly solved. For heavy atoms or molecular targets the situation become more complicated. Hence the quantum mechanical investigation of collision process for microscopic particles need some approximate methods. The choice an approximation depends up on the tractability of the calculations and its accuracy is checked by comparing the results with others approximations and with available experimental results. Various approximate methods are applied here to different atomic and ionic target in the high-energy region.

1.2 BORN APPROXIMATION:

For the theoretical investigation of the atomic collision problem, let us consider the scattering of an electron by a neutral atom of atomic number Z. We consider the nucleus of the atom as the origin of the coordinate system and denote the coordinate of incident particle and atomic electrons by $\vec{r}$ and $\vec{r}_j$ $(j = 1,2,3....Z)$, respectively. The wave function of the system $\psi(\underline{r},\underline{s},\underline{r}_j,\underline{s}_j)$ satisfies the Schrodinger equation.

$$[H - E]\,\psi(\underline{r},\underline{s},\underline{r}_j,\underline{s}_j) = 0 \qquad (1.2.1)$$

Where E is the total energy of the system and H is the Hamiltonian of the system.

$$H = H_t + V_{int}, \tag{1.2.2}$$

with $H_t = H_a + H_t$ Hamiltonian of the total system before the start of the potential.

Where $H_a = -\frac{1}{2}\nabla_r^2$ is the *K.E.* Operator of the incident particle and H_t is the Hamiltonian of the target atom or ion with the eigen state $\phi_n(\underline{r}_j)$ and eigen energy $\in_n$ such that

$$H_t\phi_n(\underline{r}_j) = \in_n \phi_n(\underline{r}_j) \tag{1.2.3}$$

$$H_t(\underline{r},\underline{r}_j)\Phi_{k0}(\underline{r},\underline{r}_j) = E_0\Phi_{k0}(\underline{r},\underline{r}_j) \tag{1.2.4}$$

with $E_0 = \frac{1}{2}K_0^2 + \in_0$; $\underline{K}_0$ is the initial momentum vector and

$$\Phi_{k0}(\underline{r},\underline{r}_j) = U_{k0}(\underline{r})\phi_0(\underline{r}_j) \tag{1.2.5}$$

where $U_{k0}(\underline{r})$ is the initial normalized wave function of the incident particle and $\phi_0(\underline{r}_j)$ is the initial state of the target. The interaction potential between the incident particle and target for incident electron is given by

$$V_{int} = [-\frac{Z}{r} + \sum_{j=1}^{N}\frac{1}{|r-\underline{r}_j|}] \tag{1.2.6}$$

For theoretical study of any collision problem we examine the asymptotic form of the total wave function $\psi_{r\to\infty}$. Considering neutral atom, normalized wave function of initial state is $\Phi_{k0}(\underline{r},\underline{r}_j) = (2\pi)^{-3/2}e^{i\underline{k}_0\underline{r}}\phi_0(\underline{r}_j)$ and

$$\psi_{r\to\infty} = [U_{k0}(\underline{r})\phi_0(\underline{r}_j) + \sum_n f_{no}(\hat{k}_0,\hat{k}_f)\frac{e^{ik_f r}}{r}\phi_n(\underline{r}_j)] \tag{1.2.7}$$

It is the sum of the incident plane wave along with the undisturbed target atom wave function and perturbation after the scattering which is in the form of a radialy out going spherical wave of the scattered particles with the atom in the same state (elastic scattering) or in an excited state (inelastic scattering). $f_{no}(\hat{k}_0,\hat{k}_f)$ is the scattering amplitude for the inelastic scattering from the ground state **0** to n^{th} excited state. $\underline{k}_f$ is the momentum vector of the incident particle after the scattering. In general scattering amplitude is complex and is related to the differential cross section through the relation

$$I_{no}(\theta)=\frac{k_f}{k_o}\left|f_{no}(\hat{k}_o,\hat{k}_f)\right|^2 \tag{1.2.8}$$

For elastic scattering $|\underline{k}_f|=|\underline{k}_0|=k_0$. Thus the differential cross section is given by

$$I_{00}(\theta)=\left|f_{00}(\hat{k}_0,\hat{k}_f)\right|^2 \tag{1.2.8a}$$

And according to optical theorem total cross section is given by

$$\sigma_{tot}=\frac{4\pi}{k_0}I_m f_{00}(\theta=0) \tag{1.2.9}$$

where θ is the scattering angle. Differential cross section (DCS) $I(\theta)$ and total cross section (TCS) σ_{tot} are the key quantities for the study of any collision problem. For the determination of DCS and TCS we have to solve (1.2.1). The exact solution of it is a formidable task. There are two approaches to solve this equation. One is differential equation approach, which is non-iterative and another is integral equation approach that is iterative. In integral equation approach the general solution of (1.2.1) is given as

$$\psi^+=\Phi_{k0}+\int G_0^+(\underline{r},\underline{r}_j;\underline{r}',\underline{r}'_j)V_{int}(\underline{r}',\underline{r}'_j)\psi^+(\underline{r}',\underline{r}'_j)d\underline{r}'\prod_j d\underline{r}'_j \tag{1.2.10}$$

G_0^+ is the outgoing Green function for the undisturbed system and ψ^+ is the out going scattered wave function. Here G_0^+ has the form

$$G_0^+(\underline{r},\underline{r}_j;\underline{r}',\underline{r}'_j)=\sum_n(-\frac{1}{2\pi})\frac{e^{ik_f|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|}\phi_n^*(\underline{r}'_j)\phi_n(\underline{r}_j) \tag{1.2.11a}$$

in momentum space

$$G_0^+=-\frac{2}{(2\pi)^3}\sum\int\frac{d\underline{q}\,exp[iq.(\underline{r}-\underline{r}')]}{q^2-k_n^2-i\in}\phi_n^*(\underline{r}'_j)\phi_n(\underline{r}_j) \tag{1.2.11b}$$

where $k_n^2=k_0^2-2(\in_n-\in_0)$.

