CHAPTER - V

ELECTRON SCATTERING FROM ALKALI ATOMS

5.1 Introduction :

So far in the thesis, discussions were confined to light atoms. Now we take up an altogether different class of atoms - the alkali atoms. The study of this class of atoms is important in a manyfold way. To list a few:

(1) their important applications in various fields of science.

(2) the part played by some of the alkali atoms in MHD (Magnetohydrodynamics) is very important in the present day energy crisis.

(3) the scarce data available on such atoms necessitates further studies.

(4) the increasing computational complexities involved in the study of alkali atoms thus resulting in the vacant areas regarding research on them.

(5) the additional provisions to be supplied for the study of alkali atoms due to their peculiar nature and behaviour.

(6) the establishment of the failure of certain widely used and popular methods in their study.

(7) the vast differences in the results reported on various analyses of the alkali atoms.

As mentioned earlier while discussing collision processes involving Li atom, it is impossible to take for granted that methods which are successfully applied to the study of lighter atoms can be equally successfully applied to the alkali atoms. The main reason for this conclusion is the peculiar nature of the alkali atoms. In these atoms, because of the quasi-degeneracy of the ground and first excited states, there exists a strong coupling between these states. The large polarizability which is a characteristic of alkali atoms can be accounted mainly on this coupling because 90% of the polarizability arises due to the said coupling. Further, the size of the atom progressively increases as the atomic number of the atom increases. The outermost electron in the alkali atom is a loosely bound S-electron and hence the increased activity of these atoms. Naturally, when a projectile electron approaches a target alkali atom the situation arising will be much different from that in the case of a simple atom like H or He. The effect of the target on the incident electron and vice versa starts even when the projectile is approaching the target from a large distance. The target polarisation or the dislocation in the cloud charge also will be felt increasingly in such cases.

It was understood since long that the difficulties to be encountered while studying alkali atoms are many (see for e.g. Massey et al 1969). And it was very well proved also that methods like polarised orbital calculations are deemed to be failures in the study of alkali atoms. As demonstrated during the discussion on Li scattering, absorption phenomena or removal of electrons from elastic to inelastic channels is all-important for alkali scattering. This fact was also proved by Vanderpoorten (1976) in his optical model (OM) calculations performed on Li scattering. He has explicitly shown that polarisation effects are negligible in e - Li scattering. The OM calculations accounting for polarisation gave exactly same results as in the Glauber calculations in which the real part in the second term corresponding to polarisation is absent. This hints at the fact that polarisation is a nil-effect phenomenon in the case of Li scattering. Same should be the case with other alkali atoms also.

The Li atom being the first member of the alkali atoms, the above discussed deviations from closed - shell atoms will be the least in its case. In his study on the alkali atoms, Walters (1973) has shown that the disparities are the least in the case of Li target whereas it goes on increasing progressively for Na, K etc. Further, in recent years, most of the high energy methods used to describe collision processes involving H and He could successfully be applied to Li scattering also. The HHOB method (Rao and Desai 1981,1983), eikonal Born series Method (Byron and Joachain 1973,77), Two-potential eikonal approximation (Tayal et al 1980), fixed scatterer approximation (Guha and Ghosh 1979), optical model calculations (Vander poorten 1976) etc. were some of the attempts to study $\bar{e}$ - Li scattering. Reasonable success was achieved in all the above attempts also. Motivated by this, in the present study also, a few of the high energy methods were applied to the case of $\bar{e}$ - Li elastic scattering. The work done using the modified GES approximation and the modified Born approximation were discussed in earlier sections (3.5 and 4.4) in order to retain continuity of the matter. It was shown in those sections that the results were quite satisfactory while taking into consideration all the aspects of the problem. It is needless to say that in all the studies involving scattering from Li atoms, the results obtained were not as satisfactory as those obtained in the case of H or He targets. The additional source of error in the wave function is one of the factors for this failure.

In comparison to the bulk of work reported on Li targets, the research done on Na targets can be termed as meagre. This situation is not surprising while considering the increased computational hazards to be met with as one goes over from Li to Na. The core approximation to the alkali atoms is of great help in this respect. When accurate and exact calculations are not within our reach, approximate evaluation has to be resorted to. In this process, part of the accuracy may be sacrifised. This is precisely the justification when even approximate methods are not attempted to. In this chapter, we will discuss some of the present work done on $\bar{e}$ - Na elastic scattering using different approximations and within the limits of the limited facilities - such as computer - available.

One major problem in the case of heavy atomic targets is the non-availability of handy and accurate wavefunctions. The approximation in the wavefunction creates an additional source of mistake in atomic collision analysis. This is one of the reasons for the scarce data as well as unsatisfactory results in the case of heavier atomic targets compared to that of lighter ones. The wavefunction obtained using Slater rules has the advantage that it is comparatively handy. In an earlier section of this thesis, this type of wavefunction for Li was used. In his analysis on alkali atoms, Walters (1973) has made use of the Coulson (1961) wavefunction for Li atom and the Szasz Mc Ginn wave function (1967) for Na and K. In the section (4.4) of the present thesis, it was shown that the choice of the wavefunction in the method of Coulson (1961) or in that of Szasz & Mc Ginn (1967) does not make much of a difference in the study of $\bar{e}$ - Li elastic scattering in the modified Born approximation. Comparison of the two wave functions will advocate the use of Coulson wavefunction only because of its compactness. The Szasz Mc Ginn wavefunction is readily available for Na atom also, but the analysis will be lengthy and complicated using this wavefunction. With the anticipation that the simplicity of the Coulson wavefunction provides enough justification for its choice as the target wavefunction, in the present study the same is taken as the wavefunction for Na. It can be derived as follows:

Using the Slater rules, the different orbitals can be represented as ϕ_{1S}, ϕ_{2S} - - - - such that

$$\Psi_{3S} = A\,\phi_{1S} + B\phi_{2S} + C\phi_{2P_x} + D\phi_{2py} + E\phi_{2p_z} + F\phi_{3S} \tag{5.1}$$

Where
$$\phi_{1S} = \left[\frac{10.7^3}{\pi}\right]^{1/2} e^{-10.7\ r_1}$$
$$\phi_{2S} = \left[\frac{6.85^5}{96\pi}\right]^{1/2} r_1\ e^{-3.425 r_1}$$
$$\phi_{2P_x} = \left[\frac{6.85^5}{32\pi}\right]^{1/2} e^{-3.425\ r_1}\ r_1\ \mathrm{Sin}\ \theta\ \mathrm{Cos}\ \phi$$
$$\phi_{2P_y} = \left[\frac{6.85^5}{32\pi}\right]^{1/2} e^{-3.425\ r_1}\ r_1\ \mathrm{Sin}\ \theta\ \mathrm{Sin}\phi$$
$$\phi_{2P_z} = \left[\frac{6.85^5}{32\pi}\right]^{1/2} e^{-3.425\ r_1}\ r_1\ \mathrm{Cos}\ \theta$$
$$\phi_{3S} = \left[\frac{2 \times 2.2^7}{5\pi \times 3^9}\right]^{1/2} r_1^{\,2}\ e^{-0.733\ r_1}$$

The constants A, B, - - - - can be obtained from the following conditions of orthonormalization of the valence state.

(1) Ψ_{3S} should be normalised

i.e. $$\int dV_1\ \Psi_{3S}\ \Psi_{3S}^{*} = 1 \tag{5.2}$$

(2) Ψ_{3S} should be orthogonal to the orbitals ϕ_{1S} etc.

i.e. $\langle \Psi_{3S} / \phi_{1S} \rangle = 0$

Hence $\Psi_{2S} = P\,\phi_{1S} + Q\,\phi_{2S}$ (5.3)

Where $\langle \Psi_{2S} / \Psi_{2S} \rangle = 1$

and $\langle \Psi_{2S} / \phi_{1S} \rangle = 0$

Making use of the above conditions,

$P = 0.2743 \qquad Q = -1.0369$

$\therefore \quad \Psi_{2S} = 0.2743\,\phi_{1S} - 1.0369\,\phi_{2S}$

Following the same procedure,

$\Psi_{3S} = A\,\phi_{1S} + B\,\Psi_{2S} + F\,\phi_{3S}$ (5.4)

Now using the conditions

$\langle \Psi_{3S} / \Psi_{3S} \rangle = 1$ and

$\langle \Psi_{3S} / \phi_{1S} \rangle = 0$

$\langle \Psi_{3S} / \Psi_{2S} \rangle = 0$

we get $A + F \langle \phi_{1S} / \phi_{3S} \rangle = 0$

$B + F \langle \Psi_{2S} / \phi_{3S} \rangle = 0$

and $A^2 + B^2 + F^2 + 2BF \langle \Psi_{2S} / \phi_{3S} \rangle$

$+ 2AF \langle \phi_{1S} / \phi_{3S} \rangle = 1$

The expressions of the form $\langle \phi / \phi \rangle$ are easily evaluated using (5.1). This gives finally

A = -1.22897 - 03

B = 8.58839 - 02

F = 1.003682

which when substituted in (5.4) gives

$$\Psi_{3S} = 0.44093\, e^{-10.7 r_1} - 0.62974\, r_1\, e^{-3.425\, r_1} + 0.0432\, r_1^2\, e^{-2.2 r_1/3} \qquad (5.5)$$

which is the wave function of the Na atom (in the ground state) using the method of Coulson. This wave function has been used in the following part of the present work.

Another important aspect of the description of the electron - atom collision is the interaction between the incident electron and the target. In the sodium atom with 11 extra - nuclear electrons, this interaction becomes very complicated. At this juncture, the core representation of the alkali atoms (Walters 1973) becomes useful. In the study of Li atom, the core approximation is well-established (Rao and Desai 1983, Mathur et al 1972, Guha and Ghosh 1979). In the earlier sections on Li scattering, in the present work also, the core-approximation was successfully applied and it was noted that the effect of the core compared to the valence electron increases with incident energy and the scattering angle. In the core-approximation the alkali atoms look like the hydrogen atom with the core similar to the hydrogen nucleus and the ns-electron (n=2,3---) similar to the extra-nuclear electron in hydrogen. Walters (1973) has used the core approximation to study alkali scattering. In the present work also, the interaction potential between the projectile and target Na atom is similarly written as

$$V = V_H + V_C \qquad .. (5.6)$$

Where $V_H = \frac{-1}{r_2} + \frac{1}{/\underline{r}_2 - \underline{r}_1/}$ is the hydrogen like interaction and V_C = the potential due to the core defined by

$$V_C = 2\sum_{i=1}^{5} \int \phi_i^* \left(-\frac{1}{r_2} + \frac{1}{/\underline{r}_2 - \underline{r}_1/} \right) \phi_i \, dv_1 \qquad .. (5.7)$$

where ϕ_i stands for the inner orbitals of Na defined by (5.1). It can be observed that V_c is independent of target co-ordinates and behaves like a static potential. With the simplification of V as in (5.6), the interaction becomes very much similar to that in hydrogen, the difference being the V_c term which will not introduce any further computational hazards because of the absence of the target co-ordinates.

The evaluation of V_c is a very lengthy but straightforward process using standard integration techniques. For each ϕ_i, the corresponding V_{ci} is calculated and the final sum gives

$$V_c = C_7 e^{-\alpha_1 r_2} \left(1 + \frac{2}{\alpha_1 r_2}\right) + C_9 e^{-\alpha_2 r_2} \left(r_2 + \frac{4}{\alpha_2} + \frac{6}{\alpha_2^{\,2} r_2}\right)$$
$$+ C_8 e^{-\alpha_4 r_2} \left(r_2^{\,2} + \frac{6 r_2}{\alpha_4} + \frac{18}{\alpha_4^{2}} + \frac{24}{r_2 \alpha_4^{3}}\right) \qquad .. (5.8)$$

Where $C_7 = -23.0101$ $\quad \alpha_1 = 21.4$
$C_8 = -109.1529$ $\quad \alpha_2 = 14.125$
$C_9 = 10.0063$ $\quad \alpha_4 = 6.85$

With the help of the wavefunction and interaction simplified as (5.5) and (5.6), we are now ready to undertake the study of the elastic scattering of electrons by Na atoms (ENa process).

