CHAPTER - IV

MODIFICATIONS TO BORN AND EIKONAL APPROXIMATIONS

4.1 Introduction :

In spite of a huge variety of theoretical approximations with respect to the study of electron scattering by atoms, it is rather strange that none of them explain equally successfully all the observed phenomena in scattering problems. Hence, the theoretical physicist resorts to a particular method which applies best to the problem under consideration. With the introduction of certain modifications, the range of applicability of the method can be widened. In certain cases, it is even found that simple modifications in a particular approximation improve the results tremendously. It may happen the other way round also - i.e. certain highly sophisticated calculations come out with poorer results than those of simpler approximations. In such cases, there might me some conspiracy of cancellation amongst the effects neglected by these simpler approximations. There is lot of scope for the modifications of some of the commonly used approximations such that their validity criteria are relaxed resulting in a wider range of applicability of the method. In the previous chapter, an improvement over the conventional Glauber method was proposed with the name of "MEGS method" - and was successfully applied to a variety of scattering phenomena. In the present chapter, another giant pillar in the field of the-oretical approximations - the Born approximation - is taken up and various methods of its improvement are studied in detail.

The modified Born approximation - resulting from a simple modification over the conventional Born method - is rather outstanding for its simplicity. Proposed by Junker in 1975, it was later on applied to the scattering problems concerned with simple atoms like H and He (Gupta and Mathur 1978, a, b, 1979). Recently, Kaushik et al (1982) have pointed out that the MBA completely fails to explain the scattering of electrons from complex atoms like C and O. Hence it was desirable to test the applicability of this method to some more of the scattering problems in a bid to understand its failure for heavier atoms, while the results were quite satisfactory for the simpler atoms. Keeping this in mind, the MBA was applied to two different scattering phenomena - elastic scattering (2S - 2S transition) in hydrogen and alkali scattering (electron-Lithium elastic scattering). The formulation of these studies and a detailed discussion of the results obtained constitute the first part of the current chapter.

The HHOB approximation proposed by Yates in 1979 has several attractive features. To point out a few, the expressions are obtainable in the closed form thus avoiding complex, numerical procedures, the problem of divergent integrals (like those in GES) is absent and the method as such is simple and computationally feasible. But the irony of the situation is that this systematic method, when applied to electron-atom scattering, results in spuriously large values of the DCS in the large angle region (Rao and Desai 1981, 83). Hence, it was desirable to try certain modifications on this approximation such that better results can be expected out of the application of the improved methods. The success of the two independent attempts - the Wallace correction (Wallace 1973) and the two potential formulation (Ishihara and Chen 1975) - to improve upon the Glauber method worked as a boost to the attempt of parallel modifications of the Born method. With the aim of having a deeper knowledge about the two - potential eikonal approximation such that a parallel treatment can be given to the Born approximation, few more scattering problems were studied in the two - potential eikonal approximation. Inspired by the success of these studies, two ways of improving upon the HHOB method were tried - Wallace type of trajectory correction in HHOB and two - potential formulation in HHOB. The two methods were formulated and independently applied to scattering problems.

Thus the high lights of this chapter are

(1) the study of ESEH process in the modified Born approximation (including polarisation and exchange).

(2) Study of ELi process in the MBA.

(3) Study of ESEH process in the two - potential eikonal approximation.

(4) Formulation of two-potential HHOB approximation (TPHB).

(5) Study of ESGH process in TPHB.

(6) Study of EHe process in TPHB.

(7) Wallace type of trajectory correction to HHOB and application to ESGH process.

Now, let us take up the above problems one by one.

4.2 The Modified Born Approximation (MBA) :

Amongst the first order theories used to study the scattering of electrons from atoms, the first Born approximation (FBA) is known to be inadequate in the intermediate energy regime. Attempts to improve the FBA by including the second-order effects have been made by Jhanwar et al (1975). Around the same time, Junker (1975) proposed a modification of the Born model for the study of the inelastic scattering which, while retaining the simplicity of the Born approach gives much better agreement of the theoretical calculations with the experimental data. The modification of Junker consists in taking the incident wave to be distorted instead of undistorted incident plane wave in the Born approximation. The distortion of the incident plane wave, which is represented by a Coulomb wave is produced by assuming an effective nuclear charge ζ at the nucleus. A similar procedure was used by Geltman and Hidalgo (1971 a, b, 1974) Geltman (1976) and Stauffer and Morgan (1975). An extension of the Born and the Coulomb-Born model, the distorted wave polarised-orbital approximation, has also been used successfully in electron-atom scattering by Mc Dowell et al (1973, 74, 75a, b).

Later on, Gupta and Mathur (1978) studied the ESGH process using the method of Junker. They included the effects of exchange and polarisation-corresponding to a Coulomb-projected Born-polarisation approach. Later on, this method was used successfully to study the electron-scattering from He. The results were found to be satisfactory in view of the simplicity of the method. The study of Kaushik et al (1982) on the electron scattering by complex atoms using the MBA revealed that the MBA completely fails in the case of those atoms. Hence, it was desirable to carry out work on some more scattering problems and explore the reasons of the above-mentioned failure of the MBA. Thus, in this chapter the 2S-2S scattering in Hydrogen (ESEH process) and the alkali scattering (Eli process) are taken up.

4.3 ESEH Process in the MBA :

The Hamiltonian for the electron plus hydrogen atom system is

$$H = -\frac{1}{2}\nabla_2^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} \qquad (4.1)$$

(r_1 and r_2 are the position co-ordinates of the atomic and incident electrons and ∇_1^2 and ∇_2^2 are the respective kinetic energy operators. Writing $H = H_o + V$ where H_o is the unperturbed Hamiltonian and V is the total interaction potential;

$$H_o \phi_i = E_i \phi_i, \qquad (4.2)$$

$$(H_o+V) \psi_i = E_i \psi_i \qquad (4.3)$$

In a collision in which the initial and final states of the target atom are $/ i >$ and $/ f >$, the DCS is

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} \frac{1}{4\pi^2} / < \phi_f / V / \psi_i^+ > /^2 \qquad (4.4)$$

In the first Born approximation, $\psi_i = \phi_i$, assuming that the scattering potential is weak and therefore the incident plane wave does not get distorted in the scattering region. This will be true only for high incident energies when the incident particle spends very little time in that region. For intermediate and low energies, this assumption is not valid.

Most of the contribution to the matrix element in the above DCS expression comes from the region where V is largest. Thus it is expected that a better approximation will result if, instead of replacing Ψ_i by $\emptyset_i$, one uses a scattering wave function which is closer to reality in the region which contributes most. Thus, following Junker (1975)

$$H = H_2 + W = H_o + U + W$$

where $U = -\delta/r_2, \quad W = -\frac{1-\delta}{r_2} + \frac{1}{r_{12}}$

and δ is the screening parameter. As pointed out by Junker, the breaking of H contains a certain amount of physical significance and has the advantages that the eigen functions of H_2 are known exactly and closed form expressions exist for the evaluation of the integrals needed in the calculation of the cross sections.

Assuming X_i to be the solution of the Schrodinger equation $(H_o + U)\, X_i = E_i\, X_i$ in the modified Born approximation, Ψ_i in (4.4) can be replaced by

$$\Psi_i = X_i\,(r_1, r_2) = F_o\,(r_2)\, U_o\,(r_1) \qquad (4.5)$$

Where $U_o(r_1)$ is the atomic wave function in the initial state and $F_o\,(r_2)$ is the scattered electron wave function given by

$$F_o(r_2) = \sqrt{(1-ia_i)}\ \exp\left(i\ \underline{k}_i.\underline{r}_2 + \frac{\pi a_i}{2}\right)_1 F_1(ia_i, 1,$$
$$i\ k_i r_2 - i\ \underline{k}_i.\underline{r}_2)$$

where $a_i = \delta/k_i$.

Thus (4.5) takes into account the distortion of the incident wave but ignores the effects of exchange and polarisation. Intorudcing exchange (4.5) becomes

$$\Psi_i^{\pm} = X_i(r_1, r_2) \pm X_i(r_2, r_1) \qquad ..(4.6)$$

To account for the perturbation of the target system by the incident particle, the polarised - orbital method of Temkin and Lamkin (1961) is followed. Thus including the polarisation term U_{pol} in (4.6)

$$\Psi_i^{\pm}(r_1, r_2) = F_o(r_2)\,[U_o(r_1) + U_{pol}(r_1, r_2)]$$
$$\pm F_o(r_1)\,[U_o(r_2) + U_{pol}(r_2, r_1)].$$

Ignoring the exchange polarisation term $F_o(r_1)\ U_{pol}(r_2, r_1)$

$$\Psi_i^{\pm}(r_1, r_2) = F_o(r_2)\,[U_o(r_1) + U_{pol}(r_1, r_2)]$$
$$\pm F_o(r_1)\,U_o(r_2) \qquad ..(4.7)$$

It is assumed that the neglect of the exchange polarisation term will not introduce significant errors since the polarisation of the wave-function is small at distances where exchange is most important. Using (4.7) in (4.4), the differential cross section for ESEH process will be

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2}\left[\frac{1}{4} / T^{+} /^{2} + \frac{3}{4} / T^{-} /^{2}\right] \qquad (4.8)$$

where $$T^{\pm} = \Gamma(1-i\,a_i)\,\exp\left(\frac{\pi a_i}{2}\right)\left[I_D + I_P \pm I_E\right] \qquad (4.9)$$

$$I_D = \int d\cdot r_2 \exp(i\,\underline{q}\cdot\underline{r}_2)\ {}_1F_1(ia_i, 1, i\,k_i r_2 - i\,\underline{k}_i\cdot\underline{r}_2)$$
$$< U_o(r_1)/V/U_o(r_1)> \qquad (4.10)$$

$$I_P = \int dr_2 \exp(i\,\underline{q}\cdot\underline{r}_2)\ {}_1F_1(ia_i, 1, i\,k_i r_2 - i\,\underline{k}_i\cdot\underline{r}_2)$$
$$<U_o(r_1)/V/\ U_{pol}(r_1, r_2)> \qquad (4.11)$$

$$I_E = \int dr_2 \exp\left[i\,(\underline{k}_i\cdot\underline{r}_1 - \underline{k}_f\cdot\underline{r}_2)\right]\ {}_1F_1(ia_i, 1, i\,k_i r_1 -$$
$$i\,\underline{k}_i\cdot\underline{r}_1)\ <U_o(r_1)/V/\ U_o(r_2)> \qquad (4.12)$$

Here q is the momentum transfer. Using the Ochkur (1964) procedure,

$$I_E = \frac{4\pi}{k_i^2}\int d\,r_2\, e^{i\,\underline{q}\cdot\underline{r}_2}\, U_o^{*}(r_2)\, U_o(r_2),$$
$${}_1F_1(i\,a_i,\ 1,\ i\,k_i r_2 - i\,\underline{k}_i\cdot\underline{r}_2) \qquad (4.13)$$

For the ESEH process,

$$U_o(r_1) = \frac{1}{4\sqrt{2\pi}}(2-r_1)\,e^{-r_1/2} \qquad (4.14)$$

The evaluation of U_{pol} is given in the appendix. This gives

$$U_{pol} = \frac{1}{4\sqrt{2\pi}}\ \frac{\mathrm{Cos}\,\theta}{r_2^2}\ \frac{1}{5r_1}\left(2r_1^4 - \frac{r_1^5}{3}\right) e^{-r_1/2}\,\epsilon(r_1, r_2) \qquad (4.15)$$

$$\epsilon = \begin{cases} 1, & r_2 > r_1 \\ 0 & r_1 > r_2\,. \end{cases}$$

θ is the angle between r_1 and r_2. To evaluate the integrals, the standard integral of Nordseick (1954) is followed. This gives

$$I(\lambda) = \int dv \, \frac{e^{-\lambda r}}{r} \, e^{i \underline{q} \cdot \underline{r}} \, {}_1F_1 \, (i \, a_i, \, 1, \, i \, k_i r - i \, \underline{k}_i \cdot \underline{r} \,)$$

$$= \frac{4\pi \, e^{-\pi a_i}}{(q^2 + \lambda^2)} \left(\frac{q^2 + \lambda^2}{2 i \lambda k_i - \lambda^2} \right)^{i a_i} \qquad (4.16)$$

In the evaluation of I_p, the following simplification is used:

$$1 - e^{-\pounds r_2} \left(1 + \pounds r_2 + \frac{\pounds^2 r_2^2}{2!} + \cdots\cdots \frac{\pounds^n r_2^n}{n!} \right.$$

$$= e^{-\pounds r_2} \sum_{m=n+1}^{\infty} \frac{\pounds^m r_2^m}{m!} \qquad (4.17)$$

Using this, all the integrals can be written in the form of λ-derivatives of $I(\lambda)$, thus avoiding the numerical methods and saving computer time. To check the procedure the calculations of Gupta and Mathur (1978) were repeated. It was found that three terms in the infinite series given above (4.17) are sufficient to give exactly the same results as reported by Gupta and Mathur using complicated numerical procedures (Table 4.1a).

In the evaluation of the parameter δ, the procedure of Junker was followed. First, the value of r_2 was found out for which

$$r_2^2 \int_0^\infty \int_0^\pi \int_0^{2\pi} U_o^*(r_1)\, V(r_1, r_2)\, U_o(r_1)\, r_1^2\, dr_1 \sin\theta_1\, d\theta_1\, d\phi_1$$

is maximum.

Now,

$$\delta = z - \int_0^{r_2} \int_0^\pi \int_0^{2\pi} U_o^*(r_1)\, U_o(r_1)\, r_1^2\, dr_1 \sin\theta_1\, d\theta_1\, d\phi_1 \qquad (4.18)$$

For the ESEH process, $z=1$

and δ was found to be equal to 0.93, corresponding to the value $r_2 = 2.8$.

Evaluation of I_D, I_P and I_E :

As mentioned earlier I_D, I_P and I_E were evaluated using the standard integral. This is possible if $< U_o /V/ U_o >$, $< U_o /V/ U_{pol} >$ and $U_o^*\ U_o$ can be represented in the form of $\frac{e^{-\lambda r_2}}{r_2}$ or $\frac{d^n\, e^{-\lambda r_2}}{d\lambda^n}$

(refer 4.10, 4.11, 4.13 and 4.16).

$$\text{Here}\quad V = -\frac{1}{r_2} + \frac{1}{r_{12}} \qquad (4.19)$$

and U_o and U_{pol} are given by (4.14) and (4.15).

$$\therefore < U_o(r_1) / V / U_o(r_1) > = \int dv_1 [A r_1 e^{-y_1 r_1} + B e^{-y_2 r_1}]^2 \left[-\frac{1}{r_2} + \frac{1}{r_{12}} \right] \qquad (4.20)$$

where $A = -\frac{1}{4\sqrt{2\pi}}$, $B = \frac{2}{4\sqrt{2\pi}}$

$Y_1 = 0.5 \quad Y_2 = 0.5$

Now $(Ar_1 e^{-y_1 r_1} + Be^{-y_2 r_1})^2 = C_1 e^{-\mathcal{L}_1 r_1} + C_2 \frac{de^{-\mathcal{L}_2 r_1}}{d\mathcal{L}_2}$

$$+ C_3 \frac{d^2}{d\mathcal{L}_3^2} e^{-\mathcal{L}_3 r_1} \qquad (4.21)$$

where $C_1 = B^2 \qquad \mathcal{L}_1 = 2Y_2$

$C_2 = -2AB \qquad \mathcal{L}_2 = y_1 + Y_2$

$C_3 = A^2 \qquad \mathcal{L}_3 = 2y_1$

Also, following Joachain (page 543)

$$\frac{1}{r_{12}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{(2l+1)} \frac{r_<^{l}}{r_>^{l+1}} Y_{lm} Y^*_{lm}$$

$$= 4\pi \frac{1}{r_>} \frac{1}{4\pi} \quad (\because \text{ Only } l = 0 \text{ term survives})$$

$$= \frac{1}{r_>} \qquad (4.22)$$

Using (4.21) and (4.22) in (4.20),

$$< U_o / V / U_o > = 4\pi \int_0^{\infty} r_1^2 \, dr_1 [C_1 e^{-\mathcal{L}_1 r_1} + C_2 \frac{d}{d\mathcal{L}_2} e^{-\mathcal{L}_2 r_1}$$

$$+ C_3 \frac{d^2}{d\mathcal{L}_3^2} e^{-\mathcal{L}_3 r_1}] [\frac{1}{r_>} - \frac{1}{r_2}]$$

$$= 4\pi \int_{r_2}^{\infty} r_1^2 \, dr_1 (C_1 e^{-\mathcal{L}_1 r_1} + C_2 \frac{d}{d\mathcal{L}_2} e^{-\mathcal{L}_2 r_1} + C_3 \frac{d^2 e^{-\mathcal{L}_3 r_1}}{d\mathcal{L}_3^2})$$

$$[\frac{1}{r_1} - \frac{1}{r_2}]$$

The evaluation of the above expression is lengthy but straight forward, which gives

$$< U_0/V/U_0 > = -4\pi \left\{ \frac{2C_1}{\lambda_1^{3}} \frac{e^{-\lambda_1 r_2}}{r_2} - \frac{C_1}{\lambda_1^{2}} \frac{d}{d\lambda_1} \frac{e^{-\lambda_1 r_2}}{r_2} \right.$$

$$+ 2C_2 \frac{d}{d\lambda_2} \frac{1}{\lambda_2^{3}} \frac{e^{-\lambda_2 r_2}}{r_2} - C_2 \frac{d}{d\lambda_2} \frac{1}{\lambda_2^{2}} \left(\frac{d}{d\lambda_2} \frac{e^{-\lambda_2 r_2}}{r_2} \right)$$

$$\left. + 2C_3 \frac{d^2}{d\lambda_3^{2}} \frac{1}{\lambda_3^{3}} \frac{e^{-\lambda_3 r_2}}{r_2} - C_3 \frac{d^2}{d\lambda_3^{2}} \frac{1}{\lambda_3^{2}} \left(\frac{d}{d\lambda_3} \frac{e^{-\lambda_3 r_2}}{r_2} \right) \right\}$$

Now a glance at the above expression shows that it can be substituted in (4.10) to give a number of integrals of the form I (λ) (4.16) or the λ-derivatives of I (λ).

$\therefore$ substituting $< U_0/V/ U_0 >$ in (4.10),

$$I_D = \frac{-8\pi C_1}{\lambda_1^{3}} I(\lambda_1) + \frac{4\pi C_1}{\lambda_1^{2}} \frac{d}{d\lambda_1} I(\lambda_1)$$

$$+ \frac{24\pi C_2}{\lambda_2^{4}} I(\lambda_2) - \frac{16\pi C_2}{\lambda_2^{3}} \frac{d}{d\lambda_2} I(\lambda_2)$$

$$+ \frac{4\pi C_2}{\lambda_2^{2}} \frac{d^2}{d\lambda_2^{2}} I(\lambda_2) - \frac{96\pi C_3}{\lambda_3^{5}} I(\lambda_3) + \frac{72\pi C_3}{\lambda_3^{4}}$$

$$\frac{d}{d\lambda_3} I(\lambda_3) - \frac{24\pi C_3}{\lambda_3^{3}} \frac{d^2}{d\lambda_3^{2}} I(\lambda_3) + \frac{4\pi C_3}{\lambda_3^{2}} \frac{d^3}{d\lambda_3^{3}} I(\lambda_3) \qquad (4.23)$$

$$\text{Here} \quad \left. \begin{array}{llll} C_1 = B^2 & & \lambda_1 = 2Y_2 \\ C_2 = -2AB & & \lambda_2 = Y_1 + Y_2 \\ C_3 = A^2 & & \lambda_3 = 2Y_1 \end{array} \right) = 1$$

In the evaluation of I_p, the relation (4.17) is used to obtain integrals of the form I (λ).

$$< U_o /V/U_{pol} > = \int dv_1 \; (Ar_1 \, e^{-y_1 r_1} + Be^{-y_2 r_1}) \left(- \frac{1}{r_2} + \frac{1}{r_{12}}\right) U_{pol}$$

Because of the property of ϵ in U_{pol},

$$\frac{1}{r_{12}} = \frac{1}{r_2} + \frac{r_1}{r_2^{\,2}} \operatorname{Cos} \theta + - - - - -$$

$$\therefore < U_o/V/U_{pol} > = \frac{1 \times 2\pi}{20\sqrt{2\pi}\; r_2^{\,4}} \int_0^{\infty} r_1^{\,2} \, dr_1 (Ar_1 \, e^{-y_1 r_1} + Be^{-y_2 r_1})$$

$$[2r_1^{\,4} - \frac{r_1^{\,5}}{3}] \; e^{-r_1/2} \int_0^{\pi} \operatorname{Sin} \theta \operatorname{Cos}^2 \theta \, d\theta$$

$$= \frac{\sqrt{2\pi}}{30} \frac{1}{r_2^{\,4}} \int_0^{r_2} dr_1 \; [2B \; r_1^{\,6} \; e^{-\beta r_1} - \frac{B}{3} r_1^{\,7} \, e^{7-\beta r_1}$$

$$+ 2A \; r_1^{\,7} \; e^{-f r_1} - \frac{A}{3} r_1^{\,8} \; e^{-f r_1} \;]$$

where $f = y_1 + \frac{1}{2}$; $\beta = y_2 + \frac{1}{2}$;

This evaluation is also long but straight forward which gives

$$<U_o/V/U_{pol}> = \frac{\sqrt{2\pi}}{30} \frac{1}{r_2^{\,4}} \Big\{ \; 2B \frac{6!}{\beta^7} \Big[(1- \frac{7}{6 \; \beta}) - e^{-\beta r_2} \; ((1- \frac{7}{6\beta})$$

$+($ [illegible] 7 [illegible] $) \; r_2$ $+(\beta - \frac{7}{6}) \; r_2 + (\beta - \frac{7}{6}) \; \beta \frac{r_2^2}{2!} + (\beta - \frac{7}{6}) \; \frac{\beta^2 r_2^3}{3!} + (\beta - \frac{7}{6})$

$$\frac{\beta^3 r_2^{\,4}}{4!} + (\beta - \frac{7}{6}) \; \frac{\beta^4 r_2^{\,5}}{5!} + (\beta - \frac{7}{6}) \; \frac{\beta^5 r_2^6}{6!} - \frac{7}{6} \; \frac{\beta^6 r_2^7}{7!} \;)\Big] + 2A \; \frac{7!}{f^8}$$

$$\left[\left(1 - \frac{8}{6\pounds}\right) - e^{-\pounds r_2}\left(\left(1 - \frac{8}{6\pounds}\right) + \left(\pounds - \frac{8}{6}\right) r_2 + \left(\pounds - \frac{8}{6}\right) \frac{\pounds r_2^{\,2}}{2!} + \left(\pounds - \frac{8}{6}\right) \frac{\pounds^2 r_2^3}{3!} + \left(\pounds - \frac{8}{6}\right) \frac{\pounds^3 r_2^{\,4}}{4!} + \left(\pounds - \frac{8}{6}\right) \frac{\pounds^4 r_2^{\,5}}{5!} + \left(\pounds - \frac{8}{6}\right) \frac{\pounds^5 r_2^{\,6}}{6!} + \left(\pounds - \frac{8}{6}\right) \frac{\pounds^6 r_2^{\,7}}{7!} - \frac{8}{6} \frac{\pounds^7 r_2^{\,8}}{8!} \right)\right] \Bigg\} \qquad (4.24)$$

Here, (4.17) is used for the simplification of (4.24). This gives

$$\langle U_o/V/U_{pol}\rangle = \frac{\sqrt{2\pi}}{30} \frac{1}{r_2^4} \Bigg\{ 2\,B\,\frac{6!}{\beta^7} \left[e^{-\beta r_2} \sum_{n=7}^{\infty} \frac{\beta^n r_2^{\,n}}{n!} - \frac{7}{6\,\beta} e^{-\beta r_2} \sum_{n=8}^{\infty} \frac{\beta^n r_2^{\,n}}{n!} \right] + 2A \frac{7!}{\pounds^8} \left[e^{-\pounds r_2} \sum_{n=8}^{\infty} \frac{\pounds^n r_2^{\,n}}{n!} - \frac{8}{6\pounds} e^{-\pounds r_2} \sum_{n=9}^{\infty} \frac{\pounds^n r_2^{\,n}}{n!} \right] \Bigg\}$$

$$= \frac{\sqrt{2\pi}}{30} \frac{1}{r_2^{\,4}} \Bigg\{ 2B \frac{6!}{\beta^7} \left[e^{-\beta r_2} \frac{\beta^7 r_2^7}{7!} + \left(1 - \frac{7}{6\beta}\right) e^{-\beta r_2} \sum_{n=8}^{\infty} \frac{\beta^n r_2^{\,n}}{n!} \right] + 2A \frac{7!}{\pounds^8} \left[e^{-\pounds r_2} \frac{\pounds^8 r_2^{\,8}}{8!} + \left(1 - \frac{8}{6\pounds}\right) e^{-\pounds r_2} \sum_{n=9}^{\infty} \frac{\pounds^n r_2^{\,n}}{n!} \right] \Bigg\}$$

$$= \frac{2\sqrt{2\pi}}{30} \Bigg\{ \frac{B}{7}\left[\frac{d^4}{d\beta^4} - \left(1 - \frac{7}{6\beta}\right) \frac{\beta}{8} \frac{d^5}{d\beta^5} + \left(1 - \frac{7}{6\beta}\right) \frac{\beta^2}{72} \frac{d^6}{d\beta^6} + \cdot\cdot\cdot\cdot \right] \frac{e^{-\beta r_2}}{r_2} + \frac{A}{8} \left[- \frac{d^5}{d\pounds^5} + \left(1 - \frac{8}{6\pounds}\right) \frac{\pounds}{9} \frac{d^6}{d\pounds^6}$$

$$- \left(1-\frac{8}{6\lambda}\right) \frac{\lambda^2}{90} \frac{d^7}{d\lambda^7} + - - - \Big] \frac{e^{-\lambda r_2}}{r_2} \Big\} \qquad .. (4.25)$$

The above expression may readily be substituted in (4.11) to get

$$I_p = 2\frac{\sqrt{2\pi}}{30} \left\{ \frac{B}{7} \left[\frac{d^4}{d\beta^4} - K_\beta \frac{\beta}{8} \frac{d^5}{d\beta^5} + K_\beta \frac{\beta^2}{72} \frac{d^6}{d\beta^6} + ---- \right] \right.$$

$$\left. I(\beta) + \frac{A}{8} \left[- \frac{d^5}{d\lambda^5} + K_\lambda \frac{\lambda}{9} \frac{d^6}{d\lambda^6} - K_\lambda \frac{\lambda^2}{90} \frac{d^7}{d\lambda^7} + --- \right] I(\lambda) \right\} \qquad .. (4.26)$$

where $K_\beta = 1 - \frac{7}{6\beta}$, $K_\lambda = 1 - \frac{8}{6\lambda}$.

Now, for the evaluation of I_E, $U_o^* U_o$ is given by (4.21). It may be still conveniently written as

$$U_o^* U_o = -C_1 \frac{d}{d\lambda_1} \frac{e^{-\lambda_1 r_1}}{r_1} - C_2 \frac{d^2}{d\lambda_2^2} \frac{e^{-\lambda_2 r_1}}{r_1} - C_3 \frac{d^3}{d\lambda_3^3} \frac{e^{-\lambda_3 r_1}}{r_1}.$$

Now I_E can be directly written as

$$I_E = \frac{-4\pi}{k_i^2} \left\{ C_1 \frac{d}{d\lambda_1} I(\lambda_1) + C_2 \frac{d^2}{d\lambda_2^2} I(\lambda_2) + C_3 \frac{d^3}{d\lambda_3^3} I(\lambda_3) \right\} \qquad (4.27)$$

Now the substitution of (4.23), (4.26) and (4.27) in (4.9) and (4.8) will give the differential cross sections for electron scattering from the excited state of H - atom (ESEH process) in the modified Born approximation (MBA).

Results and Discussion :

The DCS for the ESEH process obtained in MBA are calculated for different incident energies ranging from 100 eV to 800 eV (table 4.1b). The results are graphically exhibited and compared with other data in fig.4.1 and 4.2 at incident energies 200 eV and 400 eV at which data is available for comparison. The present results are compared with the EBS (Joachain et al 1977) and the optical model results (Joachain and Winters 1980) alongwith the most recently reported two-potential results (Pundir et al 1982) and HHOB results (Rao and Desai 1983). In the absence of enough experimental data, it is rather difficult to comment on the accuracy of the various approaches. Hence, it will be desirable to review the behaviour of all the approximations in regard of various scattering process and draw the conclusion with respect to the concerned ESEH process. The HHOB results are always found to be overestimating (Rao and Desai 1981, 83a,b) especially in the large angle region. Hence, the deviation of the present results from HHOB results is not at all discouraging. The present results closely agree with the data of Pundir et al (1982) and almost coincide with the results of optical model calculations (Joachain and Winters 1980) which has in other scattering problems, produced results agreeing well with the experimental data. In the small angle region, the present results are very near to the EBS results (Joachain et al 1977) but they are less than the EBS values at larger angles. This is encouraging situation since EBS results were, in previous studies found to be slightly over estimating in the large angle region whereas they showed nice agreement with experimental data at small angles. The satisfactory result of the application of the MBA to $\bar{e}$ -H(1S) scattering (Gupta and Mathur 1978) further enhances the evidences in favour of the present results.

In fig.4.3, the present results at 200 eV are compared with the corresponding results of $\bar{e}$ - H (1S) elastic scattering. The two DCS values are found to approach each other for larger angles where the interaction between the incident electron and the target nucleus progressively dominates the scattering. Similar type of behaviour was observed in the EBS (Joachain et al 1977) and two-potential (Pundir et al 1982) calculations as well as earlier in this thesis (MGES approximation). Since the $\bar{e}$ - H (1S) results in MBA have shown nice agreement with experimental data, we have all reasons to expect nice agreement of the present results with their experimental counterparts, especially in the large angle region.

The present results are bound to become better as the incident energy increases. In view of the simplicity of the present approach, we expect that it would provide reasonable description of the scattering process from the excited metastable states of the hydrogen atom.

4.4 Electron - Lithium elastic scattering in the Modified Born Approximation :

The motivations behind the application of MBA to Eli process are many. One is the desirability to test the applicability of MBA to higher atoms as discussed earlier. The success of the application of MBA to ESEH process is another factor. Moreover, a study of ELi process means the investigation on the first member of a class of atoms i.e. the alkali metal atoms which involve more practically applied collision processes. In the light of the scarce data available on electron alkali scattering, the extension of MBA to ELi process has enough justification. Moreover, by modelling the Li atom in the core-approximation (Walters 1973) the study of the effect of the core compared to the valence electron would also be interesting. It may be investigated as to how the collision process compares with the study of Walters. Moreover, the present method being simple, saves a lot of computer time which is definitely a covetable feature in modern atomic collision theories.

For lithium atom, the atomic field extends over a great distance-when compared to the case of H - and hence the incoming wave will be distorted even at a large distance from the nucleus. Hence the consideration of the distortion of the incident plane wave due to the target atomic field will definitely improve the model. This type of a treatment is given in MBA. Moreover, the effects of polarisation and exchange are also taken explicitly. There is enough reason to believe that part of the absorption effect will also be taken care of. This point will be discussed later on. Altogether, the MBA may be expected to give a reasonable model of $\bar{e}$ - Li scattering.

