Chapter 3

Elastic scattering of fast electrons by atoms

3.1 Introductory Remarks

In this chapter, we present our studies on the elastic scattering of intermediate to high energy electrons, by atoms. The importance of the elastic scattering process is easily recognised as one of the simplest processes of collision, where there is only a transfer of momentum. In the case of electron scattering, this merely results into a deflection of the projectile. Theoretical formulation is relatively simpler for elastic collisions, and a wealth of experimental data is now available on elastic collisions of electrons with various targets. Thus, today, the elastic collisions are the most widely studied processes followed by inelastic collisions of electrons by atoms and molecules, and the present knowledge about ionizing collisions is inadequate. One more theoretical view point here is that the elastic electron-atom processes are also easily studied in terms of the model (optical) potentials.

Here, we begin our study of elastic scattering of fast electrons, with hydrogen atoms as the target, which offers the simplest example of three-body collisions. For consistency, we begin with the first Born approximation. Unless otherwise mentioned we now work in a.u.

3.2 The First Born Approximation

This well known theoretical procedure is already introduced in the last chapter. The first Born amplitude for the elastic scattering of electrons by atoms is given by,

$$f_{B1} = -\frac{1}{2\pi} \int d\underline{r}\, e^{i\underline{q}.\underline{r}} V_{ii}(r) \qquad (3.1)$$

where the momentum transfer in a.u., is

$$q = |\underline{q}| = |\underline{k}_i - \underline{k}_f| = 2k_i \sin\frac{\theta}{2} \qquad (3.2)$$

'θ' is the angle of scattering.

Further,

$$V_{ii} = \langle 0 \mid V(\underline{r}, \underline{x}) \mid 0 \rangle \qquad (3.3)$$

In these eqns. $|i\rangle$ or $|0\rangle$ represents the ground state of the target atom, and $V(\underline{r}, \underline{x})$ is the potential of interaction between the incident electron and the target atom. The coordinate system is centred at the atomic nucleus. Here, 'x' represents all the target-electron coordinates. For e-H collisions, the potential

is,

$$V(\underline{r}\ ,\ \underline{r}_1) = -\frac{1}{r} + \frac{1}{|\underline{r} - \underline{r}_1|} \qquad (3.4)$$

where, $\underline{r}_1$ is the coordinate of the target electron, $\underline{r}_1 = \underline{b}_1 + \underline{z}_1$, where, as usual, $\underline{b}_1$ is in the (X, Y) plane. The quantity of eqn. (3.3) also denoted by V_{st} represents the potential of interaction averaged over the static charge distribution in the atom. This so called static potential is more effective in the range of atomic dimensions i.e, it is a short range interaction. If an incident particle comes sufficiently closer to the atom, it experiences the static potential and is deflected considerably. Thus, the first Born amplitude of eqn. (3.1) takes into account only the static potential and governs large angle scattering. On the other hand, no long range forces are explicitly considered here, which, the projectile may experience even at a large distance and that may produce a gentle deflection of its path. Due to this, the first Born amplitude is not good enough for small angle scattering. The simple first Born amplitude does not take into account also, the effects of the distortion of the projectile or the target produced due to interaction.

Now for the atomic hydrogen the static

potential is

$$V_{st} = -(1 + \frac{1}{r}) \exp(-2r) \qquad (3.5)$$

This yields the first Born direct Transition matrix as,

$$T^{d}_{Born} = -\frac{1}{2\pi^2}\left(\frac{q^2 + 8}{(q^2 + 4)^2}\right) \qquad (3.6)$$

Now, the relation between the T-martix and the scattering amplitude is the following

$$f = -4\pi^2 T \qquad (3.7)$$

Thus, the direct first Born amplitude for elastic e-H scattering reads as,

$$f_{B1} = \frac{2(q^2 + 8)}{(q^2 + 4)^2} \qquad (3.8)$$

The elastic DCS is obtained from the relation,

$$\frac{d\sigma}{dw} = |f|^2 \qquad (3.9)$$

We observe that the first Born amplitude depends only

on the magnitude of momentum transfer q and it predicts a constant value of the forward DCS, independent of the incident energy.

In the above discussion, 'direct scattering' means without exchange. The electron exchange effect can also be treated in the first Born approximation. The purpose of the present chapter is to discuss some of the higher order perturbation theories in the direct elastic scattering. We, therefore, do not discuss the exchange aspect.

It is found that, the first Born DCS agree with the experimental data only at high energies and at large angles of scattering. Clearly, it is inadequate to describe fully the Physics of the collision process and one must seek some higher order perturbation theories that are capable of doing so.

3.3 The Glauber Theory

As mentioned in the previous chapter, the generalization of the eikonal approximation for the scattering of charged particles from targets with internal structure, was given by R. J. Glauber (1959). In recent years, the well known Glauber approximation has been applied with success for simple targets and further

refinements too, have been brough about. (See e.g. Byron et al, 1977). We analyse the Glauber approximation again in this chapter to elucidate its nature. The Glauber amplitude for the electron-atom collisions is,

$$f^G(q, k_i) = \frac{ik_i}{2\pi} \int d\underline{b} \exp(i\underline{q}.\underline{b}) \langle f | 1 - \exp(iX) | i \rangle \qquad (3.10)$$

With i and f representing the initial and the final target states, $\underline{b}$ being the impact parameter, $d\underline{b}$ showing an area-element in the (x, y) plane and the Glauber phase X being given by ,

$$X = \frac{1}{k_i} \int_{-\infty}^{\infty} dz\, V(\underline{r}, \underline{x}) \qquad (3.11)$$

The evaluation of the Glauber amplitude depends thus on the expression of 'X' . Now, except for Hydrogen and Helium atoms, the Glauber phase has a complicated expression, so that the evaluation of the amplitude of eqn. (3.10) becomes difficult and even unmanagable. Thus, although it is true that the Glauber approximation takes into account, somehow, all orders of perturbation and is therefore superior to the first Born approximation,

the problem of evaluating the Glauber amplitude is not that simple. Thomas and Gerjuoy (1971) obtained the closed form expressions for the Glauber amplitude of the collisions of charged particles with Hydrogen atoms. Rather than trying to evaluate the amplitude of eqn. (3.10) as a whole, let us resort to its termwise analysis, as shown by Yates (1974). In the last chapter, too, we expressed the Glauber amplitude as a series (see eqn. (2.56) of chapter 2). Presently, we wish to write,

$$f^G(q, k_i) = \sum_{n=1}^{\infty} i^{n-1} f_{Gn}(q, k_i) \qquad m \quad (3.12)$$

where, the first term reduces to the first Born amplitude and each term is obtained from the expansion of exp (iX) in eqn. (3.10) so that, the n th term would be

$$f_{Gn} = \frac{k_i}{2\pi n!} \int d\underline{b} \exp(i\underline{q}.\underline{b}) \langle f | X^n | i \rangle \qquad (3.13)$$

Let us note that X is a function of the incident as well as the target electron coordinates. Hence, to simplify the evaluation of the matrix element of eqn. (3.13), we take the Fourier transform of X with respect to the incident electron co-ordinate $\underline{r}$, corresponding to which the Fourier variable is

$$\underline{P} = \underline{p} + \underline{p}_z$$

The variable $\underline{p}$ is two dimensional, and the (p_x , p_y) plane. The incident electron momentum $\underline{k}_i$ is along the polar axis. For e-H scattering, we write $B(\underline{p} , \underline{b}_1)$ for the two dimensional Fourier representation of the interaction potential of eqn. (3.4), so as to yield,

$$X(\underline{b},\underline{b}_1) = \frac{1}{\pi k_i} \int \frac{d\underline{p}}{p^2} \exp (i\underline{p}.\underline{b}) \; B(\underline{p} , \underline{b}_1) \qquad (3.15)$$

Thus, the 2nd Glauber term in the series of eqn. (3.12) becomes.

$$f_{G2} = \frac{1}{\pi k_i} \int \frac{d\underline{p}}{p^2 | \underline{q} - \underline{p} |^2}$$

$$< f | B (\underline{p} , \underline{b}_1) \; B(\underline{q} - \underline{p}, \underline{b}_1) | i > \qquad (3.16)$$

Notably, the coupling of $\underline{b}$ and $\underline{b}_1$ is removed by the use of the Fourier transform. The 2nd order Glauber amplitude for elastic e-H scattering has a form,

$$f_{G2} = \frac{1}{8\pi k_i Z^3} \left(\frac{d}{dZ} \right) \frac{Z^4}{1 + Z^2} \ln \left(\frac{1 + Z^2}{Z} \right) \qquad (3.17)$$

with $\underline{Z} = \underline{q} / \lambda$. The parameter $\lambda = 2$ arises from the product of the ground state wave functions for the Hydrogen atom. Let us note two p important features of the term, f_{G2} .

(1) The 2nd order Glauber amplitude is purely imaginary. In fact, the alternative terms of the full Glauber amplitude, eqn. (3.12), are real and imaginary respectively.

(2) The 2nd Glauber term of eqn. (3.16) diverges as $\ln q$ as $q \longrightarrow 0$. This is one of the main drawbacks of the Glauber theory and it has been attributed to the fact that, in the evaluation the Green's function in this case, the off-shell contributions are suppressed, i.e. the intermediate vector $\underline{k}_n$ is replaced by incident vector $\underline{k}_i$. In the 2nd order Born term also this behaviour is found if the average excitation energy is replaced by zero (Moiseiwitch and Williams 1959, Yates 1973). Further, the third Glauber amplitude is given by (Yates 1974),

$$f_{G3} = \frac{\lambda}{16\pi k_i^2 \, Z^3} \left(\frac{d}{dZ}\right) \frac{Z^4}{1+Z^2} \left[4 \left(\ln\left(\frac{1+Z^2}{Z}\right)\right)^2 + \frac{\pi^2}{3} - 2A(Z)\right] \qquad (3.18)$$

where,

$$A(Z) = 2(\ln Z)^2 + \frac{\pi^2}{6} + \sum_{n=1}^{\infty} \frac{(-Z^2)^n}{n^2} \qquad (3.18b)$$

if $Z \leq 1$

$$A(Z) = -\sum_{n=1}^{\infty} (-1/Z^2)^n / n^2 \qquad (3.18c)$$

if $Z > 1$

We find from eqns. (3.17) and (3.18) that the Glauber series of eqn. (3.12) is an expansion in the powers of $1/k_i$. It has been called the Glauber eikonal series (GES). For the elastic scattering of electrons by Hydrogen atoms, the exact Glauber amplitude f^G was evaluated by Thomas and Gerjuoy (1971). In the e-H elastic scattering it is found that (Yates, 1974) the first three terms of eqn. (3.12) are sufficient to approximate f^G very closely. Later on, Singh and Tripathi (1980) applied the GES method to the elastic and inelastic scattering of electrons from Helium atoms. These authors have elaborated the mathematical details of evaluating the second and third terms of the GES. It is observed that some of the integrals involved in the calculations of f_{G2} and f_{G3} are absolutely singular but their combinations turn out

to be such that the singularities cancel exactly. How does the Glauber approximation (or the GES) compare with experiments ? First of all, the Glauber DCS are divergent in the forward direction, for elastic scattering. And secondly, more or less at all angles, the Glauber cross-sections are lower than the experimental data. In the region of larger angles, even the first Born approximation is for better. We note here two relevent points, for the Glauber results.

(i) The second Glauber term lacks a real part, as compared to the second Born term. The real part of the second Born term represents the polarization effects in the target, and is dominent near the forward direction.

(ii) The sign of the third Glauber term f_{G3} is opposite to that of the first term. This is true for inelastic cases as well. Hence, the inclusion of f_{G3} reduces the cross-sections.

Now for inelastic processes, the problem of divergance of f_{G2} does not occur, because in that case, the momentum transfer $q \neq 0$ even in the forward direction. But there is certainly one point that deserves attention. In this case, when the incident particle is scattered exactly in the forward direction, the momentum transfer q ($\neq 0$) is in the forward direction, with no component

perpendicular to the incident direction. Now, the Glauber amplitude eqn. (3.10), assume $\underline{q}$ only in a plane perpendicular to $\underline{k}_i$! Thus, there is a contradiction. Perhaps, the way out is to remove the restriction that $\underline{q}$ must be two dimensional and in the plane normal to $\underline{k}_i$ (see Gau and Macek 1974, 1975).

A number of issues related to various aspects of the Glauber theory have been discussed and analysed in the literature of the recent past. In our present discussion, we consider two more points before switching over to the next section.

1) The importance of the Glauber theory lies in the fact that it contains all orders of a perturbation expansion hence, it satisfies the optical theorem (or unitarity relation) in its own frame work.

2) Of the improvements suggested to modify the Glauber amplitude mention must be made of the Wallace-correction (1973). This has been applied with success to e-H scattering problems by Roy and Sil (1978) and Unnikrishnan and Prasad (1982). The Wallace-correction has been further elaborated by Franco (1982) and also by Byron et al (1982). We now go over to the next section on the second Born approximation.

3.4 The Second Born Approximation

It becomes clear from the preceding discussion that, in many respects, the second Born amplitude must be superior to the second Glauber amplitude. Recalling the origin of the Born series as a perturbative expansion in the powers of the interaction potential, we write it as,

$$f_B = \sum_{n=1}^{\infty} f_{Bn} \tag{3.19}$$

of which the n = 1 term is the first Born amplitude. In the nth Born amplitude the potential appears n times and the Green's function, (n-1) times. In particular, the direct second Born term is written as,

$$f_{B2} = \frac{1}{\pi} \int d\underline{r}\ e^{i\underline{k}_f \cdot \underline{r}} \sum_n \langle f | V(\underline{r}, \underline{x}) | n \rangle$$

$$\int d\underline{r}'\ (2\pi)^{-3} \times \int d\underline{K}\ \frac{e^{i\underline{K}\cdot(\underline{r} - \underline{r}')}}{K^2 - k_n^2 - i\epsilon}$$

$$\langle n | V(\underline{r}', \underline{x}') | i \rangle\ e^{i\underline{k}_i \cdot \underline{r}'} \tag{3.20}$$

In the last equation $|n\rangle$ denotes an intermediate state of the target. '$\underline{k}_n$' is the intermediate momentum of the projectile electron. The variable $\underline{K}$ comes from

the Green's function, and whenever ϵ appears $\epsilon \longrightarrow 0^+$ is implied. The vector $\underline{k}_n$ is related to the internal energy of the target in its nth state, through the conservation of energy, i.e.

$$1/2\ k_i^2 + W_o = 1/2\ k_n^2 + W_n \qquad (3.21)$$

W_o = the ground state energy of the target. Now, upon slight rearrangement and use of eqn. (3.21), we get,

$$f_{B2} = 8\pi^2 \int d\underline{K} \sum_n \frac{\langle \underline{k}_f, f|V|\underline{K}, n\rangle\langle \underline{K}, n|V|\underline{k}_i, i\rangle}{K^2 - k_i^2 + 2(W_n - W_o) - i\epsilon} \qquad (3.22)$$

where $|\underline{k}_i, i\rangle$ = initial asymptotic state of the total system, etc.

