CHAPTER – III

SCATTERING OF ELECTRONS BY He AND He LIKE IONS

3.1 INTRODUCTION :

Inspired by the success of the He related problem with EBS and all other methods, which are presented in the previous chapter, now we concentrate on the ion problem with HHOB approximation in case of elastic scattering of electros from He like +ve ions : Li^{+}, Be^{+2}, B^{+3} and C^{+4} within the energy range 200 eV to 10 keV. The present work on the ion is initiated with large amount of data available for He atom (specifically Joachain et al & Desai H.S. and Rao) for the comparison of present theory. From the theoretical point of view the situation is nearly identical to that of He atom with only difference of nucleus charge and corresponding wave functions. Hartree-Fock parameter for the ground state wave functions given by Climenti & Roitee are used for He atom and He like ions. In this $\bar{e} - He, Li^{+1}, \ldots$ interaction process, we have evaluated first Born term, real & imaginary part of second born term, ochkur exchange approximation to calculate DCS at incident energies 200 to 10,000 eV for the elastic process. In the derivation of scattering amplitude for these problems, we consider the product of wave functions as summation of exponential terms. In general the exponetial term is operated with each term of product of Fourier transforms of the potential such that the problem carried with the He atom is generalized to He like ions with different atomic number Z. The evaluation of volume integrals is made simple with applying normalization condition for orbital wave functions before evaluating the integral with the total wave function. Symmetry occurred in various integrals are taken in to account for resultant evaluation very carefully through out these calculations. To obtain DCS, scattering amplitudes up to the order $O(k_i^{-2})$ are evaluated for He atom an ions.

3.2 FIRST BORN AMPLITUDE :

The first Born scattering amplitude is evaluated for He and He like ions . The scattering amplitude is basically developed for the case of He-atom, which can be generalized for He like ions.

Consider Elastic Scattering of electros by Ground State (1s) of He atom :[Z=2]

$$\bar{e} + He\ (1s) \rightarrow \bar{e} + He\ (1s) \tag{3.2.1}$$

HF – wave functions for the ground state of He atom :

Helium 1s (2)

Basis n, λ	Orbital Exponents α_i	Expansion Co-efficients C_i
1S	α_1	C_1
1S	α_2	C_2
1S	α_3	C_3

$$\psi_i^{He}(r_1, r_2) = \phi_{1s}^{He}(r_1)\,\phi_{1s}^{He}(r_2)\ , \tag{3.2.2}$$

where $\phi_{1s}^{He}(r) = C_1\chi_1 + C_2\chi_2 + C_3\chi_3$;

where $\chi = \mathrm{N}_x r^{n-1} e^{-\alpha r} \mathrm{Y}_{lm}(\theta,\varphi);\ n = 1, l = 0, m = 0$

$$= \mathrm{N}_x e^{-\alpha r} \frac{1}{\sqrt{4\pi}} \quad \text{and} \quad \mathrm{N}_x = \frac{(2\alpha)^{n+1/2}}{[(2n)!]^{1/2}} = 2\alpha^{3/2}$$

Now $\phi_{1s}^{He}(r) = \frac{N}{\sqrt{4\pi}}[Ae^{-\alpha_1 r} + Be^{-\alpha_2 r} + Ce^{-\alpha_3 r}];\ A = C_1 N_{\chi_1},\ B = C_2 N_{\chi_2}\ C = C_3 N_{\chi_3}$.

Now product of the initial and final state is

$$\psi^{He}\psi^{He^*} = |\psi^{He}(r_1, r_2)|^2 = |\phi_{1s}^{He}(r_1)|^2 |\phi_{1s}^{He}(r_2)|^2,$$

where $|\phi_{1s}^{He}(r)|^2 = \phi_{1s}^{He^*}(r)\phi_{1s}^{He}(r)$

$$= \frac{N^2}{4\pi}[\mathrm{A}^2 e^{-2\alpha_1 r} + \mathrm{B}^2 e^{-2\alpha_2 r} C^2 e^{-2\alpha_3 r} + 2\mathrm{AB}e^{-(\alpha_1+\alpha_2)r} + 2\mathrm{BC}e^{-(\alpha_2+\alpha_3)r} + 2\mathrm{AC}e^{-(\alpha_1+\alpha_3)r}]$$

$$= \frac{N^2}{4\pi}\sum_{i=1}^{6}\gamma_i e^{-\lambda_i r}, \tag{3.2.3}$$

where

$$\gamma_i: \quad A^2 \quad B^2 \quad C^2 \quad 2AB \quad 2BC \quad 2AC$$

$$\alpha_i: \quad 2\alpha_1 \quad 2\alpha_2 \quad 2\alpha_3 \quad \alpha_1+\alpha_2 \quad \alpha_2+\alpha_3 \quad \alpha_1+\alpha_3$$

Now the first Born scattering amplitude is given by equation (1.2.19).

$$f_{B1} = -\frac{1}{4\pi}\int e^{-iq\,r_0}\, U_{fi}^{(1)}\, d\underline{r}_0 = -\frac{1}{2\pi}\int e^{-iq\,r_0}\, V_{fi}\, d\underline{r}_0,$$

where $V_{fi} = <\psi_f \,|\, V(r_1,r_2) \,|\, \psi_i>$ is the interaction between incident electron and target..

