Chapter 5

Inelastic scattering of fast electrons by atoms and molecules

5.1 Introduction

We now turn to inelastic collisions of fast electrons by atoms and molecules. At the outset, we must clarify that though the term 'inelastic' collision means both excitation (or de-excitation in superelastic processes) as well as ionization of the target atom, we are concerned here with the electronic excitation of the target (atom), initially in the ground state. Additionally in the case of molecular targets the inelastic processes involve, in general, any one or more of rotational, vibrational ~~&~~ and electronic excitations and dissociation etc. Since we are dealing with fast electrons, the rotational and vibrational excitations are ingnored. Most of our study is centred around the atomic and molecular hydrogen.

The process of inelastic scattering involves both, transfer of energy and momentum. Another point of interest is the subsequent radiation emitted by the target as it returns (usually) to the ground state. For example, corresponding to 2p state excitation of the H-atom the prompt Lyman-α radiation is studied (Long et al 1968) and for the 2S state excitation, the

Lyman-α radiation induced by an applied electric field is observed (Kaupilla et al 1970); see also Williams, (1976). In exciting the $n = 2$ state of atomic hydrogen, electrons suffering 10.2 ev energy loss are scattered along with 10.2 ev photons. These processes are important in the energy-loss by particles in a medium. The theoretical treatment differs from that of elastic scattering, in terms of basic approximations, their successes and failures. This chapter naturally divides into the discussion on atomic and molecular targets : part A of this chapter deals with the atomic targets followed by part B, which deals with the molecular targets.

Part A

5.2 The First Born Approximation

Consider the hydrogen atom initially in the ground state $|i\rangle$ being excited to a final state $|f\rangle$ by an impinging fast electron. The first Born T-matrix is

$$T = (2\pi)^{-3} \int d\underline{r}\, e^{i\underline{q}.\underline{r}}\, A_f(\underline{r}) \qquad (5.1)$$

For the process leading to the final state 2S,

$$A_{2S}(r) = C_1\, e^{(-3/2)r} \left(r + \frac{2}{3}\right) \qquad (5.2)$$

with,

$$C_1 = \frac{2\sqrt{2}}{q} \tag{5.3}$$

Here, the use is made of the wave function of the 2S state of hydrogen atom,

$$\psi_{2S}(r_1) = \frac{1}{4\sqrt{2\pi}} (2 - r_1) e^{(-1/2)r_1} \tag{5.4}$$

The first Born amplitude for the transition 1S —— 2S due to electron impact, is,

$$f_{B1} (1S \text{ —— } 2S) = - \frac{8\sqrt{2}}{(q^2 + \frac{9}{4})^3} \tag{5.5}$$

Notably, the first Born inelastic amplitude, is negative, unlike that in the elastic case. The final momentum k_f(in a.u.) defined through,

$$\frac{1}{2} k_i^2 + W_o = \frac{1}{2} k_f^2 + W_n \tag{5.6}$$

gives the momentum transfer,

$$q = (k_i^2 + k_f^2 - 2k_i k_f \cos \theta)^{1/2} \tag{5.7}$$

The first Born amplitude, being proportional to q^{-6},

falls off much rapidly at large momentum transfers, compared to the first Born elastic scattering amplitude, eqn. (3.8). The first Born inelastic amplitude fails to describe the wide angle scattering even at high energies. The reason as can be seen from eqn. (5.1), is that the nucleus-electron interaction is ineffective in the present first Born approximation, because of the orthogonality of $|i\rangle$ and $|f\rangle$. This is an additional drawback of the first Born treatment in the present case, the other drawbacks being similar to those of elastic scattering discussed in the article no. (3.2). Clearly, the higher order amplitude must be dominating in the small as well as large angle inelastic scattering.

To calculate the first Born exchange amplitude for $1S \longrightarrow 2S$ transition, the required T-matrix is obtained in the potential V_p written below, after permuting the target and the incident electrons.

$$V_p = \frac{1}{|\underline{r} - \underline{r}_1|} - \frac{1}{r_1} \qquad (5.8)$$

Here, the first term, corresponding to the electron-electron interaction is more important, hence,

$$T_{B1}^{ex} = (2\pi)^{-3} \langle e^{-i\underline{k}_f \cdot \underline{r}_1} \psi_f(r) \left| \frac{1}{|\underline{r} - \underline{r}_1|} \right| e^{i\underline{k}_i \cdot \underline{r}} \psi_i(r_1) \rangle \qquad (5.9)$$

The general result for excitation from the ground state to any excited state 'n',

$$T_{n,o}^{och} = \frac{q^2}{k_i^2} T_{n,o}^{d} \text{ (Born)} \quad n \neq 0 \qquad (5.10)$$

where the corresponding direct matrix element of the first Born approximation is represented by $T_{n,0}^{d}$ (Born). The eqn. (5.10) is obtained in the Ochkur (1963) approximation. The exchange amplitude of 1S $\longrightarrow$ 2S transition is written below

$$g_{Born}^{och} (1S \longrightarrow 2S) = -\frac{8\sqrt{2}}{k_i^2} \frac{q^2}{(q^2 + \frac{9}{4})^3} \qquad (5.11)$$

Unlike elastic scattering, the exchange amplitude of eqn. (5.11) is of the same sign as that of the corresponding direct amplitude. The effect of exchange is to reduce the inelastic DCS. Further for elastic scattering at relatively

lower energies around 100 ev, the exchange contribution from the first order amplitude is quite significant, especially at $\theta = 0$. While, in contrast with that, the exchange amplitude of inelastic scattering, e.g. eqn. (5.11) rates poor in that, it falls off like k_i^{-4}. This is because $q_{min} = k_i - k_f$ and hence $q_{min} = 3/8\ k_i^2$ at high energies. This behaviour suggests that for inelastic scattering, at small q, higher orders of the exchange Born amplitudes must be considered.

Now, for the $1S \longrightarrow 2p$ excitation, we must consider three magnetic substates with $m = \pm 1, 0$, so that

$$A_{2po}(r) = \frac{2^{15/2}}{3^5} \frac{z}{r} \left(\frac{1}{r^2} - e^{-3/2r} \left(\frac{1}{r^2} + \frac{3}{2r} + \frac{9}{8} + \frac{27}{64} r \right) \right) \qquad (5.12)$$

And,

$$A_{2p+1}(r) = \frac{2^7}{3^5} \frac{b}{r} \left(\frac{1}{r^2} - e^{-3/2\ r} \left(\frac{1}{r^2} + 3/2r + \frac{9}{8} + \frac{27}{64} r \right) \right) \qquad (5.13)$$

A slightly different procedure may be adopted for getting the direct first Born amplitude to make use of the fact that only $m = 0$ contributes here. Quoting the final result,

$$f_{B1}\ (1S \longrightarrow 2p) = -\frac{12\sqrt{2}\ i}{q(q^2 + \frac{9}{4})^3} \qquad (5.14)$$

It can be seen that for $1S \longrightarrow 2p$ transition, the forward peak in the amplitude will be quite stronger, but will fall off much faster than the elastic first Born amplitude at large q. The transitions such as $1S \longrightarrow 2p$, which are optically allowed, dominate the total cross-sections at high energies.

Simple first Born calculations are inadequate to describe correctly the angular distribution of electrons scattered inelastically from an atom. This amply speaks for the need of higher order theories, which we now discuss.

5.3 The Glauber and the EBS approaches to the Inelastic Scattering

The excitation of hydrogen atom from 1S to 2S state is only next to $1S \longrightarrow 1S$ problem, in

order of difficulty. Let us review some pioneering work done in this area. Burke et al (1963) employed the close-coupling formalism to this process. The interest in the Glauber theory appeared in the early seventies, in view of the fact that it accounts for all possible channels, unlike the close-coupling approach. Byron (1971), (see also Ghosh and Sil 1970) explored the Glauber formulation to study the electron impact excitation of hydrogen and helium. This was perhaps the first work where an important drawback of the Glauber formulation for inelastic scattering was discussed. In the Glauber theory, the momentum transfer $\underline{q}$ is taken as perpendicular to incident vector $\underline{k}_i$. Now, for inelastic collisions, $\underline{q} = \underline{k}_i - \underline{k}_f$ is never zero physically, and in fact at $\theta = 0$, $\underline{q}$, $\underline{k}_i$ and $\underline{k}_f$ are collinear ! Hence, the assumption of $\underline{q}$ perpendicular to $\underline{k}_i$ is against simple kinematics and quite undesirable. Byron (1971) and later Gau and Macek (1974, 1975) used numerical evaluation to avoid this situation.

The Glauber amplitudes for the collisions of charged particles with hydrogen atoms were first derived in the closed form by Thomas and Gerjuoy (1971). Quoting their result for electrons,

$$F(1S \longrightarrow 2S) = \frac{4ik_i}{\sqrt{2}\,\lambda^6}\left(\frac{\lambda^2}{q^2}\right)^{1-in}\Gamma(1+in)\,\Gamma(1-in)$$

$$\times\ in\,(2in(1+in)\,{}_2F_1\,(1-in,\ 1-in;\ 1;\ -\lambda^2/q^2)$$

$$+\ 4in(1-in)^2\,(\lambda^2/q^2)\ \ {}_2F_1(2-in,\ 2-in,\ 2;\ -\lambda^2/q^2)$$

$$+\ (1-in)^2\,(2-in)^2\,(\lambda^4/q^4)$$

$$\times\ {}_2F_1\,(3-in,\ 3-in;\ 3;\ -\lambda^2/q^2)),\ \lambda = 3/2 \qquad (5.15)$$

where $n = 1/k_i$ in a.u. (see also Gerjuoy and Thomas, 1974) ${}_2F_1$ is a hypergeometric function. An interesting result of this work is that for $1S \longrightarrow 2p$ excitation, the amplitude vanishes for the magnetic substate $m = 0$. The reason for this can be traced back to the two dimensional nature of the Glauber amplitude. In general, for a transition $nlm \rightarrow n'l'm'$, the Glauber amplitude will be zero, whenever,

$$l + l' + |m| + |m'| = \text{odd integer} \qquad (5.16)$$

This constitutes an important drawback of the Glauber theory. Apart from this, the inelastic Glauber amplitude

(5.15) differs from the Galuber elastic amplitude in that, the question of singularity does not arise, as $q \neq 0$. The second order term of inelastic Glauber amplitude, on the other hand, retains the absence of a real part. Finally, the Glauber approximation works relatively better for small angles and for $S \longrightarrow S$ transitions, while it is poor in describing larger angle scattering where it highly underestimates. The Glauber approximation virtually breaks down for nonspherical final states. At this stage, one may recall the term by term analysis of the Glauber amplitude by Yates (1974). This approach, the GES formulation has not found much headway in the inelastic collisions. Singh and Tripathi (1980) have used the GES method to describe the elastic as well as inelastic scattering of fast electrons by He-atoms. Byron and Latour (1976) employed the EBS to analyse 2S and 2p excitation of atomic hydrogen by electrons. These authors find that the polarization effect, generated by the real part of the inelastic second Born term, is not as large as that in the elastic scattering. One of the reasons for this is that $q \neq 0$ at $\theta = 0$. In fact upto about 30° angle of scattering, the EBS and the Glauber results are in agreement. As already stated, the EBS approach seeks to evaluate the direct scattering amplitude in the form,

$$f^{d}_{EBS} = f_{B1} + f_{B2} + f_{G3} \qquad (5.17)$$

And for elastic scattering, the exchange amplitude can be incorporated through $O(k_i^{-2})$. The consistency of $O(k_i^{-2})$ does not hold for inelastic scattering. It is thus clear that, apart from a dependence on k_i, one has to also consider the dependence on q, in writing eqn. (5.17). In short, the DCS derived from the EBS amplitude would not be strictly $O(k_i^{-2})$ now.

The well-known method of evaluating the second Born amplitude of eqn. (5.17) makes use of the Dalitz integrals. Alternatively, following the HHOB of Yates (1979) the second Born amplitude for inelastic scattering can also be evaluated along the lines of our discussion in the ∮ chapter 3. Rao and Desai (1983) have studied 1S ⟶ 2S process in this way, but the results are good only at small angles. The previous results for elastic scattering (chapter 3) can be easily extended to 1S ⟶ 2S excitation.

Further, for the present case one would like to calculate the modified Glauber amplitude as is done for elastic scattering (Gien, 1976) i.e. by

constructing an amplitude,

$$f^{MG} = f^{G} - f_{G2} + f_{B2} \qquad (5.18)$$

This one and similar other approaches have enjoyed a great success in the elastic scatterings. However, it is not known if eqn. (5.18) is applied to study the 1S $\longrightarrow$ 2S (or 2p) excitation. Presently, an advantage of the modified Glauber amplitude is lost, since the inelastic Glauber amplitude is not singular and further, the real part of f_{B2} is now not so dominent. All the same, an essential ingradient of eqn. (5.18) lies in the higher order terms of f^{G}, which can play an effective role in the large-angle scattering. Uptill now, the theories described are 'plane-wave' approximations, i.e. no account is taken of the projectile distortion.

5.4 The Distorted Wave Methods

The T-matrix of the Born series for the direct inelastic scattering, for transition i $\longrightarrow$ f, is,

$$T_{fi} = \langle f, \underline{k}_f \,|\, V(1 + GV + GVGV + \ldots) \,|\, i, \underline{k}_i \rangle \qquad (5.19)$$

where, the symbol G is for an appropriate Green's function. Here the initial and the final states of the projectile electron are represented by the plane waves. However, as an electron approaches (recedes from) a target it experiences the field of the target even at a distance, so that it differs from a plane wave. Thus, actually the matrix element of eqn. (5.19) must be evaluated with 'distorted' waves. Let us see how, the first Born approximation can be modified with this idea. The modified first Born approximation was proposed by Juncker (1975) and has been further explored by Gupta and Mathur (1978 a, b, 1979). In this method the distortion in the projectile, represented by a coulomb wave, is produced by assuming an effective charge 'δ' on the target nucleus. The expression of the distorted wave looks like,

$$F(\underline{r}) = \sqrt{(1 - ia_i)}\ \exp\ (i\underline{k}_i.\underline{r} + \pi a_i/2)$$

$$X\ \ {}_1F_1\ (ia_i,\ 1,\ ik_i\ r - i\underline{k}_i.\ \underline{r}) \qquad (5.20)$$

This will yield plane waves if $a = 0$. Gupta and Mathur (1978b) have applied this procedure to $1S \longrightarrow 2S$

and the exchange is also included. Target polarization is not considered. The agreement with data is not quite good except below 30°. It may be noted that the DCS of n = 2 state excitation of hydrogen are obtained as a sum of 2S and 2p state cross-sections. At small angles, the 2p cross-sections in the first Born treatment are very large, so that all theories yield almost equally good results below 20° - 30° angles. Nearly 93 % of the integrated cross-section for n = 2 state is contributed by 1S $\rightarrow$ 2p transition.

A rigorous distorted wave calculation for n = 2 state of hydrogen is by Baluja et al (1978) which is quite similar to that of Galhoun et al (1976, 1977). Among the methods using high energy approximations in a distorted wave theory, mention must be made of the eikonal DWBA (distorted wave Born approximation) of Chen et al (1972). The validity of this method is limited to small angles only. In the next section, we describe a new high energy DWBA method.

5.5 A New High-Energy DWBA Method

Consider the inelastic electron-atom scattering. The hamiltonians in the channels 'i'

and 'f' are H_i and H_f so that,

$$H_i X_a = E_a X_a \tag{5.23a}$$

$$H_f X_b = E_b X_b \tag{5.23b}$$

where, E_a (E_b) is total initial (final) energy of the system. The initial and final asympotic states are given respectively by X_a and X_b, with,

$$X_a = (2\pi)^{-3/2} e^{i\underline{k}_i \cdot \underline{r}} \psi_\alpha(r_i) \tag{5.24}$$

where, ψ_α is the initial state of the target. Basically, we wish to evaluate the T-matrix element,

$$T = \langle X_b | V_f | \psi_a^{(+)} \rangle = \langle \psi_b^{(-)} | V_i | X_a \rangle \tag{5.25}$$

where, V_i (V_f) is the interaction between the target and the projectile in the initial (final) channel. Suppose that the interaction is splitted up into two parts,

$$V_i = U_i + W_i \tag{5.26a}$$

$$V_f = U_f + W_f \qquad (5.26b)$$

We assume that the corresponding state vectors, given below are known.

$$\phi^{(+)} = X_a + (E - H_i - U_i + i\varepsilon)^{-1} U_i X_a \qquad (5.27a)$$

$$\phi^{(-)} = X_b + (E - H_f - U_f - i\varepsilon)^{-1} U_f X_b \qquad (5.27b)$$

Starting from the integral representations (5.25) of the T-matrix, one can show (Gellmann and Goldberger, 1953) that,

$$T = \langle X_b | V_f - W_i | \phi_a^{(+)} \rangle + \langle \psi_b^{(-)} | W_i | \phi_a^{(+)} \rangle \qquad (5.28)$$

Suppose now that the potentials U_i and U_f depend only on the coordinate of the continuum electron, hence they cannot induce any transition. For inelastic scattering,

$$T_{ba} = \langle \phi_b^{(-)} | W_f | \psi_a^{(+)} \rangle = \langle \psi_b^{(-)} | W_i | \phi_a^{(+)} \rangle \qquad (5.29)$$

The treatment upto here is exact. The question now is how to determine the distorted waves $\phi_a^{(+)}$ and $\phi_b^{(-)}$.

