CHAPTER - III

MODIFIED GES APPROXIMATION

3.1 Introduction :

Due to the recent advances - both theoretical and experimental - in the study of electron - scattering by atoms, the search for computationally feasible as well as accurate theoretical methods has been enhanced. The Glauber Eikonal Series (GES) method proposed by Yates (1974) as an alternative method for the evaluation of the Glauber amplitude, has become very popular because of its simplicity. The GES method is very significant in the light of the fact that the lack of application of the Glauber Eikonal approximation to systems more complicated than helium can be attributed to the rapidly increasing computational complexity involved in evaluating the Glauber amplitude expression. Besides its simplicity, the GES method has an inherent advantage that the expressions can be obtained in the closed form. The GES approach involves expanding the amplitude in reciprocal powers of k_i, the momentum of the incident electron, for fixed momentum transfer $q = / \bar{q} /$, and attempting termwise analysis. Such an expansion can be expected to be a reasonable approximate to the Glauber scattering amplitude when k_i is large. This method has been applied to investigate the scattering of electrons by hydrogen and helium (Yates 1974, Singh and Tripathi 1980) and it has been shown explicitly that the first three terms of the GES are sufficient to give a very good representation of the Glauber cross sections for all values of q. As such the GES expressions can be used in analyzing the higher order correction within the framework of eikonal Born Series (EBS) and the modified Glauber method of Byron and Joachain (1973, 74, 74b), thus avoiding the numerical evaluation adopted by them.

In spite of the advantages of the GES method as cited above, it has all the disadvantages of the conventional Glauber method - appreciable underestimation of the cross-sections over the entire angular range except at very small angles where the Glauber amplitude logarithmically diverges. Hence a systematic study has been undertaken to arrive at a modified GES (MGES) method which retains the advantages and improves upon the GES method and removes the aforesaid shortcomings. This MGES method is applied to various scattering phenomena and excellent results are obtained. The improvement over the basic GES method is of special significance.

Formulation :

One way of obtaining improvements over the Glauber approximation has been proposed by Wallace (1973). For the case of potential scattering Wallace wrote down systematic corrections to the Eikonal phase. Detailed studies of the relationships between the terms of the Born, eikonal and Wallace series have been carried out by Byron et al (1975,79). In the light of these developments, Byron et al (1981) recently proposed a generalisation of the potential scattering Wallace amplitude to the multiparticle case, in the same spirit as that of Glauber's original extension of the potential scattering eikonal amplitude. This generalisation was also obtained subsequently by Franco and Iwinski (1982) and by Unnikrishnan and Prasad (1982). However, it should be noted that the resulting many-body Wallace amplitude does not eliminate all the difficulties inherent in the Glauber amplitude. In particular, the Wallace extension of the Glauber approximation is still a zero-excitation energy approximation and therefore does not account for the long-range polarisation effects at small angles and represents inadequately absorption effects in the same region. These difficulties can be eliminated by removing the term of the many-body Wallace amplitude which is of second order in the projectile-target interaction and replacing it by an appropriate second Born term. The amplitude thus obtained has all the strengths of the EBS method at small and intermediate angles where perturbation theory is rapidly convergent. It also contains the two leading terms (in powers of k_i^{-1}) of each order of perturbation theory summed to all orders so that at large angles the main feature of the scattering amplitude-which is similar to what is found in pure coulomb scattering-is dealt with satisfactorily.

In the light of the above discussions and keeping in mind the simplicity of the GES method, a parallel termwise analysis of the Wallace Corrected Glauber series (Byron et al 1982) was performed in the present study, the troublesome imaginary part was replaced by a very similar Born term (Yates 1979) and the effects of exchange were included through the Ochkur (1964) approximation. The resulting scattering amplitude was called the modified Glauber eikonal series (MGES) amplitude.

The many body Wallace amplitude is given by (Byron et al 1982)

$$f_w = \frac{k_i}{2\pi i} \int e^{i\,\underline{q}\cdot\underline{b}} < \psi_f\,(X) / \exp\left[i\,\left(\frac{x_o(b,x)}{k_i} + \frac{x_1(b,x)}{k_i^{\,3}} \right)\right] - 1 / \psi_i\,(x) > d^2 b \qquad (3.1)$$

where $r = b + z\,\hat{n}$, $\hat{n}$ being perpendicular to q, is the incident electron co-ordinate, X represents the target electron co-ordinates $r_1, r_2 - - r_z$, z being the atomic number, x_o is the usual Glauber phase, x_1 is the Wallace phase correction and ψ_i and ψ_f are the wavefunctions of the target at initial and final states.

For consistency of $O\left(\frac{1}{k_i^2}\right)$ in the DCS, f_w can be expressed in the form of a series. i.e.

$$f_w = \sum_{n=1}^{3} i^{n-1} \frac{k_i}{2\pi n!} \int d^2b \, e^{i \underline{q}\cdot\underline{b}} < \Psi_f / x_o^n / \Psi_i > + \frac{1}{2\pi k_i^2} \int d^2b \, e^{i\underline{q}\cdot\underline{b}} < \Psi_f / x_1 / \Psi_i > \qquad (3.2)$$

The first part of the above equation gives the first three terms of the GES (Yates 1974) whereas the second part is the additional real part in the second term of the series corresponding to Wallace correction. Hence (3.2) can be written as

$$f_w = f^{(1)}_{GES} + i \, f^{(2)}_{GES} - f^{(3)}_{GES} + fw_2 \qquad (3.3)$$

where $$fw_2 = \frac{1}{2\pi k_i^2} \int d^2b \, e^{i\underline{q}\cdot\underline{b}} < \Psi_f / x_1 / \Psi_i > \qquad (3.4)$$

As discussed previously, the trouble some imaginary part of the series (3.3) is now replaced by an appropriate Born term. In the present study, $f^{(2)}_{GES}$ is replaced by the $O(k_i^{-1})$ terms in $f^{(2)}_{HEA}$ in the HHOB approximation (Yates 1979) with the following justifications.

1. the $O\left(\frac{1}{k_i}\right)$ terms in $f^{(2)}_{HEA}$ (i.e. i f_{Im} and f_{Re_1}) originate from the same part of the Green's function which corresponds to $f^{(2)}_{GES}$.

2. the procedure of the linearisation of the Green's function etc. adopted in the GES and HHOB methods are very similar. (In fact, if the average excitation energy parameter β is made zero in the HHOB, the GES results will be obtained).

3. It can be shown that the $O(\frac{1}{k_i^2})$ term in $f^{(2)}_{HEA}$ (i.e. $f\,Re_2$) indirectly corresponds to the fw_2 in the present analysis.

Due to the replacement of $f^{(2)}_{GES}$ by the above mentioned Born terms, the β factor in $i\,fIm$ removes the divergence problem in $f^{(2)}_{GES}$. Since the 'frozen target' model is derived from a many-body Green's function in which closure has been applied and the average excitation energies in both the initial and final channels have been set equal to zero, the long-range dynamic polarization effects will be missing from the many-body Wallace amplitude (f_w). In particular, Byron et al (1982) have shown that the real part of the second term in f_w(i.e. Re f_{w2}) given by (3.4) is just the k_i^{-2} part of Re $\bar{f}_{SB2}$ (where SB2 denotes the simplified second Born term obtained in the closure approximation) with an average excitation energy value of zero, and thus lacks the all-important contribution of order k_i^{-1} which is characteristic of dipole polarisation effects. With the introduction of fRe_1 into the expression(3.3), it will take care of this polarisation effect which is not accounted for in the GES. It may be noted that the Born terms $i\, f\mathrm{Im}$ and $f\mathrm{Re}_1$ can also be obtained in the closed form.

Hence incorporating the Born terms, (3.3) becomes

$$f_w = f^{(1)}_{GES} + i\, f\mathrm{Im} + f\mathrm{Re}_1 - f^{(3)}_{GES} + fw_2 \qquad (3.5)$$

When the exchange effects are also included, the scattering amplitude becomes

$$f_w = f^{(1)}_{GES} + i\, f\mathrm{Im} + f\mathrm{Re}_1 - f^{(3)}_{GES} + fw_2 \pm f_{exch} \qquad (3.6)$$

The above expression gives the MGES scattering amplitude. Making use of the scattering amplitudes for different scattering phenomena, the corresponding DCS can be easily evaluated.

Evaluation of the scattering amplitude :

The GES terms in the scattering amplitude (3.6) are evaluated following the prescription of Yates (1974). The Born terms are evaluated following Yates (1979) (section 2.11). The exchange term f_{exch} in (3.6) is calculated using the Ochkur approximation (1964). In the evaluation of fw_2 given by (3.4), the static part of the potential only is taken because the neglect of the contribution of the second order effects like polarisation treated in the second order of the approximation may not make much of a difference because those effects have already been incorporated through the Born terms. Moreover, calculations become abundantly simpler with the static potentials. For the static potential V(r) the phase function

$$X_1 (b) = -\int_{-\infty}^{\infty} V_1 (r)\, dz \qquad (3.7)$$

where $V_1 (r) = V(r) \left[V(r) + r \frac{d}{dr} V(r) \right]$

This X_1 (b) is far simpler than the corresponding phase function (for the exact potential V) given by

$$X_1 (b, X) = \frac{1}{2} \int_{-\infty}^{\infty} (\nabla x_+) . (\nabla x_-)\, dz \qquad (3.8)$$

with

$$X_+ (b,z,X) = -\int_{-\infty}^{z} V (b,z',x)\, dz' \text{ ,and}$$

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

It should be stressed that because of the complexity of x_1 (b,x), the many-body Wallace amplitude (3.1) is vastly more difficult to evaluate than the many-body Glauber amplitude. Still, the attraction of (3.1) is that it is also unitary and contains phase correction. In view of the tremendous difficulty associated with the evaluation of (3.4) for higher atoms using (3.8), there is ample justification for the replacement of x_1 (b,x) by x_1(b) given by (3.7).

Thus, for static potentials, (3.4) becomes

$$fw_2 = -\frac{1}{2\pi k_i{}^2} \int d^2b \; e^{i\underline{q}\cdot\underline{b}} \int_{-\infty}^{\infty} V_1 (r)\, dz$$

$$= - \frac{1}{2\pi k_i^2} \int d^2b \; e^{i\underline{q}\cdot\underline{b}} \int_{-\infty}^{\infty} dz \int d\underline{P} \; e^{-i\underline{P}\cdot\underline{b}}$$

$$\int_{-\infty}^{\infty} dP_z \; e^{-iP_z z} \quad \bar{V}_1(P, P_z)$$

where $\bar{V}_1$ represents the Fourier transform of V_1. Here the following properties of delta functions are made use of:.

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

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

$\int d\underline{P} \; \delta(q-P) \; \bar{V}_1(P) = \bar{V}_1 \; (q)$. The analysis of the above term using these simplifications gives

$$fw_2 = - \frac{4\pi^2}{k_i^2} \; \bar{V}_1 \; (q) \tag{3.9}$$

Now all the terms in (3.6) can be easily evaluated. The feasibility and simplicity of the present MGES approach are demonstrated in the later sections of this chapter through applications to various scattering phenomena.

3.2 Elastic scattering of electrons from the ground state of hydrogen atom.

The elastic scattering of electrons from the ground state of hydrogen atom (abbreviated as ESGH process) can be termed as the simplest problem in atomic collision theory. Obviously, quite a lot of work has been reported on the above process. It will be of great interest to illustrate the above discussed MGES approach through the application to the ESGH process and to explore the position of the present results in the midst of a large amount of data arrived at through a variety of estimations.

The interaction potential for the ESGH process is given by

$$V_H = -\frac{1}{r} + \frac{1}{/\underline{r}-\underline{r}_1/} \qquad (3.10)$$

The groundstate wave function of hydrogen is

$$\psi_{IS} = \frac{1}{\sqrt{\pi}} e^{-r_1} \qquad (3.11)$$

For the ESGH process, $\psi_i = \psi_f = \psi$

The static potential for H (1S) is

$$V_{st} = < \psi / V / \psi > = -\left(1 + \frac{1}{r} \right) e^{-2r} \qquad (3.12)$$

The various terms in (3.6) are now evaluated using (3.10), (3.11) and (3.12). It will be convenient to express the product of the wave functions as

$$\psi^* \psi = \frac{1}{\pi} e^{-2r} = \frac{1}{\pi} \left(-\frac{d}{d\lambda} \right) \frac{e^{-\lambda r_1}}{r_1} /_{\lambda=2} \qquad (3.13)$$

Now introducing the dimensionless vector $z = q/\lambda$ and following the procedure of Yates (1974),

$$f^{(1)}_{GES} = \frac{1}{2\pi} \int e^{i\underline{q}\cdot\underline{r}} \left(1+\frac{1}{r}\right) e^{-2r} d\underline{v}$$

$$= \int_0^\infty \int_0^\pi e^{iqr \, Cos\theta} \left(1+\frac{1}{r}\right) e^{-2r} r^2 dr \, Sin\theta \, d\theta$$

$$= 2\frac{(q^2+\lambda^2+2\lambda)}{(q^2+\lambda^2)^2}$$

$$= \frac{2 + z^2}{\lambda(1 + z^2)^2}$$

i.e. $$f^{(1)}_{GES} = \frac{2 + z^2}{\lambda(1 + z^2)^2} \qquad (3.14)$$

Now, $$f^{(2)}_{GES} = \frac{Z^2}{\pi k_i} \int \frac{d\underline{P}}{P^2 |\underline{q}-\underline{p}|^2} \langle \psi_f | B(P)\, B(q-p) | \psi_i \rangle$$

Here $$B(P)\; B(q-p) = 1 - e^{i\underline{P}\cdot\underline{r}_1} - e^{i|\underline{q}-\underline{P}|\cdot r_1} + e^{i\underline{q}\cdot\underline{r}_1}$$

$$\therefore \langle \psi_f | B(P)\, B(q-p) | \psi_i \rangle = \left(-\frac{d}{d\lambda}\right) 4 \left[\frac{q^2 + 2\lambda^2}{\lambda^2 (q^2+\lambda^2)} - \frac{1}{P^2+\lambda^2} - \frac{1}{|q-p|^2+\lambda^2}\right]$$

$$\therefore f^{(2)}_{GES} = \frac{-4Z^2}{\pi k_i} \frac{d}{d\lambda} \int d\underline{P} \left\{ \frac{1}{P^2 |q-p|^2} \left[\frac{-q^2/\lambda^2}{q^2+\lambda^2}\right] + \frac{2}{\lambda^2} \frac{1}{|q-p|^2} \frac{1}{P^2+\lambda^2} \right\}$$

Here partial fractions of the form

$$-\int \frac{dP}{P^2 |q-p|^2 (P^2+\lambda^2)} = \int \frac{dP}{|q-p|^2} \frac{1}{\lambda^2} \left[\frac{1}{P^2+\lambda^2} - \frac{1}{P^2}\right]$$

are made use of.

Substitution of $z = q/\lambda$ gives

$|q-p|^2 = \lambda^2 |z - \frac{P}{\lambda}|$, and $\frac{d}{d\lambda}$ has to be replaced by

$$-\frac{z^2}{q} \frac{d}{dz}$$

$$\therefore f^{(2)}_{GES} = \frac{4\,Z^2}{\pi\,k_i}\,\frac{z^2}{q}\,\frac{d}{dz}\int\frac{dP}{\lambda^2}\left\{\frac{-z^2}{z^2+1}\,\frac{1}{P^2\lambda^2\,\left|z-\frac{P}{\lambda}\right|} + 2\Big/\left(\lambda^2\left|z-\frac{P}{\lambda}\right|^2(P^2+\lambda^2)\right)\right\}$$

Substitution of $\frac{P}{\lambda} = P_1$ results in

$$f^{(2)}_{GES} = \frac{4Z^2}{\pi\,k_i}\,\frac{z^2}{q}\,\frac{d}{dz}\int\frac{dP_1}{\lambda^4}\left\{\frac{-z^2}{(z^2+1)}\,\frac{-\ 1}{P^2_1\left|z-P_1\right|^2} + \frac{2}{\left|z-P_1\right|^2(1+P_1{}^2)}\right\}$$

$$= \frac{4\,Z^2}{\pi\,k_i}\,\frac{z^2}{q}\,\frac{d}{d_z}\,\frac{z^4}{q^4}\left[\frac{-z^2}{1+z^2}\,I_{21} + 2I_{22}\right]$$

where $I_{2k} = \int\frac{dP}{\left|z-P\right|^2(P^2+\ell_k)}$; $\ell_1=0$, $\ell_2=1$.

Since $Z^2 = 1$,

$$f^{(2)}_{GES} = \frac{1}{8\pi k_i z^3}\left(\frac{d}{dz}\right) z^4\left[-\frac{z^2}{1+z^2}\,I_{21} + 2I_{22}\right]$$

The evaluation of the integrals are shown in appendix. These results seem initially discouraging in that the integrals I_{2k} are absolutely divergent. However, for the particular combinations appearing in the above equation, a tedious, but straight-forward calculation shows that all infinities cancel exactly. It may be noted that similar cancellations occur in the analysis of the Massey-Mohr approximation to the second Born term as demonstrated by Moiseiwitsch and Williams (1959).

Thus the substitution of I_{2k} integrals leads to

$$f^{(2)}_{GES} = \frac{1}{2k_i z^3} \left(\frac{d}{dz} \right) \frac{z^4}{1 + z^2}{}_2 \ ln \left(\frac{1 + z^2}{z} \right) \qquad (3.15)$$

(Eventhough $f^{(2)}_{GES}$ does not figure in the MGES scattering amplitude (3.6), this term also is evaluated in all the scattering processes studied here in order to compare with the imaginary part of the Born term.)

$$f^{(3)}_{GES} = \frac{2\pi k_i^{(-z^3)}}{6\pi^3 k_i^3} \int \frac{d\underline{P}_1}{P_1^2} \int \frac{d\underline{P}_2}{P_2^2} \frac{1}{|q-(p_1+p_2)|^2}$$

$$\langle \psi_f | B(P_1) \, B(P_2) \, B\left[q - (p_1+p_2)\right] | \psi_i \rangle$$

Proceeding in the same way as in

$f^{(2)}_{GES}$,

$$\langle \psi_f | B(P_1) \, B(P_2) B(q-p_1-p_2) | \psi_i \rangle$$

$$= -4 \frac{d}{d\lambda} \left\{ \frac{1}{\lambda^2} - \frac{1}{P_1^2 + \lambda^2} - \frac{1}{P_2^2 + \lambda^2} - \frac{1}{|q-p_1-p_2|^2 + \lambda^2} \right.$$

$$\left. + \frac{1}{|q-p_1|^2 + \lambda^2} + \frac{1}{|q-p_2|^2 + \lambda^2} + \frac{1}{|p_1+p_2|^2 + \lambda^2} - \frac{1}{q^2 + \lambda^2} \right\}$$

Making use of substitutions like $q - p_1 = p_1'$, it can be shown that the integral $\int \frac{dP_1}{P_1^2} \int \frac{dP_2}{P_2^2} \frac{1}{|q-p_1-p_2|^2} X$ will have the same form for the three values of X namely,

$\frac{-1}{p_1^2+\lambda^2}$, $\frac{-1}{p_2^2+\lambda^2}$, $\frac{-1}{|q-p_1-p_2|^2+\lambda^2}$. Similar grouping can be done with the positive terms also of the above expression. Now the substitutions

$z = q/\lambda$, $\frac{p_1}{\lambda} = p_3$, $\frac{p_2}{\lambda} = p_4$ give

$$f^{(3)}_{GES} = \frac{1}{24\pi^2 k_i^2 z^3} \left(\frac{d}{dz}\right) z^4 \left[-\frac{z^2}{1+z^2} I_{31} + 3I_{32} - 3I_{33}\right]$$

where $I_{3k} = \int \frac{d\underline{p}_1}{|z-p_1|^2} \int \frac{d\underline{p}_2}{p_2^2 |p_1-p_2|^2} \Big/ \beta_k$,

$\beta_1 = 1$, $\beta_2 = 1 + p_2^2$, $\beta_3 = 1 + p_1^2$.

The I_{3k} integrals also are divergent like I_{2k} integrals. But the beauty of these calculations is the exact cancellation of divergencies. The substitution of I_{3k} into the above expression gives

$$f^{(3)}_{GES} = \frac{1}{8k_i^2 z^3} \left(\frac{d}{dz}\right) \frac{z^4}{1+z^2} \left\{ 4\left[\ln\left(\frac{1+z^2}{z}\right)\right]^2 + \frac{\pi^2}{3} - 2A(z) \right\} \qquad ..(3.16)$$

where $A(z) = 2(\ln z)^2 + \frac{\pi^2}{6_n} + \sum_{n=1}^{\infty} \frac{(-z^2)^n}{n^2}$, $z \leqslant 1$

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

Now the Born terms are evaluated following Yates (1979).

