CHAPTER - V

HHOB OPTICAL MODEL THEORY

5.1 INTRODUCTION

The elastic scattering of electrons and positrons by atoms and molecules in the intermediate energy region can be conveniently analysed by the optical model potential. For complex atomic targets it is a convenient model to describe both the effects of the distortion of the incident charged particle in the atomic field and the distortion of the target atom in the presence of the incident charged particle. Once the optical potential is determined, the original many - body elastic scattering problem reduces to a one-body problem, namely the scattering of a particle by a potential. Furthermore, depending on the way an optical potential is set up, it can also offer a computationally simpler solution of the differential equation of scattering (Joachain 1975). However this reduction is impossible at present and approximation methods are necessary. A number of calculations for the elastic scattering of electrons and positrons by H, He , Li, Be, C, N, O, F, Ne, Na, Mg, Ar, K, Kr, Xe (Jhanwar and Khare 1976 ; Jhanwar et al 1978b ; Khare and Kumar 1978 ; Khare and Raj 1979, 1980 ; Khare et al 1982 ; Kaushik et al 1982, 1983 ; Furness and Mc Carthy 1973 ; Mc Carthy et al 1977 ; Lucas and Mc Carthy 1978 ; Joachain et al 1977 ; Byron and Joachain 1977a ; Vanderpoorten 1975, 1976 ; Teubner et al 1978 ; Buckman et al 1979 ; Schwenke et al 1983). Therefore it would be interesting to apply the optical model formalism to the scattering of charged particles by complex atoms which we shall analyse by means of Higher energy Higher order Born (HHOB) approximation (Yates 1979). We have taken a study to formulate the optical HHOB approximation model in a form suitable for application to scattering by complex atoms. The HHOB approximation proposed by Yates (1979) has several attractive feature. The expressions are obtainable in the closed form thus avoiding complex numerical procedure . The method is simple and computationally feasible and the problem of divergent integrals (like those in GES) is absent.

The optical potential comprised of static, absorption and polarisation potentials. In the following sections after discussing briefly the static contribution to the HHOB phase, we analyse in detail the role of absorption and polarisation interactions. The absorption and polarisation phase shift function are written down for an arbitary atom interms of an excitation energy and other known quantities.

The optical potential so constructed is spherically symmetric, the differential equation is solved using the method of partial waves and the scattering matrix $S_l = e^{2i\delta_l}$, where δ_l is the phase shift in the l^{th} partial wave and hence the DCS are obtained. Calculations are carried out for elastic $\bar{e}$ scattering from hydrogen of energies 50 eV and 100 eV.

5.2 THEORY :

Let us consider the non-relativistic elastic scattering of an electron by a neutral atom having z electrons. We assume that the centre of mass of the atom coincides with its nucleus and choose it as the origin of our co-ordinate systems. We begin by writing the equivalent one body Schrodinger equation for elastic scattering namely,

$$(K + V_{opt} - \frac{1}{2} k^2) \psi_i^+ = 0, \qquad (5.1)$$

where ψ_i^+ is the elastic scattering wave function describing the motion of the projectile in the optical V_{opt} , we may write the optical potential,

$$V_{opt} = V^{(1)} + V^{(2)} \tag{5.2}$$

where $V^{(1)}$ is the static potential.

$$V^{(2)} = V_{pol} + i\,V_{abs} \tag{5.3}$$

where V_{pol} and V_{abs} are purely real but energy dependent.

The total optical potential thus becomes

$$V_{opt} = V_{st} + V_{pol} + iV_{abs} + V_{ex} \tag{5.4}$$

Following the method used for optical eikonal scattering amplitude (Byron et al 1977) we can write the first Born optical approximation as

$$f_{oB} = \frac{1}{2\pi} \int e^{i\underline{q}.\underline{b}} \Big[V_o X_{st} + V_o^2 X_{pol} + V_o^2 X_{abs} + \frac{i}{2} V_o^2 X_{st}^2 \Big] db \tag{5.5}$$

where $$V_o X_{st} = - \int_{-\infty}^{\infty} V_{st} (\underline{b}, z)\, dz \tag{5.6}$$

$$V_o^2 X_{pol} = - \int_{-\infty}^{\infty} V_{pol} (\underline{k}, \underline{b}, z)\, dz \tag{5.7}$$

$$V_o^2 X_{abs} = - \int_{-\infty}^{\infty} V_{abs} (\underline{k}, \underline{b}, z)\, dz \tag{5.8}$$

Here V_o is the strength of the coulomb potential and equal to 1 in atomic units. In the HHOB approximation (Yates 1979) taking the first and second terms, the amplitude is written as,

$$f_{HHOB} = -\frac{1}{2\pi} \int d\underline{b}\; e^{i\underline{q}\cdot\underline{b}} \int V_{ii}\; dz + \frac{1}{\pi} \sum_n \int d\underline{b}\; e^{i\underline{q}\cdot\underline{b}} \int_{-\infty}^{\infty} V_{fn}\; dz \int dV_o' \; G_o(r')\; V_{ni}\,(\underline{r} - \underline{r}')\; e^{-ik_i\cdot r'} \qquad (5.9)$$

where $V_{nm}\,(\underline{r}_o) = \langle\; \psi_n(\underline{x}) \mid V(\underline{r} - \underline{r}') \mid \psi_m(\underline{x}) \;\rangle$ (5.10)

Compairing the terms in (5.5) and (5.9) we find that

$$X_{st} = -\int_{-\infty}^{\infty} V_{ii}\; dz \qquad (5.11)$$

and

$$\frac{i}{2}\, X_{st}^2 + X_{pol} + X_{abs} = 2 \sum_n \int_{-\infty}^{\infty} V_{fn}\; dz \int dv_o' \; G_o(r')\; V_{ni}(\underline{r}-\underline{r}')\; e^{-i\underline{k}_i\cdot\underline{r}}$$

$$= \frac{i}{k_i}\; \langle\; f \mid \int_{-\infty}^{\infty} dz\; V \int_{-\infty}^{\infty} dz'\; H(z')\; e^{-i\beta_i z'} \; V(\underline{r} - z'\hat{y},\, \underline{r}_1) \,\Big|_{b'=0} \mid i \rangle \qquad (5.12)$$

where $H(z)$ is the Heaviside function

The above equation can be written for the ground state as

$$\frac{i}{2} X_{st}^{2} + X_{pol} + i X_{abs} = \frac{i}{k_i} \langle 0 \mid \int_{-\infty}^{\infty} V dz$$

$$\int_{-\infty}^{z} dz' \left(\cos \beta_i z' - i \operatorname{Sin} \beta_i z' \right)$$

$$V(\underline{r} - \underline{r}') \; H(z') \mid 0 \rangle \qquad (5.13)$$

Now the real part of the above can be written as

$$X_{pol} = \frac{1}{k_i} \langle 0 \mid \int_{-\infty}^{\infty} V \, dz \int_{-\infty}^{z} \operatorname{Sin} \beta_i z' \; V \, dz' \mid 0 \rangle$$

