# CHAPTER - II

## HHOB APPROXIMATION FOR Li ATOM

### 2.1 INTRODUCTION

The study of electron - alkali atom - collisions became an interesting area in recent years due to many reasons. Among them is the discovery of alkali atoms in the atmosphere. The theoretical study of this problem has been further stimulated in the intermediate and high energy ranges due to the availability of the experimental results ( Williams, 1976 ).Electron - alkli metal atom has many applications in various fields of science. The part played by some of the alkali atoms in Magneto-hydrodynamics is very important in the present day energy crisis.

It is a known fact that the metnods which apply well to the elastic scattering by light atoms with closed shells will not be effective in alkali atoms. The main reason for this is the pecular 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 polarisability of the alkali atoms can be accounted mainly due to this coupling. The outermost electron in this atom is a loosely bound S-electron hence the increased activity of these atoms. The absorption effect ( removal of electrons from the elastic to the inelastic channel ) also plays a leading role in the alkali atom scattering.

The Li atom being the first member of the alkali atoms, the above discussed deviations from closed shell atoms will be least in its case. Hence it offers an opportunity to test the theoretical models which are successfully applied to the lighter atoms, H and He . Many attempts have been made to study the elastic $\bar{e}$ - Li atom scattering in the intermediate energy region. Sarkar et al ( 1973 )used the eikonal approximation to investigate this problem for a wide energy range 0.8 eV to 500 eV. Gregory and Fink ( 1974 ) solved the relativistic Dirac equation and found out the differential cross section and total elastic cross section from 100 eV to 1.5 KeV. Chan and Chang ( 1976 ) applied the Glauber approximation to $\bar{e}$ - Li scattering to obtain DCS at 100 eV , 200 eV and 400 eV . Vanderpoorten ( 1976 ) constructed a local optical potential consisting of static, polarisation absorption and exchange effects and evaluated the DCS at 54.4 eV and 60 eV . Mukherjee and Sural

( 1979 ) have used an integral approach to the second order potential ( SOP ) for elastic $\bar{e}$ - Li scattering to obtain DCS and TECS from 10 eV to 200 eV. Gien ( 1981 ) investigated the exchange effects in the frozen core Glauber approximation from 20 eV to 1000 eV for $\bar{e}$ - Li elastic scattering. Tayal et al ( 1981 ) have calculated the DCS and TECS for elastic $\bar{e}$ - Li scattering from 10 eV to 200 eV in the corrected static approximation and in an approximation which combines the contribution of the non - static parts of the higher order terms in the Glauber approximation with the static part taken exactly. Wadehra ( 1982 ) has used the first Born approximation along with the polarised Born amplitude to obtain integrated elastic cross sections from 500 eV to 1000 eV . Dhal ( 1982 ) has evaluated DCS for elastic $\bar{e}$ - Li scattering at 60 eV , 200 eV and 400 eV using a two potential formation in which the close encounter collision are treated exactly and the polarisation, exchange and absorption effects are treated through the optical eikonal approximation. Rao and Desai ( 1983b ) have used the high energy higher order Born ( HHOB ) approximation along with the Glauber eikonal series ( GES ) method to investigate the DCS from 50 eV to 1000 eV and TCS from 100 eV to 700 eV . They have used core approximation of Walters ( 1973 ), the nucleus and the inner shell forming the core and the 2S – electron behaving as the valence electron. Tayal ( 1984 ) has applied the corrected static approximation to evaluate the TCS for $\bar{e}$ – Li scattering from 10 eV to 200 eV . Vijayshri ( 1985 ) have evaluated the DCS and TCS for $\bar{e}$ – Li at the energies 60 eV to 200 eV for the former and 20 eV to 1000 eV for latter using modified Glauber approximation (MGA ). They have done two models namely, the single particle scattering model ( SPSM ) and the Inert Core ( IC ) model. In the former they ignored the multiple scattering effects and in the latter they ignored core altogether. Chandraprabha ( 1985 ) used modified Glauber eikonal series ( MGES ) and ( GES ) to calculate the DCS for energies 100 eV to 800 eV . Very recently Yadav and Roy ( 1987 ) have calculated the DCS for $\bar{e}$ – Li from 10 eV to 20 eV using the coulomb – projected modified – Born approximation with Junker's modification.

It is seen that the only results reasonably close to the experimental data among all the above mentioned work are those of VanderpoorTen ( 1976 ) and MGA ( SPSM ) of Vijayshree ( 1985 ). In most of the above cases, lithium atom is represented as a one electron atom with an inert core. Also all these results show a great deal of divergence from each other in the large angle scattering region.

In the present study we have taken HHOB approximation which gives satisfactory results in the case of $\bar{e}$ - H and $\bar{e}$ - He scattering ( Rao and Desai 1981, 83 ). Hence the extension of this technique to Li atom is of great interest. Further we represent Li atom as a three electron system. Hence the present approach accounts for the long range polarisation effects and the absorption effects, We have calculated the DCS and TCS from energies 100 eV to 400 eV and 100 eV to 1000 eV respectively.

## 2.2 Theory

The direct scattering amplitude in the HHOB approximation can be written as ( Yates, 1979 ):

$$f_{HEA} = f^{(1)}_{HEA} + Re\, f^{(2)}_{HEA} + i\, I_m f^{(2)}_{HEA} + R_e f^{(3)}_{HEA} \qquad (2.1)$$

The first Born expression $f^{(1)}_{HEA}$ is obtained from (1.16). The expression for $R_e f^{(2)}_{HEA}$ and $I_m f^{(2)}_{HEA}$ are given in equation (1.47) and (1.48). $Re f^{(3)}_{HEA}$ is of the order of $k_i^{-2}$ and the evaluation of this is found to be tedious. If we put $\beta i = 0$ , it is found that $R_e f^{(3)}_{HEA}$ is same as third

Glauber term. Hence in the present study we have taken the third Glauber term in the place of $R_e f^{(3)}_{HEA}$. Hence the direct scattering amplitude can be written as

$$f_{HEA} = f^{(1)}_{HEA} + R_e f^{(2)}_{HEA} + i I_m f^{(2)}_{HEA} + f_{G3} \qquad (2.2)$$

The expression for $f_{G3}$ can be obtained from (1.32). knowing the scattering amplitude, the DCS can be calculated. The total cross section can be obtained through the optical theorem.

$$\sigma^{tot} = \frac{4\pi}{k_i} I_m f^{(2)}_{HEA} \ ( \theta = 0 ) \qquad (2.3)$$

2.3 CALCULATIONS

The wave function for the ground state of Li atom has been taken as that of Veselov et al.(1961 ) as quoted by Chan and Chang ( 1976 ), namely

$$\psi = \frac{1}{\sqrt{3!}} \alpha_{et} ( \phi_{1s\uparrow}, \phi_{1s\downarrow}, \phi_{2s\uparrow} ) \qquad (2.4)$$

with $$\phi_{1s} = \left(\frac{\alpha^3}{\pi}\right)^{1/2} e^{-\alpha r} \qquad (2.5)$$

$$\phi_{2s} = \left[\frac{3\beta^5}{\pi(\alpha^2-\alpha\beta + \beta^2)}\right]^{1/2} \left(1 - \frac{\alpha + \beta}{3} r\right) e^{-\beta r} \qquad (2.6)$$

where $\alpha = 2.694$ and $\beta = 0.767$

This wave function gives an energy of -7.414 a.u. against the experimental value of -7.478 a.u.

$$\psi\,\psi^* = \frac{1}{3!}\,|\,{}^{d}{}_{et}\,(\,\phi_{1s_\uparrow}, \phi_{1s_\downarrow}, \phi_{2s\uparrow}\,|^2$$

$$= \phi_{1s}^2(\underline{r}_1)\ \phi_{1s}^2(\underline{r}_2)\ \phi_{2s}^2\,(\underline{r}_3)$$

$$- \phi_{1s}^2(\underline{r}_1)\ \phi_{1s}(\underline{r}_2)\ \phi_{2s}\,(\underline{r}_2\,)\ \phi_{1s}\,(\underline{r}_3\,)\ \phi_{2s}(\underline{r}_3) \quad (2.7)$$