It is required to evaluate the Green's operators,

$$G^{\pm} = \lim_{\epsilon \longrightarrow 0^+} \frac{1}{(E - H \pm i\epsilon)} \qquad (5.30)$$

It can be shown that,

$$\phi_a^{(+)} = X_a + 2G_o^{(+)} U_i X_a \qquad (5.31a)$$

$$\phi_b^{(-)} = X_b + 2G_o^{(-)} U_f X_b \qquad (5.31b)$$

Now, even if $\phi_a^{(+)}$ and $\phi_b^{(-)}$ are known, the T-matrix of eqn. (5.29) is tremendously difficult, as it contains the exact wave functions $\psi_a^{(+)}$ and $\psi_b^{(-)}$. We then resort to the first Born approximation by setting,

$$\psi_a^{(+)} \doteq \phi_a^{(+)} , \quad \psi_b^{(-)} \doteq \phi_b^{(-)} \qquad (5.32)$$

Thus, the Distorted wave first Born transition matrix element is,

$$T^{DW1} = \langle \phi_b^{(-)} | W_i | \phi_a^{(+)} \rangle = \langle \phi_b^{(-)} | W_f | \phi_a^{(+)} \rangle \qquad (5.33)$$

This is our starting point.

Choosing the many body Green's operator, with spectral resolution and $\underline{K}$ - representation,

$$G_n^{\pm}(\underline{r}, \underline{r}', \underline{x}, \underline{x}') = -(2\pi)^{-3} \sum_{n=0}^{\infty} \int d\underline{K} \frac{\exp(i\underline{K}.(\underline{r} - \underline{r}'))}{K^2 - k_n^2 \mp i\epsilon} \times |n\rangle\langle n| \qquad (5.34)$$

Thus,

$$\phi_a^{(+)} = \left\{1 - \frac{1}{(2\pi)^3} \sum_n \iint d\underline{r}' \int d\underline{K} \frac{\exp(i\underline{K}.(\underline{r} - \underline{r}'))}{K^2 - k_n^2 - i\epsilon} \times |n\rangle\langle n| \right\} \underbrace{(2\pi)^{-3/2}}_{U_c(r-r')} e^{i\underline{k}_i \cdot \underline{r}} \psi_\alpha(\underline{x}) \qquad (5.35)$$

And a similar equation for $\phi_b^{(-)}$.

Now, from equ. (5.35), consider the following part of the Green's function,

$$G^{+} = -(2\pi)^{-3} \int d\underline{K} \frac{\exp\,(i\underline{K}.(\underline{r} - \underline{r}'))}{K^2 - k_n^2 - i\epsilon} \tag{5.36}$$

Here, we introduce,

$$\underline{p} = \underline{K} - \underline{k}_n, \quad \underline{R} = \underline{r} - \underline{r}' \tag{5.37}$$

Now, taking $\underline{k}_n$ along z-axis,

$$G^{+} = -(2\pi)^{-3} \exp\,(i\,\underline{k}_n.\,\underline{R})$$

$$\int d\underline{p} \frac{\exp\,(i\,\underline{p}\,.\,\underline{R})}{p^2 + 2k_n p_z - i\epsilon} \tag{5.38}$$

Further, expanding the denominator,

$$\frac{1}{p^2 + 2k_n\,p_z - i\epsilon} = \frac{1}{2k_n p_z - i\epsilon}$$

$$\left(1 - \frac{p^2}{2k_n p_z - i\epsilon} + \ldots.\right) \tag{5.39}$$

(The symbols p and p_z should not be confused with any Fourier transform variables). Thus the Green's function is linearized and in the high energy, small-angle approximation (chapter 3) we expect that the first two terms are

are sufficient to describe the distorted waves eqn. (5.31 a,b). Further, we need,

$$\underline{R} = \underline{B} + \underline{Z} \tag{5.40}$$

Now, we can show that by retaining the first two terms in eqn. (5.39)

$$G^{+} = -\frac{i}{2k_n} e^{ik_n Z} \delta(\underline{B}) H(Z) + \frac{1}{4k_n^2} \nabla_R^2 \left(Z e^{i\underline{k}_n \cdot \underline{R}} \delta(\underline{B}) H(Z)\right) \tag{5.41}$$

Here, H(Z) is the Heavyside function. Now, we replace $\underline{R} \longrightarrow \underline{r}'$ and go back to the eqn. (5.35), so that the outgoing distorted waves are given by,

$$\phi_a^{\oplus} = (2\pi)^{-3/2} e^{i\underline{k}_i \cdot \underline{r}} \left[1 + \frac{i}{k_i} \sum_n \left(\int_{-\infty}^{\infty} dz' e^{-i\beta_{in} z'} H(z') \; |n\rangle\langle n| \right. \right.$$

$$\left. \left. \left(1 + \frac{iz'}{2k_i} \nabla_{r'}^2 (U_i(\underline{r} - \underline{z}'))\right] \times \psi_\alpha(x) \right. \right. \tag{5.42}$$

In arriving at this final form,

* The property of $\delta(B)$ is used.

* The parameter $\beta_{in} = k_i - k_n$ is defined.

* The assumption $k_i \triangleq k_n$ is used (Yates, 1979)

Now to derive the form of the incoming distorted waves $\phi_b^{(-)}$, we have to start from,

$$G^- = -(2\pi)^{-3} \; e^{i\underline{k}_n \cdot \underline{R}} \int d\underline{p} \frac{\exp(i\underline{p}.\underline{R})}{p^2 + 2k_n p_z + i\varepsilon} \qquad (5.43)$$

We follow the previously described procedure. The incoming distorted waves look like,

$$\phi_b^{(-)} = (2\pi)^{-3/2} \; e^{i\underline{k}_f \cdot \underline{r}} \left[1 - \frac{i}{k_f} \right.$$

$$\sum_{n'} \left(\int_{-\infty}^{\infty} dz' \; e^{-i\beta_{in'} z'} \; H(z') \; X \; |n'\rangle\langle n'| \right.$$

$$\left. \left. (1 - \frac{iz'}{2k_f} \; V_r^2) \; U_f(\underline{r} - \underline{z}')) \right] \right] \psi_\beta(x) \qquad (5.44)$$

where, as done previously,

* $\beta_{fn'} = k_{n'} - k_f$; $k_f \triangleq k_n$ is assumed.

* $U_f(\underline{r})$ is the distorting potential in the final channel.

* the rest of the comments following eqn. (5.42) apply.

The expressions for the distorted waves are simplified by defining the average excitation energies through the relations,

$$\beta_{in} \triangleq \beta_1 = \bar{W}_1/k_i \qquad (5.45a)$$

$$\beta_{fn'} \triangleq \beta_2 = \bar{W}_2/k_f \qquad (5.45b)$$

with $\bar{W}_1$ and $\bar{W}_2$ as the mean excitation energies in the initial and the final states respectively of the target atom. We thus obtain,

$$\phi_a^{(+)} = (2\pi)^{-3/2} e^{i\underline{k}_i \cdot \underline{r}} \left[1 + \frac{1}{k_i} \int_{-\infty}^{\infty} dz' \right.$$

$$e^{-i\beta_1 z'} \; H(z') \; X \; \left(1 + \frac{iz'}{2k_i} \nabla_{z'}^2 \right)$$

$$\left. U_i(\underline{r} - \underline{z}') \right] \; \psi_\alpha(x) \qquad (5.46)$$

And an analogous expression of $\phi_b^{(-)}$. If the average

excitation energies vanish, eqn. (5.46) reduces to the eikonal expression plus terms from the second term of the Green's function expansion, eqn. (5.39). Finally the distorted wave first Born direct scattering amplitude in the present high energy approximation is,

$$f_{HE}^{DW1} = -4\pi^2 \langle \phi_b^{(-)} | W_i | \phi_a^{(+)} \rangle \qquad (5.47)$$

We discuss next the application of the present theory to the excitation of atomic hydrogen by electrons.

5.6 Application to Electron-Impact (1S ——— 2S) Excitation of Atomic Hydrogen

To evaluate the amplitude f_{HE}^{DW1}, for $1S \longrightarrow 2S$ we need, the distorting potentials U_i and U_f. A simple choice is that of static potentials, i.e.,

$$U_i(r) = -(1 + 1/r)\, e^{-2r} \qquad (5.48)$$

$$U_f(r) = \langle \Psi_{2S} \mid V \mid \Psi_{2S} \rangle$$

$$= -\left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{8}\right) e^{-r} \qquad (5.49)$$

Thus, in the present case, we have

$$f_{HE}^{DW1} = -\frac{1}{2\pi} \int d\underline{r}\, e^{i\underline{q}.\underline{r}} \left[1 + \frac{i}{k_f} \int_{-\infty}^{\infty} dz'\, e^{i\beta_2 z'} H(z') \times \left(1 - \frac{iz'}{2k_f} \nabla_{z'}^2\right) U_f(\underline{r} - \underline{z}')\right] \langle \psi_{2S} | W_i | \psi_{1S} \rangle \times \left[1 - \frac{i}{k_i} \int_{-\infty}^{\infty} dz''\, e^{-i\beta_1 z''} H(z'') \left(1 + \frac{iz''}{2k_i} \nabla_{z''}^2\right) \times U_i(\underline{r} - \underline{z}'')\right] \qquad (5.50)$$

Now, the orthogonality gives,

$$\langle \psi_{2S} | W_i | \psi_{1S} \rangle = A_{2S}(r) \qquad (5.51)$$

Let us write the complete amplitude as

$$\boxed{f_{HE}^{DW1}} = f_1 + f_2 + f_3 + f_4 \qquad (5.52)$$

where,

$$f_1 = f_{B1} (1S \longrightarrow 2S) \qquad (5.53)$$

is the plane wave first Born amplitude. The terms f_2, f_3 and f_4 are due to the cross terms of the products in the eqn. (5.50). The calculations of f_2 and f_3 are comparable to the second Born calculations, with the 'potential' acting twice. The calculations in the last term f_4 involve the 'potential' acting thrice and are comparable to the third Born term.

Notably, here the part of the interaction W_i responsible for transition, is treated in the first order and the projectile distortion is considered through the second order of pertubation. Potapov (1973) has shown that the high energy limit of the DWBA is the second Born approximation. This fact is confirmed here.

Proceeding for $1S \longrightarrow 2S$ calculations we have from eqns. (5.50) through (5.53),

$$f_2 = -\frac{-i}{2\pi k_i} \int d\underline{r}\; e^{i\underline{q}.\underline{r}}\; A_{2S}(r)$$

$$\int_{-\infty}^{\infty} dz'\; e^{-i\beta_1 z'}\; H(z')$$

$$X\left(1 + \frac{iz'}{2k_i} V_{z'}^2\right) U_i(\underline{r} - \underline{z}') \qquad (5.54)$$

Also,

$$f_3 = \frac{-i}{2\pi k_f} \int d\underline{r}\ e^{i\underline{q}.\underline{r}}\ A_{2S}(r)$$

$$\int_{-\infty}^{\infty} dz'\ e^{i\beta_2 z'}\ H(z')\ X\ (1 - \frac{iz'}{2k_f}\ V_{z'}^2,)$$

$$U_f(\underline{r} - \underline{z}') \qquad (5.55)$$

Now q is made two-dimensional and we use the Fourier representation of U_i, U_f and A_{2S}, in the variable $\underline{P} = \underline{p} + \underline{p}_z$. In the following the (overhead) 'bar' represents the corresponding Fourier transform,

$$\bar{A}_{2S}\ (\underline{p} + \underline{p}_z) = \frac{C_1}{2\pi^2} \left(\frac{\partial^2}{\partial\lambda_1^2} \frac{1}{p^2 + p_z^2 + \lambda_1^2} - \frac{2}{3} \frac{\partial}{\partial\lambda_1} \right.$$

$$\left. \frac{1}{p^2 + p_z^2 + \lambda_1^2} \right) . \lambda_1 = 3/2 \qquad (5.56)$$

$$\bar{U}_i\ (\underline{p} + \underline{p}_z) = -\frac{1}{2\pi^2} \left(1 - \frac{\partial}{\partial\lambda_2}\right)$$

$$\frac{1}{p^2 + p_z^2 + \lambda_2^2} . \qquad \lambda_2 = 2 \qquad (5.57)$$

$$\bar{U}_f\,(p + p_z) = -\frac{1}{2\pi^2}\left(1 - \frac{3}{4}\frac{\partial}{\partial\lambda_3} + \frac{1}{4}\frac{\partial^2}{\partial\lambda_3^2} - \frac{1}{8}\frac{\partial^3}{\partial\lambda_3^3}\right)$$

$$\times \frac{1}{p^2 + p_z^2 + \lambda_3^2} \cdot \lambda_3 = 1 \qquad (5.58)$$

By taking the Fourier transforms, the priority of integration in eqns. (5.54) and (5.55) changes and the continuum electron coordinates are integrated first. Now, we use the properties of delta functions and the following result.

$$\int_{-\infty}^{\infty} dx\, e^{-i\alpha x} H(x) = \pi\,\delta(\alpha) - i\,\mathcal{P}\left(\frac{1}{\alpha}\right) \qquad (5.59)$$

The symbol $\mathcal{P}$ denotes the principal value. Hence,

$$f_2 = \frac{-4\pi^3}{k_i}\left[i\int d\underline{p}\left(1 + \frac{1}{2k_i}\frac{\partial}{\partial\beta_1}(p^2 + \beta_1^2)\right)\right.$$

$$\bar{A}_{2S}\,(\underline{q} - \underline{p} - \underline{\beta}_1)\,\bar{U}_i\,(\underline{p} + \underline{\beta}_1) - \frac{1}{\pi}$$

$$\mathcal{P}\int d\underline{p}\int_{-\infty}^{\infty} dp_z\left(1 + \frac{p^2 + p_z^2}{2k_i}\frac{\partial}{\partial\beta_1}\right)\frac{1}{p_z - \beta_1}$$

$$\left.\bar{A}_{2S}\,(\underline{q} - \underline{p} - \underline{p}_z)\;\bar{U}_i\,(\underline{p} + \underline{p}_z)\right] \qquad (5.60)$$

The term f_2 splits up into real and imaginary parts, each of them having a term through $O(k_i^{-1})$ as well as $O(k_i^{-2})$. It is found that in the imaginary part, the term $O(k_i^{-2})$ is quite negligible. Hence we write, the imaginary part through the order k_i^{-1} only. Further, the term $O(k_i^{-2})$ in the real part here, corresponds to Re 2 of the HHOB discussed in the chapter 3. As $\beta_1 \longrightarrow 0$ this term will resemble the real part of the second order Wallace amplitude (see also Byron et al 1982). Now, the evaluation of f_3 is quite analogous to that of f_2 and all the comments of the last paragraph apply to f_3 also. The final expression of the high energy DW Born amplitude for 1S $\longrightarrow$ 2S transition is written below.

Let,

$$n_1^2 = \beta_1^2 + \lambda_1^2 \tag{5.61}$$

$$n_2^2 = \beta_1^2 + \lambda_2^2 \tag{5.62}$$

$$n_3^2 = \beta_2^2 + \lambda_1^2 \tag{5.63}$$

$$n_4^2 = \beta_2^2 + \lambda_3^2 \tag{5.64}$$

Hence,

$$f_{HE}^{DW1} = f_{B1}\ (1S \longrightarrow 2S)$$

$$+ \left(\frac{\partial^2}{\partial \lambda_1^2} - \frac{2}{3}\ \frac{\partial}{\partial \lambda_1} \right)\left(1 - \frac{\partial}{\partial \lambda_2}\right)$$

$$\left[\frac{iC_1}{\pi k_i}\ I_1\ (q,\ n_1^2\ ,\ n_2^2\ ) - \frac{C_1}{\pi^2 k_i} \right.$$

$$I_4\ (q,\ \lambda_1^2,\ \lambda_2^2\ ) - \frac{C_1}{2\pi^2 k_i^2}$$

$$X\ \frac{\partial}{\partial \beta_1}\ (I_3\ (\beta_1\ ,\ \lambda_1^2\ )$$

$$\left. - \lambda_2^2\ I_4\ (q_1,\ \lambda_1^2\ ,\ \lambda_2^2\ ))\right]$$

$$+ \left(\frac{\partial^2}{\partial \lambda_1^2} - \frac{2}{3}\ \frac{\partial}{\partial \lambda_1} \right)\left(1 - \frac{3}{4}\ \frac{\partial}{\partial \lambda_3} + \frac{1}{4}\ \frac{\partial^2}{\partial \lambda_3^2}\right.$$

$$\left. - \frac{1}{8}\ \frac{\partial^3}{\partial \lambda_3^3}\right)\ X\ \left[\frac{iC_1}{\pi k_f}\ I_1\ (q,\ n_3^2\ ,\ n_4^2\ ) \right.$$

$$- \frac{C_1}{\pi^2 k_f}\ I_4\ (q,\ \lambda_1^2,\ \lambda_3^2\ ) + \frac{C_1}{2\pi^2 k_f^2}\ \frac{\partial}{\partial \beta_2}$$

$$\left. (I_3(\beta_2, \lambda_1^2) - \lambda_3^2\ I_4\ (q,\ \lambda_1^2\ ,\ \lambda_3^2\ ))\right] \qquad (5.65)$$

The integrals I_1, I_3 and I_4 are given in the appendix. Before closing this section, let us estimate the difficulty of evaluating the term f_4. Consider from eqn. (5.50), only 1st term of f_4. To give only an outline, we drop the constants etc.

$$\frac{1}{k_i k_f} \int d\underline{r}\; e^{i\underline{q}.\underline{r}} \int_{-\infty}^{\infty} dz'\; e^{+i\beta_2 z'}$$

$$H(z')\; U_f(\underline{r} - \underline{z}')\; X\; A_{2S}(r) \int_{-\infty}^{\infty} dz''$$

$$e^{-i\beta_2 z''}\; H(z'')\; U_i(\underline{r} - \underline{z}'')$$

Here, after the Fourier transformation of U_i, U_f and A_{2S}, we are required to evaluate the following kind of integrals,

$$\int \frac{d\underline{p}}{(|\underline{q} - \underline{p}|^2 + \beta_1^2 + \lambda_1^2} \int \frac{d\underline{p}'}{(p^2 + n^2)(|\underline{p}' - \underline{p}|^2 + m^2)}$$

$$= \int_0^{\infty} \frac{dp}{((q^2+p^2+\beta_1^2+\lambda_1^2)^2 - 4p^2q^2)^{1/2}}\; X\; \frac{1}{\sqrt{c}}\; \ln\frac{a}{b}$$

where a, b and c are functions of 'p'.