(5.14)

The quantity X_{pol} is in general very complicated but if we are interested in the small momentum - transfer behaviour of f_{OB} we need large $\underline{b}$ behaviour of V. Therefore we can write V as

$$V = \frac{zz + bb_1 \operatorname{Cos}\phi_1}{r^3} \qquad (5.15)$$

Substituting the value of V in equation (5.14) we can write

$$X_{pol} = \frac{1}{k_i} \langle 0 \mid \int_{-\infty}^{\infty} \frac{(z \, z_1 + bb_1 \operatorname{Cos}\phi_1)}{r^3} \, dz$$

$$\int_{-\infty}^{z} \sin \beta_i z' \quad \frac{(z' z_1 + b b_1 \cos\phi_1)}{r^3} \, dz' \mid 0 \rangle \tag{5.16}$$

Changing the integration variables $x = \frac{z}{b}$ and $y = \frac{z'}{b}$, we can write the above equation as

$$X_{pol} = \frac{\langle 0 \mid z_1^2 \mid 0 \rangle}{k_i b^2} \left[\int_{-\infty}^{\infty} dx \int_{-\infty}^{x} dy \, (xy + 1) \frac{\sin(\beta_i y b)}{(1 + x^2)^{3/2} (1 + y^2)^{3/2}} \right] . \tag{5.17}$$

If we now insert this into expression (5.5) it will gives a contribution to f_{OB}, which we may denote by f_{OB}^{pol}. It is given by

$$f_{OB}^{pol} = \frac{1}{2\pi} \int d\underline{b} \; e^{i\underline{q}\cdot\underline{b}} \; X_{pol}$$

$$= \frac{\langle 0 \mid z^2 \mid 0 \rangle}{k_i} \int_{-\infty}^{\infty} dx \int_{-\infty}^{x} \frac{(xy + 1)}{(1 + x^2)^{3/2}} \frac{\sin(\beta_i y b)}{(1 + y^2)^{3/2}} \, dy \int_{0}^{\infty} \frac{J_0(qb) \, db}{b}$$

The above equation tends to glauber term when $\beta_i \longrightarrow 0$. We can also see that the above equation is similar to

Byron et al's f_{OB}^{pol} except that Sine term is having only one interaction term.

$$f_{OB}^{pol} = \langle 0 \mid z^2 \mid 0 \rangle \int_{-\infty}^{\infty} dx \int_{-\infty}^{x} dy \frac{\mathrm{Sin}(\eta y)(xy+1)}{(1+x^2)^{3/2}(1+y^2)^{3/2}}$$

$$\int_{o}^{\infty} J_o \left(\frac{q\eta}{\beta_i} \right) \frac{\mathrm{Sin}\ \eta t}{\eta} \qquad (5.19)$$

where $\eta = \beta_i b$

The integral involving the Bessel function can be evaluated analytically to give

$$\phi(t) = \int_{o}^{\infty} J_o \left(\frac{q\,\eta}{\beta_i} \right) \frac{\mathrm{Sin}\ (\eta t)}{\eta}$$

$$\begin{aligned} &= \frac{\pi}{2}\ , \quad \frac{q}{\beta_i} \leq t \\ &\quad \mathrm{Sin}^{-1} \left(\frac{\beta_i t}{q} \right) , \quad \frac{q}{\beta_i} \geq t \end{aligned} \qquad (5.20)$$

So we may write

$$f_{OB}^{pol} = \frac{\langle 0 \mid z^2 \mid 0 \rangle}{k_i} \int_{-\infty}^{\infty} \frac{dx}{(1 + x^2)^{3/2}} \ I_1 \qquad (5.21)$$

$$\text{where} \quad I_1 = \int_{-\infty}^{x} dy \frac{(xy + 1)}{(1 + y^2)^{3/2}} \ \phi\ (y) \qquad (5.22)$$

Integrating by parts the above equation and substituting in (5.21) we will get

$$f^{pol}_{OB} = \frac{\langle 0 \mid z^2 \mid 0 \rangle}{k_i} \Big[\pi - \frac{q}{\beta_i} \int_{-\infty}^{\infty} \frac{dx}{(1 + x^2)^{3/2}}$$

$$\int_0^{\pi/2} \frac{\text{Sin}\,\theta \;\; d\theta}{\left(1 + (\frac{q}{\beta_i}\ \text{Sin}\theta)^2\right)^{1/2}}$$

$$= \frac{\langle 0 \mid z^2 \mid 0 \rangle}{k_i} \Big[\pi - \int_0^{\infty} \frac{dx\ x\ \text{Sin}^{-1}(\frac{\beta_i x}{q})}{(1 + x^2)^2}$$

$$- \frac{q}{\beta_i} \int_{-\infty}^{\infty} \frac{dx}{(1 + x^2)^{3/2}} \int_0^{\pi/2} \frac{\text{Sin}\theta \;\; d\theta}{(1 + \frac{q}{\beta_i}\ \text{Sin}^2\theta)^{3/2}} \Big]$$

$$= \frac{\pi \langle 0 \mid z^2 \mid 0 \rangle}{k_i} \Big[1 - \frac{1}{8qa} - \frac{qa}{\left(1 + (qa)^2\right)^{1/2}} \Big] \tag{5.23}$$

where $a = \frac{1}{2\beta_i}$

It is interesting to note thatt the above expression is exactly same as that of Byron et al (1977) except one additional term which has less significant value. We can find out the V_{pol} from (5.23) as follows.

$$V_{pol} = \frac{\langle 0 \mid z^2 \mid 0 \rangle}{4\pi k_i} \int e^{i\underline{q}\cdot\underline{r}}\, dq \Big[1 - \frac{1}{8qa} \quad -$$

$$\frac{qa}{\left\{1 + (qa)^2\right\}^{3/2}} \;] \quad ,$$

$$= - \frac{1}{ka^3 \rho} < 0 \, |z^2| \, 0 > \int_0^\infty \mathrm{Sin}(\mu \rho) \left[1 - \frac{1}{8\mu} - \frac{\mu}{(\mu^2 + 1)^{1/2}} \right] \mu \, d\mu \qquad (5.24)$$

where $\rho = \frac{r}{a}$; $\mu = qa$ (5.25)