The evaluation of these terms differ from that of the GES terms mainly due to the inclusion of average excitation energy. For ESGH process,

$$U^{(2)}_{f_1}(\underline{q}-\underline{p}-\beta\hat{\chi},\underline{p}+\beta\hat{\chi}) = \frac{1}{\pi^4}\frac{1}{(P^2+\beta^2)\,(|\underline{q}-\underline{p}|^2+\beta^2)}\left(-\frac{d}{d\lambda}\right)$$

$$\left[\frac{q^2+2\lambda^2}{\lambda^2(q^2+\lambda^2)} - \frac{1}{|\underline{q}-\underline{p}|^2+\beta^2+\lambda^2} - \frac{1}{P^2+\beta^2+\lambda^2}\right]$$

The above expression reveals the correlation with the corresponding expression in $f^{(2)}_{GES}$, but for the average excitation energy parameter β. Hence fIm can be written - making use of partial fractions - as

$$fIm = \frac{-4}{\pi k_i}\frac{d}{d\lambda}\int\frac{d\underline{P}}{(|q-p|^2+\beta^2)}\frac{1}{\lambda^2}\left[\left(\frac{q^2+2\lambda^2}{q^2+\lambda^2}-2\right)\frac{1}{P^2+\beta^2}\right.$$

$$\left. + \frac{2}{P^2+\beta^2+\lambda^2}\right]$$

which may be written as

$$fIm = -\frac{4}{\pi k_i}\frac{d}{d\lambda}\frac{1}{\lambda^2}\left[2I_1(\beta^2,\lambda^2) - \frac{q^2}{q^2+\lambda^2}I_1(\beta^2,0)\right] \qquad (3.17)$$

The average excitation energy parameter $\beta = 0.465/k_i$ (Byron and Joachain 1977).

A very similar procedure can be adopted for the evaluation of the real Born term fRe_1. In this case, $U^{(2)}_{fi}$ is similar to the one given above but for the replacement of β by P_z. Thus $f\,Re_1$ becomes

$$f\,Re_1 = \frac{4\pi^3}{k_i}\frac{1}{\pi}\frac{1}{\pi^4}\frac{d}{d\lambda}\mathcal{P}\int d\underline{P}\int_{-\infty}^{\infty}dP_z\,\frac{1}{(|q-p|^2+P_z^2)(P_z-\beta)}$$

$$\frac{1}{\lambda^2}\left[\left(\frac{q^2+2\lambda^2}{q^2+\lambda^2}-2\right)\frac{1}{p^2+p_z^2}+\frac{2}{p^2+p_z^2+\lambda^2}\right]$$

which may be written as

$$f\,Re_1=\frac{4}{\pi^2 k_i}\left(\frac{d}{d\lambda}\right)\frac{1}{\lambda^2}\left[2I_2(\beta^2,\lambda^2)-\frac{q^2}{q^2+\lambda^2}I_2(\beta^2,0)\right] \quad (3.18)$$

The integrals $I_1(\beta^2,\lambda^2)$ and $I_2(\beta^2,\lambda^2)$ are given in the appendix. $I_1(\beta^2,0)$ is obtained by putting $\lambda=0$ in $I_1(\beta^2,\lambda^2)$

Now, fw_2 in (3.6) is evaluated using (3.12), (3.7) and (3.9). This gives $$fW_2=\frac{2}{k_i^2}\left[\frac{1}{(16+q^2)}+\frac{24}{(16+q^2)^2}+\frac{4(48-q^2)}{(16+q^2)^3}\right] \quad (3.19)$$

The application of Ochkur approximation in the evaluation of the exchange term gives

$$f_{exch}=-\frac{2}{k_i^2}\int e^{i\underline{q}\cdot\underline{r}}\,\psi^{*}(r)\,\psi(r)$$

$$=-\frac{32}{k_i^2}\,\frac{1}{(\lambda^2+q^2)^2} \quad ..(3.20)$$

Substitution of the terms from (3.14) to (3.20) gives the MGES scattering amplitude (3.6) for EGSH process. Now the DCS is given by

$$\frac{d\sigma}{d\Omega}=\frac{1}{4}\,/\,f_d+f_e\,/^{2}+\frac{3}{4}\,/\,f_d-f_e/^{2} \quad (3.21)$$

where $f_e=f_{exch}$ and $f_d=f_w-f_e$

The total elastic cross sections (TEC) are calculated using (1.9). This is given by a measure of the area enclosed by the curve drawn with $\frac{d\sigma}{d\Omega}$ Sinθ against θ. The total cross sections (TCS) are calculated from

$$\sigma_t = \frac{4\pi}{k_i} f_{Im} \quad (\theta = 0) \qquad (3.22)$$

Results and discussion :

The DCS for the ESGH process are calculated using (3.21) for incident energies from 100 eV to 800 eV. The TEC and TCS are also calculated using (1.9) and (3.22). The DCS at 100 and 400 eV are displayed in fig.3.1 and fig.3.2 alongwith other theoretical and experimental data for comparison. The individual terms of the MGES amplitude (3.6) are exhibited in tables 3.1a and 3.1b at the incident energies 200 eV and 400 eV. In table 3.2, the DCS at the sample energies are given. The TEC values in the present study along with the data of other workers is reported in table 3.3. Similarly, table 3.4 displays the TCS values.

A glance at fig.3.1 and 3.2 reveals that all the DCS curves lie close to one another in the small angle region and they depart from each other as θ increases. The real test of a particular approximation is in its satisfactory description of the scattering process in the entire angular range. Fig.3.1 shows that the present MGES results agree very nicely with the experimental data and perhaps they are nearest to the experiments. They improve upon the basic GES results considerably. The present results closely agree with the OM results (Byron and Joachain 1981). The disagreement of these results with the HHOB results (Yates 1979) is not at all discouraging because the HHOB results are proved to be very much overestimating in the large angle region (Rao and Desai 1981, 1983). The present results agree very nicely-for all θ - with the sophisticated DWSBA calculations of Kingston and Walters (1980) (not shown here); and also almost coincide with the recent UEBS results (Byron et al 1982) in the small angle region.

The present MGES method (3.6) may in general be considered as a termwise analysis of the UEBS method in the same spirit of the GES analysis. Hence, if the inequality $k_i >> 1$ is satisfied such that the MGES (3.6) can be anticipated to be rapidly convergent, the present termwise analysis should give a very good representation of the UEBS cross section for all values of q. From Fig.3.1, it can be seen that the MGES results differ from the UEBS results in the large angle region. This difference is mainly due to the difference in the treatment of exchange in the two methods. In UEBS, Byron et al have used a new non-perturbative approximation for the exchange scattering amplitude which leads to lower differential cross sections at large angles, whereas in the present MGES, Ochkur approximation is used for exchange calculations. However, excluding exchange effects, the MGES and UEBS methods give very nearly the same results. The agreement of the two sets of results becomes better at large energies because the present amplitude series (3.6) becomes more rapidly convergent then. It may be noted in fig.3.2 that at 400 eV, the MGES and UEBS results are very close to each other, even with the different treatments for exchange. Thus the MGES (3.6) proves to be a satisfactory representation of the UEBS for all values of q, even when the inequality $k_i >> 1$ is only marginally satisfied.

However, it may be noted that the UEBS evaluation is tremendously difficult even in the case of hydrogen (Byron et al 1982). It is bound to be more and more complicated for other atoms like He, Li etc. But the present MGES analysis, which represents the UEBS series satisfactorily, may be easily evaluated even in the case of higher atoms, as shown in the subsequent sections of this chapter. This is precisely the most important advantage of the present method.

The present method, which is a high-energy-approximation method, should be naturally expected to give better results at higher incident energies. This fact is explicitly clear from fig.3.2. It is encouraging to note the improvement over the basic GES (Yates 1974) results here also eventhough the improvement is less than in fig.3.1.

Table 3.1a shows the individual terms of (3.6) for the ESGH process at 200 eV. The similarity between the imaginary terms $f^{(2)}_{GES}$ and fIm is striking. $f^{(2)}_{GES}$ comes from a zero-excitation energy approximation whereas the excitation energy parameter is present in fIm. Their similarity is another point in favour of the replacement of $f^{(2)}_{GES}$ by the HEA Born terms in the present study. In Table 3.2 the present DCS values at certain sample energies are exhibited.

Table 3.3 throws light upon the similarity of the TEC values calculated in the MGES and UEBS methods. It is obvious that the agreement improves as the energy increases. This supports the argument that the MGES satisfactorily represents the UEBS as found in the DCS comparisons. The table also shows that the present results agree nicely with all other theoretical calculations whereas all of them differ from the experimental values. In the light of the excellent agreement between the theoretical predictions, it is difficult to see what effects could be invoked on the theoretical side to explain the differences between theory and experiment.

The table (3.4) of total cross sections also shows such a behaviour as is qualitatively similar to the one shown by table 3.3. Remembering equation (3.22), it can be easily understood that the present values of TCS should be the same as those obtained in the HHOB method of Yates (1979) because both the methods have identical imaginary terms. Naturally, the present results compare better with the other sets of data for higher energies.

Through the above discussions, the feasibility, simplicity and significance of the MGES approach are brought to light. The satisfactory representation of the sophisticated UEBS amplitude, the ease of calculations in comparison with the UEBS evaluation and the highly encouraging results obtained in the ESGH process provide enough motivation to extend the present MGES approach to other scattering phenomena.

3.3. Elastic scattering of electrons from the excited (2S) state of Hydrogen atom :

In spite of its numerous applications in astrophysics, plasma physics and various gaseous phenomena - besides the intrinsic theoretical interest associated with it -, very less work has been reported on the study of electron scattering from excited metastable states of atoms, when compared with the bulk of estimations of similar process from the ground state. The same is true even in the case of hydrogen atom. Electron-scattering from 2S state of hydrogen - abbreviated as ESEH - is a fundamental process for which it is reasonable to assume that experimental data will become available in the near future. A recent revival of theoretical interest on this scattering problem has resulted in the extension of many a theoretical method to study the above problem. Even then, the available data can be considered as scarce. Added to this, the motivating factors cited at the end of section 3.2 are enough for an exploration of the ESEH process from the dimensions of the MGES approach.

The interaction potential for the ESEH is the same as for ESGH (3.10). The H (2S) wavefunction is known as

$$\Psi_{2S} = \frac{1}{4\sqrt{2\pi}} (2-r_1)\, e^{-r_1/2} \qquad (3.23)$$

The static potential is evaluated as $V_{st} = < \Psi_f / V / \Psi_i >$

$$= -\left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{8} \right) e^{-r} \qquad (3.24)$$

because $\Psi_f = \Psi_i = \Psi_{2S}$.

(3.10), (3.23) and (3.24) may be used for the evaluation of the individual terms of (3.6). For similarity with the ESGH process, the product $\Psi^* \Psi$ may be represented as

$$\Psi^* \Psi = C_1 \left(\frac{-d^3}{dy_1^3}\right) \frac{e^{-y_1 r_1}}{r_1} + C_2 \left(\frac{d^2}{dy_2^2}\right) \frac{e^{-y_2 r_1}}{r_1} + C_3 \left(-\frac{d}{dy_3}\right) \frac{e^{-y_3 r_1}}{r_1} \qquad (3.25)$$

where $y_1 = y_2 = y_3 = 1$,

$C_1 = \frac{1}{32\pi}$, $C_2 = \frac{-1}{8\pi}$, $C_3 = \frac{1}{8\pi}$

$f^{(1)}_{GES}$ is essentially the same as first Born term (Yates 1979), the evaluation of which is straight forward. This gives

$$f^{(1)}_{GES} = 16\pi \left\{ \frac{C_3 (q^2 + 2\alpha_3^2)}{\alpha_3^3 (q^2+\alpha_3^2)^2} + C_2 \left(\frac{-d}{d\alpha_2}\right) \frac{q^2 + 2\alpha_2^2}{\alpha_2^3 \, (q^2+\alpha_2^2)^2} + C_1 \frac{d^2}{d\alpha_1^2} \frac{q^2 + 2\alpha_1^2}{\alpha_1^2 (q^2+\alpha_1^2)^2} \right\} \qquad (3.26)$$

where $\alpha_n = y_n$.

Now proceeding in the same way as in ESGH process, the second and third GES terms may be obtained.

The expression for $f^{(2)}_{GES}$ in the ESEH process can be easily obtained by considering the similarity of the wave-function product (3.25) with the corresponding expression (3.13) in the ESGH process. Corresponding to the three terms in the $\psi^* \psi$ (3.25), three expressions will constitute the $f^{(2)}_{GES}$. Hence

$$f^{(2)}_{GES} = f^{(2)}_{1} + f^{(2)}_{2} + f^{(2)}_{3}$$

Corresponding to the term $C_3 \left(\frac{-d}{dy_3}\right) \frac{e^{-y_3 r_1}}{r_1}$,

$$f^{(2)}_{3} = C_3 \pi \left(\frac{-4}{\pi k_i q^4} \right) D^1 \, f_2(z_3)$$

where D^1 is the differentiation w.r.t. z as transformed from $\frac{d}{dy_3}$

$$\left[ie \; \frac{d}{dy_3} f(y_3) = - \frac{z_3^2}{q} \frac{d}{dz_3} f(z_3) \right]$$ and

$$f_2(z_3) = 4\pi \frac{z_3^4}{1+z_3^2} \ln \frac{1+z_3}{z_3} \text{ with } z_3 = \frac{q}{y_3}$$

Similarly, for the other terms in (3.25),

$$f^{(2)}_{2} = C_2 \pi \left(\frac{-4}{\pi k_i q^4} \right) D^{11} \, f_2(z_2)$$ and

$$f^{(2)}_{1} = C_1 \pi \left(\frac{-4}{\pi k_i q^4} \right) D^{111} f_2(z_1)$$

where D^{11} and D^{111} denote differentiations of the second and third orders w.r.t. z as transformed from $\frac{d^2}{dy^2}$ and $\frac{d^3}{dy^3}$. Using the expressions

$$\frac{d^2}{dy^2} f(y) = \frac{z^3}{q^2}\left[2\frac{d}{dz} f(z) + z\frac{d^2}{dz^2} f(z)\right] \text{ and}$$

$$\frac{d^3}{dy^3} f(y) = -\frac{z^4}{q^3}\left\{ 6\frac{d}{dz} f(z) + 6z\frac{d^2}{dz^2} f(z) + z^2\frac{d^3}{dz^3} f(z)\right\}$$

in the above expressions, $f^{(2)}_{GES}$ becomes

$$f^{(2)}_{GES} = \frac{16\pi}{k_i q^3}\left\{ \frac{C_1}{y_1^4}\left[6\frac{d}{dz_1} f_2(z_1) + 6z_1\frac{d^2}{dz_1^2} f_2(z_1) + z_1^2\frac{d^3}{dz_1^3} f_2(z_1)\right] + \frac{C_2}{y_2^3}\left[2\frac{d}{dz_2} f_2(z_2) + z_2\frac{d^2}{dz_2^2} f_2(z_2)\right] + \frac{C_3}{y_3^2}\frac{d}{dz_3} f_2(z_3)\right\} \qquad (3.27)$$

where $z_1 = \frac{q}{y_1}$, $z_2 = \frac{q}{y_2}$, $z_3 = \frac{q}{y_3}$ and $f_2(z) = \frac{z^4}{1+z^2} \ln \frac{1+z^2}{z}$

A similar argument follows in the evaluation of $f^{(3)}_{GES}$ which may also be split as

$$f^{(3)}_{GES} = f^{(3)}_1 + f^{(3)}_2 + f^{(3)}_3$$

By analogy with similar expression in ESGH process,

$$f^{(3)}_3 = C_3\pi\left(\frac{-4}{k_i^2 q^4}\right) D^1 f_3(z_3)$$

$$f^{(3)}_{2} = C_2 \pi \left\{ \frac{-4}{k_i^2 q^4} \right\} D^{11} f_3(z_2) \quad \text{and}$$

$$f^{(3)}_{1} = C_1 \pi \left(\frac{-4}{k_i^2 q^4} \right) D^{111} f_3(z_1)$$

where D^1, D^{11} and D^{111} have the same meaning as in the previous case, and $f_3(z)$ is as defined below. After performing the differentiations, $f^{(3)}_{GES}$ becomes

$$f^{(3)}_{GES} = \frac{4\pi}{k_i^2 q^3} \left\{ \frac{C_1}{y_1^4} \left[6 \frac{d}{dz_1} f_3(z_1) + 6 z_1 \frac{d^2}{dz_1^2} f_3(z_1) + z_1^2 \frac{d^3}{dz_1^3} f_3(z_1) \right] + \frac{C_2}{y_2^3} \left[2 \frac{d}{dz_2} f_3(z_2) + z_2 \frac{d^2}{dz_2^2} f_3(z_2) \right] + \frac{C_3}{y_3^2} \frac{d}{dz_3} f_3(z_3) \right\} \qquad (3.28)$$

where $f_3(z) = \frac{z^4}{1 + z^2} \left\{ 4 \left[\ln \frac{1 + z^2}{z} \right]^2 + \frac{\pi^2}{3} - 2A(z) \right\}$

where $A(z)$ is same as in (3.16)

In the expressions (3.27) and (3.28), by putting $C_3 = \frac{1}{\pi}$ and $y_3 = 2$, $f^{(2)}_{3}$ and $f^{(3)}_{3}$ get reduced to the $f^{(2)}_{GES}$ and $f^{(3)}_{GES}$ for the ESGH process (3.15) and (3.16). This provides an indirect check to the present calculations.

The evaluation of fIm and fRe_1 are now done following Yates (1979). The average excitation energy parameter for the ESEH process is taken as $0.0556/k_i$. Using (3.10) and (3.23) fIm and fRe_1 may easily be obtained.

As in the case of the GES terms, the evaluations of the Born terms are also made easier by making use of the correlation between the $\psi^* \psi$ in the ESGH and ESEH processes. As a result, fIm will be constituted by the sum of fIm^1, fIm^2 and fIm^3 - the contributions arising from the three parts of $\psi^* \psi$ (3.25). In comparison with the ESGH process, fIm^3 may directly be written as

$$fIm^3 = C_3 \overline{\Lambda} \left[fIm \text{ for ESGH process (3.17)} \right]$$

with $\lambda = y_3$ and $\beta = 0.0556/k_i$. Similarly fIm^2 and fIm^1 may be obtained by replacing C_3, y_3 and $\frac{d}{dy_3}$ by C_2, y_2 and $\frac{d^2}{dy_2^2}$ and C_1, y_1 and $\frac{d^3}{dy_1^3}$ respectively. Thus the imaginary Born term in (3.6) may be written as

$$fIm = C_3\left(-\frac{d}{dy_3}\right) f_2(\beta^2, q^2, y_3^2) + C_2 \frac{d^2}{dy_2^2} f_2(\beta^2, q^2, y_2^2)$$
$$+C_1\left(-\frac{d^3}{dy_1^3}\right) f_2(\beta^2, q^2, y_1^2) \qquad (3.29)$$

where $f_2\ (\beta^2, q^2, y^2) = +\frac{4}{k_i}\frac{1}{y^2}\left[2I_1(\beta^2, y^2) - \frac{q^2}{q^2+y^2} I_1(\beta^2, 0)\right]$

The type of shortcut mentioned in connection with the evaluation of fIm is equally successfully applicable to the evaluation of the real Born term fRe_1. Thus it follows that

$$fRe_1 = fRe_1^1 + f\ Re_1^2 + f\ Re_1^3$$

With $f\,Re_1^3$ = $C_3 \pi x$ [fRe_1 for ESGH process (3.18)] with the same λ and β as in fIm^3. Similarly, the expressions for fRe_1^1 and fRe_1^2 are obtained by substituting C_2, y_2, $\frac{d^2}{dy_2^2}$ and C_1, y_1, $\frac{d^3}{dy_1^3}$ in the place of C_3, y_3, $\frac{d}{dy_3}$. Hence, the final form of fRe_1 for the ESEH process becomes

$$f\,Re_1 = C_3 \left(\frac{-d}{dy_3}\right) f_3(\beta^2, q^2, y_3^2) + C_2 \frac{d^2}{dy_2^2} f_3(\beta^2, q^2, y_2^2) + C_1 \left(\frac{-d^3}{dy_1^3}\right) f_3(\beta^2, q^2, y_1^2) \qquad (3.30)$$

where

$$f_3(\beta^2, q^2, y^2) = -\frac{4}{\pi k_i} \frac{1}{y^2} \left[2I_2(\beta^2, y^2) - \frac{q^2}{q^2+y^2} I_2(\beta^2, 0)\right]$$

Now f_{w2} is obtained using (3.24), (3.7) and (3.9). The evaluation of this term is quite straight forward and gives

$$fW_2 = \frac{1}{2k_i^2}\left[1 - \frac{7}{4}\frac{d}{d\lambda} + \frac{1}{2}\frac{d^2}{d\lambda^2} - \frac{1}{2}\frac{d^3}{d\lambda^3} + \frac{3}{8}\frac{d^4}{d\lambda^4} - \frac{1}{16}\frac{d^5}{d\lambda^5} + \frac{1}{16}\frac{d^6}{d\lambda^6}\right]\frac{1}{\lambda^2+q^2} \qquad (3.31)$$

where $\lambda = 2$

Using Ochkur approximation, similar to the ESGH process,

$$f_{exch} = \frac{8\pi}{k_i^2} \left\{ C_1 \frac{d^3}{dy_1^3} \frac{1}{q^2+y_1^2} + C_2 \frac{d^2}{dy_2^2} \frac{1}{q^2+Y_2^2} + C_3 \frac{d}{dy_3} \frac{1}{q^2+y_3^2} \right\} \qquad (3.32)$$

Again, the similarity between the wave function products is made use of here. Now the MGES scattering amplitude (3.6) for the ESEH process can be obtained using equation (3.26) to (3.32). Here also, the DCS is given by (3.21).

Results and discussion :

The differential scattering cross sections in the framework of the MGES approach for the ESEH process are calculated for incident energies ranging from 100 eV to 800 eV. In each case, the DCS in the GES method were separately evaluated using (3.26) to (3.28) in order to compare with the corresponding Glauber cross-sections. Such comparison had not been made previously eventhough Yates (1974) had mentioned that the determination of the validity of the GES analysis for collision processes other than ESGH requires further study. Moreover, a comparison of the present MGES results with the UEBS results (as in the case of ESGH process) for the ESEH process is not possible because the UEBS results for the same are not available so far.