When a model is applied to electron-alkali scattering, special care should be given to the peculiar nature of this scattering. As discussed elsewhere, it cannot be assumed that methods that apply well to the study of elastic scattering by atoms with closed shells will be equally effective in dealing with alkali atoms because they have a single outer electron loosely bound in an S-orbital of large radius, have large polarizability and there exists a strong coupling between the ground and first excited states. These disparities are the least in the case of Li and increase as we go to Na, K etc. The atomic radius of Li is not very high (compared to H) and the valence electron is not very loosely bound. Hence, it may be assumed that the Lithium atom, with its core and valence electron by and large resembles the H atom. In the study of alkali atoms by walters, the Li results were reasonable whereas Na and K showed large discrepancies. Similarly, many theories which were applied to the scattering by H and He atoms, were equally successfully applied to the Li atom without any changes which account for the special nature of electron Li scattering (Eg : TPE, HHOB, EBS etc.). The present MBA being a high energy approximation like them, there is enough support for the feeling that it can also be effectively applied to the $\bar{e}$ - Li scattering.

Calculation Part :

As mentioned previously, the core-approximation of Walters (1973) is used to represent the Li atom. According to this, the Li atom consists of a core at the centre and one electron in the outer orbit. Hence, the electron target interaction can be represented as

$$V = - \frac{1}{r_2} + \frac{1}{r_{12}} + V_c (r_2) \tag{4.28}$$

where $V_c = -2 \left(\frac{1}{r_2} + 2.7 \right) e^{-5.4 r_2}$

Keeping in mind the suggestion of Mathur (1972) that the difference between the scattering parameters by using one or three electron wave function of Li atom is not very appreciable at intermediate and high energies, the one-electron wave function for the Li atom was derived following Coulson. This gives

$$U_o (r_1) = C r_1 e^{-0.65 r_1} + D e^{-2.7 r_1} \tag{4.29}$$

where C = 0.11252, D = -0.42204 so that U_o is orthogonal to the 1S orbital and is normalised. The extent of simplification which the complicated expressions - for the total interaction and the exact wave function of Li atom - have undergone is quite clear from the expressions (4.28) and (4.29) which are the approximated values for the interaction and wave function.

Now the total Hamiltonian of the electron plus target system becomes $H = H_o + U + W$ where

$$U = -\frac{\delta}{r_2}, \quad W = -\frac{1-\delta}{r_2} + \frac{1}{r_{12}} + V_c(r_2)$$

The derivation for the differential cross section for the ELi process follows in a way very similar to the ESEH process with only the above-mentioned change in the Hamiltonian. As a result, expressions (4.8) to (4.13) are obtained with V, U_o and U_{pol} being replaced by the corresponding new values. It will be convenient to represent the wave function product as

$$U_o^* \, U_o = K_1 e^{-\lambda_1 r_1} + K_2 \frac{d}{d\lambda_2} e^{-\lambda_2 r_1} + K_3 \frac{d^2}{d\lambda_3{}^2} e^{-\lambda_3 r_1} \qquad (4.30)$$

where $K_1 = D^2$ $\quad\lambda_1 = 5.4$

$K_2 = -2CD$ $\quad\lambda_2 = 3.35$

$K_3 = C^2$ $\quad\lambda_3 = 1.3$

As in the case of ESEH process, the δ for E LI process is obtained as

$$\delta = 0.98.$$

In the evaluation of U_{pol}, the H (2S) wave function has been taken as an approximation to the one-electron wave function of Lithium. This procedure simplifies the mathematical analysis in a manyfold way as will be clear from a glance at the derivation of U_{pol} for ESEH process given in the appendix. Any way, this type of an approximation will definitely not result in any serious error because the effect of polarisation is almost negligible in the case of ELi process when compared to the all important excitation effects. This will be clear from an analysis of the study of Vanderpoorten (1976). There, it is found that the optical potential results almost coincide with the Glauber results in which polarisation effects are not taken care of. This provides a clue to the fact that the contribution due to polarisation should be negligible in the case of ELi process. Moreover, it has been explicitly shown that the calculations without the real part of $V^{(2)}$ in the optical potential, which corresponds to polarisation part - gave results which differ by about 10% at small angles and 1% at 90^{o}. All these results point to the not - so - significant roll of polarisation effect in the ELi process. Hence, there is all reason to believe that slight approximation - as the replacement of one electron wave function of Li by H (2S) - wave function can amply be justified in the evaluation of the polarisation effects when the extent of simplification brought about by such an approximation is thought of. Moreover, the contribution due to the core (V_c) is also negligibly small at small angles at which polarisation is important. This fact also will be explicitely proved in a later section. Introducing this approximation also in the evaluation of U_{pol}, it can be seen that the same value as (4.15) will be obtained for U_{pol} in the ELi process in the present study. However, it should be remembered that these approximations are taken only for the evaluation of U_{pol} and that I_p will be different for ESEH and ELi processes due to the difference in U_o, V and δ for the two processes.

In the ELi process also, the standard integral of Nordseick (1954) can be used for the evaluation of I_D, I_P and I_E. To evaluate I_D, $< U_o / V / U_o >$ can be written as $< U_o / (\frac{-1}{r_2} + \frac{1}{r_{12}}) / U_o > + V_c (r_2)$ because of the property of the wavefunction. The evaluation of the first term is similar to that in ESEH process, thus giving

$$
\begin{aligned}
< U_o/V/U_o > = - 4\pi \Bigg(& \frac{2K_1}{\lambda_1^3} \frac{e^{-\lambda_1 r_2}}{r_2} - \frac{K_1}{\lambda_1^2} \frac{d}{d\lambda_1} \frac{e^{-\lambda_1 r_2}}{r_2} \\
& + 2K_2 \frac{d}{d\lambda_2} \frac{1}{\lambda_2^3} \frac{e^{-\lambda_2 r_2}}{r_2} - K_2 \frac{d}{d\lambda_2} \frac{1}{\lambda_2^2} \left(\frac{d}{d\lambda_2} \frac{e^{-\lambda_2 r_2}}{r_2} \right) \\
& + 2K_3 \frac{d^2}{d\lambda_3^2} \frac{1}{\lambda_3^3} \frac{e^{-\lambda_3 r_2}}{r_2} - K_3 \frac{d^2}{d\lambda_3^2} \frac{1}{\lambda_3^2} \frac{d}{d\lambda_3} \frac{e^{-\lambda_3 r_2}}{r_2} \Bigg) \\
& + K_4 \frac{e^{-\lambda_4 r_2}}{r_2} + K_5 \frac{d}{d\lambda_4} \frac{e^{-\lambda_4 r_2}}{r_2}
\end{aligned}
\qquad (4.31)
$$

where $K_4 = -2$, $K_5 = 5.4$ $\lambda_4 = 5.4$.

All the terms in (4.31) are such that in the evaluation of I_D (4.10) the standard integral (4.16) can be made use of.

Thus the substitution of (4.31) in (4.10) gives

$$I_D = \left[\left(K_4 - \frac{8\pi K_1}{\lambda_1^3}\right) + \left(K_5 + \frac{4\pi K_1}{\lambda_1^2}\right) \frac{d}{d\lambda_1} \right] I(\lambda_1)$$

$$+ \left[\frac{24\pi K_2}{\lambda_2^4} - \frac{16\pi K_2}{\lambda_2^3} \frac{d}{d\lambda_2} + \frac{4\pi K_2}{\lambda_2^2} \frac{d^2}{d\lambda_2^2} \right] I(\lambda_2)$$

$$+ \left[\frac{-96\pi K_3}{\lambda_3^5} + \frac{72\pi K_3}{\lambda_3^4} \frac{d}{d\lambda_3} - \frac{24\pi K_3}{\lambda_3^3} \frac{d^2}{d\lambda_3^2} + \frac{4\pi K_3}{\lambda_3^2} \frac{d^3}{d\lambda_3^3} \right]$$

$$I(\lambda_3) \quad .. \qquad .. \qquad .. \qquad (4.32)$$

In the evaluation of I_P, $< U_0 / V / U_{pol} >$ is written in such a way that the standard integral may be used here also.

$$< U_0/V/U_{pol}> = \int dv_1 \left[Cr_1 e^{-0.65r_1} + De^{-2.7r_1} \right]$$

$$\left[- \frac{1}{r_2} + \frac{1}{r_{12}} + V_c \right] U_{pol}$$

$$= \frac{1}{20\sqrt{2\pi}\, r_2^2} \int dv_1 \left[Cr_1 e^{-0.65r_1} + De^{-2.7r_1} \right]$$

$$\left[\frac{r_1}{r_2^2} \cos\theta + Vc \right] \cos\theta \left(2r_1^3 - \frac{r_1^4}{3}\right) e^{-r_1/2}$$

It can be seen that the Vc part becomes zero because $\int_0^\pi \sin\theta \cos\theta \, d\theta = 0$.

The remaining part becomes very much similar to that in ESEH process with only a few changes. Thus

$$< U_0/V/U_{pol}>^* = \frac{\sqrt{2\pi}}{30} \frac{1}{r_2^4} \left\{ 2D \frac{6!}{\beta^7} \left[\left(1 - \frac{7}{6\beta}\right) - e^{-\beta r_2} \right. \right.$$

$$+ A_\beta \frac{\beta^2 r_2^3}{3!}$$

$$((1 - \frac{7}{6\beta}) + A_\beta r_2 + A_\beta \frac{\beta r_2^2}{2!} {}_\wedge + A_\beta \frac{\beta^3 r_2^4}{4!} + A_\beta \frac{\beta^4 r_2^5}{5!}$$

$$+ A_\beta \frac{\beta^5 r_2^6}{6!} - \frac{7}{6} \beta^6 \frac{r_2^7}{7!})] + 2C \frac{7!}{\pounds}\cancel{8} [(1- \frac{8}{6\pounds}) - e^{-\pounds r_2}$$

$$((1- \frac{8}{6\pounds}) + A_\pounds r_2 + A_\pounds \frac{\pounds r_2^2}{2!} + A_\pounds \frac{\pounds^2 r_2^3}{3!} + A_\pounds \frac{\pounds^3 r_2^4}{4!} + A_\pounds \frac{\pounds^4 r_2^5}{5!}$$

$$+ A_\pounds \frac{\pounds^5 r_2^6}{6!} + A_\pounds \frac{\pounds^6 r_2^7}{7!} - \frac{8}{6} \frac{\pounds^7 r_2^8}{8!})] \Big\} \qquad (4.33)$$

where $\pounds = 0.65 + 0.5$, $\beta = 2.7 + 0.5$

$$A_\beta = \beta - \frac{7}{6} , \quad A_\pounds = \pounds - \frac{8}{6} .$$

Now using (4.17) for the simplification of the above expression,

$$< U_o/V/U_{pol} > = 2 \frac{\sqrt{2\pi}}{30} \Big\{ \frac{D}{7} [\frac{d^4}{d\beta^4} - K_\beta \frac{\beta}{8} \frac{d^5}{d\beta^5} + K_\beta \frac{\beta^2}{72}$$

$$\frac{d^6}{d\beta^6} + \cdots] \frac{e^{-\beta r_2}}{r_2} + \frac{C}{8} [- \frac{d^5}{d\pounds^5} + K_\pounds \frac{\pounds}{9} \frac{d^6}{d\pounds^6} - K_\pounds \frac{\pounds^2}{90} \frac{d^7}{d\pounds^7}$$

$$+ \cdots] \frac{e^{-\pounds r_2}}{r_2} \Big\} \qquad (4.34)$$

where $K_\beta = 1 - \frac{7}{6\beta}$, $K_\pounds = 1 - \frac{8}{6\pounds}$.

It can be seen that this expression is very similar to (4.25), but there is difference of the values of certain parameters only. The above expression is in a directly substitutable form for the standard integral (4.16), from which we get

$$I_P = 2\frac{\sqrt{2\pi}}{30}\left\{\frac{D}{7}\left[\frac{d^4}{d\beta^4} - K_\beta\frac{\beta}{8}\frac{d^5}{d\beta^5} + K_\beta\frac{\beta^2}{72}\frac{d^6}{d\beta^6} + ---\right]\right.$$

$$\left. I(\beta) + \frac{C}{8}\left[-\frac{d^5}{d\pounds^5} + K_\pounds\frac{\pounds}{9}\frac{d^6}{d\pounds^6} - K_\pounds\frac{\pounds^2}{90}\frac{d^7}{d\pounds^7} + ---\right]I(\pounds)\right\}$$

$$\ldots\ldots(4.35)$$

where $C = 0.11252$, $D = -0.42204$,

$\pounds = 1.15$, $\beta = 3.2$.

The evaluation of I_E for ELi process is also easy because of the analogy with the ESEH process. The product of wave functions (4.30) can still further be expressed as

$$U_o^* U_o = -K_1\frac{d}{d\lambda_1}\frac{e^{-\lambda_1 r_1}}{r_1} - K_2\frac{d^2}{d\lambda_2^2}\frac{e^{-\lambda_2 r_1}}{r_1} - K_3\frac{d^3}{d\lambda_3^3}\frac{e^{-\lambda_3 r_1}}{r_1}$$

Using this, I_E can be evaluated as in the ESEH process to give

$$I_E = -\frac{4\pi}{k_i^2}\left\{K_1\frac{d}{d\lambda_1}I(\lambda_1) + K_2\frac{d^2}{d\lambda_2^2}I(\lambda_2)\right.$$

$$\left. + K_3\frac{d^3}{d\lambda_3^3}I(\lambda_3)\right\} \qquad \ldots\ldots(4.36)$$

Now using the expressions (4.32), (4.35) and (4.36) for I_D, I_P and I_E, the differential cross sections for the electron scattering from Lithium atom (ground state) can be obtained.

To see the effect of the core with respect to that of the valence electron of the Li atom, the above studies were conducted neglecting the V_c part of the contribution. Because the V_c part becomes zero in the evaluation of $\langle U_o/V/U_{pol}\rangle$, it can be easily understood that the suppression of the core potential will not affect the contribution due to polarisation. This is true from the physical point of view also because polarisation, being the distortion in the charge cloud, should be vastly affected by the outer most electrons only, since they will be subjected to the strong interaction with the incoming electron.

To suppress the core-contribution in the I_D part K_4 and K_5 can be directly made zero in (4.32). Incidentally this does not amount to any irregularity like divergencies. The resulting expression will give the contribution of the valence electron to I_D. The expressions so obtained can be used to find the DCS for E Li process in MBA, neglecting the core effect.

Szasz and McGinn (1967) have given a more sophisticated calculation for the Lithium wavefunction than that of Coulson (4.29). Walters (1973), in his study of Li atom has taken only the simpler Coulson wave function with a comment that both the wave functions should give more or less the same results. To explore whether there will be any improvement on using this sophisticated wave function, in the present study, the DCS in MBA are also calculated using the wave function of Szasz and Mc Ginn after orthonormalizing the valence state explicitly.

According to the work of Szasz and McGinn (1967), the one-electron wave function of Li is given as

$$\Psi(nlm) = \Sigma\, C^{(P)}_{nl} \cdot A^{(P)}_{nl} \cdot R^{(P)}_{nl} \; Y_{lm} \qquad (4.37)$$

where $A^{(P)}_{nl} = \left[\left(2\, \xi^{(P)}_{nl}\right)^{2n+1} \big/ (2n)! \right]^{1/2}$

and $R^{(P)}_{nl} = r_1^{\,n-1} \exp\left(-\xi^{(P)}_{nl} \; r_1 \right)$

The functions $\xi^{(P)}_{nl}$, $A^{(P)}_{nl}$ and $C^{(P)}_{nl}$ are tabulated in table (4.2).

Hence the total wave function can be written as

$$\Psi = (A\, R_{2S} + B\, R_{1S}) \frac{1}{\sqrt{4\pi}} \qquad (4.38)$$

where R_{1S} and R_{2S} correspond to the core and valence electrons respectively and are given by

$$R_{1S} = 2.4723 \; e^{-4.4r_1} + 6.7989 \; e^{-2.4r_1} - 0.4185\, r_1\, e^{-4.40r_1} - 0.3047 r_1\, e^{-2.4r_1} \; ;$$

$$R_{2S} = 0.0651\, e^{-2.48r_1} + 0.0488\, e^{-4.71r_1} - 0.399\, r_1\, e^{-1.735r_1} + 0.1014\, r_1\, e^{-r_1} + 0.3969\, r_1 \; e^{-0.66r_1} + 2.66 \times 10^{-4}\, r_1 e^{-0.35r_1}$$

For the orthonormalization of the valence state, the following properties are used :

$$\int \Psi^* \Psi \, dv_1 = 1, \quad \int \Psi^* \frac{R_{1S}}{\sqrt{4\pi}} \, dv_1 = 0$$

From these conditions, A and B are obtained as

$A = 1.0448$;

$B = -0.2031$ so that the one electron wave function for Li becomes

$$\psi = \sum_{i=1}^{4} C_i \, e^{-\lambda_i r_1} + \sum_{j=1}^{6} D_j r_1 \, e^{-\beta_j r_1} \qquad (4.39)$$

the leading terms of which give

$$\psi = 0.117 r_1 \, e^{-0.66 r_1} - 0.3894 \, e^{-2.4 \, r_1}$$

which is very near to the Coulson wave function (4.29). This is an indirect check of the procedure adopted to obtain the wavefunction (4.39). The constants C_i, λ_i, D_j and β_j are tabulated in table (4.3). Using this wavefunction instead of (4.29), the whole calculation can be repeated to get the DCS for ELi process in the MBA. However, in the present study, polarisation and exchange are neglected in this part and only I_D is taken because the purpose of this study is only the comparison of these results with those obtained using the wave function (4.29). Hence in both cases, I_P and I_E are neglected in (4.9) and the results are compared.

The evaluation of I_D using wave function (4.39) is rather more cumbersome than the earlier evaluation using (4.29). In the present case

$$U_o^{*} U_o = \sum_{i=1}^{4} \sum_{m=1}^{4} C_i C_m e^{-\lambda_i r_1 -\lambda_m r_1} + \sum_{j=1}^{6} \sum_{n=1}^{6} D_j D_n r_1^2 e^{-\beta_j r_1 -\beta_n r_1} + 2 \sum_{i=1}^{4} \sum_{j=1}^{6} C_i D_j r_1 e^{-\lambda_i r_1 -\beta_j r_1} \qquad (4.40)$$

which is definitely more complicated than the corresponding expression (4.30). Using the simplification $r_1 e^{-\lambda r_1} = \frac{-d}{d\lambda} e^{-\lambda r_1}$ the expressions for $<U_o/V/U_o>$ and I_D can be obtained in a same way as (4.32) is derived. The analysis is very lengthy and the result is given by

$$I_D = -4\pi \sum_{i=1}^{4} \sum_{m=1}^{4} C_i C_m \left\{ \frac{2}{(\lambda_i+\lambda_m)^3} - \frac{1}{(\lambda_i+\lambda_m)^2} \frac{d}{d(\lambda_i+\lambda_m)} \right\} I(\lambda_i+\lambda_m) + 8\pi \sum_{i=1}^{4} \sum_{j=1}^{6} C_i D_j \left\{ \frac{-6}{(\lambda_i+\beta_j)^4} I(\lambda_i+\beta_j) + \frac{4}{(\lambda_i+\beta_j)^3} I_1(\lambda_i+\beta_j) - \frac{1}{(\lambda_i+\beta_j)^2} I_2(\lambda_i+\beta_j) \right\} - 4\pi \sum_{j=1}^{6} \sum_{n=1}^{6} D_j D_n \left\{ \frac{6}{(\beta_j+\beta_n)^3} I_2(\beta_j+\beta_n) - \frac{18}{(\beta_j+\beta_n)^4} I_1(\beta_j+\beta_n) + \frac{24}{(\beta_j+\beta_n)^5} I(\beta_j+\beta_n) - \frac{1}{(\beta_j+\beta_n)^2} I_3(\beta_j+\beta_n) \right\} -2I(\lambda_1) + 5.4 \frac{d}{d\lambda_1} I(\lambda_1) \qquad (4.41)$$

where $\lambda_1 = 5.4$; $I(\lambda)$ is the standard integral (4.16); $I_1(\lambda) = \frac{d}{d\lambda} I(\lambda)$; $I_2(\lambda) = \frac{d^2}{d\lambda^2} I(\lambda)$ etc. Now, the DCS can be obtained by substituting (4.41) in (4.9). Similarly, using the I_D value (4.32) in (4.9) and neglecting I_P and I_E also, the DCS is taken which corresponds to the Coulson wavefunction.

Results and Discussion :

The DCS for ELi process in the MBA is calculated for different energies varying from 20 eV to 700 eV. The present results at 20 eV, 100 eV and 200 eV are exhibited in figure (4.4), (4.5) and (4.6) along with the available experimental data of Williams et al (1976) and the recent theoretical values (HHOB results of Rao and Desai (1983), close coupling results of Issa (1977), EBS results and Two potential - Eikonal results (Tayal et al 1980), corrected static results of Tayal et al 1981).

The present approximation, being a high energy approximation, should not be expected to give good results below 100 eV. Hence, 20 eV is definitely too low, but the results are shown because experimental data is available only at such low energies. The comparison of the present results with experimental values is quite encouraging, when considering the energy region.

The disagreement of the present results with the most recent HHOB results need not be looked upon as a bad omen because, as discussed earlier the HHOB results have been found to be higher than the corresponding experimental values. At 100 and 200 eV, the present DCS at small angles almost coincide with the EBS and CS results. Naturally, the present results are bound to be better at higher incident energies. The DCS values for certain sample energies are shown in table (4.4).

In order to see the effect of the core compared to the valence electron, the present results, with and without core potential are shown in Figure (4.7)., at the incident energy 60 eV. For comparison purpose the present values of first Born results are also shown (taken from calculation in the previous chapter). It can be seen that the effect of the core increases with the scattering angle. As Θ increases, the interaction between the core and the incident electron progressively dominates the scattering and the effect of the core becomes more and more significant. In the present study, it is found that at 60 eV, the ratio of the contributions of the valence electron to the first Born amplitude for the scattering angles 10^{o} and 150^{o} is 40.3: 1 whereas the corresponding ratio for the core contributions is 1.9:1, which illustrates the less repid variation of the core-contribution with angle.

Similarly, it was observed that when k_i increases, the core-contribution to the DCS also increases. As we go from 60 eV to 700 eV, the ratio of the DCS with and without core changes from 6.7:1 to 9.1:1 at the scattering angle 150^{o}. The corresponding ratios in the first Born Calculations are 5:1 and 9.3:1. This is actually what is expected because, as the incident energy increases, the projectile penetrates deeper into the target system and the projectile - core interaction becomes more significant. In table (4.5), the DCS values in first Born and MBA for ELi process (with and without core potential) are given at energies 60 eV and 700 eV.

In figure (4.8) comparison is made between the DCS at 60eV calculated using the two wavefunctions - the simple wave function of Coulson (4.29) and the sophisticated Szasz McGinn wavefunction (4.39). As discussed earlier, polarisation and exchange effects are neglected in this calculation in both methods. It can be seen that the cross-sections do not differ much, as anticipated by Walters (1973).

It may be concluded from the above analysis that in view of the simplicity of MBA, it gives reasonable results in the study of $\bar{e}$ - Li elastic scattering. However, the results are much less satisfactory when compared with the observations in electron scattering from H and He.

The table of total elastic cross sections obtained in the present study (table 4.6) also displays satisfactory results. It is also clear that the results improve with increasing incident energy.

In the case of Lithium, because of the quasi-degeneracy of the ground and first excited states, 98% of the polarizability arises from the interaction between these states. As a result, excitation effects become much more important than polarisation and exchange effects. Earlier it was pointed out that the contribution due to polarisation is very little in this process. Hence, eventhough methods like polarised orbital calculations will have difficulties in electron - alkali scattering, the error in the polarisation part of the present study taken through the polarized orbitals will be very insignificant.

It looks unclear why the MBA should be expected to model the absorption effect. In the comparative study of the scattering amplitudes in the optical potential approach and the EBS method, Byron and Joachain (1977) have pointed out that the absorptive part V_{abs} of the optical potential treated in first Born combined with the static part V_{st} treated twice in the perturbative theory gives the imaginary part Im f_{B_2} of the EBS amplitude. Same will be the case in the Born series also, because of the comparison between eikonal and Born imaginary parts. In the MBA analysis, which is in fact the modified first Born approximation with the second order effects like polarisation included, we get an imaginary part in the direct scattering amplitude. This imaginary part in the first Born frame work, may be attributed to the absorptive effect. Of course, the contribution of the static part V_{st} treated twice in the perturbative theory will be very small at angles at which absorptive effects are maximum. The above argument is evidenced by the fact that the present MBA results at small angles almost coincide with the EBS results which explicitly account for the absorption effects. Thus there is some logic behind the presumption that the loss of electron flux from the elastic channel which plays an important role in alkali scattering is implicitly taken in the MBA, unless some unknown conspiracy of cancellations works. However, rough calculations taking absorptive effects explicitly, have given results which are very near to the previous results.

In Vanderpoorten's (1976) work, it has been shown that the optical potential results almost coincide with the Glauber results. The table (4.6) of total elastic cross sections shows that the present MBA results also almost coincide with the Glauber results. Hence, the MBA results can be anticipated to be very near to the optical potential results at these energies. This is another evidence for the fact that the present study accounts for all important effects taken in the optical potential approach.

Anyway, in view of the complexity of the $\bar{e}$ - Li scattering process studied here, the present results are definitely not poor. Considering the agreement with the results of existing sophisticated methods, the present results can be termed as quite good especially when we think of the results given by a recent modification over the Born series, namely HHOB, which explicitly takes care of all the effects like polarisation and absorption. As such, the present studies of the ESEH and ELi processes in the MBA do not provide any clue towards the unsatisfactory results reported by Kaushik et al (1982) when MBA was applied to complex atoms like C and O. More rigorous investigations have to be undertaken in the search of the missing link between the present results and the disappointing results of Kaushik et al. However, a comparative study of the scattering of electrons from H, He and Li using the modified Born approximation reveals that the higher the atomic number of the target, the poorer the results. This sort of cumulative effect may be responsible for the predictions of Kaushik et al (1982).

With so much discussions on the modified Born Approximation, let us now switch over to the next part of the current chapter.

4.5 Two-potential eikonal approximation :

As mentioned in the introductory part of the present chapter, the search for an improvement over the HHOB approximation (Yates 1979) led to further studies on the two-potential eikonal approximation of Ishihara and Chen (1975). Hence, the same is incorporated in the current chapter which deals mainly with improvements over Born approximation. In an attempt to formulate a parallel two-potential Born approximation, an indepth analysis of the two-potential eikonal approximation (TPE) was undertaken. For this purpose, the TPE was formulated in such a way that it may be applied to the elastic scattering of electrons from any of the nlm states of H atom. This formulation was afterwards applied to $\bar{e}$ - H (2S) scattering and the results are discussed in detail. It is noteworthy to mention here that, as stated in an earlier section, the study of the above scattering process bears a certain amount of significance. Recent revival of theoretical interest on this scattering problem is evident from the reports of work done regarding the problem (Joachain et al 1977, Ho and Chan 1978, Joachain and Winters 1980, Pundir et al 1982, Rao and Desai 1983).

TPE approximation for $\bar{e}$ - H (nlm) scattering :

The Glauber approximation is known to be in appreciable error at all angles when applied to the elastic electron-atom scattering at medium and lower energies. Ishihara and Chen (1975) have shown that this is mainly due to the inadequate semiclassical treatment of close-encounter collisions. TheTPE approximation provides an effective method to treat such collisions properly.

The basic idea underlying this approximation is to pull out an arbitrary potential V_1 from the interaction potential V such that the rest of the interaction potential i.e. $V_o = V - V_1$ satisfies the semiclassical conditions $(\frac{|V_o|}{E} \ll 1$ for all values of r, where E is the energy of the system and V_o being a slowly varying function.).

To start with, let us consider the scattering by a central field V (r). Now V (r) = V_o (r) + V_1 (r). In the two-potential form given by Rodberg and Thaler (1967), the scattering amplitude can be written as

$$F\ (\Theta) = \frac{1}{k_i}\sum_{\ell}\,(2\ell+1)\,e^{i\delta_\ell^{(o)}}\,\sin\delta_\ell^{(o)}\,P_\ell(\cos\Theta) + \frac{1}{k_i}\sum_{\ell}\,(2\ell+1)\,e^{2i\delta_\ell^{(o)}}\,e^{i\delta_\ell^{(1)}}\,\sin\delta_\ell^{(1)}\,P_\ell(\cos\Theta) \qquad (4.42)$$

where δ_ℓ and $\delta_\ell^{(1)}$ are the ℓ^{th} phase shifts for the potentials V and V_1 and Θ is the scattering angle.

$\delta_\ell^{(o)} = \delta_\ell - \delta_\ell^{(1)}$. With our choice of V_1, $\delta_\ell^{(o)}$ may be evaluated by the JWKB (Jeffreys - Wenzel - Kramers - Brillouin) approximation to the first order in V_o.

$$\text{Then}\quad \delta_\ell^{(o)} = -\frac{1}{k_i}\int_{r_1}^{\infty} dr\, V_o(r)\Big/\left[1-\left(\frac{\ell+\frac{1}{2}}{k_i r}\right)^2-\frac{V_1}{E}\right]^{1/2} \qquad (4.43)$$

where r_1 is the classical turning point for the potential V_1. If we neglect the quantity of order V_oV_1, the above equation reduces to the usual form of the Glauber (or Moliere) phase shift for V_o.

Since most of the effect of V_1 is included in the second term of f (Θ), the contribution of the first term is concentrated in the forward direction and may be evaluated by using the asymptotic formula (Ford and Wheeler 1959).

$$P_\ell\ (\cos\Theta) \simeq J_o((2\ell+1)\ \sin\frac{\Theta}{2})$$

$$\text{and}\quad \sum_{\ell=0}^{\infty} \simeq \int_0^{\infty} d\ell.$$

Thus we have

$$F(\Theta) = \frac{k_i}{i} \int_0^\infty b\, db\, (e^{iX(b)} - 1)\, J_0(2 k_i b \sin \frac{\Theta}{2}) + \frac{1}{k_i} \sum_{\ell} (2\ell + 1) e^{2i\delta_\ell^{(o)}} \sin \delta_\ell^{(1)} e^{i\delta_\ell^{(1)}} P_\ell(\cos \Theta) \qquad (4.44)$$

where the impact parameter is introducted by

$$b_\ell = (\ell + \frac{1}{2}) / k_i \text{ and } X(b_\ell) = 2\delta_\ell^{(o)}.$$

Now generalizing the above formula to the case of electron-atom scattering in the frozen target approximation, the inter-action V depends on the position $\bar{r}$ of the projectile as well as the Coordinates of the target electrons. The equation for $\delta_\ell^{(o)}$ may further be approximated as

$$X(b, b_1, z_1) = X_o(b, b_1 z_1) + \Delta X(b, b_1, z_1) \qquad (4.45)$$

with $X_o = -\frac{1}{k_i} \int_{-\infty}^{\infty} V_o \, dz$

and $\Delta X = \frac{2}{k_i} V_o(z=0) \times \int_0^\infty (1 - \frac{z}{[z^2 - \frac{V_1}{E} r^2]^{1/2}}) \, dz$

where it is assumed that V_1 is attractive and short range. X_o is the glauber (straight-line) phase for $V_o = V - V_1$ and ΔX is the correction due to the separation of V_1.