The above V_{pol} is different from the Byron et al by an additional term $\frac{1}{8\mu}$. Integrating by parts twice we find that the expression for V_{pol} is same as that of Byron et al. The contribution of the term $(\frac{1}{8\mu})$ is not present because it amounts to an additional constant which when differentiate twice for tthe evaluation of the integral will be zero. Hence the expression for V_{pol} will be

$$V_{pol} = - \frac{1}{k_i \, a^3 \rho} < 0 \, |z^2| \, 0 > \left[3 \int_0^\infty \frac{\mathrm{Sin}(\rho\mu) \, d\mu}{(\mu^2 + 1)^{5/2}} - \int_0^\infty \frac{\mathrm{Sin} \, (\rho\mu)}{(\mu^2 + 1)^{3/2}} \right] \qquad (5.26)$$

Integrating the above expression we will get

$$V_{pol} = - \frac{\pi}{2k_i \, a^3} < 0 \, |z^2| \, 0 > [\; I_0(\rho) - L_0(\rho)$$

$$- \frac{1}{\rho} \left\{ I_1(\rho) - L_1(\rho) \right\}] \qquad (5.27)$$

Where L_n and I_n are modified struve and Bessel functions. Using the asymptotic expansion of $(I_o - L_o)$ and $(I_1 - L_1)$ the large r - behavior of V_{pol} is obtained.

$$V_{pol} = - \frac{\alpha}{2r^4} \left[1 + \frac{6a^2}{r^2} + \frac{135a^4}{r^4} \right] \qquad (5.28)$$

Where α is the polarisability.

The V_{pol} thus obtained is exactly the same as that of Byron et al (1974).

Now we will turn our attention to the imaginary part of equation (5.13).

$$\frac{1}{2} X_{st}^2 + X_{abs} = \frac{1}{k_i} < 0 \mid \int_{-\infty}^{\infty} V \, dz \int_{-\infty}^{z} dz' \, Cos(\beta_i z') \, V(r-r') \, H(z') \mid 0 >$$

$$= \frac{1}{k_i} < 0 \mid \int_{-\infty}^{\infty} V \, dz \int_{-\infty}^{z} dz' \, Cos \, (\beta_i z') \, V(r - z' y, r_1) \mid 0 > \qquad (5.29)$$

In order to simplify the above equation we will write the interaction potential in Fourier form given in equation (1.41). Hence the above equation can be written as

$$-\frac{1}{2} X_{st}^{2} + X_{abs} = \frac{1}{k_i} < 0 | \int V dz \int_{-\infty}^{\infty} H (z') dz' e^{-\beta_i z'} \int \int_{-\infty}^{\infty} dp\, dp_z\, e^{-ip.r + ip_z z'} \bar{V} (p + p_z \hat{y} , r_1)$$

$$= \frac{1}{k_i} < 0 | \int V d_z I_n | 0 > \qquad (5.30)$$

Here $$I_n = \int dz' H(z') e^{-\beta_i z'} \int \int_{-\infty}^{\infty} dp\, dp_z\, e^{-ip.r + ip_z z'} \bar{V} (p + p_z \hat{y} , r_1) \qquad (5.31)$$

Using the result $$\int_{-\infty}^{\infty} dx\, e^{-ix\alpha} H (x) = \pi \delta (\alpha) - i \mathcal{P}\left(\frac{1}{\alpha}\right) \qquad (5.32)$$

We can write the equation (5.31) as

$$I_n = \int dp_z \int dp\, e^{-ip.r} \bar{V} (p + p_z \hat{y} , r_1) \left[\pi \delta (p_z - \beta_i) - i \mathcal{P}\left(\frac{1}{(p_z - \beta_i)} \right) \right]$$

$$= \pi \int d\underline{p} \; e^{-i\underline{p}.\underline{b} - i\beta_i z} \; \overline{V} (\underline{p} + \beta_i \hat{y} \, , \underline{r}_1)$$

$$- i \mathcal{P} \int \frac{dp_z}{(p_z - \beta_i)} \int d\underline{p} \; e^{-i\underline{p}.\underline{b} - ip_z z}$$

$$\overline{V}(\underline{p} + p_z \hat{y} \, , z_1) \quad (5.33)$$

From X_{ABS} we can find out the value of V_{abs} using the below formula,

$$V_{abs} = \frac{1}{\pi} \int_r^\infty (b^2 - r^2)^{1/2} \frac{d}{db} (X_{abs}) \, db \qquad (5.34)$$

The first Born scattering amplitude for V_{pol} as given by (5.28) is

$$f^{B1}_{pol} = \frac{\pi}{4d} \left[\frac{\alpha(3 - q\,d)}{4} \right] e^{-qd} \qquad (5.35)$$

$$d = \frac{3a}{4}$$

The static potential is $V_{st} = - \sum_{j=1}^{3} \gamma_i \frac{e^{-\lambda_i r}}{r}$ (5.36)

values of λ -s and γ - s are given in earlier chapter. The first Born scattering amplitude for V_{st} is

$$f^{B1}_{st} = 2 \sum_{j=1}^{3} \frac{\gamma_j}{(q^2 + \lambda_j^2)} \qquad (5.37)$$

For the inclusion of exchange effects we have taken the equivalent local exchange potential.following Vanderpoorten (1975). According to him, V_{ex} is given as

$$V_{ex}(r) = \frac{1}{2}(k_i^2/2 - V_o) - \left\{ (\frac{1}{2} k_i^2 - V_o)^2 + \frac{8 (2 + 1)}{\pi} e^{-2r} \right\}^{1/2}] \qquad (5.38)$$

with $V_o = V_{st} + V_{pol}$

For the determination of the exact phase shift we have to solve the second order differential equation. We have employed the Numerov method for the step by step integration of the radial Schrodinger equation out from the origin into the asymptotic region where the potential has a negligible effect. In this region $x > x_A$, the range of the potential, we know the values of the unknown variable and its derivative. So the phase shifts can be computed. The details of this procedure is given below .

Consider the second order ordinary differential equation of the form

$$Y^n = F (x) Y_j \qquad (5.39)$$

It can be written as

$$Y_j^n = F (x_j) Y_j \qquad (5.40)$$

Using Newton's formula for forward interpolation and the method of replacing the derivative of a function by a polynomial over an interval we get the Numerov formula.

$$\left(1 - \frac{h^2}{12} F_{j+1}\right) Y_{j+1} = 2\left(1 - \frac{h^2}{12} F_j\right) Y_j - \left(1 - \frac{h^2}{12} F_{j-1}\right) Y_{j-1} + h^2 F_j Y_j \qquad (5.41)$$

Thus for $j = 1$ we have a formula for determining Y_2 provided we know the two previous ordinates y_o and y. Here h denote the step interval.