Further,

$$\phi_{1s}^*\,\phi_{1s} = \frac{\lambda_1^3}{8\pi}\,e^{-\lambda_1 r}\ , \quad \lambda_1 = 2\alpha \qquad (2.8a)$$

$$\phi_{2s}^*\ \phi_{2s} = 8N^2\ \mathrm{DOP}\,(\,\lambda_3, \lambda_2\,)\,\frac{1}{\lambda_2^3}\ \frac{\lambda_2^3}{8\pi}\,e^{-\lambda_2 r} \qquad (2.8b)$$

$$\text{where}\ N^2 = \frac{3\beta^5}{(\alpha^2 - \alpha\beta + \beta^2)}\ , \quad \lambda_2 = 2\beta,\ \lambda_3 = \alpha + \beta \quad (2.8c)$$

$$\text{and}\ \ \mathrm{DOP}\,(\,\lambda_3, \lambda_2\,) = (\,1 + \frac{2\,\lambda_3}{3}\ \frac{\partial}{\partial\lambda_2} + \frac{\lambda_3^2}{9}\ \frac{\partial^2}{\partial\lambda_2^2}\,) \qquad (2.8c)$$

The interaction between the incident electron and the target lithium atom can be written as

$$V_d = -\frac{3}{r_o} + \frac{1}{|\underline{r}_o - \underline{r}_1|} + \frac{1}{|\underline{r}_o - \underline{r}_2|} + \frac{1}{|r_o - r_3|} \qquad (2.9)$$

where $\underline{r}_o$, $\underline{r}_1$, $\underline{r}_2$, $\underline{r}_3$ are the position vectors of the incident and target electrons with respect to the target nuclei.

Now the closed form of the first Born approximation can be obtained as

$$f^{(1)}_{HEA} = -\frac{1}{2\pi}\int d\underline{r}_o \exp.\,(i\underline{q}.\underline{r}_o)\int dr_i$$

$$\psi_i \left[ -\frac{3}{r_o} + \frac{1}{|\underline{r}_o - \underline{r}_1|} + \frac{1}{|\underline{r}_o - \underline{r}_2|} + \frac{1}{|\underline{r}_o - \underline{r}_3|}\right]\phi^*$$

(2.10)

Substituting (2.8) in the above expression the final form can be obtained as

$$f^{(1)}_{HEA} = 4\,\frac{(q^2 + 2\lambda_1^{\ 2})}{(q^2 + \lambda_1^{\ 2})^2} + 8\,N^2\,\mathrm{DOP}\,(\lambda_3, \lambda_2)$$

$$\frac{2}{2^3}\left(\frac{q^2 + 2\lambda_2^{\ 2}}{q^2 + \lambda_2^{\ 2}}\right) \qquad (2.11)$$

The expression for $I_m\, f_{HEA}$ can be written as

$$I_m\, f_{HEA} = \frac{4\pi^3}{k_i}\int d\underline{p}\; Uf_i^{(2)}(\underline{q} - \underline{p} - \beta_i\hat{y}\;,\; \underline{p} + \beta_i\hat{y})$$

(2.12)

where

$$U^{(2)}_{f_i}\,(q - p - \beta_i\hat{y},\ \underline{p} + \beta_i\hat{y}) = \langle\, \psi_f^*\,(\underline{r}_1, \underline{r}_2, \underline{r}_3)$$

$$|\overline{V}(\underline{q} - \beta_i\hat{y}, \underline{r}_1, \underline{r}_2, \underline{r}_3)\ \overline{V}(q-p - \beta_i\hat{y},$$

$$\underline{r}_1, \underline{r}_2, \underline{r}_3)|\psi_i\,(\underline{r}_1, \underline{r}_2, \underline{r}_3)\rangle \qquad (2.13)$$

Substituting the value of $\overline{V}$ from (1.44) and $\psi\,\psi^*$ from (2.8) we will get

$$U_{f_i}^{(2)} ( q - p - \beta_i \hat{y} , p + \beta_i \hat{y} ) = \frac{1}{4\pi^2(|q-p|^2+\beta_i^2)(p^2+\beta_i^2)} \quad x$$

$$\iiint [ dv_1 dv_2 dv_3 \, \phi_{1s}^2(\underline{r}_1) \, \phi_{1s}^2(\underline{r}_2)$$

$$\phi_{2s}^2(\underline{r}_3) - \phi_{1s}^2(\underline{r}_1) \, \phi_{1s}(\underline{r}_2) \, \phi_{2s}(\underline{r}_2)$$

$$\phi_{2s}(\underline{r}_3) \, \phi_{1s}(\underline{r}_3)] \; x \sum_{j=1}^{3} \sum_{i=1}^{3}$$

$$( e^{ip.b_j} e^{ip_z z_j} - 1)(e^{ip.b_i} e^{ip_z z_i} -$$

(2.14)

carrying out the integration of (2.12) using (2.14) we will get the value as

$$I_m f_{HEA}^{(2)} = \frac{1}{\pi k_i} \left[ -3 + \frac{16\alpha^3 \lambda_1}{(_1^2 + q^2)^2} + 4N^2 \text{ DOP } (- \frac{\partial}{\partial \lambda_2} ) \right.$$

$$( \frac{1}{\lambda_2^2 + q^2} ) I_1(q^2, \beta_i^2 , \beta_i^2 ) + 32\alpha^6 (- \frac{\partial}{\partial \lambda_1} )$$

$$\frac{1}{\lambda_1^2} ( - \frac{\partial}{\partial \lambda_1} ) \frac{1}{\lambda_1^2} I_1( q^2, \gamma_1^2, \gamma_1^2 )+16\alpha^3(-\frac{\partial}{\partial \lambda_1} )$$

$$\frac{1}{\lambda_1^2} I_1( q^2, \gamma_1^2, \beta_i^2) + 8N^2 \text{DOP } (- \frac{\partial}{\partial \lambda_2} )\frac{1}{\lambda_2^2}$$

$$I_1(q^2, \gamma_2^2, \beta^2) + 64N^2\alpha^2 \left(-\frac{\partial}{\partial\lambda_1}\right) \frac{1}{\lambda_1^2} \mathrm{DOP}\left(-\frac{\partial}{\partial\lambda_2}\right)$$

$$\frac{1}{2^2} I_1(q^2, \gamma_1^2, \gamma_2^2) ] - \frac{32}{\pi k_i} [ \frac{4}{(\lambda_3)^8} \quad B^2 - \frac{6BB^1}{\lambda_3}$$

$$+ \frac{9B'^2}{\lambda_3^2} \quad I_1 (q^2, \beta_i^2, \beta_i^2) - \frac{4}{\lambda_3^2} \left\{ \left( \frac{8BB'}{\lambda_3^3} + \frac{12B'^2}{\lambda_3^4} \right) \right.$$

$$\left. \frac{\partial}{\partial\beta} \frac{1}{\lambda_3^2} \right\} I_1(q^2, u^2, \beta_i^2) + B^2\left(-\frac{\partial}{\partial\beta}\right) \frac{1}{\lambda_3^2}$$

$$\left(-\frac{\partial}{\partial\beta}\right) \frac{1}{\lambda_3^2} + 2BB' \left(-\frac{\partial}{\partial\beta}\right) \frac{1}{\lambda_3^2} \frac{\partial^2}{\partial\beta^2} \frac{1}{\lambda_3^2}$$

$$+ B'^2 \frac{\partial^2}{\partial\beta^2} \frac{1}{\lambda_3^2} \quad \frac{\partial^2}{\partial\beta^2} \frac{1}{\lambda_3^2} \quad I_1(q^2, u_1^2, u_2^2) ] \tag{2.15}$$