Now, an average over the direction ϕ of b_ℓ in the second term of (4.44) is made. This is reasonable if the range of V_1 (given by d) is chosen to be shorter than the atomic size. Moreover, we need only a few terms in the second term of equation (4.44) if d is chosen small enough. Thus the evaluation of (4.44) will not add any further practical difficulties to the usual Glauber approximation calculations. Hence, in the two-potential eikonal approximation, the transition amplitude from the initial state /i> of the target to the final state /f> is given by

$$F_{fi}(\theta) = \frac{k_i}{2\pi i} \int d^2b \, e^{i \cdot \underline{g} \cdot \underline{b}} \left[\Gamma_{fi}(\bar{b}) - 1 \right] + \frac{1}{k_i} \sum_{l} (2l+1) P_l(\cos\theta) \, e^{i\delta_l^{(1)}} \sin \delta_l^{(1)} \int \frac{d\phi}{2\pi} \Gamma_{fi}(b_l^-) \qquad (4.45)$$

Here $\Gamma_{fi}(b) = \langle f / e^{iX} / i \rangle$ (4.46)

and $X = X_o + \Delta X$ where X_o is the usual Glauber phase function.

$$X_o = - \frac{1}{k_i} \int_{-\infty}^{\infty} dz \quad V_o \,.$$

For the scattering from H atom, the interaction potential is given by

$V(\underline{r}, \underline{r}_1) = - \frac{1}{r} + \frac{1}{/\underline{r}-\underline{r}_1/}$. In the present study, the short range central potential V_{st} which is the static potential of the target atom, is chosen for V_1.

$$\therefore \; V_o = V - V_{st}$$

Hence from equation (4.45) it is clear that V_o is treated in the Glauber approximation and the contribution of V_{st} is calculated quantum - mechanically by taking few partial waves.

In order to make use of the above equation (4.45) to study the electron scattering from any of the excited states (nlm) of H, it is necessary to have th V_{st} and X_o corresponding to those states. The general form of V_{st} for elastic scattering is given by

$$V_{st}^{nlm} = \int d\,v_1\, \Psi^*_{nlm}\, \Psi_{nlm} \left(-\frac{1}{r} + \frac{1}{|\underline{r} - \underline{r}_1|}\right) \qquad (4.47)$$

where Ψ_{nlm} represents the standard form of wave function given by

$$\Psi_{nlm} = \frac{2}{n^2}\left[\frac{(n-l-1)!}{((n+l)!)^3}\right]^{1/2} \left(\frac{2r_1}{n}\right)^{l} e^{-r_1/n}$$

$$L_{n-l-1}^{2l+1}\left(\frac{2r_1}{n}\right) Y_{lm}(\theta,\phi) \quad .. \qquad (4.48)$$

Now, $L_{n-l-1}^{2l+1}\left(\frac{2r_1}{n}\right) = \sum_{m=0}^{n-l-1} (-1)^m\, (n+l)!\, \left(\frac{m+l}{n-l-1-m}\right)$

$$\frac{\left(\frac{2}{n}\right)^m r_1^m}{m!}$$

Using this, V_{st}^{nlm} can be deducted through a lengthy procedure which gives

$$V_{st}^{nlm} = -\frac{1}{r} + \sum_{P=0}^{\infty} \sum_{m=0}^{n-\ell-1} \sum_{j=0}^{n-\ell-1} (-1)^{m+j} \sqrt{\frac{4\pi}{2P+1}}$$

$$\binom{n+\ell}{n-\ell-1-m} \binom{n+\ell}{n-\ell-1-j} \frac{\left(\frac{2}{n}\right)^{m+j+2\ell}}{m!\; j!} \frac{4}{n^4} \frac{(n-\ell-1)!}{(n+\ell)!}$$

$$\left[\frac{(2\ell+1)^2(2P+1)}{4\pi}\right]^{1/2} \begin{pmatrix} \ell & P & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & P & \ell \\ m & 0 & m \end{pmatrix}$$

$$\left\{ \frac{1}{r^{P+1}} \left[\frac{s_1!}{\left(\frac{2}{n}\right)^{s_1+1}} - e^{-\frac{2r}{n}} \sum_{k=0}^{s_1} \frac{s_1!}{k!} \frac{r^k}{\left(\frac{2}{n}\right)^{s_1-k+1}} \right] \right.$$

$$\left. + r^P e^{-\frac{2r}{n}} \sum_{k=0}^{s_2} \frac{s_2!}{k!} \frac{r^k}{\left(\frac{2}{n}\right)^{s_2-k+1}} \right\} \tag{4.49}$$

where $s_1 = p + 2 + m + j + 2\ell$

$s_2 = 1 + m + j + 2\ell - P$

and $\begin{pmatrix} l & P & l \\ 0 & 0 & 0 \end{pmatrix}$ are usual Wigner notations.

The general form of X_o^{nlm} is

$$X_o^{nlm} = -\frac{1}{k_i} \int_{-\infty}^{\infty} V\, dz + \frac{1}{k_i} \int_{-\infty}^{\infty} V_{st}^{nlm}\, dz \tag{4.50}$$

For all states of H, the interaction potential

$$V(b,z,b_1,z_1) = -\frac{1}{r} + \frac{1}{|\underline{r}-\underline{r}_1|}$$

so that $$-\frac{1}{k_i} \int_{-\infty}^{\infty} v\, dz = \frac{2}{k_i} \ln \frac{|\underline{b} - \underline{b}_1|}{b} \tag{4.51}$$

Now $\int_{-\infty}^{\infty} V_{st}^{nlm}\, dz$ may be calculated from (4.49) using standard integration techniques. Since this is a very lengthy expression, we may take up the (ns) states. Deriving V_{st}^{ns} from (4.49) and performing the integration over dz,

$$\int_{-\infty}^{\infty} V_{st}^{ns}\, dz = \frac{8}{n^4} \frac{(n-1)!}{n!} \sum_{m=0}^{n-1} \sum_{j=0}^{n-1} (\mp 1)^{m+j}$$

$$\binom{n}{n-1-m} \binom{n}{n-1-j} \left(\frac{2}{n}\right)^{m+j} \frac{1}{m!\, j!} \left\{ \sum_{k=0}^{S_3} \right.$$

$$\frac{(S_3)!}{k!\, \left(\frac{2}{n}\right)^{S_3+k+1}} (\mp 1)^{k+1} \frac{d^{k+1}}{d\lambda^{k+1}} K_0(b\lambda) - \sum_{k=0}^{S_3+1}$$

$$\left. \frac{(S_3+1)!}{k!\, \left(\frac{2}{n}\right)^{S_3+2-k}} (-1)^{k} \frac{d^{k}}{d\lambda^{k}} K_0(b\lambda) \right\} \qquad (4.52)$$

where $S_3 = m + j + 1$ and $\lambda = \frac{2}{n}$.

Using (4.51) and (4.52), one can find the general expression for X_o^{ns} for any (ns) state of H.

4.6 $\bar{e}$ - H(2S) elastic scattering (ESEH) :

As a special case, ψ, V_{st} and X_o are derived from (4.48), (4.49), and (4.52) for the E S E H process. Thus

$$\psi_{2S} = \frac{1}{4\sqrt{2\pi}} (2 - r_1)\, e^{-r_1/2} \qquad (4.53)$$

$$V_{st} = -\left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{8} \right) e^{-r} \qquad (4.54)$$

$$\text{and} \quad X_o = \frac{2}{k_i} \ln \frac{|\underline{b} - \underline{b}_1|}{b} - \frac{2}{k_i} \left[1 - \frac{3}{4} \frac{d}{d\lambda} + \frac{1}{4} \frac{d^2}{d\lambda^2} \right.$$

$$\left. - \frac{1}{8} \frac{d^3}{d\lambda^3} \right] K_0 (b\lambda] \qquad (4.55)$$

where $\lambda = 1$.

The correction ΔX to the phase X_o contributes very little for energies greater than 100 eV and hence can be neglected. Now $\Gamma(b)$ given by (4.46) may be evaluated to give

$$\Gamma(b) = \frac{Y\, e^{-\beta_o X_e K_o(b\lambda)}}{b^{\beta_o}} \qquad (4.56)$$

where $\beta_o = \frac{2\quad i}{k_i}$, $X_e = 1 - \frac{3}{4}\frac{d}{d\lambda} + \frac{1}{4}\frac{d^2}{d\lambda^2} - \frac{1}{8}\frac{d^3}{d\lambda^3}$,

$$Y = -\frac{1}{8}\left(4\frac{d}{d\lambda} + 4\frac{d^2}{d\lambda^2} + \frac{d^3}{d\lambda^3}\right) 2^{\beta_o} \lambda^{-\beta_o - 2}$$

$$\Gamma(1 + i/k_i) \quad \Gamma(1 + i/k_i)$$

Evaluation of the eikonal part of the scattering amplitude (4.45) gives

$$f_{eik} = \frac{q^{\beta_o - 2}}{4} \quad \frac{\pi/k_i}{\sinh \pi/k_i}\left[8 - \frac{20}{k_i^{\,2}} + i\left(\frac{20}{k_i} - \frac{8}{k_i^{\,3}}\right)\right]$$

$$-2Y \times X_e \left[\frac{\Gamma(1-i/k_i)\,\Gamma(1-i/k_i)}{2^{\beta_o}\,\lambda^{2-\beta_o}}\, F\left(1 - i/k_i,\ 1 - i/k_i;\ 1; -\frac{q^2}{\lambda^2}\right)\right] \qquad (4.57)$$

where F (a; b;c;z) represents the hypergeometric function, in the simplification of which, following expression is used:

$$F\,(a,\ b;\ c;z) = (1-z)^{-a}\ F\left(a,\ c-b; c; \frac{z}{z-1}\right).$$

After simplification,

$$f_{eik} = \frac{q^{\beta_o - 2}}{4} \frac{\lambda/k_i}{\mathrm{Sinh}\,\lambda/k_i} \left[\left(8 - \frac{20}{k_i^{\,2}}\right) + i \left(\frac{20}{k_i} - \frac{8}{k_i^{\,3}} \right) \right]$$

$$- \frac{1}{4} \left[\frac{\lambda/k_i}{\mathrm{Sinh}\,\lambda/k_i} \right]^2 \left[\left(8 - \frac{20}{k_i^{\,2}}\right) + i \left(\frac{20}{k_i} - \frac{8}{k_i^{\,3}} \right) \right]$$

$$\left[1 - \frac{3}{4} \frac{d}{d\lambda} + \frac{1}{4} \frac{d^2}{d\lambda^2} - \frac{1}{8} \frac{d^3}{d\lambda^3} \right] (G + iH) \qquad (4.58)$$

where $G = \dfrac{CE - DF}{\lambda^2}$

$H = \dfrac{DE + CF}{\lambda^2}$

$E = e^{-\ln Q} \operatorname{Cos} \left(\dfrac{1}{k_i} \ln Q \right); \; Q = 1 + q^2/\lambda^2$

$F = e^{-\ln Q} \operatorname{Sin} \left(\dfrac{1}{k_i} \ln Q \right)$

$C = A \operatorname{Cos} T - B \operatorname{Sin} T$

$D = A \operatorname{Sin} T + B \operatorname{Cos} T; \; T = \dfrac{2}{k_i} \ln \lambda$

$A = 1 + \dfrac{1}{k_i^{\,2}} S + \dfrac{\left(1 + \frac{1}{k_i 2}\right)}{4k_i^{\,2}} S^2$

$B = \dfrac{1}{k_i} S + \dfrac{\left(1 + {}^{1}/k_i^{\,2}\right)}{2k_i} S^2; \; S = \dfrac{q^2/\lambda^2}{1 + q^2/\lambda^2}$

The summation of partial waves in the evaluation of the scattering amplitude is done similar to the procedure adopted by Jhanwar et al (1978). According to this,

$$\frac{1}{k_i}\sum_{\ell=0}^{\infty}(2\ell+1)\,P_\ell(\mathrm{Cos}\,\Theta)\,e^{i\delta_\ell}\,\sin\delta_\ell$$

$$=\frac{1}{k_i}\sum_{\ell=0}^{N}(2\ell+1)\,P_\ell\,(\mathrm{Cos}\,\Theta)\,e^{i\delta_\ell}\,\sin\delta_\ell$$

$$+\,f_{B1}-\frac{1}{k_i}\sum_{\ell=0}^{N}(2\ell+1)\,P_\ell\,(\mathrm{Cos}\,\Theta)\,\delta_\ell^{(B)}\,. \qquad (4.59)$$

where f_{B1} is the first Born amplitude for the potential V ; δ_ℓ and $\delta_\ell^{(B)}$ are the exact and Born - approximation phase shifts for the same potential. Thus the contribution of those partial waves $\sum_{\ell=N}^{\infty}$ is taken through the Born approximation to the phase shifts. The value of N is so chosen that the values of exact and Born phase shifts differ by only a small percentage (say 3%) beyond this N value.

For the central potential $V_{st}(r)$, the Born approximation to the phase shift is given as (Schiff 1968)

$$\delta_\ell^{(B)} = -2k_i\int_0^\infty V_{st}(r)\,j_\ell^{\,2}(k_i r)\,r^2\,dr \qquad (4.60)$$

where $j_\ell(k_i r) = \sqrt{\frac{\pi}{2k_i r}}\;J_{\ell+1/2}\,(k_i r)$.

The exact phase shifts were calculated solving the second order differential equation for $V_{st}(r)$ by the Numerov method etc. This procedure will be discussed in detail later on. With the knowledge of the phase shifts the evaluation of the partial wave part of the scattering amplitude (4.45) is easy by using the simplification (4.59).

The following approximation is again used that, for the partial wave summation $\sum_{\ell=N}^{\infty}$, the $\Gamma_{fi}(b)$ becomes approximately 1, because X_0 is very small for ℓ values greater than N. This is very much justified in the sense that for higher ℓ values, the phase shift becomes less and less significant. Since $X_0 = 2\,\delta_\ell^{(0)}$ where $\delta_\ell^{(0)}$ is the phase shift for the potential $V_0 = V - V_{st}$, the significance of $\delta_\ell^{(0)}$ and hence that of X_0 becomes less and less when compared with the phase shift corresponding to the total interaction V. Using this, the partial wave part of (4.45) can be written as

$$f_{PW} = \frac{1}{k_i} \sum_{\ell=0}^{N} (2\ell+1)\, P_\ell(\cos\Theta)\, e^{i\delta_\ell^{(1)}} \sin\delta_\ell^{(1)} \int \frac{d\phi}{2\pi}\, \Gamma_{fi}(b_\ell^-) + f_{B1} - \frac{1}{k_i}\sum_{\ell=0}^{N}(2\ell+1)\, P_\ell(\cos\Theta)\, \delta_\ell^{(B)} \qquad (4.61)$$

Thus the scattering amplitude $F_{fi}(\Theta)$ (4.45) is evaluated from (4.58) and (4.61). The DCS may be found out as

$$\frac{d\sigma}{d\Omega} = |f(\Theta)|^2 .$$

Results and Discussion :

The $\bar{e}$ - H (2S) elastic differential cross sections are calculated at the sample energies 100 eV, 200 eV and 400 eV at which data is available for comparison. It should be remembered that during the evaluation of the scattering amplitude (4.45) for different energies, each time the Born and exact phase shifts are to be calculated, their values are to be matched to fix the N value etc. Since all this procedure consumes considerable computer time, the results were taken only for the above three specific energies. It can be noted that in almost all of the reports of the work done on this problem, the results are given only at 200 eV. The present results at these energies are represented graphically in figure (4.9) and figure (4.10) and compared with the results of eikonal Born series (EBS) approximation, optical model (OM) and the Galuber (G) results alongwith the most recently reported two-potential results (Pundir et al 1982) and high energy higher order Born (HHOB) results (Rao and Desai 1983).

As mentioned earlier, in the absence of sufficient experimental data, it is rather difficult to criticise the accuracy of the various approaches. Earlier, in the study of electron-scattering from H, He and Li, the two-potential eikonal approximation has provided reasonably good agreement with the experimental data and other sophisticated theories (Ishihara and Chen 1975, Tayal et al 1980). The HHOB results are found to be overestimating in the large angle region whereas the Glauber approximation is well-known for its shortcoming of under estimation (except at small angles). The present TPE results lie between the above two results and nearer to the EBS results which has given good agreement with experiments in other scattering processes.

As in the case of $\bar{e}$,- H (1S) elastic scattering (Ishihara and Chen, 1975), here also the two potential eikonal approximation should improve the conventional Glauber results because of two reasons:

(1) the singularity in interaction V_{st} is properly taken care of by partial wave analysis.

(2) The semi classical condition necessary for the Glauber approximation is better for the interaction V_o than for V.

The above aspect is clearly brought out by the comparison of the eikonal phase function $\Gamma(b)$ for the interaction potentials V and V_o (fig.4.11). $\Gamma(b)$ for V_o is a smooth function of b while that for V oscillates strongly for small b values. Practically, the smooth function $\Gamma(b)$ makes the numerical b integral much easier than in the Glauber approximation. The first term of (4.55) is the usual Glauber phase for the scattering process considered here. The singularity of this term at $b = 0$ is cancelled by the second term. Hence, in contrast to Glauber approximation, $\Gamma(b)$ varies smoothly in the two-potential formulation. Similar behaviour is observed in the electron-scattering from H(1S), He and Li (Ishihara and Chen 1975, Tayal et al ,1980). It may be noted that as in the case of $\bar{e}$ - H (1S) scattering, here also Re $\Gamma(b)$ >> Im $\Gamma(b)$ everywhere. Since a real Γ corresponds to an imaginary phase shift, $\Gamma(b)$ contains almost no scattering, but mostly absorption. Since ΔX is a relatively small correction, $\Gamma(b)$ with the approximation $X \simeq X_0$ behaves similarly. Therefore, the Glauber approximation, roughly speaking, contains the scattering by the static potential, the treatment of which is the motivation of the two-potential eikonal approximation as such.

The present $\bar{e}$ - H (2S) scattering cross sections at 100 eV are compared with the corresponding $\bar{e}$ - H (1S) cross sections and are found to approach each other for larger angles where the incident electron - target nucleus interaction becomes more and more significant. Similar type of behaviour was discussed in an earlier section.

The Glauber approximation when applied to electron-atom collisions encounters difficulties coming primarily from; (a) the frozen target approximation, (b) the semi classical treatment of small angular momentum contributions. The frozen target approximation which neglects the long-range polarisation effect gives rise to inadequacies at forward scatterings and improper treatment of the small angular momentum contribution gives rise to errors in a wide range of scattering angles. The electron atom interaction behaves like $-\frac{Z}{r}$ as $r \longrightarrow 0$ and the condition $/V/ \ll E$ for the eikonal approximation does not hold for low energies. As is well known it is this nuclear coulomb interaction that predominates in large angle scattering, and for lower energies it effects the cross section at all angles. The observed discrepancy of the Glauber approximation in elastic electron-atom collisions is largely due to the above reason. The TPE approximation provides an effective method to treat the close-encounter collisions properly. Hence, the present method may hold good for little lower energies also. As is evident from the small angle behaviour of the present results, we have to go beyond the frozen target in order to improve the forward angle scattering. Anyway, in view of the simplicity of the present method, the results are quite reasonable, and it definitely leads to substantial improvement over the ordinary Glauber approximation.

4.7 Two-Potential Formulation in HHOB :

The High energy higher order Born approximation proposed by Yates (1979) has recently been applied to various scattering problems (Rao and Desai 1981, 83). It being a computationally simple approximation gives reasonably good results at small angles for the scattering parameters in the electron-atom scattering process. In this approximation, no question of divergent interals arise as in the case of the GES approximation (Yates 1974). The main shortcoming of the HHOB approximation is the appreciable over-estimation of the cross sections in the large angle region. As the scattering angle increases, the differential cross sections deviate more and more from the corresponding experimental values.

It is well-known that the Born approximation gives better results for weaker interaction potentials. Keeping this in mind, the present two-potential HHOB approximation is formulated in the same line as the two-potential eikonal approximation (TPE) of Ishihara and Chen (1975). As discussed in the previous section, the success of the TPE approximation in the study of various scattering phenomena provided enough motivation for the present formulation. Moreover, it was quite logical and reasonable to believe that the present formulation, in which the interaction potential V treated in the Born approximation will be replaced by V - V_1, V_1 being given a better treatment through partial wave analysis, would definitely give better results. As in the case of TPE approximation, in the present study, the basic formula is derived for potential scattering and is generalized to thecase of a target. In order to see the usefulness of this method, it is applied to elastic scattering of electrons from H and He at intermediate energies. The improvement over the basic HHOB approximation (Yates 1979) is quite appreciable, as expected.

Formulation of Two-potential HHOB approximation (TPHB):

Consider the scattering by a central field V(r) which may be singular at r = 0. An arbitrary potential V_1 is so chosen that $V_o = V - V_1$ satisfies the semiclassical conditions. (V_o being a slowly varying function and $V_o/E \ll 1$ for all values of r, where E is the energy of the system).

Now $V(r) = V_o(r) + V_1(r)$ (4.62)

We write the scattering amplitude in the two potential form of Rodberg and Thaler (1967):

$$F(\Theta) = \frac{1}{k_i} \sum_{\ell} (2\ell+1)\, T_\ell P_\ell(\mathrm{Cos}\,\Theta) \tag{4.63}$$

with $T_\ell = e^{i\delta_\ell^{(o)}} \mathrm{Sin}\,\delta_\ell^{(o)} + e^{2i\delta_\ell^{(o)}} e^{i\delta_\ell^{(1)}}$

$\mathrm{Sin}\,\delta_\ell^{(1)}$ and $\delta_\ell^{(o)} = \delta_\ell - \delta_\ell^{(1)}$,

where δ_ℓ and $\delta_\ell^{(1)}$ are the ℓth phase shifts for the potentials V and V_1, k_i is the asymptotic momentum and Θ is the scattering angle. Hence

$$F(\Theta) = \frac{1}{k_i} \sum_{\ell} (2\ell+1)\, e^{i\delta_\ell^{(o)}} \mathrm{Sin}\,\delta_\ell^{(o)}\, P_\ell(\mathrm{Cos}\,\Theta) + \frac{1}{k_i} \sum_{\ell} (2\ell+1)\, e^{2i\delta_\ell^{(o)}} \mathrm{Sin}\,\delta_\ell^{(1)}\, e^{i\delta_\ell^{(1)}} P_\ell(\mathrm{Cos}\,\Theta) \quad \ldots(4.64)$$

We now evaluate $\delta_\ell^{(o)}$ by Born approximation. The radial part of the Schro"e- dinger equation for $V_o(r)$ is

$$\frac{d^2U_\ell^{(o)}}{dr^2} + \left\{ k_i^2 - \frac{\ell(\ell+1)}{r^2} - U_o(r) \right\} U_\ell^{(o)} = 0 \tag{4.65}$$

where $U_o(r) = \frac{2m}{\hbar^2} V_o(r)$.

The solution of this equation is

$$U_\ell^{(o)}(r) = F_\ell(k_i r) + \int_0^\infty dr'\, g_\ell(r,r')\, U_o(r')\, U_\ell^{(o)}(r') \tag{4.66}$$

where $g_l\ (r, r')$ represents the green's function. Now the exact phase shift is given by

$$\tan \delta_l^{(o)} = -\frac{1}{k_i} \int_0^\infty dr\ F_l\ (k_i r)\ U_o(r)\ U_l^{(o)}(r) \tag{4.67}$$

In the second Born approximation

$$U_l^{(o)} = F_l\ (k_i r) + \int_0^\infty dr'\ g_l\ (r, r')\ U_o(r')\ F_l\ (k_i r') \tag{4.68}$$

Thus phase shift (4.67) becomes

$$\tan \delta_l^{(o)} = \frac{-1}{k_i} \int_0^\infty dr\ F_l\ (k_i r)\ U_o(r)\ \Big\{ F_l(k_i r) + \int_0^\infty dr'\ g_l\ (r, r')\ U_o(r')\ F_l(k_i r')\Big\} \tag{4.69}$$

The first part of (4.64) is the amplitude factor for the potential U_o. When $\delta_l^{(o)}$ is small, we have

$$F_l^{(o)} = \frac{1}{k_i} \sum_l (2l+1)\ \delta_l^{(o)}\ P_l\ (\mathrm{Cos}\ \theta).$$

Substituting for $\delta_l^{(o)}$ from (4.69),

$$F_l^{(o)} = \frac{1}{k_i} \sum_l (2l+1)\ P_l\ (\mathrm{Cos}\ \theta) \Big\{ -\frac{1}{k_i} \int_0^\infty dr\ /F_l\ (k_i r)/^2\ U_o(r) \Big\} + \frac{1}{k_i} \sum_l (2l+1)\ P_l\ (\mathrm{Cos}\ \theta) \Big\{ -\frac{1}{k_i} \int_0^\infty dr\ F_l\ (k_i r)\ U_o(r) \int_0^\infty dr'\ g_l\ (r, r')\ U_o(r')\ F_l\ (k_i r') \Big\} \tag{4.70}$$

i.e. $F_l^{(o)} = F_{l1}^{(o)} + F_{l2}^{(o)}$.

Now, consider the first part of (4.70).

$$F^{(o)}_{\ell 1} = -\frac{1}{k_i^2}\sum_\ell (2\ell+1)\,(P_\ell(\cos\theta)\int_0^\infty dr\, /F_\ell(k_i r)/^2 U_o(r)$$

$$= -\sum_\ell (2\ell+1)\, P_\ell(\cos\theta)\int_0^\infty dr\, r^2/j_\ell(k_i r)/^2 U_o(r)$$

$$= -\sum_\ell (2\ell+1)\, P_\ell(\cos\theta)\int_0^\infty dr\, \frac{\pi}{2k_i r}\, r^2/J_{\ell+1/2}(k_i r)/^2 U_o(r)$$

$$= -\int_0^\infty dr\, r^2 U_o(r)\,\frac{\text{Sin } qr}{qr}$$

We know that

$$\int e^{i\underline{q}\cdot\underline{r}}\, U_o(r)\, dv = 4\pi\int_0^\infty dr\, r^2 U_o(r)\,\frac{\text{Sin } qr}{qr}$$

Thus $F^{(o)}_{\ell 1} = -\frac{1}{4\pi}\int e^{i\underline{q}\cdot\underline{r}}\, U_o(r)\, dv$ which is first Born amplitude. A very similar but lengthy procedure will give

$F^{(o)}_{\ell 2}$ = second Born amplitude, a slight modification on which will give the corresponding term in HHOB. Hence, $F^{(o)}_{\ell}$ can be shown to be equivalent to the Born series, for the potential scattering.

$$\therefore\ f(\theta) = F^{(o)}_\ell + \frac{1}{k_i}\sum_\ell (2\ell+1)\, P_\ell(\cos\theta)\, e^{2i\delta_\ell^{(o)}}\, e^{i\delta_\ell^{(1)}}\ \text{Sin}\ \delta_\ell^{(1)} \tag{4.71}$$

Generalising this to the case of target,

$$F_{fi}(\theta) = \langle f / F^{(o)}_\ell / i\rangle + \frac{1}{k_i}\sum_\ell (2\ell+1)\, P_\ell(\cos\theta)\, e^{i\delta_\ell^{(1)}}\ \text{Sin}\ \delta_\ell^{(1)}\, \langle f/e^{2i\delta_\ell^{(o)}}/i\rangle$$

$$\text{i.e. } F_{fi}(\theta) = F_{HHOB} + f_{PW} \tag{4.72}$$

where $F_{HHOB} = f^{(1)}_{i \to f} + f^{(2)}_{i \to f} + \cdots\cdots$ as given by Yates (1979) for the potential $V_o(r, r_1, r_2 --- r_Z)$ where Z is the atomic number of the target.

$\delta_\ell^{(1)}$ and $\delta_\ell^{(0)}$ are the phase shifts for V_1 and V_o. When $\delta_\ell^{(0)}$ is small, $< f / e^{2i \delta_\ell^{(0)}} / i>$ can be approximated as $1 + 2i < f / \delta_\ell^{(0)} / i >$ (4.73)

An interesting consequence of this arises if we choose V_1 as the exact static potential. Now, $V_o(r, r_T) = V\ (r, r_T) - V_{st}(r)$ where r_T represents target co-ordinates. If $\delta_\ell^{(0)}$ is taken in the Born approximation,

$$< f / \delta_\ell^{(0)} / i> = -2k_i \int dv_T\ \psi^* \psi \int_0^\infty r^2 dr\ \ j_\ell^2 (k_i r)$$

$$(V(r, r_T) - V_{st}(r))$$

$$= -2k_i \int_0^\infty r^2 dr\ j_\ell^2 (k_i r) \int dv_T\ \ \psi^* \psi \left[V(r, r_T) - V_{st}(r) \right]$$

This becomes zero since $\int dv_T\ \psi^* \psi\ V = V_{st}$, the static potential by definition. This happens only when V_{st} is chosen for V_1. Hence, in such cases,

$< f / e^{2i \delta_\ell^{(0)}} / i > = 1$, as a rough approximate.

This reduces computational complexities also. However, if one is particular about retaining the contribution arising from this term, in the evaluation of the second part of (4.72), $\delta_\ell^{(0)}$ may be evaluated by the JWKB approximation to first order in V_o, as is done in the case of the TPE approximation.

Thus (4.72) gives the two potential formula in the high energy higher order Born approximation. It is obvious that the basic idea underlying this formulation is to pull out a static potential $V_{st}(r)$ from the total interaction potential $V\ (r,\ r_T)$. The rest of the inter-action $V_o=V-V_{st}$ is treated in the HHOB approximation and the contribution of V_{st} to the scattering amplitude is calculated through partial wave analysis. When we compare this with the simple HHOB approximation of Yates (1979), it can be seen that in the present two-potential formulation, the Born approximation is applied to a weaker interaction V_o when compared to V, and that part of the interaction, V_{st} is given proper treatment via taking partial waves. Thus, the two potential results should be better than the HHOB results. To demonstrate this, the present two-potential HHOB formulation is applied to electron scattering from H and He in the subsequent sections.

4.8 $\bar{e}$ - H elastic scattering in TPHB

In this section, the elastic scattering of electrons from H atom will be studied in the newly formulated two-potential HHOB (TPHB) approximation. Whenever a new theory is demonstrated, the application to the Hydrogen atom system will be convenient because of many reasons like computational ease, availability of large amount of data - both experimental and theoretical - for comparison, and less scope for mistakes from other sources like choice of wavefunction. Moreover, with respect to this scattering process, the accuracies of various approaches can be criticised with more confidence. Hence if a theory produces better results (in comparison with available data) when applied to this scattering process, the theory can be considered to be a successful one. Hence, naturally, the choice for the demonstration of the TPHB approximation discussed in the previous section fell on $\bar{e} - H$ elastic scattering.

In order to find out the differential cross sections for the ESGH process using the TPHB approximation, it is necessary to evaluate the scattering amplitude (4.72) such that

$$\frac{d\sigma}{d\Omega} = / F_{fi}(Q) /^2 \qquad (4.74)$$

For the ESGH process, the interaction potential

$$V(r, r_1) = -\frac{1}{r} + \frac{1}{/\underline{r} - \underline{r}_1/} \qquad (4.75)$$

$$\text{and } V_o(r, r_1) = V(r, r_1) - V_1(r) \qquad (4.76)$$

In the present study, for the arbitrary central potential $V_1(r)$, the static potential given by Bonham and Strand (1963) is chosen because of the simplicity in calculations and the ease with which the theory may be extended to other atoms. (For all atoms, using this static potential the formulation remains the same with changes only in the coefficients and exponential parameters.).

Thus (4.76) becomes

$$V_o (r, r_1) = V (r, r_1) - V_{st}(r) \qquad (4.77)$$

Now it is obvious that the F_{HHOB} in the scattering amplitude (4.72) represents the amplitude factor evaluated in the HHOB approximation of Yates (1979) for the potential V_o given by (4.77).

$$\therefore F_{HHOB} = f^{(1)}_{i \to f} + f^{(2)}_{i \to f} + \ldots.$$

$$= F_{B1} + i \text{ Im } f B_2 + \text{Re}_1 f B_2 + \text{Re}_2 f B_2$$

$$+ f B_3 + \ldots \qquad (4.78)$$

In the present study, the third Born term is neglected because of the following reasons :

(1) It is found that even for the whole interaction V, the contribution due to this term is very small. Hence, in the present case where the interaction is only $V - V_{st}$, the contribution of the term will be still less.

(2) In order to have a comparison of the present TPHB results with the simple HHOB results, the TPHB results excluding the contribution of the third Born term may be compared with the HHOB results excluding the contribution of the same term. Thus the comparison is justified.