The last integral could not be handled

confidently, hence f_4 is not evaluated at present. The term f_4 may be approximated by a plane wave third order Glauber term.

5.7 Inclusion of the Electron Exchange

Considering the 1S $\longrightarrow$ 2S transition, we attempt to obtain the higher order exchange amplitude in the high energy distorted wave method. The transition matrix is obtained after properly permuting the incident electron coordinate $\underline{r}$ and the (initial) target electron co-ordinate $\underline{r}_1$. Thus, we need the exchange amplitude,

$$\overline{g^{DW1}_{HE}} = -4\pi^2 < \phi^{(-)}_{Pb} \; |W_i| \; \phi^{(+)}_a > \qquad (5.66)$$

where P stands for the permutation of $\underline{r}$ and $\underline{r}_1$. Comparing this with (5.50) the exchange amplitude splits up into four terms, i.e.

$$g^{DW1}_{HE} = g_1 + g_2 + g_3 + g_4 \qquad (5.67)$$

The second order amplitude g_2 is

$$g_2 = -\frac{i}{2\pi k_i}\left[\iint d\underline{r}\, d\underline{r}_1\, e^{i\underline{k}_i\cdot\underline{r} - i\underline{k}_f\cdot\underline{r}_1}\right.$$

$$\Psi_{2S}(r)\ \ \Psi_{1S}(r_1)\ \ X\ (V - U_i)$$

$$\left. X \int_{-\infty}^{\infty} dz'\, e^{-i\beta_1 z'}\ H(z')\ U_i(\underline{r} - \underline{z}') + O(k_i^{-2})\right] \qquad (5.68)$$

Further, $g_2 = \text{Im}\ g_2 + \text{Re}\ g_2$ (5.69)

First we discuss the evaluation of the imaginary part of (5.69) and we call it g_{21}. Thus after taking the Fourier transforms of potentials,

$$g_{21} = C_2 \iiiint d\underline{p}\ \ d\underline{K}\ \ d\underline{r}\ \ d\underline{r}_1$$

$$X\ (2 - r)\ e^{-l_2 r + i\underline{k}_i\cdot\underline{r} - i\underline{P}\cdot\underline{r}}$$

$$X\ e^{-l_1 r_1 - i\underline{k}_f\cdot\underline{r}_1}\ \ X\ e^{-i\underline{K}\cdot\underline{r}}$$

$$X\left(\frac{e^{i\underline{K}\cdot\underline{r}_1} - a}{K^2} - \bar{U}_i(\underline{K})\right)\bar{U}_i(\underline{P}) \qquad (5.70)$$

in which

$$C_2 = \frac{i}{8\sqrt{32}\ \pi^5 k_i}$$

In the eqn. (5.70) a = 1 for the H-atom shows the nuclear term in the exchange integral. The most dominent contribution comes from the electron-electron term of the direct potential V. In writing eqn. (5.70) we have used,

$$\frac{1}{|\underline{r} - \underline{r}_1|} = \frac{1}{2\pi^2} \int d\underline{K} \frac{\exp(i\underline{K}.(\underline{r} - \underline{r}_1))}{K^2} \qquad (5.71)$$

This leads to the first and the most dominent term of g_{21}. The next two terms are the contributions of the (direct) electron-proton interaction and of $\bar{U}_1(K)$.
Let us further write,

$$g_{21} = C_2 \iiiint d\underline{p}\, d\underline{K}\, d\underline{r}\, d\underline{r}_1 (2 - r)$$

$$(-\frac{\partial}{\partial l_2}) \frac{e^{-l_2 r}}{r} \times e^{+i(\underline{k}_i - \underline{K} - \underline{P}).\underline{r}}$$

$$\times e^{-i\underline{k}_f.\underline{r}_1} (-\frac{\partial}{\partial l_1}) \frac{e^{-l_1 r_1}}{r_1}$$

$$\times \left(\frac{e^{i\underline{K}.\underline{r}_1} - a}{K^2} + (1 - \frac{\partial}{\partial \lambda_3}) \frac{1}{K^2 + \lambda_3^2} \right)$$

$$\times (1 - \frac{\partial}{\partial \lambda_3}) \frac{1}{p^2 + p_z^2 + \lambda_3^2} \qquad (5.72)$$

where; $l_1 = 1$, $l_2 = 1/2$ and $\lambda_3 = 2$,

For the electron-electron term from (5.72), we use,

$$\int d\underline{r}_1 \; e^{-i(\underline{k}_f - \underline{K})\cdot\underline{r}_1} \times \frac{e^{-l_1 r_1}}{r_1}$$

$$= \frac{4\pi}{|\underline{k}_f - \underline{K}|^2 + l_1^2} \tag{5.73}$$

and a similar result for $\underline{r}$ - integral. Thus, in the first term of (5.72), two out of the four integrals are solved. Turning now to the $\underline{K}$-integral, we have

$$\int \frac{d\underline{K}}{K^2} \frac{1}{(|\underline{k}_i - \underline{K} - \underline{P}|^2 + l_2^2)(|\underline{k}_f - \underline{K}|^2 + l_1^2)}$$

$$= \frac{\pi^2}{k_f^2} \left(-\frac{\partial}{\partial n}\right) \frac{1}{(q'^2 + n^2)} \tag{5.74}$$

with $n = 3/2$, and $\underline{q}' = \underline{q} - \underline{p}$.

The last result follows from the Ochkur approximation to higher order terms in the $\underline{K}$-integral. Finally, the $\underline{p}$-integral,

$$\int d\underline{p} \; \frac{1}{(p^2 + \beta_1^2 + \lambda_3^2)(|\underline{q} - \underline{p}|^2 + \beta_1^2 + n^2)}$$

$$= I_1 \; (q, \beta_1^2 + \lambda_3^2, \beta_1^2 + n^2) \qquad (5.75)$$

Thus, the first term of g_{21} of eqn. (5.72) finds an expression as,

$$g_{211} = \frac{i\sqrt{8}}{6 \, k_i k_f^2} \left(-\frac{\partial}{\partial n}\right)\left(1 - \frac{\partial}{\partial \lambda_3}\right)$$

$$I_1 \; (q, \beta_1^2 + \lambda_3^2, \beta_1^2 + n^2) \qquad (5.76)$$

The next term on our list of evaluation is the nuclear contribution to g_{21}, with $a = 1$, in the eqn. (5.72). The nuclear term, would look like

$$g_{212} = C_2 \iiiint d\underline{p} \, d\underline{K} \, d\underline{r} \, d\underline{r}_1 \, (2 - r)$$

$$\left(-\frac{\partial}{\partial l_2}\right) \frac{e^{-l_2 r}}{r} \times e^{i(\underline{k}_i - \underline{K} - \underline{P}) \cdot \underline{r}}$$

$$\times e^{-i\underline{k}_f \cdot \underline{r}_1} \left(-\frac{\partial}{\partial l_1}\right) \frac{e^{-l_1 r_1}}{r_1}$$

$$\times \left(-\frac{1}{K^2}\right)\left(1 - \frac{\partial}{\partial \lambda_3}\right)\left(\frac{1}{p^2 + \beta_1^2 + \lambda_3^2}\right)$$

$$= C_2 \left(\frac{1_1}{(k_f^2 + 1_1^2)^2} \right)\left(2 + \frac{\partial}{\partial 1_2}\right)\left(- \frac{\partial}{\partial 1_2}\right)^2$$

$$\left(1 - \frac{\partial}{\partial \lambda_3}\right) \times I_1 \left(q, \beta_1^2 + \lambda_3^2, \beta_1^2 + 1_2^2\right) \qquad (5.77)$$

In the recent literature there has been a lot of discussion about the contribution of the nuclear term to the exchange integrals. It has been often shown that the said contribution is zero, under certain assumptions (see e.g. Mishra and Pradhan, 1982). In the present case, however, it would appear that the term g_{212} showing a nuclear contribution is $O(k_i^{-5})$ as against the electron-electron term g_{211} which is $O(k_i^{-3})$, see eqn. (5.76). But a basic insight is required into the evaluation of the nuclear term. In the eqn. (5.77),, the $\underline{r}_1$-integral must vanish if we invoke the argument that the wave functions of the bound electron and the continuum electron must be orthogonal. In other words, the sum of all terms in the exchange Born series, which do not depend on the electron-electron interaction must add up to zero. (Shakeshaft, 1978).

An interesting consequence of the derivation of the term g_{211}, is that, there has been no need of the assumption that the momentum transfer $\underline{q}$ must be two dimensional and perpendicular, to $\underline{k}_i$. This is so, because

the explicit form $\underline{q} = \underline{k}_i - \underline{k}_f$ occurs only in the $\underline{K}$-integral. Now going back to the main track of our discussion, we have evaluated the dominent term of the imaginary part of the second order exchange amplitude g_2 of eqn. (5.67). It is denoted by g_{211}. All the previous discussion applies to the amplitude g_3 of eqn. (5.67). We have to only worry about the dominent term g_{311}, which is similar to g_{211}. Thus, $(g_{211} + g_{311})$ is the main contribution of the imaginary part of the second order exchange amplitude $(g_2 + g_3)$ in the present high energy DWBA. Now, for the real part of the present second order exchange amplitudes, we have to go back to eqns. (5.68) and (5.69) and write for the real part of g_2,

$$g_{22} = C_2 \mathcal{P} \int d\underline{p} \int_{-\infty}^{\infty} dp_z \int d\underline{K}$$

$$\iint d\underline{r}\, d\underline{r}_1\, (2 - r)\, e^{i\underline{k}_i \cdot \underline{r} - l_2 r}$$

$$\times\ e^{-i\underline{P}\cdot\underline{r} - i\underline{K}\cdot\underline{r}} \left(\frac{e^{i\underline{K}\cdot\underline{r}_1} - 1}{K^2} - \bar{U}_i(\underline{K}) \right)$$

$$\times\ \left(1 + \frac{p^2 + p_z^2}{2k_i} \frac{\partial}{\partial \beta_1}\right) \frac{1}{p_z - \beta_1} \bar{U}_i(\underline{P}) \qquad (5.78)$$

Now, we denote by g_{221}, the part of g_{22} containing the electron-electron interaction. Hence,

$$g_{221} = C_2 \mathcal{P} \int d\underline{p} \int_{-\infty}^{\infty} dp_z \frac{1}{p_z - \beta_1} \bar{U}_i(\underline{p} + \underline{p}_z)\left(2 + \frac{\partial}{\partial l_2}\right)\left(-\frac{\partial}{\partial l_2}\right)\left(-\frac{\partial}{\partial l_1}\right) \int \frac{d\underline{K}}{K^2} \times 16\pi^2 \frac{1}{(|\underline{k}_f - \underline{K}|^2 + l_2^2)(|\underline{k}_i - \underline{K} - \underline{P}|^2 + l_1^2)} \quad (5.79)$$

Thus, the term g_{221} will contain, apart from the numerical constants and derivatives, the integral I_4. The derivation of all other terms of g_{22} is not shown here as it involves more or less similar procedure. This completes the evaluation of g_{HE}^{DW1}, emmitting g_4. Finally, the DCS with exchange,

$$\frac{d\sigma}{dw} = \frac{k_f}{k_i}\left(\frac{1}{4}\left|\overline{f_{HE}^{DW1}} + \overline{g_{HE}^{DW1}}\right|^2 + \frac{3}{4}\left|\overline{f_{HE}^{DW1}} - \overline{g_{HE}^{DW1}}\right|^2\right) \quad (5.80)$$

We finish with an important remark that, while most of the DWBA calculations of the other workers end up with numerical procedures for integration, our method does not need any such procedure and all the final integrals are done analytically.

Now, we exhibit the results of our calculations. The DCS of electron-impact 1S $\longrightarrow$ 2S excitation in the inelastic e-H scattering obtained from the eqn. (5.80) are shown in Tables 5.1 and 5.2, for the incident energies 50 and 100 ev. In these tables we show the values of the plane-wave first Born approximation (f_{B1}), the two terms Re 1 and Re 2 of the real part of the present DWBA amplitudes, the imaginary part of the present amplitude (Imf) and the DCS including the exchange. Table 5.3 shows a comparison of the plane wave first Born DCS, the DCS calculated by Calhoun et al (1976) and those of our DWBA method, all at 100 ev. In the graphical plots of figs. (5.1) to (5.4), we have exhibited the following results.

1. The DCS in the plane wave first Born approximation.
2. The DCS of the distorted wave approximation of Calhoun et al (1977).
3. The DCS obtained in the present high energy distorted

Table 5.1

DWBA results (1S —— 2S) at 50 ev

θ (deg)	f_{B1}	Imf	Re 1	Re 2	(DCS) with exchange*
0	-0.939	0.556	-0.119	0.292	0.89
10	-0.826	0.277	-0.076	0.153	0.52
20	-0.582	0.027	0.007	0.05	0.24
30	-0.354	-0.057	0.043	0.027	0.045
40	-0.20	-0.079	0.0015	-0.084	0.051
50	-0.11	-0.081	0.0055	-0.056	0.02
60	-0.065	-0.076	0.0064	-0.043	0.01
80	-0.025	-0.063	0.0059	-0.029	0.0046
100	-0.011	-0.052	0.005	-0.024	0.0027
120	-0.0063	-0.044	0.004	-0.021	0.002

*without polarization.

Table 5.2

DWBA results (1S ——— 2S) at 100 ev

θ (deg)	f_{B1}	Imf	Re 1	Re 2	(DCS) with exchange
0	-0.967	0.441	-0.65	0.15	0.90
10	-0.74	0.10	-0.023	0.046	0.43
20	-0.376	-0.038	0.026	0.015	0.11
30	-0.16	-0.057	0.0023	-0.028	0.029
40	-0.067	-0.053	0.0036	-0.016	0.0064
50	-0.03	-0.045	0.003	-0.011	0.0027
60	-0.014	-0.038	0.0028	-0.09	0.0017
80	-0.004	-0.027	0.002	-0.0064	0.00076
100	-0.0017	-0.02	0.0016	-0.005	0.00045
120	-0.00091	-0.017	0.0013	-0.0047	0.00028

Table 5.3

The DCS (a_o^2 Sr^{-1}) of 1S — 2S excitation in inelastic e-H scattering at 100 ev

Scattering angle (deg)	First Born	Calhoun et al	Present*
0	8.9 - 01	8.8 - 01	9.0 - 01
5	7.1 - 01	6.8 - 01	7.1 - 01
10	4.5 - 01	3.8 - 01	4.3 - 01
20	1.3 - 01	8.9 - 02	1.1 - 01
30	2.4 - 02	1.6 - 02	2.8 - 02
40	4.0 - 03	5.1 - 03	6.4 - 03
60	8.0 - 05	1.9 - 03	1.7 - 03
90	-	6.6 - 04	5.6 - 04
120	-	3.1 - 04	2.9 - 04

*including exchange, without polarization.