The next step to simplify the above exact expression, many times employed, is to approximate,

$$W_n - W_o \triangleq \overline{W} \qquad (3.23)$$

adiabatic sum rule

This turns out to be a good approximation above, say 50 eV incident energy, (Walters and Ermolaev, 1980). The use of average excitation energy simplifies the expression (3.22). The simplified second Born

approximation obtained in this way is,

$$f_{SB2} = \int d\underline{K} \; \frac{1}{K^2 - k_i^2 + 2\overline{W} - i\epsilon}$$

$$\langle f | (\langle \underline{k}_f | V | \underline{K} \rangle \langle \underline{K} | V | \underline{k}_i \rangle) | i \rangle \qquad (3.24)$$

Here, the closure relation has been used for the target states. The way of writing eqn. (3.24) shows that we first evaluate the plane wave part of the matrix element.

The simplified second Born term (3.24) has been evaluated using the Dalitz integrals (see e.g. Joachain, 1975).

The subsequent discussion naturally leads us to the eikonal Born series (EBS) theory, an elegant approach developed by Byron and Joachain (1973, 1974) to describe the scattering of intermediate and high energy electrons by atoms. The aim of the EBS is to write the leading terms of the Born series to obtain accurate DCS of electron-atom collisions. Now, in the third Born term of the series, the real part is of order $1/k_i^2$, but the calculation of the third Born term is quite difficult. On the other hand, the third term of the Glauber series, i.e. f_{G3}, is relatively easily computed, as we have

seen in the previous section. Both the terms f_{G3} and f_{B3} are zero for elastic scattering in the forward direction. (Dewangan, 1980). They are both $O(k_i^{-2})$. Hence f_{B3} is approximated by f_{G3} and a direct amplitude given below is constructed, (Byron and Joachain, 1973)

$$f^{d}_{EBS} = f_{B1} + f_{B2} + f_{G3} \qquad (3.25)$$

The direct EBS amplitude of eqn. (3.25) is consistent through the order (k_i^{-2}). In the last ten years or so, the EBS theory has been successfully applied to several elastic and inelastic processes in the light and complex atoms (Byron and Joachain 1973, 1974; Byron and Latour 1976). We are now going to discuss, in detail , an alternative approach to the EBS.

3.5 The High Energy Higher Order Born Approximations (HHOB)

This approach was developed by A. C. Yates (1979) and has been further explored by our group. The HHOB is a Born theory based on the assumptions and evaluation methods of the Glauber approximation. Let us consider the Second Born amplitude, which we can write from eqn. (3.20), by defining a variable $\underline{R} = \underline{r} - \underline{r}'$. We introduce, the elements,

$$V_{fn}(\underline{r}) = \langle f | V(\underline{r}, \underline{x}) | n \rangle \qquad (3.26)$$

And a similar symbol, $V_{ni}(\underline{r} - \underline{r}')$.

Thus,

$$f_{B2} = \frac{1}{\pi} \sum_n \int d\underline{r}\, e^{i\underline{q}.\underline{r}}\, V_{fn}(\underline{r})\, (2\pi)^{-3}$$

$$X \int d\underline{r}' \int d\underline{K}\, \frac{e^{i\underline{K}.\underline{r}'}}{K^2 - k_n^2 - i\epsilon}\, V_{ni}(\underline{r} - \underline{r}')\, e^{-i\underline{k}_i.\underline{r}'} \qquad (3.27)$$

where, now $\underline{r}'$ replaces $\underline{R}$. Further evaluation consists in considering the basic integral,

$$I_n = (2\pi)^{-3} \int d\underline{r}'\, e^{-i\underline{k}_i.\underline{r}'}\, V_{ni}(\underline{r} - \underline{r}')$$

$$\int d\underline{K}\, \frac{e^{i\underline{K}.\underline{r}'}}{K^2 - k_n^2 - i\epsilon} \qquad (3.28)$$

Defining,

$$\underline{S} = \underline{K} - \underline{k}_n\,, \qquad (3.29)$$

We have,

$$K^2 - k_n^2 = S^2 + 2\underline{S}.\underline{k}_n \ ,$$

so that

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

$$\times \int d\underline{S} \frac{e^{i\,\underline{S}.\underline{r}'}}{S^2 + 2\underline{S}.\underline{k}_n - i\epsilon} \qquad (3.30)$$

Now, to linearize the Green's function, we assume that, (I) V_{ni} varies slowly over the distance of wavelength of the scattering electron i.e. $k_n a \gg 1$ with 'a' as the range of V_{ni} . (II) $\underline{k}_n$ does not differ much from $\underline{k}_i$ either in magnitude (which means $\frac{E_{in}}{k_i} \ll 1$) or in direction ' (i.e. the momentum transfer is also small). The principal contribution to $\underline{r}'$ integral, then, comes from small $\underline{S}$ and the following expansion should be rapidly convergent.

$$\int d\underline{S} \frac{e^{i\underline{S}.\underline{r}'}}{S^2 + 2\underline{S}.\underline{k}_n - i\epsilon}$$

$$= \int d\underline{S} \frac{1}{2\underline{S}.\underline{k}_n - i\epsilon} \left(1 + \frac{\nabla^2_{r'}}{2\underline{S}.\underline{k}_n - i\epsilon} + \ldots \right) e^{i\underline{S}.\underline{r}'} \qquad (3.31)$$

In the eikonal and Glauber theories a similar expansion is employed and only the first term is retained. Here, the first two terms are retained and the $\underline{S}$ integral is evaluated following the standard integration techniques. The result is,

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

$$X \; (\delta(\underline{b}') \; H(z') + \frac{i}{2k_n} \; \nabla^2_{r'}, \; \delta(\underline{b}') \; z' \; H(z')) \qquad (3.32)$$

where $|\underline{k}_i| = k_i$. In arriving at eqn. (3.32) use has been made of the result

$$\int d\underline{S} \; \frac{e^{i\underline{S}.\underline{r}'}}{2\underline{S}.\underline{k}_n - i\varepsilon} = \frac{i}{2k_n} \; \delta(\underline{b}') \; H(z') \qquad (333)$$

with the assumption, that,

$$\underline{k}_n \doteq \underline{k}_i \qquad (3.34)$$

In eqn. (3.33), $\delta(b')$ is for the Dirac delta function and the Heavyside function (or the step function) is defined by

$$H(x) = 1, \qquad x > 0$$

$$= 0, \qquad x < 0 \qquad (3.35)$$

Now choosing $\underline{k}_n$ as the polar axis, and using our basic assumptions, the following (approximate) result is obtained.

$$I_n \doteq \frac{i}{2k_i} \int_{-\infty}^{\infty} dz' \; e^{-i\beta_{in} z'}$$

$$H(z')(1 + \frac{iz'}{2k_i} \nabla_{z'}^2) \, V_{ni}^2 (\underline{r} - \underline{z}') \qquad (3.36)$$

where,

$$\beta_{in} = k_i - k_n = (W_n - W_o)/ k_i \qquad (3.37)$$

Let us recall that in the Glauber theory $k_i = k_n$. Thus the second Born direct amplitude in Yates' HHOB, is written as,

$$f_{HEA}^{(2)} = \frac{i}{2\pi k_i} \sum_n \int d\underline{r} \; e^{i\underline{q}.\underline{r}} \; V_{fn} (\underline{r})$$

$$X \int_{-\infty}^{\infty} dz' \, e^{i\beta_{in} z'} \, H(z')(1 + \frac{iz'}{2k_i} \nabla_z^2) V_{ni}(\underline{r}-\underline{z}') \qquad (3.38)$$

To carry out the sum over states here, we define the parameter β, through

$$\beta_{in} \triangleq \beta = \bar{W} / k_i \qquad (3.39)$$

This gives us the simplified second Born approximation of the present case. Further, to evaluate the second Born term of eqn. (3.38) the z-axis is chosen along $\underline{k}_i$ and $\underline{q}$ is made two dimensional, as in the Glauber formulation. Also observe that under z'-integral, the coordinates of the incident electron and the target electrons are coupled. To uncouple them, it is required to take the Fourier transform of the interaction potential, with respect to the incident electron variables $\underline{r}$ and $\underline{r}'$ by taking their Fourier variables as,

$$\underline{P} = \underline{p} + \underline{p}_z \qquad (3.40)$$

$$\underline{P}' = \underline{p}' + \underline{p}'_z \qquad (3.41)$$

Throughout our work, these variables have been used, for Fourier transformation. Here $\underline{p}$ and $\underline{p}'$ are both two dimensional, while p_z and p'_z lie along z-axis. After some mathematics, we are left with the present second Born term as follows,

$$f^{(2)}_{HEA} = i\ I_m\ f^{(2)}_{HEA} + Re\ f^{(2)}_{HEA} \qquad (3.42)$$

The imaginary part of the second Born amplitude of HHOB is given by,

$$Im\ f^{(2)}_{HEA} = \frac{4\pi^3}{k_i} \int d\underline{p}\ (1 + \frac{1}{2k_i} \frac{\partial}{\partial\beta} (p^2 + \beta^2))\ U^{(2)}_{fi} \qquad (3.43)$$

where,

$$U^{(2)}_{fi} = \langle f | \bar{V}\ (\underline{q} - \underline{p} - \underline{\beta}, \bar{x})\ \bar{V}(\underline{p} - \beta, \underline{x}) | i \rangle \qquad (3.44)$$

with $\bar{V}$ indicating the Fourier transform of the potential V, In such expressions $\underline{\beta}$ is the vector along z-axis and is obtained through $p_z = \beta$. The second term of the eqn. (3.43) comes from the 2nd term of the expansion in eqn. (3.32) and it is of order $1/k_i^2$. We have shown below how it is to be evaluated, but due to its higher order in k_i^{-1}, we will not consider it for calculating the DCS, and the term $Im\ f^{(2)}_{HEA}$ will now mean only the first term of eqn. (3.43). Now, we go back to eqn. (3.42), win which the real part of $f^{(2)}_{HEA}$ is, to be given by,

$$Ref^{(2)}_{HEA} = Re\ 1 + Re\ 2 \qquad (3.45)$$

with,

$$\text{Re } 1 = \frac{4\pi^2}{k_i} \mathcal{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{p_z - \beta} \; U_{fi}^{(2)} (\underline{q} - \underline{p} - \underline{p}_z , \underline{p} + \underline{p}_z) \qquad (3.46)$$

$$\text{Re } 2 = -\frac{2\pi^2}{k_i^2} \frac{\partial}{\partial\beta} \mathcal{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z \, (p^2 + p_z^2)}{p_z - \beta} \cdot U_{fi}^{(2)} (\underline{q} - \underline{p} - \underline{p}_z , \underline{p} + \underline{p}_z) \qquad (3.47)$$

where, the symbol $\mathcal{P}$ means the principal value. Again we note that the term Re 2 originates from the 2nd term of expansion in eqn. (3.32).

Finally, the direct scattering amplitude, consistent through $O(k_i^{-2})$ is written as

$$f_{HEA}^{d} = f_{B1} + i \, \text{Im} \, f_{HEA}^{(2)} + \text{Re} \, f_{HEA}^{(2)} + f_{G3} \qquad (3.48)$$

The theory discussed above is a blending of the Born and the Glauber theories. It differs from the direct amplitude of the EBS approach of Byron and Joachain (1975) eqn. (3.25) in that,

(i) Unlike the case of f_{B2} of the EBS, here the momentum transfer $\underline{q}$ is two dimensional. And the assumptions of the HHOB make the theory valid only for small angles of scattering.

(ii) Unlike the previous EBS case, here the final integrals (over the variable $\underline{p}$) are two dimensional making the evaluation easier.

The present theory differs from the Glauber approximation in the following points.

(i) We have mentioned earlier that, the integrals for the evaluation of f_{G2}, eqn. (3.16), are individually singular. For the HHOB, this problem does not arise. All the integrals occuring here are absolutely covergent (see the apprendix).

(ii) Because of the presence of the average excitation energy of the target through the parameter β, the imaginary part of the second Born term here, does not diverge for forward elastic scattering. In fact, if we put $\beta = 0$ all the present results go over to those of the Glauber theory. Further the real part of f_{B2} exists in the present case, unlike the Glauber approximation.

(iii) The terms arising out of the second term

of the Green's function expansion, eqn. (3.32) are similar to the Wallace-correction (1973) to the Glauber amplitude. Now we apply the present theory to the elastic e-H scattering. It can be further extended to any atom for which the wave function can be expressed as an antisymmetrized product of one electron orbitals.

3.6 Application of HHOB to e-H Elastic Scattering

3.6.1 Basic results

The evaluation of the direct amplitude for e-H elastic scattering in the present theory is discussed by Yates (1979) and can be carried out by using the intergals defined in the appendix. Presently, we evaluate the second term of eqn. (3.43) which is not discussed in that paper. We write it as,

$$\text{Im } 2 = \frac{2\pi^3}{k_i^2} \frac{\partial}{\partial\beta} \int d\underline{p} \; (p^2 + \beta^2) \; U_{fi}^{(2)} \; (\underline{q} = \underline{p} - \underline{\beta}, \; \underline{p} + \underline{\beta}) \qquad (3.49)$$

where, in the case of e-H scattering,

$$U_{fi}^{(2)} = \frac{1}{\pi^4 \; (p^2 + \beta^2)(|\underline{q} - \underline{p}|^2 + \beta^2)} \; (-\frac{\partial}{\partial\lambda}) \; (\frac{q^2 + 2\lambda^2}{\lambda^2(\lambda^2+q^2)} - \frac{1}{(|\underline{q}-\underline{p}|^2 + \underline{\beta}^2+\lambda^2} - \frac{1}{p^2 + \beta^2 + \lambda^2}) \qquad (3.50)$$

The product of the ground state wave functions is written as

$$\Psi^* \Psi = \frac{1}{\pi} \left(- \frac{\partial}{\partial \lambda} \right) \frac{e^{-\lambda r}}{r} \qquad \lambda = 2.$$

We note that the interchange of $|\underline{q} - \underline{p}|$ and $|\underline{p}|$ does not change the outcome.