Here $\gamma_1^2 = \beta_i^2 + \lambda_1^2$ ; $\gamma_2 = \beta_i^2 + \lambda_2^2$ ; $u^2 = \beta_i^2 + \lambda_3^2$

$$B = \left(\frac{\alpha^3}{\pi}\right)^{1/2} \left[ \frac{3\beta^5}{\pi(\alpha^2 - \alpha\beta + \beta^2)} \right]^{1/2}$$

and $B' = \left(\frac{\lambda_3}{3}\right) B$ . The integrals $I_1$ is defined and evaluated in the appendix

$$\beta_i = \frac{\Delta E}{k_i} , \quad \Delta E \text{ is the excitation energy.}$$

We have taken the value of $\Delta E$ = .08825 which was calculated by Vijayshri ( 1985 ). The expression for $\mathrm{Re}\, f_{HEA}^{(2)}$ = can be written as

$$\text{Re}\ f^{(2)}_{HEA} = \text{Re}\ 1\ f^{(2)}_{HEA} + \text{Re}\ 2\ f^{(2)}_{HEA} \tag{2.16}$$

where

$$\text{Re}\ 1\ f^{(2)}_{HEA} = -\frac{4\pi^2}{k_i}\ \mathcal{P}\int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{(p_z-\beta_i)}\ U^{(2)}_{f_i} \tag{2.17}$$

and

$$\text{Re}\ 2f^{(2)}_{HEA} = \frac{-2\pi^2}{k_i}\ \left(\frac{\partial}{\partial \beta_i}\right)\ \mathcal{P}\int dp \int_{-\infty}^{\infty} dp_z\ (p^2 + p_z^2)\ U^{(2)}_{f_i} \tag{2.18}$$

The notations are defined in Chapter I .

Carrying out integration using (2.17) we will get

$$\text{Re}\ 1\ f^{(2)}_{HEA} = \frac{1}{\pi^2 k_i}\ \Big[\ -3 + \frac{16\ \alpha^3 \lambda_1}{(\lambda_1^2 + q^2)^2} +$$

$$4N^2\ \text{DOp}\left(-\frac{\partial}{\partial \lambda_2}\right) \frac{1}{(\lambda_2^2 + q^2)} \qquad I_2(q^2, \beta_i^2, o)$$

$$+\ 24\ \alpha^3\ \left(-\frac{\partial}{\partial \lambda_1}\right) \frac{1}{\lambda_1^2}\ I_2(q^2\ ,\ \beta_i^2\ ,\ \lambda_1^2)$$

$$+\ 8N^2\ \text{Dop}\ \left(-\frac{\partial}{\partial \lambda_2}\right) \frac{1}{\lambda_2^2}\ I_2\ (q^2,\ \beta_i^2,\ \lambda_2)$$

$$-\ 32\ \alpha^6\ \left(-\frac{\partial}{\partial \lambda_1}\right) \frac{1}{\lambda_1^2}\ \left(-\frac{\partial}{\partial \lambda_1}\right) \frac{1}{\lambda_1^2}$$

$$I_4\ (q^2,\ \beta_i^2,\ \lambda_1^2,\ \lambda_2^2)\ +\ 64\ \alpha^6\ \left(-\frac{\partial}{\partial \lambda_1}\right)$$

$$\frac{1}{\lambda_1^2}\ \left(-\frac{\partial}{\partial \lambda_1}\right) \frac{1}{\lambda_1^2}\ I_2(q^2,\ \beta_i^2,\ \lambda_1^2)\ -\ 64\ \alpha^3 N^2$$

$$(-\frac{\partial}{\partial\lambda_1})\frac{1}{\lambda_1^2}\ \mathrm{Dop}\ (-\frac{\partial}{\partial\lambda_2})\frac{1}{\lambda_2^2}\ I_4(q^2,\beta_i^2,\lambda_1^2,\lambda_2^2)$$

$$-2 \times (4\pi)^2 \left\{ \frac{4}{\lambda_3^6} \left(B^2 - \frac{6\ B\ B'}{\lambda_3} + \frac{9\ B'^2}{\lambda_3}\right)\right.$$

$$\left. I_2\ (q^2,\ \beta_i{}^2,\ o)\right\} - \frac{2}{\lambda_3^3}\left(B^2 - \frac{6BB'}{\lambda_3}\right)$$

$$\left\{(-\frac{\partial}{\partial\ \beta})\ \frac{1}{\lambda_3^2}\ I_2\ (q^2,\ \beta_i{}^2,\ \lambda_3^2)\ +\right.$$

$$\left.\frac{6\ \beta'^2}{\lambda_3^2}\ (-\frac{\partial}{\partial\beta})^2\ \frac{1}{\lambda_3^2}\ I_2\ (q^2,\ \beta_i^2, 0, \lambda_3^2)\right\}$$

$$-\frac{2\ B^2}{(\alpha+\beta)^3}\ (-\frac{\partial}{\partial\beta})\ \frac{1}{(\alpha+\beta)^2}\ I_4\ (q^2, \beta_i^2, 0, \lambda_3^2)$$

$$+\ B^2\ (-\frac{\partial}{\partial\beta})\ \frac{1}{\lambda_3^2}\ (-\frac{\partial}{\partial\beta})\ \frac{1}{\lambda_3^2}$$

$$I_4\ (q^2,\ \beta_i{}^2,\ \lambda_3^2,\ \lambda_3^2)\ +\ \frac{4\ B\ B'}{\lambda_3^2}\ (-\frac{\partial}{\partial\beta})^2$$

$$I_4\ (q^2,\ \beta_i{}^2,\ 0,\ \lambda_3^2)\ -\ 2\ B\ B'\ (-\frac{\partial}{\partial\beta})\ \frac{1}{\lambda_3^2}$$

$$(-\frac{\partial}{\partial\beta})^2\ \frac{1}{\lambda_3^2}\ I_4\ (q^2,\ \beta_i{}^2, \lambda_3^2,\ \lambda_3^2)$$

$$-\ \frac{6\ B'^2}{\lambda_3^2}\ (-\frac{\partial}{\partial\beta})\ \frac{1}{\lambda_3^2}\ (-\frac{\partial}{\partial\beta})\ \frac{1}{\lambda_3^2}$$

$$I_4(q^2,\ \beta_i{}^2,\ \lambda_3^2, \lambda_3^2) \qquad (2.19)$$

For the calculation of $Re\ 2\ f_{HEA}^{(2)}$ we have omitted the cross terms in $U_{f_i}^{(2)}$ whose contributions are negligibly small. Hence

$$Re\ 2\ f_{HEA}^{(2)} = \frac{1}{2\pi^2 k^2} \Big[ -6\alpha^2 \left(\frac{\partial}{\partial\beta_i}\right)\left(-\frac{\partial}{\partial\lambda_1}\right) I_2(q^2, \beta_i^2, \lambda_1^2) + 32\,\alpha^6 \left(\frac{\partial}{\partial\beta_i}\right)\left(\frac{\partial^2}{\partial\lambda_1^2}\right) \frac{1}{\lambda_1^2}\ I_2(q^2, \beta_i^2, \lambda_1^2) - I_4(q^2, \beta_i^2, \lambda_1^2, \lambda_1^2)$$

$$- 16\, N^2 \left(\frac{\partial}{\partial\beta}\right) \text{Dop} \left(-\frac{\partial}{\partial\lambda_2}\right) I_2(q^2, \beta_i^2, \lambda_2^2)$$

$$- 64\,\alpha^3 N^2 \left(\frac{\partial}{\partial\beta}\right) \text{Dop} \left(-\frac{\partial}{\partial\lambda_2}\right) \frac{-\partial}{\partial\lambda_1} \frac{1}{\lambda_1^2}\ I_4(q^2, \beta_i^2, \lambda_1^2, \lambda_1^2) \tag{2.20}$$

The integrals $I_2$ and $I_4$ are defined and calculated in the appendix.