The present results at 200 eV and 400 eV are displayed in fig.3.3 and 3.4 alongwith the data of other theoretical methods. It should be remembered that absolute experimental measurements on the ESEH process have not been reported so far. In tables 3.5a and 3.5b the constituent terms of the amplitude series are listed separately. The present DCS results for certain sample energies of incidence are given in table 3.6.

In fig.3.3, along with the present MGES results for the ESEH process (curve a) the corresponding MGES results for the ESGH process (curve b) at the same energy are given for the sake of comparison between the two. It is seen that beyond 50°, they almost coincide. This is actually what is expected since the nuclear part of the interaction progressively dominates the scattering as θ increases. Similar type of coincidence was previously mentioned in the EBS and two-potential approaches to the ESEH process (Joachain et al 1977, Pundir et al 1982). The same may be expected to be true in the case of UEBS approximation also. Such a situation allows a rough estimate of the UEBS cross section for the ESEH process in the large angle region (say above 50°) even though the exact calculations have not been performed. It may be anticipated that the large angle cross sections will be nearly the same for ESGH and ESEH processes. The UEBS results for ESGH process - for large θ - may be compared with the present MGES results. The nice agreement between the two further strengthens the argument that the MGES satisfactorily reproduces the UEBS results.

A study of fig.3.3 and 3.4 reveals that the MGES results compare with other data in a way similar to the one found in section 3.2. At small angles, all of them show close agreement and they depart in the large angle region. The HHOB results (Rao and Desai 1983) depart the most from the MGES values - sometimes even an order of magnitude. The present results lie between the OM (Joachain and Winters 1980) and two-potential results (Pundir et al 1982). Since all the cited results agree with each other in the small angle region where perturbation theory is rapidly convergent, the real test of the accuracy of a particular method is in the large angle DCS. In the absence of experimental data to support the theoretical predictions, it is rather difficult to comment on the accuracies of the various approaches. In the light of the results obtained in the ESGH process and the comparison between the ESGH and ESEH processes, it is only reasonable to expect nice agreement of the present MGES results with experimental data when it becomes available.

As in the case of ESGH study, here also the imaginary terms $f^{(2)}_{GES}$ and fIm show striking similarity (table 3.5). The present method is expected to give better results for higher incident energies.

Table 3.7 shows a comparison between the DCS values obtained in the present study in the GES approximation and their Glauber counterparts (section 4.4). It may be noted that such a comparison has not been reported earlier. It is clear from the table that the GES and Glauber results are approximately the same and the proximity of the results increases with incident energy. Thus, it can be concluded that the first three terms of the Glauber eikonal series are sufficient to represent the Glauber amplitude in the case of ESEH process.

Table 3.8 lists the total cross sections obtained in the present study using the optical theorem. It should be noticed that these TCS values are proportionate to those obtained in the case of ESGH process (table 3.4). Similar behaviour is discussed in detail by Pundir et al (1982).

From the above discussions, the general conclusion drawn is that the MGES is a successful method in describing the ESGH and ESEH processes. Stimulated by the encouraging results, we now take up the study of electron scattering from helium target using this method.

3.4 Elastic scattering of Electrons from the ground state of Helium atom :

Recently Singh and Tripathi (1980) studied the electron-scattering from helium atom within the framework of the GES method. They concluded that the inclusion of only the first three terms in GES gives a good representation of the Glauber differential cross-section for elastic scattering from the ground state of helium (abbreviated as EHe process). However, the DCS were too low in comparison with experimental data at all angles (except very near the forward direction where they diverge). Hence, it was desirable to study the EHe process using the MGES method which has given improvement over the GES results in the case of electron scattering from hydrogen.

The interaction potential for the EHe process is given by

$$V\,(r,\ r_1,\ r_2) = \frac{-2}{r} + \frac{1}{/\underline{r} - \underline{r}_1/} + \frac{1}{/\underline{r} - \underline{r}_2/} \qquad (3.33)$$

The ground-state wavefunction of He is chosen as the Hartree-fock wave function of Byron and Joachain (1966).

$$\psi\,(r_1, r_2) = \phi_{1s}\,(r_1)\ \phi_{1s}\,(r_2) \qquad (3.34)$$

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

where $A = 2.60505,$

$B = 2.08144,$

$Y_1 = 1.41$

$Y_2 = 2.61.$

The static potential of He, V_{st}, was chosen following Cox and Bonham (1967). Thus,

$$V_{st} = -2 \sum_{j=1}^{5} \gamma_j \frac{e^{-\lambda_j r}}{r} \qquad (3.35)$$

Here $\lambda_1 = 2.4908$ $\gamma_1 = 1.0030$

$\lambda_2 = 3.8608$ $\gamma_2 = -0.6146$

$\lambda_3 = 6.1256$ $\gamma_3 = -0.1840$

$\lambda_4 = 2.8522$ $\gamma_4 = 0.6116$

$\lambda_5 = 5.1284$ $\gamma_5 = 0.1841$

and $\sum_j \gamma_j \simeq 1$.

The validity of these type of potentials in the range of energies studied here, was discussed in an earlier section. Now the equations (3.33) to (3.35) may be used in the evaluation of (3.6).

$f^{(1)}_{GES}$ is given by

$$f^{(1)}_{GES} = -\frac{1}{2\pi} \int\int\int dv\, e^{i\underline{q}\cdot\underline{r}}\, \psi^{*} \left[-\frac{2}{r} + \frac{1}{|\underline{r}-\underline{r}_1|} + \frac{1}{|\underline{r}-\underline{r}_2|}\right] \psi\, dV_1 dv_2$$

Substituting $\psi^{*}\psi = \frac{1}{16\pi^2} \sum_{k=1}^{9} D_k\, e^{-K_{1k}r_1 - K_{2k}r_2}$

and $\int \frac{e^{i\underline{q}\cdot\underline{r}}}{|\underline{r}-\underline{r}_1|} = \frac{4\pi}{q^2} e^{i\underline{q}\cdot\underline{r}_1}$, we get

$$f^{(1)}_{GES} = \sum_{k=1}^{9} \frac{8D_k}{q^2} \left[\frac{2}{K_{1k}^3 K_{2k}^3} - \frac{K_{1k}}{k_{2K}^3 (q^2+k_{1K}^2)^2} - \frac{k_{2K}}{k_{1K}^3 (q^2+k_{2K}^2)^2} \right] \qquad (3.36)$$

where the values of D_K, k_{1K} and k_{2K} are listed in table (3.9).

$f^{(2)}_{GES}$ and $f^{(3)}_{GES}$ for the EHe process using the same wave function (3.34) were earlier reported by Singh and Tripathi (1980). They had given the numerical results at 200 and 400 eV also. In the present study, the same procedure was followed.

The lengthy expressions for these GES terms are not given here because they will be unnecessary reproduction of earlier results.

In the evaluation of the Born terms, Yates' (1979) procedure was followed. For the case of helium target,

$$\bar{V}(P+P_z\hat{\chi};r_1r_2) = \frac{1}{2\pi^2(P^2+P_z^2)}\left[e^{i\,\underline{P}\cdot\underline{r}_1} + e^{i\,\underline{P}\cdot\underline{r}_2}-2\right]$$

The β parameter was chosen as $\beta = 1.2/\ k_i$ (Byron and Joachain 1977). For the Helium target,

$$U_{fi}^{(2)} = <\psi/\bar{V}(P+P_z\hat{\chi};r_1,r_2)\ \bar{V}(q-P-P_z\hat{\chi};r_1,r_2)/\psi>$$

$$= \frac{1}{64\pi^6}\ \frac{1}{(P^2+P_z^2)\ (/q-p/^2+P_z^2)}\iint\sum_{K=1}^{9} D_K\ e^{-k_{1K}r_1-k_{2K}r_2}$$

$$\Big[e^{i\underline{q}\cdot\underline{b}_1} + e^{i\underline{q}\cdot\underline{b}_2} -2e^{i\underline{P}\cdot\underline{r}_1} -2e^{i\underline{P}\cdot\underline{r}_2} -2e^{i/\underline{q}-\underline{p}/\cdot r_1}$$

$$-2e^{i/\underline{q}-\underline{p}/\cdot\underline{r}_2} + e^{i(\underline{P}\cdot\underline{r}_1+/\underline{q}-\underline{P}/\cdot\underline{r}_2)} + e^{i(\underline{P}\cdot\underline{r}_2+/\underline{q}-\underline{P}/\cdot\underline{r}_1)} +4\Big]$$

Now taking each term and integrating,

$$U_{fi}^{(2)} = \frac{1}{4\pi^4}\sum_{K=1}^{9} D_K\Big\{\left(-\frac{d}{dk_{1K}}\right)\left[\frac{2}{k_{2K}^3\ (q^2+k_{1K}^2)} - \frac{4}{k_{2K}^3\ B_1}\right.$$

$$\left.-\frac{4}{k_{2K}^3\ A_1}\right] + \left(-\frac{d}{dk_{2K}}\right)\left[\frac{2}{k_{1K}^3\ (q^2+k_{2K}^2)} - \frac{4}{k_{1K}^3\ B_2}\right.$$

$$\left.-\frac{4}{k_{1K}^3\ A_2}\right] + \left(\frac{-d}{dk_{1K}}\right)\left(\frac{-d}{dk_{2K}}\right)\left[\frac{1}{B_1A_2}+\frac{1}{A_1B_2}\right] + \frac{16}{k_{1K}^3\ k_{2K}^3}\Big\}$$

$$\frac{1}{(P^2+P_z^2)\ (/q-P/^2+P_z^2)} \tag{3.37}$$

where $A_1 = /q-p/^2 + P_z^2 + k_{1K}^2$, $B_1 = P^2 + P_z^2 + k_{1K}^2$,

$A_2 = /q-p/^2 + P_z^2 + k_{2K}^2$, $B_2 = P^2+P_z^2 + k_{2K}^2$,

The following method of partial fractions was used in the calculations.

$$\frac{1}{(P^2+P_z^2+\lambda^2)\;(P^2+P_z^2)} = \frac{1}{\lambda^2}\left[\frac{1}{(P^2+P_z^2)} - \frac{1}{(P^2+P_z^2+\lambda^2)}\right]$$

since $fIm = \frac{4\pi^3}{k_i} \int d\underline{P}\; U^{(2)}_{fi}$, the above simplification has to be used repetitively.

Thus fIm becomes

$$\begin{aligned} fIm = \frac{1}{\pi k_i}\sum_{K=1}^{9} D_K \Bigg\{ \Bigg[& \frac{4k_{1K}}{k_{2K}^3\,(q^2+k_{1K}^2)^2} + \frac{4k_{2K}}{k_{1K}^3\,(q^2+k_{2K}^2)^2} \\ & + \frac{16}{k_{1K}^3\;k_{2K}^3}\Bigg] I_1(\beta^2,0) + \frac{4}{k_{2K}^3}\left(\frac{d}{dk_{1K}}\right)\frac{1}{k_{1K}^2} \\ & \left[2\,I_1(\beta^2,0) - 2\,I_1(\beta^2,k_{1K}^2)\right] + \frac{4}{k_{1K}^3}\left(\frac{d}{dk_{2K}}\right)\frac{1}{k_{2K}^2} \\ & \left[2I_1(\beta^2,0) - 2I_1(\beta^2,k_{2K}^2)\right] + \left(\frac{d}{dk_{1K}}\right)\cdot\left(\frac{d}{dk_{2K}}\right) \\ & \frac{1}{k_{1K}^2\;k_{2K}^2}\Big[2I_1(\beta^2,0) - 2I_1(\beta^2,k_{2K}^2) + 2I_4(\beta^2,k_{1K}^2,k_{2K}^2) \end{aligned}$$

$$-2I_1(\beta^2, k_{1K}2)]\Big\}$$

Performing some of the differentiations and simplifying the above expression, the imaginary part of (3.6) was thus derived as

$$fI_m = \frac{1}{\pi k_i} \sum_{K=1}^{9} D_K \Big\{ \Big[\frac{4k_{1K}}{k_{2K}3(q^2+k_{1K}2)^2} + \frac{4k_{2K}}{k_{1K}3\,(q^2+k_{2K}2)^2}$$

$$-\frac{8}{k_{1K}3\,k_{2K}3} \Big] I_1(\beta^2, 0) - \frac{4}{k_{2K}3} \left(\frac{d}{dk_{1K}}\right) \frac{1}{k_{1K}2}\; I_1(\beta^2, k_{1K}2)$$

$$-\frac{4}{k_{1K}3} \left(\frac{d}{dk_{2K}}\right) \frac{1}{k_{2K}2}\; I_1\;(\beta^2, k_{2K}2\;) + 2\left(\frac{d}{dk_{1K}}\right)$$

$$\left(\frac{d}{dk_{2K}}\right) \frac{1}{k_{1K}2\; k_{2K}2}\; I_4\;(\beta^2, k_{1K}2, k_{2K}2) \Big\} \qquad (3.38)$$

Here $I_1\;(\beta^2,\; y^2)$ and $I_1(\beta^2, 0)$ are similar to those given in (3.17). $I_4\;(\beta^2,\; k_{1K}2\;,\; k_{2K}2\;)$ is given in the appendix. Proceeding in a fashion similar to the above one, f Re_1 is obtained as

$$f\;Re_1 = \frac{-4\pi^2}{k_i} \mathbb{P} \int d\underline{P} \int_{-\infty}^{\infty} \frac{dP_z}{P_z-\beta} \sum_{k=1}^{9} D_k \frac{1}{4\pi^4(P^2+P_z^2)(|q-p|^2+P_z^2)}$$

$$\Big\{ \Big[\frac{4K_{1k}}{K_{2k}3(q^2+K_{1k}2)^2} + \frac{4K_{2k}}{K_{1k}3\,(q^2+K_{2k}2)^2} + \frac{16}{K_{1k}3\;\;K_{2k}3} \Big] + \frac{4}{K_{2k}3}$$

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

$$\left[\frac{1}{B_1A_2} + \frac{1}{A_1B_2}\right] \Big\}$$

$$= -\frac{1}{\pi^2 k_i} \sum_{k=1}^{9} D_k \Big\{\Big[\frac{4K_{1k}}{K_{2k}3\ (q^2+K_{1k}2)^2} + \frac{4K_{2k}}{K_{1k}3(q^2+K_{2k}2)^2} + \frac{16}{K_{1k}3\ K_{2k}3}\Big]$$

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

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

$$\frac{1}{K_{1k}2\ K_{2k}2}\big[2I_2(\beta^2,0)-2\ I_2(\beta^2,K_{1k}2)\ -2I_2(\beta^2,K_{2k}2)$$

$$+\ 2\ I_5(\beta^2,K_{1k}2,K_{2k}2)\big]\ \Big\}$$

The simplication of some of the terms as in the case of fIm results in

$$f\ R_{el} = \frac{-1}{\pi^2 k_i} \sum_{k=1}^{9} D_k \Big\{\Big[\frac{4K_{1k}}{K_{2k}3\ (q^2+K_{1k}2)^2} + \frac{4K_{2k}}{K_{1k}3\ (q^2+K_{2k}2)^2}$$

$$-\frac{8}{K_{1k}3\ K_{2k}3}\Big]\ I_2(\beta^2,0) - \frac{4}{K_{2k}3}\left(\frac{d}{dK_{1k}}\right)\frac{1}{K_{1k}2}\ I_2(\beta^2,K_{1k}2)$$

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

$$\frac{1}{K_{1k}2\ K_{2k}2}\ I_5(\beta^2,K_{1k}2,\ K_{2k}2)\ \Big\} \qquad \ldots(3.39)$$

Here $I_2\ (\beta^2,\ y^2)$ and $I_2(\beta^2, 0)$ are similar to those given in (3.18). The integral $I_5\ (\beta^2,\ K_{1k}2,\ K_{2k}2)$ is given in the appendix. Now f_{w2} is calculated using (3.9) and (3.35).

$$f_{w2} = \frac{8}{k_i 2} \sum_{i=1}^{5} \sum_{j=1}^{5} \frac{\gamma_i \gamma_j \lambda_j}{[(\lambda_i+\lambda_j)^2+q^2]} \qquad \ldots(3.40)$$

The Ochkur approximation for the evaluation of f_{exch} in (3.6) gives

$$f_{exch} = -\frac{2}{k_i^2} \iint dv_1\, dv_2\, e^{iq \cdot r_1} \,/\Psi_i\, \Psi_f/ \qquad \ldots(3.41)$$

which can be easily evaluated using standard integration techniques. Now the substitution of the various terms in (3.6) gives the MGES scattering amplitude for EHe process from which the DCS can be calculated. Here also the TCS and TEC may be calculated similar to the ESGH process.

Results and discussion :

The differential cross sections for the EHe process are calculated as above at intermediate energies. The results at 200 and 400 eV are represented graphically (fig. 3.5 and fig. 3.6 respectively), and compared with the data of other workers.

A perusal of fig.3.5 reveals that the present results improve over the basic GES results quite significantly and they show very nice agreement with the experimental data. As in the case of ESGH and ESEH process, here also, the HHOB results overestimate the present results in the large angle region. But the two sets of results exhibit close agreement in the small angle region (upto 60°). In the case of EHe process, there is no UEBS result available in order to compare with the present MGES results. The complexity involved in the evaluation of the UEBS scattering amplitude is obvious from the experience with the EHe process. The beauty of the MGES method is the comparative ease of evaluation of the scattering amplitude, all the terms of which are obtainable in the closed form. Hence, there is no need for the complex numerical methods similar to those used in the UEBS method. However, there is enough reason to believe that the present MGES results will satisfactorily represent the UEBS results for the EHe process when they become available.

The present results should naturally give better results for larger incident energies. The comparison of figures 3.5 and 3.6 prove this. It may also be noted that the deviation among the various results obtained through different approximations narrows down as the incident energy increases.

In table 3.10, the present DCS results at certain sample energies are given. Table 3.11 shows the TCS values. Here also, the TCS values should be the same as in the HHOB approximation. Tables 3.12a and 3.12b show the individual terms of the amplitude series (3.6) at 200 eV and 400 eV. The similarity between $f_{GES}^{(2)}$ and f Im is repeated in the EHe process also. From a tabulation of the above form (table 3.12), an idea about the convergence of the series can be obtained. It should be remembered that the wavefunction used for helium (3.34) is approximate, thereby introducing an additional source of error into the calculations. However, the agreement of the present DCS with the experimental observations is definitely a matter of encouragement.

3.5 Elastic scattering of electrons from the ground state of Lithium atom :

Motivated by the successful application of the MGES method to the elastic scattering of electrons from the ground states of hydrogen and helium, an attempt was made to study the similar process from the ground state of Lithium atom. The study of alkali atoms has special significance in certain specific areas like magneto-hydrodynamics. A knowledge of the scattering cross-sections is an important design parameter. However, it is difficult to believe that methods which apply well in the study of atoms with a closed shell can be equally successfully applied to the case of alkali atoms. The reasons for this are elaborated in the later chapter on alkali scattering. However, the most important point to be kept in mind is that the absorption effect (removal of electrons from the elastic to the inelastic channel) plays a leading role in the alkali scattering. A comparative study of the optical potential model and EBS type of approach has revealed that the absorption part

Vabs of the optical potential treated in the first Born along with the contribution arising from the treatment of the static part V_{st} twice in the second order of perturbation will give the imaginary part of the EBS amplitude. This takes proper care of the absorption effects. Since the present MGES method is, in one sense, an EBS type of approach, there is enough reason to believe that the MGES amplitude will account for the absorptive part quite satisfactorily. Hence, there is no much scope for hesitation to extend the MGES method to the elastic scattering of electrons from the Lithium atom (ELi process). Moreover, Lithium being the lower extreme of the array of alkali atoms, the discrepancies arising in the study of these atoms will be the least in the case of Lithium. In spite of the main features of alkali atoms - the loosely bound S - electron, the large polarizability and the quasi-degeneracy of the ground and first excited states -, the Lithium atom may, by and large, be considered similar to the hydrogen atom when it is modelled in the core - approximation of Walters (1973) - the nucleus and the inner shell forming the core and the 2S - electron behaving as the valence electron.