Thus,

$$\text{Im } 2 = \frac{4}{\pi k_i^2} \left(\frac{-\partial^2}{\partial \beta \, \partial \lambda} \right) \int d\underline{p} \, (p^2 + \beta^2) \times \left(\frac{-q^2}{\lambda^2 + q^2} \times \frac{1}{(p^2+\beta^2)(|\underline{q}-\underline{p}|^2 + \beta^2)} + \frac{2}{\lambda^2} \times \frac{1}{(p^2 + \beta^2 + \lambda^2)(|\underline{q}-\underline{p}|^2 + \beta^2)} \right) \tag{3.51}$$

Let us evaluate this for forward elastic scattering, in which case the first term vanishes, and we get,

$$\text{Im } 2 \; (q = 0) = \frac{2\beta}{3k_i^2} \left(\frac{1}{4(\beta^2+4)} + \frac{1}{(\beta^2 + 4)^2} \right) \tag{3.52}$$

Since $= \bar{W}/k_i$, this term is actually $O(k_i^{-3})$. It is much smaller than the dominent first term of eqn. (3.43) in its contribution. Note that, as $\beta \longrightarrow 0$ Im 2 $\longrightarrow$ 0 i.e. there is no such term in Im f_{G2}.

Again we remark that the imaginary part of the second Wallace-amplitude is the same as Im f_{G2} . Now for the purpose of obtaining the DCS through $O(k_i^{-2})$, we require the imaginary part of the second Born term through $O(k_i^{-1})$ and the real part through $O(k_i^{-2})$. The expressions of these terms in the case of elastic e-H scattering are given below.

$$\text{Im } f^{(2)}_{HEA} = \frac{-4}{\pi k_i} \left(\frac{\partial}{\partial \lambda}\right) \frac{1}{\lambda^2} \left(2I_1(\beta^2, \lambda^2) - \frac{q^2}{\lambda^2 + q^2} I_1(\beta^2, 0)\right) \tag{3.53}$$

$$\text{Re } 1 = \frac{4}{\pi^2 k_i} \frac{\partial}{\partial \lambda} \int d\beta \frac{1}{\lambda^2} \left[2I_2(\beta, \lambda^2) - \frac{q^2}{\lambda^2 + q^2} I_2(\beta, \lambda^2)\right] \tag{3.54}$$

$$\text{Re } 2 = \frac{2}{\pi^2 k_i^2} \frac{\partial^2}{\partial \lambda \partial \beta} \left(\frac{I_3(\beta, 0)}{\lambda^2 + q^2} + \frac{1}{\lambda^2} I_3(\beta, \lambda^2) - I_2(\beta, \lambda^2)\right) \tag{3.55}$$

where, I_j's are defined in the appendix. Now, we consider the properties of the HHOB in the case of the forward elastic e-H scattering.

3.6.2 Forward Elastic e-H Scattering

Given below are the expressions of the various terms of the HHOB for the elastic scattering of electrons from Hydrogen atoms in the forward direction. At $q = 0$, the imaginary part of the present second Born amplitude, through $O(k_i^{-1})$ obtained from eqn. (3.53) is

$$\text{Im } f^{(2)}_{HEA} \ (q = 0) = \frac{2}{k_i} (\ln k_i + \ln 4 - \frac{1}{4}) \quad (3.56)$$

which agrees with imaginary part of the simplified second Born approximation f_{sB2} of Byron and Joachain (1973) and has a dependence of $(\ln k_i)/k_i$ on the incident energy. The last equation is derived by substituting the definition, $\beta = \bar{W}/k_i$ and $\bar{W} = 0.5$ a.u. for the hydrogen atom. On the other hand, if $\bar{W}$ and hence β is taken as zero, the present second Born term shows the familiar $\ln q$ divergence of the second Glauber term at $q = 0$.

We also learn from the eqn. (3.56) that the total cross-sections (σ^{tot}) obtained from the present second Born term and from f_{sB2} will be identical.

Considering next the real part eqns. (3.54),

(3.55) we find that

$$\text{Re } f^{(2)}_{HEA} = \frac{\pi}{k_i} + \frac{3}{2k_i^2} - \frac{5\bar{W}}{4k_i^2}, \quad q = 0 \qquad (3.57)$$

Again it is observed that in the HHOB as well as in the EBS of Byron and Joachain (1973) the real parts of second Born amplitudes are identical at $q = 0$. This means that in the forward direction, the two-term Green's function expansion, eqn. (3.31) is so rapidly convergent as to be fairly accurate. Further, the contribution of Re 2 is quite small compared to Re 1 at $q = 0$, as can be seen from the eqn. (3.57). Also from eqn. (3.57) we find that, if the average excitation energy is reduced to zero, we have,

$$\text{Re } 2\ (\bar{W} = 0) = 3/2k_i^2 \qquad (3.58)$$

This is exactly the real part of the second term of the Wallace amplitude at $q = 0$, obtained recently by Byron et al (1982).

Lastly, an interesting comment is worth making. The EBS expression of the direct scattering amplitude, eqn. (3.25) or (3.48) is the leading part of an exact amplitude, in that, it is $O(k_i^{-2})$. The exact amplitude must contain all orders of perturbation. But,

it has been shown (Dewangan, 1980) that the higher odd order Glauber terms,

$$f_{G(2n+1)} = 0, \ (q = 0) \quad n = 1, 2, 3.. \qquad (3.59)$$

Also if the closure approximation or eqn. (3.23), is applied the higher odd order Born terms,

$$f_{B(2n+1)} = 0, \quad q = 0, \ n = 1, 2, 3.. \qquad (3.60)$$

In that case, for the forward elastic scattering, the amplitude of eqn. (3.48) is quite fairly accurate. It is therefore, of interest to compare the elastic e-H results at $q = 0$, obtained in the HHOB, with a few other theoretical calculations. It is clear that the σ^{tot} results obtained from the optical-theorem using the HHOB or the EBS with simplified second Born amplitude are identical.

In table 3.1, comparisons of the total cross-sections are made with the following theories.

1. The Modified Glauber (MG) calculations of σ^{tot} (Jhanwar et al 1982a) are done by deriving analytical expressions for the forward elastic amplitudes in Glen's (1976) modified Glauber approximation, in which the amplitude is,

Table 3.1

Total cross-sections, σ^{tot} in a_o^2 units for e-H scattering

Energy eV	EBS or HHOB	MG (a)	UEBS (b)	DWSBA (c)
50	11.86	10.09	-	-
100	7.34	6.84	7.19	7.40
200	4.38	4.18	4.27	4.34
300	3.11	3.06	3.10	3.11
400	2.47	2.43	2.45	2.46

a, the MG results are given by Jhanwar et al (1982 a)

b, the UEBS results are given by Byron et al (1982)

c, the DWSBA results are given by Kingston and Walters (1980).

$$f^{MG} = f^{G} - f_{G2} + f_{B2} \qquad (3.61)$$

2. The uniterised eikonal Born series (UEBS) is obtained by Byron et al (1982) as a generalization of the potential scattering eikonal expansion given by Wallace (1973). In the following, the subscript 'W' denotes the corresponding Wallace amplitude, so that the UEBS scattering amplitude is,

$$f_{UEBS} = f_{W} - f_{W2} + f_{B2} \qquad (3.62)$$

3. The DWSBA results of Kingston and Walters (1980) are obtained in the formulation of distorted wave second Born approximation.

3.6.3 The differential cross-sections

We now obtain in DCS for elastic e-H scattering using the HHOB. To afford a better comparison, at intermediate energies, one must always consider the effect of the electron exchange. For the present purpose, it suffices to consider the first order exchange amplitude given in the Ochkur approximation (1963) which for the present case, gives the amplitude,

$$g = \frac{-32}{k_i^2} \frac{1}{(q^2 + 4)^2} \qquad (3.63)$$

The differential cross-section obtained by consideration of the Pauli-exclusion principle is given below.

$$\frac{d\sigma^{-}(\theta)}{dw} = \frac{1}{4} \left| f^{d}_{HEA} + g \right|^2 + \frac{3}{4} \left| f^{d}_{HEA} - g \right|^2 \quad (3.64)$$

Because we are not considering the direct amplitudes, beyond $O(k_i^{-2})$ in the HHOB, we only take into account here the first order exchange amplitude in the Ochkur approximation. Explicitly in our case, the DCS is,

$$\frac{d\sigma^{-}(\theta)}{dw} = (f_{B1})^2 + \left| \text{Im } f^{(2)}_{HEA} \right|^2 + (\text{Re } 1)^2$$

$$+ \frac{1}{4} (2 f_{B1} (\text{Re } 1 + \text{Re } 2 + f_{G3} + g))$$

$$+ \frac{3}{4} (2 f_{B1} (\text{Re } 1 + \text{Re } 2 + f_{G3} - g)) \quad (3.65)$$

The DCS is through $\varnothing\, O(k_i^{-4})$.

In the figs. 3.1 through 3.5 we present the DCS of HHOB theory at different scattering angles and different incident energies. In each graph, the number in theb bracket at the top-left is the present DCS at $q = 0$, e.g. at 100 eV, the forward DCS is 7.6 a_o^2 Sr^{-1}. Further, in the tables 3.2 and 3.3, the numerical values of the first Born term (f_{B1}), imaginary part of the

Table 3.2

e-H Elastic Scattering at 100 ev (HHOB)

θ_{deg}	f_{B1}	Im $f^{(2)}_{HEA}$	Re 1	Re 2	f_{G3}	DCS
5	0.9794	1.313	0.4155	0.1959	-0.0236	4.265
10	0.0220	0.9217	0.1397	0.1809	-0.0634	2.419
15	0.7442	0.4619	0.0181	0.1405	-0.1177	0.9640
30	0.5594	~~0.5594~~ 0.2836	~~0.2836~~ 0.0085	0.1090	-0.1221	0.4497
40	0.4132	0.2092	0.0108	0.0934	-0.1175	0.2361
50	0.3095	0.1723	0.0121	0.0880	-0.1053	0.1381
60	0.2381	0.1487	0.0119	0.0873	-0.0938	0.0896
80	0.1544	0.1188	0.0099	0.0896	-0.0768	0.0476
100	0.1117	0.1003	0.0081	0.0921	-0.0662	0.0313
1200	0.0885	0.0877	0.0068	0.0938	-0.0593	0.0235

Table 3.3

e-H Elastic Scattering at 200 ev (HHOB)

θ_{deg}	f_{B1}	Im $f^{(2)}_{HEA}$	Re 1	Re 2	f_{G3}	DCS
5	0.9595	0.8664	0.1141	0.0956	-0.0200	2.172
10	0.8543	0.4713	0.0164	0.0817	-0.0460	1.135
20	0.5863	0.2095	0.0018	0.0553	-0.0643	0.4175
30	0.3787	0.1377	0.0053	0.0452	-0.0560	0.1712
40	0.2513	0.1085	0.0059	0.0433	-0.0480	0.0801
50	0.1758	0.0898	0.0053	0.0443	-0.0410	0.0439
60	0.1298	0.0780	0.0044	0.0456	-0.0354	0.0276
80	0.0806	0.0587	0.0032	0.0474	-0.0283	0.0137
100	0.0573	0.0473	0.0024	0.0483	-0.0240	0.0086
120	0.0450	0.0399	0.0019	0.0489	-0.0212	0.0063

second Born term (Im $f^{(2)}_{HEA}$), the real part of the present present theory i.e. Re 1 and Re 2, the third Glauber term f_{G3} and the DCS are tabulated, at 100 eV and 200 eV for various angles. The DCS includes exchange. The real parts of the second Born term of HHOB and the EBS, both with f_{sB2}, at 200 eV are compared in table 3.5. The table 3.4 shows the present DCS compared with the first Born values, at 700 eV. An extensive comparison is made with recent calculations of other workers. The following are the theories with which we compare our results.

1. The EBS with the simplified second Born approximation, f_{sB2} (Byron and Joachain 1973) is quite akin to our present theory for nearly forward scattering, as discussed in the section (3.6.2). But the differences will be there in the prediction of large angle scattering.

2. In the EBS of Byron and Joachain (1977) a more accurate second Born amplitude is obtained by treating exactly the first term of the sum over states in eqn. (3.22) and employing closure to the rest of them. This procedure exactly treats the static potential of the atom and hence improves the large angle results. The second Born amplitude, thus obtained is denoted by $\bar{f}_{B2}$. The difference between f_{sB2} and f_{B2} decreases with energy.

3. The fixed scatterer approximation (FSA),

introduced by Ghosh (1977) and successfully applied to simple systems, assumes a fixed or static configuration of the target as it interacts with an incident particle. This theory thus neglects the excitation energies of the target, in the second Born term, but still, it differs from the Glauber theory in that, here $\underline{q}$ is not two dimensional and the three dimensional nature of the Born theory is preserved. However, in the FSA of Ghosh, the real part of the second Born term is absent, so also in the Glauber approximation, due to the absence of 'virtual excitations'. In a simplified FSA, the single and the double scattering terms only, are retained. Thus apart from constants, the double scattering direct amplitude in the FSA looks like,

$$f^D = \int\int d\underline{K}\ d\underline{r}_2\ \Psi^*(r_2)\ \Psi(r_2)$$

$$\frac{\langle \underline{k}_f \mid V \mid \underline{K} \rangle \langle \underline{K} \mid V \mid \underline{k}_i \rangle}{K^2 - k_i^2 - i\epsilon}$$

Let us mention the all important connection among the theories being discussed presently. In an exact 2nd Born approximation, the sum over infinite set of intermediate target states appears explicitly. In the simplified second Born approximation an average excitation energy $\bar{W}$ is defined and the sum rule is applied. In the FSA, the

intermediate excited states do not appear and $\bar{W} = 0$. Further, from the FSA, upon linearizing the Green's function, we arrive at the Glauber approximation. Alternatively, if we do not resort to FSA (i.e. keep $\bar{W} \neq 0$) and expand the Green's function, retaining the first two terms, we obtained the HHOB.