(3) The computational complexity increases tremendously with the attempt to include the third Born term. This type of practical difficulty was felt during the evaluation of the similar third GES term, in the course of the present study.

(4) It was observed during the process of evaluation of the various terms in (4.78) that the contribution due to the Re_2 term in the second Born expression is spuriously large. Hence, the inclusion or exclusion of the less significant third Born term does not make much of a difference because Re_2 and fB_3 are of the same order.

Taking into account the above points, the evaluation of F_{HHOB} reduces to the evaluation of the first and second Born terms in the HHOB approximation, for the interaction potential given by (4.77).

Here $$V_{st}(r) = -\sum_{j=1}^{3} \gamma_j \frac{e^{-\lambda_j r}}{r} \qquad (4.79)$$

where $\lambda_1 = 164.564$ $\gamma_1 = 0.0126671$

$\lambda_2 = 1.3060$ $\gamma_2 = 0.0580612$

$\lambda_3 = 1.48219$ $\gamma_3 = 0.927968$

The evaluation of first Born amplitude is simple.

$$f\,B_1 = -\frac{1}{2\pi} \int dv\, e^{i\underline{q}\cdot\underline{r}} \int \psi^* V_o \psi\, dv_1$$

$$= \frac{2(q^2+8)}{(q^2+4)^2} - 2\sum_j \gamma_j \frac{1}{(q^2+\lambda_j^2)} \qquad (4.80)$$

During the evaluation of the fB_1, it can be noted that the first Born amplitude itself should be very small in the large angle region because of the presence of $\int \psi^* V_o \psi \, dv_1$ because $\int \psi^* V \psi \, dv_1$ is the static potential by definition. Naturally, the contribution due to the higher order Born terms should be proportionately small, which shows the insignificance of the third Born term which is left out in the present study. Moreover, the V_{st} part in the interaction, which is treated through partial wave analysis, should be contributing more to the scattering amplitude. This treatment should improve the present results over the basic HHOB results which overestimate appreciably in the large angle region.

In the evaluation of the second Born term,

$$
\begin{aligned}
U_{fi}^{(2)} &= \langle \psi / \bar{V}_o (P + P_z \hat{\chi}) \, \bar{V}_o (/\underline{q}-\underline{p}/ - P_z \hat{\chi}) / \psi \rangle \\
&= \langle \psi / \bar{V} \, (P + P_z \hat{\chi}) \, \bar{V} \, (/\underline{q}-\underline{p}/ - P_z \hat{\chi}) / \psi \rangle \\
&\quad - 2 \langle \psi / \bar{V} \, (P + P_z \hat{\chi}) \, \bar{V}_{st} \, (/\underline{q}-\underline{p}/ - P_z \hat{\chi}) / \psi \rangle \\
&\quad + \langle \psi / \bar{V}_{st} (P + P_z \hat{\chi}) \, \bar{V}_{st} (/\underline{q}-\underline{p} / - P_z \hat{\chi}) / \psi \rangle
\end{aligned}
\qquad (4.81)
$$

As a result, in the evaluation of the imaginary and two real parts of the second Born term, three terms each will be there, the first term corresponding to the second Born amplitude for the total interaction $V(r, r_1)$, the last term corresponding to the amplitude using the static potential V_{st} and the middle term which is a cross term of V and V_{st}.

Thus $\mathrm{Im}\, fB_2 = \mathrm{Im}_1 + \mathrm{Im}_2 + \mathrm{Im}_3$ (4.82)

$$\mathrm{Re}_1\, fB_2 = \mathrm{Re}_{11} + \mathrm{Re}_{12} + \mathrm{Re}_{13} \qquad (4.83)$$

$$\mathrm{Re}_2\, fB_2 = \mathrm{Re}_{21} + \mathrm{Re}_{22} + \mathrm{Re}_{23} \qquad (4.84)$$

Im_1 for ESGH process is given by (3.17)

$$\mathrm{Im}_2 = \frac{4\pi^3}{k_i} \times (-2) \times \int d\underline{P} < \psi / \bar{V} (P + P_z \hat{\chi}) \; \bar{V}_{st} (q - P - P_z \hat{\chi}) / \psi > \qquad (4.84a)$$

Here

$$\bar{V}_{st} (q - P - P_z \hat{\chi}) = \sum_{i=1}^{3} \frac{-\gamma_i}{2\pi^2} \frac{1}{(/q-p/^2 + P_z{}^2 + \lambda_i{}^2)} \qquad (4.85)$$

Now,

$$\bar{V} (P + P_z \hat{\chi}) = \frac{1}{2\pi^2} \left[\frac{-1}{(P^2 + P_z{}^2)} + \frac{e^{i\,\underline{P}\cdot\underline{r}_1}}{(P^2 + P_z{}^2)} \right]$$

$$\therefore < \psi / \bar{V} (P + P_z \hat{\chi}) / \psi >$$

$$= \frac{-2}{\pi^2 (P^2 + P^2{}_z)} \frac{d}{d\lambda} \frac{1}{P^2 + P_z{}^2 + \lambda^2} - \frac{1}{2\pi^2 (P^2 + P_z{}^2)} \qquad (4.86)$$

$$\therefore \mathrm{Im}_2 = \frac{8\pi^3}{k_i} \sum_j \frac{\gamma_j}{2\pi^2} \int d\underline{P} \left[\frac{-2}{\pi^2 (P^2 + P_z{}^2)} \frac{d}{d\lambda} \frac{1}{P^2 + P^2{}_z + \lambda^2} - \frac{1}{2\pi^2 (P^2 + P_z{}^2)} \right] \frac{1}{(/q-p/^2 + P_z{}^2 + \lambda_j{}^2)}$$

$$= -\frac{8\pi^3}{k_i} \Big\{ \sum_j \frac{\gamma_j}{\pi^4} \int d\underline{P} \frac{d}{d\lambda} \frac{1}{\lambda^2} \frac{1}{(P^2 + \beta^2)} \frac{1}{(/q-p/^2 + \beta^2 + \lambda_j{}^2)}$$

$$+ \sum_j - \frac{\gamma_j}{\pi^4} \int d\underline{P} \frac{d}{d\lambda} \frac{1}{\lambda^2} \frac{1}{(P^2 + \beta^2 + \lambda^2)\; (/q-P/^2 + \beta^2 + \lambda_j{}^2)}$$

$$+ \sum_j \frac{\sqrt{\gamma_j}}{4\pi^4} \int d\underline{P} \, \frac{1}{(P^2+\beta^2)\,(|q-p|^2+\beta^2+\lambda_j^2)} \Big\}$$

$$= -\frac{8\pi^3}{k_i} \sum_j \frac{-\sqrt{\gamma_j}}{\pi^4} \frac{d}{d\lambda} \frac{1}{\lambda^2} \int d\underline{P} \, \frac{1}{(P^2+\beta^2+\lambda^2)(|q-p|^2+\beta^2+\lambda_j^2)}$$

Thus

$$Im_2 = \frac{8\pi^3}{k_i} \sum_j \frac{\sqrt{\gamma_j}}{\pi^4} \frac{d}{d\lambda} \frac{1}{\lambda^2} I_4(\beta^2, \lambda^2, \lambda_j^2) \qquad (4.87)$$

where the integral of the type $I_4\ (\beta^2,\ \lambda^2,\ \lambda_j^2)$ has been come across earlier and is given in the appendix. Now, Im_3 given in (4.82) is the contribution arising from V_{st} only.

$$\therefore\ Im_3 = \frac{4\pi^3}{k_i} \int d\underline{P}\ \bar{V}_{st}(P + P_z \hat{\chi})\ \bar{V}_{st}(q-P-P_z \hat{\chi})$$

$$= \frac{4\pi^3}{k_i} \int d\underline{P}\ \frac{1}{4\pi^4} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\sqrt{\gamma_i}\ \sqrt{\gamma_j}}{(P^2+P_z^2+\lambda_i^2)\ (|q-p|^2+P_z^2+\lambda_j^2)}$$

$$= \frac{1}{\pi k_i} \sum_{i=1}^{3} \sum_{j=1}^{3} \sqrt{\gamma_i}\ \sqrt{\gamma_j}\ I_4\ (\beta^2, \lambda_i^2, \lambda_j^2) \qquad (4.88)$$

Thus Im fB_2 in (4.78) will be the sum of Im_1, Im_2 and Im_3 given by (3.17), (4.87) and (4.88).

A similar procedure can be adopted for $Re_1\ fB_2$ given by

$$Re_1\ fB_2 = -\frac{4\pi^2}{k_i} \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z-\beta}\ U_{fi}^{(2)}$$

On glancing through (4.81), (4.83) and (3.18), it can be easily understood that Re_{11} for the ESGH studied here will be given by the expression (3.18).

Now, $\mathrm{Re}_{12} = + \frac{4\pi^2}{k_i} \times 2 \times \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z - \beta}$

$$\Big\{ \Big[\frac{-2}{\pi^2 (P^2 + P_z^2)} \frac{d}{d\lambda} \frac{1}{P^2 + P_z^2 + \lambda^2} - \frac{1}{2\pi^2 (P^2 + P_z^2)} \Big] \times \sum_{j=1}^{3} \frac{-\gamma_j}{2\pi^2 \left(|q-p|^2 + P_z^2 + \lambda_j^2 \right)} \Big\}$$

Now splitting the terms using partial fraction method and simplifying, $\mathrm{Re}_{12} = \frac{8\pi^2}{k_i} \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z - \beta} \sum_j \Big\{ \frac{\gamma_j}{\pi^4} \frac{d}{d\lambda}$

$$\frac{1}{\lambda^2} \frac{1}{P^2 + P_z^2} \frac{1}{|q-p|^2 + P_z^2 + \lambda_j^2} + \frac{-\gamma_j}{\pi^4} \frac{d}{d\lambda} \frac{1}{\lambda^2} \frac{1}{P^2 + P_z^2 + \lambda^2}$$

$$\frac{1}{|q-p|^2 + P_z^2 + \lambda_j^2} + \frac{\gamma_j}{4\pi^4} \frac{1}{P^2 + P_z^2} \frac{1}{|q-p|^2 + P_z^2 + \lambda^2} \Big\}$$

$$= -8 \frac{\pi^2}{k_i} \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z - \beta} \sum_j \frac{\gamma_j}{\pi^4} \frac{d}{d\lambda} \frac{1}{\lambda^2} \frac{1}{P^2 + P_z^2 + \lambda^2}$$

$$\frac{1}{|q-p|^2 + P_z^2 + \lambda_j^2}$$

$$= \sum_{j=1}^{3} \frac{-8\gamma_j}{\pi^2 k_i} \frac{d}{d\lambda} \frac{1}{\lambda^2} I_5(\beta^2, \lambda^2, \lambda_j^2) \qquad (4.89)$$

where $I_5(\beta^2, \lambda^2, \lambda_j^2)$ has been defined earlier and is shown in the appendix.

By analogy with the imaginary part expressions, Re_{13} can be directly written as

$$\mathrm{Re}_{13} = \frac{-4\pi^2}{k_i} \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z - \beta} \bar{V}_{st} (P + P_z \hat{\chi})$$

$$\bar{\bar{V}}_{st}(/q-p/ - P_z\hat{\chi})$$

$$= \frac{-4\pi^2}{k_i} \; \frac{1}{4\pi^4} \sum_{i=1}^{3} \sum_{j=1}^{3} \gamma_i \; \gamma_j \; \mathcal{P}\!\!\int d\underline{P} \int_{-\infty}^{\infty} dP_z$$

$$\frac{1}{(P_z-\beta).(P^2+P_z^{\,2}+\lambda_i^{\,2}) \; (/q-p/^2+P_z^{\,2}+\lambda_j^{\,2})}$$

$$= \frac{-1}{\pi^2 k_i} \sum_{i=1}^{3} \sum_{j=1}^{3} \gamma_i \; \gamma_j \; I_5(\beta^2,\; \lambda_i^{\,2},\; \lambda_j^{\,2}) \qquad (4.90)$$

where $I_5(\beta^2, \lambda_i^{\,2}, \lambda_j^{\,2})$ is of the same type as the integral defined in (4.89).

Hence the $Re_1 \, fB_2$ term of the F_{HHOB} part (4.78) is the sum of Re_{11}, Re_{12}, Re_{13} given by (3.18), (4.89) and (4.90).

Next is the evaluation of $Re_2 \, fB_2$ in (4.78), for the three terms in $U^{(2)}_{fi}$ given by (4.81).

$$Re_{21} = -\frac{2\pi^2}{k_i^{\,2}} \mathcal{P}\!\!\int d\underline{P} \int_{-\infty}^{\infty} dP_z \; (P^2+P_z^{\,2}) \frac{d}{d\beta} \frac{1}{P_z-\beta}$$

$$< \psi \,/\, \bar{\bar{V}} \,(P + P_z\hat{\chi}) \; \bar{\bar{V}} \,(q - p - P_z\hat{\chi}) \,/\, \psi >$$

$$= \frac{2\pi^2}{k_i^{\,2}} \; \frac{d}{d\lambda} \; \frac{1}{\pi^4} \mathcal{P}\!\!\int d\underline{P} \int_{-\infty}^{\infty} dP_z \; \frac{d}{d\beta} \; \frac{1}{P_z - \beta}$$

$$\frac{(P^2+P_z^{\,2})}{(P^2+P_z^{\,2}) \; (/q-p/^2+P_z^{\,2})} \left[\frac{q^2 + 2\lambda^2}{\lambda^2 \; (q^2+\lambda^2)} - \frac{1}{P^2+P_z^{\,2}+\lambda^2} \right.$$

$$\left. - \frac{1}{/q-p/^2 + P_z^{\,2}+\lambda^2} \right]$$

$$= \frac{2}{\pi^2 k_i^2} \frac{d}{d\lambda} \frac{d}{d\beta} \oint \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z - \beta} \left[\frac{q^2 + 2\lambda^2}{\lambda^2 (q^2+\lambda^2)} \frac{1}{/q-p/^2 + P_z^2} \right.$$

$$\left. - \frac{1}{(P^2+P_z^2+\lambda^2)\ (/q-p/^2+P_z^2)} - \frac{1}{\lambda^2 (P^2+P_z^2)} + \frac{1}{\lambda^2} \frac{1}{P^2 + P_z^2 + \lambda^2} \right]$$

$$= \frac{2}{\pi^2 k_i^2} \frac{d}{d\lambda} \frac{d}{d\beta} \left[\left(\frac{q^2 + 2\lambda^2}{\lambda^2 (q^2+\lambda^2)} - \frac{1}{\lambda^2} \right) I_3(\beta, 0) + \frac{1}{\lambda^2} \right.$$

$$\left. I_3(\beta,\lambda) - I_2(\beta^2,\lambda^2) \right]$$

$$= \frac{2}{\pi^2 k_i^2} \frac{d}{d\lambda} \frac{d}{d\beta} \left[\frac{1}{\lambda^2} I_3(\beta,\lambda) - I_2(\beta^2,\lambda^2) \right] \qquad (4.91)$$

The integrals $I_3(\beta, \lambda)$ and $I_2(\beta^2,\lambda^2)$ are discussed in the appendix. It may be noted that $\frac{d}{d\beta} I_3(\beta, 0) = 0$ since $I_3(\beta, \lambda) = -\pi^3 \left(1 - \frac{2}{\pi} \tan^{-1} \frac{\lambda}{\beta}\right)$

Now taking the second term in $U_{fi}^{(2)}$,

$$Re_{22} = \frac{4\pi^2}{k_i^2} \oint \int d\underline{P} \int_{-\infty}^{\infty} dP_z \, (P^2+P_z^2) \frac{d}{d\beta} \frac{1}{P_z-\beta} \sum_j \left\{ \frac{\gamma_j}{\pi^4} \right.$$

$$\frac{d}{d\lambda} \frac{1}{(P^2+P_z^2)\ (P^2+P_z^2+\lambda^2)} \frac{1}{(/q-p/^2+P_z^2+\lambda_j^2)} + \frac{\gamma_j}{4\pi^4} \frac{1}{P^2+P_z^2}$$

$$\left. \frac{1}{/q-p/^2 + P_z^2 + \lambda_j^2} \right\}$$

After partial fractioning and simplification of the terms,

$$Re_{22} = \frac{4\pi^2}{k_i^2} \oint \int d\underline{P} \int_{-\infty}^{\infty} dP_z \, (P^2+P_z^2) \frac{d}{d\beta} \frac{1}{P_z - \beta} \sum_j$$

$$\frac{-\gamma_j}{\pi^4}\;\frac{d}{d\lambda}\;\frac{1}{\lambda^2}\;\frac{1}{P^2+P_z^{\,2}+\lambda^2}\;\frac{1}{/q-p/^2+P_z^{\,2}+\lambda_j^{\,2}}$$

$$= \sum_j -\frac{4\gamma_j}{\pi^2 k_i^{\,2}}\;\frac{d}{d\lambda}\;\frac{1}{\lambda^2}\mathcal{P}\int d\underline{P}\int_{-\infty}^{\infty} dP_z\,\frac{d}{d\beta}\;\frac{1}{P_z-\beta}$$

$$\frac{P^2+P_z^{\,2}}{(P^2+P_z^{\,2}+\lambda^2)\;(/q-p/^2+P_z^{\,2}+\lambda_j^{\,2})}$$

Now writing $P^2+P_z^{\,2} = (P^2+P_z^{\,2}+\lambda^2)-\lambda^2$ and splitting the above integral into two,

$$Re_{22} = \sum_j \frac{-4\gamma_j}{\pi^2 k_i^{\,2}}\;\frac{d}{d\lambda}\;\frac{1}{\lambda^2}\;\frac{d}{d\beta}\mathcal{P}\int d\underline{P}\int_{-\infty}^{\infty}\frac{dP_z}{P_z-\beta}$$

$$\left[\frac{1}{/q-p/^2+P_z^{\,2}+\lambda_j^{\,2}} - \frac{\lambda^2}{(P^2+P_z^{\,2}+\lambda^2)\;(/q-p/^2+P_z^{\,2}+\lambda_j^{\,2})}\right]$$

$$= \sum_j \frac{-4\gamma_j}{\pi^2 k_i^{\,2}}\;\frac{d}{d\lambda}\;\frac{1}{\lambda^2}\;\frac{d}{d\beta}\left[I_3(\beta,\lambda_j) - \lambda^2 I_5(\beta^2,\lambda^2,\lambda_j^{\,2})\right] \quad (4.92)$$

where $I_3(\beta, \lambda_j)$ is derived in the appendix. $I_5(\beta^2,\lambda^2, \lambda_j^{\,2})$ has also been defined earlier.

Now, Re_{23} arising purely from the static part of $V_o(r, r_1)$ can be evluated using the above principles.

$$Re_{23} = -\frac{2\pi^2}{k_i^{\,2}}\mathcal{P}\int d\underline{P}\int_{-\infty}^{\infty} dP_z\;(P^2+P_z^{\,2})\;\frac{d}{d\beta}\;\frac{1}{P_z-\beta}$$

$$\bar{V}_{st}(P+P_z\hat{\chi})\;\bar{V}_{st}\;(q-p-p_z\hat{\chi})$$

$$= -\frac{2\pi^2}{k_i^{\,2}}\;\frac{1}{4\pi^4}\sum_{i=1}^{3}\sum_{j=1}^{3}\;\gamma_i\;\gamma_j\;\mathcal{P}\int d\underline{P}\int_{-\infty}^{\infty} dP_z$$

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

Again writing $P^2 + P_z^{\ 2}$ as $(P^2 + P_z^{\ 2}+ \lambda_i^{\ 2}) - \lambda_i^{\ 2}$;

$$Re_{23} = - \frac{1}{2\pi^2 k_i^{\ 2}} \sum_{i=1}^{3} \sum_{j=1}^{3} \gamma_i \gamma_j \frac{d}{d\beta} \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z-\beta}$$

$$\left[\frac{1}{/q-p/^2 +P_z^{\ 2}+\lambda_j^{\ 2}} - \frac{\lambda_i^2}{(P^2+P_z^{\ 2}+\lambda_i^{\ 2})\ (/q-p/^2+P_z^{\ 2}+\lambda_j^{\ 2})}\right]$$

$$= - \frac{1}{2\pi^2 k_i^{\ 2}} \sum_{i=1}^{3} \sum_{j=1}^{3} \gamma_i \gamma_j \frac{d}{d\beta} \left[I_3(\beta,\lambda_j) -\lambda_i^{\ 2} \right.$$

$$\left. I_5(\beta^2,\lambda_i^{\ 2},\lambda_j^{\ 2}) \right] \qquad (4.93)$$

where the integrals $I_3(\beta, \lambda_j)$ and $I_5(\beta^2,\lambda_i^{\ 2}, \lambda_j^{\ 2})$ have the same meaning as in (4.92) but for some changes in the values of certain parameters. Hence, the sum of Re_{21}, Re_{22} and Re_{23} given by (4.91), (4.92) and (4.93) will give the Re_2 fB_2 in the HHOB scattering amplitude (4.78). With all the terms evaluated term by term, the F_{HHOB} is now known, for the evaluation of the TPHB scattering amplitude (4.72). Now the task remains only to evaluate the partial wave part of (4.72).

The important part in the partial wave analysis is the evaluation of the phase shifts. Since it is difficult to carry out the infinite summation of the partial waves, the method described earlier was used throughout this study. By this way of summing of the partial waves, the contribution of the less significant higher partial waves also is taken care of through the Born approximation (4.59). For such a type of analysis, the evaluation of the Born and exact phase shifts becomes necessary. The evaluation of the Born phase shift is simple as given in (4.60), whereas the determination of the exact phase shift involves the solution of second order differential equation. In the present study, the Numerov method was developed for the step by step integration of the radial Schro"dinger equation out from the origin into the asymptotic region where the potential has a negligible effect. In this region, $x \geqslant x_A$, 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 equations of the form $Y'' = F(x)\,Y$ (4.94)
It can be written as

$$Y''_j = F\,(x_j)\;Y_j$$

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

$$\left(1-\frac{h^2}{12}F_{j+1}\right)Y_{j+1} = 2\left(1-\frac{h^2}{12}F_j\right)Y_j - \left(1-\frac{h^2}{12}F_{j-1}\right)Y_{j-1} + h^2 F_j Y_j \qquad (4.95)$$

Thus for j=1, we have a formula for determining Y_2 provided we know the two previous ordinates Y_o and Y_1. Here h denotes the step - interval.

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

$$\left(\frac{d^2}{dx^2} + k_i^2 - \frac{\ell(\ell+1)}{x^2} - 2V(x) \right) F_\ell (k_i x) = 0 \qquad (4.96)$$

where k_i is the incident momentum and $V(x) = -(1 + \frac{1}{x})e^{-2x}$

Comparing equations (4.94) and (4.96) $Y = F_\ell (k_i x)$ and

$$F(x) = \frac{\ell(\ell+1)}{x^2} - k_i^2 + 2V(x) \qquad (4.97)$$

Thus if the original two values of

$F_\ell (k_i x)$ at $x = 0$ and $x = 0 + h$ are known, using the Numerov's formula (4.95), the value of $F_\ell (k_i x)$ at $x = x_A$ can be computed. For $x \geqslant x_A$, the potential $V(x)$ can be neglected. At such distances, the differential equation being solved is simply Bessel's equation with the solutions

$$F_\ell (k_i x) \underset{x\to\infty}{\sim} k_i x (A_\ell (k_i) j_\ell (k_i x) - B_\ell (k_i) n_\ell (k_i x)) \qquad (4.98)$$

At $x = x_A$, our algorithm for solving the radial equation (4.96) using Numerov method repetitively out from the origin to $x = X_A$ yields numbers for $F_\ell (x_A)$ and $\frac{dF_1}{dx} \Big/_{x_A}$. The functions $j_\ell (k_i x_A)$ and $n_\ell (k_i x_A)$ can be obtained, for example, from tables. Therefore, the unknown coefficients

$A_\ell(k_i)$ and $B_\ell(k_i)$ of (4.98) can be determined from the pair of equations

$$\frac{F_\ell(x_A)}{k_i x_A} = A_\ell(k_i)\, j_\ell(k_i x_A) - B_\ell(k_i)\, n_\ell(k_i x_A) \qquad (4.99)$$

$$\left[\frac{d}{dx}\left(\frac{F_\ell}{k_i x}\right)\right]_{x_A} = A_\ell(k_i)\left[\frac{dj_\ell}{dx}\right]_{x_A} - B_\ell(k_i)\left[\frac{dn_\ell}{dx}\right]_{x_A} \qquad (4.100)$$

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

$$\tan \delta_\ell(k_i) = \frac{B_\ell(k_i)}{A_\ell(k_i)} \qquad (4.101)$$

Thus, it is obvious that if the two initial values of the solution $F_\ell(k_i x)$ of (4.96) are known, the phase shifts for different ℓ values for corresponding energies can be computed using (4.101) through the procedure discussed 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.

$$F_\ell(k_i x) = \sum_{n=0}^{\infty} a_n\, x^{n+\sigma} \qquad (4.102)$$

Substitution of this in (4.96) yields

$F_\ell(k_i x) \underset{x\to 0}{\sim} x^{\ell+1}$, 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,

$$F_\ell(0) = 0 \qquad \ldots \qquad (4.103)$$

If the numerical integration is begun at $x = 0$, for $\ell > 1$, then $F_\ell(k_i x)$ and $\frac{dF_l}{dx}$ are zero and we get the trivial solution $F_\ell(x) = 0$ 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 term of their series expansion (4.102). Hence $F_\ell(k_i x) = a_o h^{\ell+1}$. However to obtain greater accuracy in the solution than that offered by the leading term at h, one can retain the next terms in expansion.

In the above discussion of the numerical procedure to solve second order differential equation, we have assumed that the potentials V(x) tend to zero exponentially and that at x_A, the value of the independent variable beyond which V (x) can be neglected, the numerical solutions can be fitted to the Bessel functions. However, for potentials which vanish at infinity as x^{-s}, $S \geqslant 1$, x_A value would be very great indeed if we adopt the step by step procedure discussed above. This would have the following undesirable consequences: (1) greater amount of computer time required (2) the accumulative effects of truncation in the numerical formulas. Hence for such long range potentials some corrections like the WKB method or the numerical procedure due to Burke and Schey (1962) should be made after stopping the integration at some x_A. However, for exponential potentials - which are used in the present study - the inaccuracy due to the above mentioned reasons will be negligible. This fact is obvious from the later analysis of the phase shift values obtained in the present study.

The two principal disadvantages of the above - discussed Numerov method are (1) the process of getting the method started (2) the difficulty in changing the mesh-size. In the Runge-Kutta Method of solving the differential equation, both the above disadvantages are absent. It is a self-starting method and the step-size can be changed at any point in the integration. (Refer Kenneth Smith). Hence, in the present study, both the procedures - i.e. Numerov method and Runge Kutta method - were used to find the phase shifts for the Yukawa type of potentials. It was found that the results almost coincide.

For the purpose of checking the computer programme set up in the present study for the evaluation of the Born (4.60) and exact (4.101) phase 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 4.7. It may be noted that for higher values of , both the phase-shifts approach each other. The exact phase shifts are calculated in two ways: using the Numerov method and the Runge-Kutta method for solving the differential equation (4.96). It can be seen that the results (second and third columns of table (4.7) almost coincide.

Thus for the Yukawa type of static potential (4.79), the phase shift in the Born approximation (4.60) is given by

$$\delta_{\ell}^{(1)} = \frac{1}{k_i} \sum_{j=1}^{3} \gamma_j \, Q_{\ell}\left(\frac{2k_i^2 + \lambda_i^2}{2k_i^2} \right) \tag{4.105}$$

where Q_{ℓ} represents the defined polynomials tabulated as

$$Q_o(x) = \frac{1}{2} \ln \frac{1+x}{1-x}$$

$$Q_1(x) = \frac{x}{2} \ln \frac{1+x}{1-x} - 1 \quad \text{etc.}$$

The exact phase shifts for the static potential (4.79) are determined using the Numerov method described earlier. Both the phase shifts are compared and the ℓ value is so fixed that beyond this value of ℓ, the phase shifts differ by less than 3%.

Now, another major step in the evaluation of the F_{pw} (4.72) is the evaluation of the quantity $\langle f/e^{2i\delta_{\ell}^{(o)}}/i\rangle$. Here, taking the JWKB approximation,

$$2\delta_{\ell}^{(o)} = X = X_o + \Delta X \text{ as given in (4.45)}$$

Here $$X_o = \frac{2}{k_i}\left[\ln \left| \frac{b-b_1}{b} \right| - \sum_{j=1}^{3} \gamma_j \, K_o(b\lambda_j)\right] \tag{4.106}$$

where K_o is defined earlier.

Now $$\Delta x = \frac{2}{k_i} V_o^{(z=0)} \left\{ \int_0^{\infty} dz - \int_0^{\infty} dz + \int_o^{\infty} \sum_j \frac{\gamma_j}{2E} e^{\frac{-\lambda_j r}{z^2}} r \, dz \right\}$$

$$= \frac{1}{k_i E} \left\{ \frac{1}{(|b-b_1|^2 + z_1^2)^{1/2}} - \frac{1}{b} + \sum_j \gamma_j \frac{e^{-\lambda_j b}}{b} \right\} \sum_j \gamma_j \left(\frac{d}{d\lambda_j}\right) \lambda_j K_0 (b\lambda_j) \tag{4.107}$$

Now $\Gamma = \langle f / e^{i(x_o + \Delta x)} / i \rangle$

$$= e^{-\frac{2i}{k_i} \sum_j \gamma_j K_o (b \lambda_j) + \frac{i x_1}{k_i E} [\sum_j \gamma_j \frac{e^{-\lambda_j b}}{b} - \frac{1}{b}]}$$

$$\langle f / e^{(\frac{2i}{k_i} \ln \frac{/b-b_1/}{b} + \frac{ix_1}{k_i E} \frac{1}{(/b-b_1/^2+z_1{}^2)^{1/2}})} / i \rangle \quad (4.108)$$

where

$$x_1 = \sum_i \gamma_i (\frac{d}{d\lambda_i}) \lambda_i K_o (b \lambda_i)$$

$$\therefore \Gamma = Y \langle f / (\frac{/b-b_1/}{b})^{2i/k_i} [1 + \frac{i}{k_i E} \frac{x_1}{(/b-b_1/^2+z_1^2)^{1/2}}] / i \rangle$$

where

$$Y = e^{(-\frac{2i}{k_i} \sum_j \gamma_j K_o (b \lambda_j) + \frac{ix_1}{k_i E} [\sum_j \gamma_j \frac{e^{-\lambda_j b}}{b} - \frac{1}{b}])}$$

In the evaluation of the above expression, the assumption is taken that $b << b_1$

so that $(\frac{/b-b_1/}{b})^{2i/k_i} = (\frac{b_1}{b})^{2i/k_i}$

Now the evaluation of Γ is possible using the standard integration techniques which is little lengthy, thus giving

$$\Gamma = \frac{Y}{b^{\mathcal{L}}} \left\{ \frac{\Gamma(2 + \frac{\mathcal{L}}{2}) \Gamma(1 + \frac{\mathcal{L}}{2}) + \frac{i}{k_i E} x_1 \Gamma(1 + \frac{\mathcal{L}}{2})}{\Gamma(1 + \frac{\mathcal{L}}{2})} \right. \quad (4.109)$$

where $\mathcal{L} = \frac{2i}{k_i}$ and X_1 and Y are same as defined above. The expression for Γ can further be simplified using some simple mathematical conversions.