As mentioned previously, the computational complexity involved in the evaluation of scattering amplitudes goes on increasing with the atomic number of the target atom. Hence, the decrease in the available data. In order to reduce the computational difficulties, the lithium atom is modelled in the core-approximation. Earlier, Walters (1973, 1980) has used this approximation to study the alkali scattering. It is anticipated that this approximation results in an error which is insignificant in the light of the diminished labour and the computer time saved. According to the core approximation, the total interaction between the incident electron and target atom can be written as

$$V = V_H + V_C \qquad (3.44)$$

where V_H is the hydrogen - like term (3.10) and V_C is the potential due to the core of the atom, given by

$$V_c(r) = 2 \sum_{i=1}^{n} \int dv_1 \, \phi_i^*(r_1) \left[-\frac{1}{r} + \frac{1}{|\underline{r} - \underline{r}_1|} \right] \phi_i(r_1) \qquad (3.45)$$

for an alkali atom with (2n+1) extra-nuclear electrons. Here $\phi_i(r_1)$ are the spatial wavefunctions of the core electrons. For lithium atom, n = 1 and

$$\phi_{1s}(r_1) = \left[\frac{(2.7)^3}{\pi} \right]^{1/2} \exp(-2.7 r_1).$$

Hence, from (3.45),

$$V_c(r) = -2 \left[\frac{1}{r} + 2.7 \right] \exp(-5.4 r).$$

$$\text{So that } V = -\frac{1}{r} + \frac{1}{|\underline{r} - \underline{r}_1|} - 2\left(\frac{1}{r} + 2.7 \right) e^{-5.4r} \qquad (3.46)$$

Similarly, the valence electron wave function is written as (following Coulson 1961)

$\psi_{2S}(r_1) = C\,\phi_{2S} + D\phi_{1S}$ such that

$$\int \psi^*_{2S}(r_1)\,\psi_{2S}(r_1)\,d\underline{r}_1 = 1,$$

$$\int \psi^*_{2S}(r_1)\,\phi_{1S}(r_1)\,d\underline{r}_1 = 0, \text{ and}$$

$$\int \phi^*_{1S}(r_1)\,\phi_{1S}(r_1)\,d\underline{r}_1 = 1.$$

$$\therefore\ \psi_{2S}(r_1) = A\,r_1\,e^{-\lambda_1 r_1} + B\,e^{-\lambda_2 r_1} \qquad (3.47)$$

where $A = 0.11252,\quad B = -0.42204$

$\lambda_1 = 0.65 \qquad \lambda_2 = 2.7$

The remark of Walters (1973) should be remembered at this juncture that the calculations involving the wavefunction (3.47) give much the same results as those obtained using the more sophisticated one - electron wavefunction of Szasz and Mc Ginn (1967). The same will be provėd explicitly in a later chapter of this thesis. The static potential for lithium atom is taken similar to that of Heliumfollowing Cox and Bonham (1967). Thus

$$V_{st}(r) = -3 \sum_{j=1}^{6} \gamma_j \frac{e^{-\lambda_j r}}{r} \qquad (3.48)$$

where

$\lambda_1 = 0.8737 \qquad \lambda_2 = 7.9222 \qquad \lambda_3 = 2.2685$

$\lambda_4 = 3.8024 \qquad \lambda_5 = 1.3839 \qquad \lambda_6 = 2.7056$

$\gamma_1 = 1.3215 \qquad \gamma_2 = -0.2273 \qquad \gamma_3 = 1.3369$

$\gamma_4 = 1.1407 \qquad \gamma_5 = -1.6110 \qquad \gamma_6 = -0.9567$

so that $\sum_j \gamma_j \simeq 1.$

Equations (3.46), (3.47) and (3.48) are now used in the evaluation of (3.6) for ELi process. The calculation is made simple by considering the analogy between the wavefunctions of Li and H (2S) (Equations (3.47) and (3.23)), and their interaction potentials (equations (3.46) and (3.10)). In the case of Li also, it will be convenient to express the product of the wavefunctions $\Psi^* \Psi$ in a form similar to that of ESEH process (3.25). In both the cases, only the coefficients and exponential parameters of the terms will differ. For ELi process,

$Y_1 = 1.3$ $\quad Y_2 = 3.35$ $\quad Y_3 = 5.4$
$C_1 = 0.01266$ $\quad C_2 = 0.09498$ $\quad C_3 = 0.17812$

It has been pointed out by Mathur (1972) that the difference between the scattering parameters obtained using one or three electron wavefunction of Li atom is not very appreciable at intermediate and high energies. He has arrived at this conclusion by using the Glauber approximation. Since the present MGES method is another way of representation of the Glauber amplitude with certain modifications, the use of one electron wavefunction in the present study is justified. Moreover, it was also pointed out that the inclusion of the core potential in the double scattering terms will not affect the cross sections appreciably. Later on, the same assumption was followed in the study of ELi process in the fixed scatterer approximation - FSA - (Guha and Ghosh 1979) and in the HHOB approximation (Rao and Desai 1983). Hence, in the present study also, the effect of core is taken into account only in the first term of the series (3.6) and is neglected in the higher order terms. As a result, $f^{(1)}_{GES}$ can be written as

$$f^{(1)}_{GES} = f_a + f_b \tag{3.49}$$

where f_a is thecontribution arising from the treatment of the hydrogen - like term V_H of the interaction potential (3.44) and f_b is the term originating from V_c. Considering the analogy between (3.23) and (3.47), it can be easily understood that the expression for f_a will have essentially the same form as $f^{(1)}_{GES}$ in the ESEH process (equation 3.26). Only difference will be in the values of C's and Y's. These values are defined earlier. The evaluation of f_b arising from the core part of the interaction is quite straight forward giving

$$f_b = 4 \left\{ \frac{1}{q^2 + \lambda^2} + \frac{\lambda^2}{(q^2 + \lambda^2)^2} \right\} \tag{3.50}$$

where $\lambda = 5.4$

Thus $f^{(1)}_{GES} = f_a + f_b$ can be easily obtained. In the evaluation of $f^{(2)}_{GES}$ and $f^{(3)}_{GES}$, because of the neglect of the core effect (V_c) of the interaction potential (3.44) and the analogy between the wavefunctions (3.23) and 3.47), the resulting expressions will have the same form as the $f^{(2)}_{GES}$ and $f^{(3)}_{GES}$ in ESEH process (equations 3.27 and 3.28) with new values for C_i and Y_i.

To find out the average excitation energy parameter β for the ELi process used in the evaluation of the Born terms f Im and f Re_1 of (3.6), the prescription of Byron and Joachain (1977) is followed. Accordingly

$$\bar{\omega} = \beta k_i = \frac{2 < \psi / z^2 / \psi >}{\bar{\alpha}} \qquad (3.51)$$

where $\bar{\omega}$ is the excitation energy, $\bar{\alpha}$ is the dipole polarizability of the target atom, ψ is the ground state wavefunction and β is the average excitation energy parameter.

Using the wavefunction (3.47) $< \psi / z^2 / \psi > = 6.055$ a.u. Using the experimentally determined value of $\bar{\alpha}$ for Li ($\bar{\alpha} = 167$ a.u.) (Sternheimer 1969), $\bar{\omega}$ (given by 3.51) works out to be 0.0723. Using the Hartreefock wavefunctions of Clementi (1965), Vanderpoorten (1976) has, in his optical model approach to the ELi process, worked out the value of $< \psi / z^2 / \psi >$ as 6.211 a.u. resulting in $\bar{\omega} = 0.0745$ using the same value of $\bar{\alpha}$. The agreement between the two values is another point in favour of the choice of the wavefunction (3.47).

As in the case of the GES terms in (3.6), the Born terms f Im and f Re_1 also become similar to their counterparts in the ESEH process (3.29 and 3.30). Of course, the values of C_i, Y_i and β should be changed accordingly.

The evaluation of $f\,w_2$ becomes simpler in the light of the comparison between the static potentials for helium and lithium (equations 3.35 and 3.48). Hence

$$f\,w_2 = \frac{18}{k_i^2} \sum_{i=1}^{6} \sum_{j=1}^{6} \frac{\gamma_i\,\gamma_j\,\lambda_j}{[(\lambda_i+\lambda_j)^2+q^2]} \qquad (3.52)$$

The γ's and λ's are defined under (3.48).

The exchange term f_{exch} also becomes similar to the corresponding term (3.32) in ESEH process, but for the constants. Now that the scattering amplitude is ready, DCS may be easily evaluated for the Eli process.

Results and discussion :

The differential cross sections for the ELi process within the frame work of the MGES method are exhibited in fig 3.7 and 3.8 (at 100 and 200 eV) in order to enable the comparison between the present results and the data reported by other workers. It is quite unfortunate that the experimental data is not available for comparison at these energies. Experiments have been performed on the Eli process, but the results are reported for incident energies 20 eV and 60 eV which are too low for the present approximation. It should be remembered that the convergence of the GES amplitude series is poor at energies less than 100 eV. Hence there is no other choice but to wait till experimental data becomes available at higher energies in order to have a comparison with the present results.

An observation of the figures reveals that at small angles, all the cited results agree nicely with each other and they start departing from each other with the increase in the scattering angle. As in the previous sections, here also the HHOB results give the highest values. It is also observed that the present results almost coincide with the EBS and corrected static results at small angles (upto 40^{o}). In the large angle region, the present results are in between the two sets of data. In the absence of experimental values, it is difficult to ascertain the validity of the different theoretical results. However, from experience of the results arrived at in foregoing few sections, it is reasonable to predict that the present MGES results may show nice agreement with their experimental counterparts when the latter become available.

It should be noted that the applicability of the GES method to the ELi process has not been tested so far. Hence, in the present study, the GES DCS were also calculated (table 3.15) to have a comparison with the conventional Glauber results. A comparison of the present GES results with the corresponding Glauber results reported earlier, points out that as in the case of hydrogen and helium atoms, the ELi process can also be successfully applied to the GES method and that the first three terms of the series are sufficient to have a satisfactory representation of the Glauber amplitude. A comparison of the present GES and MGES results (table 3.14 & 3.15) shows that the MGES values are much higher than the corresponding GES values. This is an encouraging situation since the GES/ Glauber results are well-known for their appreciable underestimation at large angles. This, indirectly, is another point in favour of the present MGES results.

As mentioned earlier, the most important effect of absorption governing the alkali scattering problems, is taken proper care of through the imaginary part of the second term of the series. The table (3.13) exhibiting the individual terms of the MGES scattering amplitude throws light upon the leading role of the imaginary part of the scattering amplitude. Also, the terms $f^{(2)}_{GES}$ and f Im are nearly equal, thus providing an indirect check for the present calculations. In the course of his study of the ELi process, Vanderpoorten (1976) has compared the optical model and Glauber results. The very fact that these two results almost coincide in the small angle region, indirectly reveals that the polarization effect which is important near the forward direction is quite insignificant in alkali scattering (Glauber results do not account for the polarization effect). This statement also is made clear through survey of Table (3.13), which shows the lower values of fRe_1 compared to those of fIm.

The convergence of an expansion series of the form (3.6) should naturally improve with the increase in the incident energy. But the simultaneously increasing effect of the core contributions should also not be forgotten. It can be seen that the effect of the core increases for large momentum transfers (for large Θ at fixed k_i and for large k_i at fixed Θ). This is explicitly shown in a later chapter. Thus, for large k_i even though the MGES converges more and more, the error due to the neglect of core effect in the second and third order terms of the perturbative series becomes more and more prominent. Hence, the present results can be taken to be ideal for intermediate energy and small angle scatterings. Table (3.14) lists the present DCS results for certain sample energies.

3.6 Inelastic scattering of electrons from hydrogen atom (1S - 2S transitions) :

So far, the applications of MGES approximation were confined to elastic processes. In the light of the remark of Joachain (1977) that in the case of inelastic (S-S) transitions for the large momentum transfer, the higher order cross terms become more important than the lower order cross term (such as $f_1 f_3$ as included in the present method), it is a real challenge to test the applicability of the present method to inelastic transitions as well. Hence, in the current section, the inelastic scattering of electrons from H(1S) to H (2S) (abbreviated as IHSS process) is studied using the MGES approximation.

In the inelastic processes, the initial and final momenta are not same as in the case of elastic processes. For the IHSS process, the final momentum becomes

$$k_f = (k_i^2 - 3/4)^{1/2}$$

where k_i is the initial momentum. Thus, the momentum transfer is given as $q = [k_i^2 + k_f^2 - 2k_i k_f \cos\theta]^{1/2}$ (3.53)

where θ is the angle between k_i and k_f. The interaction potential for the IHSS process is the same as that for the ESGH process (3.10). The wavefunctions for the initial and final states of the target are given by

$$\psi_{1s} = \frac{1}{\sqrt{\pi}} e^{-r_1} \quad \text{and}$$

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

The product of the wave functions may conveniently be represented as

$$\psi^*_{1s}\,\psi_{2s} = \frac{1}{4\pi\sqrt{2}}(2-r_1)\, e^{-1.5r_1}$$

$$= A\left(\frac{d^2}{d\lambda^2}\right) \frac{e^{-\lambda r_1}}{r_1} + B\left(-\frac{d}{d\lambda}\right) \frac{e^{-\lambda r_1}}{r_1} \qquad (3.54)$$

where $A = \frac{-1}{4\pi\sqrt{2}}$; $B = \frac{1}{2\pi\sqrt{2}}$; $\lambda = 1.5$

The evaluation of the various terms of the scattering amplitude (3.6) can be done using the procedures adopted in the earlier sections. Hence the details of the derivations are not given here.

The evaluation of the first term of the series gives

$$f^{(1)}_{GES} = - \frac{8\sqrt{2}}{(q^2+\frac{9}{4})^3}$$

Following the procedure adopted by Yates (1974), the $f^{(2)}_{GES}$ and $f^{(3)}_{GES}$ terms are obtained for the IHSS process as

$$f^{(2)}_{GES} = \frac{16\pi}{k_i\, q^3} \left\{ \frac{A}{\ell^3}\, z \frac{d^2}{dz^2}\, f_2(z) + \left[\frac{2A}{\ell^3} + \frac{B}{\ell^2}\right] \frac{d}{dz}\, f_2(z) \right\} \qquad (3.55)$$

and

$$f^{(3)}_{GES} = \frac{4\pi}{k_i^2\, q^3} \left\{ \frac{A}{\ell^3}\, z\, \frac{d^2}{d_z{}^2} f_3(z) + \left[\frac{2A}{\ell^3} + \frac{B}{\ell^2}\right] \frac{d}{d_z}\, f_3(z) \right\} . \qquad (3.56)$$

where $z = \frac{q}{\ell}$

$$f_2(z) = \frac{z^4}{1 + z^2}{}^2 \ln \frac{1+z^2}{z} \quad \text{and}$$

$$f_3(z) = \frac{z^4}{1 + z^2}{}^2 \left\{ 4 \left[\ln \frac{1+z^2}{z}\right]^2 + \frac{\pi^2}{3} - 2A(z) \right\}$$

where A(z) is defined previously in the ESGH process.

As in the previous sections, the imaginary and real Born terms f Im and f Re_1 for the IHSS process are obtained following Yates (1979). The average excitation energy parameter β for this process is chosen as $\beta = 0.375/k_i$. The analysis of the Born terms results in

$$f\ Im = B\left(-\frac{d}{d\ell}\right) f_2(\beta^2, q^2, \ell^2) + A\left(\frac{d^2}{d\ell^2}\right) f_2(\beta^2, q^2, \ell^2) \qquad (3.57)$$

and

$$f\,Re_1 = B\left(-\frac{d}{d\ell}\right) f_3(\beta^2,q^2,\ell^2) + A\left(\frac{d^2}{d\ell^2}\right) f_3(\beta^2,q^2,\ell^2) \quad (3.58)$$

where

$$f_2(\beta^2,q^2,\ell^2) = \frac{4}{k_i}\ \frac{1}{\ell^2}\left[2I_1(\beta^2,\ell^2) - \frac{q^2}{q^2+\ell^2}\, I_1(\beta^2,0)\right]$$

and

$$f_3(\beta^2,q^2,\ell^2) = \frac{-4}{\pi k_i}\ \frac{1}{\ell^2}\left[2I_2(\beta^2,\ell^2) - \frac{q^2}{q^2+\ell^2}\, I_2(\beta^2,0)\right]$$

Using the Ochkur approximation similar to the ESGH process,

$$f_{exch} = \frac{8\pi}{k_i{}^2}\left\{A\,\frac{d^2}{d\ell^2}\ \frac{1}{q^2+\ell^2}{}^2 + B\left(-\frac{d}{d\ell}\right)\ \frac{1}{q^2+\ell^2}{}^2\right\} \quad (3.59)$$

Now, in the MGES scattering amplitude (3.6), all the terms except fw_2 are obtained in the closed form. The evaluation of fw_2 for the IHSS process in the present formulation is rather tricky, because in the present work the static part of the interaction only is considered in the evaluation of fw_2 because of the justifications given in section 3.1. An inspection of (3.4) reveals that a similar treatment invites difficulties in the IHSS process due to the orthogonality of the initial and final states. On the contrary, talking in terms of static potentials, excitation becomes virtually meaningless. Because of these reasons, the contribution due to the real part fw_2 is neglected in the present study. Of course, the exact treatment of the term(3.4) - similar to the one adopted by Byron et. al (1982) for the ESGH process - is a remedy for the above-mentioned defect. But this analysis is bound to be rather more cumbersome and has not therefore been attempted here. Without the inclusion of fw_2 in the amplitude series (3.6), the following types of study are possible in the IHSS process.

(1) A GES analysis of the IHSS process and comprison with the conventional Glauber amplitude.

(2) The effects of replacement of the second GES term by the Born terms.

(3) The comparison of the present MGES (excluding fw_2) results with relevant data available.

It should be kept in memory that the DCS calculation in the inelastic processes involves the multiplication by a factor k_f/k_i unlike in the elastic processes where k_f and k_i were taken to be of equal magnitudes. As in the previous studies TCS and TEC for the IHSS process can be found out making use of the amplitude terms.

Results and discussion :

The differential cross sections for the IHSS process are calculated for the incident energies 100 eV to 800 eV. In fig.(3.9), the present results at 200 eV are given along with the data of other workers. Unfortunately experimental data is not available for 1S-2S transitions only. The available experimental data (Williams and Willis 1975) considers the transition from n=1 to $n=2^*$ (i.e. 2S+2P) level. Hence, at present, no experimental data can be compared with the present data for the IHSS process. However, if the differential cross sections for the 1S-2P transition in hydrogen atom can be calculated within the framework of the same approach, the sum of the cross sections may be compared with the available experimental data.

The fig (3.9) shows that the present results agree nicely with the compared data. The additional weightage of the present simple method is its ability to reproduce the results of such highly sophisticated calculations as the one adopted in the distorted wave method of Kingston and Walters (1980).

As mentioned elsewhere in this chapter, one of the aims of the present study was to test the applicability of the GES method to this inelastic process. As per the formalism of the GES method, it may as well be applied to inelastic processes also. But the real threat is the problem of the convergence of the series. From tables (3.16 and 3.17) the GES DCS for the IHSS process for the incident energies 100 eV and 400 eV may be calculated and compared with their Glauber counterparts. Rough calculations show that the GES with the first three terms of the series describes the Glauber amplitude reasonably well for the IHSS process.

In tables (3.16 and 3.17) the individual terms of the present scattering amplitude are displayed. The notable similarity between the $f^{(2)}_{GES}$ and f Im is another indirect check for the correctness of the present calculations. These imaginary terms also agree with the corresponding term of Byron and Latour (1976). Another interesting feature of these tables is the relatively low contribution due to polarization and the significance of the absorption effect, which is expected in the case of inelastic scattering. In table (3.18), the DCS obtained in the present study for the IHSS process at various energies of incidence, are given.

From the foregoing discussion, it is clear that the GES analysis of 1S-2S transition in hydrogen is interesting and it will be useful to have a generalisation for the inelastic scattering in hydrogen (1S -- nS transitions), which is attempted in the following section.

3.7 GES for (1S-nS) transitions in H atom :

The wave function for nS state of hydrogen atom is

$$\psi_{noo} = \frac{2}{n^2}\left[\frac{(n-1)!}{(n!)^3}\right]^{1/2} e^{-r_1/n} L^{1}_{n-1}\left(\frac{2r_1}{n}\right) Y_{oo}(\theta,\phi)$$

where $Y_{oo}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$ and

$$L^{1}_{n-1}\left(\frac{2r_1}{n}\right) = \sum_{m=o}^{n-1} (-1)^m \, n! \, \overset{n}{(n-1-m)} \, \frac{\left(\frac{2r_1}{n}\right)^m}{m!}$$

$\therefore \psi_{noo}$ can be written as

$$\psi_{noo} = \sum_{m=o}^{n-1} A_m \, r_1^m \, e^{-r_1/n}$$

Where $A_m = \frac{2}{n^2}\left[\frac{(n-1)!}{(n!)^3}\right]^{1/2} \frac{1}{\sqrt{4\pi}} \frac{(-1)^m}{m!} n! \overset{n}{(n-1-m)} \left(\frac{2}{n}\right)^m$

Since $\psi_{1s} = \frac{1}{\sqrt{\pi}} e^{-r_1}$,

$$\psi_{1s}\,\psi^{*}_{nS} = \sum_{m=0}^{n-1} B_m\, r_1^{\,m}\, e^{-\lambda_n r_1}$$

$$= \left[B_o\left(-\frac{d}{d\lambda_n}\right) + B_1 \frac{d^2}{d\lambda_n^{\,2}} + \dots + B_{n-1} (-1)^n \frac{d^n}{d\lambda_n^{\,n}} \right] \frac{e^{-\lambda_n r_1}}{r_1} \qquad \dots(3.60)$$

where $B_m = \frac{A_m}{\sqrt{\pi}}$ and $\lambda_n = 1 + \frac{1}{n}$

The first Born term is

$$f_{B1}\ (n \neq 1) = \frac{-2}{q^2} \int dv_1\, e^{i\underline{q}\cdot\underline{r}_1}\, \psi_{1S}\, \psi^{*}_{nS}$$

$$= \frac{-8\pi}{q^2} \left[B_o\left(-\frac{d}{d\lambda_n}\right) + B_1\left(\frac{d^2}{d\lambda_n^{\,2}}\right) + \dots + B_{n-1}(-1)^n \frac{d^n}{d\lambda_n^{\,n}} \right] \frac{1}{q^2 + \lambda_n^2} \qquad \dots(3.61)$$

Now, $f^{(2)}_{GES}$ for 1S - nS transitions will be

$$f^{(2)}_{GES} = \frac{1}{\pi k_i} \int \frac{d\underline{P}}{P^2 / q-P /^2} \langle\langle \psi_{nS} / B(P)\, B\, (q-p) / \psi_{1S} \rangle,$$

following Yates (1974).