Tayal et al (1979) have considered the FSA for obtaining the modified Glauber (MG) amplitude, which we have mentioned previously in eqn. (3.61).

4. Again, the MG amplitude of eqn. (3.61) can be calculated using $\bar{f}_{sB2}$, or $\bar{f}_{B2}$ (see, Tayal et al 1979). In the caption of the figures, 3.1 through 3.5 a clear mention has been made regarding this.

5. The UEBS theory of Byron et al (1982) has also been mentioned previously through eqn. (3.62). Both the MG and the UEBS approaches can be considered to be superior to any of the present theories, in the sense that both are non-perturbative i.e. they take into account all orders of perturbation. The basic aim of the MG, in subtracting f_{G2} and adding f_{B2} has been to remove the divergence of the Glauber amplitude and to account for the absorption and polarization effect through f_{B2}. The UEBS approach goes a step further to take into account the Wallace correction to the Glauber amplitudes. The

Table 3.4

Elastic e-H scattering at 700 ev

Scattering angle (deg)	Present DCS	First Born DCS
0	2.8	1.0
5	0.87	0.76
10	0.40	0.38
20	0.079	0.074
30	0.022	0.019
40	0.0086	0.0066
60*	0.0025	0.0015

*At large angles the present DCS are overestimating.

subtraction of f_{w2} and addition of f_{B2} here follow the same reasoning as that given for the MG approximation.

6. At 700 eV and above, experimental data for e-H scattering are not available. We have, therefore, used the (inverted) independent atom model (see chapter 4) to estimate e-H DCS from the available e-H_2 data of Van Wingerden et al (1977).

3.7 Discussion of the e-H Results

We must now discuss the results exhibited here for the TCS as well as the DCS. Table 3.1 shows a comparative statement for the e-H TCS in various approaches, between 50 eV and 400 eV. One finds that the results of the EBS and the HHOB theories, both using f_{sB2} are somewhat higher than the results of MG or UEBS theories. This is because of the inclusion of the negative higher order terms, Im f_{G4} etc., in the MG amplitudes, and of similar Wallace amplitude terms in the UEBS. Hence within their frameworks, both MG and UEBS theories satisfy the optical theorem exactly. The difference between the TCS of the e EBS (or HHOB) and the above two theories decreases with energy, showing that the higher order terms, beyond $O(k_i^{-2})$, are unimportant above 400 eV. Let us note again that, the present (HHOB)

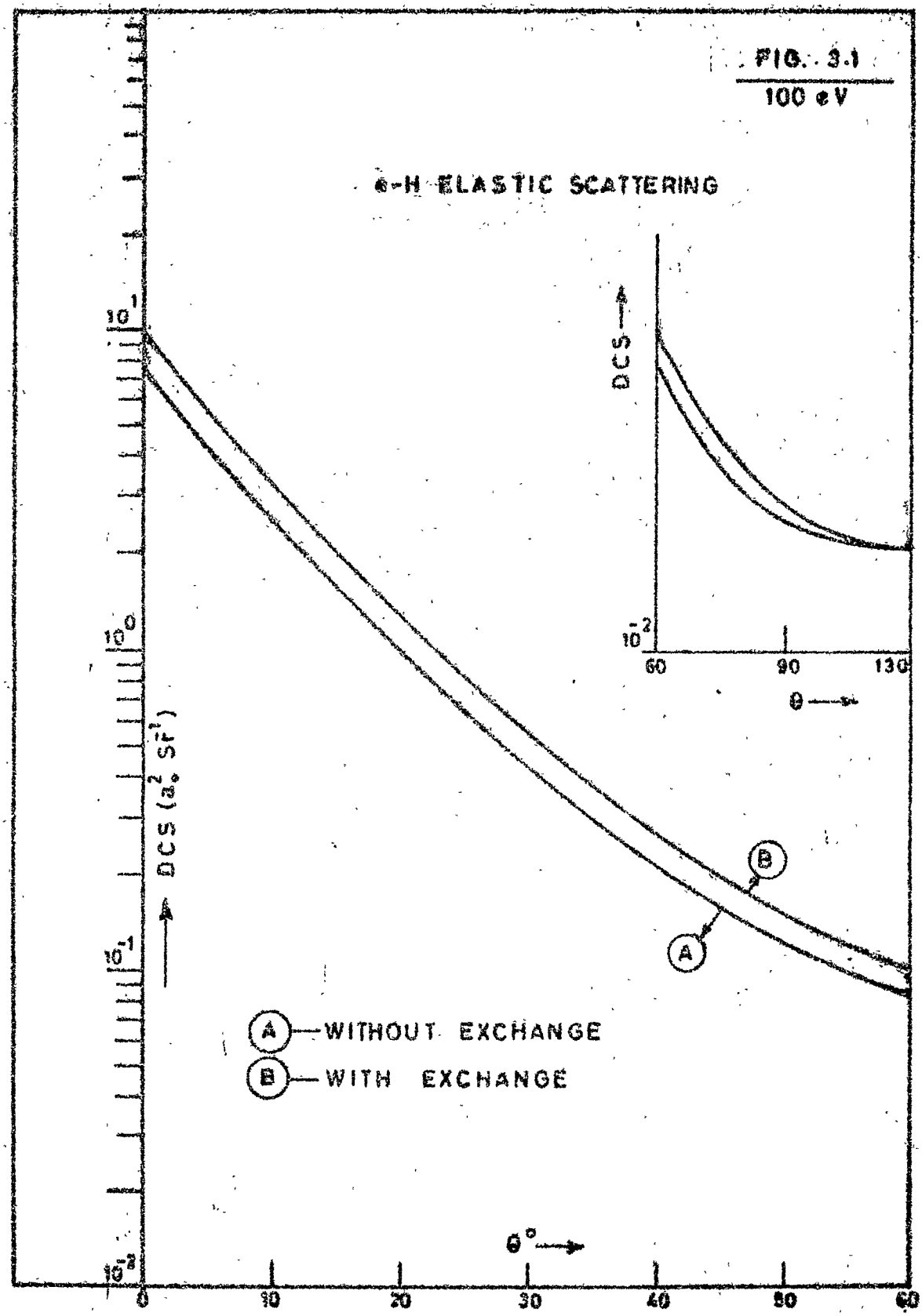
FIG. 3.1
100 eV
e-H ELASTIC SCATTERING
DCS
10^{-2}
60
90
130
θ
10^{1}
10^{0}
10^{-1}
10^{-2}
DCS (a_0^2, SR^{-1})
A
B
A—WITHOUT EXCHANGE
B—WITH EXCHANGE
θ°
0
10
20
30
40
50
60

theory also predicts a term $O(k_i^{-2})$ in the form of Im 2, eqn. (3.49), but its contribution is negligible. Further at high energies, the distortion of the incident electron is considerably small (see also chapter 5) so that the DWSBA results of Kingston and Walters (1980) are close to the other plane-wave results.

Now we discuss the graphical plots of the DCS exhibited in figs. 3.1 through 3.6. The main points emerging are a s follows.

1. Consider first the region of small and intermediate scattering-angles. The effect of exchange (fig. 3.1) is considerable at 100 eV. Further the DCS of the present work (fig. 3.2 curve A) agree with the results of the EBS with f_{sB2} at all energies in the angular range between 0^o and about 25^o, beyond which, the present results are higher than the EBS results (figs. 3.2, 3.3). Both these theories are in good agreement with the experimental measurements (Williums 1975), Van Wingerden et al 1977) in the intermediate angular range. The HHOB is occasionally closere to experimental points.

2. We have shown in this section previously that the TCS of the EBS and the HHOB, both with f_{sB2}, are identical showing that the absorption effects predicted by both these theories are of equal magnitude near $q = 0$.

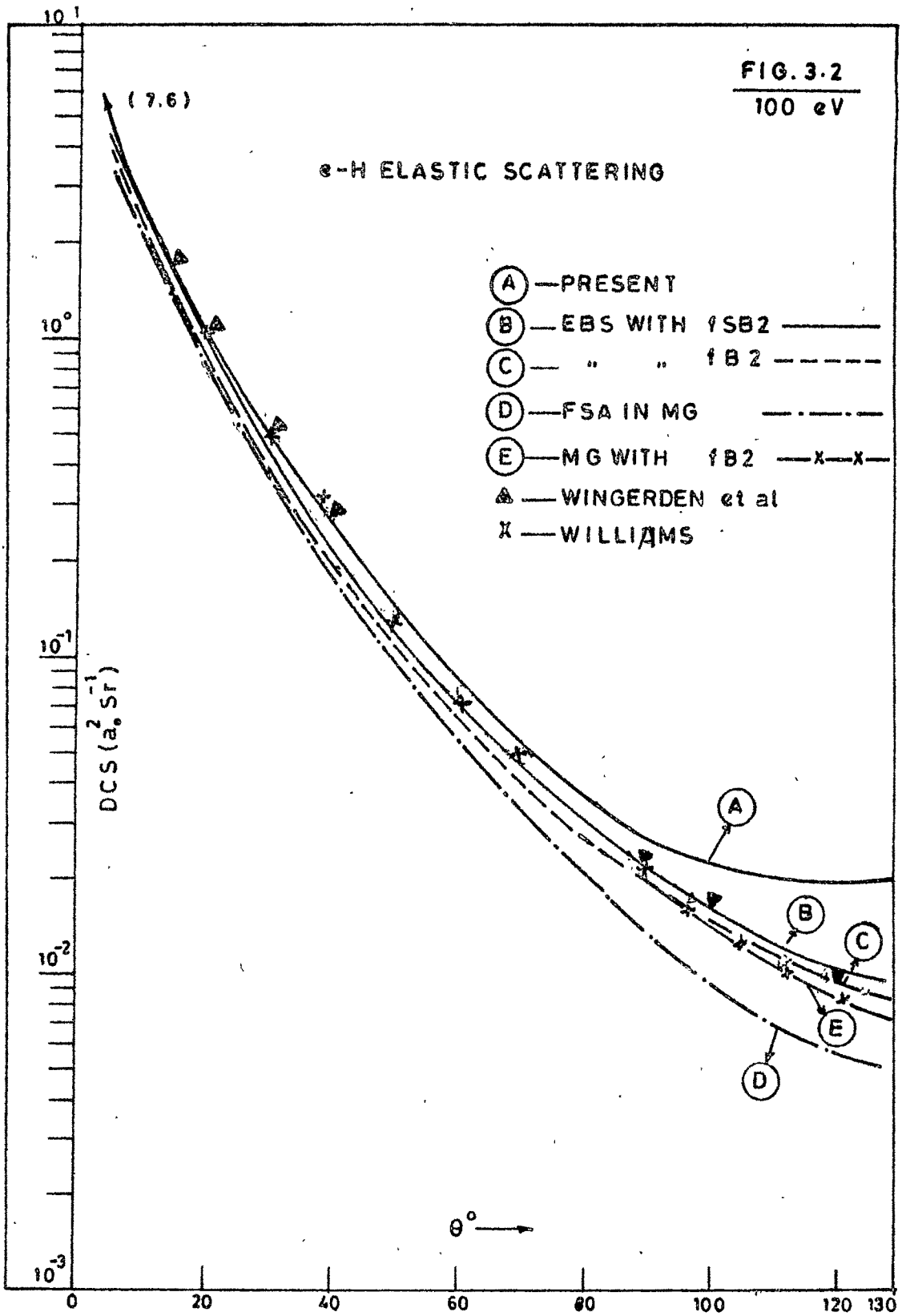
FIG. 3.2
100 eV
e-H ELASTIC SCATTERING
(7.6)
A —PRESENT
B —EBS WITH fSB2
C — " " fB2
D —FSA IN MG
E —MG WITH fB2
WINGERDEN et al
WILLIAMS
DCS (a₀² Sr⁻¹)
θ°
10¹
10⁰
10⁻¹
10⁻²
10⁻³
0
20
40
60
80
100
120
130

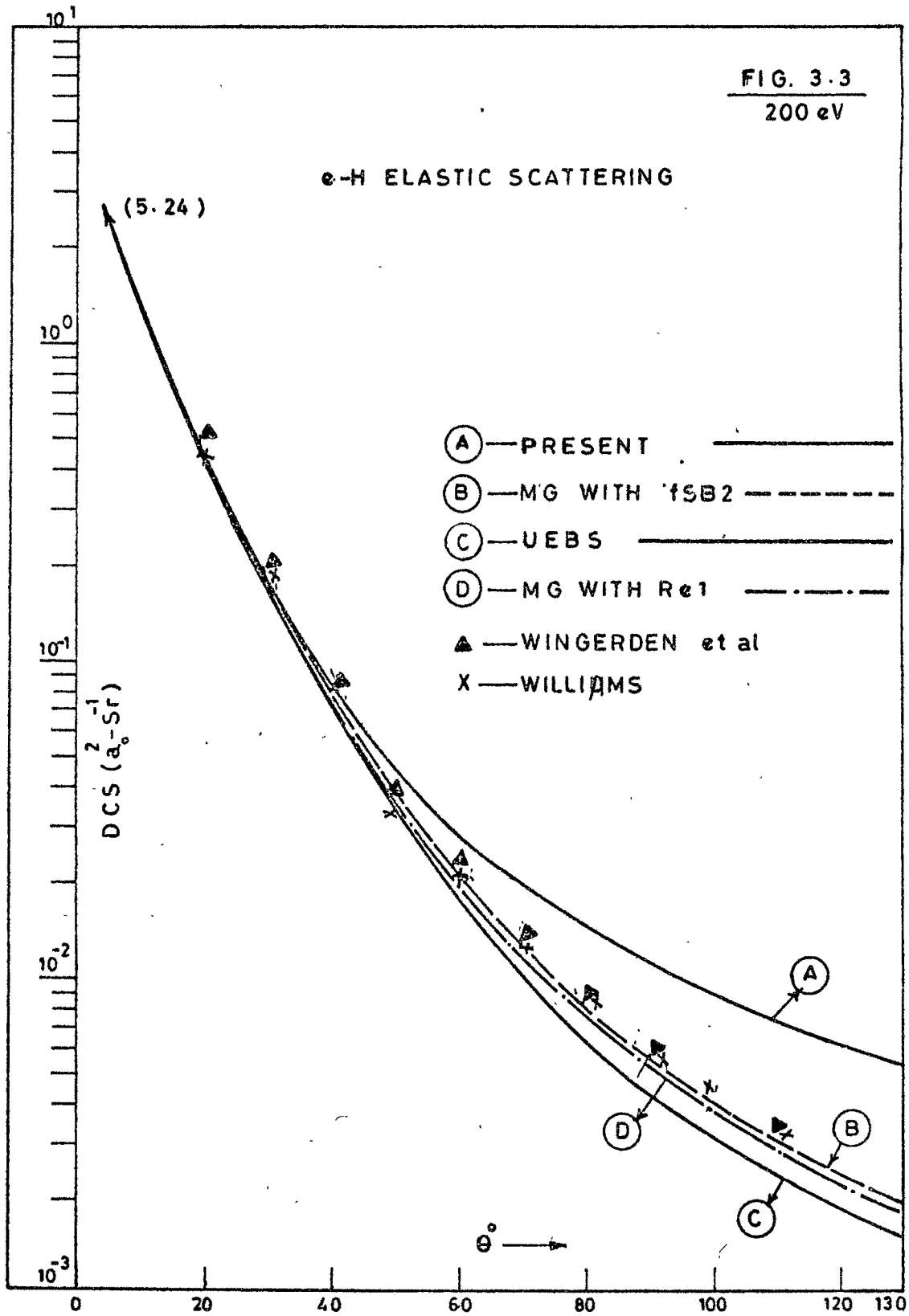
FIG. 3.3
200 eV
e-H ELASTIC SCATTERING
(5.24)
A —PRESENT
B —M'G WITH 'fSB2
C —UEBS
D —MG WITH Re1
▲ —WINGERDEN et al
X —WILLIAMS
DCS (a_o^2-Sr^{-1})
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
0
20
40
60
80
100
120
130
θ°

