CHAPTER - V

SCATTERING OF ELECTRONS BY LITHIUM ATOMS

5.1 Introduction :

Inspired by the success of the techniques employed to calculate the scattering parameters the study of scattering of electrons by lithium (Li) (z = 3) atom is continued in this chapter. In contrast with hydrogen and helium, very meagre data is available both in the theoretical studies, (Mathur et al, 1971, 1972 ; Walters, 1973 ; Vanderpoorten , 1976, Guha and Ghosh, 1979 ; Tayal et al, 1981) and the experimental results. Most of the theoretical studies, were done by using Glauber frozen core approximations for the alkali atoms. Walters (1973) used these types of approximations for the study of (2N + 1) electron system of the alkali atoms. He reduced the (2N + 1) electron systems of the alkali atoms to the hydrogen atom like problem. This was done by splitting the total interaction (equation 2.24) into two parts, one corresponding to the valance electron and the other part due to the inner (core) electrons of the target with respect to the incident electron, and considering for one electron (valance)

Slater (Coulson, 1961) type of wave functions for the alkali atoms. In this chapter we would like to study the Born terms (equation 2.47) using the Walters method of the interaction at the incident energies E = 20 to 800 eV. We consider the $\bar{e}$ - Li collision processes in the present chapter. The plan of the investigation is described below :

i) Elastic scattering of electrons by the ground state one electron wave function of the lithium atom, using the Slater type of orbitals.

ii) An analytical study of higher order Born terms in the static field with an example of $\bar{e}$ - Li elastic process.

iii) An analytical study of elastic and inelastic scattering of electrons by lithium atoms using Clementi (1965) type of wave functions.

5.2.1 Elastic scattering of electrons by the ground (2s) state of lithium atom (ESGLi) :

(Rao and Desai, 1983c)

$$\bar{e} + \mathrm{Li}\ (2s) \longrightarrow \bar{e} + \mathrm{Li}\ (2s) \qquad \dots (5.1)$$

As in the processes of ESGH (Sec. 3.2.1) and ESGHe (Sec. 4.2.1) here also the final state wave function of the target lithium atom is same as the initial ground state function (Guha and Ghosh , 1979; Walters 1973). The ground state wave function of the lithium atom corresponding to the valance electron can be given as

$$\psi_{2s} (\underline{r}_1) = A' r_1 \exp (- y_1' r_1) + B' \phi_{1s} (r_1) \quad \text{....(5.2)}$$

where

$$\phi_{1s} (\underline{r}_1) = \left[\frac{(2.7)^3}{\pi} \right]^{1/2} \exp (- y_2' r_1) \quad (5.3)$$

here $y_1' = 0.65$, $y_2' = 2.7$, A' and B' are constants so chosen that $U_{2s} (\underline{r}_1)$ is orthogonal to $\phi_{1s} (\underline{r}_1)$ and also normalised. The normalisation constants A' and B' can be obtained by solving the following integrals.

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

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

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

upon the substitution of equations (5.2, 5.3) in the above integrals we obtained the constants given as

$A' = 0.11252$, $B' = -0.16861$. Now the product of the initial and final state wave functions of the lithium atom can be obtained as

$$\Psi_i(\underline{r}_1)\,\Psi_f^*(\underline{r}_1) = [\; A\, r_1 \exp(-y_1'\, r_1) - B \exp(-y_1'\, r_1)\;]^2$$

$$= B^2 \exp(-2\,y_2'\, r_1) - 2\,A\,B\, r_1 \exp(-(y_1' + y_2')\, r_1) + A^2\, r_1^2 \exp(-2y_1'\, r_1) \qquad \ldots.(5.4)$$

$$= B^2 \exp(-2\,y_2'\, r_1) + 2\,A\,B\; D(y_2') \exp(-y_3'\, r_1) + A^2\, D^2(y_1') \exp(-2\,y_1\, r_1) \qquad (5.5)$$

$$= -\Big[\; B^2\, D(y_1)\, \frac{\exp(-y_1\, r_1)}{r_1} + 2\,A\,B\,D^2(y_2)\, \frac{\exp(-y_2\, r_1)}{r_1} + A^2\, D^3(y_3)\, \frac{\exp(-y_3\, r_1)}{r_1}\;\Big] \qquad \ldots\ldots(5.6)$$

$$= -\sum_{n=1}^{3} B_n'\, D^n(y_n)\, \frac{\exp(-y_n\, r_1)}{r_1} \qquad (5.7)$$

where $A = A'$, $B = 0.42204$, and the constants B_n's and y_n's can be obtained through the equation (5.4). Final form of the wave function product (equation 5.7) is similar to that of ESEH (Sec. 3.3.1) process (equation 3.21). So the derivations of the ESEH process scattering amplitudes (equations 3.22, 3.24, 3.25, 3.27, 3.28) can be easily extended to the present ESGLi process, as follow . The interaction between the incident electron and the target lithium atom can be written as

$$V_d = -\frac{3}{r_o} + \frac{1}{|\underline{r}_o - \underline{r}_1|} + \frac{1}{|\underline{r}_o - \underline{r}_2|} + \frac{1}{|\underline{r}_o - \underline{r}_3|} \quad .....(5.8)$$

$$= -\frac{1}{r_o} + \frac{1}{|\underline{r}_o - \underline{r}_1|} + \frac{1}{|\underline{r}_o - \underline{r}_2|} + \frac{1}{|\underline{r}_o - \underline{r}_3|} - \frac{2}{r_o}$$

where $\underline{r}_o$ and $\underline{r}_1$, $\underline{r}_2$, $\underline{r}_3$ are the position vectors of the incident and target electrons w.r.t. the target nuclei. Following the procedure of Walters (1973) this interaction can be written as

$$= -\frac{1}{r_o} + \frac{1}{|\underline{r}_o - \underline{r}_1|} + V_c (r_o) \qquad (5.9)$$

where $V_c(r_o)$ is the core potential due to the two electrons of the 1s orbital of lithium atom. This core potential can be obtained as (Walters , 1973),

$$V_c(r_o) = 2 \sum_{i=1}^{N} \int d\underline{r}\ \phi_i^*(\underline{r}) \left[-\frac{1}{r_o} + \frac{1}{|\underline{r}_o - \underline{r}|} \right] \phi_i(\underline{r}) \qquad (5.10)$$

where N = 1 for the lithium atom. Substituting equation (5.3) in the above integral we will obtain the core contribution to equation (5.9),

$$= 2 \int d\underline{r}_1\ \phi_{1s}(\underline{r}_1) \left[-\frac{1}{r_o} + \frac{1}{|\underline{r}_o - \underline{r}_1|} \right] \phi_{1s}(\underline{r}_1) \qquad (5.11)$$

By analogy with the integral procedure of equation (4.9) the closed form of the above integral can be obtained as

$$V_c(r_o) = -2 \left[\frac{1}{r_o} + 2.7 \right] \exp(-5.4\, r_o) \qquad (5.12)$$