Hence (1.210) yields

$$\psi^+=\Phi_{k0}+\sum_n(-\tfrac{1}{2\pi})\int\frac{e^{ik_f|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|}\phi_n^*(\underline{r}'_j)\phi_n(\underline{r}_j)V_{int}(\underline{r}',\underline{r}'_j)\psi^+(\underline{r}',\underline{r}'_j)d\underline{r}'\prod_j d\underline{r}'_j \tag{1.2.12}$$

If we take the asymptotic behavior of term $\frac{e^{ik_f|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|}$ coming in Green's function, the asymptotic behavior of ψ^+ can be given as

$$\psi^{+}_{r\to\infty} = \Phi_{k0} + \sum_{n}(-\tfrac{1}{2\pi})\frac{e^{ik_f r}}{r}\phi_n(\underline{r}_j)[(-\tfrac{1}{2\pi})\int e^{-i\underline{k}_f\cdot\underline{r}'}\phi_n^{*}(\underline{r}_j)V_{int}(\underline{r}',\underline{r}'_j)\psi^{+}(\underline{r}',\underline{r}'_j)d\underline{r}'\prod_j d\underline{r}'_j \quad (1.2.13)$$

Comparing equation (1.2.13) with (1.2.7) yields

$$f_{no}(\hat{k}_0,\hat{k}_f) = -\frac{(2\pi)^{3/2}}{2\pi}\int e^{-i\underline{k}_f\cdot\underline{r}'}\phi_n^{*}(\underline{r}'_j)V_{int}(\underline{r}',\underline{r}'_j)\psi^{+}(\underline{r}',\underline{r}'_j)d\underline{r}'\prod_j d\underline{r}'_j \quad (1.2.14)$$

represented by

$$f_{no}(\hat{k}_0,\hat{k}_f) = -(2\pi)^2\left\langle\Phi_{kf}\middle|V_{int}\middle|\psi^{+}\right\rangle \quad (1.2.15)$$

where $\left|\Phi_{kf}\right\rangle = (2\pi)^{-3/2}e^{i\underline{k}_f\cdot\underline{r}}\phi_n(\underline{r}_j)$.

The integral equation (1.2.10) when solved by iteration and ψ^{+} substituted in (1.2.15) gives the Born series expansion for the direct scattering amplitude given by

$$f_{no}(\hat{k}_0,\hat{k}_f) = -(2\pi)^2\left\langle\Phi_{kf}\middle|V_{int} + (V_{int}G_o^{+}V_{int}) + (V_{int}G_0^{+}V_{int}G_o^{+}V_{int}) + \ldots\middle|\Phi_{k0}\right\rangle \quad (1.2.16)$$

$$f_{no}(\hat{k}_0,\hat{k}_f) = \sum_{n=1}^{\infty}\overline{f}_{Bn} \quad (1.2.17)$$

where $\overline{f}_{Bn} = -(2\pi)^2\left\langle\Phi_{kf}\middle|V_{int}\sum_{j=0}^{n}(G_0^{+}V_{int})^j\middle|\Phi_{k0}\right\rangle$. (1.2.18)

The sum of the first n terms on the right hand side of (1.2.17) yields the n^{th} Born approximation to scattering amplitude given by

$$f_{Bn} = \sum_{j=1}^{n}\overline{f}_{Bj}.$$

For elastic scattering $\left|\underline{k}_f\right| = \left|\underline{k}_0\right| = k_0$ and momentum transfer vector $\underline{K} = \underline{k}_0 - \underline{k}_f$ and $\left|\underline{k}_0 - \underline{k}_f\right| = 2k_0 Sin\theta/2$. If we take only first term of (1.2.16) we get first Born approximation.

$$f_{B1} = -(2\pi)^2\left\langle\Phi_{kf}\middle|V_{int}\middle|\Phi_{k0}\right\rangle$$

$$= -(1/2\pi)\int e^{i\underline{K}\cdot\underline{r}}\left\langle\phi_0\middle|V_{int}\middle|\phi_0\right\rangle d\underline{r} \quad (1.2.19)$$

In this approximation the distortion of incident particle as well as that of the target atom due to the presence of each other are completely ignored. Thus it is a weak interaction approximation and its validity increases with the increase of energy. When incident particle stays in the vicinity of target polarization, absorption and distortion of incident particle effects occurs.

The inclusion of polarization, absorption and distortion of incident particle effects to first Born is the second Born approximation.

$$f_{B2} = f_{B1} + \bar{f}_{B2}, \tag{1.2.20}$$

with $\bar{f}_{B2} = -(2\pi)^2 \langle 0, \underline{k}_f | V_{int} G_0^+ V_{int} | 0, \underline{k}_0 \rangle$. (1.2.21)

Yields $\bar{f}_{B2} = 2(2\pi)^2 \sum_n \int \frac{d\underline{q} \langle 0, \underline{k}_f | V_{int} | n, \underline{q} \rangle \langle n, \underline{q} | V_{int} | 0, \underline{k}_0 \rangle}{q^2 - k_n^2 - i\epsilon}$ (1.2.22)

where $|n, q\rangle = \frac{1}{(2\pi)^{3/2}} e^{i\underline{q}.\underline{r}} \phi_n(\underline{r}_j)$.

Performing the integration of the plane wave parts of matrix elements

$$\bar{f}_{B2} = \frac{2}{\pi^2} \sum_n \int \frac{d\underline{q} \langle 0 | \sum_{l=1}^{Z} (e^{i\underline{K}_1 \underline{r}_l} - 1) | n \rangle \langle n | \sum_{l=1}^{Z} (e^{i\underline{K}_2 \underline{r}_j} - 1) | 0 \rangle}{K_1^2 K_2^2 [q^2 - k_0^2 + 2(\epsilon_n - \epsilon_0) - i\epsilon]} \tag{1.2.23}$$

with $\underline{K}_1 = \underline{k}_0 - \underline{q}$; $\underline{K}_2 = \underline{q} - \underline{k}_f$.

The above equation involves the infinite summation and is difficult to solve. So further approximation is required and it is simplified by replacing $\epsilon_n - \epsilon_0$ by mean excitation energy Δ. Then performing summation by closure relation

$$\bar{f}_{B2} = \frac{2}{\pi^2} \sum_n \int \frac{d\underline{q} \langle 0 | \sum_{l=1}^{Z} (e^{i\underline{K}_1 \underline{r}_l} - 1) \times \sum_{l=1}^{Z} (e^{i\underline{K}_2 \underline{r}_j} - 1) | 0 \rangle}{K_1^2 K_2^2 [q^2 - p^2 - i\epsilon]} \tag{1.2.24}$$

where $p^2 = k_0^2 - 2\Delta$.

The second Born term provides significant improvement to first Born results, therefore inclusion of higher order Born terms will also improve the results.