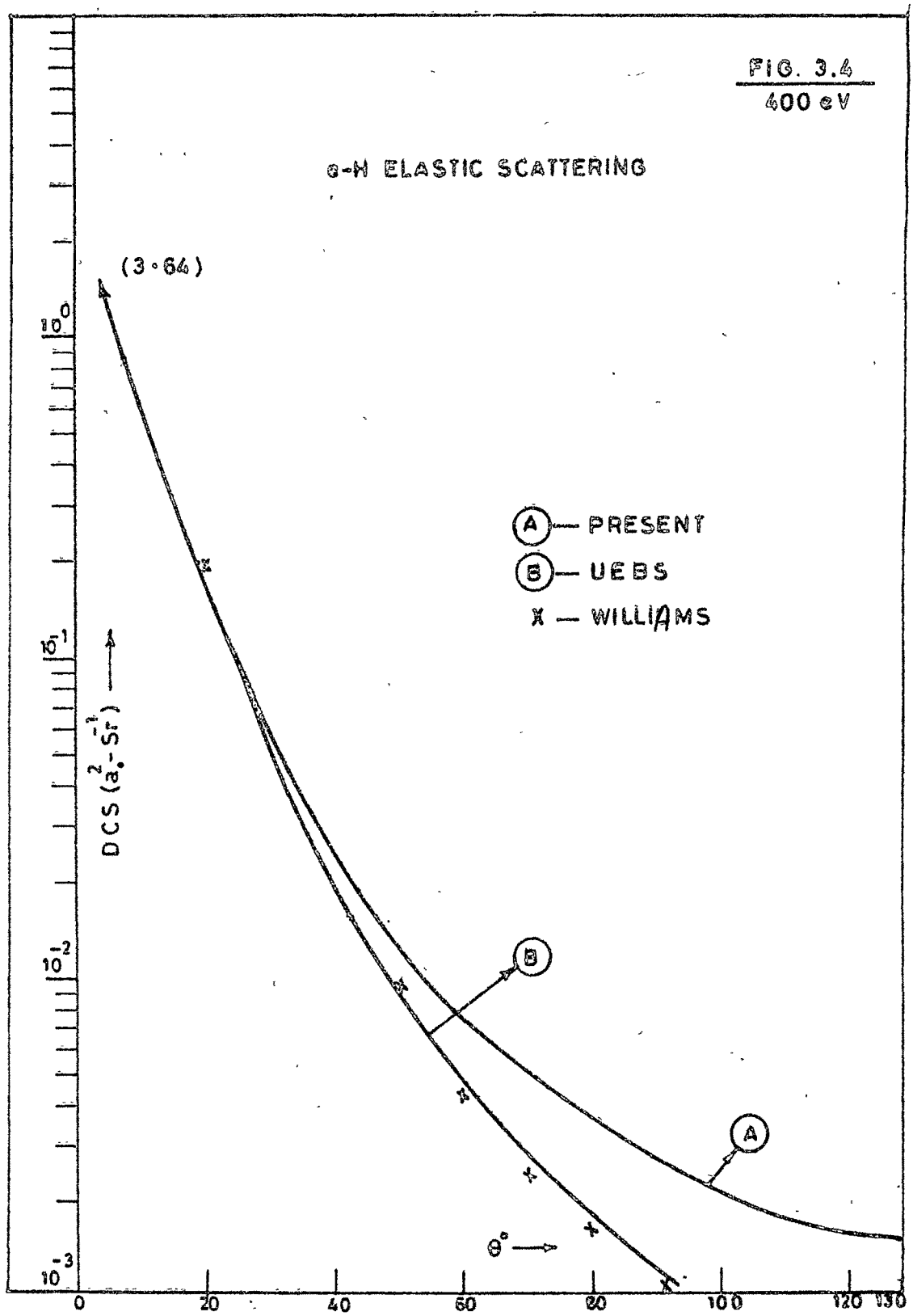
FIG. 3.4
400 eV
e-H ELASTIC SCATTERING
(3·64)
A — PRESENT
B — UEBS
X — WILLIAMS
DCS (a_0^2-Sr^{-1})
10^0
10^{-1}
10^{-2}
10^{-3}
θ°
0
20
40
60
80
100
120
130

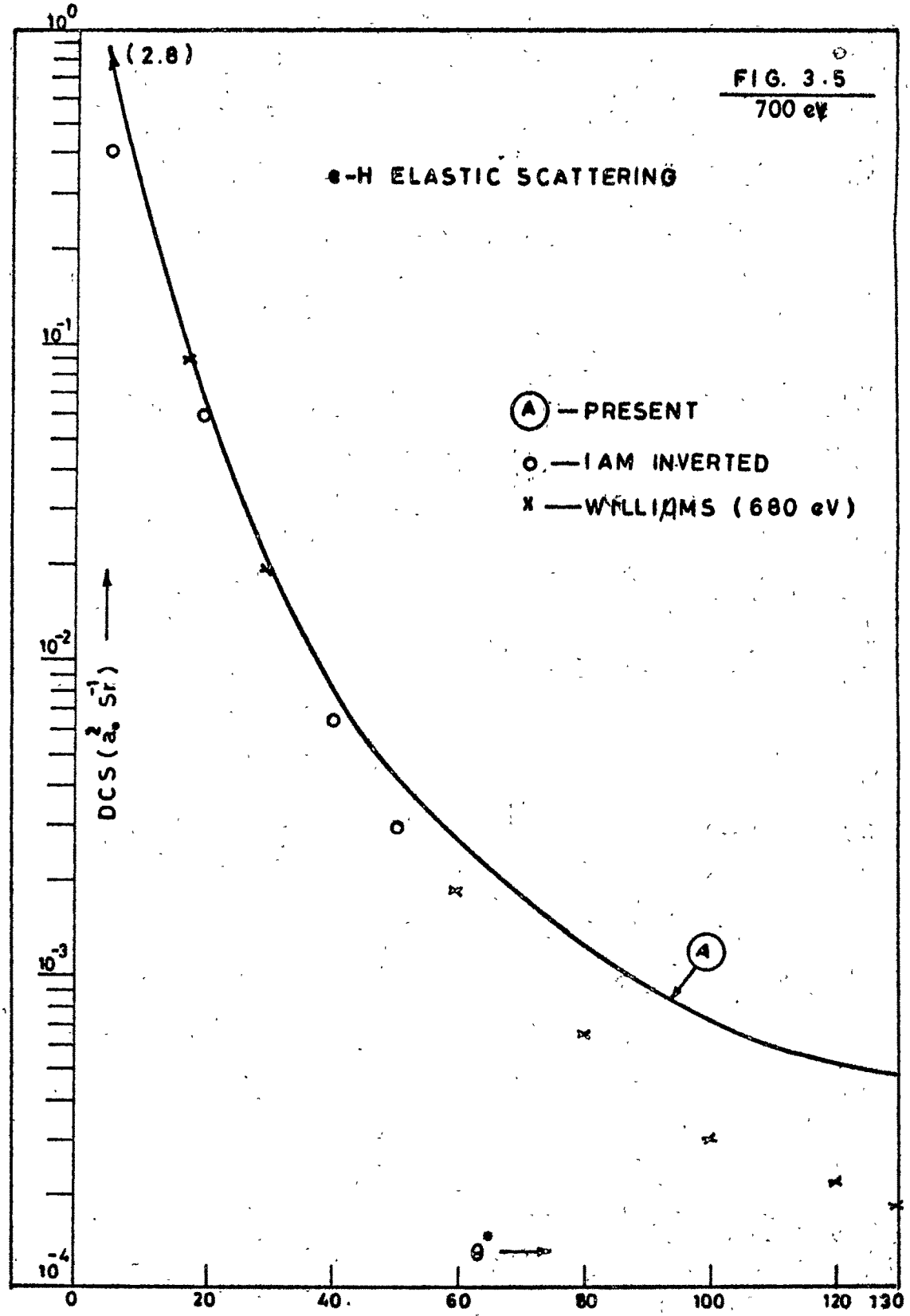
FIG. 3.5
700 eV
e-H ELASTIC SCATTERING
(2.8)
A — PRESENT
o — I AM INVERTED
x — WILLIAMS (680 eV)
DCS (a_0^2 Sr^{-1})
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
θ^*
0
20
40
60
80
100
120
130

Also the polarization effects in both of them, represented by the real parts of the second Born amplitude, are the same near q = 0. But the dependence of the real parts in these theories on q at large angles is different. The term $Ref^{(2)}_{HEA}$ varies rather slowly with 'q' at large angles.

3. The higher order approaches like the MG theory are found to be somewhat underestimating, between 100 eV and 400 eV (see also fig. 3.6). The reason lies in the negative higher order terms in them as already discussed.

4. It has been recognized that, near the forward direction the effects of polarization of the target, induced by the incident particle are dominent so that the contribution of the Re f_{B2} is quite large. The FSA, lacks in this regard, so that when the FSA is used in the framework of the MG approximation (Tayal et al 1979), it further underestimates the DCS towards the forward direction (fig. 3.2, curve D).

5. Below 60^{o}, the present DCS compare favourably with the experimental results of Van Wingerden et al (1977). However, these experimental results are not available above 200 eV, and the agreement with the measurements of Williums (1975) is not so close. In fig. 3.5 for 700 eV we have shown the available data of Williums (1975)

at 680 eV.

6. At all energies considered, the situation is quite different whenever $q > k_i$ ($\theta > 60^o$). The present DCS increasingly overestimate as q increases e.g. at 100 eV and $\theta = 100^o$, the present DCS is 35 % higher than the EBS result as well as the experimental value. This large-angle overestimation is common to all the systems that have been studied under the HHOB by us. Onthe other hand, the EBS with f_{sB2} or f_{B2}, is fairly accurate even at large angles. This suggests that the convergence of the Green's function expansion eqn. (3.31) is quite slow for large momentum transfers. However, it must be borne in mind in discussing this point that, the third order term we have used is the f_{G3}. For a more accurate amplitude $O(k_i^{-2})$, we must use the corresponding third Born term of Yates' (1979) theory. Still however, we are guided by the fact that the present approach is a high energy,small angle approximation. At $q = 0$, both f_{B3} and f_{G3} are zero and for small q, they would not differ very much from each other. This is the justification for writing the present direct scattering amplitude as in eqn. (3.48). Yates (1979) has suggested,

Table 3.5

Real parts of $f^{(2)}_{HEA}$ and f^{EBS}_{SB2} in a.u. for 200 ev

θ_{deg}	Re f_{SB2}	Re $f^{(2)}_{HEA}$
40	0.028	0.048
60	0.016	0.050
90	0.008	0.048
120	0.006	0.049

$$f^{d}_{HEA} = f_{B1} + i\ \mathrm{Im}\ f^{(2)}_{HEA} + \mathrm{Re}\ 1$$

$$+ \mathrm{Re}\ 2 + \mathrm{Re}\ f^{(3)}_{HEA} \qquad (3.66)$$

7. To look further into the large angle behaviour of the present DCS, we have compared in the table 3.5 , the real parts of the second Born amplitude of HHOB and the EBS at 200 eV, the expression of Re f_{sB2} of EBS is given below,

$$\mathrm{Re}\ f_{sB2} = 2\pi \frac{q^2 + 8}{(q^2 + 4)^2} \left(\frac{1}{k_i} - \frac{q}{(k_i^2 q^2 + 4\bar{W}^2)^{1/2}} \right)$$

$$+ \frac{4 + 6\bar{W}}{2k_i^2 (q^2 + 4)} + \frac{16}{k_i^2 (q^2 + 4)^2}$$

$$- \frac{128\ \bar{W}}{k_i^2 (q^2 + 4)^3} \qquad (3.67)$$

At once one sees from the table 3.5 that for $q > k_i$, these quantities in the HHOB are larger than corresponding EBS values and the difference widens with q. Thus, we conclude that the present large-angle overestimation results from Re $f^{(2)}_{HEA}$ and further, from tables 3.2 and 3.3, we find that the real culprit for this behaviour is the term Re 2. We recall here, that the term Re 2 originates

from the second term of the Green's function expansion, eqn. (3.31). With the parameter $\beta = 0$, it resembles the real part of the second order Wallace amplitude Re f_{W2}. It is worth mentioning here that the eikonal expansion of Wallace (1973) was proposed for small momentum transfers and its validity ø criterion has been discussed by Gerjuoy and Thomas (1974) (see also Glauber, 1959). In the derivation of the basic results of the HHOB, the assumption of small angle scattering is already made, following eqn. (3.30). Therefore, a good outcome is expected only for small angles. At this stage, we quote an observation made by Unnikrishnan and Prasad (1982), who have calculated $1S \longrightarrow 2S$ excitation cross-sections for e-H scattering in the second order eikonal approximation (i.e. with the Wallace-correction). These authors find that at large angles, their DCS values steadily increase with θ. Hence they have reported only upto $\theta = 30^{o}$.