Considering the first term of the $\psi_{1S}\,\psi^{*}_{nS}$ above, and the procedure adopted by Yates (1974) for the evaluation of the GES amplitude for the ESGH process, the $f^{(2)}_{GES}$ for $B_o\left(-\frac{d}{d\lambda_n}\right) \frac{e^{-\lambda_n r_1}}{r_1}$ (denoted as $f^{(2)}_{0}$) will be B_o times the corresponding term in Yates (1974) treatment.

$$\therefore\ f_0^{(2)} = B_o \pi \times \frac{16}{k_i q^4} \left(-\frac{d}{d\lambda_n}\right) \frac{z_n^4}{1 + Z_n^2} \ln \frac{1 + z_n^2}{z_n}$$

changing $\frac{d}{d\lambda_n}$ to $\frac{d}{dz_n}$ Using $\frac{d}{d\lambda_n} = \frac{-z_n^2}{q} \frac{d}{dz_n}$,

$$f_0^{(2)} = B_o \pi \times \frac{16}{k_i z_n^3 \lambda_n^5} \left(\frac{d}{dz_n}\right) \frac{z_n^4}{1 + z_n^2} \ln \frac{1 + z_n^2}{z_n}$$

i.e. $f_o^{(2)} = B_o \pi \times$equation (3.15) with $\lambda_n=2$. Hence

$$f_o^{(2)} = B_o\left(-\frac{d}{d\lambda_n}\right) f_2(z_n)$$

where $f_2(z_n) = \frac{16\pi}{k_i q^4} \frac{z_n^4}{1 + z_n^2} \ln \frac{1 + z_n^2}{z_n}$

This procedure can be adopted for all the terms in (3.60), thus obtaining $f_{GES}^{(2)}$ for 1S-nS transitions as

$$f_{GES}^{(2)} = \left[B_o\left(-\frac{d}{d\lambda_n}\right) + B_1 \frac{d^2}{d\lambda_n^2} + \dots + B_{n-1}(-1)^n \frac{d^n}{d\lambda_n^n}\right] f_2(z_n) \qquad \dots(3.62)$$

Here all λ_n derivatives should be converted to corresponding z_n derivatives as done in (3.27) because $z_n = \frac{q}{\lambda_n}$

All the above arguments hold good in the evaluation of the third GES term for 1S - nS transitions in hydrogen.

Considering the analogy of $B_o \left(\frac{-d}{d\lambda_n}\right) \frac{e^{-\lambda_n r_1}}{r_1}$ with the wavefunction used in the treatment of Yates (1974), it can be seen that with $B_o = \frac{1}{\pi}$ and $\lambda_n = 2$, one gets the third GES term as given by Yates (1974). Generalising, this to the case of different B_n and λ_n values, the $f^{(3)}_{GES}$ for 1S-nS transitions can be written down, Hence

$$f^{(3)}_0 = B_o \pi \times \frac{4}{k_i^2 q^4} \left(-\frac{d}{d\lambda_n}\right) \frac{z_n^4}{1 + z_n^2} \left\{ 4\left[\ln \frac{1 + z_n^2}{z_n}\right]^2 + \frac{\pi^2}{3} - 2A\,(z_n) \right\}$$

where $A\,(z_n)$ is defined in (3.16).

$$\text{Now} \quad \frac{4}{k_i^2 q^4} \left(-\frac{d}{d\lambda_n}\right) = \frac{4}{k_i^2 z_n^3 \lambda_n^5} \left(\frac{d}{dz_n}\right)$$

Putting $\lambda_n = 2$,

$$f^{(3)}_0 = B_o \pi \times \text{eqn} \quad (3.16)$$

$$\text{Thus} \quad f^{(3)}_{GES} = \left[B_o\left(-\frac{d}{d\lambda_n}\right) + B_1 \frac{d^2}{d\lambda_n^2} + \dots + B_{n-1}(-1)^n \frac{d^n}{d\lambda_n^n}\right] f_3(z_n) \qquad (3.63)$$

$$\text{where} \quad f_3(z_n) = \frac{4\pi}{k_i^2 q^4} \frac{z_n^4}{1+z_n^2} \left\{4\left[\ln \frac{1+z_n^2}{z_n}\right]^2 + \frac{\pi^2}{3} - 2A\,(z_n)\right.$$

Here also λ_n differentiations have to be converted into corresponding differentiations with respect to z_n.

The second term in the HHOB series (Yates 1979) can also be evaluated for the 1S-nS transitions as follows:

f Im for 1S-nS transitions is given as

$$f\ Im = \frac{4\pi^3}{k_i} \int d\underline{P} \ < \psi_{ns} / \bar{V}\ (P+P_z \hat{\chi})\ \bar{V}\ (q-P-P_z\hat{\chi}) / \psi_{1s} >$$

Here also the expression for $\psi_{1s}\ \psi^*_{nS}$ in the form (3.60) can be made use of. Following the above discussed methods, fIm can be directly written down using the corresponding terms in Yates (1979).

$$\text{Thus } f\ Im = [B_o(\frac{-d}{d\lambda_n}) + B_1(\frac{d^2}{d\lambda_n^2}) + \ldots. + B_{n-1}(-1)^n \frac{d^n}{d\lambda_n^n}] f_2(\lambda_n) \qquad \ldots. \quad (3.64)$$

$$\text{where } f_2(\lambda_n) = \frac{4}{k_i}\ \frac{1}{\lambda_n^2} [2I_1(\beta_n^2, \lambda_n^2) - \frac{q^2}{q^2+\lambda_n^2} I_1(\beta_n^2, o)] \qquad ($$

Substitution of $B_o = \frac{1}{\pi}$ gives the corresponding imaginary term for ESGH process as given by Yates (1979). This is a direct check to the above expression.

$$f\ Re_1 = [B_o(\frac{-d}{d\lambda_n}) + B_1 \frac{d^2}{d\lambda_n^2} + ----+ B_{n-1}(-1)^n \frac{d^n}{d\lambda_n^n}] f_3(\lambda_n) \quad (3.65)$$

where

$$f_3(\lambda_n) = -\frac{4}{\pi k_i}\ \frac{1}{\lambda_n^2} [2I_2(\beta_n^2, \lambda_n^2) - \frac{q^2}{q^2+\lambda_n^2}\ I_2(\beta_n^2, o)]$$

For checking purpose, taking ESGH process and substituting $B_o = \frac{1}{\pi}$, $B_1, B_2 \ldots = 0$, the corresponding real term is obtained as given by Yates.

Thus the general expressions for the GES and HHOB terms in the MGES scattering amplitude for 1S - nS transitions are derived above. The substitution of n=2 will result in the 1S-2S transition in hydrogen atom. Substituting $B_o = \frac{1}{2\pi\sqrt{2}}$, $B_1 = -\frac{1}{4\pi\sqrt{2}}$ and $\lambda_n = 1.5$, $B_2, B_3 - - - = 0$ in the above set of expressions, we get the corresponding terms (3.55, 3.56, 3.57 and 3.58) obtained in the study of 1S - 2S inelastic scattering, thus proving the correctness of these equations. Hence, they may be used for the study of the transitions involving n=3, 4 etc. states in the case of hydrogen atom.

We may now take up the more complicated generalisation for tne 1S - np transitions in H atom, from which we can arrive at the expressions for 1S - 2p transitions.

3.8 GES for 1S - np transitions :

As in the case of 1S - nS scattering in hydrogen atom, it will be interesting to study the 1S - np transitions also. For this we have to consider

$$\psi_{nlm} = \frac{2}{n^2}\left[\frac{(n-2)!}{((n+1)!)^3}\right]^{1/2} \frac{2r_1}{n} e^{-r_1/n} L^3_{n-2}\left(\frac{2r_1}{n}\right) Y_{lm}(\theta,\phi)$$

where $L^3_{n-2}\left(\frac{2r_1}{n}\right) = \sum_{S=0}^{n-2} (-1)^s (n+1)! \binom{n+1}{n-2-S} \frac{\left(\frac{2r_1}{n}\right)^s}{s!}$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\,\mathrm{Cos}\theta, \quad Y_{1,1} = \sqrt{\frac{3}{4\pi}}\,\mathrm{Sin}\theta\ \mathrm{Cos}\phi$$

$$Y_{1,-1} = \sqrt{\frac{3}{4\pi}}\,\mathrm{Sin}\theta\ \mathrm{Sin}\phi$$

Thus corresponding to the three values of m, the wave function for np state of hydrogen becomes

$$\left.\begin{aligned} \psi_{n,1,0} &= \sum_{s=0}^{n-2} A_s\, r_1^{1+S}\, e^{-r_1/n}\ \mathrm{Cos}\theta_1 \\ \psi_{n,1,\pm1} &= \sum_{S=0}^{n-2} A_s\, r_1^{1+S}\, e^{-r_1/n}\ \mathrm{Sin}\theta_1\ \phi_\pm \end{aligned}\right\} \qquad (3.66)$$

where $\phi_+ = \mathrm{Cos}\phi_1$ and $\phi_- = \mathrm{Sin}\ \phi_1$.

Here $A_S = \frac{2}{n^2}\left[\frac{(n-2)!}{((n+1)!)^3}\right]^{1/2} \frac{2}{n} \sum_{S=0}^{n-2} \frac{(-\frac{2}{n})^S}{S!}\ (n+1)!\,\overset{n+1}{(n-2-S)} \sqrt{\frac{3}{4\pi}}$

In the first Born approximation,

$$f_{B1} = -\frac{1}{2\pi}\int dv \int dv_1\ \psi^*_{np}(r_1)\ V(r,r_1)\ \psi_{1s}(r_1)\ e^{i\underline{q}\cdot\underline{r}}$$

Here, contrary to the methods adopted in the previous chapters, it will be convenient to evaluate, the dv integral first because of the orthogonality of the initial and final state wavefunctions. The following integral may be made use of :

$$\int \frac{e^{i\underline{q}\cdot\underline{r}}}{|\underline{r} - \underline{r}_1|}\, dv = \frac{4\pi}{q^2}\, e^{i\underline{q}\cdot\underline{r}_1}$$

Hence $f_{B1} = -\frac{1}{2\pi}\int dv_1 \psi^*_{np}(r_1)\ \frac{4\pi}{q^2}\ e^{i\,\underline{q}\cdot\underline{r}_1}\ \psi_{1s}(r_1)$

The above integral is readily performed by choosing the quantization axis to be along the momentum transfer q. Then the factors exp $(\pm i\phi_1)$ that appear in the wave functions for the magnetic substates m = ± 1 of the state /np> prevent these substates from being excited - by integration over ϕ_1. Thus, within the frame work of the FBA, the state $nP_z(m=0)$ is the only final substate which is excited.

Thus $$f_{B_1} = -\frac{1}{2\pi}\int dv_1 \frac{4\pi}{q^2} e^{i\mathbf{q}\cdot\mathbf{r}_1}\Psi^*_{n,1,o}\,\Psi_{1S}$$

$$= -\frac{2}{q^2}\int dv_1\, e^{iqr_1\cos\theta_1}\sum_{S=0}^{n-2} B_s r_1^{1+S}\, e^{-\lambda_n r_1}\cos\theta_1$$

where $B_s = \frac{A_s}{\sqrt{\pi}}$, $\lambda_n = 1 + \frac{1}{n}$

It is convenient to write

$$r_1^{1+S}\, e^{-\lambda_n r_1} = (-1)^S \frac{d^S}{d\lambda_n^S}\, e^{-\lambda_n r_1}\, r_1$$

The above substitution combined with the application of a few standard integrals gives f_{B1}. Thus, the final result for f_{B_1} can be obtained as

$$f_{B1}\,(1S\text{-}np) = -\frac{6\;4\pi i}{q}\sum_{S=0}^{n-2} B_s(-1)^s \frac{d^S}{d\lambda_n^S}\left[\frac{\lambda_n}{(q^2+\lambda_n^2)^3}\right] \qquad (3.\ 67)$$

The substitution of $B_S = \frac{1}{4\pi\sqrt{2}}$ and $\lambda_n = 1.5$ gives the well-known first Born amplitude for 1S -2P transitions. This is a direct check for the evaluation procedure.

Thus $f^{B}_{1}(1S \longrightarrow 2P) = -i \frac{12\sqrt{2}}{q} \frac{1}{(q^2 + \frac{\underline{q}}{4})^3}$ (3.68)

It may be noted that the first Born amplitude in 1S - np transitions is purely imaginary and in the large angle region; it falls off like q^{-7} i.e. much faster than the elastic or 1S - 2S first Born amplitudes in hydrogen target.

Now we will take up the evaluation of the second term of the GES series for 1S - np transitions.

$$f^{(2)}_{GES} = \frac{1}{\pi k_i} \int \frac{d\underline{P}}{P^2 /q-p/^2} < \Psi_{np}/B(P)\, B(q-p)/ \Psi_{1S}>$$

where $B(P)B(q-p) = 1 - e^{i\,\underline{P}\cdot\underline{r}_1} - e^{i\,/\underline{q}-\underline{p}/\cdot\underline{r}_1} + e^{i\underline{q}\cdot\underline{r}_1}$ (3.69)

Becuase of our choice of the quantization axis, it can be seen that here also

$< \Psi_{np}/ e^{i\,\underline{x}\cdot\underline{r}_1} / \Psi_{1S} >$ survives only for Ψ_{np_z}

Thus $< \Psi_{n\,P_z} / e^{iq\cdot r_1} / \Psi_{1S} >$

$$= \int dv_1 \; e^{i\,\underline{q}\cdot\underline{r}_1} \sum_{S=0}^{n-2} B_s\, r_1^{1+S}\, e^{-\lambda_n r_1} \cos\theta_1 \;.$$

Here it will be convenient to represent

$r_1^{1+S}\, e^{-\lambda_n r_1} = (-1)^S \frac{d^{2+S}}{d\lambda_n^{2+S}} \frac{e^{-\lambda_n r_1}}{r_1}$ so that

integration process is simplified.

Again making use of standard integrals and undertaking a lengthy procedure,

$$< \psi_{np} / e^{i\underline{q}\cdot\underline{r}_1} / \psi_{1S} > = -4\pi i \sum_{S=0}^{n-2} B_S (-1)^S \frac{1}{q}$$

$$\left[\frac{d^{2+S}}{d\lambda_n^{2+S}} \frac{\lambda_n}{q^2 + \lambda_n^2} + \frac{d^{1+S}}{d\lambda_n^{1+S}} \frac{1}{q^2 + \lambda_n^2} \right]$$

Similar expressions can be written for other terms of (3.69) also

whereas $< \psi_{np} / 1 / \psi_{1S} > = 0$

Thus $f^{(2)}_{GES}(1S-np) = -\frac{4i}{k_i} \sum_{S=0}^{n-2} B_s (-1)^S \int \frac{d\underline{P}}{P^2 / \underline{q} - \underline{P}/^2}$

$$\left\{ \frac{d^{2+S}}{d\lambda_n^{2+S}} \left[\frac{\lambda_n}{q(q^2+\lambda_n^2)} - \frac{\lambda_n}{P(P^2+\lambda_n^2)} - \frac{\lambda_n}{/q-p/(/q-p/^2+\lambda_n^2)} \right] \right.$$

$$\left. + \frac{d^{1+S}}{d\lambda_n^{1+S}} \left[\frac{1}{q(q^2+\lambda_n^2)} - \frac{1}{P(P^2+\lambda_n^2)} - \frac{1}{/q-p/(/q-p/^2+\lambda_n^2)} \right] \right\}$$

As in the analysis of the GES terms in the earlier sections, here also the substitutions $z = \frac{q}{\lambda_n}$ and $\frac{P}{\lambda_n} = P_1$ are made.

Hence $f^{(2)}_{GES} = \frac{-4\ i}{k_i} \sum_{S=0}^{n-2} B_s (-1)^s \left\{ \frac{d^{2+S}}{d\lambda_n^{2+S}} \frac{1}{\lambda_n^4} \int \frac{d\underline{P}_1}{P_1^2 / z - P_1/^2} \right.$

$$\left[\frac{1}{z(1+z)^2} - \frac{1}{P_1(1+P_1)^2} - \frac{1}{/z-P_1/(/z-p_1/^2+1)} \right] + \frac{d^{1+S}}{d\lambda_n^{1+S}} \frac{1}{\lambda_n^5}$$

$$\left. \int \frac{dP_1}{P_1^2 / z-p_1/^2} \left[\frac{1}{z(1+z^2)} - \frac{1}{P_1(1+P_1)^2} - \frac{1}{/z-p_1/(/z-p_1/^2+1)} \right] \right\}$$

Grouping some of the above terms and simplifying,

$$f^{(2)}_{GES} = \frac{-4\,i}{k_i} \sum_{S=0}^{n-2} B_S(-1)^S \left\{ \frac{d^{2+S}}{d\lambda_n^{1+S}} \frac{1}{\lambda_n^4} \left[\frac{1}{z(z^2+1)} I_a - 2I_b\right] + \frac{d^{1+S}}{d\lambda_n^{1+S}} \frac{1}{\lambda_n^5} \left[\frac{1}{z(1+z^2)} I_a - 2I_b\right] \right\} \qquad (3.70)$$

where $I_a = \int \frac{dP_1}{P_1^2 /z-P_1/^2} = \lim_{\nu \to 0} \frac{2\pi}{z^2} \ln \frac{z^2}{\nu^2}$ and

$$I_b = \int \frac{dP_1}{P_1^2 |z-P_1|^2} \Big/ P_1(1+P_1^2)$$

$$= \lim_{\nu \to 0} \left\{ \frac{4\pi}{z^3}\left[\frac{1}{2} \ln \frac{2z}{\nu} - 1\right] - \frac{4\pi}{1+z^2} \left[\frac{1}{2z} \ln \frac{2z}{\nu} - \frac{\pi}{2} + \tan^{-1} z\right] \right\}$$

It is seen that the integrals Ia and I_b are divergent separately, but the divergences cancel exactly for the combination of the integrals appearing in the equation (3.70). This, is proved explicitly below:

We consider $\frac{1}{z(1+z^2)} I_a - 2I_b$

Taking the divergent terms in the integrals,

$$\text{i.e. } \lim_{\nu \to 0} \frac{1}{z(1+z^2)} \left[- \frac{2\pi}{z^2} \ln \nu^2\right] -2 \left[\frac{-4\pi}{2z^3} \ln \nu + \frac{4\pi}{2z(1+z^2)} \ln \nu\right]$$

$$= \lim_{\nu \to 0} \ln\nu \left[\frac{-4\pi}{z^3(1+z^2)} + \frac{4\pi}{z^3} - \frac{4\pi}{z(1+z^2)}\right] = 0.$$

Thus the divergent terms cancel exactly.

Now in order to derive the imaginary term in the GES i.e. $f^{(2)}_{GES}$ for 1S -- 2P transitions, the substitution of $B_S = \frac{1}{4\pi\sqrt{2}}$ and $\lambda_n = 1.5 = \lambda$ in equation (3.70) is sufficient. This gives

$$f^{(2)}_{GES}(1S-2P) = -\frac{i}{\sqrt{2}\,\pi k_i}\left\{\frac{d^2}{d\lambda^2}\frac{1}{\lambda^4}\left[\frac{1}{z(1+z^2)}I_a - 2I_b\right] + \frac{d}{d\lambda}\frac{1}{\lambda^5}\left[\frac{1}{z(1+z^2)}I_a - 2I_b\right]\right\} \qquad (3.71)$$

An important feature of $f^{(2)}_{GES}$ for 1S-np transitions is that it is imaginary. Thus the second term $O\left(\frac{1}{k_i}\right)$ of the GES series becomes real, in contrast to the situation in the earlier studies. It may be noted that the same combination of I_a and I_b integrals appear in $f^{(2)}_{GES}$ (1S - 2p) also, hence no need to worry about the divergence problem. This type of exact cancellations of the divergences is a peculiar character of the GES series and it provides an indirect assessment of the correctness of the expressions derived above.