1.3 EIKONAL APPROXIMATION:

The evaluation of higher order Born terms is quite involved. Thus to include higher order terms semiclassical approximation is used which practically include the higher order Born terms. In this approximation the relative coordinate $\underline{r}$ of the two particles and coordinates $\underline{r}_j$ of the target particles are decomposed in as

$$\underline{r} = \underline{b} + z\hat{\underline{n}} \;\; ; \;\; \underline{r}_j = \underline{b}_j + z_j \hat{\underline{n}} \tag{1.3.1}$$

where $\underline{b}$ and z are the perpendicular and parallel components, respectively and unit vector $\underline{n}$ is chosen either along $\underline{k}_0$ or $\underline{k}$. Using $k_n^2 = k_o^2 - 2\Delta$ in (1.2.11) and assuming

$\epsilon_n - \epsilon_0 = 0$ and then summing over intermediate states of the target using closure relation with intermediate momentum $\underline{P} = \underline{q} - \underline{k}_0$. Equation (1.2.11b) becomes

$$G_0^+(\underline{r},\underline{r}_j;\underline{r}',\underline{r}'_j) = -\frac{2}{(2\pi)^3} exp[i\underline{k}_0.(\underline{r}-\underline{r}')]\delta(\underline{r}_j - \underline{r}'_j) \times \int \frac{d\underline{p}\, exp[i\underline{p}.(\underline{r}-\underline{r}')]}{p^2 - 2\underline{p}.\underline{k}_0 - i\epsilon} \quad (1.3.2)$$

Now linearizing the Green's function by neglecting p^2 and carrying out the integration using (1.3.1)

$$G_0^+(\underline{r},\underline{r}_j;\underline{r}',\underline{r}'_j) = -\frac{1}{k_0} exp[i\underline{k}_0.(z-z')\delta(b-b')\theta(z-z')\delta(\underline{r}_j - \underline{r}'_j) \quad (1.3.3)$$

Putting this in (1.2.10)

$$\psi^+ = \Phi_{k0}(\underline{r},\underline{r}_j) - \frac{i}{k_0} e^{ik_0 z} \int_{-\infty}^{z} dz'\, d\underline{b}'\, \delta(\underline{b}-\underline{b}') e^{-ik_0 z'} V_{int}(\underline{r}',\underline{r}_j)\psi^+(\underline{r}',\underline{r}_j) \quad (1.3.4)$$

Let

$$\psi^+ = \Phi_{k0}\, F(\underline{r}) = \left(\frac{1}{(2\pi)^{3/2}} e^{i\underline{k}_0.\underline{r}} \phi_0(\underline{r}_j) \right) F(\underline{r}) \quad (1.3.5)$$

where $F(\underline{r})$ is determined from

$$F(\underline{r}) = 1 - \frac{i}{\underline{k}_0} \int_{-\infty}^{z} dz'\, d\underline{b}'\, \delta(\underline{b}-\underline{b}') V_{int}(\underline{r}',\underline{r}_j)\psi^+(\underline{r}',\underline{r}_j)\, F(\underline{r}) \quad (1.3.6)$$

Inserting $F(\underline{r})$ from (1.3.6) in (1.3.5), the eikonal approximation to ψ^+ is obtained.

$$\psi^+ = \phi_0(\underline{r}_j) \frac{1}{(2\pi)^{3/2}} exp[i\underline{k}_0.\underline{r} - \frac{i}{\underline{k}_0} \int_{-\infty}^{z} dz'\, d\underline{b}'\, \delta(\underline{b}-\underline{b}') V_{int}(\underline{r}',\underline{r}_j)] \quad (1.3.7)$$

$$f_E = -\frac{1}{2\pi} \int d\underline{r}\, e^{i\underline{k}.\underline{r}} \int \prod_j d\underline{r}_j \phi_f^*(\underline{r}_j)\phi_0(\underline{r}_j) V_{int}(\underline{r},\underline{r}_j) \times exp[i\underline{k}_0.\underline{r} - \frac{i}{\underline{k}_0} \int_{-\infty}^{z} dz'\, d\underline{b}'\, \delta(\underline{b}-\underline{b}') V_{int}(\underline{r}',\underline{r}_j)] \quad (1.3.8)$$

1.4 EIKONAL BORN SERIES METHOD:

Consider the non-relativistic scattering of a particle of mass m by a real, spherically symmetric potential V(r) of range a . The Glauber eikonal scattering amplitude is given by

$$f_E = \frac{k}{i} \int_0^{\infty} db\, b\, J_0(\Delta b)\left[e^{i\chi_0(b)/k} - 1\right] = Re\, f_E + i\, Im\, f_E \quad (1.4.1)$$

where $Re\, f_E$ and $Im\, f_E$ are real and imaginary parts of f_E.

The magnitude of momentum transfer $\Delta = |\vec{k}_f - \vec{k}_i| = 2k\,Sin\theta/2$, and eikonal phase

$$\chi_0(b) = -\frac{1}{2}\int_{-\infty}^{\infty} U(b,z)dz \tag{1.4.2}$$

with $U(r) = 2V(r)$ the reduced potential, where $r = (b^2 + z^2)^{1/2}$.

Now Born and eikonal multiple scattering series are as follow

$$f_B(k,\Delta) = \sum_{n=1}^{\infty} \bar{f}_{Bn} = \bar{f}_{B1} + \bar{f}_{B2} + \bar{f}_{B3} + \ldots.$$

$$= \bar{f}_{B1}(\Delta) + \left[\frac{A(\Delta)}{k^2} + i\frac{B(\Delta)}{k}\right] + \left[\frac{C(\Delta)}{k^2} + i\frac{D(\Delta)}{k^3}\right] + \ldots.$$

$$f_E(k,\Delta) = \sum_{n=1}^{\infty} \bar{f}_{En} = \bar{f}_{E1} + \bar{f}_{E2} + \bar{f}_{E3} + \ldots. \quad ;$$

where $\bar{f}_{En} = -\frac{i^{n+1}k}{n!}\int_0^{\infty} J_0(\Delta b)[\chi(k,b)]^n\, b\,db$

$$= \bar{f}_{E1}(\Delta) + \left[\qquad + i\frac{B(\Delta)}{k}\right] + \ldots., \text{ where } Re\,\bar{f}_{E2} = 0.$$

Here the term of order k_i^{-2} is missing in f_E. Thus to include all the terms corrected up to the order of k_i^{-2}, one must include $Re\,\bar{f}_{B2}$ which also gives contribution to this order. A marked improvement over the eikonal amplitude f_E was obtained by adding the quantity $Re\,\bar{f}_{B2}$. So that scattering amplitude

$$f_{EBS} = f_E + Re\,\bar{f}_{B2}\,. \tag{1.4.3}$$

Another way of improving eikonal amplitude in potential scattering has been proposed by Wallace [12]. Applying the Wallace correction to eikonal phase shift, scattering amplitude is given by

$$f_W = \frac{k}{i}\int_0^{\infty} db\, b\, J_0(\Delta b)\{\exp[i(\frac{\chi_0(b)}{k} + \frac{\chi_1(b)}{k^3})] - 1\}, \tag{1.4.4}$$

where $\chi_0(b)$ is the eikonal phase given by equation (1.4.2) and

$$\chi_1(b) = -\frac{1}{4}\int_{-\infty}^{+\infty} U(r)\,[U(r) + r\frac{d}{dr}U(r)]\,dz \tag{1.4.5}$$

We rewrite equation (1.4.3) as

$$f_{EBS} = f_W + Re\,\bar{f}_{B2}. \tag{1.4.6}$$

Thus differential cross section is given by

$$\frac{d\sigma}{d\Omega} = |f_{EBS}|^2 = \left|\mathrm{Re}\, f_E + \mathrm{Re}\,\overline{f}_{B2}\right|^2 + \left|\mathrm{Im}\, f_E\right|^2 . \tag{1.4.7}$$