We may obtain $f_{G_3}$ by simplifying (1.32) with n = 3 for Li atom.

$$f_{G_3} = f_{G_3}^{1} + f_{G_3}^{2} \tag{2.21}$$

where
$$f_{G_3}^{1} = 2f_{G_3}^{H}(\lambda_1, q) + 8N^2\ \text{Dop}(\lambda_3, \lambda_2)\ \frac{1}{3}\ f_{G_3}^{H}(\lambda_2, q) \tag{2.22}$$

$$f^{H}_{G_3}(\lambda_1, q) = \frac{\lambda_1}{16(\frac{\lambda}{2})^3 k_i^2 x^3} \frac{\partial}{\partial x}\left(\frac{x^4}{1+x^2}\right)$$

$$\left\{ 4\left[l_n\left(\frac{1+x^2}{x}\right)\right]^2 + \frac{\pi^2}{3} - 2A(x) \right\} \qquad (2.23)$$

$$\text{with} \quad A(x) = 2(\ln x)^2 + \frac{\pi^2}{6} + \sum_{n=1}^{\infty} \frac{(-x^2)^n}{n^2}, \quad x \leqslant 1$$

$$= -\sum_{n=1}^{\infty} \frac{(-1/x^2)^n}{n^2}, \quad \text{for} \quad x > 1 \qquad (2.24)$$

x being equal to $q/\lambda_1$.

$f^{2}_{G_3}$ can be obtained as

$$f^{2}_{G_3} = -\frac{1}{k_i^2} \int_0^{\infty} b \, db \, J_0(q\,b) \left[I_1 I_2 + I_2 I_3 + I_4 I_1 + I_1^2 I_3 - I_5 I_6 - I_1 I_5^2\right] \qquad (2.25)$$

where

$$I_1 = \langle \phi_{1s} | A\,I | \phi_{1s} \rangle$$

$$I_2 = \langle \phi_{1s} | A\,II | \phi_{2s} \rangle$$

$$I_3 = \langle \phi_{2s} | A\,I | \phi_{2s} \rangle \qquad (2.26)$$

$$I_4 = \langle \phi_{2s} | A\,II | \phi_{2s} \rangle$$

$$I_5 = \langle \phi_{1s} | A\,I | \phi_{2s} \rangle$$

$$I_6 = \langle \phi_{1s} | A\,II | \phi_{2s} \rangle$$

with

$$A\,I = \ln\left(1 - \frac{2\,b_1}{b}\cos\phi_1 + \frac{b_1^2}{b^2}\right) ;$$

$$A\,II = \ln^2\left(1 - \frac{2\,b_1}{b}\cos\phi_1 + \frac{b_1^2}{b^2}\right) \qquad (2.27)$$

Substituting the values of $\phi_{1s}$ and $\phi_{2s}$ from (2.5) and (2.6) and carrying out the integral over z we obtain

$$I_1 = \frac{\lambda_1^3}{4\pi} \int_0^\infty b_1^2\, db_1\; K_1(\lambda_1 b_1)\; ALN1\,(b_1, b) \qquad (2.28a)$$

$$I_2 = \frac{\lambda_1^2}{4\pi} \int_0^\infty b_1^2\, db_1\; K_1(\lambda_1 b_1)\; ALN_2\,(b_1, b) \qquad (2.28b)$$

$$I_3 = \frac{2\,N^2}{\pi} \int_0^\infty b_1^2\, db_1\; Dop\,(\lambda_3, \lambda_2) K_1(\lambda_2 b_1) ALN_1(b_1, b) \qquad (2.28c)$$

$$I_4 = \frac{2\,N^2}{\pi} \int_0^\infty b_1^2\, db_1\; Dop\,(\lambda_3, \lambda_2)\; K_1(\lambda_2 b_1)\; ALN_2(b_1, b) \qquad (2.28d)$$

$$I_5 = \frac{1}{\pi}\left(\frac{\lambda_1^3 N^2}{2}\right)^{1/2} \int_0^\infty b_1^2\, db_1\left(1 + \frac{\lambda_3}{3}\frac{\partial}{\partial\lambda_3}\right) K_1(\lambda_3 b_1)\; ALN_1\,(b_1, b) \qquad (2.28e)$$

$$I_6 = \frac{1}{\pi}\left(\frac{N^2}{2}\right)^{1/2} \int_0^\infty b_1^2\, db_1\left(1 + \frac{\lambda_3}{3}\frac{\partial}{\partial\lambda_3}\right) K_1(\lambda_3 b_1)\; ALN_2\,(b_1, b) \qquad (2.28f)$$

where

$$ALN_1\ (b_1, b) = \int_0^{2\pi} \ln\left(1 - \frac{2b_1}{b}\cos\phi_1 + \frac{b_1^2}{b^2}\right) d\phi_1 \quad (2.28g)$$

$$ALN_2\ (b_1, b) = \int_0^{2\pi} \ln^2\left(1 - \frac{2b_1}{b}\cos\phi_1 + \frac{b_1^2}{b^2}\right) d\phi_1 \quad (2.28h)$$

and $K_1\ (\lambda b)$ are the modified Bessel functions of the second kind. The integral (2.24) to (2.25) are performed using suitable numerical integration techniques (Vijayshree 1985 ).

Thus using the above equations we have obtained the DCS and the TCS for elastic scattering by Li atom from 100 eV to 400 eV and from 100 eV to 1000 eV respectively.

## 2.4 RESULTS AND DISCUSSIONS

The present DCS calculations for the elastic scattering of electrons by Li atoms from 100 eV to 400 eV are given in table (2.1) to (2.3) along with other available theoretical data. The results are also shown in figures (2.1) to (2.4). It is quite unfortunate that the experimental data is not available for comparison at these energies. The experimental results are reported for incident energies 20 eV and 60 eV which are too low for the present approximation.

As mentioned earlier the main advantage of the present approximation is that it is computationally simple. More over the problem of divergent integral is not there. All the integrals are convegent due to the presence of $\beta_i$ term. If we put $\beta_i = 0$ in the present HHOB terms we will get the corresponding terms in GES ( Glauber eikonal Series ). The imaginary part of the second HHOB term will not diverg for forward elastic scattering due to $\beta_i$ term.

Here we have compared our results with those theoretical data which are agreeable with the experimental data in low energy region. Vijayshri's (1985) are quite agreeable with the experimental data. For 300 eV other results are not available except Rao and Desai (1983). For 400 eV we compared our results with those of Rao and Desai (1983) and Chandra Prabha (1985).

From Table-1 we can see that the present results are quite agreeable with the MGA (SPSM) than MGA (IC) of Vijayshri (1985) for all angles. In MGA (IC) she had ignored the core altogether. Hence the results are lower in all angles. In Table - 2 also we can see that the present calculations are more close to MGA (SPSM). These supported the fact that in any model the inclusion of core is necessary due to the deeper penetration of the incident particle into the atomic core ( Chan and Chang, 1976 ). The results of Yadav and Roy ( 1986 ) also used single electron system. Hence their results decreases our results for 100 eV and 200 eV in all angles. In figures (2.1) and (2.2) we have shown the results of 100 eV and 200 eV alongwith other results. From figure ( 2.3 ) we can see that Rao and Desai's results are lower than that of ours for all angles. They also considered Li atom as single electron system and calculated the DCS using HHOB approximation. This again emphesis the need of considering Li atom as 3 electron system. In figure ( 2.4 ) we compared our results with the MGES of Chandraprabha ( 1985 ) and Rao and Desai ( 1983 ). Up to $70^{o}$ our present results are greater than that of their's . After that our results decreases.