Thus if Γ can be written as e^{iy} ($e + if$) where

$$Y = -\frac{2}{k_i} \sum_j \gamma_j \; K_o(b\lambda_j) + \frac{X_1}{k_i E} \left[\sum_j \gamma_j \frac{e^{-\lambda_j b}}{b} - \frac{1}{b} \right] - \frac{2}{k_i} \ln b,$$

..(4.110)

$$\text{then } F_{PW} = \frac{1}{k_i} \sum_{\ell} (2\ell + 1)\, P_{\ell}\, (\cos \Theta)\, \sin \delta_{\ell}^{(1)}$$

$$\left[(e \cos \mathcal{L} - f \sin \mathcal{L}) + i\,(f \cos \mathcal{L} + e \sin \mathcal{L}) \right] \qquad (4.111)$$

where $\mathcal{L} = \delta_{\ell}^{(1)} + Y$ where $\delta_{\ell}^{(1)}$ is the phase shift for $V_1 = V_{st}^{(r)}$. Now using different values of phase shifts in the exact and Born methods, the ℓ value upto which the above series may be summed is fixed at N and the summation is carried out as described in (4.59). With the help of the tabulated values for the polynomials P $(\cos \Theta)$ such as $P_o(\cos \Theta) = 1, P_1(\cos \Theta) = \cos \Theta$ etc. the evaluation of F_{PW} in (4.72) becomes easy. From the knowledge of the complete expression for the scattering amplitude (4.72), the DCS may be computed.

In order to obtain the total cross sections in the TPHB approximation, the usual expression for TCS may be used.

$$\text{Thus} \quad \sigma^{tot} = \frac{4\pi}{k_i} \operatorname{Im} F_{fi} (\Theta) \Big|_{q=0}$$

$$= \frac{4\pi}{k_i} \left\{ \operatorname{Im} FB_2 \Big/_{q=0} + \operatorname{Im} F_{PW} \Big/_{q=0} \right\}$$

$$= \frac{4\pi}{k_i} \left\{ \mathrm{Im}_1 /_{q=0} + \mathrm{Im}_2 /_{q=0} + \mathrm{Im}_3 /_{q=0} + \frac{1}{k_i} \sum_{\ell} (2\ell+1) \sin \delta_\ell^{(1)} \right.$$

$$\left. (f \cos \mathcal{L} + e \sin \mathcal{L}) \right\} \qquad (4.112)$$

From the expression (3.17) for Im_1, it is obvious that

$$\mathrm{Im}_1 /_{q=0} = \frac{-4}{\pi k_i} \frac{d}{d\lambda} \frac{1}{\lambda^2} 2 \int \frac{d\underline{P}}{(P^2+\beta^2)(P^2+\beta^2+\lambda^2)}$$

which may be simplified using the substitution $P^2+\beta^2 = x$ to give $\mathrm{Im}_1 /_{q=0} = \frac{1}{k_i} \left(\ln \frac{\beta^2+4}{\beta^2} - \frac{2\beta^2}{\beta^2+4} \right)$ (4.113)

From the expression for Im_2 (4.87),

$$\mathrm{Im}_2 /_{q=0} = \sum_{j=1}^{3} \frac{8 \gamma_j}{\pi k_i} \frac{d}{d\lambda} \frac{1}{\lambda^2} \int \frac{d\underline{P}}{(P^2+\beta^2+\lambda^2)(P^2+\beta^2+\lambda_j^2)}$$

where the substitution $P^2+\beta^2+\lambda^2 = x$ will be convenient. Thus using standard integrals,

$$\mathrm{Im}_2 /_{q=0} = \sum_{j=1}^{3} \frac{8 \gamma_j}{k_i} \left\{ \frac{-1}{(\lambda_j^2-4)(\beta^2+4)} + \ln \frac{\beta^2+\lambda_j^2}{\beta^2+4} \right.$$

$$\left. \left[\frac{1}{(\lambda_j^2-4)^2} - \frac{1}{4(\lambda_j^2-4)} \right] \right\} \qquad (4.114)$$

Further, making use of expression (4.88) and proceeding similarly as in the previous cases,

$$\mathrm{Im}_3 /_{q=0} = \frac{4\pi^3}{k_i} \int d\underline{P} \frac{1}{4\pi^4} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\gamma_i \gamma_j}{(P^2+\beta^2+\lambda_i^2)(P^2+\beta^2+\lambda_j^2)}$$

$$= \begin{cases} \frac{1}{k_i} \sum_i \sum_j \frac{\gamma_i \gamma_j}{\lambda_j^2 - \lambda_i^2} \ln \left(\frac{\beta^2 + \lambda_j^2}{\beta^2 + \lambda_i^2} \right) & \text{when } \lambda_i \neq \lambda_j \\ \frac{1}{k_i} \sum_i \sum_j \frac{\gamma_i \gamma_j}{\beta^2 + \lambda_j^2} & \text{when } \lambda_i = \lambda_j \end{cases} \qquad \ldots(4.115)$$

Substitution of the expressions (4.113), (4.114) and (4.115) in (4.112) will give the total cross sections for the ESGH process in the two-potential HHOB approximation.

Another study performed in the present work was with regard to the significance of ΔX in the phase shift. For this, the differential cross sections were obtained after suppressing the ΔX part in the expression for X and using only X_o. The resulting Γ for this case will be

$$\Gamma = e^{\left(-\frac{2i}{k_i} \sum_j \gamma_j K_o(b \lambda_j) \right)} < f / e^{\frac{2i}{k_i} \ln \frac{|b-b_1|}{b}} / i >$$

which is much simpler compared to the Γ given by (4.108). But in actual practice, the inclusion of ΔX part in the expression for X resulted in only a negligible contribution for energies greater than 100 eV. Similar was the case reported in two-potential eikonal approximation (Ishihara and Chen 1975) also. Thus it was concluded that ΔX can be neglected for computations involving incident energies greater than 100 eV without any significant error.

Another important scattering parameter, the total elastic cross-section (TEC) can be calculated using

$$\sigma_{el} = 2\pi \int_0^{\pi} \frac{d\sigma}{d\Omega} \sin \theta \, d\theta \qquad \text{----} \qquad (4.116)$$

Results and Discussion :

The differential cross sections, total cross-sections and total elastic cross sections are calculated for the ESGH process in the two-potential HHOB approximation as discussed above for a variety of incident energies and a wide range of scattering angles. In figures (4.12) and (4.13) the present TPHB DCS are shown at incident energies 100 eV and 400 eV alongwith other theoretical and experimental data (experimental data of Williams (1975) and Van Wingerden et al (1977), EBS results of Byron and Joachain (1977), and HHOB (Yates 1979) results). From the figures, it is obvious that the present results agree with experimental values nicely over the entire angular region. Since the present TPHB formulation was basically an attempt to improve upon the HHOB method of Yates (1979), the real comparison should be made between the results produced in both the methods i.e. curves A and B. It may be noted that in the present TPHB calculations, the contribution due to third Born term is neglected on the basis of the assumptions drawn earlier. However, this type of reasonable comparison between the curves asserts that the improvements whatsoever obtained are due to the approximation introduced and not due to the inclusion or exclusion of any particular term. Thus the avoiding of the laborious third Born evaluation finds enough justification.

In the HHOB approximation, Re $f_{HEA}^{(3)} = f_1^{(3)} + f_2^{(3)}$ and if $\beta = 0$, then only $f_1^{(3)}$ remains such that Re $f_{HEA}^{(3)}$ $(\beta = 0) = f_1^{(3)} (\beta = 0) = f_{GES}^{(3)}$. In the high energy approximation, $\beta = \frac{\Delta E}{k_i}$ being very small, it can be approximated as zero in practical situations for the sake of simplicity. The contribution of β in the scattering amplitudes is small (as seen in the comparison between the imaginary terms in the GES and Born methods) when compared to the important part played by it in saving some of the integrals from divergence problem (comparison between GES and HHOB integrals). Hence the significance of the β factor. Keeping all these points in mind, third Born term can be approximated to the third GES term within a certain accuracy. Thus in the present study the HHOB calculations were done incorporating the third GES term. However, it was observed that, curve A, only gives better agreement with experimental values reported in the recent past.

The main attraction of present TPHB results is that it gives reasonably good results even at lower energies, for the entire angular range. Since the total interaction V is replaced by a reduced interaction $V - V_1$ in the TPHB approximation, the lower limit of E can also be pulled down slightly such that $\frac{V}{E} << 1$. Hence the approximation should give better results than in the simple HHOB approximation in the case of lower energy of incidence also. From the comparison between the two figures (4.12) and (4.13) at 100 eV and 400 eV, it can be readily observed that as expected the results improve with higher incident energies. But the most covetable feature of the present TPHB results is the very satisfactory cross sections in the large angle region. The general experience is that many a theory which gives quite good results at small angles, gives poorer results at large angles. Same is the case with the HHOB approximation of Yates (1979). Hence, the improvement of the present TPHB results over the Yates' method is most significant in the large angle region. At all energies, the two-potential HHOB results are far better than the simple HHOB approximation at large angles.

In table (4.8) the present DCS in the two potential formulation are given at certain sample energies 100 eV, 200 eV and 400 eV. Since the summation of the partial waves as described elsewhere 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 chosen values of incident energies, at which quite a lot of data is available for comparison. However, the present work can be carried out for other energies also if required, without much difficulty. Since the motivation behind the present TPHB formulation was the necessity to modify the HHOB approximation, the prime interest in the present study was only comparison between the two sets of results, which can be carried out with two or tnree sets of data.

In tables (4.9) and (4.10), the total collision cross sections (TCS) and total elastic cross sections (TEC) for the ESGH process calculated in the two potential HHOB approximation using expressions (4.112) and (4.116) are given, alongwith other data for comparison. The present results are quite encouraging and as in the case of DCS, the TCS and TEC results also improve with higher incident energies.

4.9 $\bar{e}$ - He elastic scattering in TPHB :

The success of the TPHB approximation in describing the ESGH process as demonstrated in the previous section is the main motivation behind the application of this approximation to EHe process. The study of EHe process is computationally rather more cumbersome than the ESGH process. Naturally, with an increasing atomic number, the interaction potential as well as the wave function of the atom are bound to become more and more complicated. This increasing complexity results in studies which are centred on lighter atoms - sometimes even the lightest atom, hydrogen. With the advent of the hydrogen - like representations of the alkali atoms through core approximations, the study of such atoms is rendered easier. But the helium atom, with no such facility for simplification, remains a computational hurdle in the atomic collision theory. A comparison of the expressions to be given in this section with their counterparts in the previous section will give a quick idea regarding the increasing computational complexity as we go from H to He. However, inspired by the results of the previous section, a study of the more complicated EHe process using the TPHB approximation is undertaken in this section.

For the EHe process, the interaction potential is given by

$$V\ (r, r_1, r_2) = -\frac{2}{r} + \frac{1}{/\underline{r} - \underline{r}_1/} + \frac{1}{/\underline{r} - \underline{r}_2/} \qquad (4.117)$$

and $V_o\ (r,\ r_1,\ r_2) = V\ (r,\ r_1,\ r_2) - V_1(r)$. Here also, for the arbitrary central potential $V_1(r)$, the static potential of Bonham and Strand (1963) is chosen, considering the simplicity rendered by this choice as well as the reliability of this potential as experienced in the previous section.

$$\text{Thus } V_o\ (r,\ r_1, r_2) = V\ (r, r_1, r_2) - V_{st}(r) \qquad (4.118)$$

$$\text{where } V_{st}(r) = -\ 2 \sum_{j=1}^{3} \gamma_j \frac{e^{-\lambda_j r}}{r} \qquad (4.119)$$

The procedure for the evaluation of the scattering amplitude in the TPHB approximation can be carried out exactly parallel to the study of the ESGH process. Hence, the first problem is the evaluation of F_{HHOB} given by (4.78). For this purpose, the ground state wave function of He is taken as the Hartree - Fock wave function given by Byron and Joachain (1966).

$$\Psi(r_1, r_2) = \phi_{1s}(r_1)\ \phi_{1s}(r_2) \qquad (4.120)$$

$$\text{with}\quad \phi_{1s}(r) = \frac{1}{\sqrt{4\pi}}\left(A\ e^{-Y_1 r} + B\ e^{-Y_2 r}\right)$$

where $A = 2.60505$, $B = 2.08144$

$Y_1 = 1.41$, $Y_2 = 2.61$

The evaluation of the first Born amplitude in (4.78) is simple which comprises of two parts resulting from the two parts of V_o(4.118). The first part has been evaluated in an earlier section whereas the evaluation of the second part is exactly similar to its counterpart in the previous section, but for the numerical values of certain parameters. Hence the first Born amplitude can be derived as

$$f\,B_1 = \sum_{k=1}^{9} \frac{8\,D_k}{q^2}\left[\frac{2}{K_{1k}^3 K_{2k}^3} - \frac{K_{1k}}{K_{2k}^3(q^2+K_{1k}^2)^2} - \frac{K_{2k}}{K_{1k}^3(q^2+K_{2k}^2)^2}\right] - 4\sum_{j=1}^{3}\frac{\gamma_j}{(q^2+\lambda_j^2)} \quad .. \qquad (4.121)$$

where D_k, K_{1k} and K_{2k} are same as given in table (3.9), γ_j and λ_j are defined constants and q is the momentum transfer.

As in the case of ESGH process in the present EHe process also, $U^{(2)}_{fi}$ which appears in the second Born amplitude is given by (4.81). As a result, each term (imaginary, Real 1 and Real 2) in the second Born expression will consist of three terms each and can be written as

$$\left.\begin{aligned} \mathrm{Im}\ fB_2 &= \mathrm{Im}_1 + \mathrm{Im}_2 + \mathrm{Im}_3 \\ \mathrm{Re}_1\ fB_2 &= \mathrm{Re}_{11} + \mathrm{Re}_{12} + \mathrm{Re}_{13} \\ \mathrm{Re}_2\ fB_2 &= \mathrm{Re}_{21} + \mathrm{Re}_{22} + \mathrm{Re}_{23} \end{aligned}\right) \qquad (4.122)$$

For the $\bar{e}$ - He scattering,

$$\bar{V}\,(P + P_z\hat{\chi}) = \frac{1}{2\pi^2(P^2+P_z^2)}\,\left(e^{i\,\underline{p}\cdot\underline{r}_1} + e^{i\underline{p}\cdot\underline{r}_2} - 2\right)$$

$$\text{and } \bar{V}_{st}\,(q - p - P_z\hat{\chi}) = \sum_{i=1}^{3} \frac{-\gamma_j}{\pi^2(/q-p/^2+p_z^2+\lambda_i^2)} \qquad (4.123)$$

The evaluation of Im_1 involves the first term in (4.81), which is the $U^{(2)}_{fi}$ defined by (3.37)

Since $\mathrm{Im}\ fB_2 = \frac{4\pi^3}{k_i} \int d\underline{P}\ U^{(2)}_{fi}$, Im_1 is given by (3.38).

$$\text{Now } \mathrm{Im}_2 = -\frac{8\pi^3}{k_i} \int d\underline{P} < \psi \,/\, \bar{V}\,(P + P_z\hat{\chi}) / \,\psi > \bar{V}_{st}\,(q-P-P_z\hat{\chi})$$

$$= -\frac{8\pi^3}{k_i} \int d\underline{P} \left\{ \frac{-1}{4\pi\,(P^2+P_z^2)} \sum_{k=1}^{9} \sum_{j=1}^{3} D_k\, \gamma_j \left[\frac{1}{K_{2k}^3} \left(-\frac{d}{dK_{1k}}\right) \frac{1}{P^2+P_z^2+K_{1k}^2} + \frac{1}{K_{1k}^3}\left(-\frac{d}{dK_{2k}}\right) \frac{1}{(P^2+P_z^2+K_{2k}^2)} - \frac{4}{K_{1k}^3\ K_{2k}^3} \right] \frac{1}{(/q-p/^2 + P_z^2+\lambda_j^2)} \right\}$$

which can be simplified using partial fraction method and can be broken up into integrals come across earlier.

Thus $$\mathrm{Im}_2 = \frac{8}{\pi k_i} \sum_{k=1}^{9} \sum_{j=1}^{3} D_k \gamma_j \left\{ \frac{1}{K_{2k}^3} \left(\frac{d}{dK_{1k}} \right) \frac{1}{K_{1k}^2} I_4(\beta^2, K_{1k}^2, \lambda_j^2) + \frac{1}{K_{1k}^3} \left(\frac{d}{dK_{2k}} \right) \frac{1}{K_{2k}^2} I_4(\beta^2, K_{2k}^2, \lambda_j^2) \right\} \qquad (4.124)$$

Here D_k, K_{1k} and K_{2k} are same as defined above. The constants originating from the static potential are given as

$\lambda_1 = 85.4037$ $\gamma_1 = 4.0832\text{-}03$
$\lambda_2 = 7.8945$ $\gamma_2 = 1.1249\text{-}01$
$\lambda_3 = 1.4502$ $\gamma_3 = 8.8296\text{-}01$

Now, $\mathrm{Im}_3 = \frac{4\pi^3}{k_i} \int d\underline{P}\ \bar{V}_{st}(P + P_z\hat{\chi})\ \bar{V}_{st}(q - P - P_z\hat{\chi})$

Considering the analogy between the $\bar{V}_{st}$ for ESGH process and EHe process (given by 4.85 and 4.123) it can be seen that there is change only in the values of the coefficients and the exponential parameters. Thus the derivation of Im_3 should be similar to the Im_3 for ESGH process, but for the above changes. Thus Im_3 for EHe process can straightway be written as

$$\mathrm{Im}_3 = 4 \frac{1}{\pi k_i} \sum_{i=1}^{3} \sum_{j=1}^{3} \gamma_i \gamma_j I_4(\beta^2, \lambda_i^2, \lambda_j^2) \qquad (4.125)$$

where λ_i and γ_i are as defined above.

Now the real part I of (4.78) is evaluated. From (4.81)

$$Re_{11} = -\frac{4\pi^2}{k_i} \wp \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z-\beta} < \psi / \bar{V} (P+P_z \hat{\chi}) \bar{V} (q-P-P_z \hat{\chi})/\psi>$$

which is same as the $\wp Re_1$ evaluated in section (3.4). Thus Re_{11} is given by (3.39).

$$Re_{12} = \frac{8\pi^2}{k_i} \wp \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z-\beta} < \psi / \bar{V} (P+P_z \hat{\chi})/\psi > \bar{V}_{st} (q-P-P_z \hat{\chi})$$

$$= \frac{8\pi^2}{k_i} \wp \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z-\beta} \left\{ \sum_{k=1}^{9} \sum_{j=1}^{3} \frac{D_k \gamma_j}{\pi^4 (P^2+P_z^2)(/q-p/^2+P_z^2+\lambda_j^2)} \right.$$

$$\left[\frac{1}{K_{2k}^3} \frac{d}{dK_{1k}} \frac{1}{P^2+P_z^2+K_{1k}^2} + \frac{1}{K_{1k}^3} \frac{d}{dK_{2k}} \frac{1}{P^2+P_z^2+K_{2k}^2} \right.$$

$$\left. \left. + \frac{4}{K_{1k}^3 \; K_{2k}^3} \right] \right\}$$

This can be also brought to the integrals of known form by the method of partial fractions. Finally,

$$Re_{12} = \frac{-8}{\pi^2 k_i} \sum_{k=1}^{9} \sum_{j=1}^{3} D_k \gamma_j \left\{ \frac{1}{K_{2k}^3} \left(\frac{d}{dK_{1k}} \right) \frac{1}{K_{1k}^2} I_5 \right.$$

$$\left. (\beta^2, K_{1k}^2, \lambda_j^2) + \frac{1}{K_{1k}^3} \left(\frac{d}{dK_{2k}} \right) \frac{1}{K_{2k}^2} I_5 (\beta^2, K_{2k}^2, \lambda_j^2) \right\}$$

... (4.126)

Here D_k, K_{1k}, K_{2k}, λ_j, γ_j etc. have the same values as in their counterparts in imaginary terms.

$$Re_{13} = \frac{-4\pi^2}{k_i} \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z - \beta} \bar{V}_{st}(P + P_z \hat{\chi}) \bar{V}_{st}(q - P - P_z \hat{\chi})$$

can be compared with similar Re_{13} in ESGH process. Thus in the present case

$$Re_{13} = \frac{-4}{\pi^2 k_i} \sum_{i=1}^{3} \sum_{j=1}^{3} \gamma_i \gamma_j \, I_5 \, (\beta^2, \lambda_i^2, \lambda_j^2) \tag{4.127}$$

Thus $Re_1 fB_2$ term of the F_{HHOB} part (4.78) for the E He process will be the sum of Re_{11}, Re_{12} and Re_{13} given by (3.39), (4.126), and (4.127).

In order to evaluate $Re_2 fB_2$, a parallel procedure as was used in the ESGH process may be adopted. Thus,

$$Re_{21} = \frac{-2\pi^2}{k_i^2} \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} dP_z \, (P^2 + P_z^2) \frac{d}{d\beta} \frac{1}{P_z - \beta}$$

$$< \psi / \bar{V} (P + P_z \hat{\chi}) \bar{V} (q - P - P_z \hat{\chi}) / \psi >$$

Using the expression (3.37) for $< \psi / \bar{V} \bar{V} / \psi >$ in the above term,

$$Re_{21} = \frac{-2\pi^2}{k_i^2} \mathcal{P} \int d\underline{P} \int_{-\infty}^{\infty} dP_z (P^2 + P_z^2) \frac{d}{d\beta} \frac{1}{P_z - \beta}$$

$$\frac{1}{(P^2 + P_z^2)(/q-p/^2 + P_z^2)} \frac{1}{4\pi^4} \sum_{k=1}^{9} D_k \left\{ \frac{4K_{1k}}{K_{2k}^3 (q^2 + K_{1k}^2)^2} \right.$$

$$\left. + \frac{4K_{2k}}{K_{1k}^3 (q^2 + K_{2k}^2)^2} + \frac{16}{K_{1k}^3 K_{2k}^3} + \left(\frac{d}{dK_{1k}} \right) \left[\frac{4}{K_{2k}^3 B_1} + \frac{4}{K_{2k}^3 A_1} \right] \right.$$

$$+\left(\frac{d}{dK_{2k}}\left[\frac{4}{K_{1k}^3\,B_2}+\frac{4}{K_{1k}^3\,A_2}\right]+\frac{d}{dK_{1k}}\,\frac{d}{dK_{2k}}\left(\frac{1}{B_1\,A_2}+\frac{1}{A_1\,B_2}\right)\right\}$$

where A_1, B_1, A_2, B_2 are defined in (3.37).

$$\therefore\ Re_{21} = -\frac{1}{2\pi^2 k_i^2}\sum_{k=1}^{9} D_k \frac{d}{d\beta}\left\{\left[\frac{4K_{1k}}{K_{2k}^3\,(q^2+K_{1k}^2)^2}\right.\right.$$

$$\left.+\frac{4K_{2k}}{K_{1k}^3(q^2+K_{2k}^2)^2}+\frac{16}{K_{1k}^3\;K_{2k}^3}\right] I_3(\beta,0)+\frac{4}{K_{2k}^3}\left(\frac{d}{dK_{1k}}\right)$$

$$\left[I_2(\beta^2,K_{1k}^2)+\frac{1}{K_{1k}^2}I_3(\beta,0)-\frac{1}{K_{1k}^2}I_3(\beta,K_{1k}^2)\right]+\frac{4}{K_{1k}^3}\left(\frac{d}{dK_{2k}}\right)$$

$$\left[I_2(\beta^2,K_{2k}^2)+\frac{1}{K_{2k}^2}I_3(\beta,0)-\frac{1}{K_{2k}^2}I_3(\beta,K_{2k}^2)\right]+\frac{d}{dK_{1k}}$$

$$\frac{d}{dK_{2k}}\left[\frac{1}{K_{2k}^2}I_2(\beta^2,K_{1k}^2)-\frac{1}{K_{2k}^2}I_5(\beta^2,K_{1k}^2,K_{2k}^2)\right.$$

$$\left.\left.-\frac{1}{K_{1k}^2}I_5(\beta^2,K_{1k}^2,K_{2k}^2)+\frac{1}{K_{1k}^2}I_2(\beta^2,K_{2k}^2)\right]\right\}$$

Since $\frac{d}{d\beta}\,I_3(\beta,0)=0$, simplification of the above expression yields

$$Re_{21} = -\frac{1}{2\pi^2 k_i^2}\sum_{k=1}^{9} D_k\frac{d}{d\beta}\left\{\frac{2}{K_{2k}^3}\left(\frac{d}{dK_{1k}}\right)\right.$$

$$\left[I_2(\beta^2,K_{1k}^2)-\frac{2}{K_{1k}^2}I_3(\beta,K_{1k}^2)\right]+\frac{2}{K_{1k}^3}\left(\frac{d}{dK_{2k}}\right)$$

$$\left[I_2(\beta^2,K_{2k}^2)-\frac{2}{K_{2k}^2}I_3(\beta,K_{2k}^2)\right]-\left(\frac{d}{dK_{1k}}\right)\left(\frac{d}{dK_{2k}}\right)$$

$$\left.\left[\frac{1}{K_{2k}^2}I_5(\beta^2,K_{1k}^2,K_{2k}^2)+\frac{1}{K_{1k}^2}I_5(\beta^2,K_{1k}^2,K_{2k}^2)\right]\right\} \qquad (4.128)$$

$$\text{Now } Re_{22} = \frac{4\pi^2}{k_i^2}\,\mathcal{P}\int d\underline{P}\int_{-\infty}^{\infty} dP_z\,(P^2+P_z^2)\,\frac{d}{d\beta}\,\frac{1}{P_z-\beta}$$

$$\left\{\sum_{k=1}^{9}\sum_{j=1}^{3}\frac{D_k\gamma_j}{\pi^4(P^2+P_z^2)\,(/q-P/^2+P_z^2+\lambda_j^2)}\left[\frac{1}{K_{2k}^3}\frac{d}{dK_{1k}}\frac{1}{P^2+P_z^2+K_{1k}^2}+\frac{1}{K_{1k}^3}\frac{d}{dK_{2k}}\frac{1}{P^2+P_z^2+K_{2k}^2}+\frac{4}{K_{1k}^3\,K_{2k}^3}\right]\right\}$$

$$=\frac{4}{\pi^2k_i^2}\sum_{k=1}^{9}\sum_{j=1}^{3}D_k\,\gamma_j\,\frac{d}{d\beta}\left\{\frac{1}{K_{2k}^3}\frac{d}{dK_{1k}}I_5(\beta^2,K_{1k}^2,\lambda_j^2)+\frac{1}{K_{1k}^3}\frac{d}{dK_{2k}}I_5(\beta^2,K_{2k}^2,\lambda_j^2)+\frac{4}{K_{1k}^3\,K_{2k}^3}I_3(\beta,\lambda_j)\right\} \qquad \ldots (4.129)$$

$$Re_{23}=-\frac{2\pi^2}{k_i^2}\,\mathcal{P}\int d\underline{P}\int_{-\infty}^{\infty}dP_z\,(P^2+P_z^2)\,\frac{d}{d\beta}\,\frac{1}{P_z-\beta}\,\bar{V}_{st}(P+P_z\hat{\chi})\,\bar{V}_{st}(q-P-P_z\hat{\chi})$$

Considering the analogy between the $\bar{V}_{st}$ for H and He(4.85) and (4.123) Re_{23} can be directly written from (4.93) as

$$Re_{23}=-\frac{2}{\pi^2k_i^2}\sum_{i=1}^{3}\sum_{j=1}^{3}\gamma_i\,\gamma_j\,\frac{d}{d\beta}\left[I_3(\beta,\lambda_j)-\lambda_i^2\,I_5(\beta^2,\lambda_i^2,\lambda_j^2)\right] \qquad \ldots .(4.130)$$

Now $Re_2\,fB_2 = Re_{21}+Re_{22}+Re_{23}$ given by (4.128),(4.129) and (4.130).

Now, with all the terms in (4.78) being evaluated, F_{HHOB} is known for the evaluation of the TPHB amplitude for E He process. Now the partial wave part F_{PW} of (4.72) has to be evaluated for the same process. For this

$$X_o(\underline{b}, \underline{b}_1, \underline{b}_2) = \frac{2}{k_i}\left[\ln \frac{/\underline{b}-\underline{b}_1/\cdot/\underline{b}-\underline{b}_2/}{b^2} - \sum_j 2\,\gamma_j\,K_o(b\lambda_j)\right] \qquad (4.131)$$

ΔX is neglected assuming that it will not be much significant.

$$\therefore \quad \Gamma_{fi}(b_l) = \langle \psi_i / e^{i X_o} / \psi_i \rangle$$

Assuming that for large momentum transfers, b is small compared to b_1 and b_2

$$\Gamma_{fi}(b_1) = e^{\left(-\frac{4i}{k_i} \sum_j \gamma_j\, K_o(b\lambda_j)\right)} \langle \psi_i / \left(\frac{b_1 b_2}{b^2}\right)^{\mathcal{L}} / \psi_i \rangle$$

where $\mathcal{L} = \dfrac{2i}{k_i}$.

Using standard integration techniques, the above expression can be re-written as

$$\Gamma_{fi}(b_l) = \frac{4Y}{b^{2\mathcal{L}}} \sum_{k=1}^{9} D_k\, 2^{2\mathcal{L}}\, (K_{1k}\,K_{2k})^{-(3+\mathcal{L})}$$

$$\left\{ \Gamma\left(1 + \frac{\mathcal{L}}{2}\right) \Gamma\left(2 + \frac{\mathcal{L}}{2}\right) \right\}^{2} \qquad (4.132)$$

where $Y = e^{\left(-\frac{4i}{k_i} \sum_j \gamma_j\, K_o(b\lambda_j)\right)}$

The constants D_k, K_{1k} and K_{2k} were defined earlier in this section. Writing $\left\{\Gamma\left(1 + \frac{\mathcal{L}}{2}\right) \Gamma\left(2 + \frac{\mathcal{L}}{2}\right)\right\}^2$ as $E + iF$

$$\Gamma_{fi}(b_l) = \sum_{k=1}^{9} \frac{4\,D_k}{K_{1k}^3\;K_{2k}^3}\;\frac{e^{iY}\,(E + iF)}{e^{\mathcal{L}\ln(K_{1k}\,K_{2k})}}$$

where $Y = -\frac{4}{k_i}\sum_j \gamma_j\, K_0\,(b\lambda_j) + \frac{4}{k_i}\ln 2 - \frac{4}{k_i}\ln b.$

Writing the above expression in a convenient form

$$\Gamma_{fi}\,(b_l) = e^{ig}\,(e + if) \qquad (4.133)$$

Using this in the scattering amplitude F_{PW} (4.72),

$$F_{PW} = \frac{1}{k_i}\sum_l (2l+1)\, P_l\,(\cos\theta)\,\sin\delta^{(1)}\,[e\cos\mathcal{L} - f\sin\mathcal{L}]$$

$$+ \frac{i}{k_i}\sum_l (2l+1)\, P_l\,(\cos\theta)\,\sin\delta_l^{(1)}\,[f\cos\mathcal{L} + e\sin\mathcal{L}] \qquad \ldots \quad (4.134)$$

where $\mathcal{L} = \delta_l^{(1)} + g$.

Here $\delta_l^{(1)}$ is the Born phase shift for the interaction given by (4.119). Hence

$$\delta_l^{(1)} = \frac{2}{k_i}\sum_j \gamma_j\, Q_l\left(\frac{2k_i^2 + \lambda_j^2}{2k_i^2}\right)$$

Thus having computed the F_{HHOB} and F_{PW} for the E He process, the scattering amplitude for this process in the TPHB approximation can be calculated using (4.72). From this DCS can be evaluated at different incident energies and angles.