The total interaction to be considered in the present study is

$$V_d = -\frac{1}{r_o} + \frac{1}{|\mathbf{r}_o - \mathbf{r}_1|} - 2\left[\frac{1}{r_o} + 2.7\right]$$

$$\exp(-5.4\, r_o) \qquad (5.13)$$

Substituting the equations (5.7, 5.13) in the scattering amplitudes (equations 2.12, 2.57, 2.43) we will obtain the corresponding scattering contributions for the DCS (equation 3.2). Now the closed form of the first Born approximation for the ESGLi process can be obtained as

$$f^{(1)}_{i \to f} = -\frac{1}{2\pi} \int d\,\mathbf{r}_o \exp(i\,\mathbf{q}\cdot\mathbf{r}_o) \int d\,\mathbf{r}_1$$

$$\Psi_i(\mathbf{r}_1)\left[-\frac{1}{r_o} + \frac{1}{|\mathbf{r}_o - \mathbf{r}_1|}\right.$$

$$\left. + V_c(r_o)\right] \Psi^*_f(\mathbf{r}_1)$$

$$= -\frac{1}{2\pi} \sum_{n=0}^{2} A_n'\, D^n(y_n) \int d\,\mathbf{r}_o \exp(i\,\mathbf{q}\cdot\mathbf{r}_o)$$

$$\int d\,\mathbf{r}_1\left[-\frac{1}{r_o} + \frac{1}{|\mathbf{r}_o - \mathbf{r}_1|} - \right.$$

$$\left.\left(\frac{2}{r_o} + 5.4\right) \exp(-5.4\, r_o)\right]$$

$$\exp(-y_n r_1)$$

Using the first Born results of ESEH process (equation 3.22) the above integral form can be written in the closed form

$$f^{(1)}_{i\to f} = \sum_{n=0}^{2} A_n D^n (y_n) \left[\frac{(q^2 + 2 y_n^2)}{y_n^3 (q^2 + y_n^2)^2} + \frac{2}{y_n^3 (q^2 + y_4^2)} + \frac{(5.4) y_4}{y_n^3 (q^2 + y_4^2)^2} \right] \qquad \ldots\ldots (5.14)$$

where the constants A_n's and y_n's are obtained as

$A_o = 8.95318$, $A_1 = 4.7740$, $A_2 = 0.63640$ and

$y_o = 5.4$, $y_1 = 3.4$, $y_2 = 1.3$, $y_4 = 5.4$.

Now in the derivations of second Born (equation 2.57) and third GES (equation 2.43) approximations we will neglect the core potential contribution (equation 5.12) in the interaction of $\bar{e}$ - Li elastic process (equation 5.13) (Guha and Ghosh , 1979) . The imaginary and the real parts of the second Born approximation equations(2.60, 2.59, 2.58) and third GES term (equation 2.43) can be obtained by substituting the equations (5.7, 5.13) in the corresponding scattering amplitudes (equation 2.60, 2.59, 2.58, 2.43).

The closed form of all these scattering amplitudes can be readily obtained from the final forms of the ESEH process (Sec. 3.3.1) for the present ESGLi process.

$$\mathrm{Im}\ f^{(2)}_{\mathrm{HEA}} = -\frac{1}{k_i} \sum_{n=1}^{3} B_n D^n (y_n) \frac{1}{y_n^2} \left[2 I_1 (\beta_i^2 , y_n^2) - \frac{q^2}{(q^2 + y_n^2)} I_1' (\beta_i^2 , 0) \right] \qquad (5.15)$$

$$\mathrm{Re1}\ f^{(2)}_{\mathrm{HEA}} = \frac{1}{\pi k_i} \sum_{n=1}^{3} B_n D^n (y_n) \frac{1}{y_n^2} \left[2 I_2 (\beta_i^2 , y_n^2) - \frac{q^2}{(q^2 + y_n^2)} I_2' (\beta_i^2 , 0) \right] \qquad (5.16)$$

$$\mathrm{Re2}\ f^{(2)}_{\mathrm{HEA}} = \frac{1}{2 \pi k_i^2} \sum_{n=1}^{3} B_n D^n (y_n) D' \left[\frac{I_3 (\beta_i , y_n)}{y_n^2} - \frac{I_3' (\beta_i , 0)}{(q^2 + y_n^2)} - I_2 (\beta_i^2 , y_n^2) \right] \qquad (5.17)$$

where $I_1(\beta_i^2, y_n^2)$, $I_1'(\beta_i^2, 0)$, $I_2(\beta_i^2, y_n^2)$, $I_2'(\beta_i^2, 0)$, $I_3(\beta_i, y_n)$, $I_3'(\beta_i, 0)$, are defined differentiable integral solutions (ESEH Sec.3.3.1) And B_n's , y_n's are constants can be obtained through the equations (5.4, 5.7 , 2.60).

$B_1 = 0.71247$, $B_2 = 0.3799$, $B_3 = 0.05064$

$y_1 = 5.4$, $y_2 = 3.4$, $y_3 = 1.3$

In a similar way third GES term can be derived making use of the equations (3.16, 3.28).

$$f_{GES}^{(3)} = -\frac{\pi}{16\,k_i^2}\sum_{n=1}^{3} y_n^4\, B_n'\, D^n(y_n)\, F(q, y_n) \qquad \ldots\ldots (5.18)$$

$$= -\frac{1}{k_i^2}\sum_{n=1}^{3} C_n\, D^n(y_n)\left(\frac{1}{q^2+y_n^2}\right)\left[4\left\{\log\left(\frac{q^2+y_n^2}{y_n\, q}\right)\right\}^2+\frac{\pi^2}{3} - 2A(q, y_n^2)\right] \qquad (5.19)$$

where the constants are obtained as $C_1 = 29.73803$,

$C_2 = 2.49206$, $C_3 = 0.00710$. And a typical function $A(q, y_n^2)$ was defined previously (equation 3.16) . Finally the expression for TCS, and exchange scattering amplitude (equations 3.3 , 2.36) can be obtained by substituting the equations (5.15, 5.5) in(3.3 , 3.17) And making use of the ESEH results (equations 3.12, 3.29), the corresponding expressions for the present case can be written as

$$\sigma_{tot}^{.Li} = - \frac{8\pi^2}{k_i^2} \sum_{n=1}^{3} \left[B_n D^n(y_n) \frac{1}{y_n^4} \log \frac{y_n^2 + \beta_i^2}{\beta_i^2} \right] \qquad (5.20)$$

and the exchange contribution can be obtained as

$$g_{och} = - \frac{1}{k_i^2} \sum_{n=0}^{2} A_n D^n(y_n) \left[\frac{y_n}{(q^2 + y_n^2)^2} \right]$$

..... (5.21)

Using these expressions(equations (5.14, 5.15, 5.16, 5.17, 5.19), we have calculated the DCS and TCS at incident energies E = 20 to 700 eV. Exchange term equation (5.21) is neglected in the calculation of DCS (equation 3.2).