1.5 DAS METHOD:

The evaluation of higher order Born term is very difficult. In 1978 Das has suggested a method for the consideration of higher order terms. In this method the Born series is represented by Fredholm integral equation for the scattering amplitude. The substitution of equation (1.2.10) in (1.2.15) yields scattering amplitude for scattering from initial state **0** to final state f.

$$\begin{aligned} f_{fo}(\hat{k}_f,\hat{k}_o) = &-(2\pi)^2\left\langle \Phi_{kf}(\underline{r},\underline{r}_j)\middle|V_{int}(\underline{r},\underline{r}_j)\middle|\Phi_{ko}(\underline{r},\underline{r}_j)\right\rangle \\ &-(2\pi)^2\left\langle \Phi_{kf}(\underline{r},\underline{r}_j)\middle|V_{int}(\underline{r},\underline{r}_j)G_0^+V_{int}(\underline{r}',\underline{r}'_j)\middle|\psi^+(\underline{r}',\underline{r}'_j)\right\rangle \end{aligned} \tag{1.5.1}$$

Substituting G_0^+ from (1.2.11b) Fredholm integral equation is obtained

$$f_{fo}(\hat{k}_f,\hat{k}_o) = f_{fo}^{B1}(\hat{k}_f,\hat{k}_o) + (2\pi)^2\frac{2}{(2\pi)^3}\sum_n \int \Phi^*_{kf}(\underline{r},\underline{r}_j)V_{int}(\underline{r},\underline{r}_j)\times$$

$$exp[+iq.(r-r')]\phi_n(\underline{r}'_j)\phi_n(\underline{r}_j)\times\frac{V_{int}(\underline{r}',\underline{r}'_j)\psi_o^+(\underline{r}',\underline{r}'_j)\,d\underline{r}\prod_j d\underline{r}_j\prod_j d\underline{r}'_j d\underline{q}\,d\underline{r}'}{q^2-k_n^2-i\in}$$

$$= f_{fo}^{B1}(\hat{k}_f,\hat{k}_o) + \frac{1}{\pi}\sum_n \int \Phi^*_{kf}(\underline{r},\underline{r}_j)V_{int}(\underline{r},\underline{r}_j)\,e^{iq.\underline{r}}\phi_n(\underline{r}_j)\,d\underline{r}\,d\underline{r}_j$$

$$\times\int\frac{e^{-iq.\underline{r}'}\phi_n^*(\underline{r}'_j)\,V_{int}(\underline{r}',\underline{r}'_j)\psi_o^+(\underline{r}',\underline{r}'_j)\,d\underline{r}'\,d\underline{r}'_j\,d\underline{q}}{q^2-k_n^2-i\in}$$

$$= f_{fo}^{B1}(\hat{k}_f,\hat{k}_o) + \frac{1}{\pi}\frac{(2\pi)^3}{(4\pi^2)^2}\sum_n\int\frac{d\underline{q}}{q^2-k_n^2-i\in}$$

$$\times[-(4\pi)^2\int\Phi^*_{kf}(\underline{r},\underline{r}_j)V_{int}(\underline{r},\underline{r}_j)\,\Phi_{kn}(\underline{r},\underline{r}_j)d\underline{r}\,d\underline{r}_j]$$

$$\times[-(4\pi)^2\int\Phi^*_{kn}(\underline{r}',\underline{r}'_j)V_{int}(\underline{r}',\underline{r}'_j)\,\psi_0^+(\underline{r}',\underline{r}'_j)d\underline{r}'\,d\underline{r}'_j]$$

$$= f_{fo}^{B1}(\hat{k}_f,\hat{k}_o) + \frac{1}{(2\pi)^2}\sum_n\int\frac{f_{fn}^{B1}(\hat{k}_f,\hat{q})\,f_{no}^{B1}(\hat{q},\hat{k}_o)\,d\underline{q}}{q^2-k_n^2-i\in} \tag{1.5.2}$$

Where $f_{fo}^{B1}(\hat{k}_f,\hat{k}_o)$ is the first Born scattering amplitude. The evaluation of this equation by iteration methods gives the scattering amplitude in Born series. For elastic scattering equation (1.5.2) becomes.

$$f_{oo}^{B1}(\hat{k}_f,\hat{k}_o)=f_{oo}^{B1}(\hat{k}_f,\hat{k}_o)+\frac{1}{(2\pi)^2}\sum_n\int\frac{f_{on}^{B1}(\hat{k}_f,\hat{q})\,f_{no}(\hat{q},\hat{k}_o)\,dq}{q^2-k_n^2-i\in} \qquad (1.5.3)$$

To solve this equation Das replaced $f_{no}(\hat{q},\hat{k}_o)$ by trial input scattering amplitude $f_{no}^{(in)}(\hat{q},\hat{k}_o)$ and output scattering amplitude $f_{oo}^{(out)}(\hat{k}_f,\hat{k}_o)$ was used to obtain differential and total cross sections. The scattering amplitude $f_{oo}(\hat{k}_f,\hat{k}_o)$ for finite values of k_0 satisfies the limiting conditions

$$f_{oo}(\hat{k}_f,\hat{k}_o)\underset{k_f\to 0}{\approx}c(k_o)\,f^{B1}(\hat{k}_O) \quad \text{and}$$

$$\underset{k_f\to\infty}{\approx}d(k_o)\,f^{B1}(\hat{k}_O) \qquad (1.5.4)$$

Where c and d are complex quantities which depend on k_o. The input trial scattering function is considered as

$$f_{no}^{(in)}(\hat{q},\hat{k}_o)=(a^D+ib^D)\,f_{no}^{B1}(\hat{q},\hat{k}_o) \qquad (1.5.5)$$

Where a^D and b^D are energy dependent parameters. With the choice of input trial function the out put scattering amplitude is obtained as

$$f_D^{(out)}=f_{oo}^{(out)}=f_{oo}^{B1}(\hat{k}_f,\hat{k}_o)+(a_D+i\,b_D)\,\overline{f}_{oo}^{B2}(\hat{k}_f,\hat{k}_o) \qquad (1.5.6)$$

Denoting $f_{oo}^{B1}(\hat{k}_f,\hat{k}_o)$ and $\overline{f}_{oo}^{B2}(\hat{k}_f,\hat{k}_o)$ by f_{B1} and $\overline{f}_{B2}$ respectively.

$$f_D^{(out)}=f_{oo}^{B1}+(a_D+ib_D)\,\overline{f}_{B2} \qquad (1.5.7)$$

The parameters a_D and b_D are obtained by minimizing the norm $\left|f_D^{(out)}-f_{oo}^{(in)}\right|^2$ integrated over the whole angular region of the scattering angle with respect to a_D and b_D. The calculation of a_D and b_D with equation (1.5.5) and (1.5.6) yields

$$a_D=\frac{\int d\theta\,Sin\theta\;f_{B1}(f_{B1}-\overline{f}_{B2R})}{\int d\theta\,Sin\theta\;[(f_{B1}-\overline{f}_{B2R})^2+\overline{f}_{B2I}^{\,2}]} \qquad (1.5.8)$$

$$b_D = \frac{\int d\theta \, Sin\theta \, \bar{f}_{B2I}}{\int d\theta \, Sin\theta \, I(f_{B1} - \bar{f}_{B2R})^2 + \bar{f}_{B2I}^2 I} \tag{1.5.9}$$

Thus in this method partial contribution of higher Born terms are taken in account by multiplying second order Born term by energy dependent complex parameter.