The analysis of the third GES term $f^{(3)}_{GES}$ for 1S - np transitions proceeds on a similar track as in the case of $f^{(2)}_{GES}$

$$f^{(3)}_{GES}(1S-np) = \frac{2\pi k_i}{6\pi^3 k_i^3}\int\frac{d\underline{P}_1}{P_1^2}\int\frac{d\underline{P}_2}{P_2^2\,|\underline{q}-\underline{P}_1-\underline{P}_2|^2}$$

$< \psi_{np} / B(P_1)\; B(P_2)\; B\,(q-P_1-P_2) / \psi_{1S} >$

Here $< \psi_{np} / B\,(P_1) \;---\; / \psi_{1S} >$

$$\begin{aligned}
&= 4\pi i \sum_{S=0}^{n-2} B_S (-1)^S \Big\{ \frac{d^{2+S}}{d\lambda_n^{\,2+S}}\, \lambda_n \Big[\frac{1}{P_1(P_1^2+\lambda_n^2)} + \frac{1}{P_2(P_2^2+\lambda_n^2)} \\
&\quad + \frac{1}{(q-p_1-p_2)\,(/q-p_1-p_2/^2+\lambda_n^2)} - \frac{1}{(q-p_1)\,(/q-p_1/^2+\lambda_n^2)} \\
&\quad - \frac{1}{(q-p_2)(/q-p_2/^2+\lambda_n^2)} - \frac{1}{(p_1+p_2)}\; \frac{1}{((p_1+p_2)^2+\lambda_n^2)} \\
&\quad + \frac{1}{q(q^2+\lambda_n^2)} \Big] + \frac{d^{1+S}}{d\lambda_n^{\,1+S}} \Big[\frac{1}{p_1(p_1^2+\lambda_n^2)} + \frac{1}{p_2(p_2^2+\lambda_n^2)} \\
&\quad + \frac{1}{(q-p_1-p_2)\,(/q-p_1-p_2/^2+\lambda_n^2)} - \frac{1}{/q-p_1/\,(/q-p_1/^2+\lambda_n^2)} \\
&\quad - \frac{1}{/q-p_2/\,(/q-p_2/^2+\lambda_n^2)} - \frac{1}{(p_1+p_2)\,((p_1+p_2)^2+\lambda_n^2)} \\
&\quad + \frac{1}{q(q^2+\lambda_n^2)} \Big] \Big\}
\end{aligned}$$

Substitution of this expression in $f^{(3)}_{GES}$ will result in integrals of the form $\int \frac{dP_1}{P_1^2} \int \frac{dP_2}{P_2^2 /q-P_1-P_2/^2}\, \mathcal{Y}$. These integrals are same for $\mathcal{Y} = \frac{1}{P_1(P_1^2+\lambda_n^2)}, \; \frac{1}{P_2(P_2^2+\lambda_n^2)},$

$\frac{1}{|q-p_1-p_2|\,(|q-p_1-p_2|^2+\lambda_n^2)}$. Hence these terms can be grouped together. Similar is the case with the negative terms in $<\psi|(x)|\psi>$. Thus grouping the terms and applying certain simplifications like $|\underline{q}-\underline{p}_1| = \underline{P}_1$, we get

$$f^{(3)}_{GES} = \frac{1}{3\pi^2 k_i^2}\, 4\pi i \sum_{S\neq 0}^{n-2} B_S\, (-1)^S \left\{ \frac{d^{2+S}}{d\lambda_n^{2+S}}\, \lambda_n \left[3I_9 - 3I_{10} + \frac{1}{q(q^2+\lambda_n^2)}\, I_{11}\right] + \frac{d^{1+S}}{d\lambda_n^{1+S}} \left[3I_9 - 3I_{10} + \frac{1}{q(q^2+\lambda_n^2)}\, I_{11}\right] \right\} \quad (3.72)$$

where $I_9 = \int \frac{d\underline{P}_1}{|q-p_1|^2} \int \frac{d\underline{P}_2}{P_2^2\,|P_1-P_2|^2}\; \frac{1}{P_2(P_2^2+\lambda_n^2)}$

$$I_{10} = \int \frac{d\underline{P}_1}{|q-P_1|^2} \int \frac{d\underline{P}_2}{P_2^2\,|p_1-p_2|^2}\; \frac{1}{P_1(P_1^2+\lambda_n^2)}$$

$$I_{11} = \int \frac{d\underline{P}_1}{|q-p_1|^2} \int \frac{d\underline{P}_2}{P_2^2\,|P_1-P_2|^2}$$

As in the previous cases, putting $z = \frac{q}{\lambda_n}$

$\frac{P_1}{\lambda_n} = P_3$ and $\frac{P_2}{\lambda_n} = P_4$ in I_9

$$I_9 = \frac{1}{\lambda_n^5} \int \frac{dP_3}{|z-p_3|^2} \int \frac{dP_4}{p_4^2\,|p_3-p_4|^2}\; \frac{1}{p_4(1+p_4^2)}$$

Similar simplifications are possible for I_{10} and I_{11}. Hence the final-expression for $f^{(3)}_{GES}$ is arrived at as

$$f^{(3)}_{GES}(1S - np) = \frac{4 \cdot i}{3\pi k_i^2} \sum_{S=0}^{n-2} B_S (-1)^S \left\{ \frac{d^{2+S}}{d\lambda_n^{2+S}} \frac{1}{\lambda_n^4} \cdot \left[3 I_{31} - 3 I_{32} + \frac{1}{z(1+z^2)} I_{33}\right] + \frac{d^{1+S}}{d\lambda_n^{1+S}} \frac{1}{\lambda_n^5} \left[3 I_{31} - 3 I_{32} + \frac{1}{z(1+z^2)} I_{33}\right] \right\} \qquad (3.73)$$

where $I_{3k} = \int \frac{d\underline{P}_3}{|z-P_3|^2} \int \frac{d\underline{P}_4}{P_4^2 |P_3-P_4|^2} \frac{1}{\beta_k}$

where $\beta_1 = \frac{1}{P_4(1+P_4^2)}$, $\beta_2 = \frac{1}{P_3(1+P_3^2)}$, $\beta_3 = 1$.

In all the above cases, it is obvious that λ_n should be converted to corresponding z_n and $\frac{d}{d\lambda_n}$ to corresponding $\frac{d}{dz_n}$.

A quick glance at the expression (3.73) reveals that $f^{(3)}_{GES}$ is imaginary for 1S - np transitions. It may be noted that in other scattering phenomena studied earlier, the corresponding term was a real one. Also, the combination of the integrals appearing in $f^{(2)}_{GES}$ and $f^{(3)}_{GES}$ in 1S - np transitions carry the same form as in the analysis of Yates (1974). It is to be presumed that the individual integrals I_{3k} should be divergent. But from previous experience, it can be anticipated that the combinations of these integrals are such that the divergences cancel out exactly. This can be shown explicitly also.

From the equation (3.73), the particular case of $f^{(3)}_{GES}$ for 1S-2p scattering can be derived as in the case of $f^{(2)}_{GES}$. Now, that the first three terms of the GES series are known, the DCS for 1S-2p scattering in the GES approximation can be calculated. However, these calculations are not included in this work.

To summarise the third chapter, the MGES formulation was discussed and it was applied to a variety of scattering phenomena. In the case of the electron scattering from H(1S), H(2S), He and Li, the present MGES method was found to improve upon the basic GES approximation quite significantly. Thereafter, the case of inelastic scattering in hydrogen in the GES approximation was studied with generalisations to 1S - ns and 1S - np transitions in hydrogen. The 1S - 2S scattering cross sections were compared with available data. In brief, the third chapter has been dealing with the GES as well as modified GES approximations. In the next chapter, we take up the study based upon Born approximation and its associated approximations.

Table 3.1a - Behaviour of the individual terms of the MGES (3.6) for ESGH process at 200 eV (atomic units)

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	f_{Im}	Re_1	$f^{(3)}_{GES}$	f_{w_2}	f_{exch} -Ve
10	0.8543	0.4416	0.4737	0.1639 -01	0.4598 -01	0.2615 -01	0.110 00
20	0.5863	0.2017	0.2090	0.1812 -02	0.6429 -01	0.2246 -01	0.653 -01
30	0.3787	0.1364	0.1378	0.5168 -02	0.5603 -01	0.1805 -01	0.345 -01
40	0.2513	0.1083	0.1084	0.5899 -02	0.4807 -01	0.1404 -01	0.184 -01
50	0.1759	0.9000 -01	0.8979 -01	0.5299 -02	0.4081 -01	0.1087 -01	0.103 -01
70	0.1003	0.6574 -01	0.6554 -01	0.3749 -02	0.3145 -01	0.6810 -02	0.399 -02
90	0.6701 -01	0.5119 -01	0.5104 -01	0.2728 -02	0.2592 -01	0.4685 -02	0.195 -02
110	0.5023 -01	0.4231 -01	0.4219 -01	0.2130 -02	0.2245 -01	0.3539 -02	0.115 -02
130	0.4115 -01	0.3688 -01	0.3679 -01	0.1782 -02	0.2025 -01	0.2903 -02	0.795 -03

Table 3.1b - Behaviour of the individual terms of the MGES (3.6) for ESGH process at 400 eV (atomic units)

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	fIm	Re_1	$f^{(3)}_{GES}$ -Ve	fw_2	f_{exch} -Ve
10	0.7427	0.2126	0.2204	0.1124 -02	0.2949 -01	0.1240 -01	0.454 -01
20	0.4054	0.1010	0.1018	0.2163 -02	0.2912 -01	0.9368 -02	0.191 -01
30	0.2249	0.7233 -01	0.7232 -01	0.2869 -02	0.2285 -01	0.6509 -02	0.771 -02
40	0.1379	0.5582 -01	0.5573 -01	0.2324 -02	0.1824 -01	0.4479 -02	0.345 -02
50	0.9273 -01	0.4435 -01	0.4428 -01	0.1771 -02	0.1515 -01	0.3173 -02	0.174 -02
70	0.5121 -01	0.3031 -01	0.3026 -01	0.1085 -02	0.1133 -01	0.1804 -02	0.596 -03
90	0.3386 -01	0.2273 -01	0.2269 -01	0.7469 -03	0.9129 -02	0.1193 -02	0.276 -03
110	0.2527 -01	0.1838 -01	0.1835 -01	0.5684 -03	0.7773-02	0.8873 -03	0.158 -03
130	0.2066 -01	0.1582 -01	0.1579 -01	0.4694 -03	0.6932 -02	0.7230 -03	0.107 -03

Table 3.2 - Differential Cross sections (in units of $a_0^2 \, s_r^{-1}$) in the MGES approximation at different incident energies.

θ / EeV	100 eV		200 eV		400 eV		600 eV		800 eV	
10	0.221	01	0.104	01	0.607	00	0.446	00	0.349	00
20	0.831	00	0.379	00	0.168	00	0.951	-01	0.606	-01
30	0.377	00	0.151	00	0.515	-01	0.254	-01	0.150	-01
40	0.190	00	0.654	-01	0.195	-01	0.905	-02	0.518	-02
50	0.104	00	0.322	-01	0.883	-02	0.400	-02	0.227	-02
70	0.385	-01	0.106	-01	0.271	-02	0.120	-02	0.676	-03
90	0.184	-01	0.475	-02	0.118	-02	0.524	-03	0.293	-03
110	0.107	-01	0.268	-02	0.661	-03	0.291	-03	0.163	-03
130	0.729	-02	0.180	-02	0.442	-03	0.195	-03	0.109	-03

Table 3.3 - Total elastic cross sections (in units of a_o^2) for the ESGH process.

E eV	Present MGES	UEBS (a)	OM (b)	DWSBA (c)	Williams (1975)
100	1.473	1.43	1.54	1.45	1.75
200	0.623	0.613	0.631	0.609	0.669
300	0.385	0.382	0.391	0.380	-
400	0.280	0.276	0.282	0.276	-

(a) Byron et al (1982)
(b) Byron and Joachain (1981)
(c) Kingston and Walters (1980)

Table 3.4 - Total cross sections (in units of a_o^2) for the ESGH Process.

E eV	Present MGES	(a) UEBS	(b) OM	(c) DWSBA	(d) Semi-empirical
100	7.56	7.19	7.68	7.40	6.85
200	4.37	4.27	4.38	4.34	4.18
300	3.14	3.10	3.14	3.11	3.06
400	2.48	2.45	2.48	2.46	2.43

(a) Byron et al (1982)
(b) Byron and Joachain (1981)
(c) Kingston and Walters (1980)
(d) de Heer et al (1977)

Table 3.5a - Behaviour of individual terms of the MGES (3.6) for the ESEH process at 200 eV

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	fIm	Re_1	$f^{(3)}_{GES}$	fw_2	f_{exch}
10	0.4416 01	0.1638 01	0.1601 01	0.3241 -01	0.8005 00	0.5449 -01	-0.1821 -02
20	0.1089 01	0.9133 00	0.9067 00	0.2315 -01	0.4229 00	0.1489 -01	-0.4530 -02
30	0.4903 00	0.5164 00	0.5132 00	0.1090 -01	0.2906 00	0.7415 -02	-0.4618 -02
40	0.2849 00	0.3355 00	0.3333 00	0.6331 -02	0.2135 00	0.4779 -02	-0.2645 -02
50	0.1883 00	0.2401 00	0.2385 00	0.4188 -02	0.1655 00	0.3288 -02	-0.1476 -02
70	0.1029 00	0.1468 00	0.1458 00	0.2299 -02	0.1120 00	0.1825 -02	-0.5483 -03
90	0.6786 -01	0.1040 00	0.1034 00	0.1519 -02	0.8467 -01	0.1199 -02	-0.2611 -03
110	0.5061 -01	0.8145 -01	0.8093 -01	0.1135 -02	0.6919 -01	0.8894 -03	-0.1519 -03
130	0.4136 -01	0.6874 -01	0.6831 -01	0.9287 -03	0.6010 -01	0.7241 -03	-0.1040 -03

Table 3.5b - Behaviour of individual terms of the MGES (3.6) for the ESEH process at 400 eV

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	fIm	Re_1	$f^{(3)}_{GES}$	fw_2	f_{exch}
10	0.2252 01	0.9279	0.9151	0.1809 -01	0.1696	0.1538 -01	+0.4419 -03
20	0.5433	0.3954	0.3930	0.6046 -02	0.1534	0.4018 -02	-0.2469 -02
30	0.2496	0.2132	0.2119	0.2776 -02	0.9854 -01	0.2128 -02	-0.1110 -02
40	0.1443	0.1368	0.1359	0.1609 -02	0.6984 -01	0.1274 -02	-0.4845 -03
50	0.9484 -01	0.9704 -01	0.9642 -01	0.1061 -02	0.5304 -01	0.8405 -03	-0.2377 -03
70	0.5161 -01	0.5854 -01	0.5818 -01	0.5794 -03	0.3507 -01	0.4536 -03	-0.7879 -04
90	0.3398 -01	0.4116 -01	0.4091 -01	0.3822 -03	0.2615 -01	0.2964 -03	-0.3579 -04
110	0.2533 -01	0.3206 -01	0.3186 -01	0.2851 -03	0.2119 -01	0.2197 -03	-.2035 -04
130	0.2069 -01	0.2696 -01	0.2679 -01	0.2331 -03	0.1830 -01	0.1789 -03	-0.1376 -04

Table 3.6 - Differential cross sections (in units of $a_o^2\ Sr^{-1}$) for the ESEH process in the MGES approximation.

Θ / E eV	100 eV	200 eV	400 eV	600 eV	800 eV
10	0.2539 02	0.1164 02	0.4029 01	0.1591 01	0.8751 00
20	0.4985 01	0.9793 00	0.2382 00	0.1051 00	0.5921 -01
30	0.9168 00	0.2146 00	0.5113 -01	0.2245 -01	0.1254 -01
40	0.3301 00	0.7360 -01	0.1744 -01	0.7594 -02	0.4217 -02
50	0.1472 00	0.3280 -01	0.7706 -02	0.3330 -02	0.1841 -02
70	0.4630 -01	0.1030 -01	0.2371 -02	0.1013 -02	0.5563 -03
90	0.2128 -01	0.4675 -02	0.1057 -02	0.4483 -03	0.2451 -03
110	0.1239 -01	0.2686 -02	0.5998 -03	0.2529 -03	0.1378 -03
130	0.8558 -02	0.1836 -02	0.4063 -03	0.1707 -03	0.9281 -04

Table 3.7 - Comparison between the DCS obtained in the GES and Glauber approximations for the ESEH Process.

θ / E	100 eV		200 eV		400 eV	
	GES	Glauber	GES	Glauber	GES	Glauber
20	4.497 00	3.957 00	0.909 00	1.114 00	0.2283 00	0.297 00
30	0.801 00	0.802 00	0.198 00	0.226 00	0.4893 -01	0.602 -01
40	2.881 -01	2.629 00	6.786 -02	7.401 -02	0.1671 -01	0.197 -01
50	1.279 -01	1.128 -01	3.029 -02	3.175 -02	0.7396 -02	0.846 -02
70	4.036 -02	3.325 -01	9.567 -03	9.358 -03	0.2281 -02	0.249 -02
90	1.871 -02	1.439 -02	4.361 -03	4.052 -03	0.1019 -02	0.108 -02
110	1.097 -02	1.045 -02	2.514 -03	2.249 -03	0.5786 -03	0.583 -03

Table 3.8 - TCS for ESEH process

E eV	TCS
100	150.2
200	83.4
300	58.8
400	45.8
500	37.7
600	32.2

Table 3.9 - Constants of wavefunction product for the He target

k	D_k	K_{1k}	K_{2k}
1	46.0536709	2.82	2.82
2	18.7696245	5.22	5.22
3	29.4008522	2.82	5.22
4	29.4008522	5.22	2.82
5	117.6034086	4.02	4.02
6	46.9826758	4.02	5.22
7	46.9826758	5.22	4.02
8	73.5939445	2.82	4.02
9	73.5939445	4.02	2.82

Table 3.10 - Differential cross sections (in units of a_o^2 Sr^{-1}) for the EHe process in the MGES approximation.

θ / E	200 eV	400 eV
10	1.285 00	6.790 -01
20	6.219 -01	2.940 -01
30	3.195 -01	1.291 -01
40	1.859 -01	6.254 -02
50	1.027 -01	3.337 -02
70	4.557 -02	1.195 -02
90	2.357 -02	4.864 -03
110	1.388 -02	2.393 -03
130	9.029 -03	1.382 -03

Table 3.11 - TCS - EHe Process

E eV	Present MGES	Blaauw et al (1980)	Dalba et al (1979)	Byron and Joachain (1977)	Byron and Joachain (1975)	de Heer and Jansen (1975)
100	4.94	3.97	4.15	6.16	4.68	4.05
200	2.93	2.58	2.73	3.37	2.92	2.68
300	2.14	1.98	2.02	2.38	2.15	2.03
400	1.69	1.64	1.61	1.86	1.71	1.66
500	1.42	1.35	1.35	1.56	1.43	1.39

Table3.12a - Behaviour of the individual terms of the MGES (3.6) for the EHe process at 200 eV

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	fIm	Re_1	$f^{(3)}_{GES-Ve}$	fw_2	$f_{exch-Ve}$
10	0.7373	0.631	0.6572	0.1359	-0.129	6.556 -02	0.1248 00
20	0.6103	0.378	0.4006	0.0370	-0.126	6.159 -02	0.9919 -01
30	0.4743	0.273	0.2818	0.0218	0.137	5.598 -02	0.7246 -01
40	0.3622	0.223	0.2276	0.0195	0.117	4.968 -02	0.5127 -01
50	0.2793	0.193	0.1955	0.0185	0.123	4.348 -02	0.3626 -01
70	0.1775	0.154	0.1610	0.0157	0.102	3.299 -02	0.1921 -01
90	0.1247	0.129	0.1376	0.0128	0.094	2.560 -02	0.1135 -01
110	0.0958	0.112	0.1165	0.0107	0.086	2.077 -02	0.7526 -02
130	0.0794	0.100	0.1009	0.0094	0.080	1.774 -02	0.5572 -02

Table 3.12 b - Behaviour of the individual terms of the MGES (3.6) for the EHe process at 400 eV.

Θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	fIm	Re_1		$f^{(3)}_{GES\ -Ve}$		fw_2		$f_{exch\ -Ve}$	
10	0.6893	0.351	0.3678	2.739	-02	6.78	-02	3.209	-02	5.753	-02
20	0.4944	0.201	0.2060	0.931	-02	6.89	-02	2.846	-02	3.818	-02
30	0.3350	0.150	0.1522	0.927	-02	6.57	-02	2.391	-02	2.313	-02
40	0.2310	0.124	0.1284	0.857	-02	5.80	-02	1.950	-02	1.396	-02
50	0.1660	0.106	0.1113	0.749	-02	5.19	-02	1.576	-02	8.711	-03
70	0.0975	0.080	0.0835	0.545	-02	4.32	-02	1.054	-02	3.871	-03
90	0.0660	0.064	0.0602	0.407	-02	3.74	-02	0.753	-02	2.052	-03
110	0.0497	0.053	0.0470	0.322	-02	3.34	-02	0.581	-02	1.272	-03
130	0.0409	0.047	0.0390	0.273	-02	3.07	-02	0.482	-02	9.042	-04

Table 3.13a - Behaviour of the individual terms of the MGES (3.6) for the ELi process at 200 eV.