5.2.2 Comparison of present ESGLi results with the other data :

ESGLi scattering amplitudes (equations 5.14, 5.15 5.16,5.17, 5.19) derived in the preceding section (5.2.1) are employed to calculate DCS and TCS in the incident energy range E = 20 to 700 eV . We have used an average excitation energy DE = 0.0745 a.u (Vanderpoorten,1976) in the calculation of second Born term (equation 2.57). These results are listed in the Tables (5.1, 5.2) and shown in Figs. (5.1 to 5.4) along with the other theoretical and experimental data. The present DCS results are found to be in good agreement with the available data in the angular region $\theta \leq 50^{\circ}$. The details of the Tables and Figs.are as follows .

Fig. (5.1) shows, DCS for ESGLi at incident energy E = 20 eV . Solid curves a' and b' are the present results, with and without real part (equation 5.17) in the DCS calculations. Other representations correspond to theoretical results -.- - - C C (Close coupling) of Issa (1977), + — EBS of Byron and Joachain (taken from the abstract book of IIIrd National Workshop on Atomic and Molecular Physics Roorkee , 1981) and experimental data ● — of Williams (1976).

Fig. (5.2) shows DCS for ESGLi at incident energies E = 100 eV (set A) and 200 eV (set B). Set A shows present DCS (solid curves a' and b') at incident energy E = 100 eV along with the compared theoretical results, ● — CS (Corrected Static) of Tayal et al (1981), + — EBS of Byron and Joachain (taken from the paper of Tayal et al , 1981) and O — of present work (Corresponding to Static results, Sec. 5.3.1). Set B shows DCS at incident E = 200 eV. All the representations in this set B are same as given in set A.

Fig. (5.3) shows present DCS (Solid curves a' and b' (Sec. 5.2.1)) and small circles (Sec. 5.3.1) for ESGLi at incident energy E = 400 eV.

Fig. (5.4) shows the TCS (equation 5.20) at incident energy range E = 80 to 700 eV.

It can be observed from the Figs. (5.1, 5.2, 5.3) that the variation in DCS (solid curves a' and b') due to real part (equation 5.17) gradually decreases from E = 20 to 400 eV. This behaviour shows that the convergence of equation (5.17) is more rapid at higher incident energies (400 eV) than at lower incident energies (100, 200 and 20 eV). And the curve

b' approaches the compared EBS and CS results (Tayal et al, 1981) in the angular region $\theta \leq 60^o$ and lies in between these compared results for $\theta > 60^o$ (Rao and Desai , 1983c). The present DCS results (curves a' and b') agree well with the compared theoretical results in the small angle region. Similar to ESEH (Sec. 3.3.2) process, here also it was difficult to make exact comparison of our DCS results due to the unavailability of experimental data at higher incident energies. A lot of similarities between ESEH (Fig. 3.3) and the present ESGLi (Fig. 5.2) process can be observed . These similarities are due to the wave functions (equations 3.19 and 5.2) used in these two targets which are similar to each other . Fig. (5.4) shows the general pattern of the variation of TCS with respect to the incident energy.

In Table (5.1) we have listed ESGLi scattering contributions (equations 5.14, 5.16, 5.17, 5.19, 5.15) to the DCS (equation 3.2) at 400 eV incident energy. Similar to ESEH process (Table 3.8) here also fluctuations are observed in the real part equation (5.17) and the contribution of this term to the DCS was greater than real part equation (5.16) and third GES (equation 5.19) term. In Table (5.2) we have listed only DCS results at incident energies E = 80 to 700 eV.

In anticipation of experimental and theoretical results, we are expecting that the present ESGLi results will compare nicely at small angles and high incident energies.

5.3.1 An analytical study of higher order Born terms in the static field :

(Rao and Desai, 1983b)

So far, first and second Born terms (equations 2.12, 2.57) for elastic process of hydrogen (Secs. 3.2.1 , 3.3.1),helium (Sec. 4.2.1) and lithium (Sec. 5.2.1) atoms are studied for the direct and exchange interactions (equations 2.24, 2.36) by considering the structure of the target atoms. These studies will be combursome if one goes beyond a certain limit of the atomic number z of the target atom. In order to overcome this difficulty for complex system we would like to extend the HEA approximation (Sec. 2.3.5) for the fields. The analytical expressions for the static field of various atoms can be obtained by the pioneer workers (Tietz , 1965; Cox and

Bonham, 1967 ; Bonham and Strand, 1963, 1964). In this Section an attempt is made to derive three Born terms (equations 2.12, 2.57, 2.62) of HEA (Sec. 2.3.5) for the known static fields. These derived amplitudes can be used for any atom, as an example elastic scattering of electrons by the static field of lithium atom is considered.

Consider the non - relativistic scattering of a spinless electron by a potential field $V_{st}(\underline{r}_o)$ of an z - electron atom with initial and final states and energies given (Ψ_i, E_i) and (Ψ_f, E_f) respectively. The static field can be defined as

$$V_{st}(r_o) = \langle \Psi_i | V_d | \Psi_f \rangle = V_{fi}(r_o) \qquad \ldots\ldots(5.22)$$

V_d is the interaction between the incident electron and the target atom (equation 2.24). The static potential for different atoms can be obtained (Cox and Bonham, 1967 ; Tietz, 1965 ; Bonham and Strand , 1963, 1964) in the analytical form. A general form of this can be given as

$$V_{st}(r_o) = z \sum_{i=1}^{N} R_i \frac{\exp(-y_i r_o)}{r_o} \qquad (5.23)$$

where z is the atomic number and R_i's and y_i's are constants. For lithium atom these constants (Tietz , 1965) can be given as

$R_1 = 1.2197$, $R_2 = -0.2197$, $R_3 = 1.6368$

$R_4 = 0.9508$, $R_5 = -1.6368$, $R_6 = -0.9508$

and $y_1 = 0.8776$, $y_2 = 7.9510$, $y_3 = 2.4948$

$y_4 = 3.9701$, $Y_5 = 1.4948$, $y_6 = 2.9701$

$z = 3$, and $N = 6$.

Similarly for various atoms, the analytical expression (equation 5.23) for the field and related constants can be obtained (Tietz, 1965 ; Cox and Bonham, 1967 ; Bonham and Stand , 1963, 1964). The fourier transform of equation (5.23] can be obtained as

$$V_{st} (r_o) = \int d \underline{p} \exp (- i \underline{p} \cdot \underline{b}_o) \int_{-\infty}^{\infty} d p_Z \exp (- i p_Z Z_o) \bar{V}_{st} (\underline{p} + p_Z \hat{y}) \qquad .....(5.24)$$

where

$$\bar{V}_{st} (\underline{p} + p_Z \hat{y}) = \frac{z}{2 \pi^2} \sum_{i=1}^{N} \frac{R_i}{(p^2 + p_Z^2 + y_i^2)} \qquad .....(5.25)$$

With these defined quantities (equations 5.22 to 5.25), first, second and third Born amplitudes for elastic process can be derived easily. The basic approximations and the computation procedure adopted in the second (equation 2.57) and the equation(2.62) Born terms are same as given in HEA (Sec. 2.3.5).