1.6 HIGH ENERGY HIGHER ORDER BORN APPROXIMATION:

The high energy higher order Born approximation procedure is adopted here to developed expansion of the second Born term in powers of k_i^{-2}. The second term of generalized Born series for the scattering amplitude, which describes the collision of an electron with an N-electron atom with initial and final atomic states and energies (ψ_i, E_i) and (ψ_f, E_f) respectively is given by [10]. For the evaluation of second Born term, interaction between electron and atom and the Green's function $V(\underline{r}_0, \ldots \underline{r}_n) = -\frac{N}{r_0} + \sum_{i=1}^{N} \frac{1}{|\underline{r}_0 - \underline{r}_i|}$, and $G_n(\underline{r}_0 - \underline{r}'_0) = \frac{1}{(2\pi)^3} \int \frac{d\underline{k}' e^{i\underline{k}'.(\underline{r}_0 - \underline{r}'_0)}}{k'^2 - k_n^2 - i\epsilon}, \epsilon \to 0^+$ are considered respectively.

$$f_{i\to f}^{(2)} = \frac{1}{\pi} \sum_n \int d\underline{r}_0 \, e^{-i\underline{k}_f . \underline{r}_0} V_{fn}(r_0) \int d\underline{r}'_0 \, G_n(r_0 - r'_0) V_{ni}(r'_0) e^{i\underline{k}_i \underline{r}'_0} \tag{1.6.1}$$

A more convenient form can be obtained by transforming the integration variables $(\underline{r}_0, \underline{r}'_0)$ to the set $(\underline{r}_0, \underline{\rho})$; $\underline{\rho} = \underline{r}_0 - \underline{r}'_0$; and replacing $\underline{\rho}$ by $\underline{r}'_0$, then the term reduces in the following form

$$f_{i\to f}^{(2)} = \frac{1}{\pi} \sum_n \int d\underline{r}_0 \, e^{i\underline{q}.\underline{r}_0} V_{fn}(\underline{r}_0) I_n \tag{1.6.2}$$

where

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

The basic approximations are introduced by the transformation of variable

$\underline{s} = \underline{k}' - \underline{k}_n$, in I_n ,

$$I_n = \frac{1}{(2\pi)^3} \int d\underline{r}'_0 e^{i(\underline{k}_i - \underline{k}_n)\underline{r}'_0} V_{ni}(\underline{r}_0 - \underline{r}'_0) \int \frac{d\underline{s} \, e^{i\underline{s}.\underline{r}'_0}}{s^2 + 2\underline{s}.\underline{k}_n - i\epsilon} \tag{1.6.3}$$

and assuming that $k_n >> 1$, $k_n = k_i$, then expanding $(s^2 + 2\underline{s}.\underline{k}_n - \epsilon)^{-1}$ in powers of s^2, the $d\underline{s}$ integral of (1.6.3) can be obtained as

$$\int \frac{d\underline{s}\, e^{i\underline{s}.\underline{r}'_0}}{s^2 + 2\underline{s}.\underline{k}_n - i\in} = \int \frac{d\underline{s}}{2\underline{s}.\underline{k}_n - i\in}\left[1 + \frac{\nabla^2_{\underline{r}'_0}}{2\underline{s}.\underline{k}_n - i\in}\right] e^{i\underline{s}.\underline{r}'_0}$$

where $\nabla_{\underline{r}'_0}$ is differential operator w.r.t. $\underline{r}'_0$ 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 definition of delta function and ds_z integral can be evaluated using contour integral techniques for first and second order poles to obtain the closed form. Using this equation (1.6.3) can be written as

$$I_n = \frac{i}{2k_n}\int d\underline{r}'_0\, e^{-i[(\underline{k}_l - \underline{k}_n).\underline{r}'_0]} V_{nl}(\underline{r}_0 - \underline{r}'_0)\left[1 + \frac{i}{2k_n}\nabla^2_{\underline{r}'_0} z'_0\right]\delta(\underline{b}'_0) H(z'_0)$$

$$= \frac{i}{2k_n}[I_{n1} + I_{n2}] \qquad (1.6.4)$$

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

$$\underline{r}'_0 = \underline{b}'_0 + \underline{z}'_0 \hat{k}_n \ .$$

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

$$I_{n1} = \int_{-\infty}^{\infty} e^{-i(\underline{k}_l - \underline{k}_n).\hat{k}_n z'_0} H(z'_0) V_{nl}(\underline{r}_0 - \underline{r}'_0) dz'_o \Big|_{\underline{b}'_0 = 0}$$

Now consider the integral I_{n2}

$$I_{n2} = \frac{i}{2k_n}\int d\underline{r}'_0\, e^{i(\underline{k}_l - \underline{k}_n).\underline{r}'_0} V_{nl}(\underline{r}_0 - \underline{r}'_0)\nabla^2_{\underline{r}'_0}\delta(\underline{b}'_0) z'_0 H(z'_0)$$

Integrating by parts twice

$$= \frac{i}{2k_n}\int d\underline{r}'_0\, \delta(\underline{b}'_0) z'_0 H(z'_0)\nabla^2_{\underline{r}'_0} e^{i(\underline{k}_l - \underline{k}_n).\underline{r}'_0} V_{nl}(\underline{r}_0 - \underline{r}'_0)$$

After the $\nabla^2_{\underline{r}'_0}$ operation, the corresponding I_{n2} and I_{n1} gives I_n

$$I_n = \frac{i}{2k_n}\int_{-\infty}^{\infty} dz'_0\, e^{i(\underline{k}_l - \underline{k}_n).\hat{k}_n z'_0} H(z'_o)\left[\left(1 + \frac{iz'_0}{2k_n}\hat{O}_{ln}\right) V_{nl}(\underline{r}_0 - \underline{r}'_0)\right]_{\underline{b}'_0 = 0}$$

where $\hat{O}_{ln} = \nabla^2_{\underline{r}'_0} - 2i(\underline{k}_l - \underline{k}_n).\vec{\nabla}_{\underline{r}'_0} - |\underline{k}_l - \underline{k}_n|^2$.