It should be remembered that recently experimental measurements have appeared for the above process (Teubner et al - 1978, Srivastava and Vuskovic - 1980). But unfortunately, most of the results are for low energies of incidence.

Now we take up a systematic study of the ENa process using various methods one by one.

5.2 First Born Approximation :

This is a very basic approximation which is found useful later in many sophisticated methods like GES, HHOB etc. Walters has already analysed the ENa process within the framework of the FBA. But he has used the Szasz Mc Ginn wavefunction (1967). In the present study, we use the Coulson wavefunction derived earlier (5.5). By studying the ENa process in the FBA using core-approximation, the following advantages can be expected.

(1) The comparison of the present results can be made with that of Walters (1973).

(2) From the above, an approximate idea about the correctness of the present wavefunction and core-potential can be obtained.

(3) The first Born results so obtained can be used in later sections where higher order theories are discussed.

(4) If the present results compare favourably with that of Walters, it can be presumed that the two wavefunctions do not give much different results.

Now, $$f_B^{(1)} = -\frac{1}{2\pi}\int dv_2\, e^{i\,\underline{q}\cdot\underline{r}_2}\int \psi^* V \psi\, dv_1 \qquad (5.9)$$

Using the expression (5.5) for ψ, it is convenient to write

$$\psi^*\psi = C_1 e^{-\alpha_1 r_1} + C_2\frac{d}{d\alpha_2} e^{-\alpha_2 r_1} + C_3\frac{d^2}{d\alpha_3^2} e^{-\alpha_3 r_1} + C_4\frac{d^2}{d\alpha_4^2} e^{-\alpha_4 r_1} + C_5\frac{d^3}{d\alpha_5^3} e^{-\alpha_5 r_1} + C_6\frac{d^4}{d\alpha_6^4} e^{-\alpha_6 r_1} \qquad (5.10)$$

where the value of C_j and α_j are given in the table (5.1).

Now, $$\int \psi^* V \psi\, dv_1 = V_c + \int \psi^*\psi\left(-\frac{1}{r_2} + \frac{1}{|\underline{r}_2 - \underline{r}_1|}\right) dv_1 .$$

For the term $e^{-\alpha_1 r_1}$ in $\psi^*\psi$ (5.10),

$$\int \psi^*\psi\, V_H^{(1)}\, dv_1 = -\frac{4\pi}{\alpha_1^2} e^{-\alpha_1 r_2}\left(1 + \frac{2}{\alpha_1 r_2}\right)$$

Thus for the $\psi^*\psi$ given by (5.10),

$$\int \psi^{*} \psi V_H \, dv_1 = -4\pi \Big\{ C_1 \frac{e^{-\alpha_1 r_2}}{\alpha_1^2} \left(1 + \frac{2}{\alpha_1 r_2}\right)$$

$$+ C_2 \frac{d}{d\alpha_2} \frac{e^{-\alpha_2 r_2}}{\alpha_2^2} \left(1 + \frac{2}{\alpha_2 r_2}\right)$$

$$+ C_3 \frac{d^2}{d\alpha_3^2} \frac{e^{-\alpha_3 r_2}}{\alpha_3^2} \left(1 + \frac{2}{\alpha_3 r_2}\right) + C_4 \frac{d^2}{d\alpha_4^2} \frac{e^{-\alpha_4 r_2}}{\alpha_4^2} \left(1 + \frac{2}{\alpha_4 r_2}\right)$$

$$+ C_5 \frac{d^3}{d\alpha_5^3} \frac{e^{-\alpha_5 r_2}}{\alpha_5^2} \left(1 + \frac{2}{\alpha_5 r_2}\right) + C_6 \frac{d^4}{d\alpha_6^4} \frac{e^{-{}_6 r_2}}{\alpha_6^2} \left(1 + \frac{2}{\alpha_6 r_2}\right) \Big\} \quad (5.11)$$

Now $$f_B^{(1)} = -\frac{1}{2\pi} \int dv_2 \, e^{i \underline{q} \cdot \underline{r}_2} \int \psi^{*} V_H \psi \, dv_1 - \frac{1}{2\pi} \int dv_2 \, e^{i \underline{q} \cdot \underline{r}_2} V_c(r_2) \qquad .. \quad (5.12)$$

$$\therefore f_{BA}^{(1)} = -\frac{2}{q} \int_0^\infty dr_2 \, r_2^2 \frac{\text{Sin } q r_2}{r_2} \int \psi^{*} V_H \psi \, dv_1$$

For one representative term of (5.11) i.e. $\frac{e^{-\alpha_1 r_2}}{\alpha_1^2} \left(1 + \frac{2}{\alpha_1 r_2}\right)$, $f_{BA}^{(1)}$ is obtained as

$$f_{BA}^{(1)} \text{ (one term)} = \frac{-4}{\alpha_1^3} \frac{(q^2 + 2\alpha_1^2)}{(q^2 + \alpha_1^2)^2}$$

Hence for $\int \psi^{*} V_H \psi \, dv_1$ given by (5.11),

$$f_{BA}^{(1)} = 16\pi \Big\{ C_1 \frac{(q^2 + 2\alpha_1^2)}{\alpha_1^3 (q^2 + \alpha_1^2)^2} + C_2 \frac{d}{d\alpha_2} \frac{(q^2 + 2\alpha_2^2)}{\alpha_2^3 (q^2 + \alpha_2^2)^2}$$

$$+ C_3 \frac{d^2}{d\alpha_3^2} \frac{(q^2 + 2\alpha_3^2)}{\alpha_3^3 (q^2 + \alpha_3^2)^2} + C_4 \frac{d^2}{d\alpha_4^2} \frac{(q^2 + 2\alpha_4^2)}{\alpha_4^3 (q^2 + \alpha_4^2)^2}$$

$$+ C_5 \frac{d^3}{d\alpha_5^3} \frac{(q^2+2\alpha_5^2)}{\alpha_5^3(q^2+\alpha_5^2)^2} + C_6 \frac{d^4}{d\alpha_6^4} \frac{(q^2+2\alpha_6^2)}{\alpha_6^3(q^2+\alpha_6^2)^2} \Bigg\} \qquad (5.13)$$

Similarly by substituting V_c given by (5.8) in (5.12) and using Standard integrals and simplifications,

$$f_{BB}^{(1)} = -2 \Bigg\{ 2C_7 \frac{(q^2+2\alpha_1^2)}{\alpha_1 (q^2+\alpha_1^2)^2} + C_8 \Bigg[\frac{-24\alpha_4(q^2-\alpha_4^2)}{(q^2+\alpha_4^2)^4}$$

$$- \frac{6}{\alpha_4} \frac{2(q^2-3\alpha_4^2)}{(q^2+\alpha_4^2)^3} + \frac{18}{\alpha_4} \frac{2}{(q^2+\alpha_4^2)^2} + \frac{24}{\alpha_4^3} \frac{1}{(q^2+\alpha_4^2)} \Bigg]$$

$$+ C_9 \Bigg[\frac{-2(q^2-3\alpha_2^2)}{(q^2+\alpha_2^2)^3} + \frac{8}{(q^2+\alpha_2^2)^2} + \frac{6}{\alpha_2^2(q^2+\alpha_2^2)} \Bigg] \Bigg\} \qquad (5.14)$$

Now the first Born approximation to the ENa process is the sum of the expressions given by (5.13) and (5.14). The DCS for the ENa process within the frame work of FBA can be easily calculated now. The results so obtained are displayed in fig.(5.1) at 54.4 ev at which there is data for comparison. In the same figure, the DCS without the core - contribution to the interaction (5.6) is also shown. The following conclusions can be drawn from the study of fig.(5.1).

(1) The present results compare favourably with those of Walters (1973). This indirectly shows that the choice of the different wavefunctions in both the studies has not affected the results much.

(2) The effect of the core is very much for higher scattering angles.

(3) Even at a low energy such as 54.4 eV, the core-contribution is highly significant. The comment of Walters that core-effects are negligible below 100 eV is questionable.

The effect of the core is expected to increase for large angles where the nuclear part of the interaction predominates. It should be assumed that even at lower energies the projectile penetrates deep into the target.

In an earlier section (4.4) the simple Coulson wave function and the sophisticated Szasz Mc Ginn wave function were compared by using them to study the same process. Here also the comparison of the present results with that of Walters (1973) is similar. Since the Szasz Mc Ginn wavefunction is very unwieldy and difficult to handle, in the rest of the present work also only the Coulson wavefunction for Na is taken on the basis of the above mentioned comparison.

However, the comparison of the First Born DCS with experimental results (Teubner et al (1978), Srivastava and Vuskovic (1980), is very discouraging. In the very small angle region only there is some sort of qualitative agreement between the two results. Naturally, in the case of alkali scattering where second order effects like absorption are all-important, a first order theory like FBA cannot be expected to hold good. Hence, the inclusion of higher order terms is required. With this view, we now take up the study of ENa process in a higher order theory.

5.3 ENa process in the GES Method :

The success of the GES method as a reasonable termwise representation of the Glauber series is well established. In the earlier part of the present work also, the GES analysis was performed for some basic scattering phenomena. In the present study of ENa process, it was decided to carry out the GES analysis because of the following reasons:

(1) In the previous section, the necessity for a higher order theory was felt.

(2) The second term of the GES i.e. $f^{(2)}_{GES}$ is found to be very similar to the imaginary part of the second Born term.

(3) $f^{(2)}_{GES}$ takes care of the important absorption effect.

(4) In the study of Walters (1973) Glauber result was found to be much better than the first Born result. Hence, the GES results should also be good.

)5) Because of the representation of the interaction potential and Wavefunction as (5.6) and (5.5), the evaluation of the GES terms should not be very much difficult.

It should be borne in mind that the first term of GES series is the first Born term given by (5.12). Hence, the task is to evaluate $f_{GES}^{(2)}$ and $f_{GES}^{(3)}$. Here, we use an approximation as follows:

It was pointed out by Mahtur et al (1972) that in the core-approximation of Li atom, the core part can be neglected in the evaluation of double scattering terms. The same was followed later on by many workers such as Guha and Ghosh (1979), Rao and Desai (1983) etc. In the current study also, in the evaluation of the higher order terms, we neglect the core part of the interaction enumerating the following reasons :

(1) The second order effects like absorption and polarisation are important in the small angle region where the effect of the core is small.

(2) For the low incident energies considered here, the penetration of the projectile into the target is very little. Hence, the effects due to the core of the atom will not be significant while considering the valence electron, the distortion in the cloud charge etc.

(3) In a previous section of the study on Li scattering, the same procedure was adopted with successful outcome.