Now in the scattering problem for example electron hydrogen scattering, the second order differential equation is given as

$$\left(\frac{d^2}{dx^2} + k_i^2 - \frac{l(l+1)}{x^2} - 2V(x)\right) F_l(k_i x) = 0, \qquad (5.42)$$

where k_i is the incident momentum and $V(x)$ is the interaction potential.

Comparing equations (5.39) and (5.42)

$$Y = F_l(k_i x) \quad \text{and}$$

$$F(x) = \frac{l(l+1)}{x^2} = k_i^2 + 2V e_x \qquad (5.43)$$

Thus if the original two values of $F_l(k_i x)$ at $x = 0$ and $x = 0 + h$ are known, using the Numerov's formula (5.41), the value of $F_l(k_i x)$ at $x = x_A$ can be computed. For $x > x_A$, the potential $V(x)$ can be neglected. At such distances, the differential equation being solved is simply Bessel's equation with the solutions $F_l(k_i x) \underset{x\to\infty}{\sim} k_i x \; [A_l(k_i)\, j_l(k_i x) - B_l(k_i)\, n_l(k_i x)]$

$$(5.44)$$

At $x = x_A$, our algorahtm for solving the radial equation (5.42) using Numerou method repetitively out from the origin to $x = x_A$ yields number for $F_l(x_A)$ and $\frac{dF_l}{dx}/x_A$. The functions $j_l(k_i x)$ and $n_l(k_i x_A)$ can be obtained, for example from tables. Therefore, the unknown coefficients $A_l(k_i)$ and $B_l(k_i)$ of (5.44) can be obtained from the pair of equations

$$\frac{F_l(x_A)}{k_i x_A} = A_l(k_i)\; j_l(k_i x_A) - B_l(k_i)\; n_l(k_i x_A)$$

$$\left[\frac{d}{dx} \left(\frac{F_l}{k_i x} \right) \right]_{x_A} = A_l(k_i) \left[\frac{dj_l}{dx} \right]_{x_A} - B_l(k_i) \left[\frac{dn_l}{dx} \right]_{x_A} \qquad (5.45)$$

for each value of the energy k_i^2. The phase shift is given by

$$\tan \delta_l (k_i) = \frac{B_l(k_i)}{A_l(k_i)} \qquad (5.46)$$

Thus it is obvious that if the two initial values of the solution $F_l(k_ix)$ of (5.42) are known, the phase shift for different l values for corresponding energies can be computed, using (5.46) through the procedure disscussed above. Hence the remaining task is the computation of these initial values. For starting the solution, we assume that at small values of x it is possible to expand the solution in an ascending power series in x.

$$F_l(k_ix) = \sum_{n=0}^{\infty} a_n x^{n+\sigma} \qquad (5.47)$$

Substitution of this in (5.42) yields $F_l(k_ix)$ x^{l+1}, since it is regular at the origin and we want physically significant solutions (i.e. no infinite probabilities). Hence, the physical solution demands that at the origin, $F_l(0) = 0$.

If the numerical integration is begun at x=0, for $l > 1$ then $F_l(k_ix)$ and $\frac{dF_l}{dx}$ are zeros and we get the trival solution $F_l(x) = 0$ for all x. However, if we step a very small increment h away from the origin, then F_l and its derivative can be computed from the first few terms of their series expansion (5.47).

Hence $F_l(k_i x) = \sum_{n=0}^{3} a_n h^{n+l+1}$.

5.3 CALCULATIONS

The real analysis of any theoretical formulation should be its application to the practical problem. Now we apply this formulation to the elastic scattering of electrons by hydrogen atom. The ground state wave function for the hydrogen atom can be written as

$$\phi^{H}_{1s}(\underline{r}_1) = (\pi)^{-1/2} \exp(-r) \qquad (5.48)$$

Using (5.36) we will get X_{st} as

$$X_{st} = - \int_{-\infty}^{\infty} V_{st} \, dz$$

$$= 2 \sum_{j=1}^{3} k_o (b \lambda_j) \gamma_j \qquad (5.49)$$

For the polarisation potential given in (5.28) we have used $\alpha = 4.552$ and $\beta_i = .465$.

For the calculation of X_{abs}, the interaction potential taken is

$$V = - \frac{1}{r_o} + \frac{1}{|\underline{r}_o - \underline{r}_1|} \qquad (5.50)$$

Hence $\bar{V}(\underline{p} + pz\,\hat{y}, - - - - \underline{r}_N) = \frac{1(e^{i\underline{p}\cdot\underline{b}_1} e^{ipz\cdot z_1} - 1)}{2\pi^2 (p^2 + pz^2)}$

$$(5.51)$$

Substituting (5.51) in (5.33) and carrying out the integration we will get

$$\frac{1}{2} X_{st}^{2} + X_{abs} = \frac{1}{2k_i} \langle 0 \,|[e^{i\beta_i z_1} 2K_o(\beta_i|\underline{b}_1-\underline{b}|) -2K_o(\beta_i b) + 2 e^{-i\beta_i z_1} K_o(\beta_i|\underline{b}_1-\underline{b}|) - \frac{i}{k_i} K_o(\beta_i b) -2K_o(\beta_i b) + 2 e^{-i\beta_i z_1} K_o(\beta_i|\underline{b}_1-\underline{b}|) \;]|0\rangle \qquad (5.52)$$