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

$$(\underline{k}_i - \underline{k}_n).\hat{\underline{k}}_n = k_i \, Cos\theta_{in} - k_n$$

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

$$\therefore I_n = \frac{i}{2k_n}\int_{-\infty}^{\infty} dz'_0 \, e^{-i\beta_i z'_0} H(z'_0)(1 + \frac{iz'_0}{2k_n}\nabla^2_{\underline{r}'_0}) V_{ni}(\underline{r}_0 - \underline{r}'_0)\Big|_{\underline{b}'_0=0} \tag{1.6.5}$$

where $\beta_i = k_i - k_n \approx \Delta E_{in} / k_i$, on using the energy conservation condition, the above expression embodies the central approximation. 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 $z+1$ electron will be written as $\underline{r}_i = \underline{b}_i + z_i\hat{\zeta}$, $i = 0,1\ldots z$, where ζ is a unit vector in the $z-$direction. Denote X for target coordinates.

For the simplification of the second Born term (1.6.1), it is useful to take the Fourier form of the interaction $V(\underline{r}_0,\ldots \underline{r}_N)$

$$V(\underline{r}_0,\ldots\underline{r}_N) = \int d\underline{p}\, e^{i\underline{p}.\underline{b}_0}\int_{-\infty}^{\infty} dp_z \, e^{-ip_z z_0}\overline{V}(\underline{p} + p_z\hat{\zeta}, \underline{r}_1 \ldots \underline{r}_N) \tag{1.6.6}$$

$$\text{where } \overline{V}(\underline{p} + p_z\hat{\zeta}, \underline{r}_1 \ldots\underline{r}_z) = \frac{1}{2\pi^2(p^2 + p_z^2)}\sum_{j=1}^{z}(e^{i\,\underline{p}.\underline{b}j + i\,p_z.z_j} - 1) \tag{1.6.7}$$

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

$$V_{nm}(\underline{r}_0) = \langle\psi_n(X)|V(X)|\psi_m(X)\rangle \tag{1.6.8}$$

Now substituting (1.6.6, 1.6.5) in (1.6.1), the corresponding second Born term can be written as

$$f^{(2)}_{HEA} = \frac{i}{2\pi k_i}\sum_n \int d\underline{r}_0 \, e^{i\underline{q}.\underline{r}_0} V_{fn}(\underline{r}_0)\int_{-\infty}^{\infty} dz'_0 H(z'_0) e^{-i\beta_{in} z'_0}[V_{ni}(\underline{r}_0 - z'_0\hat{\zeta}) + \frac{iz'_0}{2k_i}\nabla^2_{\underline{r}'_0} V_{ni}(\underline{r}_0 - \underline{r}'_0)\Big|_{b'_0=0}] \tag{1.6.9}$$

The infinite summation over the atomic states can be treated in a simple way by Byron and Joachain, 1977.

$$\sum_n V_{fn}(\underline{r}_0)V_{ni}(\underline{r}_0 - \underline{r}'_0) = V_f(\underline{r}_0)V_i(\underline{r}_0 - \underline{r}'_0) \tag{1.6.10}$$

It is assumed that $\beta_{in} = \beta_i \approx \Delta E / k_i$, where ΔE is the average energy transferred to intermediate atomic states during the course of the collision. Now (1.6.9) can be written as

$$f_{HEA}^{(2)} = \frac{i}{2\pi k_i}\int d\underline{r}_0\, e^{i\underline{q}\cdot\underline{r}_0}\left\langle \psi_f \left| V(\underline{r}_0,\ldots.\underline{r}_N)\int_{-\infty}^{\infty} dz'_0\, H(z'_0)\, e^{-i\beta_{in} z'_0}\right.\right. [V(\underline{r}_0 - z'_0\hat{\zeta},\underline{r}_1,\ldots\underline{r}_N)$$

$$\left.\left. + \frac{iz'_0}{2k_i}\nabla^2_{\underline{r}'_0} V(\underline{r}_0 - \underline{r}'_0,\underline{r}_1\ldots.\underline{r}_N)\Big|_{b'_0=0}\right] \left| \psi_i \right\rangle \right. \qquad (1.6.11)$$

Real and imaginary parts of the above expression can be obtained by using (1.6.7) and carrying out $\nabla^2_{\underline{r}'_0}$ operation in (1.6.11). Then the corresponding terms through $O(k_i^{-2})$ for DCS can be written as

$$Re1\ \ f_{HEA}^{(2)} = -\frac{4\pi^2}{k_i}\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{p_z-\beta_i} U_{fi}^{(2)}(\underline{q}-\underline{p}-p_z\hat{\zeta},\underline{p}+p_z\hat{\zeta}) \qquad (1.6.12)$$

$$Re2\ \ f_{HEA}^{(2)} = -\frac{2\pi^2}{k_i^2}\frac{\partial}{\partial\beta_i}\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{p_z-\beta_i}(p^2+p_z^2)U_{fi}^{(2)}(\underline{q}-\underline{p}-p_z\hat{\zeta},\underline{p}+p_z\hat{\zeta}) \qquad (1.6.13)$$

$$Im\ \ f_{HEA}^{(2)} = \frac{4\pi^3}{k_i}\int d\underline{p}\ U_{fi}^{(2)}(\underline{q}-\underline{p}-\beta_i\hat{\zeta};\underline{p}+\beta_i\hat{\zeta}) \qquad (1.6.14)$$

where P is the principle value. The general form of $U_{fi}^{(2)}$ can be given as

$$U_{fi}^{(2)}(\underline{p}+p_z\hat{\zeta},\underline{p}'+p'_z\hat{\zeta}) = \left\langle \psi_f \left| \overline{V}(\underline{p}+p_z\hat{\zeta},\underline{r}_1\ldots,\underline{r}_N)\overline{V}(\underline{p}'+p'_z\hat{\zeta},\underline{r}_1\ldots,\underline{r}_N)\right|\psi_i\right\rangle.$$

The DCS through order $(1/k_i^2)$ for direct scattering can be obtained from the scattering amplitude given as

$$f_{HEA}^{d} = f_{I\to f}^{(1)} + Re1\, f_{HEA}^{(2)} + Re2\, f_{HEA}^{(2)} + i\, Im\, f_{HEA}^{(2)} \qquad (1.6.15)$$

where $f_{I\to f}^{(1)}$ is the first Born approximation. Yates (1979) has made an analytical study of equations (1.6.11, 1.6.12, and 1.6.13) for elastic scattering of electrons by hydrogen atoms. And the following behaviors of these expressions are worth noting. The assumptions in ***HEA*** were made along with the small angle approximation of Glauber (1959). ***HEA*** concerned with short wavelength i.e $ka >> 1$ and for small momentum transfers i.e. small angles. The partial expansion of equation (1.6.2) was necessitated to include a plausible and accurate description of virtual excitations (target polarization). In the second Born term (1.6.10) if $\beta_i \to 0$ the real part of order k_i^{-2} (1.6.12) remains, similarly the imaginary part (1.6.13) reduces to the second term of GES. Finally it was concluded by Yates that the ***HEA*** provides an accurate description for small q .