The table ( 2.4 ) exhibit the individual terms of the present HHOB scattering amplitude. The real part of the second term account for the polarisation effect . The absorption effects are taken care of by the imaginary term. A survey of the table (2.4) reveals the fact that the absorption effects are more important than polarisation effects in alkali atom scattering. Vanderpoorten ( 1976 ) compared the optical model and Glauber results. He has shown that the two results almost coincide in the small angle region, which reveals that the polarisation effect is quite insignificant in alkali scattering .

The EBS method which gives good result for $\bar{e}$ - H and $\bar{e}$ - He gives higher values in the case of $\bar{e}$ - Li scattering. It could be because of the non cancellation of higher Born terms in the case of $\bar{e}$ - Li scattering.

The total collisional cross sections for $\bar{e}$ - Li scattering are given in table ( 2.5 ) along with other data. It can be seen that MGA of Vijayshri ( 1985 ) is very close to our results up to 1000 eV. We have also shown the results of Tayal ( 1984 ) in the simplified second Born approximation and the corrected static approximation. Their results are higher than our results. The integral elastic cross-sections of Guha and Ghosh ( 1979b ) and Wadehra ( 1982 ) are also shown in table. A comparison of the present results with the integral elastic cross section shows that the contribution of the inelastic scattering to the total collisional cross section is important over the whole energy range considered.

In the light of above discussion we can conclude that our present formulation is good for intermediate energy range. Since the experimental results are not available in this energy region it is not possible to do a complete analysis of the present theoretical results.

Table : 2.1 : The differential cross sections ( $a_o^2 \; s_r^{-1}$ ) for the elastic scattering of electron. $E = 100$ eV

| Angle | Present | MGA ( I C ) | MGA ( S P S M ) | EBS | Rao and Desai(1983) |
|---|---|---|---|---|---|
| 5 | 5.3778(1) | 4.49(1) | 5.53(1) | 5.29(1) | - |
| 10 | 2.2760(1) | 1.75(1) | 2.22(1) | 1.82(1) | 2.797(1) |
| 15 | 9.6669 | 7.70 | 1.05(1) | 7.47 | - |
| 20 | 4.4368 | 3.48 | 5.30 | 3.73 | 7.212 |
| 25 | 2.5995 | 1.67 | 2.88 | 2.40 | - |
| 30 | 1.7316 | 8.74(-1) | 1.70 | 1.85 | 2.613 |
| 40 | 7.0060(-1) | 3.02(-1) | 7.20(-1) | - | 1.274 |
| 50 | 5.2992(-1) | 1.31(-1) | 3.66(-1) | - | 7.446(-1) |
| 60 | 4.1575(-1) | 6.66(-2) | 2.12(-1) | 8.89(-1) | 4.915(-1) |
| 70 | 2.6970(-1) | 3.80(-2) | 1.35(-1) | - | 3.538(-1) |
| 80 | 1.4017(-1) | 2.38(-2) | 9.30(-2) | - | 2.721(-1) |
| 90 | 1.2943(-1) | 1.61(-2) | 6.78(-2) | 6.16(-1) | 2.200(-1) |
| 100 | 6.4789(-2) | 1.15(-2) | 5.18(-2) | - | - |
| 110 | 3.0652(-2) | 8.74(-3) | 4.12(-2) | - | 1.605(-1) |
| 120 | 2.9647(-2) | 6.94(-3) | 3.41(-2) | 4.99(-1) | 1.430(-1) |
| 130 | 1.8923(-2) | 5.75(-3) | 2.91(-2) | - | 1.303(-1) |
| 140 | 1.1558(-2) | 4.95(-3) | 2.56(-2) | - | - |
| 150 | 1.1246(-2) | - | 2.32(-2) | 4.43(-1) | - |

Table : 2.2 : The differential cross sections ( $a_o^2 \; s_r^{-1}$ ) for the elastic scattering of electrons by Lithium atom $E = 200$ eV.

| Angle | Present | MGA ( I C ) | MGA ( S P S M ) | EBS | Rao and Desai(1983) |
|---|---|---|---|---|---|
| 5 | 3.3954(1) | 2.6 (1) | 3.12(1) | 2.86(1) | - |
| 10 | 1.3476(1) | 9.47 | 1.20(1) | 9.93 | 1.3691(1) |
| 15 | 5.6950 | 3.26 | 4.70 | 3.69 | - |
| 20 | 2.5331 | 1.20 | 2.04 | 1.36 | 2.3859 |
| 25 | 1.4557 | 5.11(-1) | 1.04 | 9.89(-1) | - |
| 30 | 9.9444(-1) | 2.51(-1) | 5.95(-1) | 6.70(-1) | 7.7251(-1) |
| 40 | 4.3140(-1) | 8.18(-2) | 2.54(-1) | 3.90(-1) | 3.6646(-1) |
| 50 | 2.7583(-1) | 3.49(-2) | 1.33(-1) | 2.70(-1) | 2.1445(-1) |
| 60 | 1.0000(-1) | 1.77(-2) | 7.95(-2) | 2.06(-1) | 1.4311(-1) |
| 70 | 9.7470(-2) | 6.02(-2) | 5.15(-2) | 1.68(-1) | 1.0411(-1) |
| 80 | 5.4285(-2) | 1.42(-3) | 3.56(-2) | 1.42(-1) | 8.0552(-2) |
| 90 | 3.5685(-2) | 4.37(-3) | 2.58(-2) | 1.24(-1) | 6.5112(-2) |
| 100 | 2.1343(-2) | 3.16(-3) | 1.96(-2) | 1.11(-1) | 4.7356(-2) |
| 110 | 1.6391(-2) | 2.4[illegible](-3) | 1.55(-2) | 1.01(-1) | - |
| 120 | 7.9070(-3) | 1.93(-3) | 1.27(-2) | 9.31(-2) | 4.2029(-2) |
| 130 | 3.9629(-3) | 1.60(-3) | 1.08(-2) | 8.71(-2) | 1.8305(-2) |
| 140 | - | 1.38(-3) | 9.47(-3) | 8.26(-2) | - |
| 150 | 1.0856(-3) | 1.24(-3) | 8.55(-3) | 7.93(-2) | - |

Table : 2.3 : The differential cross sections ( $a_o^2 \, s_r^{-1}$ ) for the elastic scattering of electron E = 400 eV.

| Angle | Present | GES | MGES | Rao and Desai |
|---|---|---|---|---|
| 5 | 2.2853(1) | - | - | - |
| 10 | 6.6259 | 4.570 | 4.905 | 5.6746 |
| 15 | 2.5377 | - | - | - |
| 20 | 1.0619 | 5.422(1) | 6.269(-1) | 7.2730(-1) |
| 25 | 6.0898(-1) | - | - | - |
| 30 | 4.3328(-1) | 1.620(-1) | 2.003(-1) | 2.3558(-1) |
| 40 | 3.1653(-1) | 7.110(-2) | 9.292(-2) | 1.1378(-1) |
| 50 | 1.1625(-1) | 3.712(-2) | 5.059(-2) | 6.7001(-2) |
| 60 | 5.3131(-2) | - | - | 4.4315(-2) |
| 70 | 2.9755(-2) | 1.339(-2) | 1.934(-2) | 3.1880(-2) |
| 80 | - | - | - | 2.4191(-2) |
| 90 | 8.3802(-3) | 6.231(-3) | 9.353(-3) | 1.9271(-2) |
| 100 | - | - | - | - |
| 110 | - | 3.534(-3) | 5.439(-3) | 1.3612(-2) |
| 120 | 5.0259(-3) | - | - | 1.1948(-2) |

Table : 2.4 : a - Behaviour of the individual terms of the HHOB (2.1) for Lithium atom scattering at 100 eV.