Substituting the value of wave function from (5.39) and carrying out the integration we will get,

$$X_{abs} = X - \frac{1}{2} X_{st}^{2} , \qquad (5.53)$$

where $$X = \frac{1}{2k_i} \Big[- \frac{4}{\pi} \left(- \frac{\partial}{\partial\lambda} \right) \frac{K_o(\beta_i b)}{\lambda^2} K_o(\beta_i b) - K_o(b\sqrt{\lambda^2+\beta_i^{2}}) + 16 \left(- \frac{\partial}{\partial\lambda}\right) \frac{1}{(\lambda^2-\beta_i^{2})} k_o(\beta_i b) - K_o(\lambda b) + 4 (K_o(\beta_i b))^{2} \Big] \qquad (5.54)$$

with $\lambda = 2$

X_{abs} for helium atom also can be find out in the same way as that of hydrogen. Using Hyllerass wave function,

$$\phi(\underline{r}_1 , \underline{r}_2) = \frac{y^3}{\pi} \exp \left(- y(r_1 + r_2) \right) \qquad (5.55)$$

with $y = 1.69$ we will get the expression as

$$\begin{aligned} X^{He}_{abs} = \frac{y^6}{k_i} \Big[& - \frac{4}{\pi} \left(- \frac{\partial}{\partial y} \right) \frac{K_o(\beta_i b)}{y^2} \quad K_o(\beta_i b) \\ & - K_o\left(b \sqrt{y^2 + \beta_i^2} \right) + 16 \Big\{ \left(- \frac{\partial}{\partial y} \right) \\ & \frac{1}{(y^2 - \beta_i^2)} \left(K_o(\beta_i b) - k_o(yb) \right) \\ & + 4 \quad K_o(\beta_i b) \Big\}^2 + 16 \Big\{ \left(- \frac{\partial}{\partial y} \right) \frac{1}{(y^2 - \beta_i^2)} \\ & \left(K_o(\beta_i b) - K_o(yb) \right) \Big\}^2 \Big] - 2 \left(\sum_{i=1}^{5} \gamma_i K_o(\lambda_i b) \right) \end{aligned}$$

(5.56)

The values of γ_i - s and λ_i- s are given in 3rd Chapter.

From X_{abs} we can find out V_{abs} using the formula

$$V_{abs} = \frac{1}{\pi} \int_r^{\infty} (b^2 - r^2)^{1/2} \frac{d}{db} (X_{abs}) \, db \qquad (5.57)$$

we have solved the above integration numerically.

Thus having the optical potential (5.38), (5.49) and (5.58), the radial equation (1.59) is solved numerically by Numerov method for the first M values of the angular momentum number l and scattering matrix S_l for the first M values are obtained. The scattering amplitude is obtained from the following relation,

$$f(\theta) = \frac{1}{2ik_i} \sum_{l=0}^{M} (2l + 1)(S_l - 1)\; P_l(\mathrm{Cos}\theta) + f^B(\theta) - \frac{1}{k_i} \sum_{l=0}^{M} (2l + 1)\, \delta_l^B\, P_l(\mathrm{Cos}\theta) \tag{5.58}$$

where δ_l^B represents the phase shifts due to the static, polarisation and absorption potentials in the first Born approximation. $f^B(\theta)$ is the scattering amplitude in the first Born approximation due to the above mentioned potentials. Here M is an integer and S_l is related to the exact phase shift δ_l as $S_l = e^{2i\delta_l}$. Since the determination of S_l matrix takes a good amount of computer time and also the contribution of S_l for higher values of l is very small, we have calculated S_l matrix upto $l = 15$. The Born phase shifts can be obtained from the relation.

$$\delta_l^B = -2 k_i \int_0^\infty dr\, r^2\, V(r)\, [\, j_l(k_i r)\,]^2 \qquad (5.59)$$

Hence the phase shift for V_{st} is obtained as

$$= \frac{1}{k_i} \sum_{j=1}^{3} \gamma_j\, Q_l \left(\frac{\lambda_j + 2k_i^2}{2k_i^2} \right) \qquad (5.60)$$

where Q_l represents the defined polynomials tabulated as

$$\begin{aligned} Q_0(x) &= \frac{1}{2} \ln \left(\frac{1+x}{1-x} \right) \\ Q_1(x) &= \frac{x}{2} \ln \left(\frac{1+x}{1-x} \right) - 1 \end{aligned} \qquad (5.61)$$

$$(n+1)\, Q_{n+1} = (2n+1) x \left(Q_n - n\, Q_{n-1} \right) \qquad (5.62)$$

Following Deo Raj (1981), we have calculated the phase shifts for polarisation from the semiclassical expression given by LaBahn and Callaway (1969). The relation is

$$\delta_l^{pol} = -\frac{1}{k_i} \int_{r_0}^{\infty} \frac{r\, V_{pol}(r)\, dr}{(r^2 - r_0^2)^{1/2}}\,, \qquad (5.63)$$

with $r_0 = (l + 0.5) \,|\, k_i$

Thus the semiclassical phase shifts are given by the analytical expression

$$= \frac{\pi}{8k_i} \left[\frac{\alpha}{c^3} - \frac{3\alpha d^2}{4c^5} \right] \qquad (5.64)$$

with $c = r_o^2 + d^2$

The phase shifts for absorption are found to be

$$\delta_l^{abs} = X_{abs}/2 \tag{5.65}$$

The first Born amplitude for absorption is

$$f_{abs} = -\frac{1}{2\pi} \int e^{i\underline{q}\cdot\underline{r}} V_{abs}\, dv \tag{5.66}$$

This we have done numerically.

The exchange amplitude is calculated using the formula

$$f_{ex} = -\frac{1}{2k_i} \sum_{p=0}^{15} (2l+1)(S_l - 1) P_l(\mathrm{Cos}\theta)$$

$$- f_{B1}^{ex} - \frac{1}{k_i} \sum_{l=0}^{15} \delta_l^{ex} P_l(\mathrm{Cos}\theta) \tag{5.67}$$

where $$\delta_l^{ex} = -2k_i \int_0^{\infty} dr\, V_{ex} \left[j_l(k_i r) \right]^2 \tag{5.68}$$

and $$f_{B1}^{ex} = -\frac{1}{q} \int_0^{\infty} dr\, r\, \mathrm{Sin}(qr)\, V_{ex} \tag{5.69}$$

We have done the above integrations numerically.

Thus having the scattering amplitude $f(\theta)$ from (5.59) the differential cross sections are obtained from the relation.

$$f^H(\theta) = \frac{1}{4} \left| f(\theta) + f_{ex} \right|^2 + \frac{3}{4} \left| f(\theta) - f_{ex} \right|^2$$

5.4 RESULTS AND DISCUSSION

The values of exact phase shifts for the elastic scattering of electrons from hydrogen atom are tabulated in tables (5.1) and (5.2). For the purpose of checking the computer programme set up in the present study for the evaluation of the Born and the exact phase~~s~~ shifts for a potential, both the phase shifts were evaluated for the Yukawa type of potential. The results obtained for different l values ranging from 0 to 10 are shown in table (5.3). It may be noted that for higher values of l both the phase shifts approach each other.