Hence, we proceed with the evaluation of $f^{(2)}_{GES}$ and $f^{(3)}_{GES}$ for the valence electron of the Na atom.

$$f^{(2)}_{GES} = \frac{z^2}{\pi k_i} \int \frac{d\underline{P}}{P^2 |\underline{q}-\underline{p}|^2} \langle \psi_f | B(P)\, B(q-p) | \psi_i \rangle \quad (5.15)$$

It will be possible to reduce some length of the calculations by considering the analogy with H-atom problem. For this purpose, it will be convenient to represent $\psi^* \psi$ in the present case as

$$\psi^* \psi = -\pi \Big\{ C_1 \frac{d}{d\alpha_1} \frac{e^{-\alpha_1 r_1}}{\pi r_1} + C_2 \frac{d^2}{d\alpha_2^{\,2}} \frac{e^{-\alpha_2 r_1}}{\pi r_1} + C_3 \frac{d^3}{d\alpha_3^{\,3}} \frac{e^{-\alpha_3 r_1}}{\pi r_1}$$

$$+ C_4 \frac{d^3}{d\alpha_4^{\,3}} \frac{e^{-\alpha_4 r_1}}{\pi r_1} + C_5 \frac{d^4}{d\alpha_5^{\,4}} \frac{e^{-\alpha_5 r_1}}{\pi r_1} + C_6 \frac{d^5}{d\alpha_6^{\,5}} \frac{e^{-\alpha_6 r_1}}{\pi r_1} \Big\} \quad (5.16)$$

The interaction pertaining to the valence electron of the Na atom is similar to that of H atom. Thus,

$$B(P)\, B(q-p) = 1 - e^{i\underline{P}\cdot\underline{r}_1} - e^{i|\underline{q}-\underline{P}|\cdot\underline{r}_1} + e^{i\,\underline{q}\cdot\underline{r}_1} \quad (5.17)$$

$$\text{Now} \quad f^{(2)}_{GES} = f_1^{\,2} + f_2^{\,2} + f_3^{\,2} + f_4^{\,2} + f_5^{\,2} + f_6^{\,2} \quad (5.18)$$

where each expression corresponds to one term in the expression (5.16) for $\psi^* \psi$.

It should be remembered now that for H - atom,

$$\psi^* \psi = C \left(- \frac{d}{d\lambda} \right) \frac{e^{-\lambda r_1}}{r_1} \quad \text{with } \lambda = 2 , \quad C = 1/\pi .$$

Hence the $\psi^* \psi$ of (5.16) is similar to the above expression, the difference being in the values of the parameters and the additional differentiations. The $f^{(2)}_{GES}$ for H atom was derived in an earlier section (3.24). Hence the f_1^2, f_2^2--- can be directly written down as

$$f_1^{(2)} = \pi C_1 \quad k_2 \quad \left(- \frac{d}{d\alpha_1}\right) f_2 (z_1)$$

$$f_2^{(2)} = \pi C_2 \quad k_2 \quad \left(- \frac{d^2}{d\alpha_2^2}\right) f_2 (z_2)$$

$$f_3^{(2)} = \pi C_3 \quad k_2 \quad \left(- \frac{d^3}{d\alpha_3^3}\right) f_2 (z_3)$$

$$f_4^{(2)} = \pi C_4 \quad k_2 \quad \left(- \frac{d^3}{d\alpha_4^3}\right) f_2 (z_4)$$

$$f_5^{(2)} = \pi C_5 \quad k_2 \quad \left(- \frac{d^4}{d\alpha_5^4}\right) f_2 (z_5)$$

$$f_6^{(2)} = \pi C_6 \quad k_2 \quad \left(- \frac{d^5}{d\alpha_6^5}\right) f_2 (z_6)$$

Where $k_2 = \dfrac{4}{\pi k_{iq}^4}$

and $f_2(z) = 4\pi \dfrac{z^4}{1 + z^2} \ln \left(\dfrac{1+z^2}{z} \right)$.

It is needless to say that the α -differentiations $\dfrac{d}{d\alpha}$, $\dfrac{d^2}{d\alpha^2}$ etc. have to be converted to the corresponding z - differentiations $\dfrac{d}{dz}$, $\dfrac{d^2}{d_z^2}$ etc. for $z = q/\alpha$.

Thus $\dfrac{d^5}{d\alpha^5}$ should be replaced by

$$- \frac{z^6}{q^5} \left(120 \frac{d}{dz} + 240 z \frac{d^2}{d_z^2} + 120 z^2 \frac{d^3}{d_z^3} + 20 z^3 \frac{d^4}{d_z^4} + z^4 \frac{d^5}{d_z^5} \right) \text{ and so on.}$$

$$\text{Hence}\quad f^{(2)}_{GES} = -\pi k_2 \Big\{ C_1 \frac{d}{d\alpha_1} f_2(z_1) + C_2 \frac{d^2}{d\alpha_2^{\,2}} f_2(z_2) + C_3 \frac{d^3}{d\alpha_3^{\,3}} f_2(z_3) + C_4 \frac{d^3}{d\alpha_4^{\,3}} f_2(z_4) + C_5 \frac{d^4}{d\alpha_5^{\,4}} f_2(z_5) + C_6 \frac{d^5}{d\alpha_6^{\,5}} f_2(z_6) \Big\} \qquad ..(5.19)$$

Similar method can be followed for the evaluation of $f^{(3)}_{GES}$ also.

$$f^{(3)}_{GES} = \frac{2\pi k_i\,(-z^3)}{6\,\pi^3 k_i^{\,3}} \int \frac{dP_1}{P_1^{\,2}} \int \frac{dP_2}{P_2^{\,2}} \frac{1}{/q-(P_1+P_2)/^2}$$

$$< \psi_f / \; B(P_1)\; B\;(P_2)\; B\;(\,q-(P_1+P_2))\; / \; \psi_i >$$

Here again making use of the convenient representation (5.16) of $\psi^* \psi$, $f^{(3)}_{GES}$ will be constituted by six terms, each term corresponding to one term in $\psi^* \psi$.

$$\text{Thus}\quad f^{(3)}_{GES} = f_1^{\,3} + f_2^{\,3} + - - - - - - - + f_6^{\,3}.$$

Here also for the term of $\psi^* \psi$ of the type $C \left(\frac{-d}{d\lambda}\right) \frac{e^{-\lambda r}}{\pi r}$ corresponding $f^{(3)}_{GES}$ will be

$$C \;x\; \frac{4}{3\pi^2 k_i^{\,2} q^4} \left(-\frac{d}{d\lambda}\right) f_3(z) \quad \text{where} \quad z = \frac{q}{\lambda}.$$

The above derivation was arrived at earlier.

$$\text{Hence}\quad f_1^{\,3} = \pi C_1 k_1 \left(-\frac{d}{d\alpha_1}\right) f_3\;(z_1)$$

$$f_2^{\,3} = \pi C_2 k_1 \left(-\frac{d^2}{d\alpha_2^{\,2}}\right) f_3\;(z_2)$$

$$f_3^{\,3} = \pi C_3 k_1 \left(-\frac{d^3}{d\alpha_3^{3}}\right) f_3\;(z_3)$$

$$f_4^{\,3} = \pi C_4 k_1 \left(- \frac{d^3}{d\alpha_4^3} \right) f_3(z_4)$$

$$f_5^{\,3} = \pi C_5 k_1 \left(- \frac{d^4}{d\alpha_5^4} \right) f_3(z_5)$$

$$f_6^{\,3} = \pi C_6 k_1 \left(- \frac{d^5}{d\alpha_6^5} \right) f_3(z_6)$$

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

and $k_1 = \frac{4}{3\pi^2 k_i^2 q^4}$. A(z) is the same as defined under equation (3.16). Here also the differentiation variable has to be changed from α to z correspondingly using conversions given earlier.

$$\text{Thus } f^{(3)}_{GES} = \frac{-\pi k_1}{} \left\{ C_1 \frac{d}{d\alpha_1} f_3(z_1) + C_2 \frac{d^2}{d\alpha_2^2} f_3(z_2) \right.$$

$$+ C_3 \frac{d^3}{d\alpha_3^3} f_3(z_3) + C_4 \frac{d^3}{d\alpha_4^3} f_3(z_4) + C_5 \frac{d^4}{d\alpha_5^4} f_3(z_5)$$

$$\left. + C_6 \frac{d^5}{d\alpha_6^5} f_3(z_6) \right\} \qquad ..(5.20)$$

Where $z_n = \frac{q}{\alpha_n}$.

Using the expressions (5.19) and (5.20), the DCS for the ENa process in the GES approximation can be written as

$$\frac{d\sigma}{d\Omega} = f_{B_1} \times f_{B_1} + f^{(2)}_{GES} \times f^{(2)}_{GES} - 2 \times f_{B_1} \times f^{(3)}_{GES} .$$

Results and discussion :

The DCS obtained for the ENa process as described above are shown in fig. (5.2) for E = 54.4 eV. The results are compared with first Born DCS as well as experimental data. It can be seen that the present DCS is quite good at small angles. This is as expected since the GES analysis is another way of representing the Glauber approximation which is necessarily a small angle approximation. The comparison of the present GES results with the Glauber results of Walters in fig.(5.2) shows that the GES method discussed above compares with the Glauber cross-sections reasonably well at small angles, considering the relative ease of evaluation of the GES method compared to that of Glauber method.

It should not be forgotten that in evaluating the Glauber amplitude, Walters has used a different wave-function than the one used here. This shows the comparison between the wave functions also. The present results should not be expected to hold good at large angles for the energies considered here. This fact is obvious from the table (5.2) giving the individual GES terms. It can be seen that at 100 eV for $\Theta > 70^{\circ}$, $f^{(3)}_{GES} > f^{(2)}_{GES}$ i.e. the series is no longer convergent. For the energy E = 54.4 eV, it can be seen that upto the $\Theta = 40^{\circ}$, $f^{(3)}_{GES} < f^{(2)}_{GES}$ i.e. the validity of the present method is better at higher energies. Unfortunately, since experimental data is available only at small energies, we have to stretch the high energy methods also down to lower energies. Anyway, there is enough evidence to believe that the GES results, should be reasonably good at higher incident energies.

The improvement of the GES results over the first Born results is also notable. This is also in accordance with our earlier anticipation that the GES results should be good because the Glauber results are better than their First Born counterparts provided the GES can satisfactorily represent the Glauber series. Thus we can conclude that the first three terms of the GES series gives satisfactory representation of the Glauber Series for ENa process and the inclusion of higher order terms has improved the approximation.

5.4 Inclusion of Polarisation Effect :

One major defect of the Glauber as well as the GES methods is the logarithmic divergence of the cross sections for very small angles. Another shortcoming is the absence of the real part in the second term corresponding to polarisation. In the proposition of a modified GES method in section (3.1) a remedy for these disadvantages was suggested i.e. replacement of $f^{(2)}_{GES}$ by the $O(\frac{1}{k_i})$ terms of HHOB such that the scattering amplitude becomes

$$f = f_{B1} + f\,\mathrm{Im} + f_{Re_1} - f^{(3)}_{GES}$$

In earlier sections it was explicitly shown that $f\,\mathrm{Im}$ is almost equal to $f^{(2)}_{GES}$. But the beauty of the present term f Im is that it is not divergent even at $q = 0$, because of the average excitation energy term β. Hence, the net result of the replacement of the GES term by HHOB term is the inclusion of polarisation effects taken through fRe_1. As mentioned earlier, polarisation effects should not be significant when compared to the grossly effective absorptive part. However, it would be interesting to study the effects of inclusion of polarisation effect.

Incorporation of HHOB terms necessitates the evaluation of the β parameter for ENa process. This was done as follows; as given by Byron and Joachain (1977).

$$\bar{W} = \beta k_i = 2 \frac{< \psi / z_1^2 / \psi >}{\bar{\alpha}}$$

Where $\bar{\alpha}$ is the dipole polarisability of the target atom and $\underline{r}_1 = \underline{b}_1 + z_1 \hat{\lambda}$. This method of evaluation of β was checked first for ELi process. For that, the Coulson wavefunction (1961) was taken for ψ and the recent and accurate value of $\bar{\alpha}$ = 167 a.u was taken from Sternheimer (1969). This gave $\bar{W} =$ 0.0723 for ELi process. For the same process, Vanderpoorten (1976) obtained $\bar{W} = 0.0745$ using the same $\bar{\alpha}$ but with a better established Hartree fock wavefunction of Clementi (1965). This indirectly marks the correctness of the present method of evaluation of $\bar{W}$ or β as well as the dependability of the Coulson wavefunction. Hence, the same procedure was adopted for the evaluation of β for ENa process.