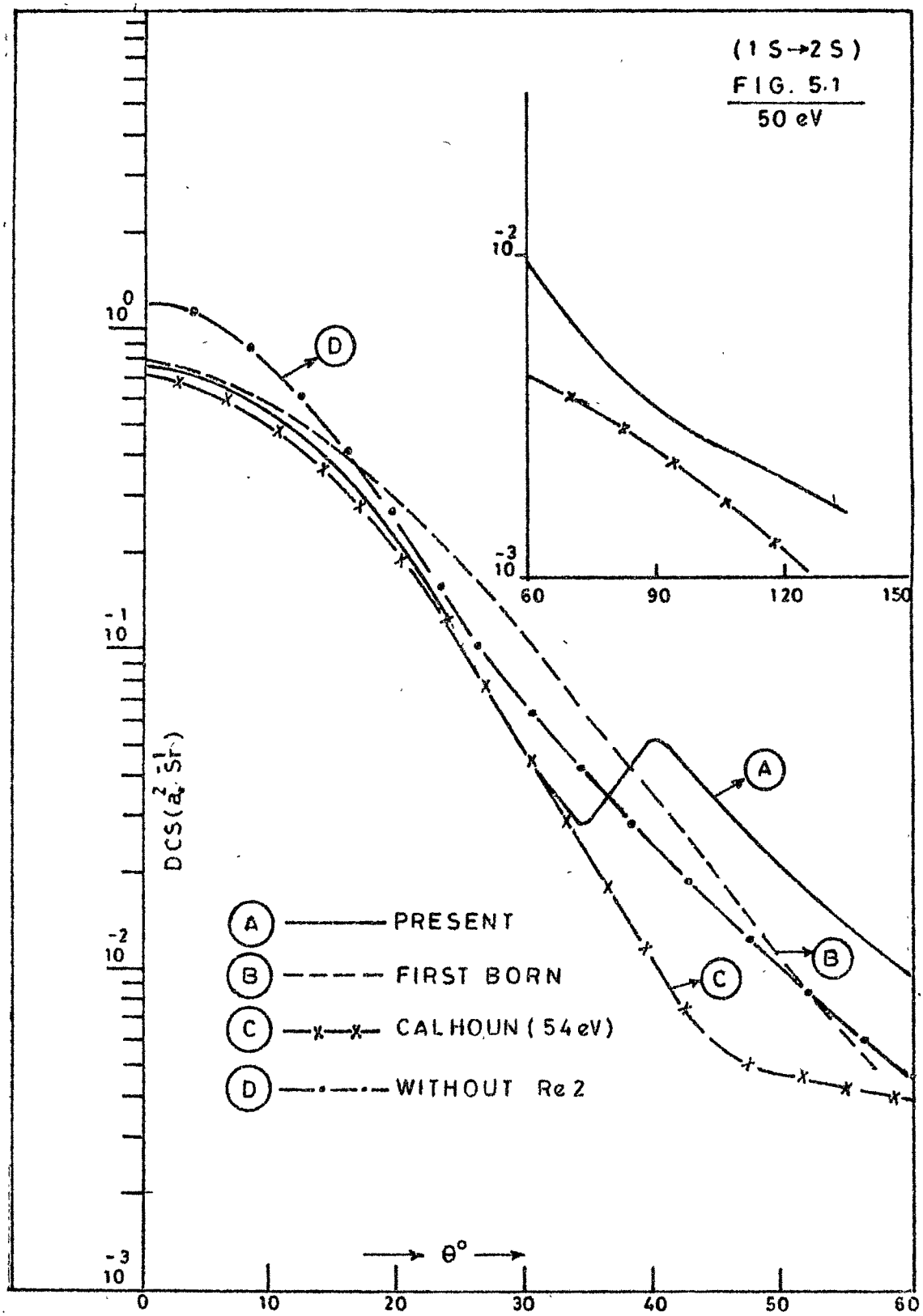
wave Born approximation (Joshipura and Desai, 1982). ✱. A comparison with some of the recent works has been made later in this chapter.

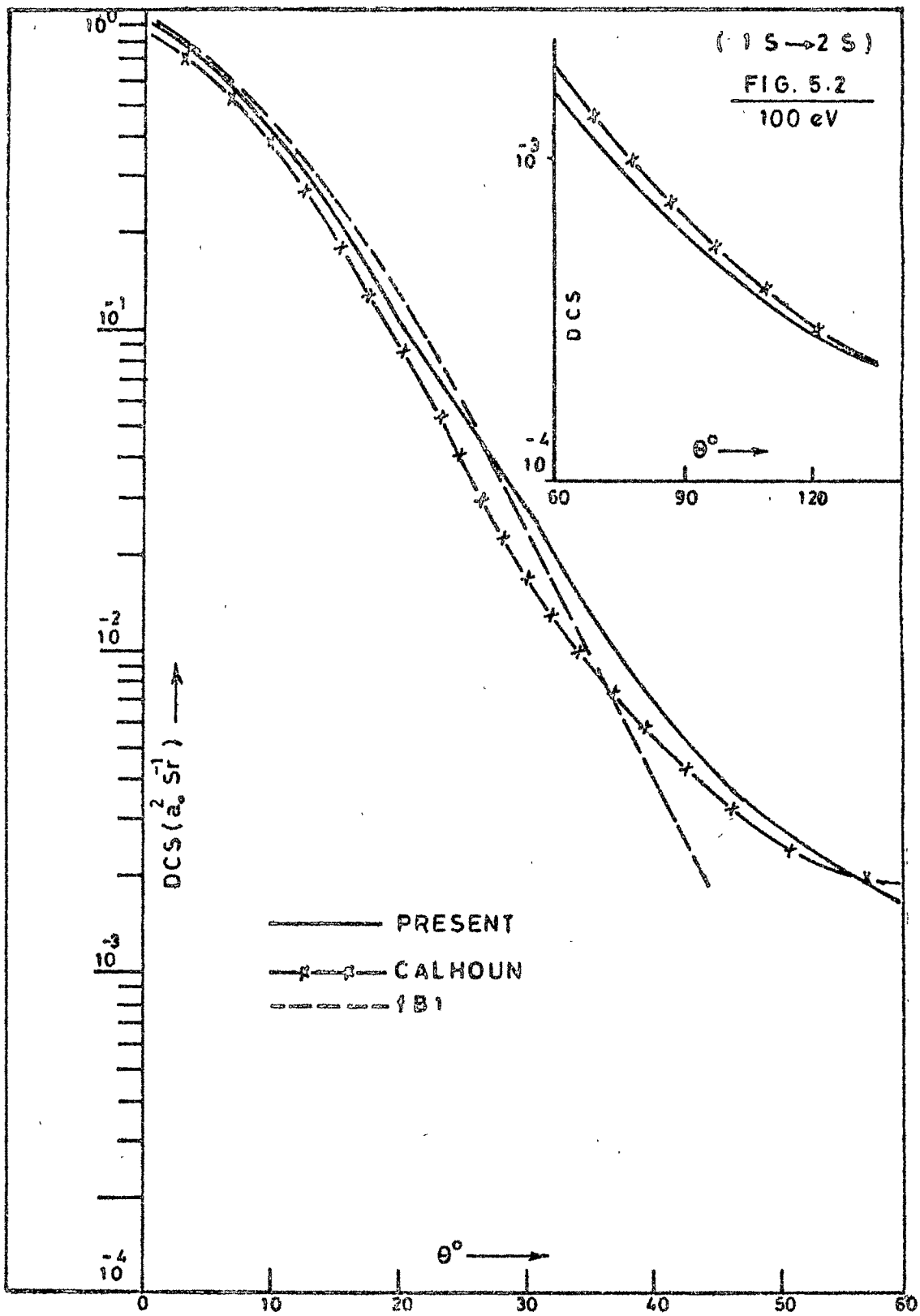
An examination of the results presented in these tables and graphs stimulates the following interesting points of discussion:

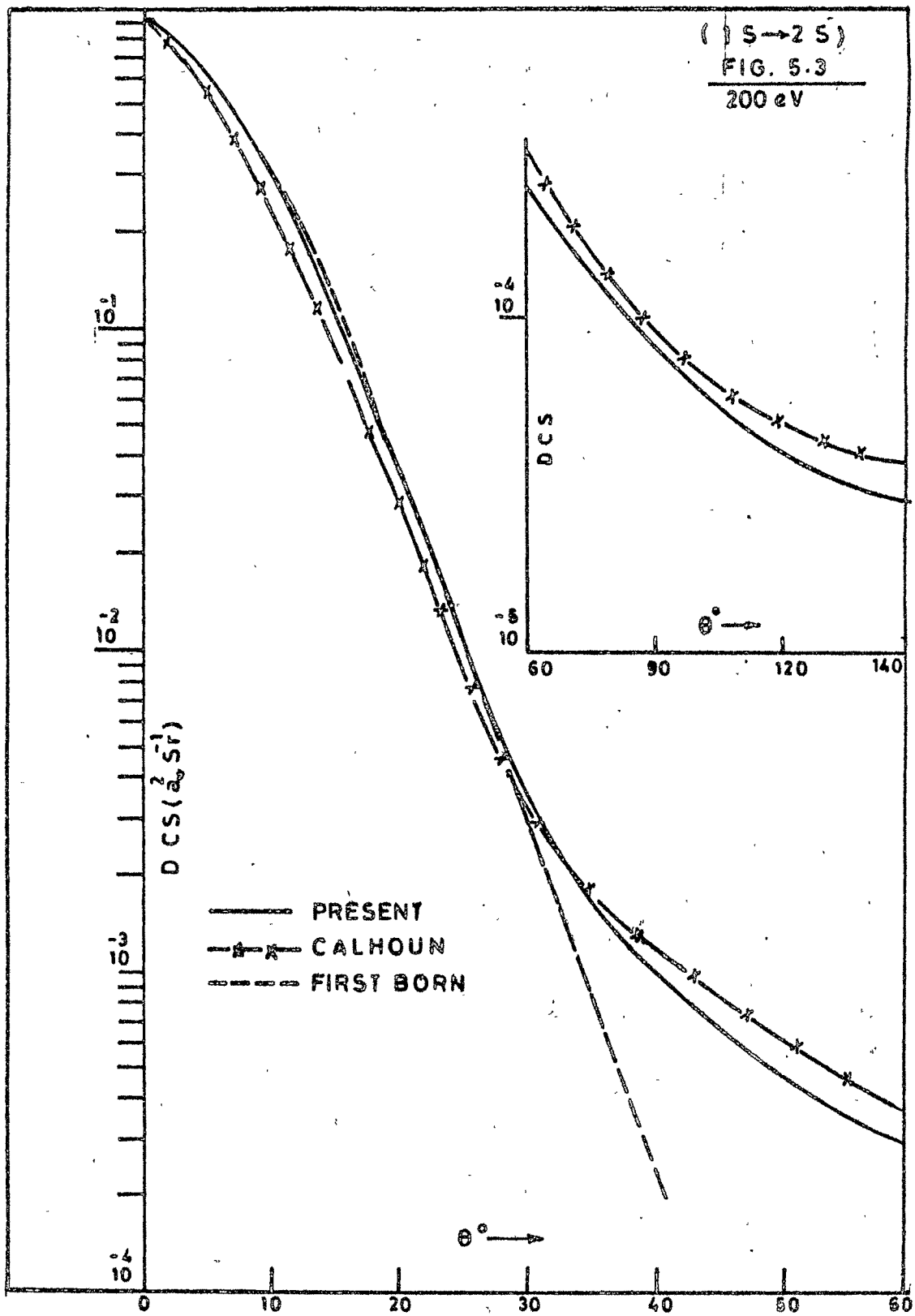
1. A general observation about the DCS of inelastic scattering is that the DCS towards the forward direction are found to increase with energy. This must be due to two reasons; the ✱ inelastic DCS (eqn. 5.80) contain a front factor k_f/k_i. This is effectively less than 1 towards lower energies. And secondly the minimum momentum transfer $\underline{q}_{min} = k_i - k_f$ is also energy dependent, approaching zero only at high energies. This behaviour is in contrast with the forward elastic DCS.

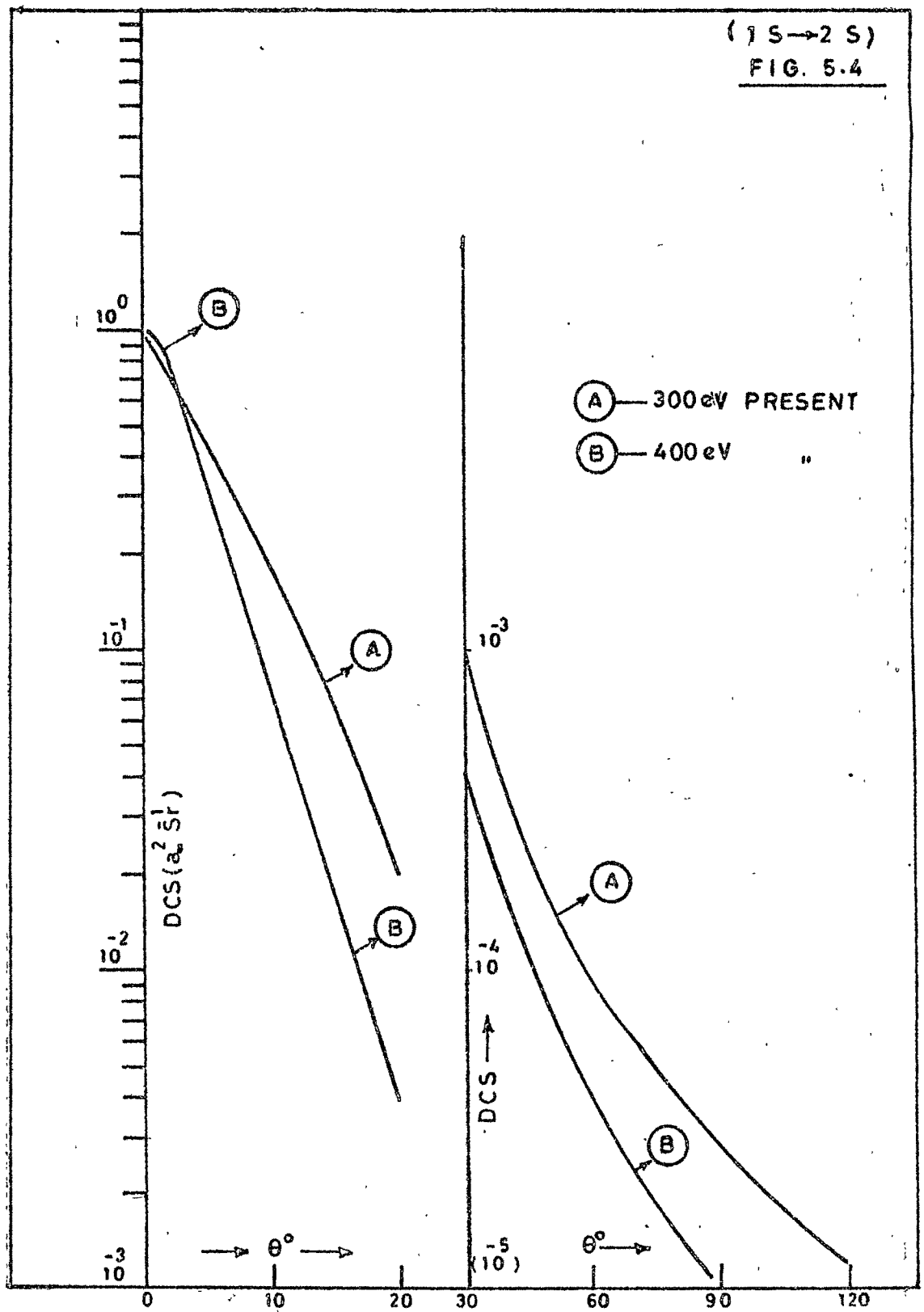
2. The results exhibited are the DCS of 1S ⟶ 2S excitation, for which, Williams (1981) ⟶ has obtained the experimental DCS separately, but these data are at low energies, upto 54.4 ev. Presently, the comparison of our results with experiments is not done. Please see also section (5.9).

3. Also not shown are the DCS without exchange. It


(1S→2S)
FIG. 5.1
50 eV
DCS(a₀² sr⁻¹)
θ°
A PRESENT
B FIRST BORN
C CALHOUN (54 eV)
D WITHOUT Re 2


(1 S → 2 S)
FIG. 5.2
100 eV
DCS
θ°
60
90
120
DCS (a_0^2 Sr^{-1})
θ°
0
10
20
30
40
50
60
PRESENT
CALHOUN
IBI


(1 S→2 S)
FIG. 5.3
200 eV
DCS
θ°
60
90
120
140
DCS (a₀² Sr⁻¹)
PRESENT
CALHOUN
FIRST BORN
θ°
0
10
20
30
40
50
60


(1S→2S)
FIG. 5.4
A — 300 eV PRESENT
B — 400 eV "
DCS (a_0^2 Sr^{-1})
DCS
θ°
θ°
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-3}
10^{-4}
10^{-5}
0
10
20
30
60
90
120

is found that the inclusion of the exchange reduces the cross-sections and the effect is appreciable near the forward direction. But compared to the elastic e-H scattering the exchange is less effective, even at 100 ev. The comments on the first order exchange term are already made.

4. The present DWBA is a high energy approximation, so one may not expect it to be good at a low energy of about 50 ev. However, we show our 50 ev results in fig. 5.1. The behaviour of the DCS at 50 ev is quite remarkable. In the region of 35 to 50° a dip-bump structure is observed. This is also observed by Buckley and Walters (1975); see also Kingston and Walters (1980). However, the DCS of the DW approximation of Calhoun et al (1976, 1977) are rather flat in this angular region. There is a remarkable disparity in different theories as regards this behaviour.

5. The distortion effect reduces the DCS near forward direction. The amount of distortion in the forward direction differs among the different theories. In this regard our theory closely agrees with the work of Calhoun et al (1976, 1977). The forward DCS obtained by these authors are

slightly less than the Born value. The earlier eikonal DWBA theory of Chen et al (1972) produced a considerable distortion of the plane waves in the forward direction. Our forward DWBA cross-sections are quite close to the first Born values, as seen from the graphs and tables. The distortion decreases with energy.

6. 100 ev is the most suitable energy for the comparison of various theories. At this energy, the effects of the inelastic process are still observable. The effects of the exchange and the projectile distortion are also appreciable. Finally our high energy DWBA method can be expected to be reasonably good at 100 ev, if not below. At this energy, we find (fig. 5.2) that our DCS coinside with the first Born value below 5°, above which the present DCS fall below the Born value, due to the distortion. Calhoun's theory produces some what more distortion here. Above 30°, the first Born DCS rapidly fall off compared to the present DCS. We could not compare our results with some of the latest calculations, for want of tabulated results. It is difficult to read off the values from the published graphs. Now, at large angles, the DCS of Calhoun's work are higher than the present results. The first Born DCS fall off very rapidly. All these comments

equally apply to the results at 200 ev.

7. Above 200 ev, the forward DCS are a little higher than the corresponding lower-energy results, as already mentioned. But as q increases, the cross-sections fall off in a nose-dive fashion. Thus, the forward and the backward DCS differ by a factor of 10^5 or more. The DCS above 400 ev, therefore, may not be of interest except near the forward direction. Now, before making some basic improvements in the present theory, let us observe once again that the term $\theta(k_i^{-2})$ in the present DWBA amplitude does not behave smoothly at lower-energies. This arises from the second term of eqn. (5.39). If we choose to retain only the first term of that expansion, the resultant amplitude will be of order k_i^{-1}. In fig. 5.1 drawn for 50 ev, we have shown curve D for the DCS without Re 2. The dip-bump structure disappears and the fall of the DCS is smooth. At the same time, the distortion in the forward direction is also inadequately produced.