In table (5.4) and (5.5) the present results are given at certain sample energies 50 eV and 100 eV. Since the summation of the partial waves requires the evaluation of the phase shifts in two ways, comparison of the values etc it takes more computer time and hence the present studies were carried out only at certain energies, at which quite a lot of data is available for comparison. Since the motivation behind our study is to calculate the absorption potential using HHOB approximation and finding out the DCS including that also, two data will be sufficient to compare the present results with other data. However the present work can be carried out for other energies also if required without much difficulty.

In Table (5.4) we have compared our results for 50 eV with the results of EBS , MG, PI (Kusum Lata 1984) and the experimental results of Williams (1975). We can see that the present results are slightly higher than the experimental results in the whole angular region. EBS results increases our results up to 20°. After that EBS results are lower than our present results. PI results are lower than our results in the whole angular region. Same is the case of MG. But the differences between the various results are found to be less than 10 %. We can see from the Table (5.4) that other theoretical values are less than the experimental values except small angles. But our results are higher may be due to the fact we have included the absorption potential for the present calculation .

In Table (5.5) we have compared the present results for 100 eV with the other theoretical and experimental results. Here also we can see that present results are quite comparable with the experimental results in the whole angular region. Our results are higher than the EBS results from 10° onwards. The MG and PI results are also slightly lower than our present calculations.

Thus from the above presented results and discussion, we can conclude that the inclusion of absorption potential for the calculation of DCS in the partial wave analysis method is justified.

Table : 5.1 : The values of the exact phase shifts for elastic scattering of electrons by hydrogen atom. E = 50 eV.

l	δ_l^{st}	δ_l^{pol}	δ_l^{abs}
0	0.7079	0.6716(-1)	0.1563(-1)
1	0.2192	0.7358(-1)	0.1715(-1)
2	0.7584(-1)	0.6245(-1)	0.1796(-1)
3	0.2774(-1)	0.4602(-1)	0.1803(-1)
4	0.1037(-1)	0.3222(-1)	0.1654(-1)
5	0.3935(-2)	0.2231(-1)	0.1485(-1)
6	0.1476(-2)	0.1575(-1)	0.1252(-1)
7	0.5632(-3)	0.1124(-1)	0.1075(-1)
8	0.2144(-3)	0.8346(-2)	0.8729(-2)
9	0.1476(-3)	0.6180(-2)	0.7468(-2)
10	0.6434(-4)	0.4841(-2)	0.5983(-2)
11	0.3841(-4)	0.3825(-2)	0.5193(-2)
12	0.1424(-4)	0.3151(-2)	0.4151(-2)
13	0.7097(-5)	0.2962(-2)	0.3662(-2)
14	0.3667(-5)	0.1135(-2)	0.2959(-2)
15	0.1437(-5)	0.1017(-2)	0.2101(-2)

Table : 5.2 : The values of exact the phase shifts.

E = 100 eV.

l	δ_l^{st}	δ_l^{pol}	δ_l^{abs}
0	0.6024	-0.1269	0.1504
1	0.2458	0.7087(-1)	0.4588(-1)
2	0.1125	0.2795(-1)	0.6941(-2)
3	0.5378(-1)	0.1858(-1)	0.9370(-2)
4	0.2602(-1)	0.1459(-1)	0.6555(-2)
5	0.1295(-1)	0.1103(-1)	0.7868(-2)
6	0.6458(-2)	0.1286(-1)	0.7247(-2)
7	0.3195(-2)	0.5166(-2)	0.3645(-2)
8	0.1582(-2)	0.1036(-2)	0.3145(-2)
9	0.8136(-3)	0.6351(-3)	0.1635(-2)
10	0.3656(-3)	0.2188(-3)	0.1393(-2)
11	0.2045(-3)	0.7154(-4)	0.1298(-2)
12	0.1021(-3)	0.6021(-4)	0.1117(-2)
13	0.2093(-4)	0.2102(-4)	0.1012(-2)
14	0.3277(-4)	0.4947(-4)	0.0925(-2)
15	0.2925(-4)	0.2562(-4)	0.0853(-2)

Table : 5.3 : Phase shift analysis for the Yukawa potential $-\frac{e^{-r}}{r}$ for the wave number 5.

	Born phase shift	Exact phase shift
0	0.2308	0.2384
1	0.1354	0.1383
2	9.1739(-2)	9.2820(-2)
3	6.5710(-2)	6.6315(-2)
4	4.8488(-2)	4.8843(-2)
5	3.6456(-2)	3.6629(-2)
6	2.7766(-2)	2.7618(-2)
7	2.1348(-2)	2.1254(-2)
8	1.6533(-2)	1.6498(-2)
9	1.2878(-2)	1.2776(-2)
10	1.0078(-2)	1.0076(-2)

Table : 5.4 : The differential cross section ($a_o^2 \ s_r^{-1}$) for the elastic scattering of electrons by the hydrogen atom.

E = 50 eV

Angle	Present	EBS	MG	PI	Williams
5	8.2406	9.43	8.81	5.91	-
10	5.5903	6.20	5.62	4.11	5.04
15	3.5855	3.95	3.60	2.82	3.18
20	2.2386	2.55	2.34	1.95	2.17
30	8.5163(-1)	1.14	1.10	9.97(-1)	1.12
40	5.4870(-1)	5.76(-1)	5.82(-1)	5.46(-1)	5.51(-1)
50	3.4959(-1)	3.21(-1)	3.33(-1)	3.16(-1)	3.08(-1)
60	2.1115(-1)	1.93(-1)	2.02(-1)	1.92(-1)	2.05(-1)
70	1.6086(-1)	1.26(-1)	1.29(-1)	1.22(-1)	1.46(-1)
80	8.5724(-2)	8.71(-2)	8.60(-2)	8.22(-2)	9.93(-2)
90	6.3867(-2)	6.43(-2)	6.00(-2)	5.79(-2)	7.16(-2)
100	5.2746(-2)	5.01(-2)	4.38(-2)	4.29(-2)	5.58(-2)
110	4.5856(-2)	4.09(-2)	3.33(-2)	3.32(-2)	4.21(-2)
120	3.9494(-2)	3.47(-2)	2.64(-2)	2.69(-2)	3.49(-2)

Table : 5.5 : The differential cross sections ($a_o^2\ s_r^{-1}$) for the elastic scattering of the electrons by the hydrogen atom. E = 100 eV.