8. In the preceding discussion, excluded is the fact that, our scattering amplitude is consistent only through $O(k_i^{-2})$. The picture would change if higher orders of perturbation are included in the scattering amplitude. This means that a modified Glauber amplitude (MG) with the present second Born term, should improve the present results.

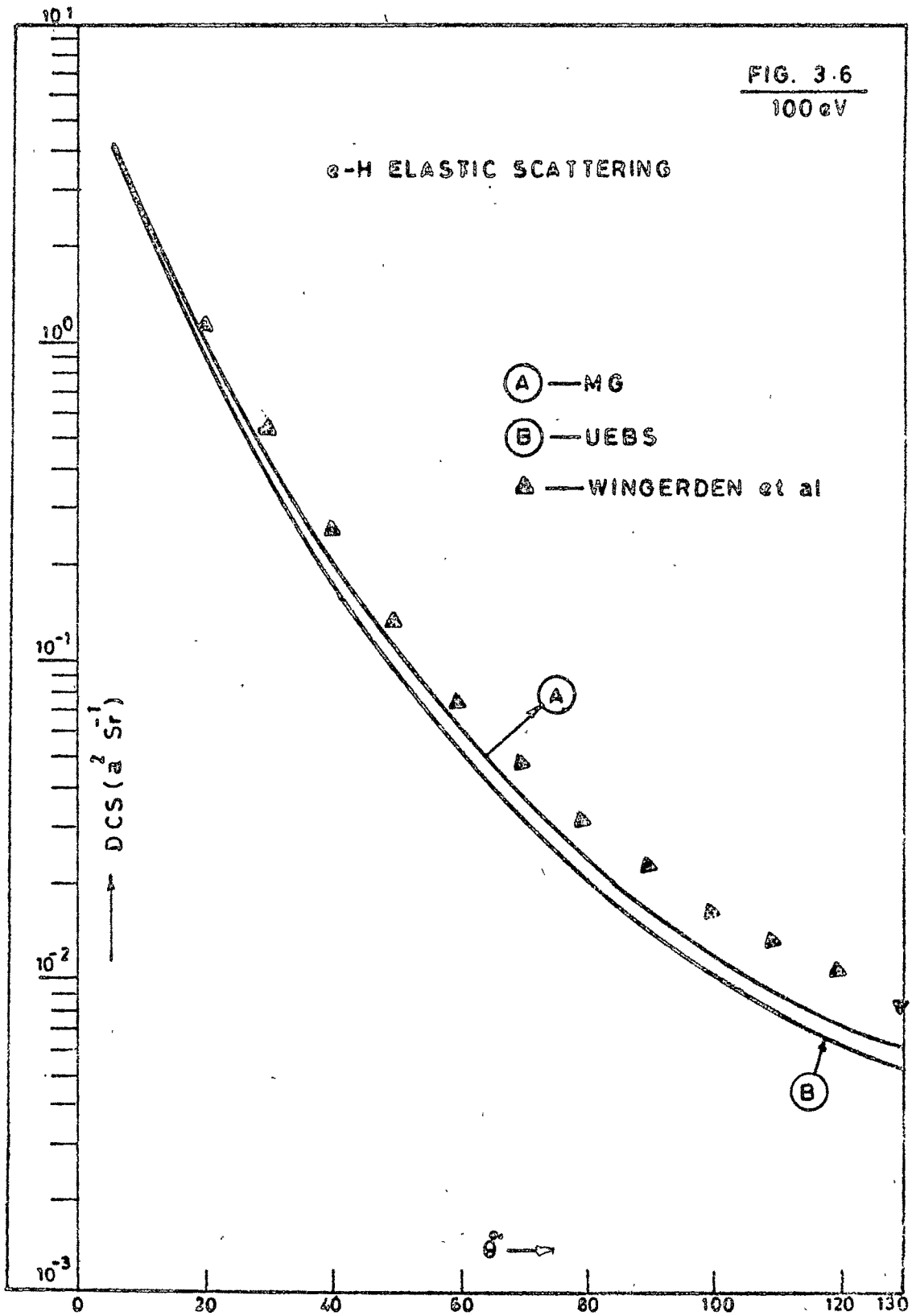
FIG. 3.6
100 eV
e-H ELASTIC SCATTERING
A —MG
B —UEBS
—WINGERDEN et al
DCS (a² Sr⁻¹)
θ°
10¹
10⁰
10⁻¹
10⁻²
10⁻³
0
20
40
60
80
100
120
130

9. In this dicsussion, it is interesting to compare the USBS theory of Byron et al (1982) with the MG theory of Glen (1977), as both these have explored the higher orders of perturbation. This comparison is made at 100 eV in fig. 3.6 . The difference between the MG and the UEBS results arises from the fact that, unlike the Glauber amplitudes f_{Gn} , the Wallace amplitudes f_{wn} $(n \geq 2)$ are complex and contain both real and imaginary parts. Both the approaches are underestimating the experimental results, more so at large angles. The effect of higher order terms dwindles at high energies. At 100 eV and 200 eV the MG and UEBS results are 20 % to 30 % lower than the experimental results. At present, there seems to be no effect which would improve upon the theoretical results, in order to bring an agreement with experiments. To sum up, we are led to conclude that the HHOB theory is accurate in its predictions at small and intermediate angles, i.e. for $q < k_i$, in the entire energy range considered. It appreciably deviates from other theories and experiments at $q > k_i$.

10. While it would be an ideal thing to have the scattering amplitude evaluated in the Born series for all orders, it is an impossible task. So, it is resorted to have higher order terms in the Glauber series and the

usefulness of the second Born term is exploited through the modified Glauber approximation. Now, the HHOB approach paves the way for the evaluation of the third Born term relatively easily. Hence in the MG amplitude f_{G3} may be replaced by Re $f^{(3)}_{HEA}$.

3.8 Modifications in the HHOB

3.8.1 A modified Glauber approach

The discussion of the preceding article naturally leads us to think of possible modifications in the HHOB theory of Yates (1979). At least in the case of electron hydrogen atom collisions, there have been quite a few recent attempts to obtain the scattering amplitude through all orders k_i^{-1} . This point has been often discussed in connection with eqns. (3.61) and (3.62). While we do not repeat the arguments preceding those equations, let us here propose the modified form of the Glauber amplitude, with the second Born term of the HHOB, instead of the f_{sB2}.

One can aski, what motivation do we have in replacing f_{sB2} of EBS in the well known MG approximation, eqn. (3.61), by the present second Born term $f^{(2)}_{HEA}$? On the contrary one can argue that f_{sB2} is found to be superior to $f^{(2)}_{HEA}$. All the same, in

writing eqn. (3.61), to remove the drawbacks of the second Glauber term, there has been an arbitrary digression from the basic framework of the Glauber theory and use has been made of an altogether different apparatus, viz that of the Born theory. Rosendorff (1980) has critisized this new Glauber amplitude with an addition of Re f_{B2}. The advantages of the MG formulation can still be retained within the Glauber theory by making one change, and that is to retain the average excitation energy $\bar{W}$ in the second term of the Glauber series. Thus, in our proposal, the first Born term remains in tact. Further, the Green's function is linearized and the second order amplitude is obtained by 'switching on' the average excitation energy and all higher order terms f_{Gn} are obtained as usual, by 'switching off' the average excitation energy. Now, from section (3.5), we know that whenever $\bar{W} \neq 0$, f_{G2} is taken over by Im $f^{(2)}_{HEA}$ and further the first term of the real part, i.e. Re 1, appears. According to this idea then, the proposed modified Glauber amplitude should be,

$$f_{MG1} = f_G - f_{G2} + i \text{ Im } f^{(2)}_{HEA} + \text{Re } 1 \, f^{(2)}_{HEA} \qquad (3.68)$$

or, $$f_{MG1} = (f_{B1} + \sum_{n \geq 3} f_{Gn}) + i \text{ Im } f^{(2)}_{HEA} + \text{Re } 1 \, f^{(2)}_{HEA}$$

Table 3.6

DCS (a_o^2 Sr^{-1}) for elastic e-H scattering at 200 ev, in the Modified Glauber approaches

Scattering angle θ	a (present)	b
40	0.0608	0.0708
60	0.0164	0.0187
90	0.0048	0.0053
120	0.0022	0.0024

a using eqn. (3.68) of the text.

b using eqn. (3.61) (Gien, 1977).

where, the last term is the same as Re 1 of eqn. (3.45). In a more or less the same spirit, we can propose, a new UEBS amplitude,

$$f'_{UEBS} = f_w - f_{w2} + i\ Im\ f^{(2)}_{HEA} + (Re\ 1 + Re\ 2) \qquad (3.69a)$$

The amplitudes of eqns. (3.68) and (3.69) have the advantages of their original expressions (3.61) and (3.62) respectively. Additionally, each term in any one of them is derived under the same basic formulation as already discussed. At sufficiently small angles, the results with these new amplitudes are not much different from those of the corresponding amplitudes with f_{sB2}.

Presently we have used Gien's (1977) results and eqn. (3.67) to estimate the DCS from the eqn. (3.68) and these modified results estimated in this way are shown for 200 eV in the table 3.6. The fig. 3.3 shows the graphical plot (caption, curve D). It is found that the DCS obtained by the proposed amplitude f_{MG1} of eqn. (3.68) are following closely below the MG results of Gien (1977).

The modification introduced by eqn. (3.69) is not expected to improve the large-angle overestimation of the HHOB. This is because of the large magnitudes of the

term $\not$ Re 2 at large angles. The results therefore, estimated from eqn. (3.69) are not shown. A careful examination of the behaviour of Re 2 is required. Even in the Wallace amplitude, we can think of the following variant,

$$f_{w1} = f_w - f_{w2} + (\text{Im } f^{(2)}_{HEA} + \text{Re } 1\, f^{(2)}_{HEA}) + \text{Re } f_{w2} \qquad (3.69b)$$

Thus, here too, we replace only the term Im fw2 by the term in the bracket.

Our aim in proposing the above modifications has been to have a single theory capable of serving at least three purposes as follows :

1. giving all order k_i^{-1} terms,
2. yielding a nonsingular imaginary part of the second term, and
3. producing a real part in the second term corresponding to the induced polarization of the target.

Recently, a serious attempt in this direction has been made by Rosendorff (1981). He has evaluated the real part of the propagator of the second-order amplitude in the eikonal approximation by an angular momentum expansion. The new amplitude satisfies the unitarity

theorem to all orders of the coupling constant, and is free from all the shortcomings of the Glauber theory. A very attractive feature of this work is that, non-zero excitation energy is retained in all orders expect the first. This must be a most superior theory of the day.

3.8.2 Corrections to the second term of the HHOB

It follows from the above discussions that the more important task here is to improve upon the 2nd Born term of the HHOB theory. Let us recall that the 2nd term of the HHOB amplitude is derived along the lines of the Glauber theory. An important correction to the usual Glauber approximation is the second order phase correction (Wallace, 1973) in which the straight line trajectory of the incident particle is modified and systematic corrections to the T-matrix of eikonal formulation are introduced. In HHOB, Yates (1979) has followed the Glauber formulation and has allowed $\underline{k}_n \neq \underline{k}_i$, eqn. (3.34), assuming a small angle scattering. Chandraprabha et al (1982) have considered the Wallace-type correction in HHOB by taking,

$$\underline{k}_n = 1/2\ (\underline{k}_i + \underline{k}_f) \qquad (3.70)$$

which offers a better approximation to the particle

trajectory. For the moment, let us call the following, our Green's function keeping the other symbols of eqn. (3.31)

$$G = \frac{1}{S^2 + 2\underline{S} \cdot \underline{k}_n - i\epsilon} \tag{3.71}$$

Then the correction of eqn. (3.70) leads to,

$$G = \frac{1 + y}{2\underline{S} \cdot \underline{k}_n - i\epsilon} - \frac{S^2}{(2\underline{S} \cdot \underline{k}_n - i\epsilon)^2} \tag{3.72}$$

where, $y = 1 - \cos(\theta/2)$. (3.73)

Now further, the HHOB analysis can be made with eqn. (3.72), exactly as done previously, to calculate the scattering amplitudes. The term of the amplitudes of order k_i^{-1} are modified as follows

$$w \ \mathrm{Im} \ f_{HEA}^{(2)} = (1 + y) \ \mathrm{Im} \ f_{HEA}^{(2)} \tag{3.74}$$

And,

$$w \ \mathrm{Re} \ 1 \ f_{HEA}^{(2)} = (1 + y) \ \mathrm{Re} \ f_{HEA}^{(2)} \tag{3.75}$$

And the terms of $O(k_i^{-2})$ are unaltered by the said correction. Notably, the trajectory correction is zero

at $\theta = 0$ and quite small at small angles. At 100 eV, this correction is shown for the DCS of HHOB between 10^{o} and 30^{o} in fig. 3.8 .