The first Born amplitude can be obtained in the closed form through the equations (5.22, 5.23, 3.8).

$$f_{st}^{(1)} = -2\,z \sum_{i=1}^{N} \frac{R_i}{(\,q^2 + y_i^2\,)} \qquad (5.26)$$

The second Born amplitude for fields can be obtained by substituting equation (5.22) in equation (2.57). The resulting expression can be obtained in the d $\underline{p}$ integral form by using equation (5.24) and following the procedure given under equation (2.57). Then the real and imaginary terms O (k_i^{-2}) for DCS can be obtained.

$$\mathrm{Im}\; f_{HEAS}^{(2)} = \frac{4\,\pi^3}{k_i} \int d\,\underline{p}\;\; \bar{V}_{st}\,(\,\underline{q} - \underline{p} + \beta_i\,\hat{\nu}\,)\;\; \bar{V}\,(\,\underline{p} + \beta_i\,\hat{\nu}\,)$$

......(5.27)

$$= \frac{4\ \pi^3\ z^2}{4\ \pi^4\ k_i} \int d\ \underline{p} \sum_{i,J=1}^{N}$$

$$\left[\frac{R_i\ R_J}{(\ p^2 + \beta_i{}^2 + y_i{}^2\ )\ (\ |\ \underline{g} - \underline{p}\ |^2 + \beta_i{}^2 + y_J{}^2\ )} \right]$$

.... (5.28)

$$= \frac{z^2}{\pi\ k_i} \sum_{i,J=1}^{N} R_i\ R_J\ I_1\ (\ \beta_i{}^2,\ u^2\ ,\ v^2\ )$$

.... (5.29)

$$\mathrm{Re}\ f^{(2)}_{\mathrm{HEAS}} = - \frac{4\ \pi^2\ z^2}{4\ \pi^4\ k_i} \sum_{i,J=1}^{N} R_i\ R_J \left[\ \mathcal{P} \int d\ \underline{p} \int_{-\infty}^{\infty} \right.$$

$$\frac{d\ p_Z}{(\ p_Z - \beta_i\ )}$$

$$\frac{1}{(\ p^2 + p_Z{}^2 + y_i{}^2\ )\ (\ |\ \underline{g} - \underline{p}\ |^2 + p_Z{}^2 + y_J{}^2\ )}$$

$$+ \frac{D'}{2\ k_i}\ \mathcal{P} \int d\ \underline{p} \int_{-\infty}^{\infty} \frac{d\ p_Z}{(\ p_Z - \beta_i\ )}$$

$$\left. \frac{(\ p^2 + p_Z{}^2\ )}{(\ p^2 + p_Z{}^2 + y_i{}^2\ )\ (\ |\ \underline{q} - \underline{p}\ |^2 + p_Z{}^2 + y_J{}^2\ )} \right]$$

....(5.30)

$$= - \frac{z^2}{\pi^2 k_i} \sum_{i,J=1}^{N} R_i R_J \left[I_4 (\beta_i^2, y_i^2, y_J^2) + \frac{D'}{2 k_i} \left\{ I_3 (\beta_i , y_i) - y_i^2 I_4 (\beta_i^2, y_i^2, y_J^2) \right\} \right] \qquad \ldots.(5.31)$$

The evaluation of the $d \underline{p}$, $d \underline{p}_Z$ integrals in the above equations (5.28, 5.30), and the closed form of these are given in appendix. In the forward direction ($q \longrightarrow 0$), the imaginary and real parts have a finite value. Now the TES can be obtained using the equation (5.29).

$$\sigma_{tot} = \frac{4 \pi z^2}{k_i^2} \left[\sum_{i \neq J} \frac{R_i R_J}{(y_i^2 - y_J^2)} \log \frac{\beta_i^2 + y_i^2}{\beta_i^2 + y_J^2} + \sum_{i=J} \frac{R_i^2}{(\beta_i^2 + y_i^2)} \right] \qquad (5.32)$$

Similarly third Born real part can be obtained through the equations (2.62) and (5.22 to 5.24).

$$\mathrm{Re}\, f^{(3)}_{HEAS} = f^{(3)}_{1s} + f^{(3)}_{2s} \qquad (5.33)$$

where

$$f_{1s}^{(3)} = \frac{z^3}{2\,\pi^2\,k_i^2} \sum_{i,J,k=1}^{N} R_i\,R_J\,R_k\;I\,(\,q^2,\,y_i^2,\,y_J^2,\,y_k^2)$$

.....(5.34)

and

$$f_{2s}^{(3)} = -\,\frac{z^3}{2\,\pi^4\,k_i^2} \sum_{i,J,k=1}^{N} R_i\,R_J\,R_k \int d\,\underline{p}' \int d\,\underline{p}$$

$$\mathcal{P}\int_{-\infty}^{\infty} \frac{d\,p_Z'}{(\,p_Z' - \beta_i)} \int_{-\infty}^{\infty} \frac{d\,p_Z}{(\,p_Z - \beta_i\,)}$$

$$\Big[\frac{1}{(p^2 + p_Z^2 + y_i^2)(\,|\underline{q} - \underline{p} - \underline{p}'|^2 + p_Z^2 + y_J^2 - p_Z'^2\,)}$$

$$\frac{}{(\,p'^2 + p_Z'^2 + y_k^2\,)}\Big])$$

......(5.35)

In equation (5.34) , $I\,(\,q^2\,,\,y_i^2\,,\,y_J^2\,,\,y_k^2\,)$ represents an analytical expression for $d\,\underline{p}$, $d\,\underline{p}'$ integrals. This is similar to the one given by Yates (1974) [illegible] Singh and Tripathi (1980). Now the integrals in equation (5.35) can be reduced to one dimensional integral after evaluating the principal value integrals. This one dimensional integral can be evaluated using the quadrature integral technique)(Abramowitz and Stegun , 1964). The DCS $O (k_i^{-2})$ can be obtained for fields using the following amplitude.

$$F_{HEAS} = f_{st}^{(1)} + \mathrm{Re}\ f_{HEAS}^{(2)} + \mathrm{Re}\ f_{HEAS}^{(3)} + i\ \mathrm{Im}\ f_{HEAS}^{(2)} \qquad ....(5.36)$$

Using the first (equation 5.26) and second (equations 5.29, 5.31). Born amplitudes we calculated the TES, DCS $O (k_i^{-2})$ for the lithium atom (Tietz , 1965) at incident, energies 100 to 700 eV. The constants used in the analytical form of the field of lithium atom (equation 5.23) are same as given by Tietz (1965). The TES (Rao and Desai , 1983 b) and DCS are shown in Tables (5.3, 5.4, 5.5).