| Angle | $f^{(1)}_{HEA}$ | $I_m f^{(2)}_{HEA}$ | $R_{e1}$ | $R_{e2}$ | $f_{G3}$ |
|---|---|---|---|---|---|
| 5 | 5.310 | 4.618 | 1.306 | 4.041(-1) | 1.47 |
| 10 | 4.359 | 2.053 | 1.315 | 2.246(-1) | 1.79 |
| 15 | 3.286 | 1.241 | 1.173 | 7.101(-2) | 1.86 |
| 20 | 2.387 | 1.021 | 1.047 | 6.017(-2) | 1.77 |
| 25 | 1.741 | 9.527(-1) | 9.562(-1) | 3.677(-2) | 1.64 |
| 30 | 1.308 | 8.976(-1) | 8.898(-1) | 3.769(-2) | 1.53 |
| 40 | 8.283(-1) | 7.637(-1) | 7.903(-1) | 2.276(-2) | 1.43 |
| 50 | 5.983(-1) | 6.878(-1) | 7.057(-1) | 1.174(-2) | 1.16 |
| 60 | 4.690(-1) | 5.406(-1) | 6.291(-1) | 6.138(-2) | 1.10 |
| 70 | 3.861(-1) | 4.689(-1) | 5.608(-1) | 3.376(-3) | 1.00 |
| 80 | 3.286(-1) | 4.158(-1) | 5.015(-1) | 1.956(-3) | 9.56(-1) |
| 90 | 2.881(-1) | 3.758(-1) | 4.511(-1) | 1.182(-3) | 9.30(-1) |
| 100 | 2.569(-1) | 3.451(-1) | 4.091(-1) | 7.389(-4) | 9.80(-1) |
| 110 | 2.324(-1) | 3.213(-1) | 3.747(-1) | 4.738(-4) | 8.60(-1) |
| 120 | 2.121(-1) | 3.029(-1) | 3.470(-1) | 3.103(-4) | 8.60(-1) |

Table:2.4 : b – Behaviour of the individual terms (2.2) for Lithium scattering for 200 eV.

| Angle | $f_{B1}$ | $I_m f^{(2)}_{HEA}$ | $R_{e1}$ | $R_{e2}$ | $f_{G3}$ |
|---|---|---|---|---|---|
| 5 | 4.959 | 2.166 | 9.773 | 2.109(-1) | 8.170(-1) |
| 10 | 3.464 | 8.826(-1) | 8.481(-1) | 5.941(-1) | 9.300(-1) |
| 15 | 2.198 | 6.811(-1) | 7.273(-1) | 3.193(-1) | 8.670(-1) |
| 20 | 1.421 | 6.340(-1) | 6.488(-1) | 2.339(-1) | 7.810(-1) |
| 25 | 9.909(-1) | 5.742(-1) | 5.927(-1) | 9.770(-2) | 7.150(-1) |
| 30 | 7.443(-1) | 5.063(-1) | 5.447(-1) | 7.100(-2) | 6.640(-1) |
| 40 | 4.919(-1) | 3.921(-1) | 4.586(-1) | 6.900(-2) | 6.440(-1) |
| 50 | 3.647(-1) | 3.154(-1) | 3.832(-1) | 1.554(-2) | 5.340(-1) |
| 60 | 2.881(-1) | 2.642(-1) | 3.201(-1) | 6.600(-3) | 4.850(-1) |
| 70 | 2.345(-1) | 2.285(-1) | 2.693(-1) | 2.800(-3) | 4.450(-1) |
| 80 | 1.975(-1) | 2.024(-1) | 2.293(-1) | 1.220(-3) | 4.250(-1) |
| 90 | 1.703(-1) | 1.828(-1) | 1.982(-1) | 6.422(-4) | 3.920(-1) |
| 100 | 1.517(-1) | 1.676(-1) | 1.741(-1) | 3.260(-4) | 3.720(-1) |
| 110 | 1.342(-1) | 1.558(-1) | 1.555(-1) | 2.983(-4) | 3.420(-1) |
| 120 | 1.225(-1) | 1.464(-1) | 1.412(-1) | 2.594(-4) | 3.390(-1) |

Table : 2.4 : c – Behaviour of the individual terms ( 2.3 ) for Lithium scattering for 400 eV.

| Angle | $f_{B1}$ | $I_m f^{(2)}_{HEA}$ | $R_{e1}$ | $R_{e2}$ | $f_{G3}$ |
|---|---|---|---|---|---|
| 5 | 4.36 | 9.263(-1) | 6.585(-1) | 8.206(-1) | 4.48(-1) |
| 10 | 2.37 | 4.713(-1) | 5.285(-1) | 7.856(-1) | 4.41(-1) |
| 15 | 1.29 | 4.384(-1) | 4.506(-1) | 2.250(-1) | 3.81(-1) |
| 20 | 8.08(-1) | 3.689(-1) | 3.977(-1) | 1.259(-1) | 3.39(-1) |
| 30 | 5.77(-1) | 2.569(-1) | 3.515(-1) | 5.611(-2) | 2.84(-1) |
| 40 | 4.46(-1) | 1.923(-1) | 3.088(-1) | 4.200(-2) | 1.90(-1) |
| 50 | 4.26(-1) | 1.539(-1) | 2.358(-1) | 1.100(-2) | 1.85(-1) |
| 60 | 1.70(-1) | 1.287(-1) | 1.404(-1) | 2.000(-3) | 1.76(-1) |
| 70 | 1.48(-1) | 1.109(-1) | 1.119(-1) | 8.900(-4) | 1.70(-1) |
| 80 | 1.12(-1) | 9.770(-2) | 9.169(-2) | 7.500(-4) | 1.60(-1) |
| 90 | 9.46(-2) | 8.759(-2) | 7.706(-2) | 5.000(-4) | 1.52(-1) |
| 100 | 8.56(-2) | 7.971(-2) | 6.635(-2) | 1.290(-4) | 1.42(-1) |
| 110 | 7.49(-2) | 7.352(-2) | 5.841(-2) | 1.210(-4) | 1.32(-1) |
| 120 | 6.52(-2) | 6.864(-2) | 5.249(-2) | 1.110(-4) | 1.27(-1) |

Table : 2.5 : The total collisional cross sections ( in $\pi a_o^2$ ) for $\bar{e}$ – Li scattering.

| E(eV) | Present | MGA (1C) | MGA (SPSM) | Tayal (1984) a | Tayal (1984) b | Integral elastic cross – sections Guha and Ghosh (1979) |
|---|---|---|---|---|---|---|
| 100 | 18.942 | 17.70 | 19.00 | 21.5 | 20.9 | 3.32 |
| 200 | 10.464 | 10.10 | 10.80 | 12.0 | 16.1 | 1.60 |
| 400 | 5.728 | 5.61 | 6.02 | – | – | – |
| 700 | 3.501 | 3.46 | 3.70 | – | – | 4.43(-1)* |
| 1000 | 2.554 | 2.53 | 2.71 | – | – | 3.10(-1)* |

* Results of Wadehra ( 1982 ).

a Results of Tayal ( 1984 ) in corrected static Approximation

b Results of Tayal ( 1984 ) in simplified second Born Approximation.