Now as already mentioned, the term Re 2 is not well behaved at large momentum transfers. Also, at large q, the scattering of electrons is governed by the static potential of the atom, i.e. the terms with $\bar{W} = 0$ are important. Further, Byron et al have recently shown (1982) that in the limit of $\bar{W} = 0$, the term $O(k_i^{-2})$ in Re f_{SBA} goes over to Re f_{W2}. Considering all this, it is not a bad approximation to write,

$$\text{Re } 2 \doteq \text{Re } f_{W2} \qquad (3.76)$$

at large momentum transfers. In other words, it simply means that the original expression (3.55), is valid for small momentum transfers and it should not be stretched to large momentum transfers. Inclusion of eqn. (3.76) can definitely improve our present results. That this is so, can be readily seen from fig. 3.7 plotted for 100 eV with the usual HHOB and the one with the replacement of Re 2 by Re f_{W2} for $q > k_i$. The eqn. (3.76) brings down the overestimation of our previous calculations. Now, what is the significance of this change ? It means that only in the first term of the linearized propagator,

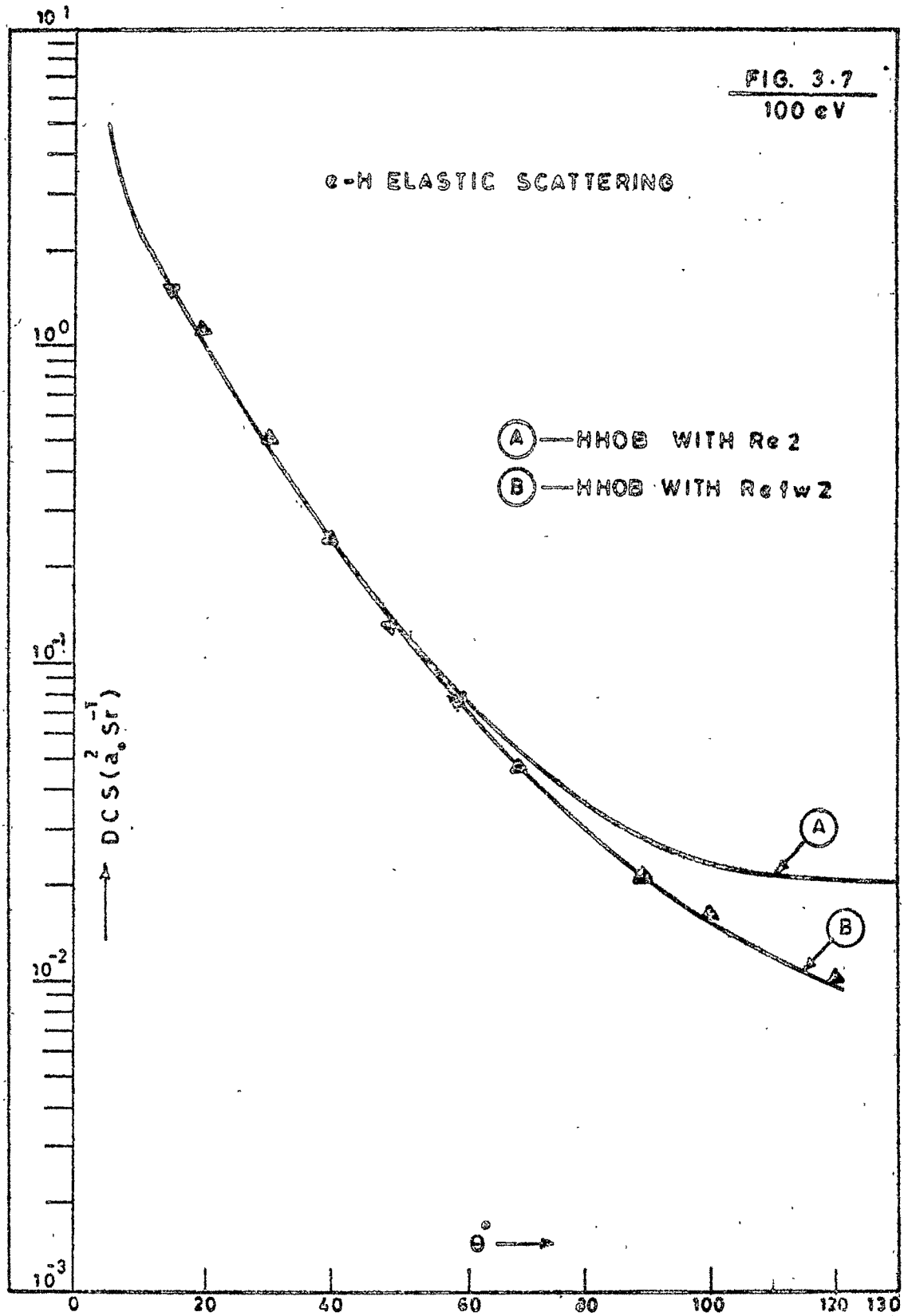
FIG. 3.7
100 eV
e-H ELASTIC SCATTERING
A—HHOB WITH Re 2
B—HHOB WITH Re1w2
DCS(a₀² Sr⁻¹)
θ°
10¹
10⁰
10⁻¹
10⁻²
10⁻³
0
20
40
60
80
100
120
130
A
B

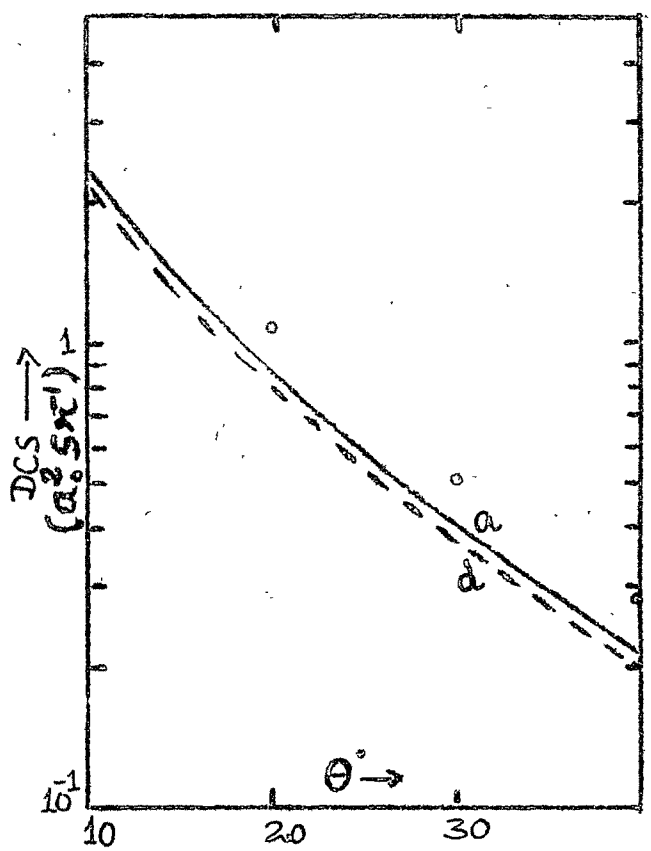

FIG. 3.8

a) HHOB with TC

d) HHOB without TC

eqn. (3.31), we retain $\bar{W} \neq 0$, to avoid the shortcomings of the second order Glauber term. The argument of eqn. (3.76) can also be extended to our previous modification given through eqn. (3.69), but at least presently, it is not attempted.

3.8.3 The third Born term

We now turn briefly to the third Born term of the HHOB (Yates, 1979) which is one of the few serious attempts ever made to evaluate f_{B3}. In the HHOB, we begin with the expression,

$$f_{if}^{(3)} = -\frac{2}{\pi} \sum_{n,n'} \int d\underline{r}\, e^{i\underline{q}\cdot\underline{r}}\, V_{fn}(\underline{r}) \int d\underline{r}'\, e^{i\underline{k}_i\cdot\underline{r}'}\, G_n(\underline{r}')\, V_{nn'}(\underline{r}-\underline{r}') \int dr''\, e^{i\underline{k}_i\cdot\underline{r}''}\, G_{n'}(\underline{r}'')\, V_{n''i}(\underline{r}-\underline{r}'-\underline{r}'') \qquad (3.77)$$

where, two intermediate-state labels n and n' and two dummy variables $\underline{r}'$ and $\underline{r}''$ appear. Here again, to develop $f_{HEA}^{(3)}$, we define the integral, 'I_n' through equation (3.30) and use presently,

$$I_n \doteq \frac{i}{2k_i} \int_{-\infty}^{\infty} dz' \, e^{-i\beta_{in} z'} \, H(z') \, V_{ni} \, (\underline{r}-\underline{z}') \qquad (3.78)$$

So that the third Born amplitude of the HHOB, has a shape,

$$f_{HEA}^{(3)} = \frac{1}{2\pi k_i^2} \int d\underline{p} \int_{-\infty}^{\infty} dp_z \int d\underline{p}' \int_{-\infty}^{\infty} dp_z'' \int d\underline{p}''$$

$$X \int_{-\infty}^{\infty} dp_z'' \; U_{fi}^{(3)} \, (\underline{X}, \underline{Y}, \underline{Z}) \; X \int d\underline{b} \; e^{i(\underline{q} - \underline{p} - \underline{p}' - \underline{p}'') \cdot \underline{b}}$$

$$X \int_{-\infty}^{\infty} dz \, e^{-i(p_z + p_z' + p_z'') z}$$

$$X \int_{-\infty}^{\infty} dz' \; e^{i(\beta - p_z' - p_z'') z'} \qquad H(z')$$

$$X \int_{-\infty}^{\infty} dz'' \; e^{i(\beta - p_z'')} \qquad H(z'') \qquad (3.79)$$

This result makes use of the average energy parameter,

$$\beta_{in} \doteq \beta_{in'} \doteq \bar{W} / k_i \qquad (3.80)$$

Also, as done previously, the Fourier representation of the

potentials is used and the following quantity is defined.

$$U_{fi}^{(3)} \quad (\underline{X}, \underline{Y}, \underline{Z}) = < f \mid \bar{V}(\underline{X})\ \bar{V}(\underline{Y})\ \bar{V}(\underline{Z}) \mid i > \qquad (3.81)$$

Further if we require the DCS through $O(k_i^{-2})$, we need only the real part of the third Born term, which in the HHOB analysis, splits up into two terms as,

$$\mathrm{Re}\ f_{HEA}^{(3)} = f_1^{(3)} + f_2^{(3)} \qquad (3.82)$$

Now, for the elastic scattering of electrons by hydrogen atoms the form of $U_{fi}^{(3)}$ is simple, so that the first term of (3.82) is expressed as,

$$f_1^{(3)} = \frac{2\pi}{k_i^2}\left(-\frac{\partial}{\partial\lambda}\right) \int d\underline{p} \int \frac{d\underline{p}'}{(p^2+\beta^2)(|\underline{q}-\underline{p}-\underline{p}'|^2+\beta^2)\ p'^2}$$

$$\times \left(-\frac{q^2}{\lambda^2(q^2+\lambda^2)} + \frac{2}{p^2+\beta^2+\lambda^2} - \frac{2}{|\underline{p}+\underline{p}'|^2+\beta^2+\lambda^2}\right.$$

$$\left. + \frac{1}{p'^2+\lambda^2} - \frac{1}{|\underline{q}-\underline{p}'|^2+\lambda^2}\right) \qquad (3.83)$$

To bring about the relation between the present treatment and the Glauber-eikonal series (GES) of Yates (1974) we

have to define $\underline{Z} = \underline{q}/\lambda$ and take $\beta = 0$. One would find then,

$$f_1^{(3)} \ (\beta = 0) \quad = f_{G3} \tag{3.84}$$

With the static potential, we have readily $\beta = 0$ and the term $f_{HEA}^{(3)}$ will reduce to the third term of the eikonal amplitude, f_{E3}. In the HHOB third Born amplitude, we get a term $f_1^{(3)}$ similar to the third Glauber term, and also another term, viz. $f_2^{(3)}$ is obtained. Again as expected, at $q = 0$,

$$\text{Re} \ f_{HEA}^{(3)} = f_1^{(3)} + f_2^{(3)} = 0, \ (q = 0) \tag{3.85}$$

The important result of Yates' theory is that in the real part of the third Born amplitude, apart from a Glauber-like term, there is a term viz., $f_2^{(3)}$, also $O(k_i^{-2})$.

The expression for the DCS $O(k_i^{-2})$ with the third Born term is already given in the eqn. (3.66). The evaluation of the terms $f_1^{(3)}$ and $f_2^{(3)}$ involves a general integral of the type,

$$I_K \ (\underline{Z}, n_1^2, n_2^2, n_3^2) = \int \frac{d\underline{p} \ (\ln \ (p^2 + n_3^2))^K}{(p^2 + n_1^2)(|\underline{Z} - \underline{p}|^2 + n_2^2)} \tag{3.86}$$

This integral is easier for $K = 0$. With $K = 1$ and the special cases $n_3 = 0$ as well as $n_1 = n_3$, the integral I_k has been evaluated by Singh and Tripathi (1980). For the third Born terms, quite general cases of I_k $(K = 1)$ are encountered and the evaluation has been far more difficult.

We have also tried to perform numerical integration of I_k $(K = 1)$ but without a reasonable success. The recent trends indicate that, rather than trying for higher Born terms, the attempts are directed towards more sophisticated 'eikonalized' theories.

3.9 Elastic Scattering from Other Atoms

3.9.1 General

The HHOB has been further applied to e-He scattering (Rao and Desai, 1981) and e-H(2s) scattering (Rao and Desai, 1983) and the behaviour, as discussed in the article 3.7 is observed. These calculations are open to corrections suggested in our previous analysis. In the case of atoms other than Hydrogen, an additional source of error comes from the use of approximate wave functions. Also, due to the complexity of wave functions and many target electrons involved in the case of higher atoms, it becomes difficult

to generalize a method used for e-H scattering. Still however, employing optical potentials and other methods, successes have been achieved in the study of elastic scattering of electrons from atoms like He, Ne, etc. Fortunately in some the cases, experimental data are also available (Jansen et al 1976, Williums and Crowe 1975).

For the alkali atom (Li, Na etc) targets, 'inert core approximation' consists in considering the target as composed of the last (active) electron and the inert core, so as to write the interaction with an incident electron as,

$$V(\underline{r}, \underline{x}) = V_1 + V_c \qquad (3.87)$$

With this, the calculations are easier.