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	fIm	Re_1	$f^{(3)}_{GES-Ve}$	fw_2	$f_{exch-Ve}$
10	0.3373 01	0.1010 01	0.9386	0.2591 -02	0.4169	0.1695	0.3721 -01
20	0.1348 01	0.5840	0.5398	0.1289 -01	0.2582	0.1325	-0.1675 -02
30	0.7199	0.3899	0.3638	0.8283 -02	0.1859	0.1096 -	-0.1279 -02
40	0.4793	0.2708	0.2535	0.5140 -02	0.1426	0.9503 -01	0.4165 -03
50	0.3564	0.1994	0.1869	0.3459 -02	0.1146	0.8373 -01	0.1088 -02
70	0.2305	0.1248	0.1171	0.1915 -02	0.8097 -01	0.6603 -01	0.1174 -02
90	0.1672	0.8951 -01	0.8402 -01	0.1269 -02	0.6273 -01	0.5348 -01	0.9177 -03
110	0.1318	0.7055 -01	0.6624 -01	0.9496 -03	0.5205 -01	0.4494 -01	0.7035 -03
130	0.1107	0.5980 -01	0.5616 -01	0.7775 -03	0.4563 -01	0.3938 -01	0.5652 -03

Table 3.13 b - Behaviour of individual terms of the MGES (3.6) for the ELi process at 400 eV

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	fIm	Re_1	$f^{(3)}_{GES\,-Ve}$	fw_2	$f_{exch\,-Ve}$
10	0.2254 01	0.5291	0.4861	0.5029 -02	0.1752	0.7644 -01	0.4859 -02
20	0.7799	0.2934	0.2736	0.4492 -02	0.9754 -01	0.5619 -01	-0.8137 -03
30	0.4357	0.1739	0.1629	0.2272 -02	0.6659 -01	0.4574 -01	0.3489 -03
40	0.2949	0.1149	0.1079	0.1336 -02	0.4931 -01	0.3805 -01	0.6137 -03
50	0.2168	0.8274 -01	0.7765 -01	0.8842 -03	0.3854 -01	0.3178 -01	0.5672 -03
70	0.1337	0.5069 -01	0.4759 -01	0.4847 -03	0.2635 -01	0.2275 -01	0.3588 -03
90	0.9309 -01	0.3596 -01	0.3378 -01	0.3203 -03	0.2002 -01	0.1715 -01	0.2228 -03
110	0.7128 -01	0.2817 -01	0.2646 -01	0.2392 -03	0.1642 -01	0.1371 -01	0.1501 -03
130	0.5903 -01	0.2378 -01	0.2235 -01	0.1956 -03	0.1429 -01	0.1162 -01	0.1117 -03

Table 3.14 - Differential Cross sections (In units of $a_0^2 Sr^{-1}$) for the ELi process in the MGESapproximation

θ / E	100 eV	200 eV	400 eV	600 eV	800 eV
10	0.1985 02	0.1069 02	0.4905 01	0.2805 01	0.1792 01
20	0.4430 01	0.1803 01	0.6249 00	0.3417 00	0.2258 00
30	0.1531 01	0.5516 00	0.2003 00	0.1124 00	0.7420 -01
40	0.7037 00	0.2535 00	0.9292 -01	0.5071 -01	0.3229 -01
50	0.3969 00	0.1428 00	0.5059 -01	0.2639 -01	0.1619 -01
70	0.1769 00	0.6111 -01	0.1934 -01	0.9341 -02	0.5455 -02
90	0.1013 00	0.3249 -01	0.9353 -02	0.4314 -02	0.2459 -02
110	0.6719 -01	0.2015 -01	0.5439 -02	0.2448 -02	0.1379 -02
130	0.5001 -01	0.1426 -01	0.3699 -02	0.1643 -02	0.9213 -03

Table 3.15 - Differential cross sections for the ELi process in the GES approximation.

θ/E	100 eV	200 eV	400 eV	600 eV
10	0.1678 02	0.9586 01	0.4570 01	0.2654 01
20	0.3073 01	0.1462 01	0.5422 00	0.3045 00
30	0.9218 00	0.4025 00	0.1620 00	0.9536 -01
40	0.3626 00	0.1663 00	0.7110 -01	0.4153 -01
50	0.1714 00	0.8510 -01	0.3712 -01	0.2108 -01
70	0.5156 -01	0.3138 -01	0.1339 -01	0.7215 -02
90	0.2003 -01	0.1499 -01	0.6231 -02	0.3267 -02
110	0.9109 -02	0.8579 -02	0.3534 -02	0.1832 -02
130	0.4718 -02	0.5725 -02	0.2363 -02	0.1222 -02

Table 3.16 - Behaviour of the various terms of (3.6) for the IHSS Process at 100 eV

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	$f^{(3)}_{GES}$	fIm	Re_1	f_{exch}
10	-0.7389	-0.3362 00	-0.1452 00	-0.3285 00	-0.4383 -01	-0.2334 -01
20	-0.3753	-0.1363 00	-0.1392 00	-0.1163 00	-0.1824 -01	-0.4399 -01
30	-0.1595	-0.1166 00	-0.8536 -01	-0.9449 -01	-0.2260 -01	-0.4100 -01
40	-0.0667	-0.9788 -01	-0.6839 -01	-0.8108 -01	-0.1829 -01	-0.2983 -01
50	-0.0296	-0.7701 -01	-0.5335 -01	-0.6469 -01	-0.1310 -01	-0.2019 -01
70	-0.0075	-0.4724 -01	-0.3835 -01	-0.3979 -01	-0.6925 -02	-0.9443 -02
90	-0.0026	-0.3175 -01	-0.3009 -01	-0.2649 -01	-0.4289 -02	-0.5044 -02
110	-0.0012	-0.2364 -01	-0.2502 -01	-0.1951 -01	-0.3061 -02	-0.3122 -02
130	-0.0007	-0.1923 -01	-0.2189 -01	-0.1573 -01	-0.2435 -02	-0.2212 -02

Table 3.17 Behaviour of the various terms of (3.6) for the IHSS Process at 400 eV

Θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	$f^{(3)}_{GES}$	fIm	Re_1	f_{exch}
10	-0.3659	-0.6747 -01	-0.3443 -01	-0.5652 -01	-0.3759 -02	-0.1105 -01
20	-0.0591	-0.4741 -01	-0.1638 -01	-0.4065 -01	-0.4543 -02	-0.7069 -02
30	-0.0111	-0 .2734 -01	-0.1050 -01	-0.2354 -01	-0.2127 -02	-0.2963 -02
40	-0.0028	-0.1629 -01	-0.7645 -02	-0.1383 -01	-0.1122 -02	-0.1315 -02
50	-0.0009	-0.1065 -01	-0.5848 -02	-0.8879 -02	-0.6892 -03	-0.6559 -03
70	-0.0002	-0.5668 -02	-0.3820 -02	-0.4587 -02	-0.3501 -03	-0.2218 -03
90	-0.0001	-0.3679 -02	-0.2796 -02	-0.2912 -02	-0.2239 -03	-0.1017 -03
110	-	-0.2720 -02	-0.2229 -02	-0.2118 -02	-0.1646 -03	-0.5813 -04
130	-	-0.2212 -02	-0.1902 -02	-0.1704 -02	-0.1335 -03	-0.3940 -04

Table 3.18 Differential cross sections $(a_o^2 s_{\hbar}^{-1})$ for the IHSS process.

θ/E	100 eV		200 eV		400 eV		600 eV		800 eV	
10	0.4680	00	0.2502	00	0.1105	00	0.5307	-01	0.2757	-01
20	0.4972	-01	0.2195	-01	0.3897	-02	0.1182	-02	0.4899	-03
30	0.1230	-01	0.3634	-02	0.6482	-03	0.2089	-03	0.9083	-04
40	0.5394	-02	0.1474	-02	0.2314	-03	0.7120	-04	0.3023	-04
50	0.3788	-02	0.7418	-03	0.1033	-03	0.3079	-04	0.1292	-04
70	0.1699	-02	0.2450	-03	0.3075	-04	0.8982	-05	0.3749	-05
90	0.8387	-03	0.1083	-03	0.1319	-04	0.3844	-05	0.1605	-05
110	0.4865	-03	0.6011	-04	0.7266	-05	0.2118	-05	0.8853	-06
130	0.3297	-03	0.3998	-04	0.4823	-05	0.1407	-05	0.5885	-06

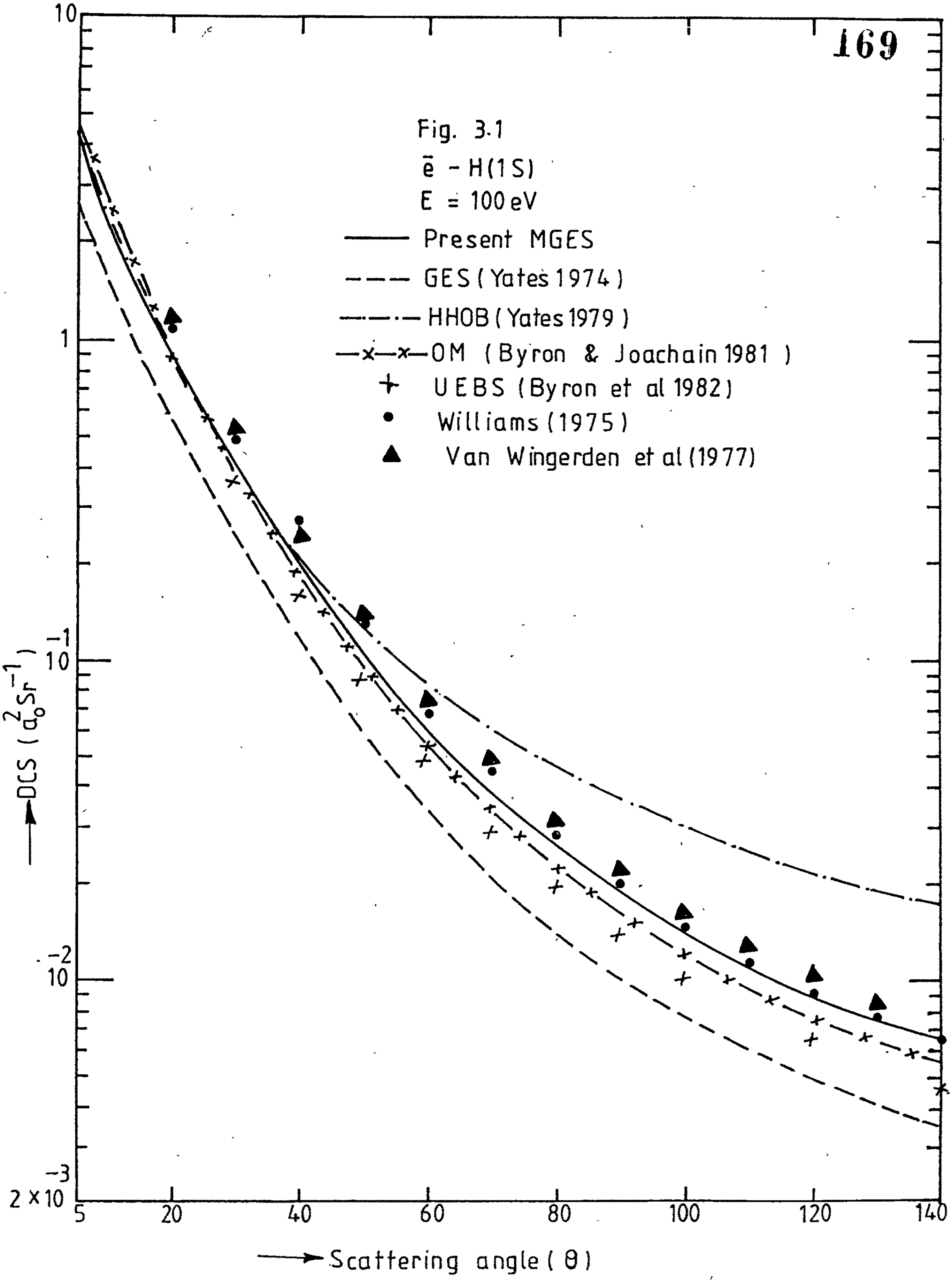

Fig. 3.1
$\bar{e}$ - H(1S)
E = 100 eV

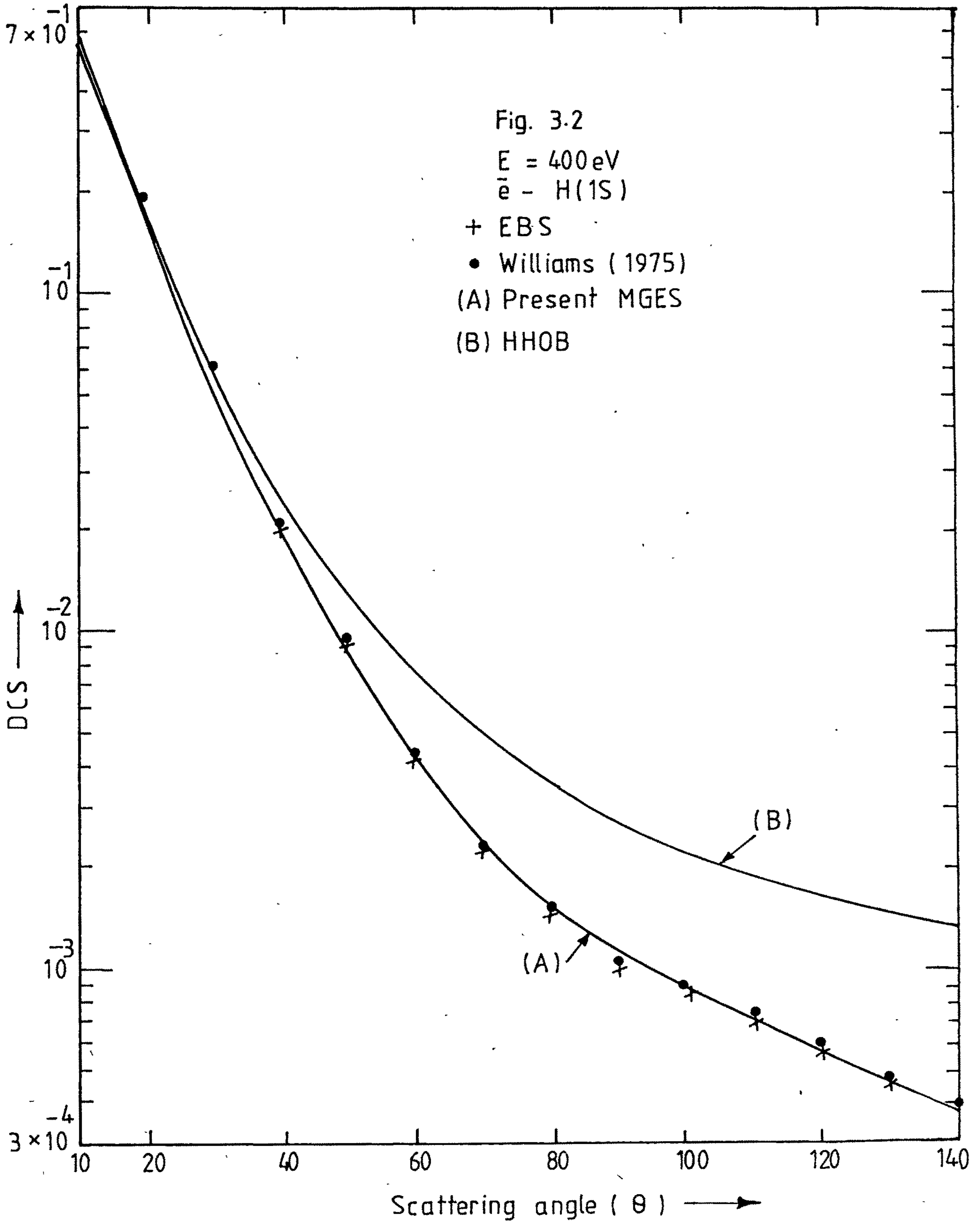
Fig. 3.2
E = 400 eV
e⁻ - H(1S)
+ EBS
● Williams (1975)
(A) Present MGES
(B) HHOB
(A)
(B)
DCS
7 × 10⁻¹
10⁻¹
10⁻²
10⁻³
3 × 10⁻⁴
10
20
40
60
80
100
120
140
Scattering angle (θ)

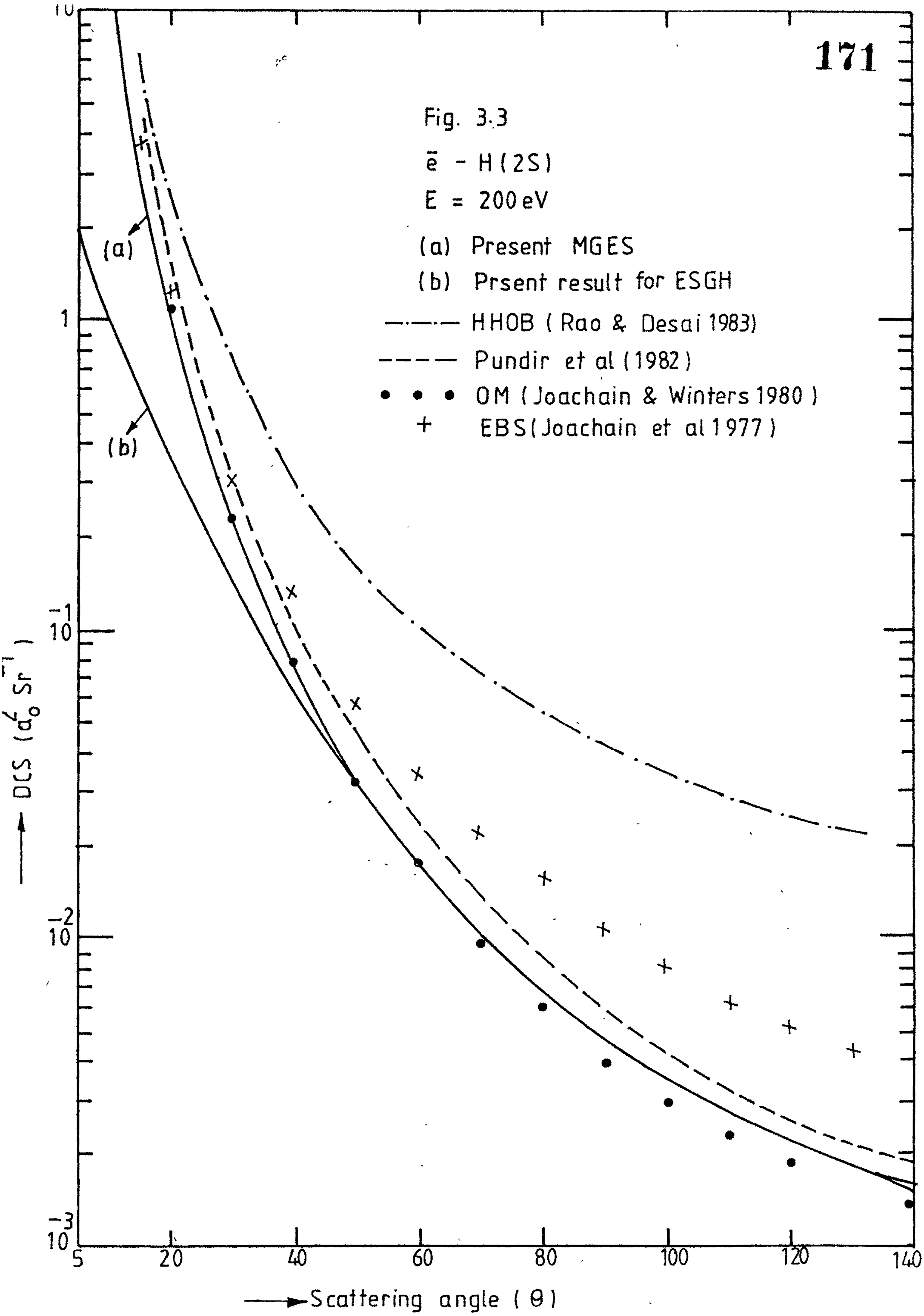

Fig. 3.3

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

E = 200 eV

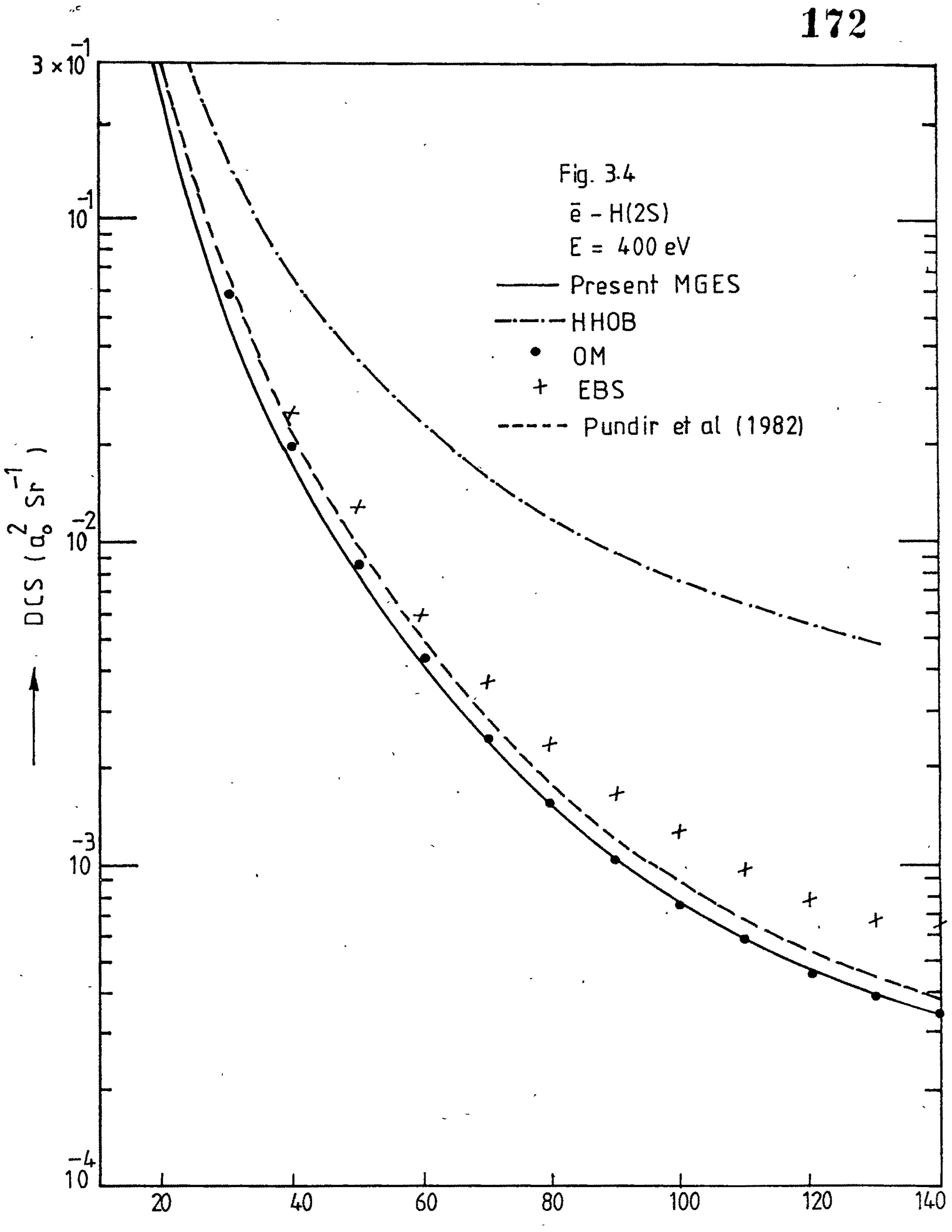
Fig. 3.4
ē - H(2S)
E = 400 eV
Present MGES
HHOB
OM
EBS
Pundir et al (1982)
3 × 10⁻¹
10⁻¹
10⁻²
10⁻³
10⁻⁴
DCS (a₀² Sr⁻¹)
20
40
60
80
100
120
140
Scattering angle (θ)