For this process

$$\bar{\alpha} = 22.59\ (A^{o})^{3} = 152.6 \text{ a.u.}$$

Using the Coulson wavefunction (5.5) for ψ and evaluating $< \psi / z_1^{2} / \psi >$ and substituting,

$$\bar{W} = 0.1313 \text{ a.u.}$$

Hence for the ENa process, $\beta = 0.1313/k_i$. Now we can take up the evaluation of f Im and f Re_1 terms of ENa process.

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

For the evaluation of this, the expression (5.16) for $\psi^{*}\ \psi$ will be very useful. Now one can consider that

$f\ Im = f\ Im^{(1)} + f\ Im^{(2)} + \ldots\ldots + f\ Im^{(6)}$, each term corresponding to one term in (5.16). For our choice of the interaction potential, $\bar{V}$ becomes similar to the one given in section (3.2). By considering one term $C_1 (- \frac{d}{d\alpha_1}) \frac{e^{-\alpha_1 r_1}}{r_1}$ and comparing it with the $\psi^{*}\ \psi$ for ESGH process, it will be easy to derive $f\ Im^{(1)}$, $f\ Im^{(2)}$ - - - similar to the derivation given to arrive at the expression (3.17). Since all this process is very lengthy, we consider here only the final results namely

$$f\ Im^{(1)} = \frac{-4}{k_i}\ C_1\ \frac{d}{d\alpha_1}\ \frac{1}{\alpha_1^{2}}\ \left(2\ I_1\ (\beta^{2}, \alpha_1^{2}) - \frac{q^{2}}{q^{2}+\alpha_1^{2}}\ I_1(\beta^{2},0)\right)$$

$$f\ Im^{(2)} = -\frac{4}{k_i}\ C_2\ \frac{d^{2}}{d\alpha_2^{2}}\ \frac{1}{\alpha_2^{2}}\ \left(2\ I_1(\beta^{2},\alpha_2^{2}) - \frac{q^{2}}{q^{2}+\alpha_2^{2}}\ I_1(\beta^{2},0)\right)$$

etc. such that

f Im for ENa process

$$= - \frac{4}{k_i} \left\{ C_1 \frac{d}{d\alpha_1} I_{N1} + C_2 \frac{d^2}{d\alpha_2^2} I_{N2} + C_3 \frac{d^3}{d\alpha_3^3} I_{N3} + C_4 \frac{d^3}{d\alpha_4^3} \right.$$

$$\left. I_{N4} + C_5 \frac{d^4}{d\alpha_5^4} I_{N5} + C_6 \frac{d^5}{d\alpha_6^5} I_{N6} \right\} \qquad (5.21)$$

Where I_{N1}, I_{N2} - - - I_{N6} are obtained by putting α_1, α_2 - - - α_6 for the α_n in

$$I_{Nn} = \frac{1}{\alpha_n^2} \left[2 I_1(\beta^2, \alpha_n^2) - \frac{q^2}{q^2+\alpha_n^2} I_1(\beta^2, 0) \right].$$

$I_1(\beta^2, \alpha_n^2)$ has the same meaning as defined in earlier sections.

For the evaluation of $f Re_1$ also, a shortcut similar to the above one can be used. $f Re_1$ can also be represented as $f Re_1 = f Re_1^{(1)} + f Re_1^{(2)} + - - - + f Re_1^{(6)}$, corresponding to the six terms in (5.16) for $\psi^* \psi$. The derivation for $f Re_1$ for the ESGH is given earlier wherein the $\psi^* \psi$ has the same form as the first term of (5.16)

Thus the expressions for $f Re_1^{(1)}$, $f Re_1^{(2)}$ etc. can be derived in the same lines. With a view to save space, the lengthy derivation is not given here but only the results. Thus one can obtain for the various terms in $f Re_1$

$$f Re_1^{(1)} = \frac{4}{\pi k_i} C_1 \frac{d}{d\alpha_1} \frac{1}{\alpha_1^2} \left[2 I_2(\beta^2, \alpha_1^2) - \frac{q^2}{q^2+\alpha_1^2} I_2(\beta^2, 0) \right]$$

$$f\,Re_1^{(2)} = \frac{4}{\pi k_i} C_2 \frac{d^2}{d\alpha_2^2} \frac{1}{\alpha_2^2} \left[(2\, I_2(\beta^2, \alpha_2^2) - \frac{q^2}{q^2+\alpha_2^2} I_2(\beta^2, 0) \right]$$

etc.

Thus the final form of $f\,Re_1$ for ENa process will be

$$f\,Re_1 = \frac{4}{\pi k_i} \left\{ C_1 \frac{d}{d\alpha_1} I_{M1} + C_2 \frac{d^2}{d\alpha_2^2} I_{M2} + C_3 \frac{d^3}{d\alpha_3^3} I_{M3} + C_4 \frac{d^3}{d\alpha_4^3} I_{M4} + C_5 \frac{d^4}{d\alpha_5^4} I_{M5} + C_6 \frac{d^5}{d\alpha_6^5} I_{M6} \right\} \quad (5.22)$$

where I_{M1}, I_{M2} etc. are obtained by putting $\alpha_1, \alpha_2 \ldots \alpha_6$ for the α_n in $I_{Mn} = \frac{1}{\alpha_n^2} \left[2\, I_2(\beta^2, \alpha_n^2) - \frac{q^2}{q^2+\alpha_n^2} I_2(\beta^2, 0) \right]$.

Here also the integrals $I_2\,(\beta^2, \alpha_n^2)$ have the same form as used earlier and given in appendix.

With the expressions for f Im and $f\,Re_1$ available now, the DCS for the ENa process can be written as

$$\frac{d\sigma}{d\Omega} = f_B \times f_B + f\,Im \times f\,Im + f\,Re_1 \times f\,Re_1 + 2\, f_B\,(f\,Re_1 - f^{(3)}_{GES}) \quad (5.23)$$

This will give the new DCS obtained after replacing the second GES term by the HHOB terms thereby including the polarisation effect.

Results and Discussions :

As discussed earlier, the effects of polarisation are almost negligible for the ENa process when compared to the absorption effects. The table (5.3) explicitly shows this fact. Moreover, it can be seen that $f^{(2)}_{GES} \simeq f_{Im}$ as in the earlier cases. But the advantage of taking f Im is that it is not divergent at $\theta = 0$ as $f^{(2)}_{GES}$ because of the presence of the average excitation energy parameter, and the individual integrals appearing in f Im are not divergent also. Hence it is possible to evaluate the total cross section for the ENa process from the value of f Im ($\theta = 0$) using the famous optical theorem.

The differential cross section obtained using (5.23) is also shown in fig. (5.3). It can be seen that there is no significant change in the DCS because of the replacement of the second GES term by the Born terms.

5.5 Two Potential Born Approximation :

It was shown in the earlier sections that the first Born, GES and HHOB methods are not sufficient to represent the ENa process satisfactorily especially at large angles. In this connection, we remember how the two potential Born approximation improved the simple Born approximation for large angle scattering. Specific examples were also cited by applying the two-potential HHOB approximation to the ESGH and EHe processes.

Moreover, in our study of the ENa process within the frame work of FBA, it was shown that the contribution due to the core part of the interaction varies very slowly with increasing scattering angles. This results in the high scattering cross-sections at large angles. Hence, if there is some way by which the core part of the interaction can be separated out from the total interaction and be given a better treatment, the results should improve. Hence, a partial wave treatment for V_c should be a remedy. Further, the Born approximation should be better for weaker interactions. Hence, if the total interaction V treated in FBA is replaced by $V - V_1$ where V_1 is arbitrary such that $V - V_1$ satisfies semi-classical conditions, we should get better results. With this idea in mind, we will now study the ENa process in the two-potential formulation.

We have seen earlier that the interaction potential for ENa process is $V = V_H + V_c$ where $V_H = -\frac{1}{r_2} + \frac{1}{/\underline{r}_1 - \underline{r}_2/}$. In the two potential Born formulation discussed earlier, we subtract an arbitrary potential $V_1(r_2)$ from $V\ (r_1, r_2)$ such that $V_o(r_1, r_2) = V\ (r_1 r_2) - V_1(r_2)$ satisfies semiclassical conditions. Then $V_o\ (r_1, r_2)$ is treated in the Born approximation and $V_1\ (r_2)$ is treated by partial wave method.

For the ENa process, we choose for the arbitrary potential:

$$V_1(r_2) = V_c(r_2)$$

Such that $V_o(r_1, r_2) = V_H(r_1, r_2) + V_c(r_2) - V_c(r_2) = V_H(r_1, r_2)$

.. (5.24)

Now we treat $V_H(r_1,\ r_2)$ in the Born approximation and $V_c(r_2)$

in the partial wave method described earlier.

To start with, we take only the first Born term in the Born approximation i.e. V_H should be treated in FBA and V_C by Partial waves method.

Thus we note that

(1) earlier $V_H + V_C$ was treated in FBA and we found that V_C contribution was very slowly varying thus resulting in higher cross sections.

(2) Now only V_H is treated in FBA and this being a weaker interaction should give better results.

(3) Now the contribution due to V_C is taken quantum mechanically through a few partial waves.

(4) This type of two potential method was earlier found useful and here also there are reasons to assume that the results obtained should be better than those obtained through simple Born approximation.

To evaluate the V_H part of the interaction in the FBA, we can readily take the earlier result (5.13) for $f_{BA}^{(1)}$. Now the scattering amplitude in the two-potential method will be

$$f = \sum_n f_B^{(n)} + \frac{1}{k_i} \sum_l (2l+1) \, P_l(\cos \theta) \, e^{i \delta_l^{(1)}} \sin \delta_l^{(1)} \langle \psi / e^{2 i \delta_l^{(0)}} / \psi \rangle \qquad (5.25)$$

where $f_B^{(n)}$ is the Born amplitude for the interaction V_H.

At present we take only $f_B^{(1)}$. Afterwards higher terms will be included.

$\delta_\ell^{(1)}$ and $\delta_\ell^{(0)}$ are the phase shifts for V_1 and V_o respectively. Here, since $V_1 = V_c(r_2)$, we have to find the $\delta_\ell^{(1)}$ for $V_c(r_2)$. For this, it is convenient to write (5.8) as

$$V_c(r_2) = C_7 \left[\frac{2}{\alpha_1} \frac{e^{-\alpha_1 r_2}}{r_2} - \frac{d}{d\alpha_1} \frac{e^{-\alpha_1 r_2}}{r_2} \right] + C_9 \left[\frac{6}{\alpha_2^2} \frac{e^{-\alpha_2 r_2}}{r_2} - \frac{4}{\alpha_2} \frac{d}{d\alpha_2} \frac{e^{-\alpha_2 r_2}}{r_2} + \frac{d^2}{d\alpha_2^2} \frac{e^{-\alpha_2 r_2}}{r_2} \right] + C_8 \left[\frac{24}{\alpha_4^3} \frac{e^{-\alpha_4 r_2}}{r_2} - \frac{18}{\alpha_4^2} \frac{d}{d\alpha_4} \frac{e^{-\alpha_4 r_2}}{r_2} + \frac{6}{\alpha_4} \frac{d^2}{d\alpha_4^2} \frac{e^{-\alpha_4 r_2}}{r_2} - \frac{d^3}{d\alpha_4^3} \frac{e^{-\alpha_4 r_2}}{r_2} \right]$$

Now making use of (4.105), the phase shift for the Yukawa type of potential in the Born approximation, the Born phase shift for the potential V_c is given by

$$\delta_\ell^{(B)} = -\frac{1}{k_i} \left\{ C_7 \left(\frac{2}{\alpha_1} - \frac{d}{d\alpha_1} \right) Q_\ell \left(\frac{2k_i^2 + \alpha_1^2}{2k_i^2} \right) + C_9 \left(\frac{6}{\alpha_2^2} - \frac{4}{\alpha_2} \frac{d}{d\alpha_2} + \frac{d^2}{d\alpha_2^2} \right) Q_\ell \left(\frac{2k_i^2 + \alpha_2^2}{2k_i^2} \right) + C_8 \left(\frac{24}{\alpha_4^3} - \frac{18}{\alpha_4^2} \frac{d}{d\alpha_4} + \frac{6}{\alpha_4} \frac{d^2}{d\alpha_4^2} - \frac{d^3}{d\alpha_4^3} \right) Q_\ell \left(\frac{2k_i^2 + \alpha_4^2}{2k_i^2} \right) \right. \quad (5.26)$$

The exact phase shift $\delta_\ell^{(1)}$ for the above potential can be found out using the Numerov method for the solution of the second order differential equation as described earlier. The numerical values of the exact phase shifts are obtained this way. The summation of partial waves in (5.25) is done by matching the Born and exact phase shifts etc. as discussed in section (4.5).