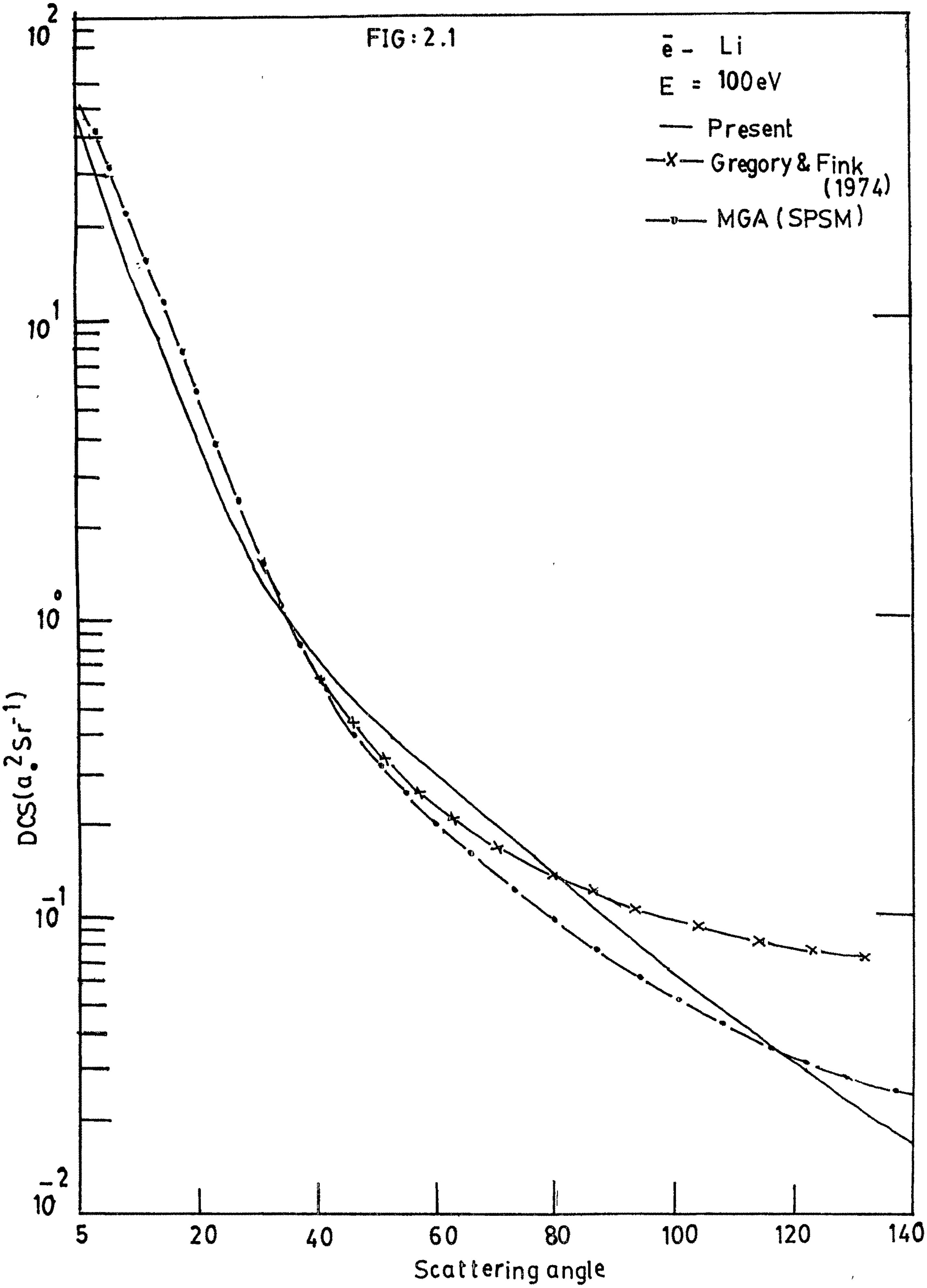
FIG: 2.1
ē - Li
E = 100eV
Present
Gregory & Fink (1974)
MGA (SPSM)
DCS(a₀²Sr⁻¹)
10²
10¹
10⁰
10⁻¹
10⁻²
5
20
40
60
80
100
120
140
Scattering angle

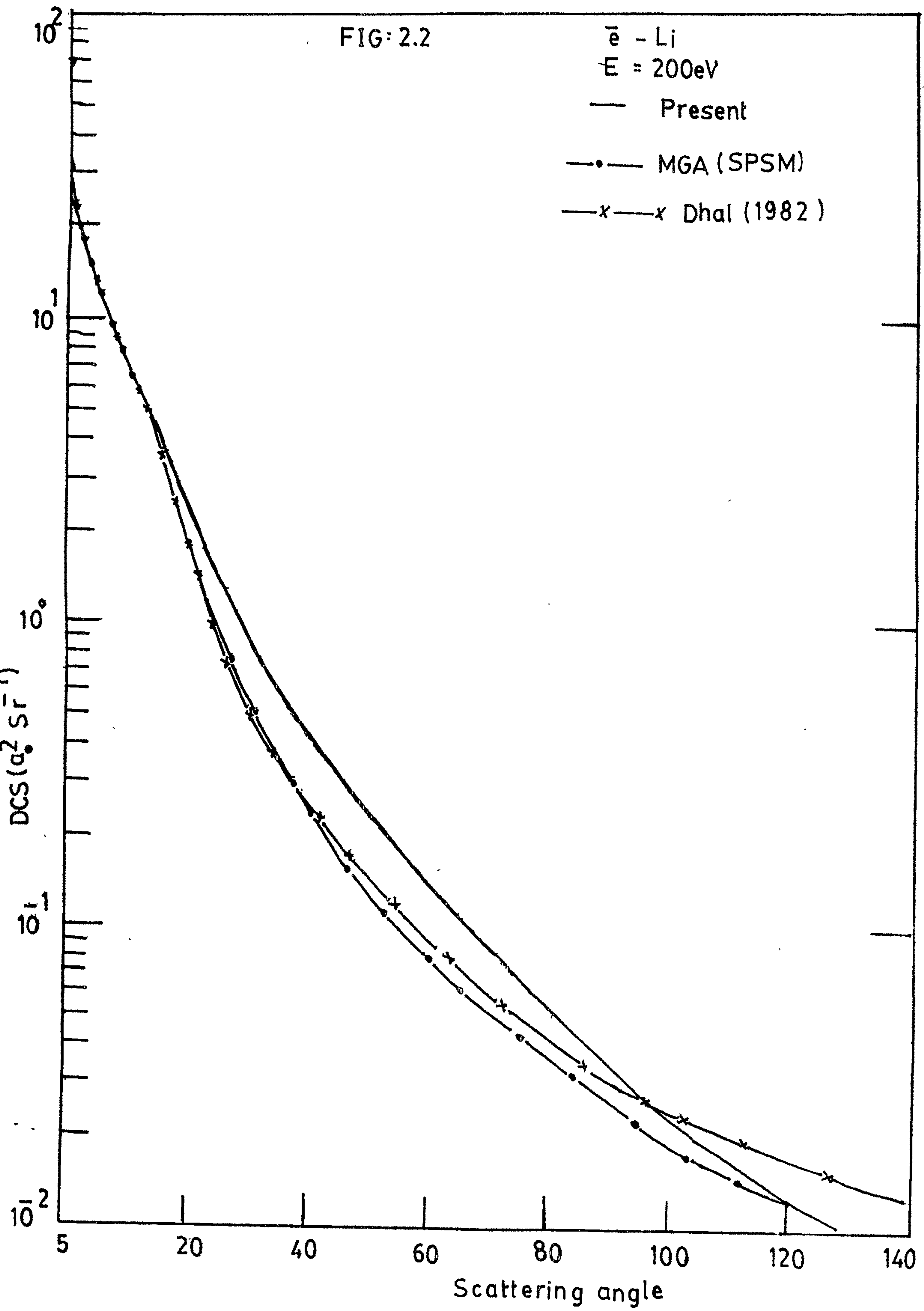

FIG: 2.2
e - Li
E = 200eV
Present
MGA (SPSM)
Dhal (1982)
DCS (a0^2 Sr^-1)
Scattering angle
10^2
10^1
10^0
10^-1
10^-2
5
20
40
60
80
100
120
140