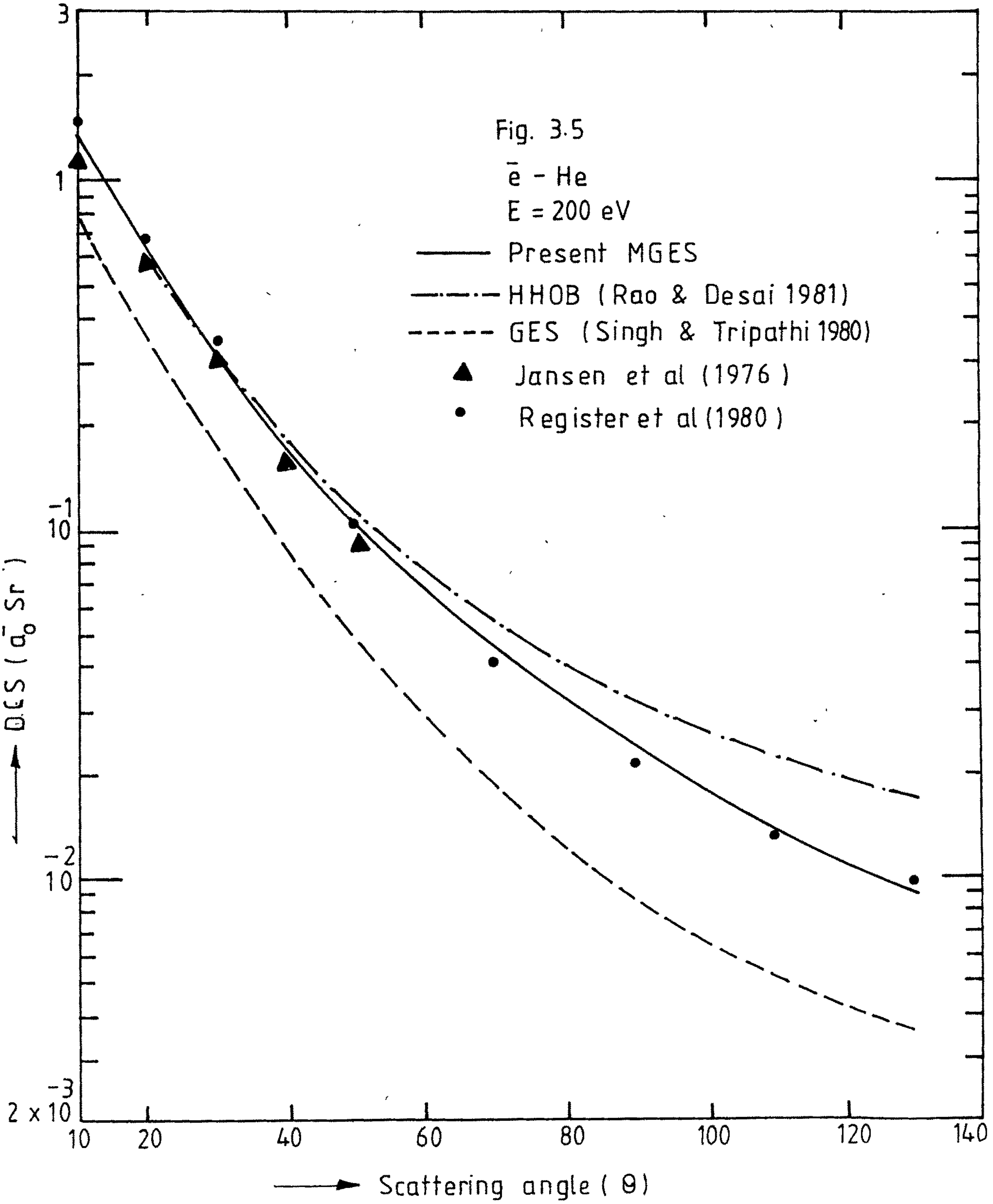
Fig. 3.5
ē - He
E = 200 eV
Present MGES
HHOB (Rao & Desai 1981)
GES (Singh & Tripathi 1980)
Jansen et al (1976)
Register et al (1980)
3
1
10⁻¹
10⁻²
2 x 10⁻³
10
20
40
60
80
100
120
140
DCS (a₀² Sr⁻¹)
Scattering angle (θ)

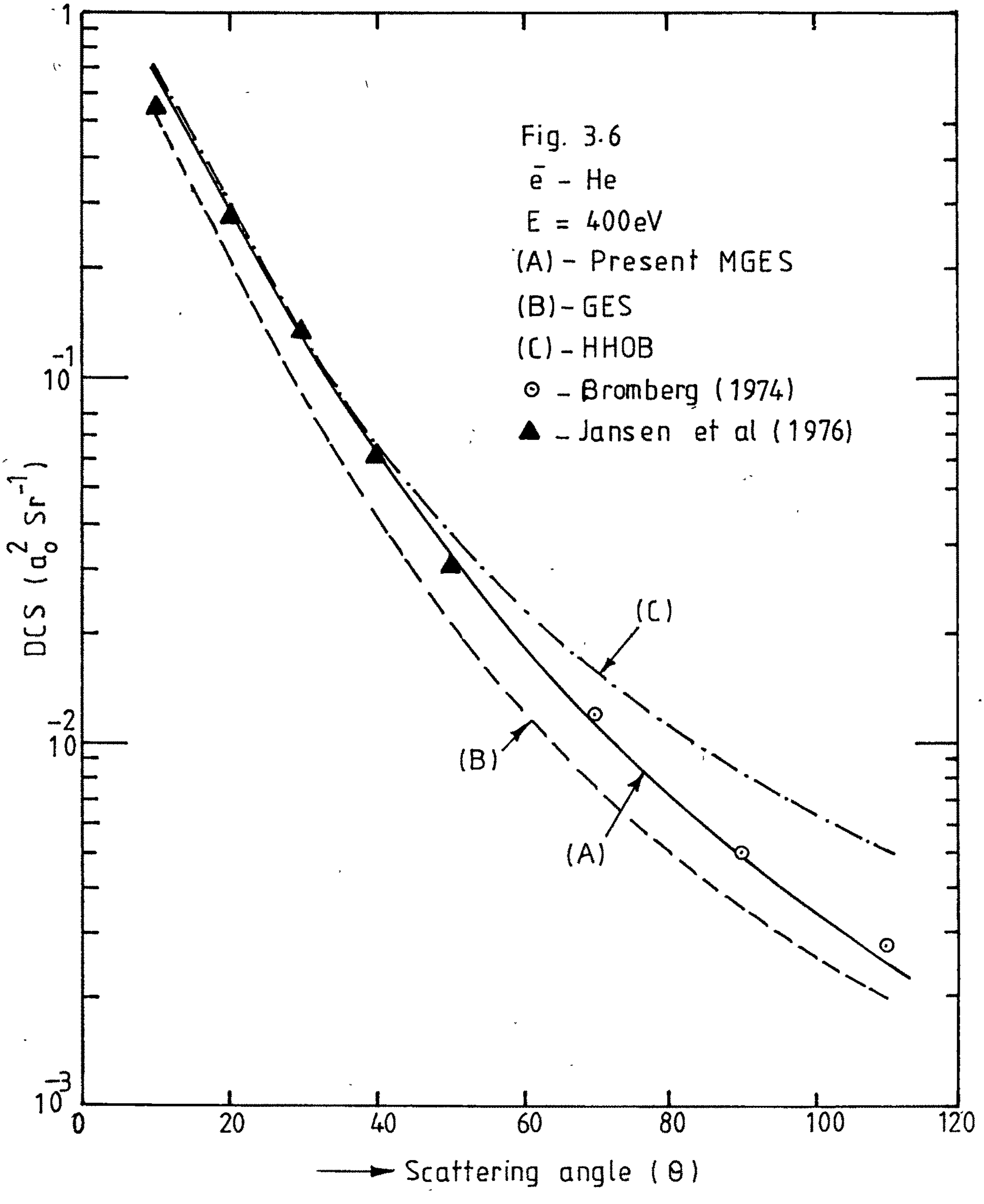
Fig. 3.6
$\bar{e}$ - He
E = 400eV
(A) - Present MGES
(B) - GES
(C) - HHOB
⊙ - Bromberg (1974)
▲ - Jansen et al (1976)
(A)
(B)
(C)
DCS ($a_o^2 \, Sr^{-1}$)
1
10^{-1}
10^{-2}
10^{-3}
0
20
40
60
80
100
120
Scattering angle (θ)

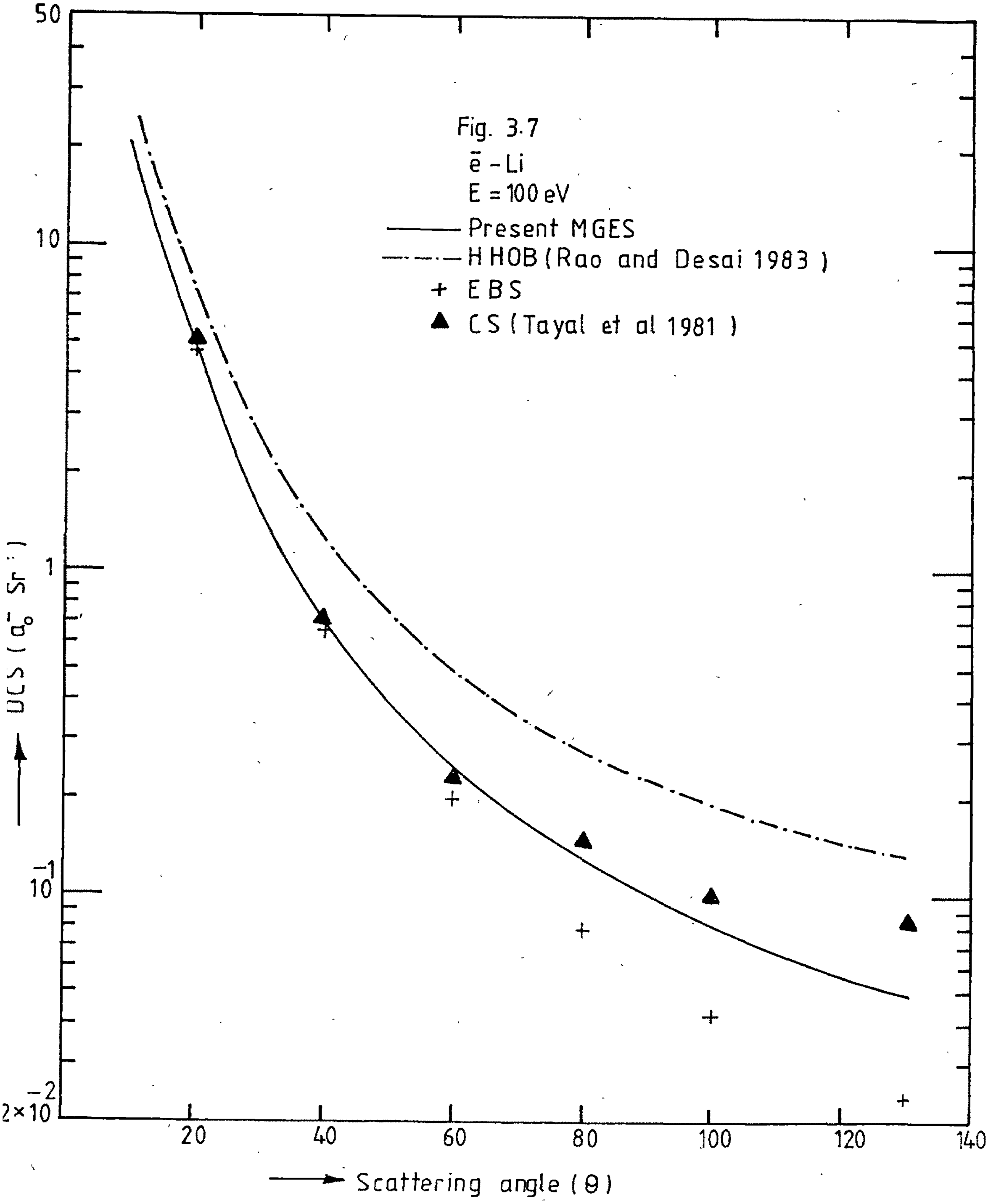
Fig. 3.7
ē - Li
E = 100 eV
Present MGES
HHOB (Rao and Desai 1983)
+ EBS
▲ CS (Tayal et al 1981)
50
10
1
10^{-1}
2×10^{-2}
DCS (a_0^2 Sr^{-1})
20
40
60
80
100
120
140
Scattering angle (θ)

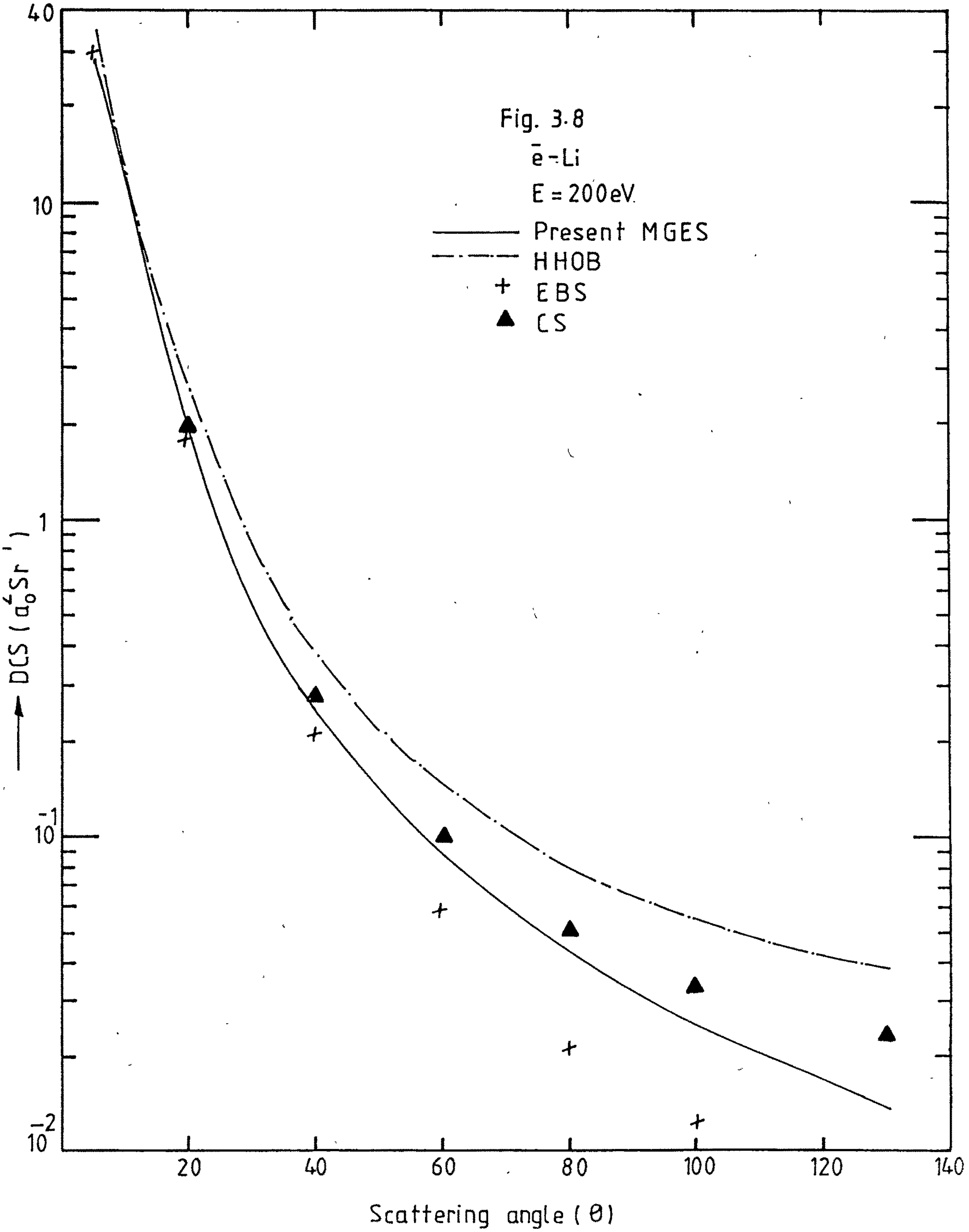
Fig. 3.8
$\bar{e}$-Li
E = 200eV
Present MGES
HHOB
+ EBS
▲ CS
DCS ($a_0^2 Sr^{-1}$)
40
10
1
10^{-1}
10^{-2}
20
40
60
80
100
120
140
Scattering angle (θ)

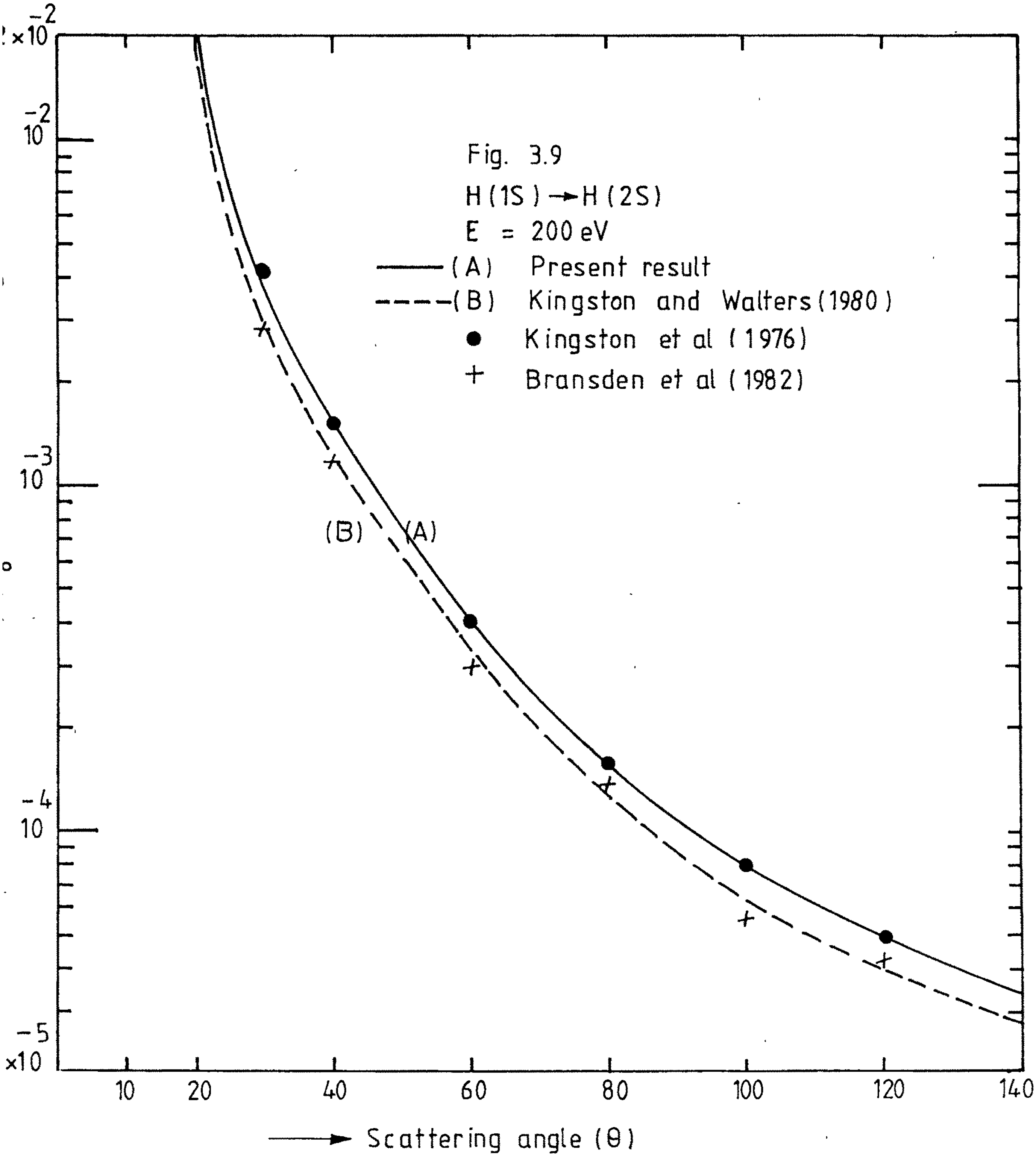
Fig. 3.9

×10^-2
10^-2
10^-3
10^-4
×10^-5
H(1S) → H(2S)
E = 200 eV
(A) Present result
(B) Kingston and Walters (1980)
● Kingston et al (1976)
+ Bransden et al (1982)
(B)
(A)
10
20
40
60
80
100
120
140
→ Scattering angle (θ)