Now knowing the scattering amplitude (5.25) the DCS may be calculated. The process may be repeated for varying incident energies.

Results and Discussion :

The DCS obtained as discussed above at 54.4 eV is shown in fig (5.4). It is compared with experimental results and first Born DCS. This is done because the above two - potential formulation can be considered as a modification over the first Born approximation due to the following reason:

The present scattering amplitude

$$f = f_B^{(1)} + f_{Pw}$$

In the first Born approximation, the interaction potential $V_H + V_C$ is treated in fBA. Here, V_H is treated in fBA and V_C by partial wave analysis through a two-potential formulation. Hence a comparison between the present results and first Born results will be most appropriate.

From the figure it can be seen that the present TPB results vastly improve the first Born DCS. The present results reproduce the shape of the experimental curve, eventhough there is some quantitative difference. The present curve shows a dip around 105° as in the case of experimentally observed results, whereas the first Born DCS does not exhibit such a dip.

It can be concluded that the present two-potential result is definitely an improvement over simple first Born results. This is what was expected also because

(1) Now a weaker interaction is treated in the FB approximation.

(2) The core part of the interaction is given a better treatment through partial wave method.

The results at 100 eV shown in fig (5.5) also display same type of behaviour as at 54.4 eV. Unfortunately experimental results are not available for high energies. So discussion lacks the crucial comparison with experiments at such energies and hence has to be confined to lower energies.

5.6 Two-potential formulation including higher order Born terms :

In the earlier section, we have seen that the two-potential formulation involving only the first term of the Born series has improved the first Born approximation.

Eventhough the results so obtained show nice qualitative agreement with experimental data, the quantitative agreement is not so good.

It was discussed elsewhere that the absorption effects are all-important in the case of alkali scattering. Earlier it was also discussed that the results have improved by the incorporation of the absorption effect through the imaginary part of the second Born term. Hence the next step taken in the present study is the incorporation of the higher order terms in the two-potential formulation described in the previous section.

The higher order terms f Im, f Re_1 and $f^{(3)}_{GES}$ are to be determined in the Born approximation for the part of interaction V_H. Now

$$f = f^{(1)}_{B} + f\ \mathrm{Im} + f\ \mathrm{Re}_1 - f^{(3)}_{GES} + F_{Pw} \qquad (5.27)$$

In the two potential formulation, the first four terms in f are to be calculated for the potential $V_H = -\frac{1}{r_2} + \frac{1}{r_{12}}$. This is done in the earlier sections of this chapter. So these expressions (5.12), (5.21), (5.22) and (5.20) can be directly made use of. f_{Pw} remains same as in the previous section.

Here, one point is worthy of mention. In the evaluation of higher order Born terms, we have taken V_H part of the interaction because the V_c part is taken care of through partial waves. In the earlier sections, in the evaluation of higher order terms, V_H part was taken after completely ignoring the core potential V_c assuming that its contribution will be less. Hence the present study will help to assess the significance of V_c in double scattering terms.

Now that the scattering amplitude (5.27) is known, the differential cross sections can be computed for various incident energies.

Results and Discussion :

The DCS obtained as explained above are shown at the energy 100 eV alongwith other data (fig.5.6). The results of the earlier section (i.e. TPB results including only first Born term) are of special significance. Contrary to the expectation, the present DCS including higher order terms in the TPB results deviate away from the experimental curve. This may be due to one of the following reasons:

(1) The Born series is not convergent at such low energies.

(2) The importance of the core part of the interaction.

In the present analysis, we are not neglecting V_c, but taking it through some other way whereas in the previously discussed GES method, we have completely neglected V_c. If we had incorporated V_c there also, perhaps the results would have been much different. In the GES/HHOB method

$$f = f_{B1}\ (\text{Core} + \text{Val.}) + f\ \text{Im}\ (\text{Val}) + f\ \text{Re}_1 (\text{Val}) - f^{(3)}_{GES} (\text{val})$$

Here

$$f = f_{B1}\ (\text{val}) + f\ \text{Im}\ (\text{val}) + f\ \text{Re}_1\ (\text{val}) - f^{(3)}_{GES}\ (\text{val}) + f_{Pw}\ (\text{core})$$

The comparison of the above two scattering amplitudes shows that earlier we had neglected the imaginary part (corresponding to absorption) due to V_c and presently we are taking this into account through partial waves. Hence, there is enough reason to believe that the difference in the two sets of values is largely due to the incorporation of the core part in the higher order terms. This in turn shows that core cannot be simply neglected without enough justification.

5.7 ENa Process in the static potential :

In the previous section, we have seen the effects of neglecting the core part of the interaction. Unfortunately, the retaining of the core-part brings in lots of computational difficulties in the methods discussed so far. Moreover, in the current discussion we have not so far come across an appropriate method to describe the ENa process for large angle scattering. Here, we resort to the partial wave analysis of the static potential of Na atom for the following reasons:

(1) The static part of the interaction is predominant in the large angle region.

(2) In the static potential there is no differentiation between the potential due to the core electrons or valence electron of Na atom. Hence, there is no question of neglecting the core effect.

(3) Partial wave analysis of the static potential for many atoms have been proved to yield satisfactory results except for small angles of scattering.

(4) Calculations are simpler with static potentials because of the absence of the target co-ordinates.

The potential given by Co x and Bonham (1967) was chosen for the static potential of Na atoms. The Cox Bonham (CB) potentials are meant for mainly high energies. Hence first of all it is necessary to try their applicability at the intermediate energies of interest for us. For this purpose, we have already undertaken the study of the total cross sections for the elastic scattering of electrons by hydrogen atoms using the static potentials given by Cox and Bonham (Section 2.12). The TCS values are found to be comparable with other intermediate energy calculations, and hence it is verified that the CB potentials hold good at intermediate energies.

Now to go back to our discussion, we have to do the partial wave analysis of the ENa process using the CB Static potential for Na atom.

i.e. $$V_{st}\ (\mathrm{Na}) = -11 \sum_{j=1}^{6} \gamma_j \frac{e^{-\lambda_j r}}{r} \tag{5.28}$$

Here, $\lambda_1 = 0.9864$ $\quad \gamma_1 = 0.8281$

$\lambda_2 = 29.1004$ $\quad \gamma_2 = -0.0809$

$\lambda_3 = 3.0015$ $\quad \gamma_3 = 1.3795$

$\lambda_4 = 10.9701$ $\quad \gamma_4 = 3.2885$

$\lambda_5 = 1.2554$ $\quad \gamma_5 = -0.9576$

$\lambda_6 = 9.9009$ $\quad \gamma_6 = -3.4600$

The scattering amplitude is

$$f = \frac{1}{k_i} \sum_{\ell} (2\ell + 1)\, P_\ell\ (\mathrm{Cos}\ \theta)\ e^{i\delta_\ell}\ \mathrm{Sin}\ \delta_\ell \tag{5.29}$$

Hence the main part of the evaluation of the above scattering amplitude is the determination of the phase shifts for the potential V_{st}. Here again, to simplify the infinite summation over ℓ, we resort to the method described earlier

i.e. $$f = \frac{1}{k_i} \sum_{\ell=0}^{N} (2\ell+1)\, P_\ell\ (\mathrm{Cos}\ \theta)\ e^{i\delta_\ell}\ \mathrm{Sin}\ \delta_\ell + f_B^{(1)} - \frac{1}{k_i} \sum_{\ell=0}^{N} (2\ell+1)\, P_\ell\ (\mathrm{Cos}\ \theta)\ \delta_\ell^{(B)} \tag{5.30}$$

through which we are considering the partial waves for $\ell = 0$ to ∞. Here $f_B^{(1)}$ is the first Born amplitude for V_{st} and δ_ℓ and $\delta_\ell^{(B)}$ are the exact and Born phase shifts respectively. The N value is obtained by matching the two phase shift values. The Born phase shift $\delta_\ell^{(B)}$ for the static potential (5.28) of Na atom is given by

$$\delta_{\ell}^{(B)} = \frac{11}{k_i} \sum_{j=1}^{6} \gamma_j \; Q_{\ell} \left(\frac{2k_i^2 + \lambda_j^2}{2k_i^2} \right) \qquad (5.31)$$

For the evaluation of the exact phase shift δ_ℓ correspondingly, the value of V(x) in (4.97) has to be taken as

$V_{(x)} = -11 \sum_j \gamma_j \frac{e^{-\lambda_j x}}{x}$. Thereafter, the same procedure should be followed for the solution of the differential equation and evaluation of the phase shift δ_ℓ. After obtaining the two phase shifts $\delta_\ell^{(B)}$ and δ_ℓ, their values may be matched to fix the value of N suitably.

The first Born amplitude $f_B^{(1)}$ for the static potential (5.28) is

$$f_B^{(1)} = -\frac{1}{2\pi} \int dv \; e^{i\underline{q}\cdot\underline{r}} \; V_{St}(r)$$

which can be evaluated using standard integration techniques as

$$f_B^{(1)} \approx 22 \sum_j \frac{\gamma_j}{(q^2+\lambda_j^2)} \qquad (5.32)$$

Hence, knowing all the quantities in the scattering amplitude (5.30), the DCS for the ENa process in the static potential can be calculated as

$$\frac{d\sigma}{d\Omega} = |f|^2$$

Results and discussion :

The DCS for the ENa process in the partial wave method using the Cox Bonham static potential of Na atom is calculated in the method discussed above. The results at 54.4 eV are shown in fig (5.7). Alongwith the present results, those of other workers are also included in the figure for the purpose of a comparative study of the various results.

From the figure, it can be seen that the present results are reasonably good at intermediate and large angles when compared to the experimentally observed values. This is expected since:

(1) At intermediate and large angles, the coulomb type of term is predominant in the interaction which is properly treated through static potential.

(2) In the static potential, the effects of polarisation, absorption etc. are not taken care of. These effects are most significant at small angles of scattering. Hence the underestimation of the present results at small angles.

The present result at large angles is quite encouraging. In view of the importance of the absorption effect in alkali scattering, the static potential treatment given to ENa process is inadequate. The need is for a method which can describe the scattering at all angles reasonably well. Taking up all the above aspects, it can be ascertained that the partial wave analysis of an optical potential will be most suitable for the ENa process. This optical potential may be written as

$$V_{opt} = V_{st} + V_{pol} + i\,V_{abs} + V_{ex} \qquad (5.33)$$

In the above study, we have taken only the first term of this potential. Similar studies with the optical potential have been carried out for ELi process by Vanderpoorten (1976). The evaluation of the various terms in the optical potential (5.33) has been discussed in the review of Byron and Joachain (1977). The same procedure may be extended to the case of ENa process. A quick glance at the mode of evaluation suggests that there should not be much difficulty in extending the calculations for ENa process. However, the same is not attempted here.