5.3.2 Comparison of static field results of ESGLi with the other data :

Using the scattering amplitudes (equations 5.26, 5.29, 5.31) for the static field of lithium atom (Tietz, 1965), we have calculated the DCS and TES in the incident energy range E = 100 to 700 eV. The DCS (small circles) results at incident energy E = 100, 200, and

400 eV are shown in Figs. (5.2 and 5.3). These results are found to be in good agreement with the compared present (solid curves a' and b') and other theoretical (EBS, CS (Tayal et al, 1981)) results. It can be observed from these Figs. (5.2, 5.3) that the present static field results for lithium atom are noted in between the DCS results (curves a' and b') of ESGLi (Sec. 5.2.2) . In Table (5.3) we have listed the first Born (equation 5.26) and second Born (equations 5.29, 5.31) results at incident energy E = 400 eV. Table (5.4) shows the present DCS at incident energies E = 100 to 700 eV. and TES results in the energy range E = 20 to 600 eV (Rao and Desai, 1983 d) are listed in Table (5.5) along with the compared results of Guha and Ghosh (1979). The present TES results are found to be slightly lower than the results of Guha and Ghosh (1979).

5.4.1 An analytical study of elastic and inelastic scattering of electrons by Lithium atoms :

(Desai and Rao, 1983 b)

The aim of the present section is only to obtain the analytical expression for DCS equation (3.2) for elastic and inelastic scattering of electrons by lithium atoms using the ground and excited state wave functions of lithium atom (Clementi , 1965 ; Mathur et al, 1972). The approximations to be used in these derivation are same as discussed in ESGLi (Sec. 5.2.1). And the first order exchange amplitude is derived using the Lewis (1956) integral technique. The present section shows only how easily the derived amplitudes (ESGH Sec. 3.2.1, ESEH Sec. 3.3.1 and ESGLi Sec. 5.2.1) can be utilized in deriving the present scattering amplitudes for elastic and inelastic processes of lithium atom. The wave functions for ground and excited states of lithium atom (Clementi, 1965 ; Mathur et al, 1972) can be written as

$$\Psi_{2s}(r_1) = \frac{1}{\sqrt{4\pi}} \left[\sum_{i=1}^{2} A_i \exp(-y_i' r_1) + \sum_{J=3}^{6} A_J r_1 \exp(-y_J' r_1) \right] \tag{5.37}$$

and for excited state

$$U_{2p}(r_1) = A r_1 \exp(-y' r_1) \tag{5.38}$$

where $A = 0.22805$, $y' = 0.5227$. The product of the wave functions for elastic (final state is same as ground state) and inelastic (final state is taken as excited 2p state) can be obtained in the derivative forms as given in ESGH (equation 3.6) and ESEH (equation 3.19) processes. Following the computation procedure adopted in ESGH (Sec. 3.2.1) process, the present scattering amplitudes can be derived. The closed form of these can be obtained as

$$\begin{aligned} \mathrm{Im}\ F^{(2)} = \frac{1}{4} \Big[& \sum_{i=1}^{4} D_i\ F(y_i) - \sum_{J=1}^{8} E_J\ D(y_J) \\ & F(y_J) + \sum_{k=1}^{16} F_k\ D^2(y_k) \\ & F(y_k) \Big] \end{aligned} \tag{5.39}$$

$$\begin{aligned} \mathrm{Re}\ F^{(2)} = \frac{1}{4} \Big[& \sum_{i=1}^{4} D_i\ G(y_i) - \sum_{J=1}^{8} E_J\ D(y_J) \\ & F(y_J) + \sum_{k=1}^{16} F_k\ D^2(y_k) \\ & F(y_k) \Big] \end{aligned} \tag{5.40}$$

$$\begin{aligned} \mathrm{GES}^{(3)} = \frac{1}{4} \Big[& \sum_{i=1}^{4} D_i\ H(y_i) - \sum_{J=1}^{8} E_J\ D(y_J) \\ & H(y_J) + \sum_{k=1}^{16} F_k\ D^2(y_k) \end{aligned}$$

$$H (y_k)] \qquad (5.41)$$

where D_i's , E_J's, F_k's and y_i's, y_J's, y_k's are constants can be obtained from the product of the ground (equation 5.37) and final state wave function of the lithium atom and F (y), G (y), H (y) are the corresponding scattering amplitudes in ESGH process (equations 3.11, 3.13, 3.15, 3.16). Similarly the first order exchange amplitude (Joachain , 1975) can be obtained using the equation (5.37) and the integral technique of Lewis (1956). The closed form of this can be given as

$$T_{ex} = -2 \sum_{i,J}^{6} A_{iJ} (- 1)^{m+n} \frac{1}{y_i \; y_J} D^m (y_J) \\ D^n (y_i) \frac{\tan^{-1}}{f_1} \left(\frac{f_1}{f_2} \right) \qquad (5.42)$$

where

$$f_1^2 = q (k_i^2 + y_J^2) (k_i^2 + y_i^2) + (y_i^2 - y_J^2)^2 k_i^2$$

$$f_2^2 = y_J (k_i^2 + y_i^2) + y_i (k_i^2 + y_J^2)$$

m and n are the powers of the target coordinate in the wave function equation (5.37). The first Born amplitude can be obtained similar to equation (5.14) of ESGLi (Sec. 5.2.1) . All these expressions (equations 5.39, 5.40, 5.41) can be easily extended to the inelastic process.

Finally, the DCS equation (3.2) can be obtained for elastic and inelastic processes using the derived scattering amplitudes (equations 5.39, 5.40, 5.41, 5.42).

Table (5.1) : Behaviour of Scattering amplitudes (Equations 5.14, 5.16, 5.17, 5.18, 5.15) in ESGLi process (Sec.5.2.1) at incident Energy E = 400 eV.

θ	$f^{(1)}_{i\rightarrow f}$	Re1 $f^{(2)}_{HEA}$	Re2 $f^{(2)}_{HEA}$	$f^{(3)}_{GES}$ (-ve)	Im $f^{(2)}_{HEA}$	DCS_1	DCS_2
5	0.451991+1	0.109619-1	0.765138-1	0.391340-2	0.10831+1	0.22359+2	0.21667+2
10	0.228190+1	0.546990-2	0.496110-1	0.314680-2	0.52215+0	0.56994+1	0.54734+1
20	0.749170+0	0.470173-2	0.619310-1	0.818030-2	0.29235+0	0.73433+0	0.64153+0
30	0.404190+0	0.236977-2	0.650218-1	0.130210-1	0.17368+0	0.23749+0	0.18493+0
40	0.269701+0	0.139309-2	0.656502-1	0.140340-1	0.11489+0	0.11453+0	0.79122-1
50	0.197900+0	0.922220-3	0.658520-1	0.127910-1	0.82693-1	0.67365-1	0.41301-1
70	0.123380+0	0.505481-3	0.660090-1	0.924690-2	0.50677-1	0.31924-1	0.15636-1
90	0.871547-1	0.334000-3	0.660840-1	0.652790-2	0.35959-1	0.19329-1	0.78099-2
110	0.674810-1	0.249430-3	0.661260-1	0.489001-2	0.28169-1	0.13646-1	0.47215-2
130	0.563230-1	0.204024-3	0.661509-1	0.393840-2	0.23785-1	0.10758-1	0.33064-2

Table (5.2) : DCS_1 for ESGLi process at incident Energies E = 80 to 700 eV.