5.8 Modifications over the Present DWBA

To any distorted wave method, the following questions must be posed.

1. Is distortion included in both the initial

and the final states ?

2. If the answer to the question (1) is yes, is the distorting potential in the initial and the final state the same or different ?

3. Are the distorting potentials obtained from the target eigenfunctions directly or in an approximate prodedure (e.g. Thomas-Fermi) employed ?

4. Is exchange included in calculations ?

5. Are there any specific assumptions concerning the orthogonality ?

6. Is there any attempt to consider higher orders of the projectile distortion ?

7. Is there any attempt to consider the target distortion i.e. polarization effect ? If so, is it included in both the initial and the final states ?

8. Finally, to what extent is the analytical evaluation possible ?

The answer to these questions can characterize different distorted wave approaches. For our high energy DW method, discussed in the sections

(5.5, 5.6 and 5.7), the answer to (1) is yes. Further the distorting potentials U_i and U_f are different in the initial and the final channels here, although many authors have chosen U_i in both the channels. The latter choice is not theoretically satisfactory.

The answer to (3) is that both U_i and U_f are obtained from the exact wave functions. The questions (4) and (5) are related. So far as we exclude the exchange, the orthogonality of the initial and the final distorted waves is obvious. But in the exchange calculations, the orthogonality plays a tricky role. This is discussed previously in connection with the contribution of the nuclear term to the exchange amplitude. Now, question (8), as already stated many of the works quoted in this chapter end up with numerical procedures in the final analysis. In the present DWBA method, a complete analytical evaluation of all the final expressions is possible.

Consider now the question of the higher orders of projectile-distortion. Let us recall that the T-matrix element,

$$T = \langle \phi_b^{(-)} \mid W_i \mid \phi_a^{(+)} \rangle \qquad (5.81)$$

takes into account to the first-order, that part (W_i) of the interaction which produces transition. Thus, eqn. (5.81) is essentially a first Born approximation. But in arriving at this, the interaction is splitted up into two parts and the 'static' part U_i (or U_f) is used to calculate the distorted waves. The distorted waves may be calculated to all orders of perturbation in U_i (and U_f) but we have achieved a good agreement with other theories by keeping the leading terms of the distorted waves (see eqns. (5.42), (5.46)). The higher orders of the projectile distortion are less important compared to other aspects such as the target distortion and the absorption effects. These aspects are treated in an exact second Born approximation. As we have mentioned already, the DW expression (5.81) has some elements of the second Born term and may be supplemented with that part of the second Born term which it lacks (Buckley and Walters, 1975, Winters 1978).

A basic improvement over eqn. (5.81) would be to consider the distorted wave second Born approximation (DWSBA) given formally by,

$$T^{DW2} = \langle \phi_b^{(-)} \mid W_f \, G^+ \, W_i \mid \phi_a^{(+)} \rangle \qquad (5.82)$$

The evaluation of this expression is made difficult by the presence of distorted waves. In the case of our high energy DW method, this amounts to calculating third Born like terms. These calculations may be simplified by neglecting distortion in the second order. (Buckley and Walters, 1975). Notably, the plane-wave part of eqn. (5.81) will still differ from the usual second Born term f_{B2} ($i \longrightarrow f$). This is so because, even with plane waves,

$$\langle X_b^{(-)} | W_f G^+ W_i | X_a^{(+)} \rangle = \langle X_b^{(-)} | (V - U_f) G^+ (V - U_i) | X_a^{(+)} = \langle X_b^{(-)} | VG^+ V | X_a^{(+)} \rangle - \langle X_b^{(-)} | U_f G^+ V | X_a^{(+)} \rangle - \langle X_b^{(-)} | VG^{(+)} U_i | X_a^{(+)} \rangle + \langle X_b^{(-)} | U_f G^+ U_i | X_a^{(+)} \rangle \qquad (5.83)$$

Of which the last term will vanish and the first term is the usual f_{B2} ($i \longrightarrow f$). Dewangan and Walters (1977) emphasized that distorted waves must be used, and they suggested an approximation. Winters (1978) on the other hand, used a local potential, generated by the plane wave second Born amplitude.

The effect of distortion in the second Born term has been exactly evaluated by Kingston and Walters (1980) for the elastic as well as inelastic e-H scattering.

A simple way of including the target distortion in the distorted wave first Born approximation is the method of polarized orbitals, introduced by Temkin and Lamkin (1961). All those methods which are based on the DWBA and the polarized-orbital method have been called DWPO methods, in the recent literature. The inclusion of the polarized orbitals can improve the DWBA results near the forward direction.

Temkin and Lamkin (1961) take the wave function of the electron-hydrogen atom system as,

$$\Psi = (\Psi_{1S}(r_1) + \phi_o(\underline{r}, \underline{r}_1)) F_o(\underline{r}) \qquad (5.84)$$

where, $F_o(\underline{r})$ is the continuum wave function of the incident electron. $\phi_o(\underline{r}, \underline{r}_1)$ represents the change in the eigen function of the 1S hydrogen atom, perturbed by the presence of the continuum electron fixed at $\underline{r}$. The term $\phi_o(\underline{r}_1, r_1)$ is evaluated by expanding the term $1/|(\underline{r} - \underline{r}_1)|$ of the potential, in the multipole expansion and retaining only the dipole term. This procedure yields (see e.g. Mott

and Massey, 1965),

$$\phi_o(\underline{r},\underline{r}_1) = -\frac{1}{\sqrt{\pi}} \frac{e(r,r_1)}{r^2} e^{-r_1} (r_1 + \tfrac{1}{2} r_1^2) \cos\theta_1 \quad (5.85)$$

where,

$$e(r, r_1) = 0, \quad r < r_1$$

$$= 1, \quad r > r_1 \quad (5.86)$$

'θ_1' is the angle between $\underline{r}$ and $\underline{r}_1$.

This method of including the polarization of the target (in the initial state) has been successfully employed by Gupta and Mathur (1978 a, b). We now incorporate the polarized orbitals in our DWBA formulation. The present amplitude f_{HE}^{DW1} does not include the target polarization i.e. the term $\phi(r, r_i)$ of eqn. (5.84). Hence, we require now the amplitude,

$$f_{pol} = -4\pi^2 \langle \phi_b^{(-)} | W_i | \phi_{pol}^{(+)} \rangle \quad (5.87)$$

so that, the total scattering amplitude is,

$$f^{DWP} = f_{HE}^{DW1} + f_{pol} \quad (5.88)$$

To obtain now 'f_{pol}', we proceed as follows.

$$- 4\pi^2 \langle \phi_b^{(-)} \mid W_i \mid \phi_{pol}^{(+)} \rangle = - \frac{1}{2\pi} \iint d\underline{r} \; d\underline{r}_1$$

$$e^{i\underline{q}.\underline{r}} \left(1 + \frac{i}{k_f} \int_{-\infty}^{\infty} dz' \; e^{+i\beta_2 z'} H(z')\right.$$

$$\times \left(1 - \frac{iz'}{2k_f} \nabla_{z'}^2\right) U_f(\underline{r} - \underline{z}'))$$

$$\times \psi_{2S}(r_1)\left(-\frac{1}{r} + \frac{1}{|\underline{r} - \underline{r}_1|}\right) \phi_o(\underline{r}, \underline{r}_1)$$

$$\times \left(1 + \frac{i}{k_i} \int_{-\infty}^{\infty} dz'' \; e^{i\beta_1 z''} H(z'')\right.$$

$$\left.\left(1 + \frac{iz''}{2k_i} \nabla_{z''}^2\right) U_i(\underline{r} - \underline{z}'')\right) \qquad (5.89)$$

where, we have substituted for the distorted waves from eqn. (5.46). Further, consider the first term of eqns. (5.89). Expanding $1/|\underline{r} - \underline{r}_1|$ and retaining only the dipole term, we get the $\underline{r}_1$ integral in the eqn. (5.89). The resulting expression is a typical r^{-4} dependent long-range polarization potential

$$g(r) = -\frac{\sqrt{2}}{3r^4}\left(\frac{4!}{l^5}\left(1 - e^{-lr}\sum_{k=0}^{4}\frac{(lr)^k}{k!}\right)\right.$$

$$\left. - \frac{6!}{4l^7}\left(1 - e^{-lr}\sum_{m=0}^{6}\frac{(lr)^m}{m!}\right)\right) \qquad (5.90)$$

$$l = 3/2.$$

For further integration it is convenient to write,

$$\sum_{k=0}^{4}\frac{(lr)^k}{k!} = e^{lr} - \sum_{k=5}^{\infty}\frac{(lr)^k}{k!} \qquad (5.91)$$

Now, we go back to f_{pol}, which we write in a way similar to eqn. (5.52),

$$f_{pol} = f_{1p} + f_{2p} + f_{3p} + f_{4p} \qquad (5.92)$$

whereas in (5.53), we have

$$f_{1p} = \frac{-\sqrt{2}}{3}\int d\underline{r}\; e^{-i\underline{q}.\underline{r}}\; g(r) \qquad (5.93)$$

as the most dominent term of the polarization amplitude f_{pol}. The next two terms are mutually similar in form, both of them involving the distorted waves. The last term

is ignored. Now, the terms f_{2p} and f_{3p} can be evaluated by using the Fourier techniques. Accordingly, let the symbol $\bar{g}(r)$ represent the Fourier transform of $g(r)$. Then by analogy with f_2 of eqn. (5.60), the term f_{2p} takes the shape,

$$f_{2p} = -\frac{4\pi^3}{k_i}\left(i\int d\underline{p}\,\bar{g}(\underline{q}-\underline{p}-\underline{\beta}_1)\,\bar{U}_i(\underline{p}+\underline{\beta}_1)\right.$$

$$-\frac{1}{\pi}\mathcal{P}\int d\underline{p}\int_{-\infty}^{\infty} dp_z\left(1+\frac{p^2+p_z^2}{2k_i}\frac{\partial}{\partial\beta_1}\right)$$

$$\left.\frac{1}{p_z-\beta_1}\,\bar{g}(\underline{q}-\underline{p}-\underline{p}_z)\,\bar{U}_i(\underline{p}+\underline{p}_z)\right) \qquad (5.94)$$

The procedure of further evaluation is very much like that of the previous calculations.

Now, the complete polarization term can also be calculated under the electron-exchange. But as pointed out by Gupta and Mathur (1978a, b) the labour is not worth doing, so we neglect the exchange-polarization terms. Thus, the DCS of electron-impact 1S $\longrightarrow$ 2S excitation of hydrogen, in present exchange DWPO method are obtained from the following experession.

$$\frac{d\sigma}{dw} = \frac{k_f}{k_i}\left(\frac{1}{4}\left|f^{DWP} + g_{HE}^{DW1}\right|^2 + \frac{3}{4}\left|f^{DWP} - g_{HE}^{DW1}\right|^2\right) \qquad (5.95)$$

5.9 Comparison and Discussion of the 1S —— 2S Results

Now we exhibit the DCS results of our present DWBA method including the exchange and polarization, as calculated from eqn. (5.95). Tables 5.4 to 5.6 show the comparison of the present DCS with recently published data. At 100 ev (table 5.5) the first Born DCS are also given. Further in the figs. 5.5 to 5.8, we give the graphical plots of the present DWPO results along with the data at 54.4, 100, 200, 300 and 400 ev. The comparisons are made with the following :

1. The DWSBA of Kingston and Walters (1980), denoted by DWSBA (KW) in the tables, graphs and in the discussion, has been mentioned previously, in sec. (5.8).

2. The second order eikonal calculation has been done in the angular range $0^\circ - 30^\circ$ by Unnikrishnan and Prasad (1982). These results are denoted by SOEA (UP), everywhere.

The separate DCS of H(2s) excitation have

Table 5.4

A comparison of the DCS of 1S —— 2S excitation in the e-H inelastic scattering. (The present DCS include exchange and polarization)

energy 54.4 ev

Scattering angle	Data of Williams	DWSBA (KW)	SOEA (UP)	Present
0	-	1.5 + 00	1.95 + 00	1.6 + 00
10	6.8 - 01	3.2 - 01	6.8 - 01	9.8 - 01
20	1.4 - 01	1.0 - 01	1.4 - 01	3.0 - 01
30	3.7 - 02	2.8 - 02	3.4 - 02	5.8 - 02
35	-	1.3 - 02	-	8.0 - 02
40	1.8 - 02	6.8 - 03	-	4.2 - 02
50	-	5.2 - 03	-	1.5 - 02
60	1.0 - 02	5.9 - 03	-	7.6 - 03
80	5.2 - 03	4.0 - 03	-	3.9 - 03
90	5.7 - 03	3.2 - 03	-	2.9 - 03
120	3.0 - 03	1.7 - 03	-	1.5 - 03