5.8 More about the core approximation of ENa process :

Recently singh et al (1983) have reported the results arrived at by them for the ENa process. They have followed the procedure proposed by Lal and Srivastava (1981) where the contribution of the static part of the interaction is evaluated exactly and the on-shell contribution of remaining part is included by using the Glauber approximation. The scattering amplitude is thus written as

$$f = f^{st} + f_G - f_G^{st} \qquad (5.34)$$

where f^{St} and f_G are respectively the scattering amplitudes corresponding to the static interaction and the total interaction. Singh et al (1983) have taken f^{St} to be the static potential of the entire atom while f_G is the Glauber contribution for only the valence electron. The results so obtained exhibit qualitatively the same shape as predicted by experimental measurements of Teubner et al (1978) and Srivastava and Vuskovic (1980).

We can study the ENa process in a similar way using the HHOB approximation instead of the Glauber approximation. Thus the present scattering amplitude will be

$$f = f^{St} + f_{HHOB} - f^{St}_{HHOB} \qquad (5.35)$$

where f^{st} is the scattering amplitude for the static interaction obtained in the partial wave analysis, f_{HHOB} is the high energy Born contribution for the valence electron and f^{St}_{HHOB} stands for the scattering amplitude obtained by treating the static interaction in the HHOB approximation.

The evaluation of f^{St} and f_{HHOB} are described earlier in section (5.7) and (5.4) respectively. The HHOB analysis using the static potentials was discussed in Section (2.12). Hence, the evaluation of f^{St}_{HHOB} is also easy. Thus, one can obtain a scattering amplitude of the form (5.35).

In the present work, rough calculations for the ENa process using the above scattering amplitude were done. It was observed that the results agree qualitatively with the experimental data with a dip as shown in figures (5.4) and (5.5), but the quantitative agreement is not as good as the one, obtained by Singh et al (1983). It should be borne in mind that in the study of Walters (1973), the Born cross sections were much higher than their Glauber counterparts. Hence, similar type of modifications in the Glauber method (5.34) and the Born approximation (5.35) may result in higher cross section in the latter case.

Further analysis of (5.34) reveals that f_G^{st} and f^{st} being approximately same, the major contribution to the scattering amplitude comes from the term f_G, which is the Glauber contribution for only the valence electron. Hence, it can be noticed that the core contribution is not taken fully in the amplitude (5.34). This partial suppression of the core part may be responsible for the quantitative agreement of the results of Singh et al (1983) with the experimental data. It should be remembered that in the present study of ENa process using the two-potential formulation (Sections 5.5 and 5.6), the core potential was explicitly taken care of through partial wave analysis.

All these comparisons point out the fact that the core contribution is quite significant even at the energies 54.4 eV and 100 eV at which most of the present work was carried out.

From the above discussions, it becomes clear that a modified Glauber approach may be a plausible method in the small angle region. The partial wave analysis of an optical potential of the form (5.33) incorporating all the important effects in the case of electron-alkali scattering will be a much better description of the ENa process over the entire angular range. This is the general conclusion drawn from the discussions on the results arrived at in the present chapter using different modes of describing the ENa process as given in the various sections. Further analysis in this direction is in progress in our research group.

Table 5.1 C_j and λ_j for the target Sodium atom

j	C_j	λ_j
1	0.1944192	21.4
2	0.5553425	14.125
3	0.0380963	11.43
4	0.3965724	6.85
5	0.0544095	4.158
6	0.0018662	1.467

Table 5.2 - Individual terms for the $\bar{e}$ - Na elastic scattering in the GES approximation at E = 54.4 eV

θ	$F^{(1)}_{GES}$	$F^{(2)}_{GES}$	$F^{(3)}_{GES}$
10	0.8747 01	0.5630 01	0.2379 01
20	0.5623 01	0.2292 01	0.2439 01
30	0.3665 01	0.1729 01	0.1687 01
50	0.2223 01	0.1094 01	0.1131 01
70	0.1705 01	0.7234 00	0.8512 00
90	0.1406 01	0.5305 00	0.6828 00
110	0.1208 01	0.4234 00	0.5784 00
130	0.1075 01	0.3616 00	0.5141 00
150	0.9942 00	0.3271 00	0.4768 00

Table 5.2a - Individual terms for the $\bar{e}$ - Na elastic scattering in the GES approximation at 100 eV

θ	$f^{(1)}_{GES}$		$f^{(2)}_{GES}$		$f^{(3)}_{GES}$	
10	0.7576	01	0.2655	01	0.1440	01
15	0.5522	01	0.1647	01	0.1313	01
25	0.3188	01	0.1169	01	0.6493	00
35	0.2296	01	0.8459	00	0.6342	00
50	0.1706	01	0.5358	00	0.4635	00
70	0.1277	01	0.3391	00	0.3339	00
90	0.1004	01	0.2446	00	0.2617	00
110	0.8234	00	0.1935	00	0.2179	00
130	0.7084	00	0.1644	00	0.1917	00

Table 5.3 Individual terms including the Born terms obtained in the case of $\bar{e}$ - Na elastic scattering at 54.4 eV

θ	$f^{(1)}_{GES}$	$f^{(2)}_{GES}$	$f^{(3)}_{GES}$	fIm	fRe_1
10	0.8747 01	0.5630 01	0.2379 01	0.4925 01	0.2111 00
20	0.5623 01	0.2292 01	0.2439 01	0.2190 01	0.1032 00
30	0.3665 01	0.1726 01	0.1687 01	0.1653 01	0.1605 00
50	0.2223 01	0.1094 01	0.1131 01	0.0965 01	0.9761 -01
70	0.1705 01	0.7234 00	0.8512 00	0.7132 00	0.5641 -01
90	0.1406 01	0.5305 00	0.6828 00	0.5296 00	0.3784 -01
110	0.1208 01	0.4234 00	0.5784 00	0.4110 00	0.2846 -01
130	0.1075 01	0.3616 00	0.5141 00	0.3599 00	0.2337 -01
150	0.9942 00	0.3271 00	0.4768 00	0.3211 00	0.2063 -01

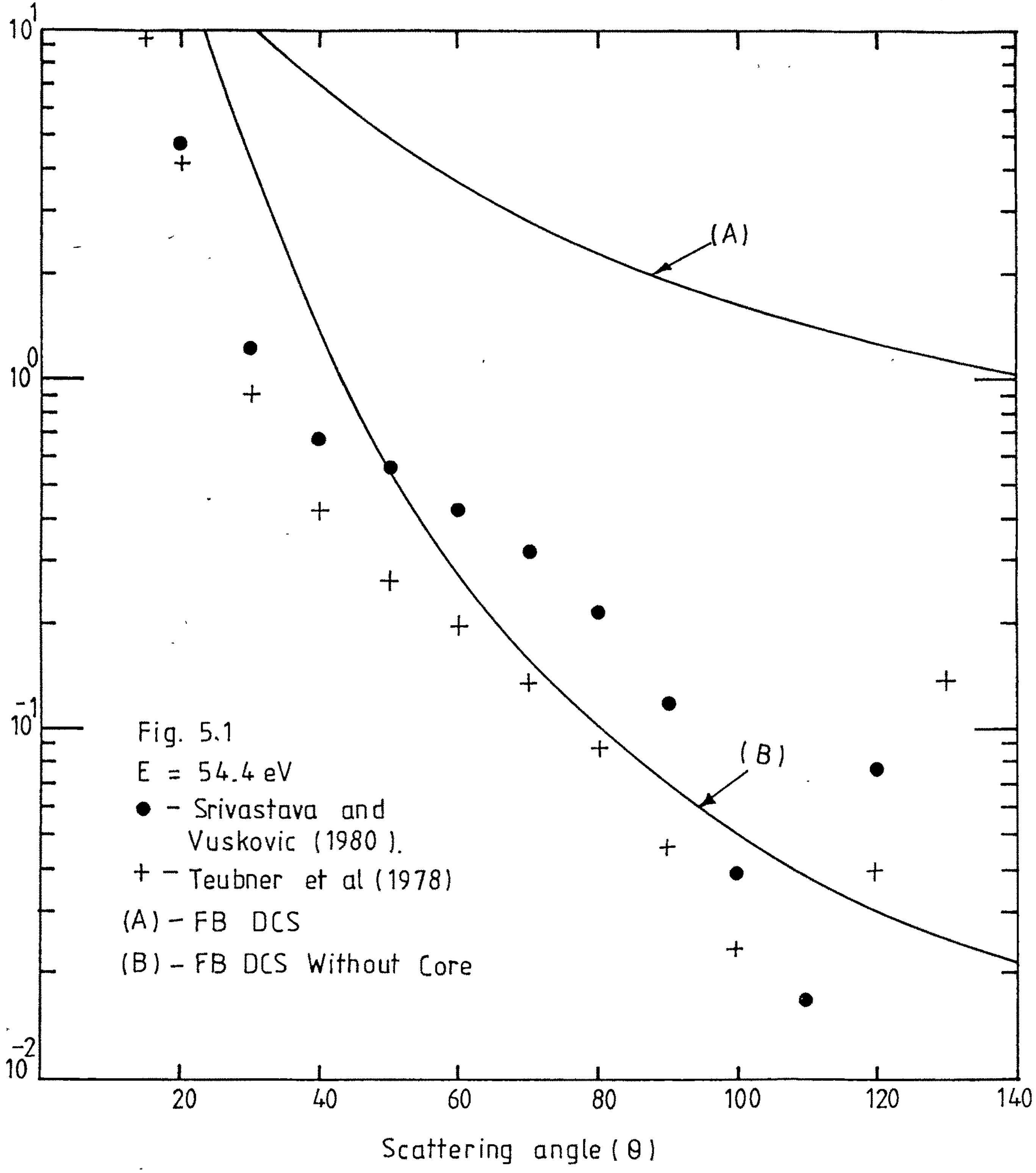

Fig. 5.1

E = 54.4 eV
● – Srivastava and Vuskovic (1980).
+ – Teubner et al (1978)
(A) – FB DCS
(B) – FB DCS Without Core
(A)
(B)
10^1
10^0
10^{-1}
10^{-2}
20
40
60
80
100
120
140
Scattering angle (θ)