1.7 PARTIAL WAVE ANALYSIS:

The scattering amplitude and cross section are determined by asymptotic behavior of stationary scattering wave function. In the case of central potential solution of Schrodinger equation $[-\frac{\hbar^2}{2m}\nabla_r^2+V(r)]\psi(r)=E\psi(r)$ may be separated in spherical polar coordinates and a simple connection between the radial solution and the asymptotic form of the stationary scattering wave function can be obtained. This procedure is called method of partial wave.

The Schrodinger time-independent equation for the stationary scattering wave function $\psi_{k_i}^{(+)}(r)$ can be written as

$$\frac{\hbar^2}{2m}[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})+\frac{1}{r^2Sin\theta}\frac{\partial}{\partial\theta}(Sin\theta\frac{\partial}{\partial\theta})+\frac{1}{r^2Sin^2\theta}\frac{\partial^2}{\partial\varphi^2}]\psi_{k_i}^{(+)}(r)+V(r)\psi_{k_i}^{(+)}(r)=E\psi_{k_i}^{(+)}(r) \quad (1.7.1)$$

Now the Hamiltonian operator H in spherical polar coordinates can be written in terms of square of the orbital angular momentum L^2 as

$$H=-\frac{\hbar^2}{2m}[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})-\frac{L^2}{\hbar^2r^2}]+V(r) \quad (1.7.2)$$

where $L^2=L_x^2+L_y^2+L_z^2=-\hbar^2[\frac{1}{Sin\theta}\frac{\partial}{\partial\theta}(Sin\theta\frac{\partial}{\partial\theta})+\frac{1}{Sin^2\theta}\frac{\partial^2}{\partial\varphi^2}]$

such that $L^2Y_{lm}(\theta,\varphi)=l(l+1)\hbar^2Y_{lm}(\theta,\varphi)$ (1.7.3)

and $L_zY_{lm}(\theta,\varphi)=m\hbar Y_{lm}(\theta,\varphi)$.

Here $[H,L^2]=[H,L_z]=0$, *i.e.* H, L^2 and L_z all commute, so there exist an eigen function common to these three operators. Thus the scattering wave function $\psi_{k_i}^{(+)}$ can be expanded in partial waves as

$$\psi_{k_i}^{(+)}(k,r)=\sum_{l=0}^{\infty}\sum_{m=-l}^{+l}C_{lm}(k)R_{lm}(k,r)Y_{lm}(\theta,\varphi) \quad (1.7.4)$$

where wave function $\psi_{k_i}^{(+)}(k,r)$, radial function R_{lm} and expansion coefficient C_{lm} are depending on wave number $k=\frac{(2mE)^{1/2}}{\hbar}$ using the expansion in the schrodinger equation and making the use of (1.7.3) and (1.7.2) radial equation is obtained as

$$-\frac{\hbar^2}{2m}[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})-\frac{l(l+1)}{r^2}]R_l(k,r)+V(r)R_l(k,r)=ER_l(k,r) \tag{1.7.5}$$

Using $u_l(k,r)=rR_l(k,r)$ and reduced potential $U=2mV/\hbar^2$, the equation becomes

$$[\frac{d^2}{dr^2}+k^2-l(l+1)/r^2-U(r)]u_l(k,r)=0 \tag{1.7.6}$$

Now consider the radial equation for a free particle *i.e.* $U(r)=0$

$$[\frac{d^2}{dr^2}+k^2-l(l+1)/r^2]y_l(k,r)=0\ . \tag{1.7.7}$$

Changing variables to $\rho=kr$ and defining $f_l(\rho)=y_l/\rho$

$$[\frac{d^2}{d\rho^2}+\frac{2}{\rho}\frac{d}{d\rho}+(1-\frac{l(l+1)}{\rho^2})]f_l(\rho)=0 \tag{1.7.8}$$

This is known as Bessel differential equation. Particular solution of this equation are the spherical Bessel function j_l and spherical Neumann function n_l. The general solution is then a linear combination of two linearly independent particular solutions.

$$y_l(k,r)=kr[C_l^{(1)}(k)j_l(kr)+C_l^{(2)}(k)n_l(kr)] \tag{1.7.9}$$

where $C_l^{(1)},C_l^{(2)}$ the pair of integration constant. But the only solution of equation (1.7.8), which is finite every where, is the function $j_l(kr)$. Therefore there exist eigenfunction $j_l(kr)Y_{lm}(\theta,\varphi)$ common to the free Hamiltonian $H_0=-\frac{\hbar^2}{2m}\nabla_r^2$ and to the operator L^2 and L_z. Now the plane wave $\exp(ik_l.r)$ which represents a free particle of momentum $p_l=\hbar k_l$ is a solution of Schrodinger equation $H_0\psi=E\psi$ such that $E=\hbar^2k^2/2m$ with $k=|k_l|$. Since the eigenfunction $j_l(kr)Y_{lm}(\theta,\varphi)$ form a complete set, the plane wave may be developed in the series of these functions. Choosing the z-axis along the direction of $\underline{k}_l$ so that $\exp(ik_l.r)=\exp(ikrCos\theta)$ is independent of φ. The partial wave expansion of the plane wave is given as

$$\exp(ik_l.r)\equiv\exp(ikz)=\sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(Cos\theta) \tag{1.7.10}$$

where function $P_l(Cos\theta)$ are the Legender polynomials.

The boundary condition must be imposed up on the radial function $u_l(k,r)$ that out side the range '*a*' of the potential it is same as the free particle solution.

$$u_l(k,r) = kr[C_l^{(1)}(k) j_l(kr) + C_l^{(2)}(k) n_l(kr)], \quad r >> a \tag{1.7.11}$$

Let us assume that r is so large that the term $U(r)$ and $l(l+1)/r^2$ may be neglected in equation (1.7.6). An 'asymptotic' solution is then obviously of the form $\exp(\pm ikr)$. Thus the general solution of equation (1.7.6) for large r is given by

$$u_l(k,r) = B_l^{(1)}(k) e^{ikr} + B_l^{(2)}(k) e^{-ikr} \tag{1.7.12}$$

Using the fact that

$$j_l(x) \xrightarrow[r\to\infty]{} \frac{1}{x} Sin(x - l\pi/2) \quad \text{and} \quad n_l(x) \xrightarrow[r\to\infty]{} -\frac{1}{x} Cos(x - l\pi/2) \tag{1.7.13}$$

We may also write equation (1.7.12) in the form (1.7.9). Thus we have

$$u_l(k,r) \xrightarrow[r\to\infty]{} kr[C_l^{(1)}(k) j_l(kr) + C_l^{(2)}(k) n_l(kr)] \tag{1.7.14}$$

Using equation (1.7.13) the boundary condition is obtained as

$$u_l(k,r) \xrightarrow[r\to\infty]{} A_l(k) Sin[kr - l\pi/2 + \delta_l(k)] \tag{1.7.15}$$

$$\text{with } A_l(k) = \{[C_l^{(1)}(k)]^2 + [C_l^{(2)}(k)]^2\}^{1/2} \text{ and } \tan\delta_l(k) = -\frac{C_l^{(2)}(k)}{C_l^{(1)}(k)} \tag{1.7.16}$$

The quantities δ_l, which are called the phase shifts, display the influence of the interaction. The effect of potential on spherical waves is given by δ_l.