E	θ = 5°	10°	20°	30°	40°	50°	60°
80	0.77689+2	0.35137+2	0.99985+1	0.38266+1	0.19074+1	0.11265+1	0.74483+0
100	0.61889+2	0.27969+2	0.72123+1	0.26129+1	0.12737+1	0.74464+0	0.49147+0
200	0.35489+2	0.13691+2	0.23858+1	0.77251+0	0.36646+0	0.21445+0	0.14311+0
300	0.27107+2	0.84102+1	0.11926+1	0.38186+0	0.18289+0	0.107901+0	0.71999-1
400	0.22359+2	0.56994+1	0.73433+0	0.23749+0	0.11453+0	0.67365-1	0.44315-1
500	0.18827+2	0.40715+1	0.49832+0	0.16368+0	0.79239-1	0.46361-1	0.30374-1
600	0.16189+2	0.30583+1	0.36809+0	0.12233+0	0.59061-1	0.34202-1	0.22150-1
700	0.14078+2	0.23814+1	0.28634+0	0.95923-1	0.46054-1	0.26414-1	0.16992-1

Table (5.3) : Behaviour of scattering amplitudes (Equations 5.26, 5.31, 5.29) in the static field of lithium atom at incident energy $E = 400$ eV.

θ	$f^{(1)}_{st}$	Re1 $f^{(2)}_{HEAS}$	Re2 $f^{(2)}_{HEAS}$	Im $f^{(2)}_{HEAS}$
5	0.45953 + 1	0.20960 − 1	0.10202	0.10019 + 1
10	0.23723 + 1	0.15177 − 1	0.11594	0.85079
20	0.81578 + 0	0.73252 − 2	0.14153	0.57514
30	0.45244 + 0	0.45119 − 2	0.16281	0.4225
40	0.30448 + 0	0.31058 − 2	0.18205	0.33424
50	0.22231 + 0	0.23879 − 2	0.19803	0.27560
70	0.13584 + 0	0.153614− 2	0.21977	0.20151
90	0.94272 − 1	0.10977 − 2	0.23192	0.15827
110	0.72094 − 1	0.85752 − 3	0.23871	0.13181
130	0.59686 − 1	0.71885 − 3	0.24253	0.11550

Re1 $f^{(2)}_{HEAS}$, Re2 $f^{(2)}_{HEAS}$, Correspond to $O(k_i^{-1})$, $O(k_i^{-2})$ in equation (3.1).

Table (5.4) : DCS for the static field in electron - lithium elastic process at incident energies E = 100 to 700 eV.

E θ =	5^{o}	10^{o}	20^{o}	30^{o}	40^{o}	50^{o}	60^{o}
100	0.32843+2	0.20697+2	0.61081+1	0.220853+1	0.106007+1	0.59263+0	0.35267+0
200	0.28285+2	0.125321+2	0.22765+1	0.72453+0	0.32048+0	0.15803+0	0.77481-1
300	0.24296+2	0.82098+1	0.11965+1	0.37184+0	0.15544+0	0.68498+0	0.27086-1
400	0.209917+2	0.57328+1	0.75346+0	0.23183+0	0.91735-1	0.36273-1	0.11078-1
500	0.182605+2	0.42087+1	0.528701+0	0.16064+0	0.601815-1	0.21448-1	0.46216-2
600	0.15991+2	0.32157+1	0.39719+0	0.11879+0	0.42253-1	0.13598-1	0.16577-2
700	0.14093+2	0.25395+1	0.31263+0	0.91816-1	0.31093+0	0.90407-2	0.19296-3

Table (5.5) : Comparison of present TES (Using the equation 5.32) with the other results (in units of a_o^2).

Incident energy E eV	Present results	(a)
20	15.6742	23.3383
30	10.4725	13.4880
50	6.2950	7.2058
60	5.2600	5.8376
70	4.4995	
100	3.1520	3.3177
150	2.1060	2.1568
200	1.5770	1.5992
300	1.0514	
400	0.7886	
500	0.6313	
600	0.5260	

(a) : Guha and Ghosh (1979).