Angle	Present	EBS	MG	PI	Williams
5	4.0538	4.54	4.34	3.51	
10	2.7906	2.41	2.28	2.00	
20	1.0753	8.86(-1)	8.63(-1)	8.21(-1)	1.10
30	4.3407(-1)	3.96(-1)	3.95(-1)	3.85(-1)	5.09(-1)
40	2.3730(-1)	1.94(-1)	1.95(-1)	1.91(-1)	2.88(-1)
50	1.4429(-1)	1.04(-1)	1.03(-1)	1.01(-1)	1.32(-1)
60	7.3374(-2)	6.03(-2)	5.83(-2)	5.77(-2)	7.22(-2)
70	4.3427(-2)	3.80(-2)	3.54(-2)	3.54(-2)	4.91(-2)
80	2.7055(-2)	2.57(-2)	2.30(-2)	2.33(-2)	2.95(-2)
90	2.0508(-2)	1.86(-2)	1.58(-2)	1.63(-2)	2.09(-2)
100	1.7275(-2)	1.42(-2)	1.15(-2)	1.21(-2)	1.55(-2)
110	1.1125(-2)	1.13(-2)	8.78(-3)	9.41(-3)	1.15(-2)
120	9.7137(-3)	9.42(-3)	7.01(-3)	7.66(-3)	9.20(-3)

FIG: 5.1

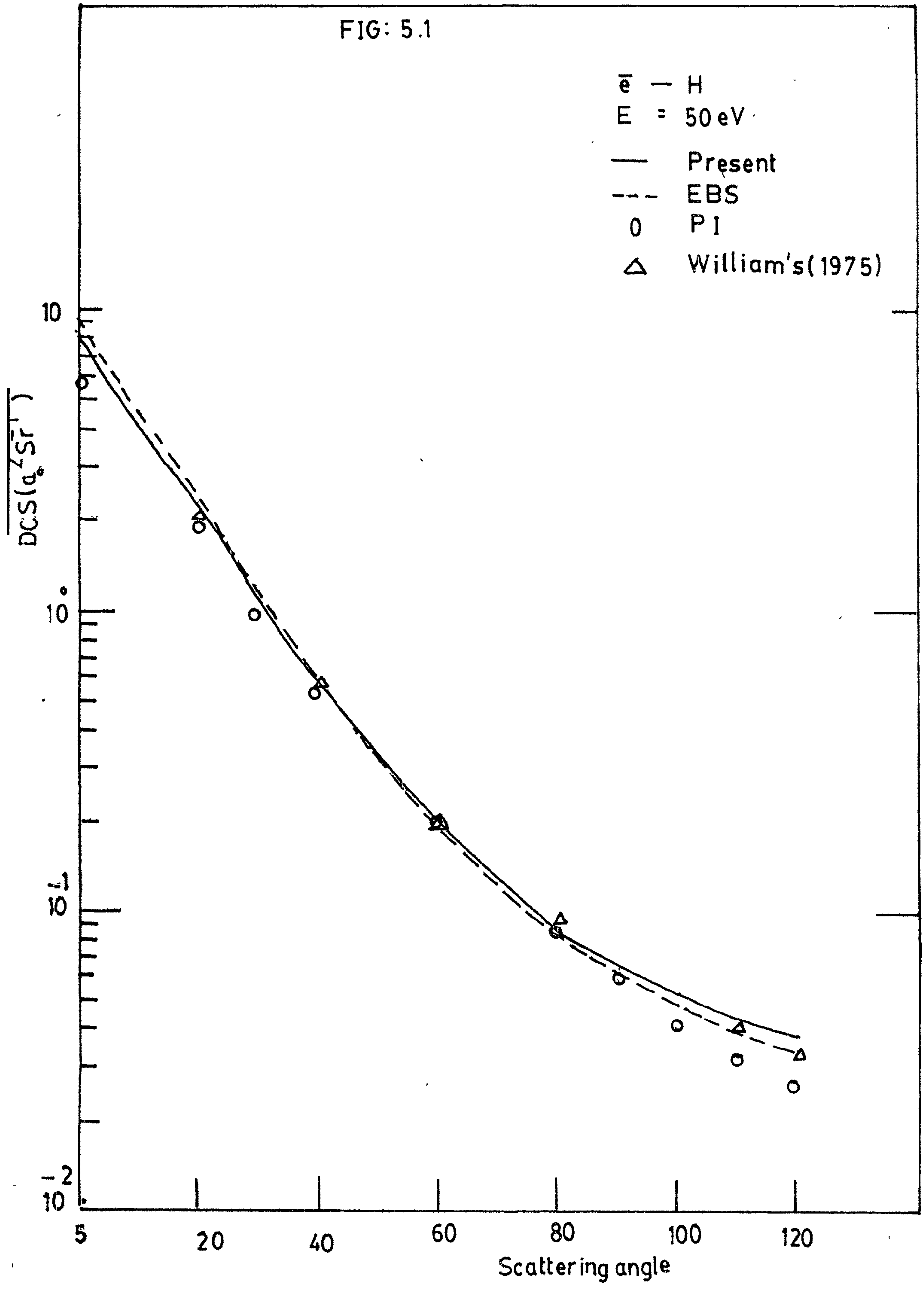
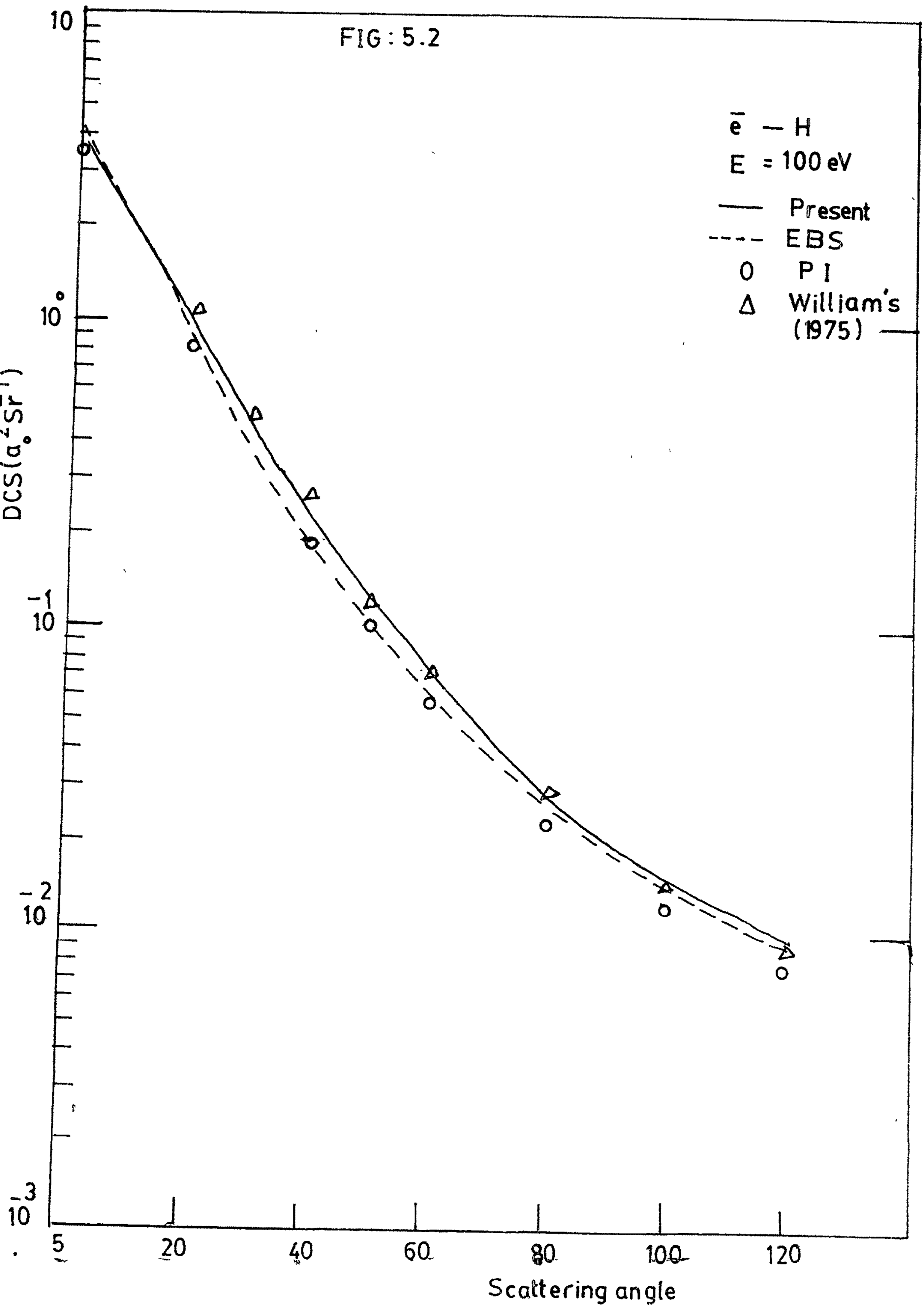