Scattering amplitude :

The asymptotic form of the scattering wave function is given as

$$\psi_{k_i}^{(+)}(k,r) \xrightarrow[r\to\infty]{} A(k)[\exp(ik_i r) + f(k,\theta,\varphi)\frac{\exp(ikr)}{r}] \tag{1.7.17}$$

Using equation (1.7.10) and (1.7.13)

$$\psi_{k_i}^{(+)}(k,r) \xrightarrow[r\to\infty]{} A(k)\left[\sum_{l=0}^{\infty}(2l+1) i^l \frac{\sin(kr - l\pi/2)}{kr} P_l(\cos\theta) + f(k,\theta,\varphi)\frac{e^{ikr}}{r}\right] \tag{1.7.18}$$

$$\psi_{k_i}^{(+)}(k,r) \xrightarrow[r\to\infty]{} A(k)\Big[\sum_{l=0}^{\infty}\sum_{m=-l}^{+l}[4\pi(2l+1)]^{1/2} i^l \frac{e^{i(kr - l\pi/2)} - e^{-i(kr - l\pi/2)}}{2ikr} \times$$

$$Y_{lm}(\theta,\varphi)\delta_{m,0} + f(k,\theta,\varphi)\frac{e^{ikr}}{r}\Big] \tag{1.7.19}$$

Considering the partial wave expansion (1.7.4) for large r and substituting $R_{lm}(k,r) \equiv R_l(k,r) = r^{-1}u_l(k,r)$ together with equation (1.7.15)

$$\psi_{k_i}^{(+)}(k,r) \underset{r\to\infty}{\to} \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} c_{lm}A_l(k)\frac{1}{2ir}\left[e^{i(kr-l\pi/2+\delta_l)} - e^{-i(kr-l\pi/2+\delta_l)}\right]Y_{lm}(\theta,\varphi) \qquad (1.7.20)$$

Comparing the coefficients of incoming spherical waves in equation (1.7.19) and (1.7.20)

$$c_{lm}(k) = \frac{A(k)}{kA_l(k)}[4\pi(2l+1)]^{1/2} i^l \exp(i\delta_l)\delta_{m,0} \qquad (1.7.21)$$

Substitute for c_{lm} in equation (1.7.20) and matching the coefficients of the out going spherical waves in equation (1.7.19) and (1.7.20)

$$f(k,\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}\sum_{m=-l}^{+l}\frac{(4\pi)^{1/2}}{(2l+1)^{1/2}}Y_{lm}\delta_{m,0}(2l+1)[\exp\{2i\delta_l(k)\}-1]$$

$$= \frac{1}{2ik}\sum_{l=0}^{\infty}\frac{(4\pi)^{1/2}}{(2l+1)^{1/2}}Y_{l,0}(\theta)(2l+1)[\exp\{2i\delta_l(k)\}-1]$$

$$\therefore f(k,\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)[\exp\{2i\delta_l(k)\}-1]P_l(\cos\theta) \qquad (1.7.24)$$

The knowledge of phase shifts allows one to obtain the scattering amplitude by means of the above relation. The differential scattering cross section and total cross section are then obtained respectively as

$$\frac{d\sigma}{d\Omega}(k,\theta) = |f(k,\theta)|^2 \text{ and } \sigma_{total}(k) = 2\pi\int_0^{\pi}\frac{d\sigma}{d\Omega}(k,\theta)\sin\theta\, d\theta\ . \qquad (1.7.25)$$

A similar analysis was made for the Dirac relativistic equations for elastic scattering of electrons is given in chapter 2.

1.8 APPROACH TO THE PRESENT INVESTIGATION:

The elastic scattering of an electron from an atom or ion is the phenomenon occurring in a wide range of physical context such as in astrophysical or atmospheric environments, fusion reactors, technical plasmas used for modifying materials such as semiconductors, etc. The work has similar importance in fundamental studies also.

Calculations of elastic collision cross sections are carried out at high energies presently is initiated from the following causes.

[1] Elastic scattering of electrons by neutral atom is of importance in different experimental technique as accurate phase shifts are required to interpret the results of low-energy electron diffraction measurements [1] .

[2] Differential cross sections are needed to analyze the effect of elastic scattering in quantitative Auger electron spectroscopy and X-ray photoelectron spectroscopy[2,3].

[3] Elastic scattering has important role in electron-photon shower theory and electron microscopy [4,5].

[4] Byron and Joachain [6-11] have reported considerable amount of work for the calculation of scattering cross sections for different atoms. High-energy range up to 40 KeV did not studied much except few workers [13-17]. During intensive study of the results of various approximations for the description of electron atom scattering processes at high energies. Following reasons are found for the present investigation.

[5] Few theoretical methods were able to reproduce the scattering cross section, which can be compared satisfactorily with the results of the experiments.

[6] Some approximations required complicated numerical techniques for the evaluation of the scattering cross sections.

[7] Divergent integral problems were common in some approximations.

[8] Much more complex calculations are required for better approximation in $\bar{e}$-atom / ion collision processes.

[9] Moreover approximations were found to be difficult in order to extend for the study of many electron system of atom or ion ($Z>1$).

During the study of EBS approach [8-12] and HHOB theory [19-21], which is applied to the actual problem in the present work it is noted that the approximations can remove the above problems. Keeping all the above points HEA approach is selected for present investigations. The HHOB approximation is extended to study different atoms and ions.

[10] Motivation behind this work is also due to experiment of Coffman-Fink. Where no peak at high-energy range [15-35 KeV] observed experimentally as reported by GML [17]. We want to evaluate the same by better approximate method. With reference to partial wave work we can verify all other methods at high energy by using Dirac relativistic wave equation.

[11] Recently the direct investigation of elastic scattering of electrons by ions [22] has created new theoretical interest other than atoms.

[12] Also certain experiments require knowledge of the elastic cross section to estimate backgrounds for inelastic channel measurements [23].

[13] In the fast ion-atom or ion-molecule studies binary encounter peak has been interpreted by elastic scattering of electrons from ion [24-26].

[14] Elastic and inelastic collision cross sectional data are applied for modeling plasma environments as well as it has crucial role in the energy and momentum transport in the plasma. Thus recent research interest has been found for the present work on He like ions.

Keeping all above mentioned points in reference the problem of elastic scattering of electrons mainly from He, Ne, and Ar targets, as well as some targets of He iso-electronic series are studied at high energies through different approaches is presented in this thesis.