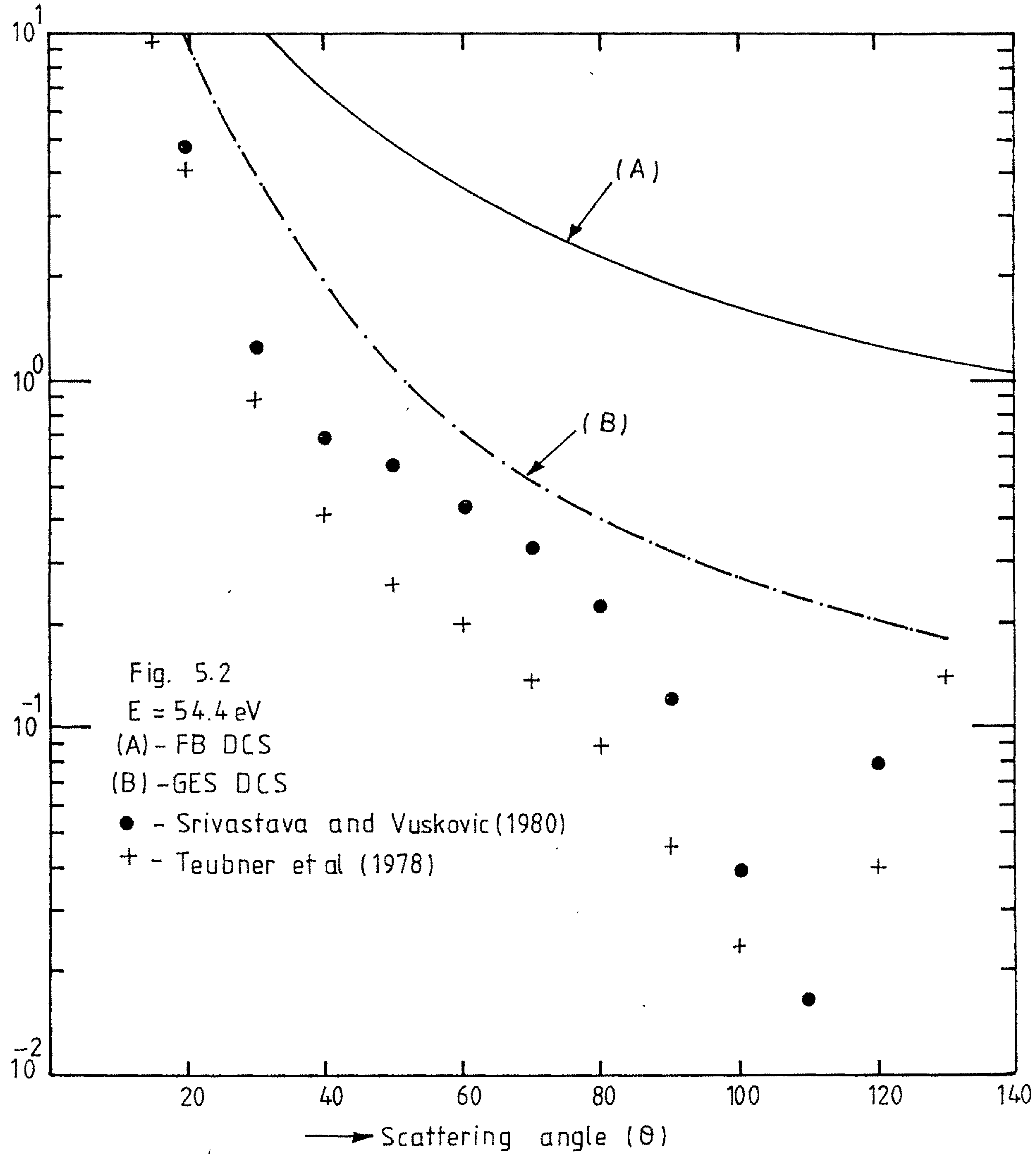

Fig. 5.2

E = 54.4 eV
(A) - FB DCS
(B) - GES DCS
● - Srivastava and Vuskovic (1980)
+ - Teubner et al (1978)
(A)
(B)
10^1
10^0
10^{-1}
10^{-2}
20
40
60
80
100
120
140
→ Scattering angle (θ)

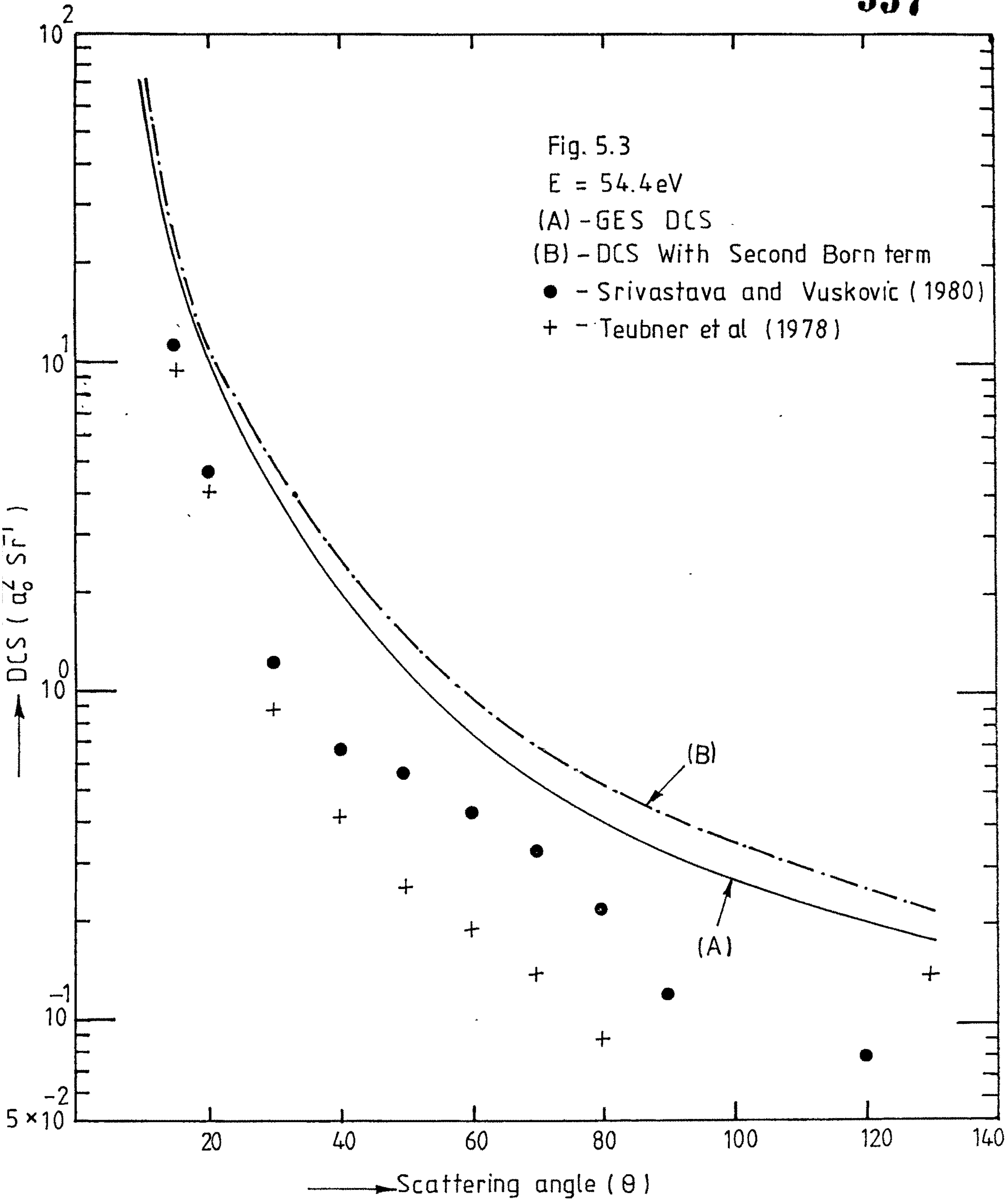
Fig. 5.3
E = 54.4eV
(A) - GES DCS
(B) - DCS With Second Born term
● - Srivastava and Vuskovic (1980)
+ - Teubner et al (1978)
(A)
(B)
10^2
10^1
10^0
10^{-1}
5×10^{-2}
20
40
60
80
100
120
140
→ DCS ($a_0^2\ Sr^{-1}$)
→ Scattering angle (θ)

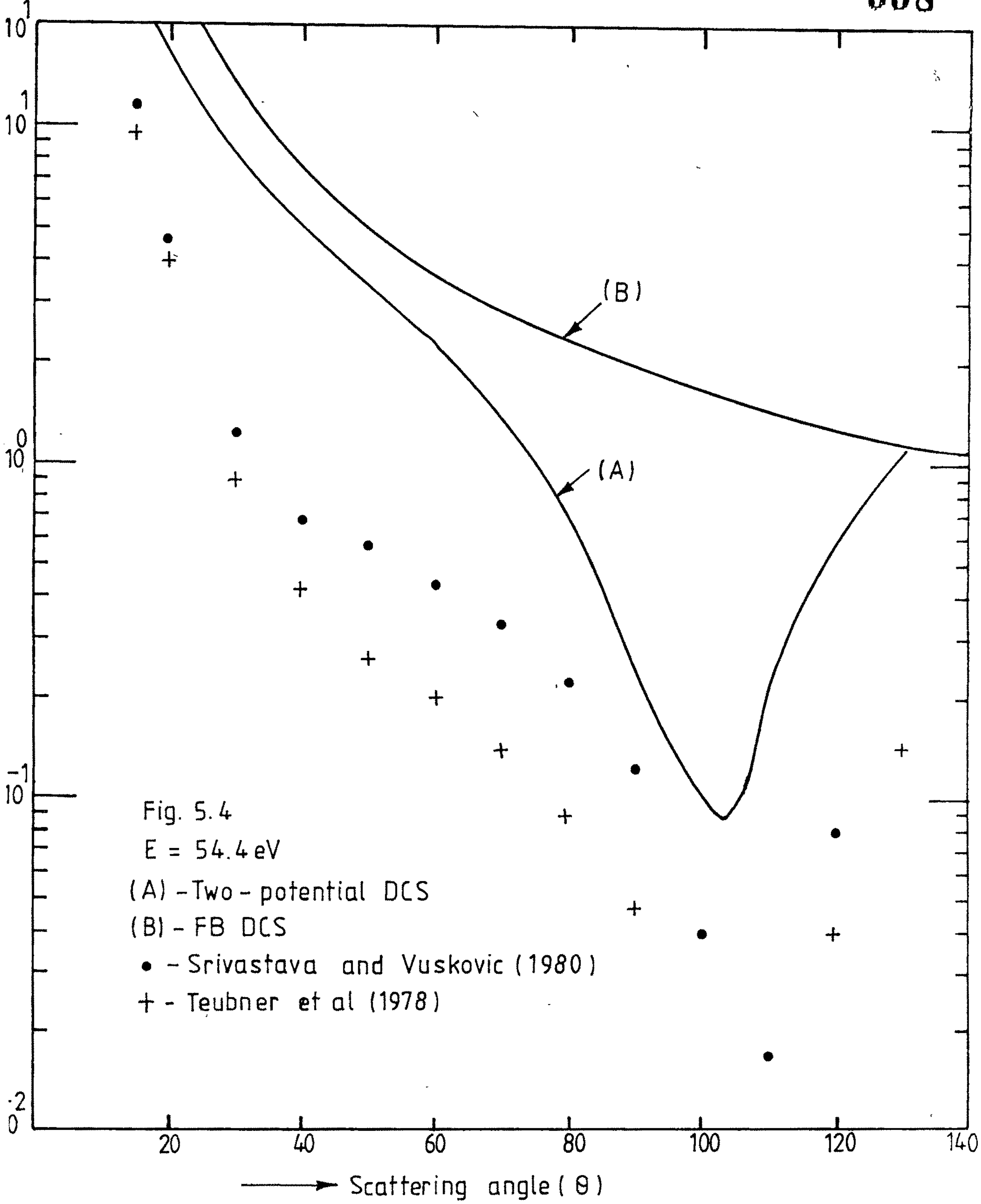

Fig. 5.4
E = 54.4 eV
(A) - Two - potential DCS
(B) - FB DCS
● - Srivastava and Vuskovic (1980)
+ - Teubner et al (1978)