In order to evaluate the total corss-sections for this process, the imaginary part of the scattering amplitude (4.72) has to be evaluated for $\theta = 0$ such that

$$\sigma^{tot} = \frac{4\pi}{k_i} \left\{ Im_1 \Big/_{q=o} + Im_2 \Big/_{q=o} + Im_3 \Big/_{q=o} \right.$$

$$\left. + \frac{1}{k_i} \sum_{\ell} (2\ell+1) \sin \delta_\ell^{(1)} (f \operatorname{Cos} \ell + e \operatorname{Sin} \ell) \right\} \qquad (4.135)$$

Evaluating the integrals occurring in (3.38), (4.124) and (4.125),

$$I_1 (\beta^2, 0) \Big/_{q=o} = \frac{\pi}{\beta^2}, \quad I_1 (\beta^2, \lambda^2) \Big/_{q=o} = \frac{\pi}{\lambda^2} \ln \frac{\beta^2+\lambda^2}{\beta^2},$$

$$I_4 (\beta^2, \lambda_1^2, \lambda_2^2) \Big/_{q=o} = \frac{\pi}{\lambda_2^2 - \lambda_1^2} \ln \frac{\beta^2+\lambda_2^2}{\beta^2+\lambda_1^2}; \quad \lambda_1 \neq \lambda_2$$

$$= \frac{\pi}{\beta^2 + \lambda_1^2}; \quad \lambda_1 = \lambda_2$$

$$\therefore \; Im_1 \Big/_{q=0} = \frac{1}{k_i} \sum_{k=1}^{9} D_k \left[- \frac{4}{K_{2k}^3} \frac{d}{dK_{1k}} \frac{1}{K_{1k}^2} \ln \frac{\beta^2+K_{1k}^2}{\beta^2} \right.$$

$$- \frac{4}{K_{1k}^3} \frac{d}{dK_{2k}} \frac{1}{K_{2k}^2} \ln \frac{\beta^2+K_{2k}^2}{\beta^2}$$

$$\left. + 2 \frac{d}{dK_{1k}} \frac{d}{dK_{2k}} \frac{1}{K_{1k}^2 K_{2k}^2} X \right] \qquad (4.136)$$

where $X = \dfrac{1}{K_{2k}^2 - K_{1k}^2} \ln \dfrac{\beta^2 + K_{2k}^2}{\beta^2 + K_{1k}^2}$ for $K_{1k} \neq K_{2k}$

$= \dfrac{1}{\beta^2 + K_{1k}^2}$ for $K_{1k} = K_{2k}$.

Similarly $Im_2 \Big/_{q=o} = \dfrac{8}{k_i} \displaystyle\sum_{k=1}^{9} \sum_{j=1}^{3} D_k \gamma_j \left\{ \dfrac{1}{K_{2k}^3} \left(\dfrac{d}{dK_{1k}}\right) \dfrac{1}{K_{1k}^2} \right.$

$$\frac{1}{\lambda_j^2 - K_{1k}^2} \ln \frac{\beta^2 + \lambda_j^2}{\beta^2 + K_{1k}^2} + \frac{1}{K_{1k}^3} \left(\frac{d}{dK_{2k}} \right) \frac{1}{K_{2k}^2} \frac{1}{\lambda_j^2 - K_{2k}^2} \ln \frac{\beta^2 + \lambda_j^2}{\beta^2 + K_{2k}^2} \Bigg\} \qquad ..(4.137)$$

and $Im_3 \, / _{q=o}$

$$= \frac{4}{k_i} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\gamma_i \gamma_j}{\lambda_j^2 - \lambda_i^2} \ln \frac{\beta^2 + \lambda_j^2}{\beta^2 + \lambda_i^2} ; \lambda_i \neq \lambda_j$$

$$= \frac{4}{k_i} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\gamma_i \gamma_j}{\beta^2 + \lambda_j^2} ; \lambda_i = \lambda_j \qquad ..(4.138)$$

The substitution of (4.136), (4.137), and (4.138) in (4.135) will give the TCS for E He process in the TPBB approximation.

The total elastic cross sections for this process also can be evaluated making use of the DCS values and the expression (4.116)

Results and discussion :

The scattering parameters DCS and TCS obtained in the present study of the elastic scattering of electrons by Helium atom using the two-potential HHOB approximation are compared with other theoretical and experimental data. The results are found to be encouraging as follows the comparison. In fig.(4.14) and (4.15), the present DCS values at 200 eV and 400 eV are compared with other recent data (HHOB results of Rao and Desai (1981), GES results of

Singh and Tripathi (1980), EBS results of Byron and Joachain (1977), experimental data of Bromberg (1974), Jansen et al (1976), Register et al (1980)).

It can be seen from the figures that the present results agree well with other data. It may be noted that as in the previous section, the two-potential formulation in HHOB approximation yields better results than the simple HHOB approximation (Rao and Desai 1981), especially at large angles. Thus the two-potential formulation is an appropriate remedy for the main disadvantage of the HHOB - approximation namely over estimation in the large angle region. From the comparison between the present results at 200 eV and 400 eV it is obvious that the results improve for higher incident energies.

In table (4.11), the present results for differential cross sections are given at few sample energies. The calculations were carried out only at these energies because of the lack of computer time, since the calculation for each energy involves the evaluation of the Born and exact phase-shifts, their comparison etc. besides the lengthy evaluation procedure for the scattering amplitude. Since the study at few chosen energies is sufficient for the prediction of the behaviour at other energies, the present study was confined to only those energies with an abundance of data available.

In table (4.12) the present TCS values are compared with the results reported by other workers. The present results are rather satisfactory, the trend being the same as discussed above. Hence better results are to be expected for higher incident energies.

In the light of the above discussion, the conclusion can be drawn that the two-potential formulation in HHOB (TPHB) as derived in an earlier section, improves the basic HHOB approximation of Yates (1979) in the study of the elastic scattering of electrons from hydrogen and helium atoms.

4.10 Wallace type of trajectory correction in HHOB approximation :

In the foregoing few sections, an attempt to modify the recent HHOB approximation of Yates (1979) - namely TPHB approximation - was discussed. In the present section, another effort is put in with a view of improving upon the HHOB approximation. The chief motivation behind such an idea is the work reported by Wallace (1973) wherein he has incorporated the trajectory correction in the expansion of the Green's function of the eikonal approximation and carried out further analysis of the perturbative series. As mentioned elsewhere in a previous section, the similarity between the modes of expansion of the Green's function in the eikonal and HHOB approximations gives much scope for a similar attempt in the HHOB approximation also. Keeping this in mind, in the present study, the HHOB analysis was carried out after incorporating the correction in the Green's function, the scattering amplitudes in the second Born approximation were derived accordingly and the new expressions were used to study the elastic scattering of electrons by hydrogen atom (ESGH process).

Theory

The second Born amplitude in the HHOB approximation is given as (Yates 1979)

$$f^{(2)}_{i \to f} = \frac{1}{\pi} \sum_n \int d\,\underline{r}_o \, e^{i\underline{q}\cdot\underline{r}_o} \, V_{fn}(\underline{r}_o) \, I_n \qquad (4.139)$$

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

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

$$\int ds \, \frac{e^{i\underline{s}\cdot\underline{r}'_o}}{s^2+2\underline{s}\cdot\underline{k}_n - i\epsilon} \, , \; \epsilon \longrightarrow 0^+ \qquad (4.140)$$

where $s = \underline{k}' - \underline{k}_n$.

It is assumed that V_{ni} is slowly varying over the distance of a wavelength of the scattering electron i.e. $k_n \, a > 1$ where a is the range of V_{ni}, and that $\underline{k}_n$ does not differ greatly from $\underline{k}_i$ in either magnitude or direction.

Let us denote $\dfrac{1}{s^2 + 2s\cdot k_n} = G$ in (4.140)

(suppressing ϵ for the time being).

i.e. $G^{-1} = s^2 + 2s\cdot k_n \longrightarrow$ (a)

Now, dropping the quadratic term in the Glauber way,

$$g^{-1} = 2s\cdot k_n \longrightarrow \text{(b)}$$

Abarbanel and Itzykson (1969) have taken

$$k_n = K = \frac{1}{2}(k_i + k_f)$$

$$\therefore G_{Al}^{-1} = 2s\cdot K \longrightarrow \text{(c)}$$

From (a) and (c), $G^{-1} = G_{Al}^{-1} + s^2 \longrightarrow$ (d)

$$g^{-1} - G_{Al}^{-1} = 2s\cdot k_n \left(1 - \frac{K}{k_n}\right) = \lambda\, 2s\cdot k_n$$

where $\lambda = 1 - \cos\frac{\theta}{2}$.

i.e. $g^{-1} = G_{Al}^{-1} + \lambda 2s\cdot k_n \longrightarrow$ (e)

From (d) and (e),

$$G^{-1} = g^{-1} - \lambda\, 2s\cdot k_n + s^2$$

i.e. $G^{-1} = g^{-1} - N \longrightarrow$ (f)

where $N = \lambda\, 2s\cdot k_n - s^2$

$$\therefore g\, G^{-1} G = g\, g^{-1} G - gNG$$

i.e. $G = g + gNG = g + gNg + gNgNg + - - -$

$$\text{i.e.} \quad \frac{1}{2s\cdot k_n+s^2} = \frac{1}{2s\cdot k_n} + \frac{1}{2s\cdot k_n}(\lambda\ 2s\cdot k_n - s^2)\frac{1}{2s\cdot k_n}$$

$$\text{i.e.} \quad \frac{1}{s^2+2s\cdot k_n} = \frac{1}{2s\cdot k_n} + \frac{\lambda}{2s\cdot k_n} - \frac{s^2}{(2s\cdot k_n)^2} \qquad (4.141)$$

It should be noted that in the HHOB analysis (Yates 1979), $\frac{\lambda}{2s\cdot k_n}$ term is absent. There it was assumed that $\underline{k}_n$ does not differ much from $\underline{k}_i$ in either magnitude or direction and hence the integrated expansion of $(s^2+2\underline{s}\cdot \underline{k}_n)^{-1}$ in powers of s^2 should be rapidly convergent. However, in the present analysis, since provision is given for $k_n = \frac{k_i + k_f}{2}$ rather than $k_n = k_i$, the present expansion (4.141) should be logically more accurate. Since $\lambda = 1\text{-Cos}\,\frac{\theta}{2}$, it may be noted that at $\theta = 0$, the additional term in the expansion (4.141) i.e. $\frac{\lambda}{2s\cdot k_n}$ becomes zero. However, the prominence of λ increases in the intermediate angles region. Now, further analysis of the second Born term using (4.141) can be carried out as follows:

Substitution of (4.141) in I_n (4.140) gives

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

$$\int \frac{d\underline{s}}{2\underline{s}\cdot\underline{k}_n - i\epsilon}\left[(1+\lambda) - \frac{s^2}{2\underline{s}\cdot\underline{k}_n - i\epsilon}\right] e^{i\underline{s}\cdot\underline{r}'_0}$$

Making use of the result

$$\int d\underline{s}\ \frac{e^{i\underline{s}\cdot\underline{r}_o}}{2s\cdot k_n - i\epsilon} = \frac{i}{2\ k_n}\ \delta(b_o')\ H\ (z_o')$$

where $\delta(b_o')$ is the Dirac delta function and $H\ (z_o')$ is the Heavyside function defined by $H\ (X) = 1,\quad x > 0$

$$= 0,\quad x < 0$$

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

$$[(1+\lambda)\ \delta(b_o')\ H\ (z_o') + \frac{i}{2k_n}\nabla^2_{r_o'}\ [\delta(b_o')\ z_o'H(z_o') + O(k_n^{-2})]\quad (4.142)$$

In performing the above $\underline{s}$ integration in cylindrical polar co-ordinates, $\underline{k}_n$ was chosen as the polar axis and $\underline{r}_o' = \underline{b}_o'+z_o'\hat{k}_n$.

Now the second term in the above equation is integrated by parts twice thus giving the approximation

$$I_n = \frac{i}{2k_n}\int_{-\infty}^{\infty} dz_o'\ e^{-i(\underline{k}_i-\underline{k}_n)\cdot\hat{k}_n z_o'}\ H\ (z_o')\ [\ (1+\lambda)+\frac{i\,z_o'}{2k_n}\ \nabla^2_{r_o'}\ ]$$

$V_{ni}\ (\underline{r}_o-\underline{r}_o')/_{\underline{b}_o'=0}$. Noting that $(\underline{k}_i - \underline{k}_n)\cdot\hat{k}_n \simeq k_i-k_n = \beta$

and $\hat{k}_n \simeq \hat{k}_i$ or $\frac{1}{k_n} = \frac{1}{k_i} + \Theta\ (\frac{1}{k_i^3})$,

I_n can be finalised as

$$I_n = \frac{i}{2k_i}\int_{-\infty}^{\infty} dz_o'\ e^{-i\beta z_o'}\ H\ (z_o')\ [(1+\lambda) + \frac{i\,z_o'}{2k_i}\ \nabla^2_{r_o'}\ ]V_{ni}\ (\underline{r}_o-\underline{r}_o')\quad (4.143)$$

Here β can be obtained using energy conservation conditions. The above equation embodies the central approximations in the trajectory corrected HHOB analysis.

Now, $$Wf^{(2)}_{HEA} = \frac{i}{2\pi k_i} \sum_n \int d\underline{r}_o \, e^{i\underline{q}\cdot\underline{r}_o} V_{fn}(\underline{r}_o)$$

$$\int_{-\infty}^{\infty} dz'_o \, e^{-i\beta z'_o} H(z'_o) \left[(1+\lambda) + \frac{iz'_o}{2k_i} \nabla^2_{\underline{r}'_o} \right] V_{ni}(\underline{r}_o - \underline{r}'_o) /_{\underline{b}'_o=0}$$

...(4.144)

The infinite summation over atomic states can be treated by the simple method of defining an average excitation energy and then employing closure. Hence $\beta \simeq \frac{\Delta E}{k_i}$

where ΔE is the average energy transferred to intermediate atomic states during the course of the collision. Thus $Wf^{(2)}_{HEA}$ can be represented in a simpler form as

$$Wf^{(2)}_{HEA} \geq \frac{i}{2\pi k_i} \int d\underline{r}_o \, e^{i\underline{q}\cdot\underline{r}_o} < \Psi_f / V(\underline{r}_o, - - - \underline{r}_n)$$

$$\int_{-\infty}^{\infty} (1+\lambda) \, dz'_o \, H(z'_o) \, e^{-i\beta z'_o} [V(r_o - z'_o \hat{\chi},$$

$$\underline{r}_1, - - - -\underline{r}_N) + \frac{iz'_o}{2k_i} \nabla^2_{\underline{r}'_o} V(\underline{r}_o - \underline{r}'_o, \underline{r}_1 --- \underline{r}_N)$$

$$/_{\underline{b}'_o=0}] / \Psi_i >$$

(4.145)

The rest of the analysis can be carried out exactly similar to that done in the HHOB analysis. The fourier transform of the interaction is written using

$$V\,(\underline{r}_0---\underline{r}_N) = \int d\underline{P}\; e^{-i\underline{P}\cdot\underline{b}_0} \int_{-\infty}^{\infty} dP_z\; e^{-iP_z z_0}$$

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

and the ∇^2 operation is carried out.

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

$$< \Psi_f / \bar{V}\; \bar{V} / \Psi_i \int d\underline{b}_0\; e^{i(\underline{q}-\underline{P}-\underline{P}')\cdot\underline{b}_0} \int_{-\infty}^{\infty} dz_0$$

$$e^{-i(P_z+P'_z)z_0} \left[(1+\lambda) + \frac{P'^2+P'^2_z}{2k_i} \frac{d}{d\beta} \right) \int_{-\infty}^{\infty} d\,z'_0$$

$$e^{-i(P'_z-\beta)\,z'_0}\; H(z'_0)$$

Making use of the following properties of δ functions,

$$\int_{-\infty}^{\infty} e^{-i\,P_z z} dz = 2\pi\,\delta(P_z)\ ,$$

$$\int d^2b\; e^{i(\underline{q}-\underline{P})\cdot\underline{b}} = (2\pi)^2\,\delta(q-P),$$

and $$\int d\underline{P}\;\delta(q-P)\;\bar{V}_1\,(P) = \bar{V}_1(q)$$

the final expression for $Wf^{(2)}_{HEA}$ can be written down as

$$Wf^{(2)}_{HEA} = \frac{4\pi^3}{k_i} \Big[i\int d\underline{P} \;\Big((1+\lambda) + \frac{1}{2K_i} \frac{d}{d\beta} (P^2+\beta^2) \Big)$$

$$U^{(2)}_{fi} (\underline{q} - \underline{P} - \beta\hat{\chi},\; \underline{P} + \beta\hat{\chi}) - \frac{1}{\pi} \mathbb{P} \int d\underline{P} \int_{-\infty}^{\infty} dP_z$$

$$\Big((1+\lambda) + \frac{P^2+P_z^2}{2k_i} \frac{d}{d\beta} \Big) \frac{1}{P_z - \beta}$$

$$U^{(2)}_{fi} (\underline{q} - \underline{P} - P_z\hat{\chi}, \underline{P} + P_z\hat{\chi}) \Big] \tag{4.146}$$

where $\mathbb{P}$ stands for the principal value of the integral and

$$U^{(2)}_{fi}(\underline{P} + P_z\hat{\chi}, \underline{P}' + P'_z\hat{\chi}) = \langle \Psi_f / \bar{V}(\underline{P}+P_z\hat{\chi}, \underline{r}_1 \ldots\ldots \underline{r}_N)$$

$$\bar{V}(\underline{P}'+P'_z\hat{\chi}, \underline{r}_1, --- \underline{r}_N) / \Psi_i \rangle$$

In arriving at the above expression the following result was used:

$$\int_{-\infty}^{\infty} dx\ e^{-i a x} H(x) = \pi\delta(a) - i\,\mathbb{P}(\frac{1}{a})$$

Comparison of the trajectory corrected $Wf^{(2)}_{HEA}$ (4.146) with the corresponding term in Yates (1979), we can see that only $O(\frac{1}{k_i})$ terms differ in both cases whereas $O(\frac{1}{k_i}2)$ terms remain same. Obviously, this should be the case since in the expansion (4.141), $O(\frac{1}{k_i})$ term is additional than in Yates (1979) where $O(\frac{1}{k_i^2})$ terms are same in both expansions. In short, the real and imaginary parts in the second Born approximation accounting for the tragectory correction can be written as

$$W\ \mathrm{Im}\ f^{(2)}_{HEA} = (1+\lambda)\mathrm{Im}\ f^{(2)}_{HEA} \tag{4.147}$$

$$W\ \mathrm{Re}\ f^{(2)}_{HEA} = (1+\lambda)\ \mathrm{Re}\ f^{(2)}_{HEA} \tag{4.148}$$

where $\mathrm{Im}\ f^{(2)}_{HEA}$ and $\mathrm{Re}\ f^{(2)}_{HEA}$ represent the $O(\frac{1}{k_i})$ terms in the second Born of Yates (1979).

Now let us apply the tragectory corrections to the ESGH process. Since $\mathrm{Im}\ f^{(2)}_{HEA}$ and $\mathrm{Re}\ f^{(2)}_{HEA}$ are positive quantities in ESGH process and λ is also positive, the corrections will increase the values of the DCS only. In view of the fact that the DCS obtained using the HHOB analysis of Yates (1979) slightly underestimates the experimental values, the above situation is really welcome. The DCS values at 100 eV obtained after incorporating the trajectory correction in HHOB are exhibited in fig.(4.16) and compared with the HHOB results without correction and experimental data. The values are shown at small angles only because

(1) HHOB is good for only small angles.

(2) The correctness of the Wallace type of trajectory correction has not been established for large angles.

It should be noted that in the work of Unnikrishnan and Prasad (1982) incorporating the Wallace correction, the results are given for angles 30° only.

On the observation of fig. (4.16) it becomes clear that eventhough there is slight improvement in the results due to the incorporation of the trajectory correction, the difference in the two results is not quite large. The present results have shifted towards the experimental points of Williams (1975). However, since the improvement brought is not that much as expected in the start of this work, further computations for incident energies other than 100eV were not carried out. However, there is enough reason to believe that the correction described in this section combined with the previously discussed modification in HHOB (viz. the two - potential HHOB formulation) will definitely give very good results. Turning back to fig.(4.12), in the small angle region, the results of the present work were underestimating the experimental values and this underestimation may to an extent be removed by taking $Wf^{(2)}_{HEA}$ instead of simple $f^{(2)}_{HEA}$ in the two potential HHOB analysis leading to the results displayed in fig.(4.12). More work in this direction is in progress in our research group.

In the foregoing few sections, the modified Born approximation, the two-potential eikonal approximation, the two-potential HHOB approximation and the trajectory correction to HHOB were discussed. In all the above cases, the applications of the various theories considered were made with respect to scattering phenomena involving light atomic targets. In the following chapter, an entirely different class of atomic targets - the alkali atoms - are taken up in the study of electron scattering from atoms.

Table 4.1a – Comparison of DCS ($a_o^2 s_r^{-1}$) for ESGH process in the MBA using different modes of evaluation of the integrals at 200 eV.

θ	Gupta and Mathur (1978)		Present study	
10	0.192	01	0.1830	01
20	0.490	00	0.5044	00
30	0.160	00	0.1623	00
40	0.650	-01	0.6550	-01
50	0.310	-01	0.3110	-01
60	0.170	-01	0.1672	-01
70	0.990	-02	0.9927	-02
90	0.440	-02	0.4407	-02
100	0.320	-02	0.3219	-02
120	0.200	-02	0.1983	-02
140	0.140	-02	0.1435	-02

Table 4.1b - Differential scattering cross sections ($a_o^2 S_r^{-1}$) for the ESEH process in the modified Born Approximation.

θ/ E_{eV}	100		200		300		400		600		800	
10	0.4472	02	0.1937	02	0.8374	01	0.4752	01	0.2082	01	0.1159	01
20	0.4289	01	0.1111	01	0.5038	00	0.2886	00	0.1318	00	0.7547	-01
30	0.8351	00	0.2268	00	0.1049	00	0.6034	-01	0.2746	-01	0.1563	-01
40	0.2767	00	0.7609	-01	0.3506	-01	0.2008	-01	0.9088	-02	0.5156	-02
50	0.1209	00	0.3307	-01	0.1517	-01	0.8665	-02	0.3911	-02	0.2216	-02
70	0.3637	-01	0.9842	-02	0.4494	-02	0.2563	-02	0.1155	-02	0.6539	-03
90	0.1585	-01	0.4271	-02	0.1948	-02	0.1110	-02	0.5000	-03	0.2832	-03
110	0.8815	-02	0.2373	-02	0.1082	-02	0.6166	-03	0.2777	-03	0.1572	-03
130	0.5885	-02	0.1584	-02	0.7222	-03	0.4115	-03	0.1853	-03	0.1049	-03
150	0.4561	-02	0.1228	-02	0.5598	-03	0.3189	-03	0.1436	-03	0.8134	-04

Table 4.2 - Various constants for the Li atom in the Szasz Mc Ginn (1967) formulation

Basis (nl)	$\xi_{nl}^{(P)}$	$C_{nl}^{(P)}$	$A_{nl}^{(P)}$
		Core Wavefunctions	
1S	4.4	0.133937	18.459
1S	2.4	0.914304	7.436
2S	4.4	-0.008925	46.89
2S	2.4	-0.029575	10.304
		Valence electron wavefunction	
1S	2.4803	0.0083285	7.812
1S	4.7071	0.0023871	20.42
2S	1.735	-0.0871464	4.578
2S	1.	0.0877919	1.1547
2S	0.6615	0.9659271	0.41
2S	0.35	0.0031811	0.08368

Table 4.3 - The constants for the Szasz Mc Ginn (1967) wavefunction for the ground state of Lithium atom.

i/j	C_i	λ_i	D_j	β_j
1	0.01919	2.48	-0.11759	1.735
2	0.01438	4.71	0.02989	1.0
3	-0.14162	4.4	0.11698	0.66
4	-0.38945	2.4	0.00008	0.35
5	-	-	0.02397	4.4
6	-	-	0.01745	2.4

Table 4.4 - Differential cross sections $(a_o{}^2 s_r{}^{-1})$ for the ELi process in the modified Born approximation.

θ/ EeV	60		100		200		400		700	
10	0.2044	02	0.1759	02	0.1163	02	0.5502	01	0.2401	01
20	0.9066	01	0.5214	01	0.1905	01	0.6403	00	0.2796	00
30	0.3274	01	0.1551	01	0.5416	00	0.2002	00	0.9099	-01
40	0.1377	01	0.6524	00	0.2434	00	0.9202	-01	0.4003	-01
50	0.7229	00	0.3551	00	0.1361	00	0.4976	-01	0.2035	-01
70	0.3098	00	0.1559	00	0.5753	-01	0.1889	-01	0.7012	-02
90	0.1801	00	0.8845	-01	0.3035	-01	0.9146	-02	0.3218	-02
110	0.1229	00	0.5827	-01	0.1877	-01	0.5351	-02	0.1831	-02
130	0.9397	-01	0.4315	-01	0.1328	-01	0.3665	-02	0.1236	-02
150	0.7896	-01	0.3547	-01	0.1062	-01	0.2878	-02	0.9634	-03

Table 4.5 - Differential cross sections for the ELi process in the first Born and Modified Born approximations revealing the core contributions to the DCS.

Θ	60 eV				700 eV			
	MBA		FBA		MBA		FBA	
	a	b	a	b	a	b	a	b
10	0.2044 02	0.1755 02	0.2436 02	0.2174 02	0.2401 01	0.1664 01	0.2217 01	0.1526 01
20	0.9066 01	0.7212 01	0.9544 01	0.7966 01	0.2796 00	0.1011 00	0.2659 00	0.9567 -01
30	0.3274 01	0.2233 01	0.3405 01	0.2518 01	0.9099 -01	0.2019 -01	0.8669 -01	0.1907 -01
40	0.1377 01	0.7601 00	0.1427 01	0.8965 00	0.4003 -01	0.6649 -02	0.3819 -01	0.6272 -02
50	0.7229 00	0.3179 00	0.7302 00	0.3832 00	0.2035 -01	0.2867 -02	0.1945 -01	0.2703 -02
70	0.3098 00	0.9129 -01	0.2927 00	0.1097 00	0.7012 -02	0.8497 -03	0.6725 -02	0.8013 -03
90	0.1801 00	0.3968 -01	0.1621 00	0.4685 -01	0.3218 -02	0.3685 -03	0.3092 -02	0.3478 -03
110	0.1229 00	0.2226 -01	0.1075 00	0.2589 -01	0.1831 -02	0.2048 -03	0.1762 -02	0.1934 -03
130	0.9397 -01	0.1499 -01	0.8079 -01	0.1727 -01	0.1236 -02	0.1367 -03	0.1190 -02	0.1291 -03
150	0.7896 -01	0.1169 -01	0.6729 -01	0.1339 -01	0.9634 -03	0.1059 -03	0.9282 -03	0.1001 -03

a = with core effect

b = without core effect

Table 4.6 - Total elastic cross sections (πa_0^2) for the ELi process - comparison of different results.

E eV	Present results	Walters (1973) Born	 Glauber	FSA[a]	HHOB[b]
100	2.9	3.08	2.58	3.379	3.152
200	1.4	1.69	1.40	1.614	1.577
400	0.8	0.82	0.78	-	-

a - Guha and Ghosh (1979)

b - Rao and Desai (1983)

Table 4.7 - Phase shift analysis for the Yukawa potential $-e^{-r}/r$ for the wavenumber k = 5

l	Born Phase shift		Exact phase shift a		 b	
0	0.2308	00	0.2384	00	0.2379	00
1	0.1354	00	0.1383	00	0.1378	00
2	9.1739	-02	9.2820	-02	9.2809	-02
3	6.5710	-02	6.6315	-02	6.6296	-02
4	4.8488	-02	4.8843	-02	4.8783	-02
5	3.6456	-02	3.6629	-02	3.6601	-02
6	2.7766	-02	2.7618	-02	2.7587	-02
7	2.1348	-02	2.1254	-02	2.1298	-02
8	1.6533	-02	1.6498	-02	1.6501	-02
9	1.2878	-02	1.2776	-02	1.2834	-02
10	1.0078	-02	1.0076	-02	1.0081	-02

a = Using Numerov's method b= Using Runge-Kutta method

Table 4.8 – Differential cross sections ($a_o^2\ S_r^{-1}$) for the elastic scattering of electrons from H (1S) in the two-potential HHOB approximation.

$\theta/_E$	100 eV	200 eV	400 eV
10	1.7899 00	1.0438 00	0.5673 00
20	0.7609 00	0.3515 00	0.1723 00
30	0.3514 00	0.1307 00	4.6908 -02
40	0.1639 00	0.5132 -01	1.8308 -02
50	8.7071 -02	2.5118 -02	7.9374 -03
70	3.2419 -02	9.2609 - 03	2.3574 -03
90	1.6488 -02	4.5803 -03	0.9940 -03
110	9.8421 -03	2.5984 -03	0.6605 -03
130	6.6353 -03	1.6781 -03	0.4850 -03

Table 4.9 Total cross sections (TCS) for ESGH process in the two potential HHOB approximation

E eV	Present results	HHOB[a]	EBS[b]	Winters[c]
100	7.95	7.56	7.49	7.73
200	4.62	4.37	4.39	4.49
400	2.61	2.48	2.50	-

a - Yates (1979)
b - Byron and Joachain (1977)
c - Winters et al (1974)

Table 4.10 Total elastic cross sections (TEC) for the ESGH process in the TPHB approximation (unit a_o^2)

E eV	Present study	EBS[b]	HHOB (with exchange)	Winters[c]	Van Wingerden et al (1977)
100	1.50	1.57	2.03	1.40	1.83
200	0.64	0.63	0.77	0.58	0.79
400	0.29	0.28	0.32	-	-

Table 4.11 - Differential cross sections for the EHe process in the TPHB approximation.

θ/E	200 eV		400 eV	
10	1.2471	00	2.248	-01
20	0.5533	00	1.937	-01
30	0.2812	00	7.608	-02
40	0.1629	00	3.016	-02
50	0.1071	00	1.453	-02
70	0.3819	-01	4.829	-03
90	0.1886	-01	2.247	-03
110	0.1122	-01	1.326	-03

Table 4.12 - Total cross sections (a_o^2) for E He process in the TPHB approximation.