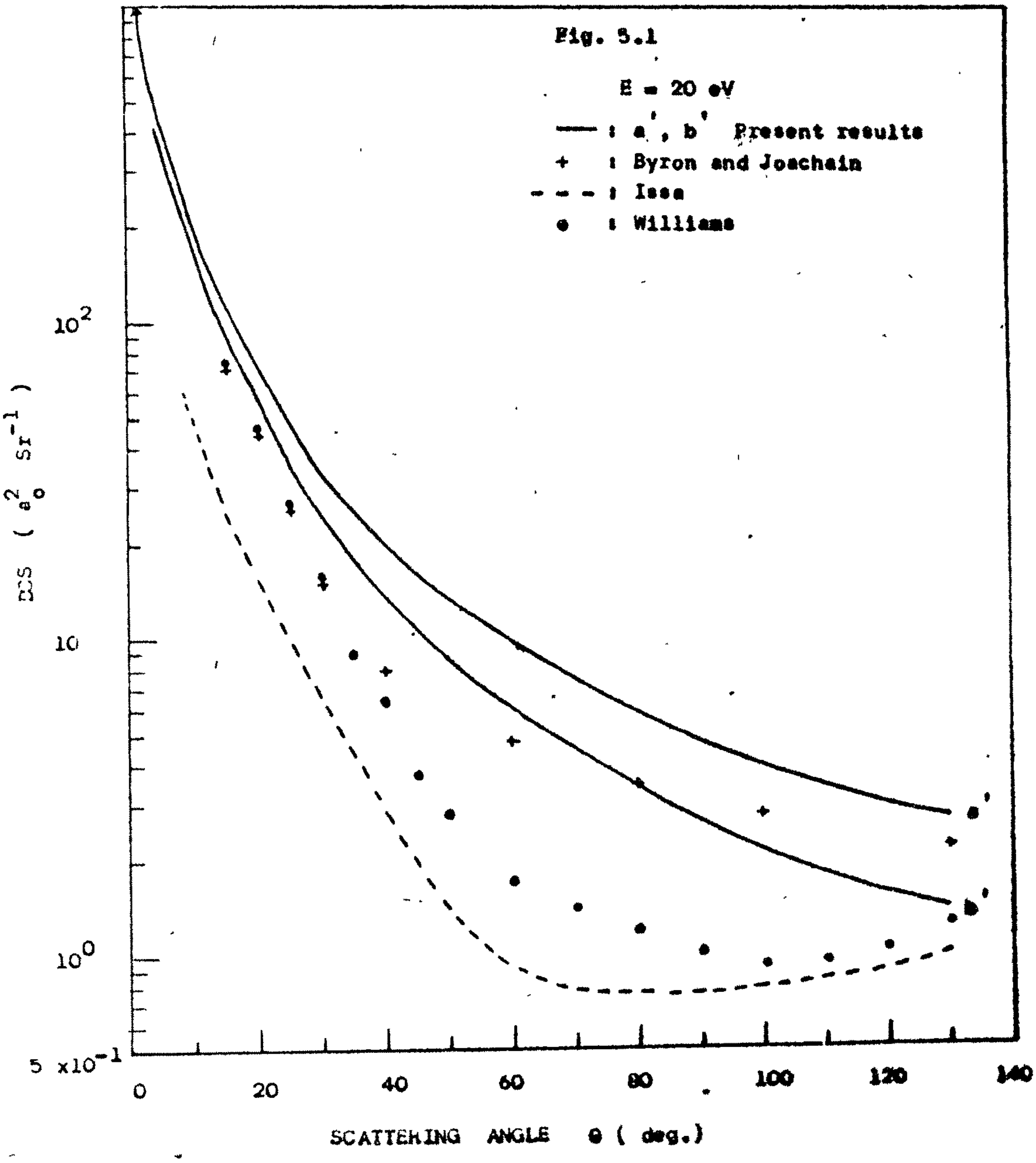

Fig. 5.1

E = 20 eV
—— : a', b' Present results
+ : Byron and Joachain
- - - : Issa
● : Williams
DCS (a_o^2 sr^{-1})
10^2
10
10^0
5 x10^{-1}
0
20
40
60
80
100
120
140
SCATTERING ANGLE θ (deg.)