Table 5.5

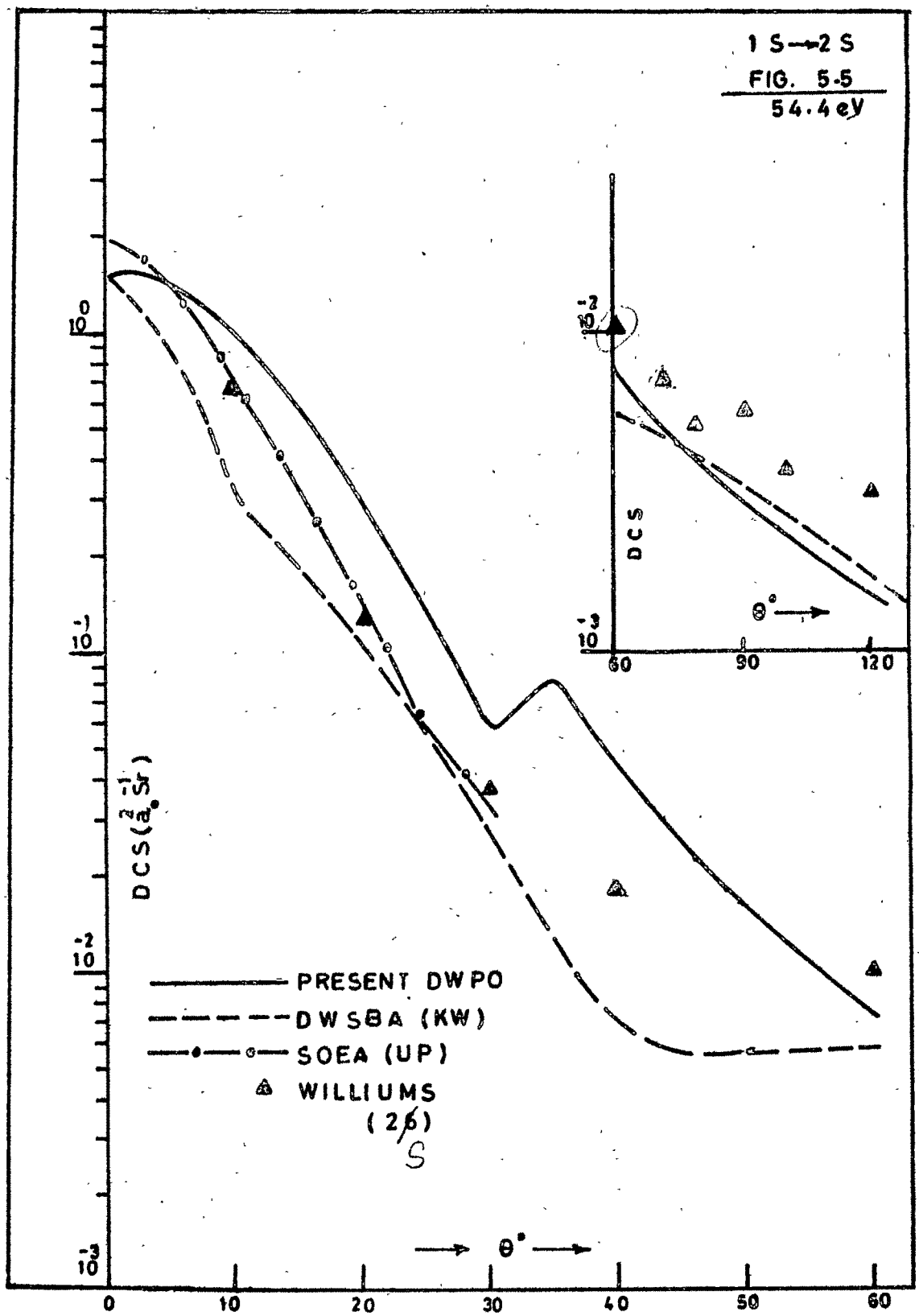
DCS of 1S —— 2S excitation 100 ev

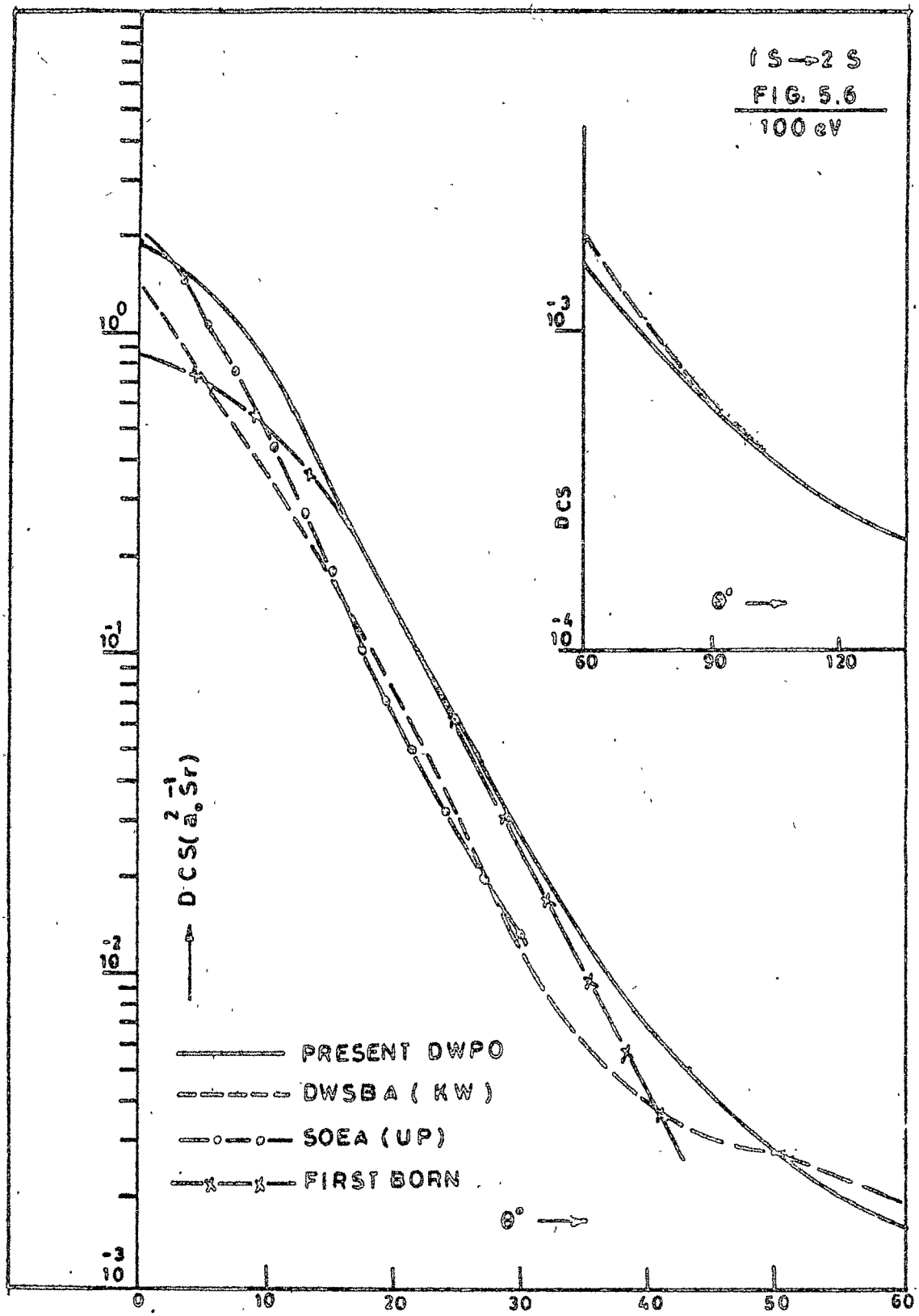
Scattering angle (deg)	SOEA (UP)	DWSBA (KW)	First Born	Present
0	2.1 + 00	1.5 + 00	8.9 - 01	1.9 + 00
10	4.7 - 01	3.8 - 01	5.2 - 01	7.8 - 01
20	6.4 - 02	7.8 - 02	1.4 - 07	1.4 - 01
40	-	3.9 - 03	4.2 - 03	6.2 - 03
60	-	1.9 - 03	-	1.6 - 03
90	-	5.6 - 04	-	5.6 - 04
120	-	2.9 - 04	-	2.9 - 04

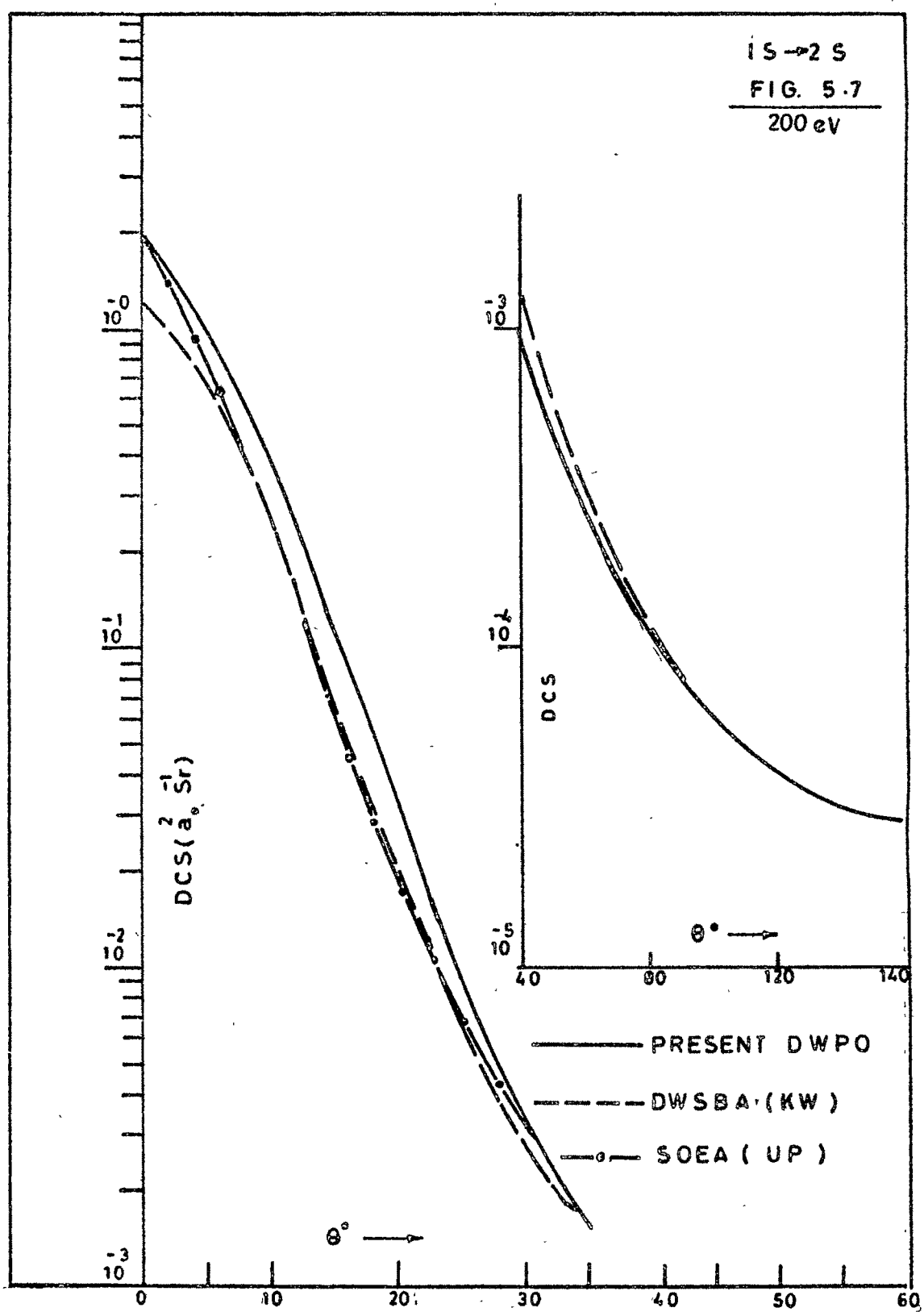
Table 5.6

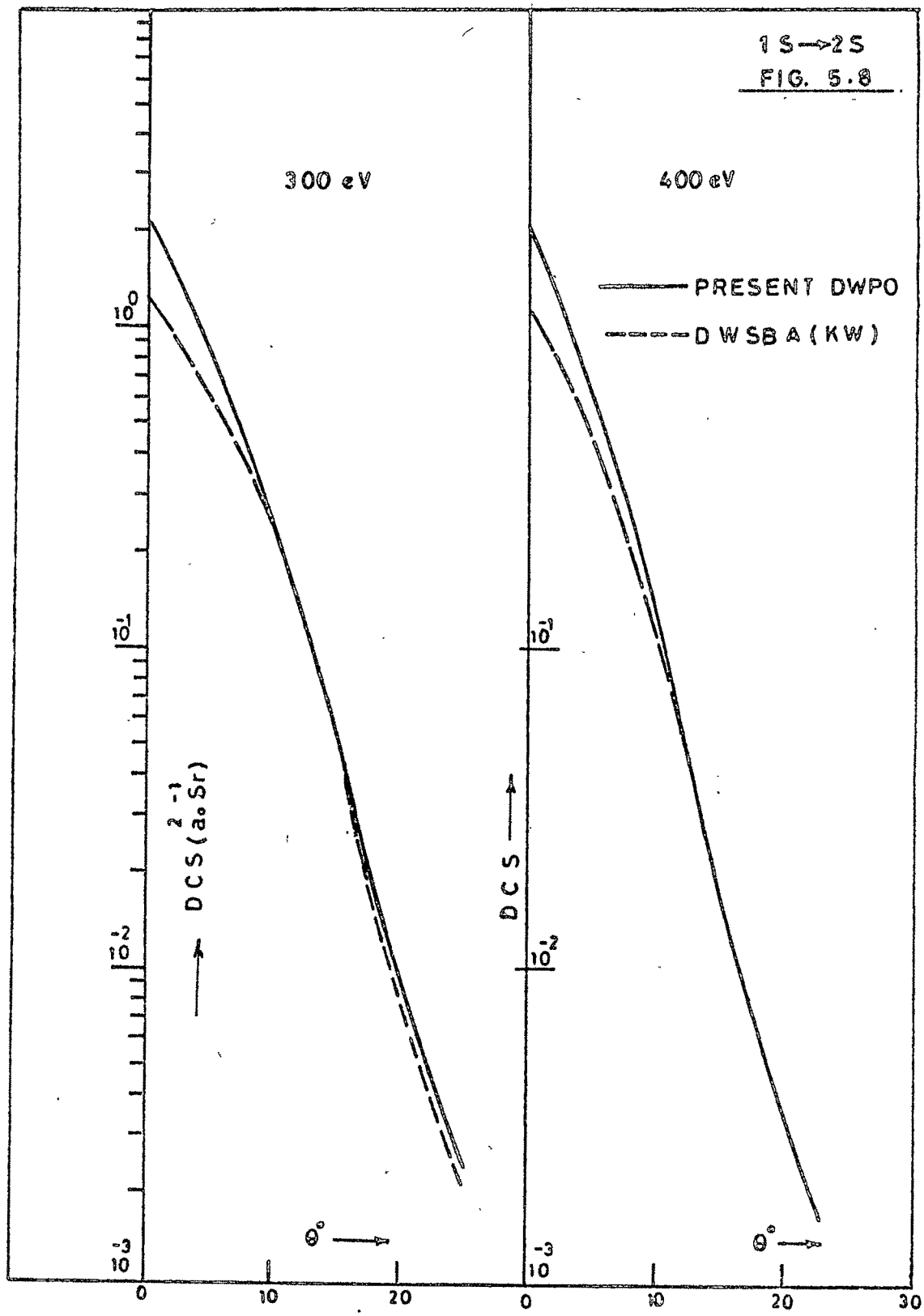
DCS of 1S —— 2S excitation 200 ev

Scattering angle (deg)	SOEA (UP)	DWSBA (KW)	Present
0	1.9 + 00	1.3 + 00	2.1 + 00
10	2.7 - 01	2.7 - 00	4.1 - 01
20	1.9 - 02	2.2 - 02	3.3 - 02
40	-	1.1 - 03	9.4 - 04
60	-	3.4 - 04	2.8 - 04
90	-	8.0 - 05	8.0 - 05
120	-	4.0 - 05	4.0 - 05


1 S→2 S
FIG. 5-5
54.4 eV
DCS ($a_0^2 Sr^{-1}$)
10^{0}
10^{-1}
10^{-2}
10^{-3}
0
10
20
30
40
50
60
θ°
PRESENT DWPO
DWSBA (KW)
SOEA (UP)
WILLIUMS
(2S)
DCS
10^{-2}
10^{-3}
60
90
120
θ°


1 S → 2 S
FIG. 5.6
100 eV
DCS(a.u.)
θ°
PRESENT DWPO
DWSBA (KW)
SOEA (UP)
FIRST BORN
DCS
θ°
0
10
20
30
40
50
60
90
120


1S→2S
FIG. 5.7
200 eV
DCS(a_0^2 Sr^{-1})
DCS
θ°
PRESENT DWPO
DWSBA·(KW)
SOEA (UP)


1S→2S
FIG. 5.8
300 eV
400 eV
PRESENT DWPO
DWSBA (KW)
DCS (a₀² Sr⁻¹)
DCS
θ°
θ°
10⁰
10⁻¹
10⁻²
10⁻³
0
10
20
30

been obtained recently by Williams (1981), but these measurements are upto 54.4 ev. Now the discussion follows.

1. First of all, at low energies, e.g. 54.4 ev, the overall behaviour of the present DCS (fig. 5.5) is similar to that without polarization (see fig. 5.1) except that here the polarization enhances the DCS near forward direction. At 54.4 ev (fig. 5.5) in our results a dip appears around 30° followed by a bump around 35°. This is also observed by Buckley and Walters (1975), at 54.4 ev. In the DWSBA (KW) this structure is flattened. Thus, we conclude that at lower energies a higher order calculation is required. Previously also we noted that the high energy theories are not successful below 100 ev. Further the 54.4 ev results of SOEA (UP) are slightly above ours in the forward direction. It must be noted that SOEA (UP) does not include any polarization effect, which would increase the DCS slightly further near the forward direction. In the region of 5° - 30°, our results are higher than the others and lie close to the DWSBA (KW) only beyond 60°. None of the theories is in accord for all angles, with the separate H(2S) measurement of Williams (1981) at 54.4 ev, SOEA (UP) is good for small angles. DWSBA (KW) more or less underestimates at all angles,

while the present results are overestimating. This overestimation at a low energy is frequently found with many high energy theories. The dip-bump part of the DCS curve is not evident in the experimental points; however, the angular interval of 10° in the measurements is not small enough to reveal any such behaviour. The experimental results show a dip-bump around 80° and 90°, a behaviour not supported by any theory. (see also table 5.4).

2. The forward DCS in different theories do not show the same behaviour. In the present case, the forward DCS show a gentle rise with respect to energy. The reason is discussed previously, in sec. 5.7.

3. Our 100 ev forward DCS lie close to SOEA (UP) but above DWSBA (KW); both of the latter results lie below the present as well as the first Born result upto about 30°, beyond which the first Born result tends to fall off. The DWSBA (KW) is higher than the present result beyond 50°. The difference between these two results is narrower at 100 ev than at 54.4 ev but the shape of the DCS curves differs. At 200 ev the agreement is better. The DWSBA is higher than the present result between 50° and 85°.

4. At 300 ev and above the cross-sections are significant only within the forward cone of about 30°. Hence, we have not shown the large angle results. The effect of polarization decreases with energy. The agreement between the present theory and the DWSBA (KW) is generally good except near the forward direction. Above 400 ev no special features of the cross-sections are revealed so we have not shown any further results.

5. Our calculations have omitted the third order amplitude (f_4 of eqn. 5.54), the inclusion of which can bring a closer agreement with the other theories.

5.10 1S —— 2p Excitation in e-H Collisions

We have studied the excitation to H(2S) by electron impact, in the various theoretical treatments. Now, the cross-sections of n = 2 excitation are given by the sum of the 2S and 2p state cross-sections, with the latter averaged over 2l + 1 (l = 1) magnetic substates. The 2p state splits up into three magnetic substates $m_1 = 0$, and $\pm$ 1; it is found that the first Born amplitude, exists only for m = 0, the Glauber (Thomas and Gerjuoy, 1971) amplitude as well as the second order eikonal or

the Wallace amplitude (Unnikrishnan and Prasad, 1982) exists only for m = $\pm$ 1. Already in section 5.2 we have emphasized the use of the first Born approximation at small angles in the 1S $\longrightarrow$ 2p transition. The first Born DCS are so overwhelmingly large at small angles that the effects like exchange, polarization and projectile distortion are not much significant for this case.

Further, as noted by Chen et al (1972), the distortion effects in the $2p_0$ and $2p_{\pm 1}$ substates are opposite and hence the net distortion is quite small. However there are no recent studies in this regard.

Here, in the table 5.7 the first Born DCS at 100, 200 and 300 ev energy are exhibited for small angles, where the strong forward peaks are apparent. Also in that table these are compared at 100 ev with the recent higher order calculations, viz, DWSBA (KW) and SOEA(UP). One can see a close agreement at small angles. The distorted wave part of the calculation in the 1S $\longrightarrow$ 2p case differs slightly from the previous (1S $\longrightarrow$ 2S) one. Presently, the term A_{2S} of eqn. (5.56) is replaced by A_{2p}, given in eqn. (5.13). Let us recall that our distorted wave approach is similar to the Glauber

Table 5.7

DCS of 1S —— 2p transition 100 ev

θ (deg)	First Born DCS	DWSRA (KW)	SOEA (UP)
0	100	98.6	91.5
5	25	24	23
10	05	4.6	3.98
15	1.3	1.0	-

1S —— 2p

θ (deg)	First Born DCS 200 ev	First Born DCS 300 ev
0	210	310
5	12	08
10	1.7	0.9

formulation, so that, the substate m = 0 does not contribute. However, the m = 0 contribution will come from the first term of our DWBA theory, which is the plane wave first Born term. The effects of exchange and polarization are not dominent in the 1S $\longrightarrow$ 2p calculations. A general trend of the 1S $\longrightarrow$ 2p cross-sections is that near the forward direction these are much larger than the 2S cross-sections, but beyond 60° the two are nearly equal. We have not shown here the 1S $\longrightarrow$ 2p cross-section of the present theory. Calculations on the higher states in the atomic hydrogen are rare. For n = 3 excitation in e-H collisions, the distorted wave calculations are done by Syms et al (1975). Exclusive distorted wave calculations have been made for excitation of Helium; see Buckley and Walters (1975), Scott and McDowell (1975 | 1976), Baluja and McDowell (1979) etc. The 2S $\longrightarrow$ 3S excitation in e-Li scattering was studied by Vanderpoorten and Winters (1977). It is interesting to note that the ground state of Li atom is similar to H(2S), under the inert core approximation, so that, the present DWBA method can be certainly extended to the 2S $\longrightarrow$ 3S process in e+Li scattering. Further, it must be mentioned that the total inelastic cross-sections (σ_{inel}) have been obtained by Inokuti (1974b) for

several atomic targets beyond H and He. Lastly there are also some attempts to study electron impact excitation in the other atoms ($Z > 3$). With this, we conclude the part A of the fifth chapter.