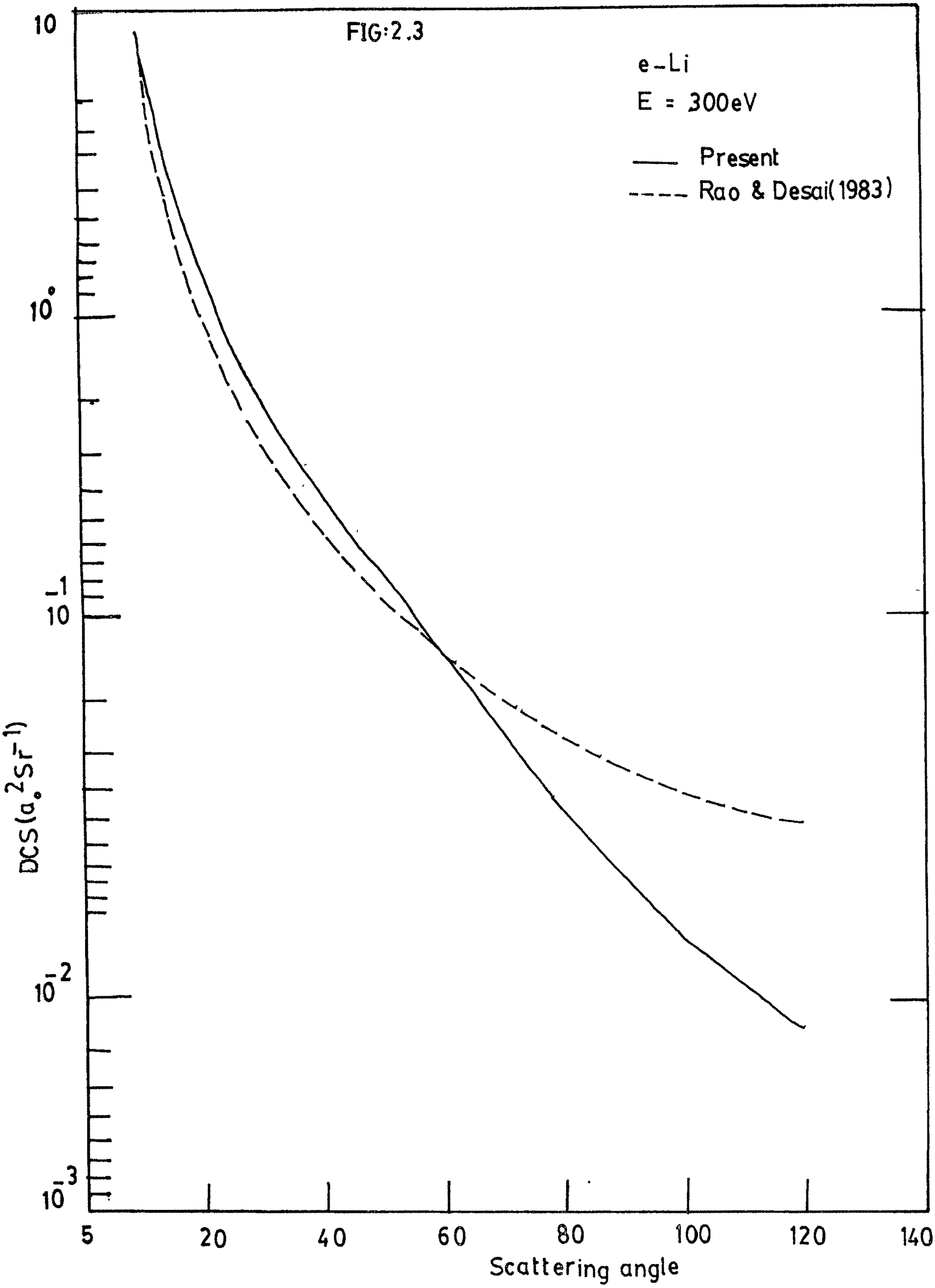
FIG:2.3
e-Li
E = 300eV
Present
Rao & Desai(1983)
10
10°
10⁻¹
10⁻²
10⁻³
DCS(a₀²Sr⁻¹)
5
20
40
60
80
100
120
140
Scattering angle

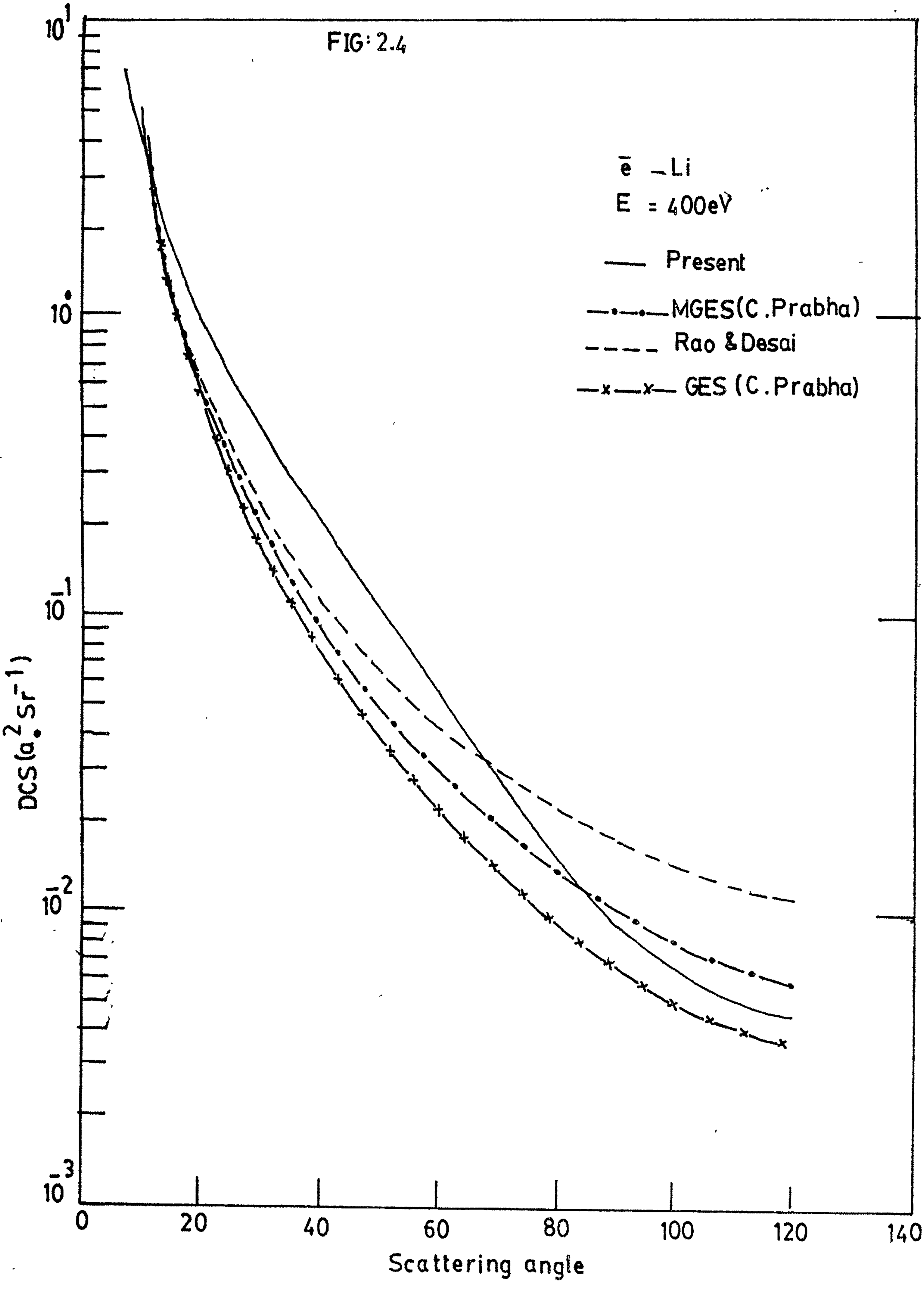

FIG: 2.4
$\bar{e}$ – Li
E = 400eV
Present
MGES(C.Prabha)
Rao & Desai
GES (C.Prabha)
$DCS(a_0^2 Sr^{-1})$
$10^1$
$10^0$
$10^{-1}$
$10^{-2}$
$10^{-3}$
0
20
40
60
80
100
120
140
Scattering angle