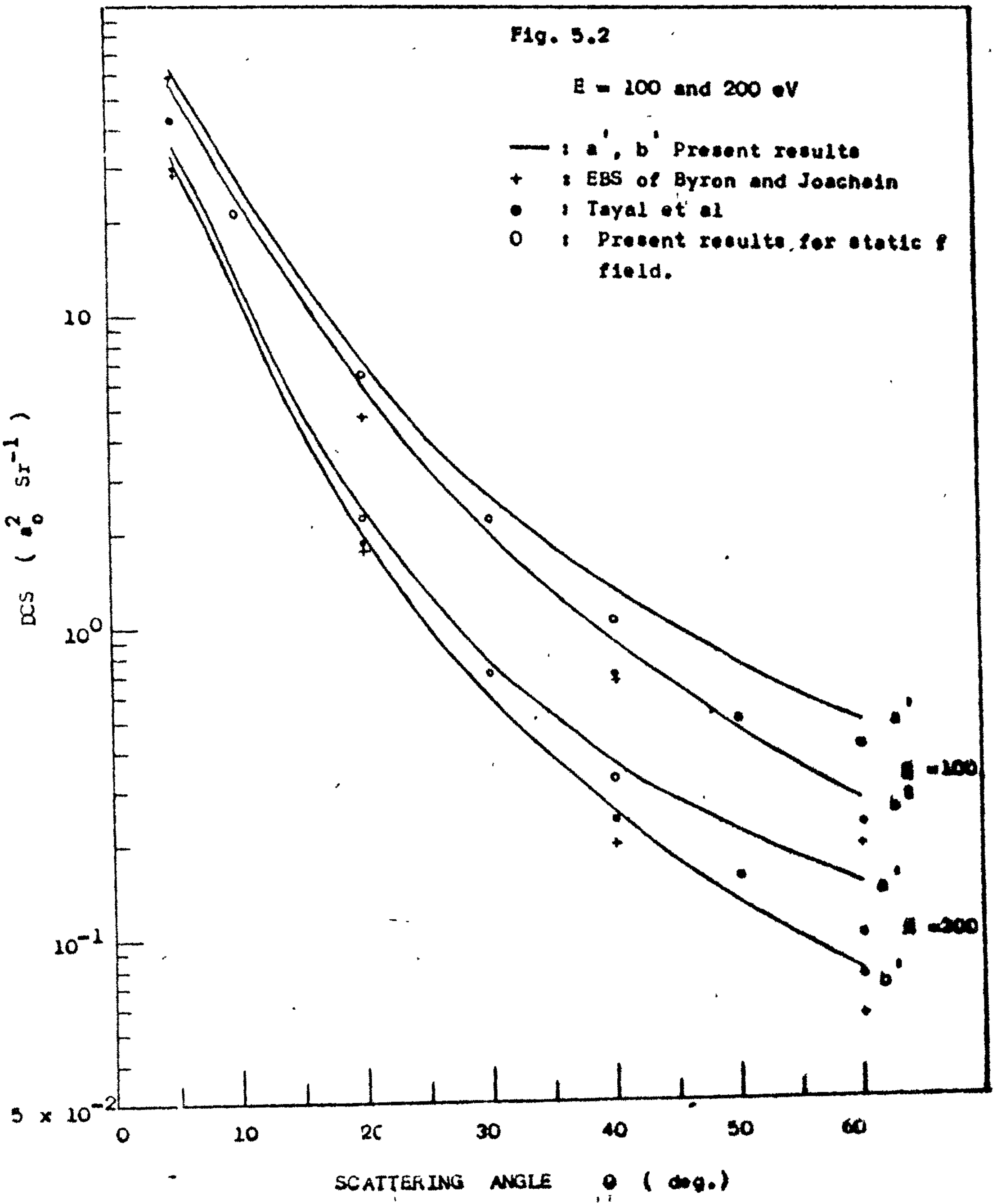

Fig. 5.2

E = 100 and 200 eV

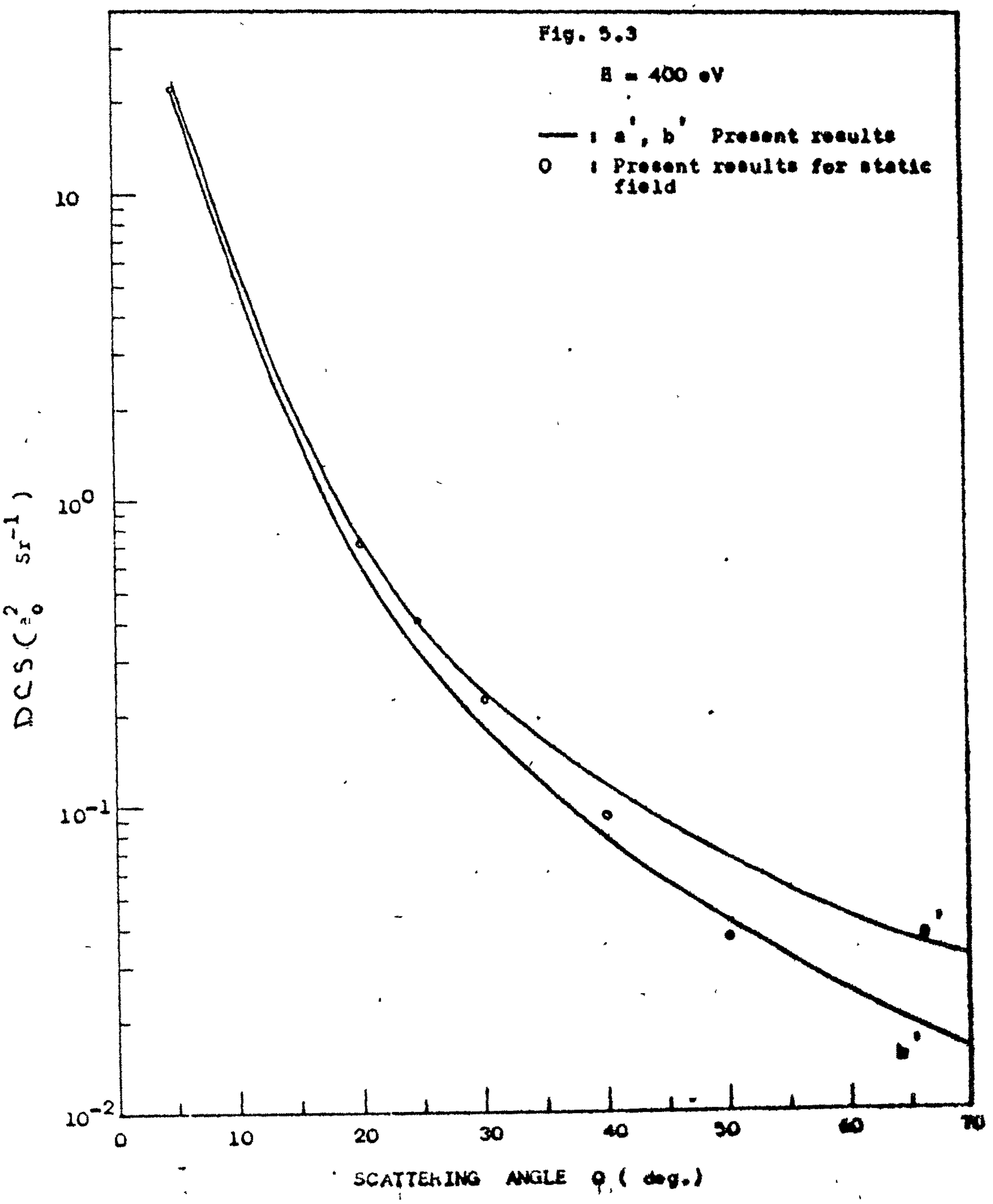

Fig. 5.3

E = 400 eV
—— : a', b' Present results
O : Present results for static field
10
10^0
10^{-1}
10^{-2}
DCS (a_0^2 sr^{-1})
0
10
20
30
40
50
60
70
SCATTERING ANGLE θ (deg.)
a'
b'

Fig. 5.4

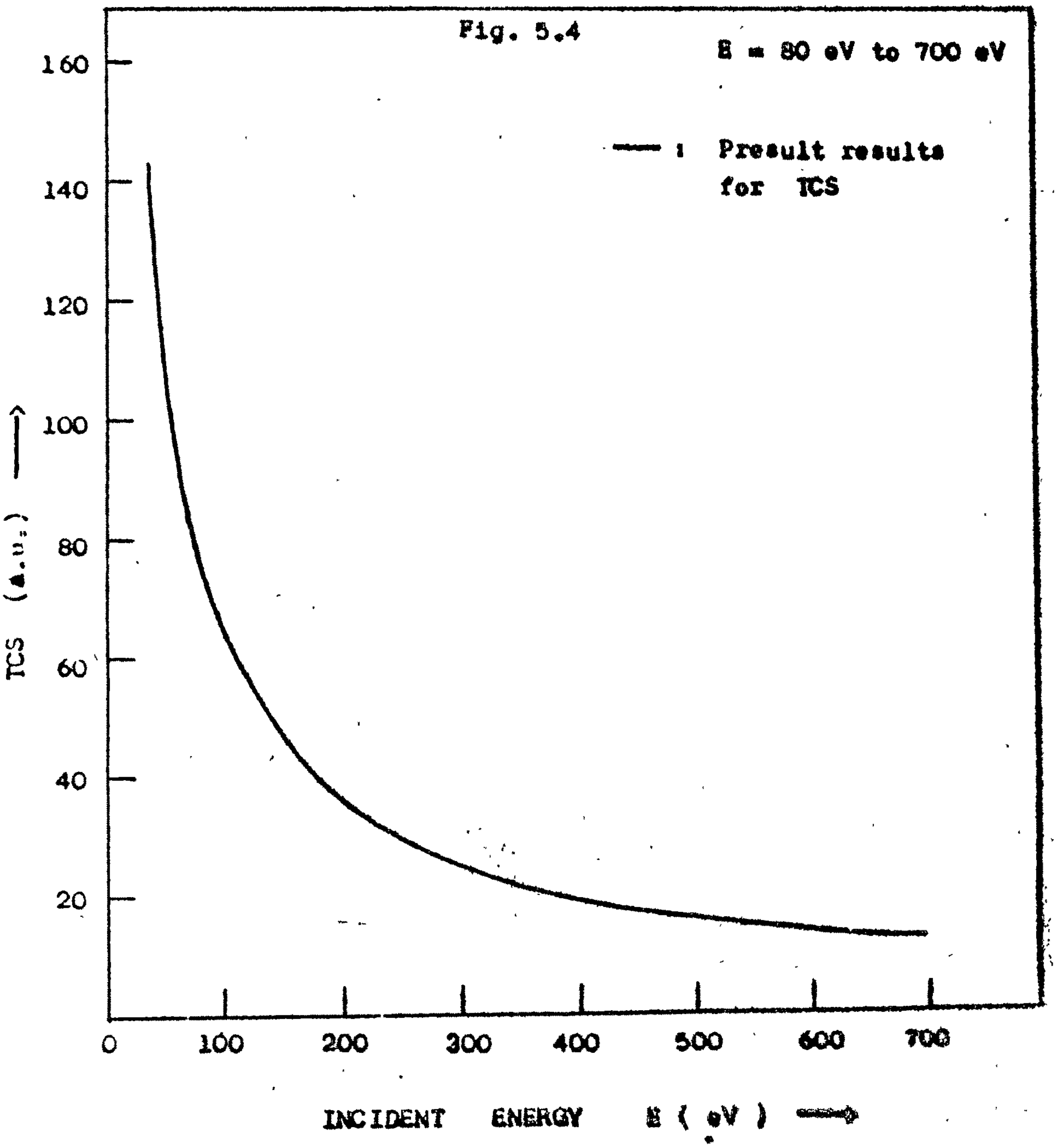
Fig. 5.4
E = 80 eV to 700 eV
—— : Presult results for TCS
TCS (a.u.) ⟶
160
140
120
100
80
60
40
20
0
100
200
300
400
500
600
700
INCIDENT ENERGY E (eV) ⟹