PART B

5.11 Electronic Excitation in Electron-Molecule Collisions

We now devote some attention to inelastic scattering of fast electrons by molecules, in which electronic states are excited; precious little has been done in this field. The target of our investigation is the H_2 molecule.

First of all a few words about the electronic states of the H_2 molecule. The ground state of H_2 is denoted by $X^1\ \Sigma_g^+$ and is made up of two 1S hydrogen atoms properly combined. Here, the term Σ corresponds to the component (along the nuclear axis) of the total electronic orbital angular momentum being zero. The right upper + sign indicates the symmetry of the molecular wave function with respect to reflection in any plane passing through the nuclear axis. Further, if an electronic state of a

homonuclear diatomic molecule will be symmetric or anti-symmetric relative to the exchange of the two nuclei. These two alternatives are denoted respectively by the suffixes 'g' (for gerade) and 'u' (for ungerade). The left upper '1' or '3' near Σ indicates the singlet or triplet state. The first excited state of H_2, i.e. $b^3\ \Sigma_u^+$ is a triplet state, with two 1S electrons having an identical spin. One of the first triumphs of the modern quantum theory was to predict that this triplet state would be dissociative. Given below are the low-laying excited states of H_2, with separated atom limit indicated at the right hand side (Massey et al 1969).

Electronic state		Separated-atom-limit
X^1	Σ_g^+	$(\sigma_g\ 1S)^2$
b^3	Σ_u^+	$(\sigma_g\ 1S\ \sigma_u\ 1S)$
B^1	Σ_u^+	$(\sigma_g\ 1S\ \sigma_u\ 2S)$
a^3	Σ_g^+	$(\sigma_g\ 1S\ \sigma_g\ 2S)$
E^1	Σ_g^+	$(\sigma_g\ 1S\ \sigma_g\ 2S)$
C^1	Σ_u^-	$(\sigma_g\ 1S\ \pi_u\ 2p)$
C^1	π_u^+	$(\sigma_g\ 1S\ \pi_u\ 2p)$
C^3	π_u	$(\sigma_g\ 1S\ \pi_u\ 2p)$

Now, we outline the work done in studying the electron-impact excitation of these states. Apart from the pioneering work of Massey (1932) and Roscoe (1941), the Born-Ochkur calculations were made by Khare and Moiseiwitch (1965, 1966) With the use of the molecular wavefunctions, the calculations are quite difficult beyond the first order. The Born-Ochkur-Rudge type of calculations were done by Cartwright and Kuppermann (1967), Chung and Lin (1972, 1974) andC Chung, Lin and Lee (1975). A close-coupling result is by Chung and Lin (1978). A sophisticated version of the distorted wave method called the L^2 basis method has been used by Rescigno et al (1975, 1976, 1979). Most of these methods are confined to energies below 50 ev, in particular around 10 to 20 ev, corresponding to the excitation energies of various states of H_2. A most recent piece of work comes from Lee-Mu Tao et al (1982) (see also Fliflet and McKoy 1980). Further, experimental results if any, are rare. Mention must be made of Geiger's (1964) experiments at very high energies, and the recent measurement of Srivastava and Jansen (1977) on $B^1\Sigma_u^+$ transition by 20 - 60 ev electrons. No cross-sections, to our knowledge, are reported in the range 100 - 1000 ev.

Now, we spell out our aim in taking up the

present study. As noted previously, most of the theoretical methods developed for electron-atom scattering have been successfully extended to molecular targets. In fact, for elastic scattering, we have used the accurately evaluated atomic scattering amplitudes to obtain the cross-sections of the electron-molecule scattering, via independent atom model. It is not known whether this model has ever been extended to inelastic scattering involving electronic excitation by fast electrons, except the electron diffraction studies (Massey et al 1969). Presently our purpose is to employ the IAM to obtain the inelastic e-H_2 cross-sections by starting from our previously derived inelastic e-H scattering amplitudes.

5.12 Independent Atom Model for Inelastic Electron Molecule Collisions

The simple IAM in this case is quite similar to that discussed in the fourth chapter, on elastic scattering. Considering the e-H_2 system, we assume that each atom scatters the incident electron, freely and independently, and further, only one of the two atoms is excited in the process. Though the final expression is similar to that of elastic scattering it is derived in a different manner.

Assume that in the inelastic process one of the two target electrons, denoted by suffix '1' is involved and the other one, given by suffix 'C', forms an inert core. The antisymmetric wave function of the molecule can be written as a product of one-electron wave functions, so we write the initial and the final state wave functions of the target as follows (Massey et al 1969).

$$\psi_i = \frac{1}{\sqrt{2}} (\phi_i (r_{1A}) \pm \phi_i(r_{1B})) \psi_C (r_c) \qquad (5.96a)$$

$$\psi_f = \frac{1}{\sqrt{2}} (\phi_f (r_{1A}) \pm \phi_f (r_{1B})) \psi_C (r_c) \qquad (5.96b)$$

where A and B denote the two nuclei. The $\pm$ sign here denotes respectively the symmetric or antisymmetric wave function of electron 1 with respect to interchange of nuclei A and B. The atomic orbitals are denoted by ϕ_i etc. Also,

$$\underline{r}_{1A} - \underline{r}_{1B} = \underline{R} \qquad (5.97)$$

Now, the first Born approximation of this case is

$$f^M_{B1} = - \frac{1}{2\pi} \int e^{i\underline{q}.\underline{r}} \, d\underline{r} \, \langle \psi_f | V | \psi_i \rangle \qquad (5.98)$$

with

$$\langle \psi_f \,|V|\, \psi_i \rangle = \iint d\underline{r}_1 \; d\underline{r}_c \; \psi_f^* \left(- \frac{1}{|\underline{r} - \underline{R}/2|} \right.$$

$$\left. - \frac{1}{|\underline{r} + \underline{R}/2|} + \frac{1}{|\underline{r} - \underline{r}_1|} + \frac{1}{|\underline{r} - \underline{r}_c|} \right) \psi_i$$

$$= \frac{1}{2} \int d\underline{r}_1 \left(\phi_i(r_{1A}) \pm \phi_i(r_{1B}) \right)$$

$$\times \frac{1}{|\underline{r} - \underline{r}_1|} \left(\phi_f(r_{1A}) \pm \phi_f(r_{1B}) \right) \qquad (5.99)$$

Here, the coordinates $\underline{r}$, $\underline{r}_1$, $\underline{R}/2$ refer to the molecular midpoint and orthonormality is used. Thus, from the last equation dropping the terms of overlap integrals,

$$f_{B1} \doteq - \frac{1}{q^2} \left[e^{i\underline{q}\cdot\underline{R}/2} \left(\int d\underline{r}_{1A} \, \phi_f^*(r_{1A}) \right. \right.$$

$$\left. e^{i\underline{q}\cdot\underline{r}_{1A}} \, \phi_i(r_{1A}) \right) \pm e^{-i\underline{q}\cdot\underline{R}/2}$$

$$\left. \int d\underline{r}_{1B} \, \phi_f^*(r_{1B}) \, e^{i\underline{q}\cdot\underline{r}_{1B}} \, \phi_i(r_{1B}) \right] \qquad (5.100)$$

Herein lies the central assumption of the independent atom model, viz. that in writing (5.100) the overlap of atomic orbitals is neglected. Now the $\pm$ sign holds for the identical or opposite nuclear symmetry in the initial and the final states. The eqn. (5.100) can also be written in terms of the atomic scattering amplitudes as

$$f^{M}_{B1} = 2\, f^{a}_{B1} \times (\cos(\underline{g}.\underline{R}/2))$$

or

$$2\, f^{a}_{B1} \times (i \sin(\underline{g}.\underline{R}/2)) \qquad (5.101)$$

where f^{a}_{B1} denotes the corresponding atomic amplitude. The factor $\cos(\underline{g}.\underline{R}/2)$ or $i \sin(\underline{g}.\underline{R}/2)$ arises according as the nuclear symmetry is unchanged or changed. The relation like (5.101) holds true for higher order Born terms also. The final result is obtained by squaring the amplitude and averaging over all orientations of $\underline{R}$, as done previously. We have the averaged e-H_2 inelastic DCS,

$$\bar{I}(\theta) = 2\, I_a(\theta)\left(1 \pm \frac{\sin qR}{qR}\right) \qquad (5.102)$$

$I_a(\theta)$ denotes the corresponding atomic inelastic DCS.

The atoms are not 'free' scatterers, so the valance bond correction is required to be applied, both in the initial and final state orbitals. For the ground state of H_2 this is given by taking $Z = 1.2005$ and in the final state, since the internuclear separation actually increases, the valance-distortion may be neglected, at least for H_2. The second important aspect is the inclusion of electron exchange.

Consider the electron-impact transition from the ground (singlet) state to an excited singlet state. The electron-exchange in this case must be in the triplet (see also Jhanwar 1980). Further the probability of a target electron of spin say α being close to a nucleus A or B is 1/2. Hence, the scattering amplitude for any atom, including exchange must be,

$$f_A = f_H(Z) - \frac{1}{2} g_H(Z) \qquad (5.103)$$

where, $f_H(Z)$ and $g_H(Z)$ are the direct and the exchange amplitudes for inelastic scattering from the target H-atom represented by orbital e^{-Zr}. Thus, the average inelastic $e\text{-}H_2$ DCS with exchange are,

$$\bar{I}(\theta) = \frac{k_f}{k_i} 2 \left| f_H(Z) - \frac{1}{2} g_H(Z) \right|^2 \times \left(1 \pm \frac{\sin qR}{qR}\right) \qquad (5.104)$$

But if the excitation leads to the final triplet state, then the exchange must occur in the singlet and hence the final expression is,

$$\bar{I}(\theta) = \frac{k_f}{k_i} 2 \left| f_H(Z) + \frac{1}{2} g_H(Z) \right|^2 \times \left(1 \pm \frac{\sin qR}{qR} \right) \qquad (5.105)$$

Now, an additional complication, not encountered in the case of elastic scattering, arises here due to vibrational aspect. The ground state of H_2 may be taken as the ground vibrational state also. But the final electronic state may be accompanied by a final vibrational state v'. Hence we have to consider the probability of the vibrational transition $0 \longrightarrow v'$. This probability is expressed in terms of the Frank-Condon factors (Allison and Dalgarno, 1970). Another related fact is that in the final state, the internuclear ' (equilibrium) separation increases. This fact is not considered in the basic expression, (5.102). One more difference between this and the IAM formula of the elastic scattering will arise in the kinematical calculation of momentum transfer q. Here, we have to use,

$$\frac{1}{2} k_i^2 = \frac{1}{2} k_f^2 + E_{fi} \qquad (5.106)$$

where E_{fi} is the energy of the vertical excitation of an electronic state of the molecule. Because of this, the present 'q' will slightly differ from the corresponding value of the atomic transition. Let us also remark in passing that if the final state is a triplet one, the scattering cannot occur without exchange and we must use eqn. (5.105).

A comparison of the diffraction factors for elastic and inelastic scattering proves to be crucial. Whenever the nuclear symmetry changes, the diffraction factor is 1-(sin qR)/qR. This factor is quite small in the forward direction though not zero. Thus, if the nuclear symmetry changes, the forward inelastic DCS are expected to be rather small. Finally the expression of the DCS is to be multiplied by (2S + 1)/2, where S = 0 for the singlet-singlet and 1 for the singlet-triplet transitions.

Apart from all these special comments high--lighting the characteristic features of the electronic excitations in the diatomic molecules, the usual corrections to the IAM can be made here also. Notable of them are the multiple scattering and the effect of nuclear vibrations. These effects are quite insignificant in the e-H_2 system, it is even more so for the excited states of the molecule. The requirements of a 'good' IAM spelled out in the

beginning of section (4.6) of the previous chapter, are well met in the case of e-H_2 system at intermediate to high emergies. In the treatment of elastic scattering of electrons by H_2 molecules, the model breaks down below 100 ev. This might also be the case presently.

5.13 Applications the IAM to Inelastic e-H_2 Scattering

Consider first the excitation of H_2 molecules from the ground state to the singlet $B^1\ \Sigma_u^+$ state, the lowest stable excited state of H_2. Here, since the nuclear symmetry changes, we have to use the diffraction factor $(1 - \frac{\sin\ qR}{qR})$. We take $R = 1.4\ a_o$, which is not a very good choice. To consider the valance-bond correction we take the orbitals in the ground state as exp (-zr), with z = 1.2005. Further, the exchange is also incorporated, using eqn. (5.104) we have obtained the averaged DCS for the transition $X^1\ \Sigma_g^+ \longrightarrow B^1\ \Sigma_u^+$ with 60 ev electrons and compared with measured values of Srivastava and Jansen (1977) for V' = 2 vibrational band of the final state. For the same state, the DCS summed over all final vibrational states are calculated by Fliflet and Mckoy (1980). Our results with IAM at 60 ev (not shown) are much lower than both of these cited results, primarily due

to the failure of the model at that low energy. Thus, the IAM must be used above, say 100 ev. At these high energies, no data are yet available. Hence, we have compared the DCS of the $B^1\ \Sigma_u^+$ state (or 'B'-state) with those of the $a^3\ \Sigma_g^+$ (or 'a'-state), both of which are extremely neighbouring stable states (Massey et al 1969). The DCS of the transition $X^1\ \Sigma_g^+ \longrightarrow a^3\ \Sigma_g^+$ are calculated from,

$$\bar{I}(\theta) = 2 \left| f_H(Z) + \frac{1}{2} g_H(Z) \right|^2 \left(1 + \frac{\sin qR}{qR}\right) \qquad (5.107)$$

The DCS of the 'B' and the 'a' states, are shown for 100, 200 and 400 ev in figs. (5.10), (5.11) and (5.12) at scattering angles between 10 and 140°. Also in the table 5.8 we have compared the DCS of these two states near the forward direction at 100, 200 and 400 ev. The diffraction-factor, $\left(1 - \frac{\sin qR}{qR}\right)$, at different angles for 100 ev, is exhibited in the table 5.9. The most significant feature to be noticed is a drop of the DCS for the B-state as against the peak for the a-state in the forward direction. Further, as seen from the DCS curves (figs. 5.10 to 5.12) the difference between the DCS of these two states decreases

Table 5.8

DCS ($a_o^2\ Sr^{-1}$) of inelastic e-H_2 scattering at small angles

$a \pm b = a \times 10^{\pm b}$

θ deg	100 ev $B^1\Sigma_u^+$	100 ev $a^3\Sigma_g^+$	200ev $B^1\Sigma_u^+$	200ev $a^3\Sigma_g^+$	400 ev $B^1\Sigma_u^+$	400 ev $a^3\Sigma_g^+$
0	1.6 - 02	1.3 + 01	9.0 -03	1.2 + 01	4.7 - 03	1.29 + 01
5	3.6 - 02	8.55 +00	5.4 -02	8.1 + 00	7 - 02	5.85 + 00
10	6.5 - 02	4.95 +00	6.85-02	2.75+ 00	4.3 - 02	8.4 - 01
15	5.5 - 02	2.1 + 00	3.45-02	6.0 - 01	1.1 - 02	9 - 02

Table 5.9

The diffraction factor ($1 - \frac{\sin qR}{qR}$)

at 100 ev ($R = 1.4\ a_o$)

θ_{deg}	$1 - \frac{\sin qR}{qR}$
0	0.01
2.5	0.014
5	0.03
10	0.06
20	0.26
40	0.78
60	1.14
80	1.21
100	1.10
120	1.01
140	1.08