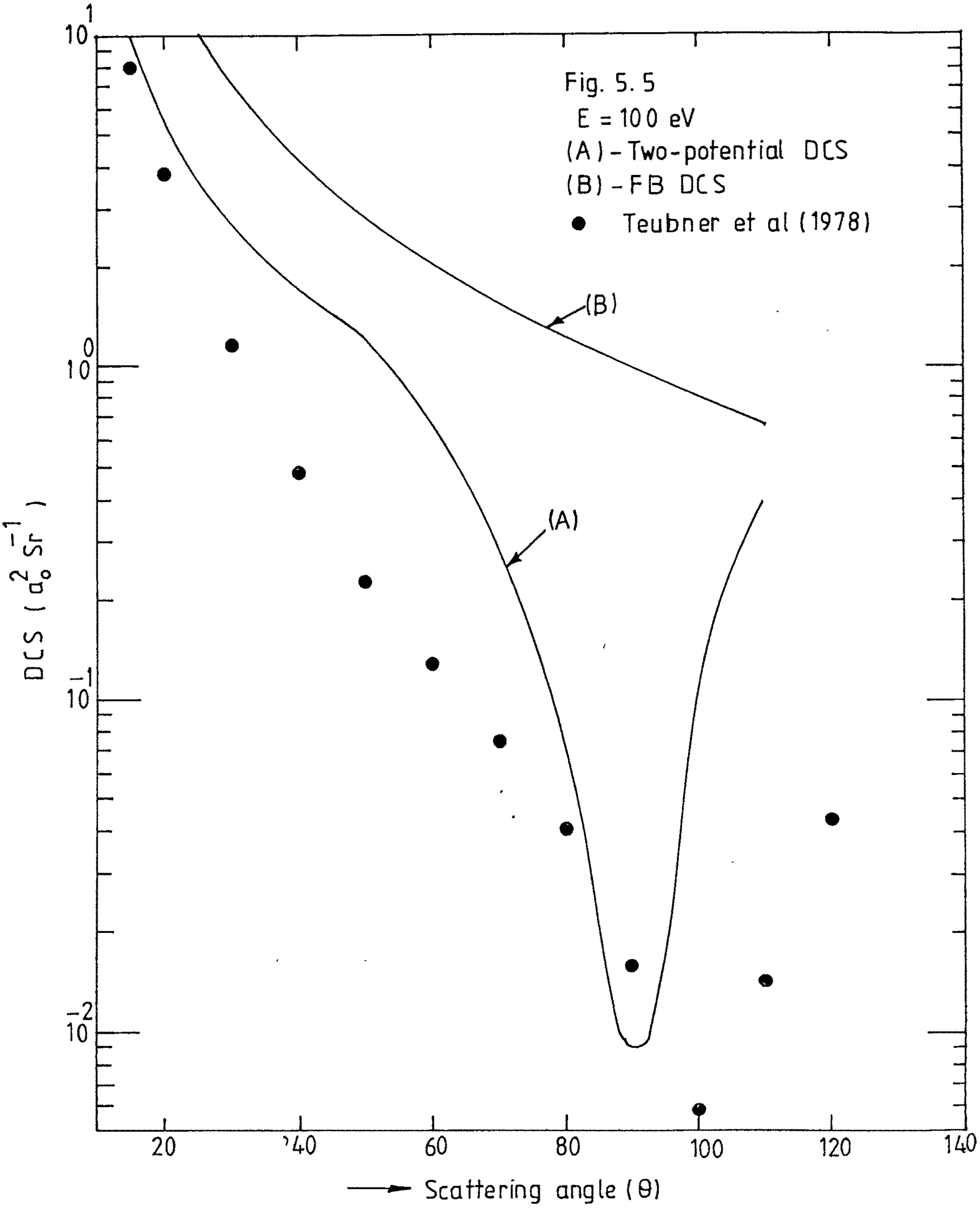
Fig. 5.5
E = 100 eV
(A) - Two-potential DCS
(B) - FB DCS
● Teubner et al (1978)
(A)
(B)
10^1
10^0
10^{-1}
10^{-2}
DCS (a_o^2 Sr^{-1})
20
40
60
80
100
120
140
Scattering angle (θ)

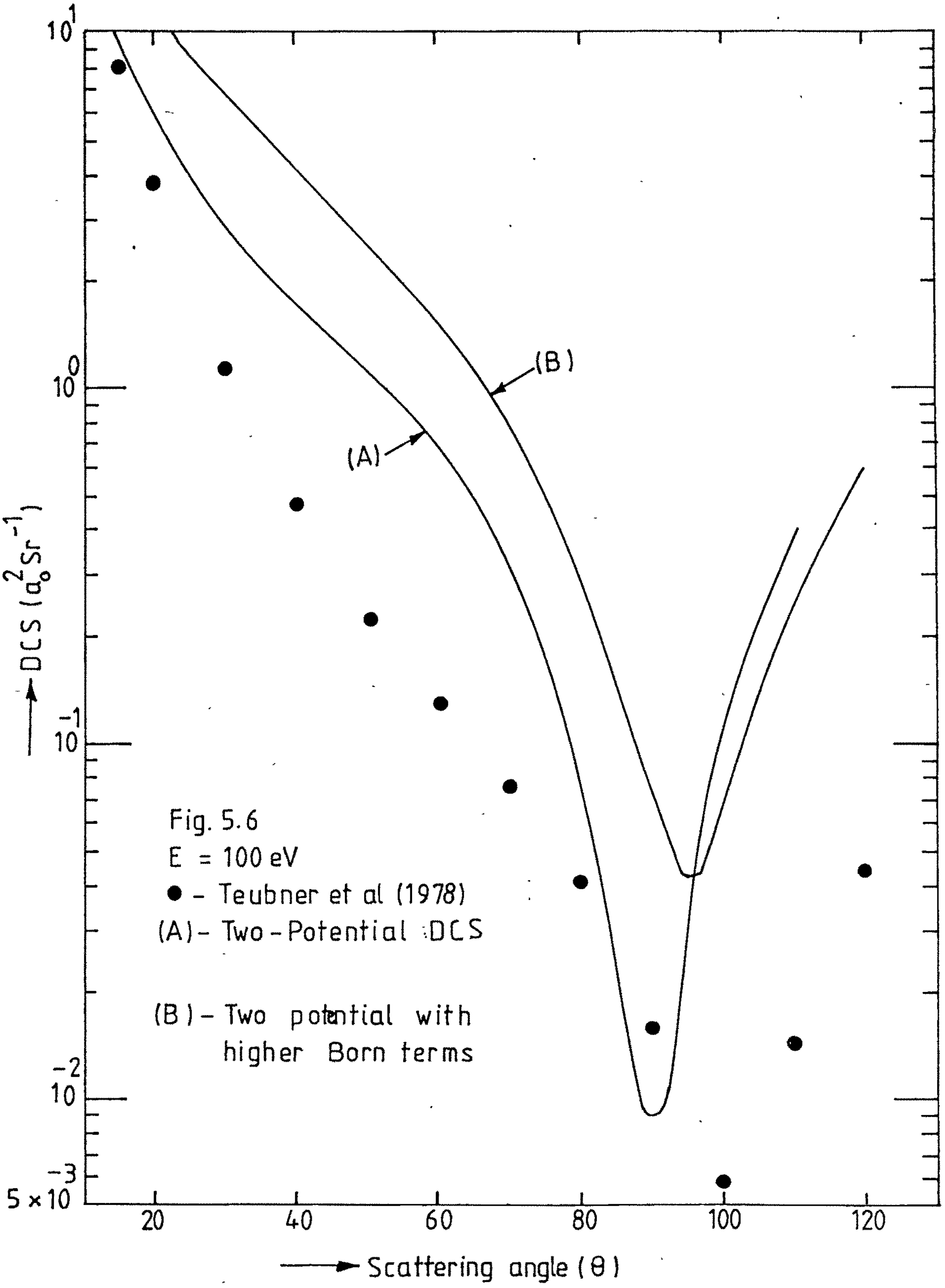
Fig. 5.6

E = 100 eV
● - Teubner et al (1978)
(A) - Two-Potential DCS
(B) - Two potential with higher Born terms
(A)
(B)
10^1
10^0
10^{-1}
10^{-2}
5×10^{-3}
20
40
60
80
100
120
→ DCS ($a_o^2 Sr^{-1}$)
→ Scattering angle (θ)

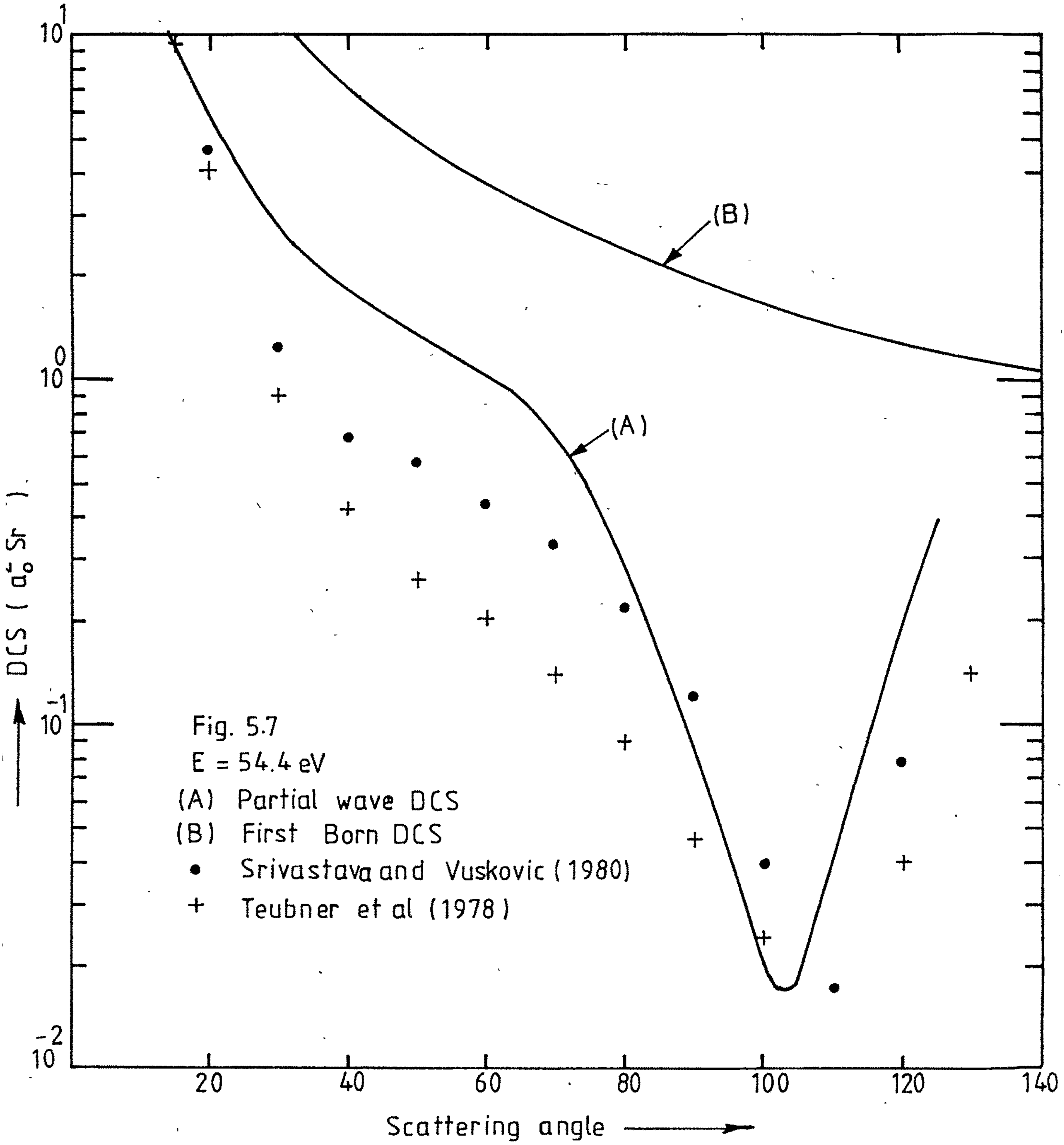

Fig. 5.7

E = 54.4 eV