E eV	Present results	HHOB[a]	Winters et al[b]	Byron and Joachain[b]	EBS[b]
200	3.58	2.93	3.55	3.37	2.92
400	2.08	1.69	2.00	1.86	1.71

a - Rao and Desai (1981)

b - Byron and Joachain (1977)

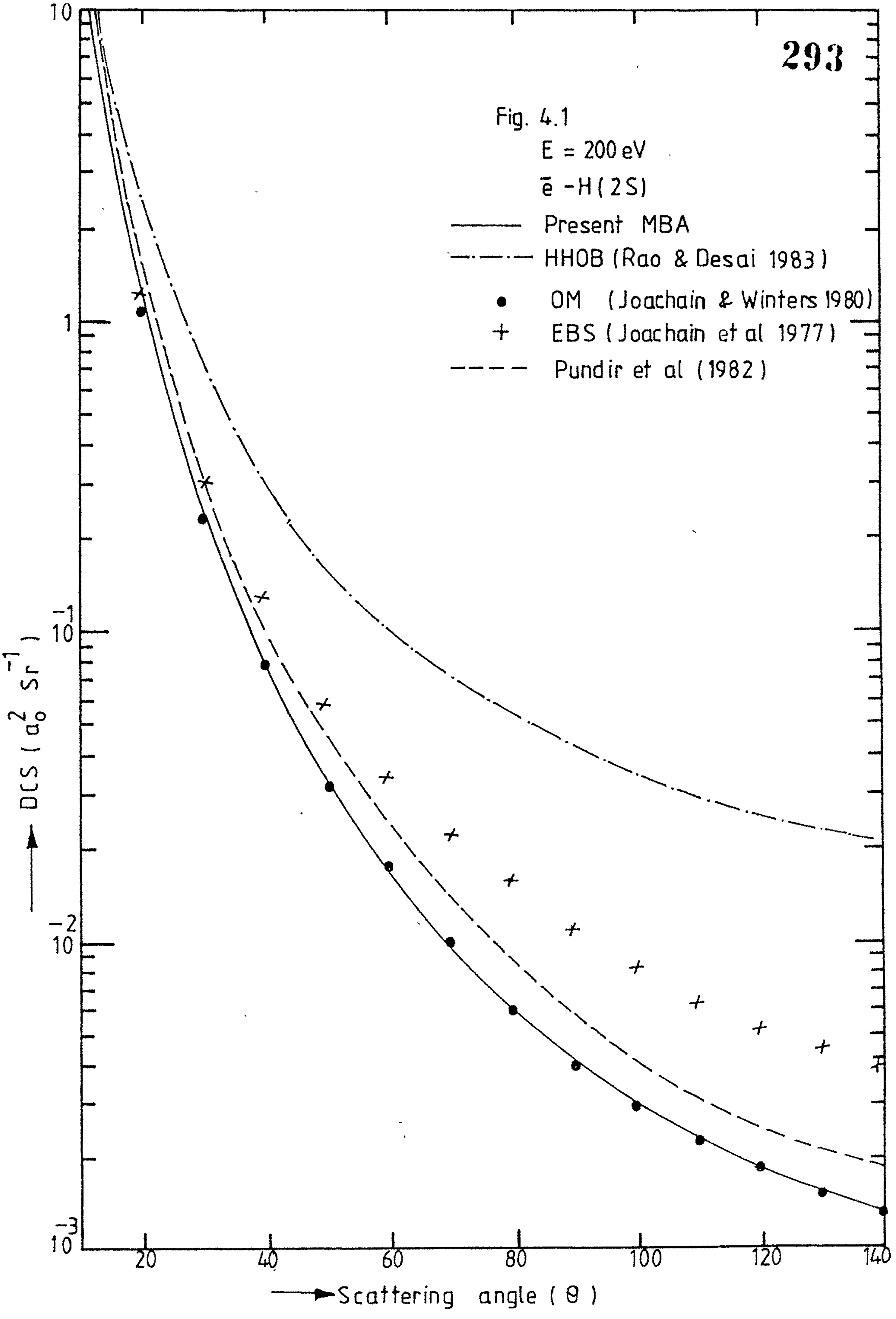


Fig. 4.1

E = 200 eV
$\bar{e}$ -H (2S)
Present MBA
HHOB (Rao & Desai 1983)
OM (Joachain & Winters 1980)
EBS (Joachain et al 1977)
Pundir et al (1982)
10
1
10^{-1}
10^{-2}
10^{-3}
DCS (a_o^2 Sr^{-1})
20
40
60
80
100
120
140
Scattering angle (θ)

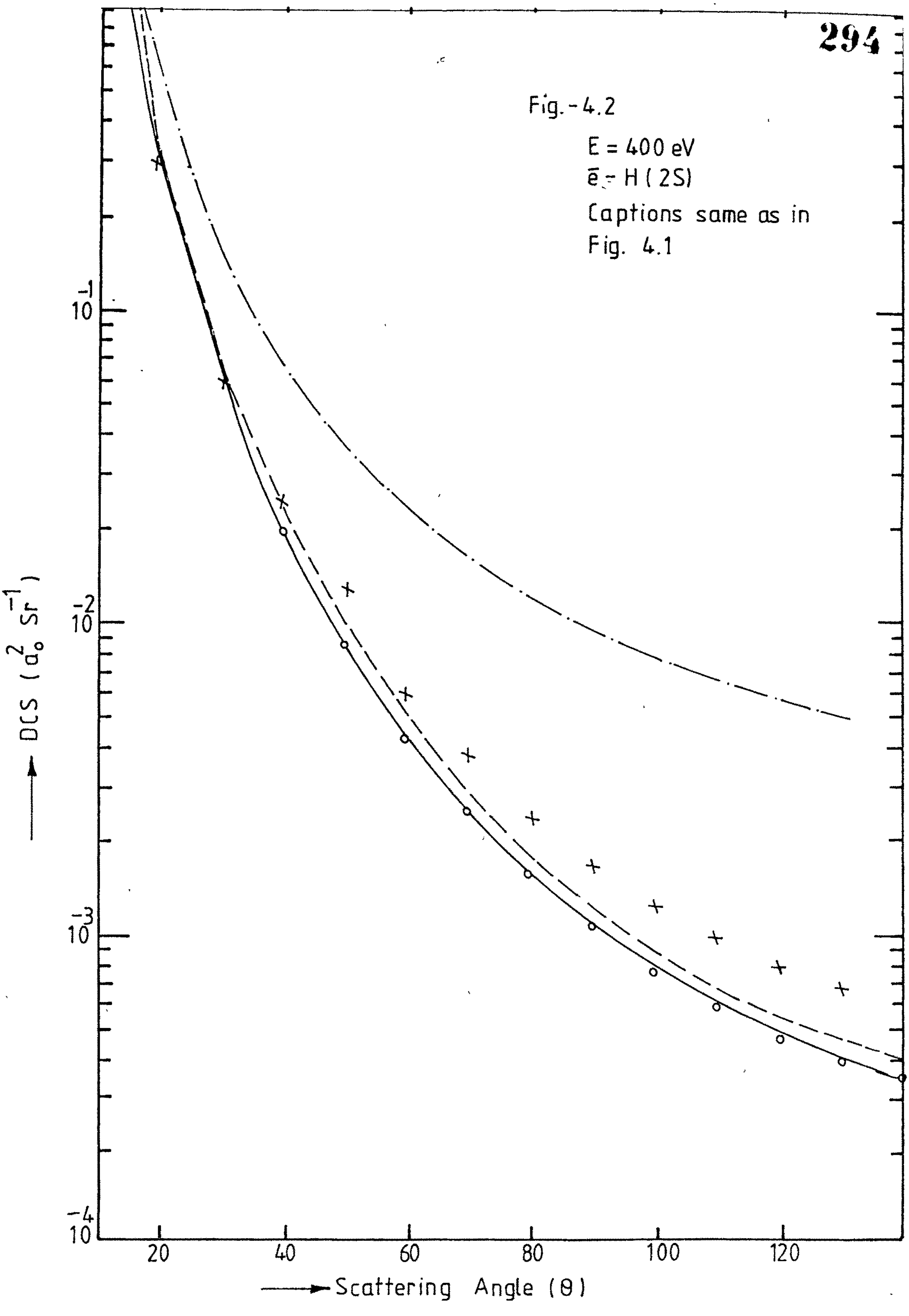


Fig.-4.2

E = 400 eV

$\bar{e}$ - H (2S)

Captions same as in Fig. 4.1

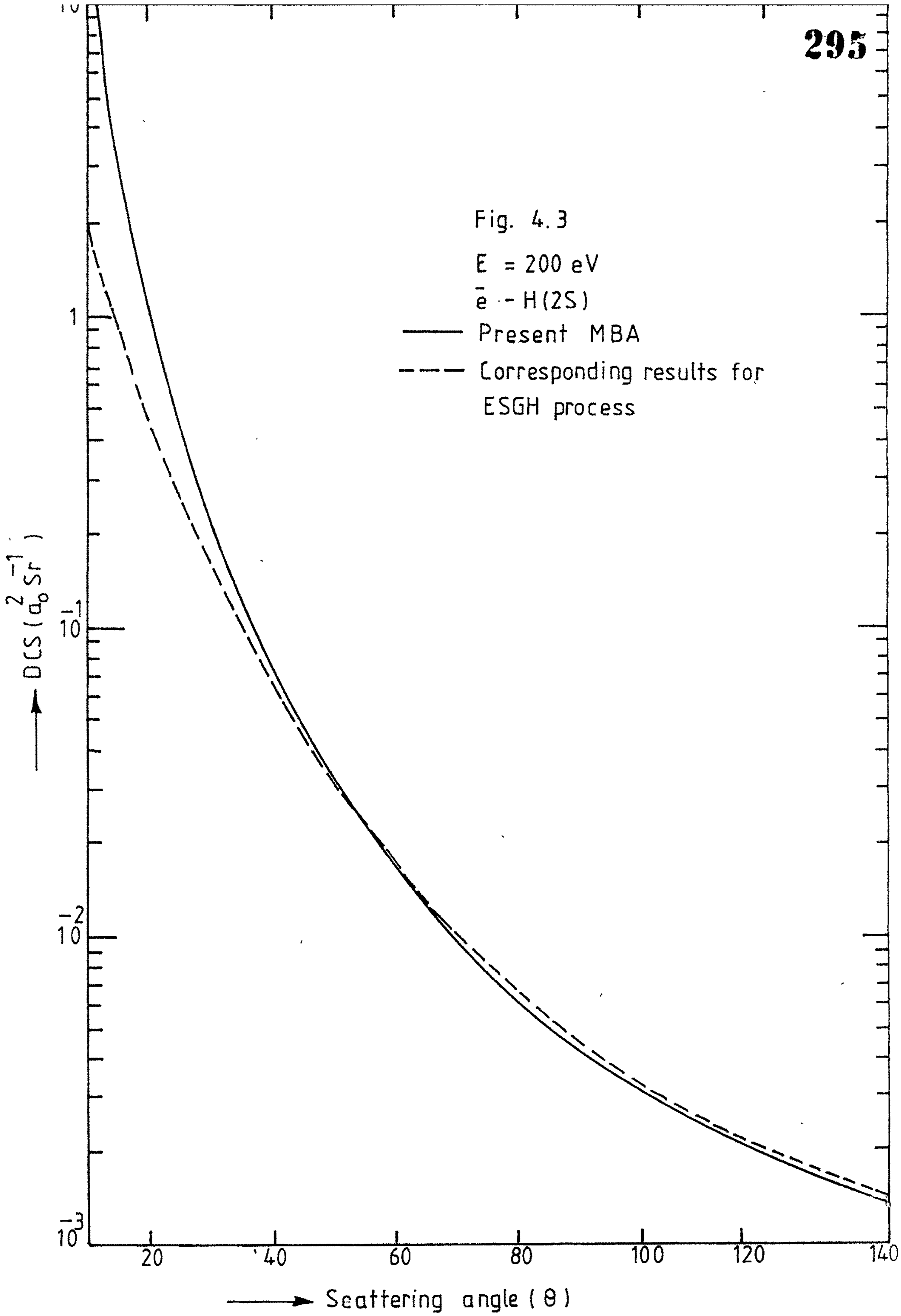


Fig. 4.3
$E = 200$ eV
$\bar{e}$ - H(2S)
Present MBA
Corresponding results for ESGH process
10
1
10^{-1}
10^{-2}
10^{-3}
→ DCS ($a_0^2 \, Sr^{-1}$)
20
40
60
80
100
120
140
→ Scattering angle (θ)

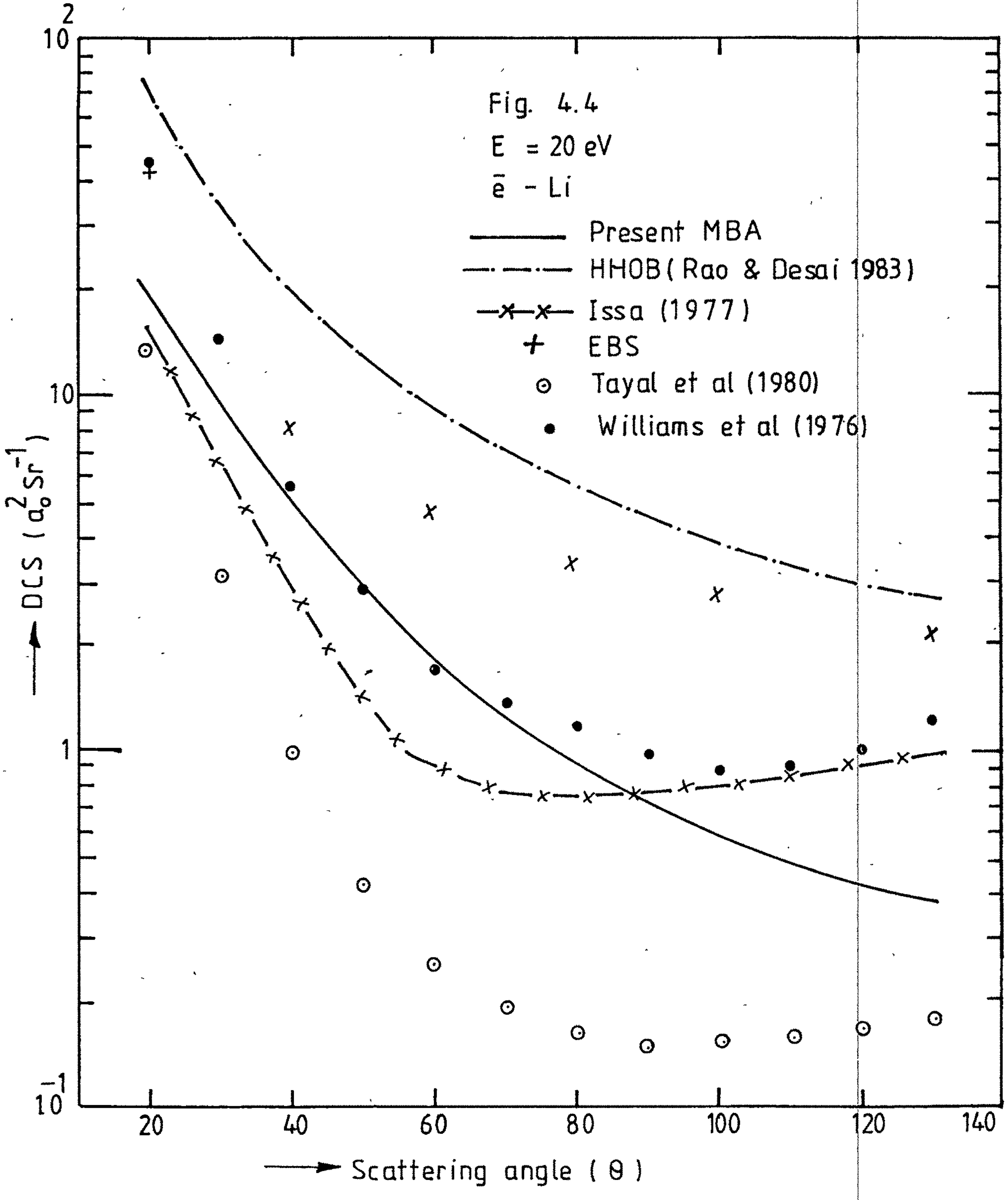


Fig. 4.4
E = 20 eV
ē - Li
Present MBA
HHOB (Rao & Desai 1983)
Issa (1977)
EBS
Tayal et al (1980)
Williams et al (1976)
DCS (a_o^2 Sr^{-1})
10^2
10
1
10^{-1}
20
40
60
80
100
120
140
Scattering angle (θ)

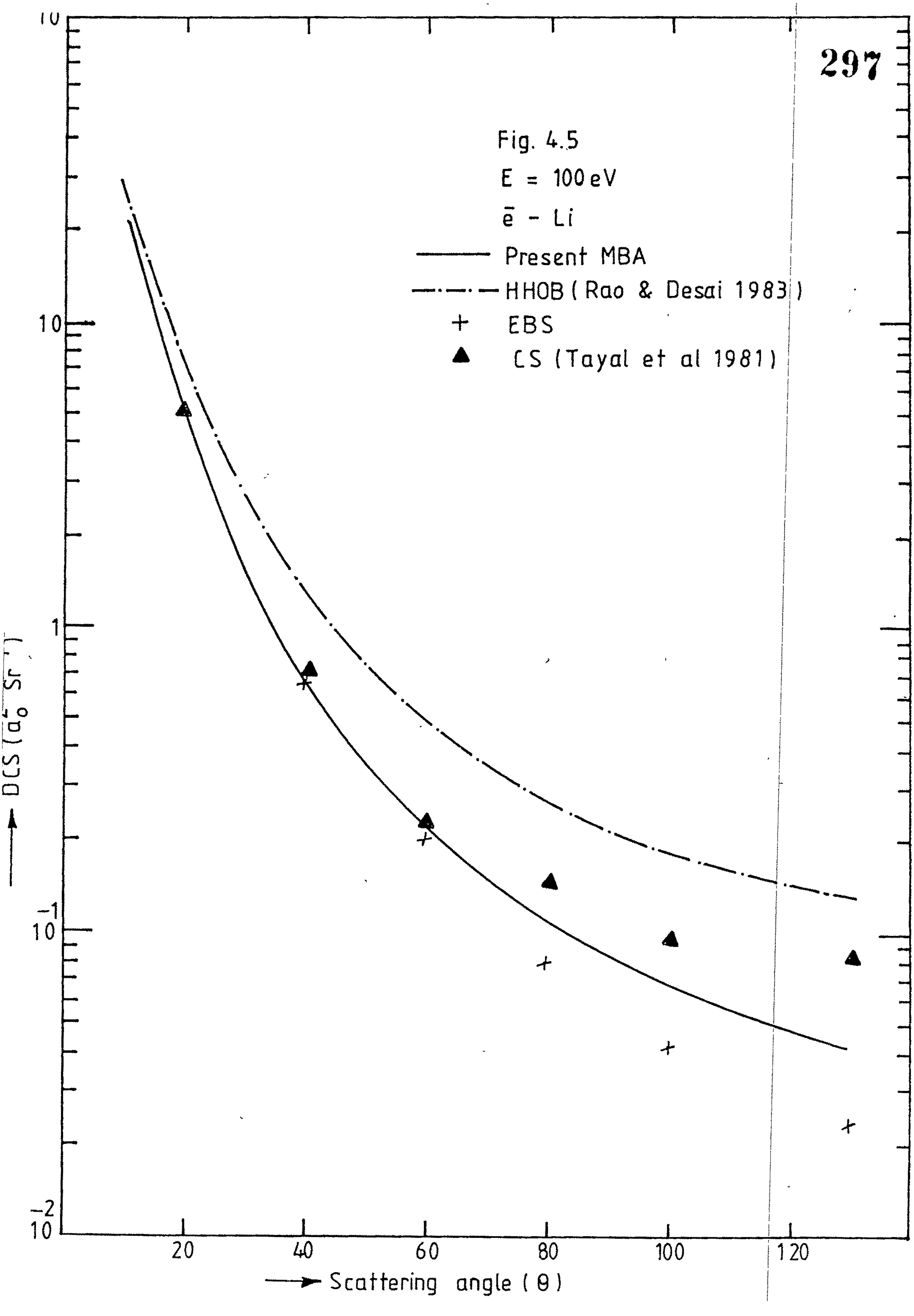


Fig. 4.5

E = 100 eV
ē - Li
Present MBA
HHOB (Rao & Desai 1983)
+ EBS
▲ CS (Tayal et al 1981)
10
10
1
-1
10
-2
10
20
40
60
80
100
120
→ Scattering angle (θ)
→ DCS (a_0^2 Sr^{-1})

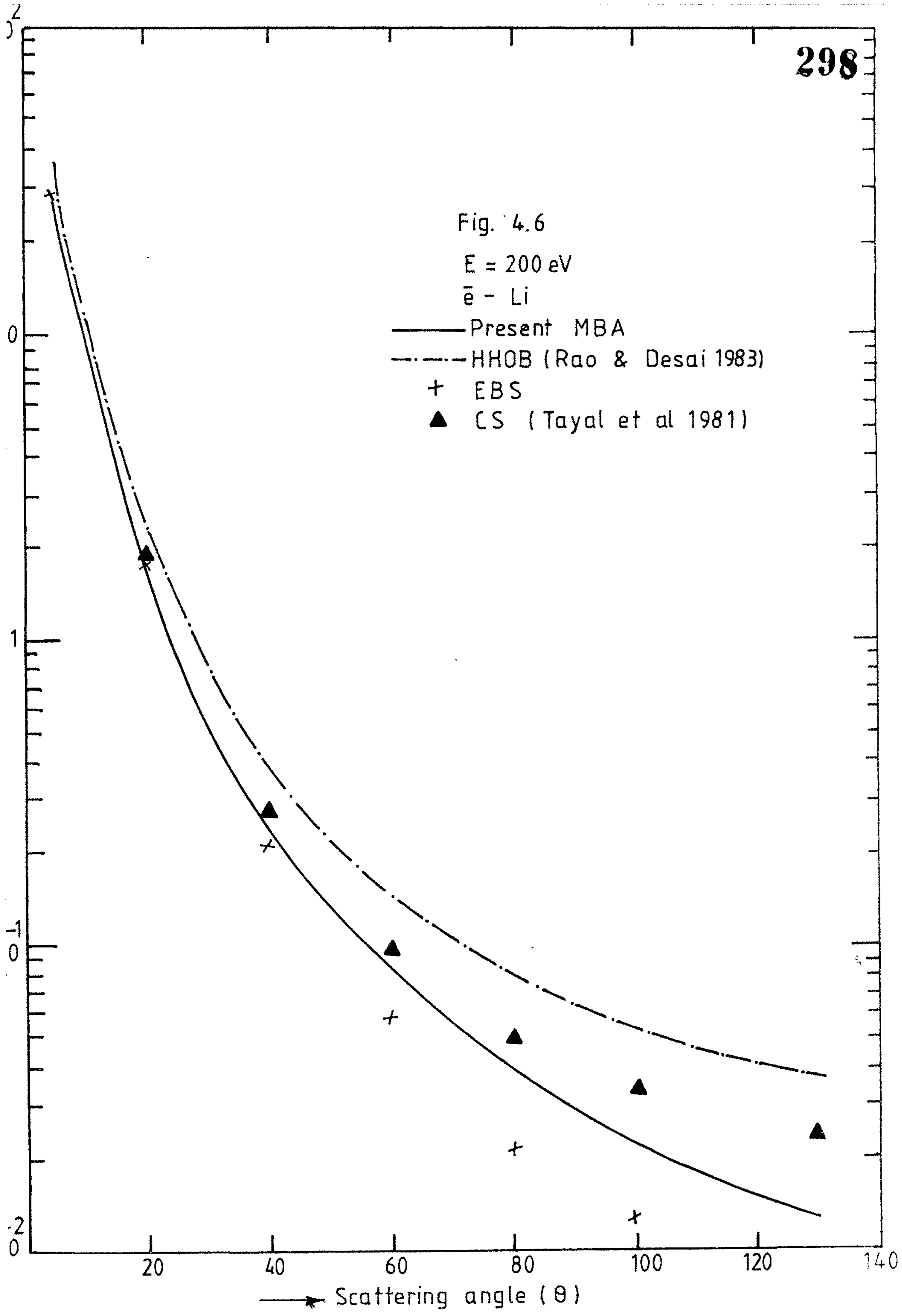


Fig. 4.6
E = 200 eV
ē - Li
Present MBA
HHOB (Rao & Desai 1983)
EBS
CS (Tayal et al 1981)
2
0
0
1
-1
0
-2
0
20
40
60
80
100
120
140
Scattering angle (θ)

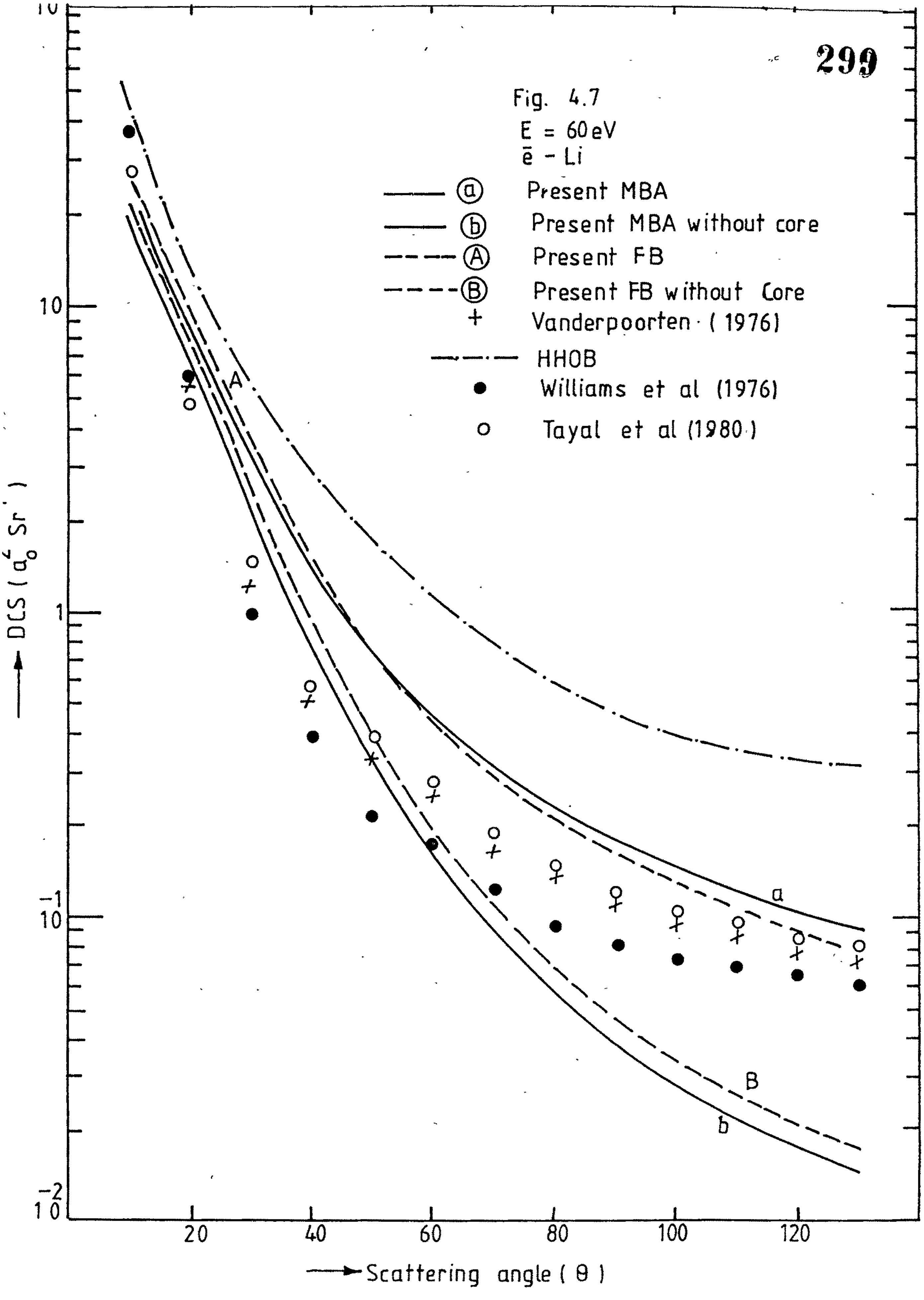


Fig. 4.7
E = 60 eV
ē - Li
ⓐ Present MBA
ⓑ Present MBA without core
Ⓐ Present FB
Ⓑ Present FB without Core
+ Vanderpoorten (1976)
HHOB
● Williams et al (1976)
○ Tayal et al (1980)
A
a
B
b
DCS (a_0^2 Sr^{-1})
10
1
10^{-1}
10^{-2}
Scattering angle (θ)
20
40
60
80
100
120

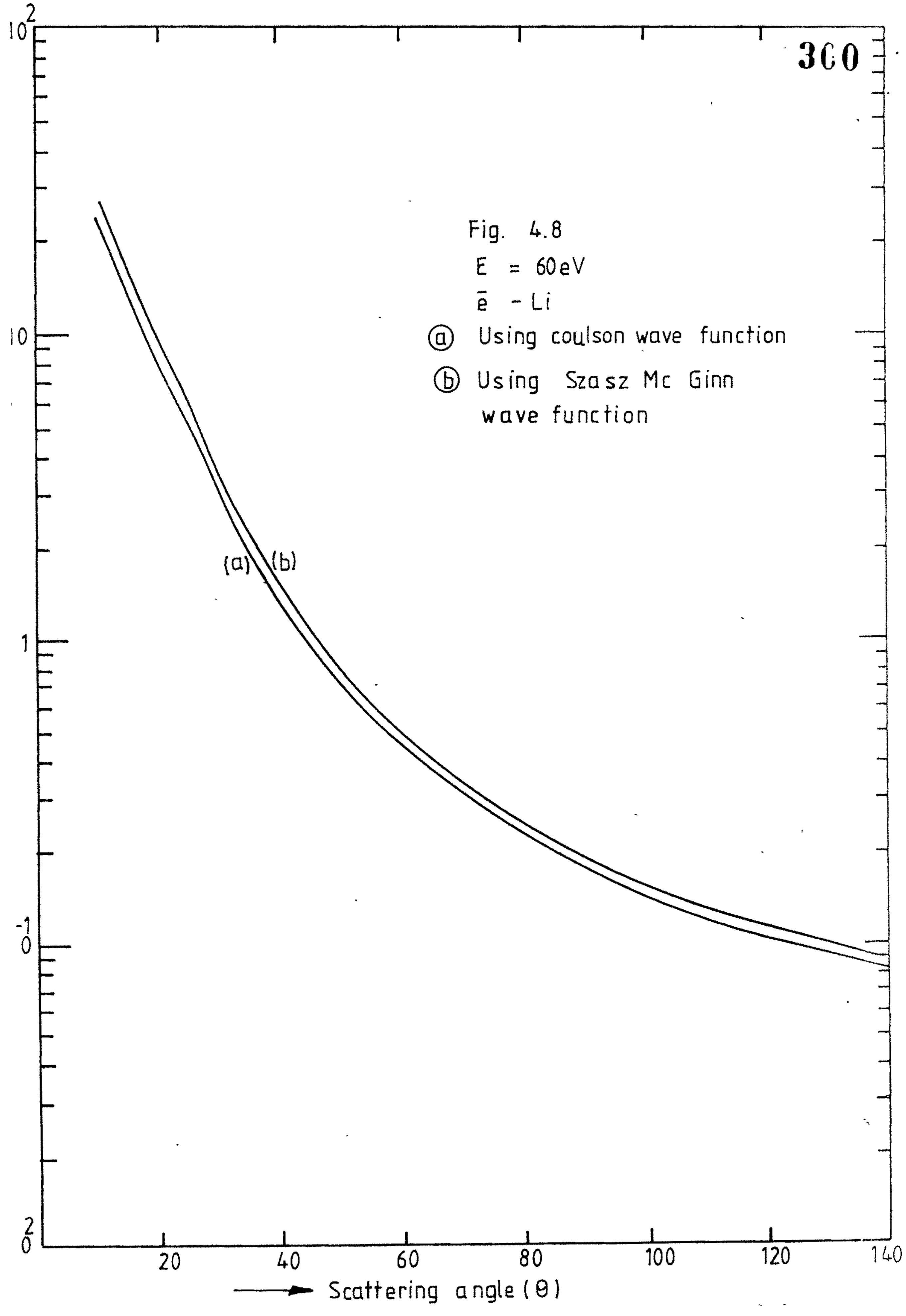


Fig. 4.8

$E = 60\,eV$
$\bar{e}$ - Li
ⓐ Using coulson wave function
ⓑ Using Szasz Mc Ginn wave function
(a)
(b)
10^{2}
10
1
10^{-1}
10^{-2}
20
40
60
80
100
120
140
Scattering angle (θ)