$\bar{e}$ — H
E = 50 eV
Present
EBS
0 PI
△ William's (1975)
$DCS(a_0^2 Sr^{-1})$
10
10^0
10^{-1}
10^{-2}
5
20
40
60
80
100
120
Scattering angle

FIG: 5.2


$\bar{e}$ — H
E = 100 eV
Present
EBS
O PI
Δ William's (1975)
DCS$(a_0^2 Sr^{-1})$
10
10^0
10^{-1}
10^{-2}
10^{-3}
5
20
40
60
80
100
120
Scattering angle

but depend on energy in this method. In HII method the parameters are calculated by making the difference between output and input scattering amplitudes equal to zero. In both the methods the terms up to the order k_i^2 are retained in the expression for scattering amplitude. In HI method only one parameter'a' is needed. The third Born term is replaced by the third Glauber term. The exchange effects are included through ochkur exchange scattering amplitude . In ωI method and ωII method $\frac{1}{k_i^2}$ term of real part of HI and HII methods are replaced by the corresponding Wallace term. In the third chapter we have applied HI, HII, ωI, and ωII methods to calculate the elastic scattering of electrons by hydrogen, helium and lithium atoms for energies varying from 100 eV to 400 ev. The following conclusions are drawn from these results.

1. The technique used for the partial inclusion of higher order Born terms is computationally simple and gives good results.

2. The comparison of results in HI and ωI shows that at large angles ωI yields better agreement with experiments.

3. The comparison of the results in HI and HII methods HII method is in better agreement with the experimental results.

4- The total elastic cross sections using Cox and Bonham static potential also show better agreement with the experimental results. Hence this method can be extend to other atoms also.

In the fourth chapter modifications to the HHOB approximation were attempted. Wallace(1973) has improved the eikonal method by applying a trajectory correction in the Green's function and carried out further analysis of the perturbation series. The similarity between the modes of expansion of the Green's function in the eikonal and HHOB approximations gives much scope for similar attempt in the HHOB approximation also. The HHOB analysis was carried out after incorporating the correction in Green's function and scattering amplitude is derived accordingly. The $\frac{1}{k_i^2}$ term in the HHOB real term is not present in the new real term. Instead second Wallace term is present in the new calculation. The real O $(\frac{1}{k_i})$ and imaginary terms of the present calculations are different from the HHOB terms by $(1 + \lambda)$ and $(1 - \lambda)$ respectively.

The Wallace corrected HHOB amplitude is applied to study the elastic scattering of electrons by hydrogen, helium and lithium atoms in chapter IV. A comparison of DCS and TCS results reveals the

1. The present results shows better agreement with the experimental results than the HHOB results in small angle region.

2. The second Wallace term is smaller than the $\frac{1}{k_i^2}$ real term in HHOB approximation. Hence the DCS obtained by the present method is lower than that due to HHOB approximation.

3. The total cross section for hydrogen atom shows better agreement with experimental results than simple HHOB .

4. The present method can be extend to other atoms also.

In the fifth chapter the elastic scattering of electrons by hydrogen atom is found out using optical potential method. In the optical potential method many body collisional problem is reduced to one body problem in which the effects of the rest of the particles is included through an equivalent potential known as optical potential. This optical potential is generally complex non spherical an non local. It consists of static, exchange ,polarisation and absorption potential . The absorption and polarisation potentials are formulated using the HHOB approximation. The second order polarisation effects are included through an energy dependent and spherically symmetric polarisation. This polarisation potential contains a cut off parameter r_0 which removes the divergency of the potential at the origin. The static potential given here is the static potential given by Cox and Bonham (1967). The exchange potential given here is the one given by Vanderpoorten (1975). With this optical potential the radial differential equations for elastic $\bar{e}$ - H scattering have been solved numerically using Numerov method to obtain scattering matrices S_l for first few partial waves. The contribution of higher order partial waves included through the Born phase shifts. With these scattering matrices S_l and Born phase shifts, the DCS for elastic $\bar{e}$ - H scattering is calculated for 50 eV and 100 eV. The following conclusions can be drawn.

1. The absorption and polarisation potentials formulated in the HHOB approximation is used for the calculation of DCS for elastic $\bar{e}$ - H scattering to test the correctness of these potentials. The absorption potential has a significant effect on DCS.

2. The results for DCS are in good agreement with the experimental data of Williams .

3. The present method can be extend to other atoms also without much difficulty when compared to the application to hydrogen atom.