3.9.2 Electron scattering from C, N and O atoms

The present knowledge about cross-sections for C, N and O - atoms is inadequate. We review here in brief the present state of affairs. First of all, one is faced with the problem of target wave functions which, even if accurate, are very difficult to handle. This can be overcome by the use of static potentials. Strand and Bonham (1964) expressed the static potential between a neutral atom of charge 'Z' and incident electron as (in a.u.).

$$V(\underline{r}) = -\frac{Z}{r}\,(Z_p\,(r)/Z) \qquad (3.88)$$

where, the quantity $Z_p\,(r)/Z$ was expressed as a superposition of Yukawa terms and derivatives of Yukawa terms. Later, Cox and Bonham (1967) expressed the potential completely in the superposition of Yukawa terms in the coordinate of the incident electron, as

$$V(\underline{r}) = -\frac{Z}{r}\sum_{i=1}^{n} \gamma_i \exp\,(-\lambda_i r) \qquad (3.89)$$

where the parameters γ_i, λ_i and n are tabulated (Cox and Bonham, 1967). These parameters successfully predict the bound-state properties of the atoms. Originally these parameters were employed in the very high energy scattering problems, but it is not clear upto what lower energy of the projectile they can be applied. With the static potential of eqn. (3.89), the first Born amplitude for the electron scattering by an atom of number 'Z', has a simple form,

$$f_{B1} = 2Z\sum_{i=1}^{n} \frac{\gamma_i}{(q^2+\lambda_i^2)} \qquad (3.90)$$

In an earlier work, Duncan et al (1972) used the eikonal approximation for Oxygen atoms at intermediate and high energies, Blaha and Davis (1975) have done distorted wa

wave calculations for that system. The static potential is only the first term of the optical potential, which must include in general the polarization, absorption and exchange terms, Recently, Kaushik et al (1982) have applied a model polarization potential having the form,

$$V_{dp}(r) = -\frac{1}{2}\left(\frac{\alpha_d\, r^2}{(r^2 + d^2)^3} + \frac{\alpha_q\, r^4}{(r^2 + d^2)^5}\right) \qquad (3.91)$$

with,

$$d = 0.375\, k_i / \bar{W} \qquad (3.92)$$

And α_d and α_q respectively are the atomic dipole and quadrupole polarizabilities. Kaushik et al (1982) have used the modified Born approximation to consider the projectile-distortion. It fails below about 500 ev and the results of partial wave analysis are remarkably different from those of other methods. Now we might have attempted the HHOB to say, electron Oxygen atom case. No computational difficulty would arise with the use of the static potential. But consider a part of eqn. (3.38) for elastic scattering i.e.

$$f^{(2)}_{HEA} = \frac{i}{2\pi k_i} \int d\underline{r}\; e^{i\underline{q}.\underline{r}} \sum_{n=o}^{\infty}$$

$$< 0 \mid V_{st} \mid n > \int_{-\infty}^{\infty} dz' \exp(-i\beta_{in} z')$$

$$H(z') < n \mid V_{st} \mid 0 > \qquad (3.93)$$

Clearly, because of the static potentials, only $n = 0$ remains and the excitation energy parameter vanishes, in eqn. (3.93). This will lead to the 2nd term of the eikonal approximation, Im f_{E2}.

However, the exact calculation of the second Born amplitude is possible using the Cox and Bonham potential of eqn. (3.89). To do this we define,

$$U(r) = 2\,V(r) \qquad (3.94)$$

And obtain the second Born amplitude,

$$f_{B2} = 2\pi^2 \int d\underline{K} < \underline{k}_f \mid U \mid \underline{K} >$$

$$\frac{1}{K^2 - k_i^2 - i\epsilon} < \underline{K} \mid U \mid \underline{k}_i > \qquad (3.95)$$

Substituting the eqn. (3.89) in eqn. (3.95) we find that the evaluation of the term f_{B2} requires the Dalitz integral,

$$I_{1,1}\ (\alpha,\ \beta,\ \underline{k}_i,\ \underline{k}_f) = \int d\underline{K}$$

$$X \quad \frac{1}{(K^2 - k_i^2 - i\epsilon)(\alpha^2 + |\underline{K} - \underline{k}_i|^2)(\beta^2 + |\underline{K} - \underline{k}_f|^2)} \qquad (3.96)$$

One finds that the second Born term consists of the real and imaginary parts as follows,

$$I_m\ f_{B2} = \sum_{i=j} \frac{4Z^2\ \gamma_i^2}{\lambda_i^2\ (\lambda_i^2 + 4k_i^2)}$$

$$+ \sum_{i \neq j} \frac{Z^2\ \gamma_i\ \gamma_j}{k_i(\lambda_i^2 - \lambda_j^2)}\ X\ \ln \frac{\lambda_i^2\ (\lambda_j^2 + 4k_i^2)}{\lambda_i^2\ (\lambda_i^2 + 4k_i^2)} \qquad (3.97)$$

And,

$$\text{Re } f_{B2} = \sum_{i=j} \frac{2Z^2 \gamma_i^2}{\lambda_i^2 (\lambda_i^2 + 4k_i^2)}$$

$$+ \sum_{i \neq j} \frac{Z^2 \gamma_i \gamma_j}{k_i (\lambda_i^2 - \lambda_j^2)} \left(\tan^{-1} \frac{2k_i}{\lambda_j} - \tan^{-1} \frac{2k_j}{\lambda_i}\right) \quad (3.98)$$

In the last two equations, $q = 0$.

The corresponding expressions using the Strand and Bonham (1964) potentials are a little more complicated. Physically, the second Born term accounts for the polarization and the absorption effects. But in the present case, we have considered the 'static' potential, which is 'flat' towards the forward direction, but as energy increases, it will be more and more accurate. Now, we use Im f_{B2} to calculate the total cross-section (TCS) via optical theorem. For C, N and O atoms experimental data are not available for σ^{tot}. So we planned to calculate this quantity employing the static potentials of Strand and Bonham (1964) (SB) as well as of Cox and Bonham (CB) (1967) and compare them. The quantities obtained in the present calculations are total elastic cross-sections (TECS).

The results with SB parameters are higher than those with CB parameters. We obtained the TECS

for e-Li scattering using the (CB) paramters, and compared with the results of Guha and Ghosh (1979), obtained in the FSA (see table 3.7). The agreement between the two is quite satisfactory and more so at high energies. Next, in the table 3.8 we have shown the TECS for the electron- Oxygen atom scattering, calculated with (CB) potentials. We include the results of Inokuti and McDowell (1974a) who have expressed the TECS in the form,

$$\sigma_{el}(k_i^2) = (ak_i^{-2} + bk_i^{-4} + ck_i^{-6}) \qquad (3.99)$$

These authors have tabulated the parameters a, b and c for various atomic targets. The results of eqn. (3.99) are also included in the table 3.8 and a very good agreement is found especially above 100 ev. The CB potentials give a more reliable value of the quantity than that given by SB-potentials at all energies (table 3.8). Towards lower energies, the actual cross-section might be reduced because of the projectile distortion etc. Finally, in the table 3.9, we have compared the TCS of electron scattering from C, N and O atoms, employing c CB potentials.

However, in the present calculations, there is no difference between the TCS and the TECS

Table 3.7

Total Elastic Cross-Sections (πa_o^2) for e-Li scattering

Energy ev	Present (a)	Ghosh (1979) (b)
100	3.11	3.32
150	-	2.16
200	1.59	1.60
300	1.07	-
400	0.80	-
500	0.65	-
600	0.54	-
700	0.46	-
800	0.41	-
900	0.36	-
1000	0.32	-

(a) Using the Cox-Bonham potentials.

(b) Using the FSA (Ghosh, 1979).

Table 3.8

Total Elastic Cross-Sections (a_o^2) for Electron-Oxygen atom scattering

Energy (ev)	Present (a)	(b)	Inokuti and McDowell
100	22.2	30	22.00
200	11.7	20	-
300	7.97	17	-
400	6.04	--	6.00
500	4.86	13	-
600	4.06	--	-
700	3.49	--	3.5
800	3.06	--	-
900	2.73	--	-
1000	2.46	--	2.5

(a) Using Cox-Bonham potentials

(b) Using Strand-Bonham potentials.

Table 3.9

Total Elastic Cross-Sections (a_o^2) for C, N and O atoms

Energy (ev)	Carbon	Nitrogen	Oxygen
100	20.0	21.0	22.2
200	10.5	11.1	11.7
300	7.1	7.5	7.97
400	5.38	5.67	6.04
500	4.32	4.56	4.86
600	3.61	3.81	4.06
700	3.10	3.27	3.49
800	2.72	2.87	3.06
900	2.42	2.55	2.73
1000	2.18	2.30	2.46

Actually to get σ^{tot}, we must obtain σ_{inel} and it must be added to our cross-sections. Inokuti (1974b) has obtained total el inelastic cross-sections for all atoms from He to Ne.

Now a good theoretical picture can be obtained by constructing an optical potential

$$V_{opt} = V_{st} + V_{pol} + iV_{abs} + V_{ex} \qquad (3.100)$$

where, V_{st} of eqn. (3.89) and V_{pol} of eqn. (3.91) can be employed. In eqn. (3.100) the terms are written in order of their difficulty value. In the case of complex atoms like Ne, Byron and Joachain (1977) have developed a second order potential, by making use of the Hartree-Fock a wave functions given by Clementi (1965). Lastly, an interesting calculations has been reported by Konaka (1982) in which a high energy limit of electron atom (or molecule) second Born term is obtained, without an explicit use of wave functions. This may prove to be quite useful for atoms beyond H, He and Li.

3.10 Chapter Summary, Further Prospects

The third chapter has mainly dealt with the elastic scattering of electrons by H-atoms in Yates' (1979) theory. The basic theory is outlined and calculations

of the DCS and the TCS are compared with theoretical and experimental data. The HHOB overcomes the shortcomings of the 2nd order Glauber amplitude in that, the imaginary part is finite at $\theta = 0$, and a real part of the second order amplitude exists. This has been made possible by considering a non-zero intermediate energy loss to the virtual target states in the second order amplitude. However, the evaluation of the third term of the HHOB has remained problematic and we have to be content with the corresponding Glauber term. The present DCS are satisfactory for small and intermediate angles, $(q < k_i)$, but are appreciably larger than experimental and other theoretical data for $q > k_i$. This is a major drawback of the HHOB. We have not tried this theory below 100 ev, since it is a high energy approximation.

The reasons for the large-angle discrepancy of the HHOB are discussed. The term $O(k_i^{-2})$ in the real part of its second order amplitude is responsible for the same. Modifications of this theory are studied. Now, in the energy range, 50 ev - 200 ev, the higher order terms in the amplitude are also important, hence an amplitude $O(k_i^{-2})$ is inadequate. The modified ~~Gauber~~ amplitude of Gien (1977) employs the full Glauber amplitude minus its second term, supplimented with the second Born term.

This procedure is not quite satisfactory. Presently we propose a better way of removing the well-known shortcomings of the Glauber amplitude. It consists in evaluating the second order term with linearized Green's function, by retaining an average excitations-energy and keeping the higher order Glauber terms unchanged. The DCS obtained in this way are not only better than the simple HHOB results, but they also compared favourably with recent works. The proposal just mentioned, can also be extended to the uniterized EBS amplitude of Byron et al (1982). As a by-product of the discussion, it becomes clear that, at least at 100 and 200 ev, more accurate theories tend to fall below the experimental data, especially at large angles.

The trajectory correction applied to the HHOB leads to only a marginal change. Further the close analogy between Re $2f^{(2)}_{HEA}$ and Re $f^{\&}_{W2}$ is used here to rectify the large angle overestimation by the HHOB.

Towards the end of the third chapter, we have turned our attention to the elastic scattering of electrons by C, N and O atoms. The TCS for these atoms are estimated in the ¢ CB and $ SB static potentials and comparisons are made. These are compared

with Inokuti (1974a). Also, we suggest improvements over the calculations available in literature, of the TCS of electron scattering from C, N and O atoms.

It will be appropriate to point out at further prospects of researches to which the chapter has been devoted. These are as follows :

1. Going through the chapter, one cannot miss the delicate issues related to the second order amplitude in the elastic electron-atom collisions. Let us point out here an aspect which has remained untouched. In the Glauber approximation as well as in the HHOB, the momentum transfer is assumed to be two dimensional. Gau and Macek (1974-75) have shown how the restriction $q_z = 0$ can be removed in the Glauber approximation. A similar treatment is required for the HHOB also. This may have its effects on the large angle scattering.

2. A simple HHOB treatment holds good for small and intermediate angles. In this chapter, we have shown a way to extend its reliability to large scattering angles also, even with DCS $O(k_i^{-2})$. This suggestion can definitely improve the results of Rao and Desai (1981, 1982), which are derived on the basis of a simple HHOB theory.

3. As mentioned, the present method of calculating the second Born (HHOB) amplitude can also be incorporated in the modified Glauber formulation. Also, the modified Glauber approximation needs the knowledge of the full Glauber amplitude, which itself is quite difficult in the case of higher atoms ($Z > 2$). In this context, the termwise expansion, (Yates, 1974) is still very much relevant, for complex cases.

It is found that the calculations with the following amplitude are reasonably good for elastic scattering from H(2S) and Li,

$$f = f_{B1} + i \text{ Im } f^{(2)}_{HEA} + \text{Re } 1\, f^{(2)}_{HEA} + \text{Re } f^{R}_{wa} + f_{G3} \qquad (3.101)$$

The results are not shown here.

4. While it would be an ideal thing to have the Born amplitude evaluated to all orders of k_i^{-1}, it is an impossible task. Hence, we resort to the Glauber series. Now, Rosendorff (1981) has evolved a Glauber formulation where the

excitation energy is retained in all orders beyond the first. More and more applications of this theory are expected.

5. The Methods like the HHOB, the EBS or the modified Glauber approximation do not yield good results below 100 ev, where there is a considerable variance with the experimental values at all angles. The reasons are that,

   i) the high energy approximation slowly becomes weaker in that region, and

   ii) the distortion of the projectile needs to be taken into account.

   It will be instructive if a distorted wave formalism is incorporated in the MG formulation, between 50 ev and 200 ev. Thus, we need a theory to account for the projectile as well as target distortion, absorption, exchange and also higher orders of perturbation.

6. The HHOB theory applied here to the electron scattering may be applied to any charged particle by hydrogen atoms, to surmount ~~charged particle by hydrogen atoms, to surmount~~ the shortcomings of the Glauber theory. Turning to higher atoms, there is a need for further

theoretical and experimental work. There is a scope of improving our present TECS results of C, N and O atoms, at least in two ways

(i) by supplimenting our results with the total inelastic cross section σ_{inel} of Inokuti (1974b) and

(ii) by carrying out the optical model calculations for these atoms.

Calculations for these atoms have not been made as yet using the wave functions. Konaka (1982) has discussed the second Born amplitude without the explicit use of the wave-functions of the target.