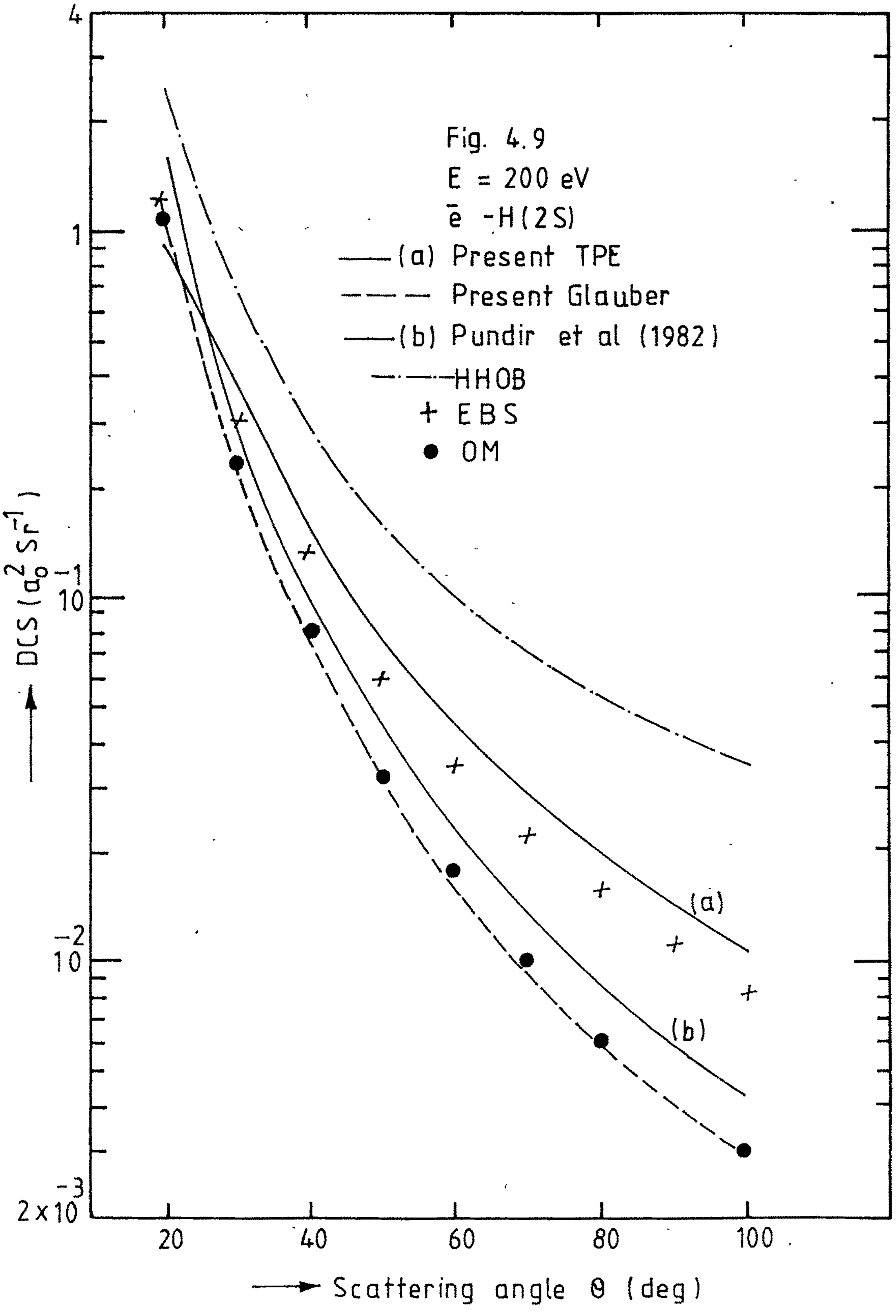


Fig. 4.9
E = 200 eV
ē -H(2S)
(a) Present TPE
Present Glauber
(b) Pundir et al (1982)
HHOB
+ EBS
● OM
(a)
(b)
DCS (a_0^2 Sr^{-1})
Scattering angle θ (deg)
4
1
10^{-1}
10^{-2}
2×10^{-3}
20
40
60
80
100

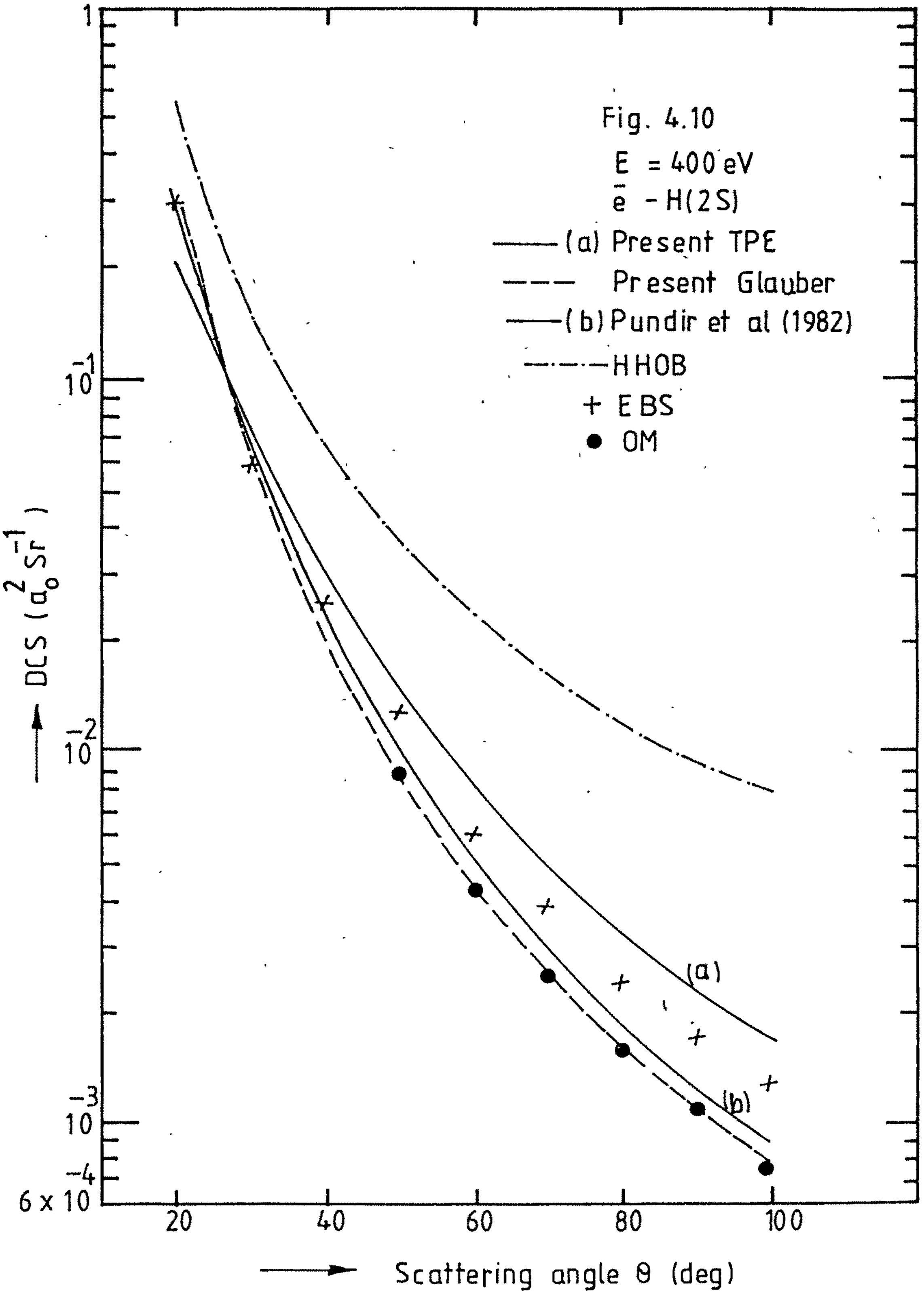
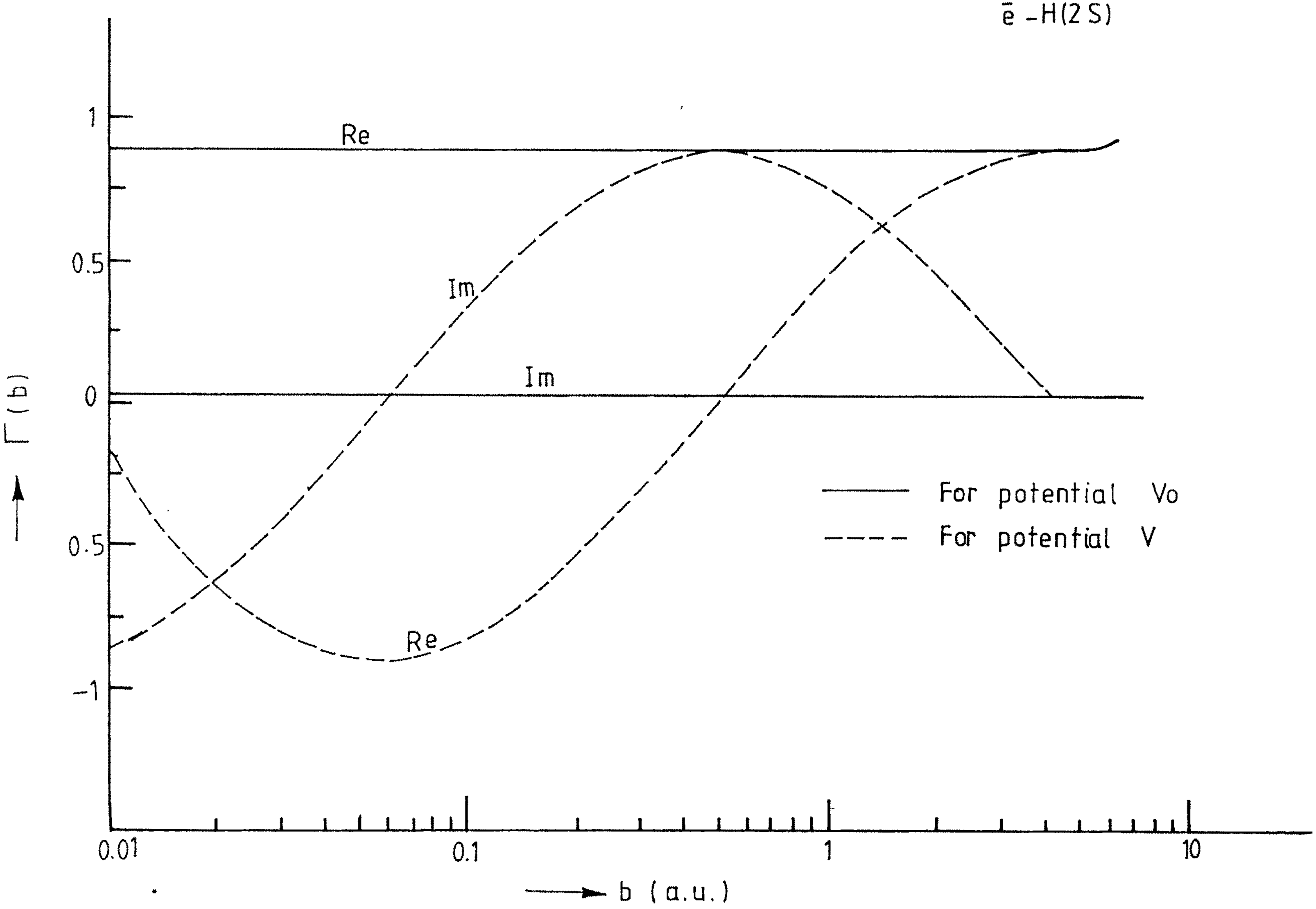


Fig. 4.10
E = 400 eV
$\bar{e}$ - H(2S)
(a) Present TPE
Present Glauber
(b) Pundir et al (1982)
HHOB
+ EBS
● OM
(a)
(b)
1
10^{-1}
10^{-2}
10^{-3}
6×10^{-4}
DCS ($a_o^2 Sr^{-1}$)
20
40
60
80
100
Scattering angle θ (deg)

Fig. 4.11
$E = 100$ eV
$\bar{e}-H(2S)$



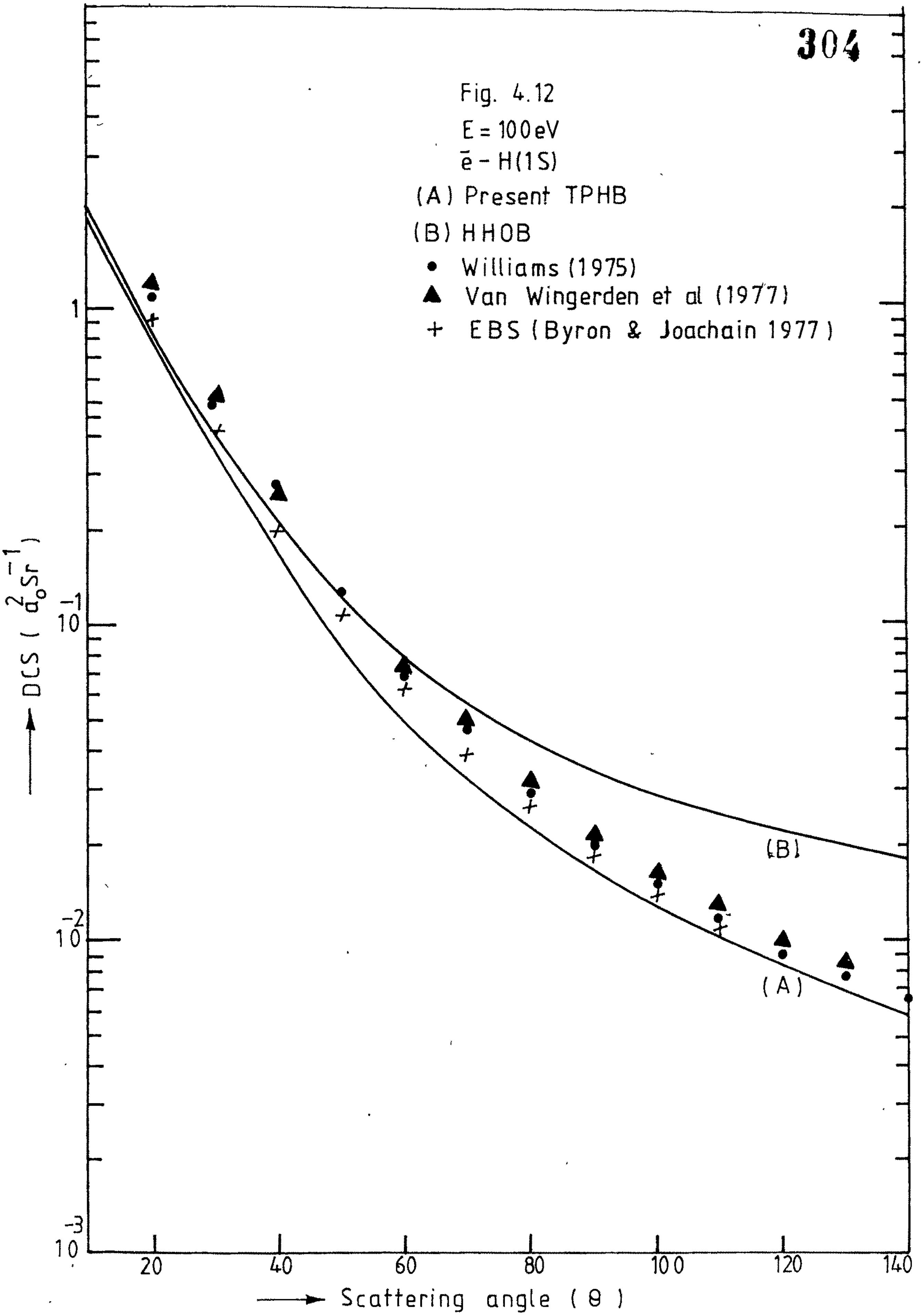


Fig. 4.12
E = 100eV
$\bar{e}$ - H(1S)
(A) Present TPHB
(B) HHOB
● Williams (1975)
▲ Van Wingerden et al (1977)
+ EBS (Byron & Joachain 1977)
(A)
(B)
1
10^{-1}
10^{-2}
10^{-3}
→ DCS ($a_o^2 Sr^{-1}$)
20
40
60
80
100
120
140
→ Scattering angle (θ)

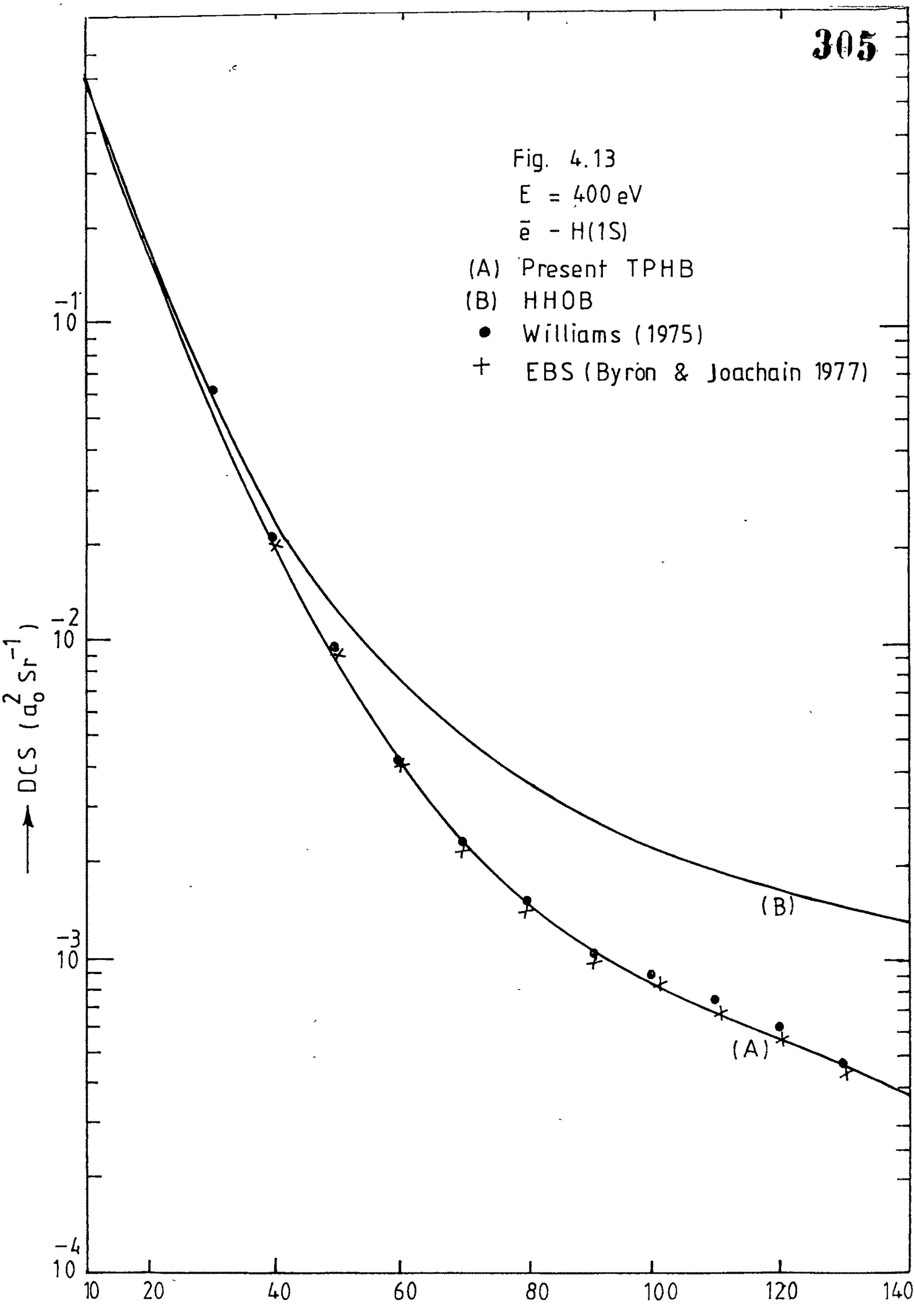


Fig. 4.13

E = 400 eV
$\bar{e}$ - H(1S)
(A) Present TPHB
(B) HHOB
● Williams (1975)
+ EBS (Byron & Joachain 1977)
(A)
(B)
10^{-1}
10^{-2}
10^{-3}
10^{-4}
→ DCS ($a_0^2\,Sr^{-1}$)
10
20
40
60
80
100
120
140
→ Scattering angle (θ)

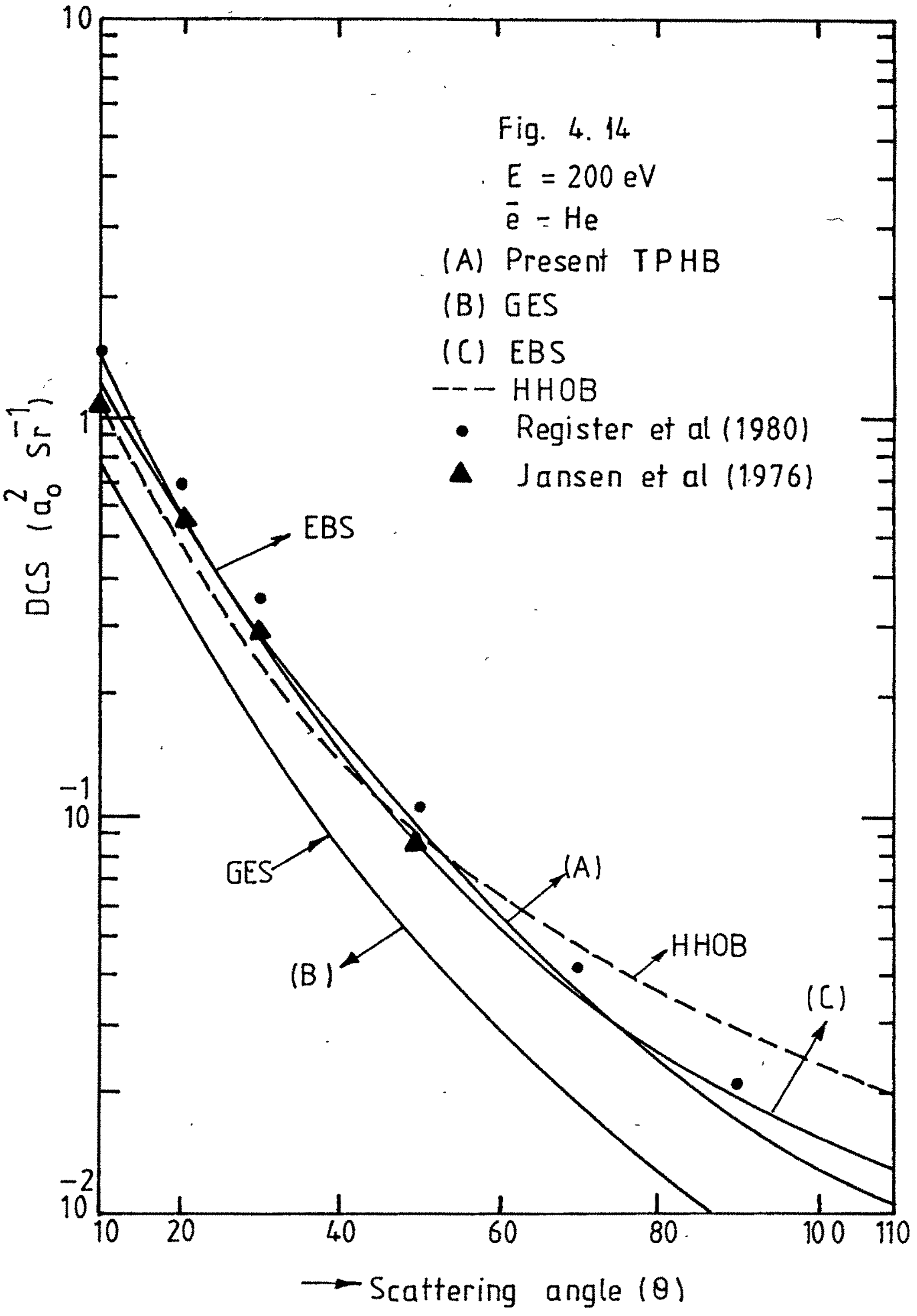


Fig. 4. 14
E = 200 eV
ē - He
(A) Present TPHB
(B) GES
(C) EBS
--- HHOB
● Register et al (1980)
▲ Jansen et al (1976)
EBS
GES
(B)
(A)
HHOB
(C)
DCS (a_o^2 Sr^{-1})
10
1
10^{-1}
10^{-2}
10
20
40
60
80
100
110
Scattering angle (θ)

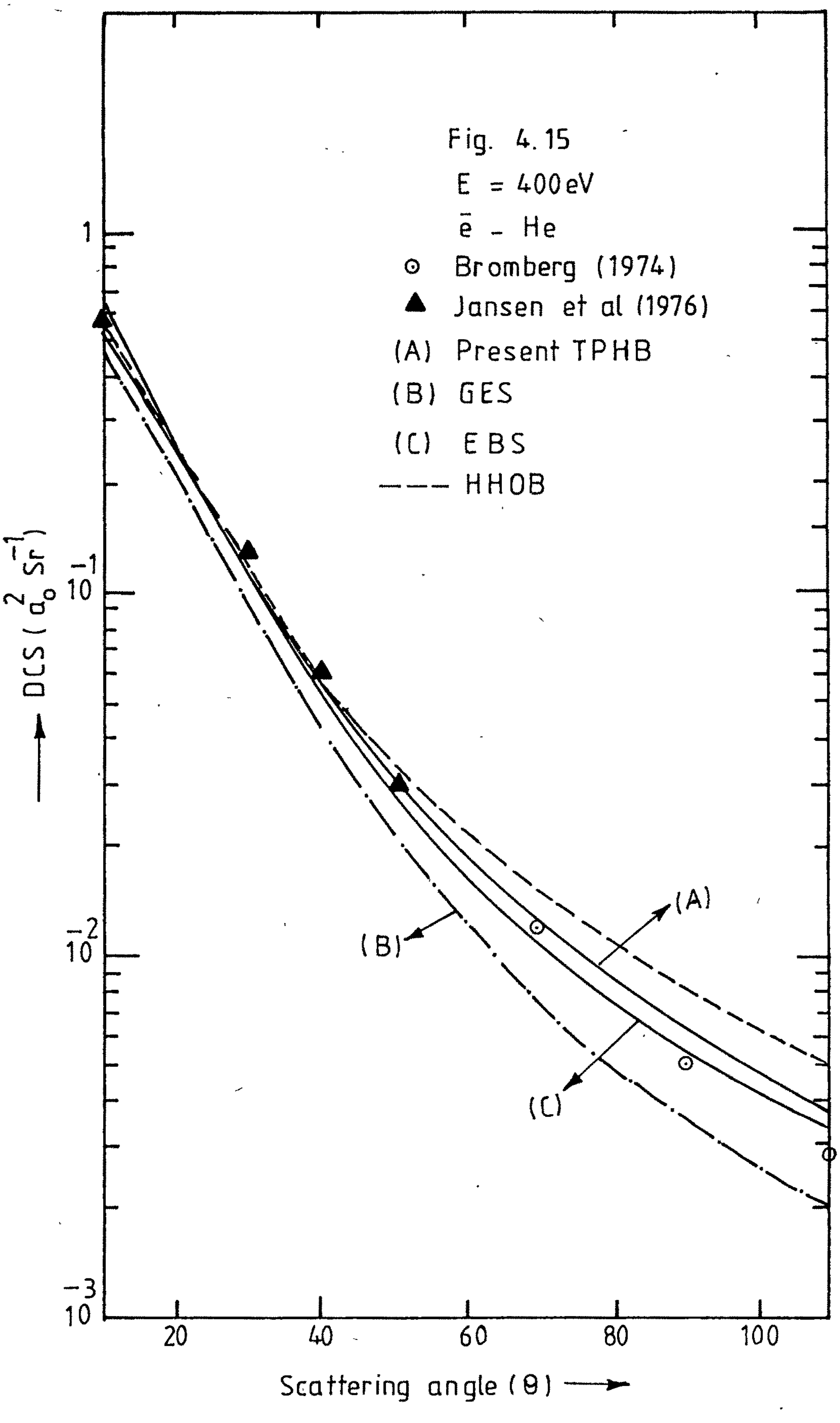


Fig. 4.15
E = 400 eV
ē – He
⊙ Bromberg (1974)
▲ Jansen et al (1976)
(A) Present TPHB
(B) GES
(C) EBS
––– HHOB
(A)
(B)
(C)
1
10^{-1}
10^{-2}
10^{-3}
DCS ($a_0^2 Sr^{-1}$) →
20
40
60
80
100
Scattering angle (θ) →

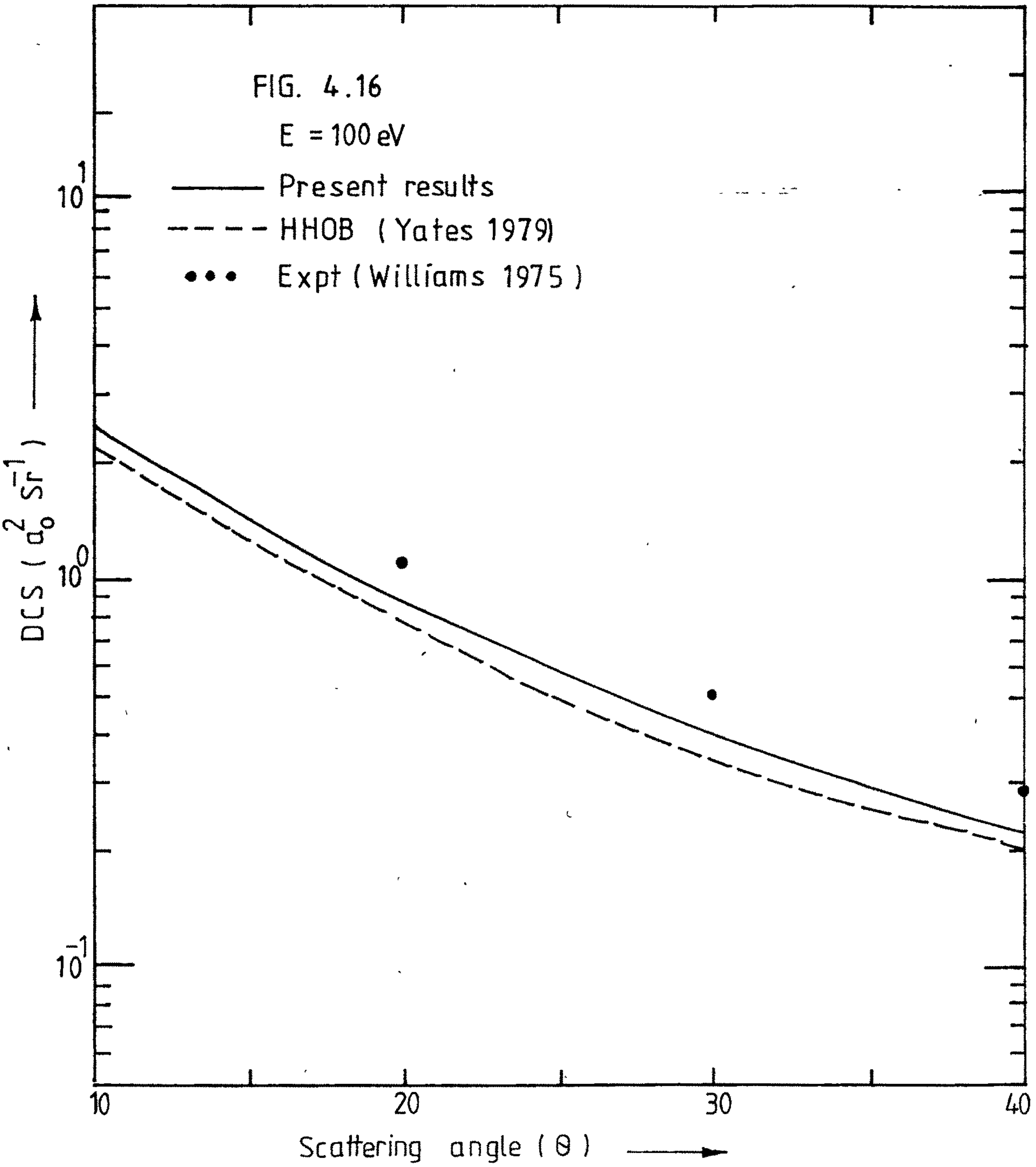


FIG. 4.16

E = 100 eV
Present results
HHOB (Yates 1979)
Expt (Williams 1975)
DCS (a_0^2 Sr^{-1})
10^1
10^0
10^{-1}
10
20
30
40
Scattering angle (θ)