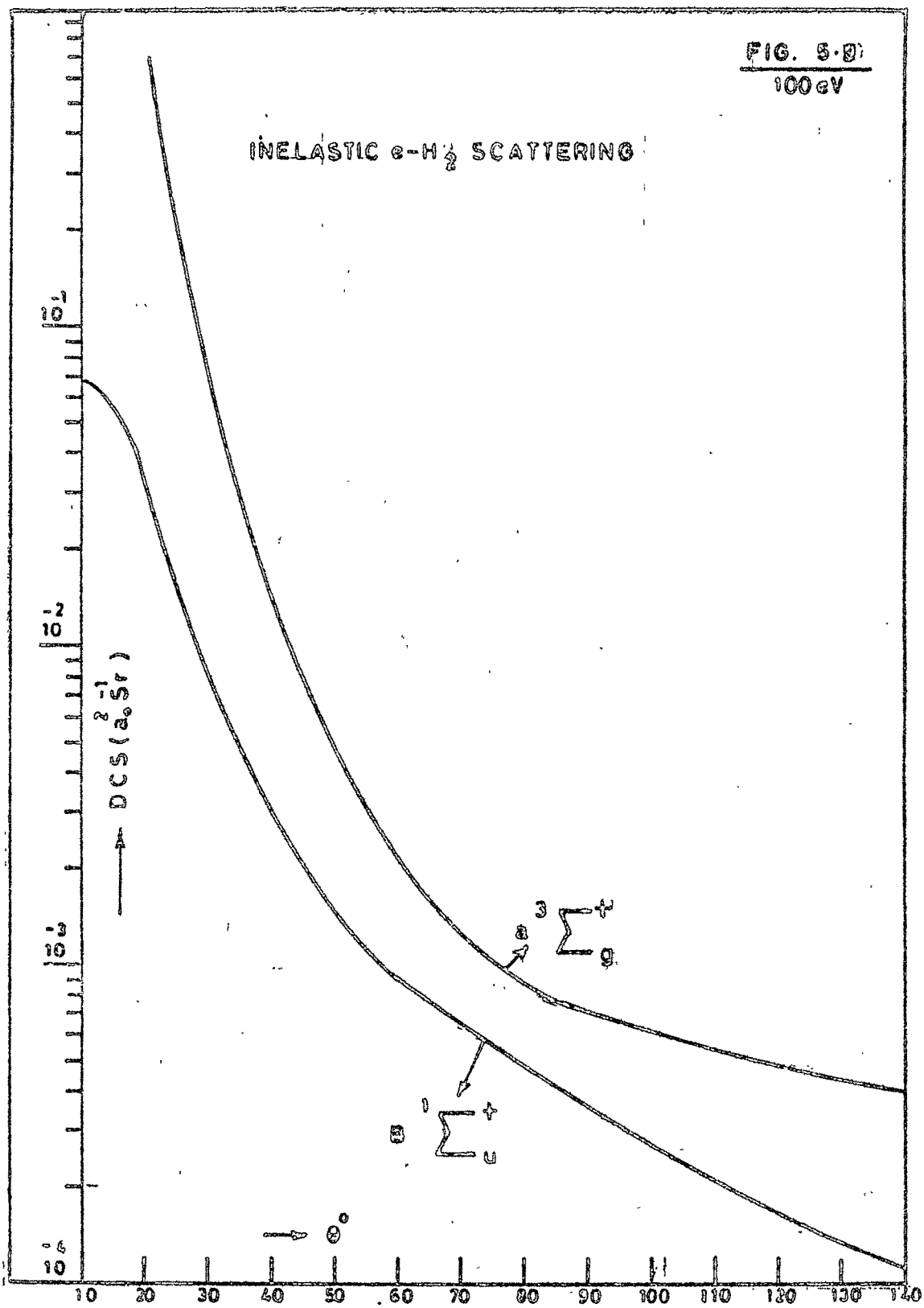


FIG. 5·9
100 eV
INELASTIC e-H2 SCATTERING
DCS (a0² Sr⁻¹)
10⁻¹
10⁻²
10⁻³
10⁻⁴
a ³Σg⁺
B ¹Σu⁺
θ°
10
20
30
40
50
60
70
80
90
100
110
120
130
140

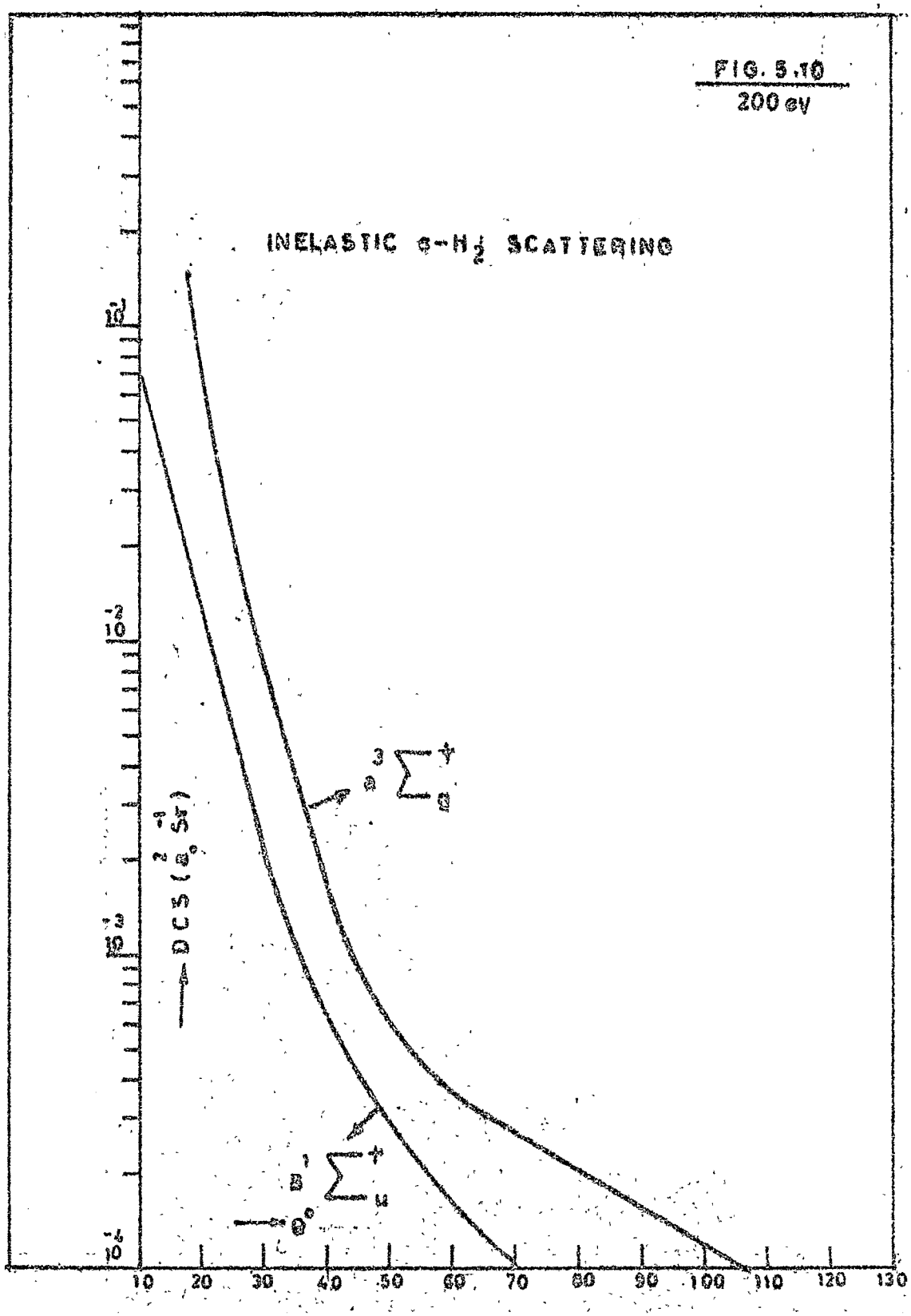


FIG. 5.10
200 ev
INELASTIC e-H2 SCATTERING
DCS (a0² Sr⁻¹)
10²
10¹
10⁰
10⁻¹
10⁻²
10 20 30 40 50 60 70 80 90 100 110 120 130
θ°
B' Σ⁺u
a' ³Σ⁺g

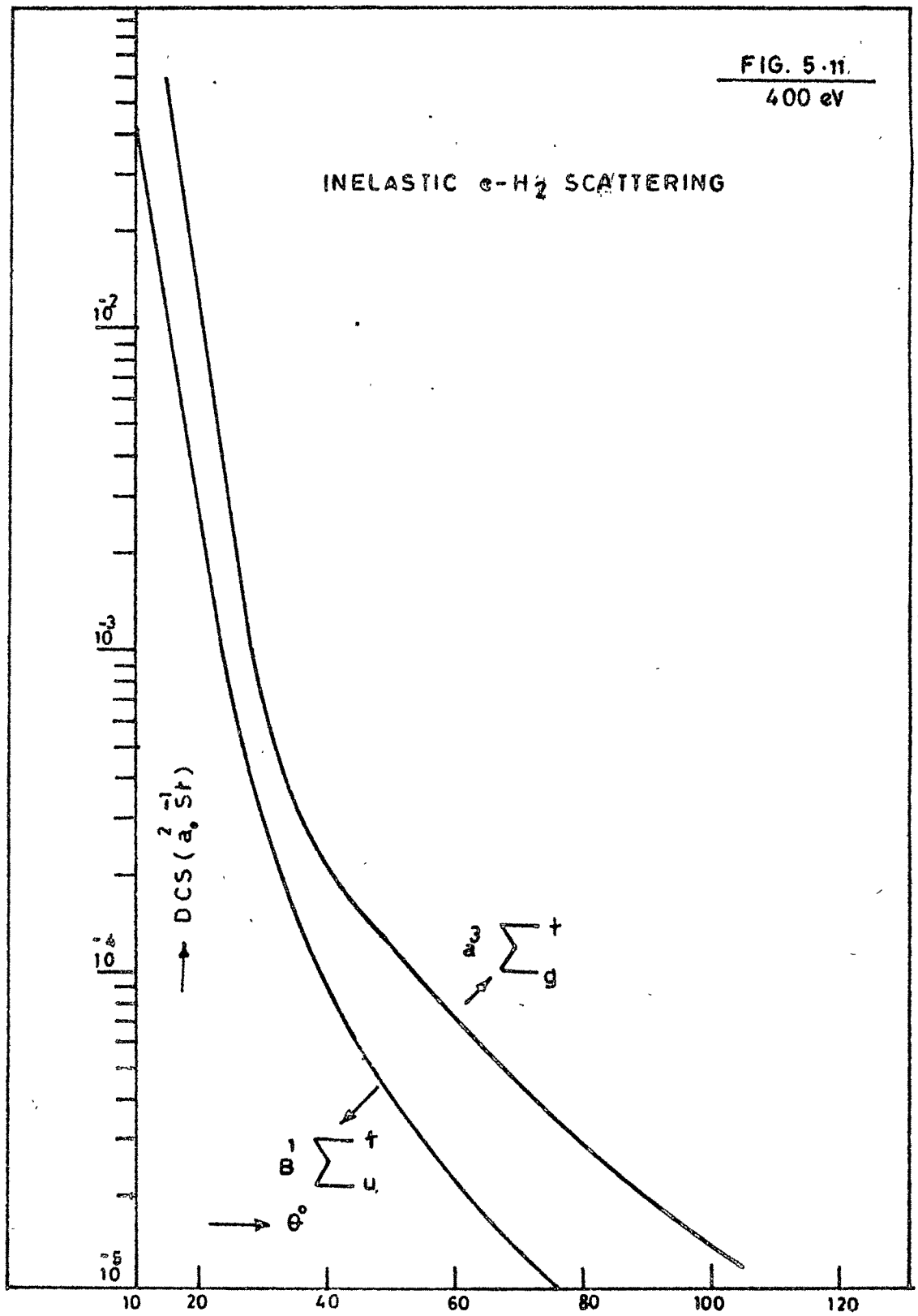


FIG. 5·11.
400 eV
INELASTIC e-H2 SCATTERING
DCS (a0² sr⁻¹)
10⁻²
10⁻³
10⁻⁴
10⁻⁵
10
20
40
60
80
100
120
θ°
a³Σg+
B¹Σu+

in the angular range 30°-50° and again it increases at large angles, but still remains smaller than that near the forward direction. This behaviour continues practically at all energies. The drop of DCS near the forward direction in the case of $b^3\ \Sigma_u^+$ (dissociative) state is noticed by Fliflet and Mckoy (1980) between 12 and 60 ev. But such a behaviour is not observed by them for $B^1\ \Sigma_u^+$ state. That the diffraction pattern is 'inverted' for transitions leading to u-symmetry states, has been confirmed by Swick and Karle (1961) for the excitation of Br_2 molecules by fast electrons. However, there are no recent studies in this regard.

Finally, using the H(2p) cross-sections in the IAM, we can study the excitations to several other electronic states of H_2. Notably, the H(2p) cross-sections in the forward direction are higher, but it will not be so for transition based on 1S $\longrightarrow$ 2p and resulting into a final u-symmetry state of H_2.

5.14 Chapter Summary, Further Prospects

The fifth chapter covering a study of the inelastic collisions of fast electrons by atoms and molecules, was divided into two main parts; part A dealing with atomic targets, while part B with molecular targets. In the part A, we have first reviewed the

fundamental aspects of the inelastic scattering of fast electrons by atomic hydrogen. This time the distorted wave methods have been at the centre of our attention. Many of the distorted wave theories end up with a numerical procedure to obtain the cross-sections, and further there is a great disparity in their outcome. Hence, we have developed presently a new high energy distorted wave (first) Born approximation for elastic collisions of electrons with atoms, based on the assumptions and evaluation methods of the Glauber approximation. The energy parameter β of this theory distinguishes it from the Glauber theory. Further, the present method employs a Green's function expansion, retaining two terms, to obtain distorted waves. The present high energy DWBA is fully illustrated for H(2S) excitation. Here are the distinct features of our basic theory.

* The distorting potentials in the initial and the final channel are appropriately chosen.

* The exchange is also accounted for

* No resort whatsoever is taken to numerical procedures.

* At a relatively low energy of 54.4 ev, the present method yields a dip-bump structure in the DCS curve, as observed with some of the other theories.

The present theory is then corrected by

including the polarized orbitals of Temkin and Lamkin. (1961). This method does not include the target polarization in the final state. The DCS are calculated for 54.4 - 400 ev and comparisons with available data are made. At 54.4 ev experimental results for 1S $\longrightarrow$ 2S process are now available but an accord is reached with no other theory except that of Kingston (1976). The present DWBA method is reliable at and above 100 ev, though at 54.4 ev, it behaves like that of Buckley and Walters (1975). At all energies, the various theories compared here, are found to yield the forward DCS at variance with each other and further, the energy-dependence of this quantity also varies. The DCS at high energies are found to fall off very rapidly.

The cross-sections of 1S $\longrightarrow$ 2p process in e-H scattering are dominated by the first-Born approximation in the forward direction, and are much higher than the 1S $\longrightarrow$ 2S cross-sections. The present DWBA theory can be applied to 1S $\longrightarrow$ 2p case also, although the results in this case are not shown here.

In the part B of the present chapter, we have dealt with electronic excitation in e-H_2 collisions. We have given some of the basic concepts of electronic states of molecules, in particular H_2. The purpose of the present chapter was two-fold viz, to develop a distorted wave theory for inelastic electron-atom collisions and to apply

it to the inelastic electron-molecule scattering via independent atom model. Accordingly in the part A we discussed a new DWBA theory. The next thing required is an IAM for electronic excitation of molecules. This is discussed in sec. (5.12). The important differences between the IAM formulations of the elastic and inelastic cases are brought forth. Now our calculations of H(2S) excitation can be employed via IAM to describe the inelastic e-H_2 scattering leading to four distinct final states, differing in symmetry and spin. They are given as, $B^1\Sigma_u^+$, $a^3\Sigma_g^+$, $E^1\Sigma_g^+$ and $^3\Sigma_u^+$. For the first of these states, experimental and theoretical data exist between 10 and 60 ev. Some calculations have also been reported for the other states, but not for energies between 100 and 1000 ev. The present DCS are obtained in this range of energy. We have tried to compare the present IAM results with the available data of 60 ev, but without success, the reason being the breakdown of the IAM. The IAM calculations indicate that although the two states $B^1\Sigma_u^+$ and $a^3\Sigma_g^+$ are quite neighbouring, the DCS for their excitation are very much different. The DCS for the excitation of a state with u-symmetry are much lower, especially near the forward direction. This can be seen from the 'inverted' diffraction factor, table 5.9. The DCS of $a^3\Sigma_g^+$ excitation are sharply peaked, in the forward direction. The difference in

the DCS of these states is small in the range of intermediate angles, but a difference of an order of magnitude or more is found, in the other regions. The behaviour of the B-state DCS near the forward direction, caused by the change of symmetry, is in accord with the observations of Swick and Karle (1961). No other recent references are available for this kind of work.

Finally, as we converge to the end of this chapter, let us conclude by giving indications of further prospects of work in the inelastic electron-atom-molecule collisions.

1. There is still a disparity among various theories as regards the DCS of the H(2S) excitation below 100 ev. This calls for an accurate distorted wave second Born approximation. This is also true for the 'sensitive' near-threshold region, which we have not attempted.

2. There is a great scope for theorietical as well as experimental work for electron impact excitation of the higher states of atomic hydrogen .e.g. n = 3.

3. We have remarked in sections (5.5) through (5.9) that the distorted wave first Born amplitude contains elements of the second and third Born terms also. Hence, such an amplitude can be used to assess the importance of

the third Born term. This idea, together with the second order distorting potentials has been very recently explored Madison et al (1983). The DWBA method of the present chapter can be extended by employing the second order potentials and/or second Born formulation.

4. The present theory can be applied to 2S ⟶ 3S excitation in the e+Li scattering. There is also a wide scope of work on excitation of other atoms, molecules and ions, by electron impact. We have not touched the more difficult problems of ionization by electron impact, which do need a lot of study.

5. The electronic excitation of molecules is gaining attention now; see e.g. Lee-Mu Tao et al (1982) for a very recent reference. The dissociation of molecules by incident electrons has been hardly studied beyond H_2. All these aspects constitute nearly vacant area, where, a lot of prospects for further work may be found. Obviously, the list of 'knowns' is smaller than that of the 'unknowns', so we stop here to come to the last chapter of the thesis.