$$\therefore f_{B1}^{He} = -\frac{1}{2\pi}\int d\underline{r}_0\, e^{iq\,r_0}\int d\underline{r}_1\int d\underline{r}_2\,[-\frac{Z}{r_0}+\frac{1}{|r_0-r_1|}+\frac{1}{|r_0-r_2|}]\,|\phi_{1s}^{He}(r_1)|^2\,|\phi_{1s}^{He}(r_2)|^2 \quad (3.2.4)$$

Let , the contribution of nucleus to the first Born is

$$f_{B1}^{P} = -\frac{1}{2\pi}\int d\underline{r}_0\, e^{iq\,r_0}\int d\underline{r}_1\int d\underline{r}_2\,[-\frac{Z}{r_0}]\,|\phi_{1s}^{He}(r_1)|^2\,|\phi_{1s}^{He}(r_2)|^2$$

$$= -\frac{1}{2\pi}\int d\underline{r}_0\, e^{iq\,r_0}[-\frac{Z}{r_0}]\int d\underline{r}_1\,|\phi_{1s}^{He}(r_1)|^2\int d\underline{r}_2\,|\phi_{1s}^{He}(r_2)|^2$$

$$= -\frac{1}{2\pi}\int d\underline{r}_0\, e^{iq\,r_0}[-\frac{Z}{r_0}]\cdot 1\cdot 1 \qquad [\because \text{Normalized orbital}]$$

$$= \frac{1}{2\pi}Z\int\frac{e^{iq\,r_0}}{r_0}\,d\underline{r}_0 = \frac{1}{2\pi}Z\times 2\pi\times\frac{2}{q}\times\frac{1}{q}$$

$$= Z\times\frac{2}{q^2}. \qquad (3.2.5)$$

The contribution of one electron to the first Born is

$$f_{B1}^{el} = -\frac{1}{2\pi}\int d\underline{r}_0\, e^{iq\,r_0}\int dr_1\int dr_2[\frac{1}{|r_0-r_1|}]\;|\phi_{1s}^{He}(r_1)|^2\,|\phi_{1s}^{He}(r_2)|^2$$

$$= -\frac{1}{2\pi}\int d\underline{r}_0\, e^{iq\,r_0}\int dr_1[\frac{1}{|r_0-r_1|}]\;|\phi_{1s}^{He}(r_1)|^2\int dr_2\,|\phi_{1s}^{He}(r_2)|^2$$

$$= -\frac{1}{2\pi}\int dr_0\,\frac{e^{iq\,r_0-iq\,r_1}}{|r_0-r_1|}\int d\underline{r}_1\, e^{iq\,r_1}\,|\phi_{1s}^{He}(r_1)|^2\times 1$$

$$f_{B1}^{el} = -\frac{1}{2\pi}I_0\times I_1$$

Now $I_0 = \int\frac{e^{iq\,(r_0-r_1)}}{|r_0-r_1|}\,d\underline{r}_0 = \int\frac{e^{iq\,r}}{|r|}\,d\underline{r}$

$$= \int_0^{2\pi}d\phi\int_0^{\infty}\int_0^{\pi}\frac{e^{iqr\cos\theta}}{r}\,Sin\theta d\theta\, r^2 dr$$

$$= 2\pi \times \frac{2}{q} \times \frac{1}{q} = 2\pi \times \frac{2}{q^2}$$

Now $I_1 = \int d\underline{r}_1 e^{iq r_1} |\phi_{1s}^{He}(r_1)|^2 = \int d\underline{r}_1 e^{iq r_1} \frac{N^2}{4\pi} \sum_{i=1}^{6} \gamma_i e^{-\lambda_i r_1}$

Considering one exponential term of $|\phi_{1s}^{He}(r_1)|^2$

$$I_1^{i_1} = \int d\underline{r}_1 e^{iq r_1} [\frac{N^2}{4\pi} \gamma_i e^{-\lambda_i r_1}] = \frac{N^2}{4\pi} \gamma_i \int e^{iq.r_1} e^{-\lambda_i r_1} d\underline{r}_1$$

$$= \frac{N^2}{4\pi} \gamma_i \int_0^{2\pi} d\varphi_1 \int_0^{\pi} e^{iq r_1 \cos\theta_1} Sin\theta_1 d\theta_1 \int_0^{\infty} e^{-\lambda_i r_1} r_1^2 d\underline{r}_1$$

$$= \frac{N^2}{4\pi} \gamma_i \times 2\pi \times \frac{2}{q} \times \frac{2\lambda_i q}{[\lambda_i^2 + q^2]^2} = N^2 \gamma_i \times \frac{2\lambda_i}{[\lambda_i^2 + q^2]^2}.$$

$$\Rightarrow I_1 = 2N^2 \sum_{i=1}^{6} \gamma_i \times \frac{\lambda_i}{[\lambda_i^2 + q^2]^2}$$

$$\Rightarrow f_{B1}^{e1} = -\frac{1}{2\pi}(2\pi \frac{2}{q^2}) \times 2N^2 \sum_{i=1}^{6} \gamma_i \times \frac{\lambda_i}{[\lambda_i^2 + q^2]^2}$$

$$= -\frac{4}{q^2} N^2 \sum_{i=1}^{6} \gamma_i \frac{\lambda_i}{(\lambda_i^2 + q^2)^2} \qquad (3.2.7)$$

We have $f_{B1}^{He} = f_{B1}^{P} + f_{B1}^{e1} + f_{B1}^{e1}$

$$= f_{B1}^{P} + 2 f_{B1}^{e1} \qquad [\because f_{B1}^{e1} = f_{B1}^{e2}]$$

$$= Z \times [\frac{2}{q^2}] + 2[-\frac{4}{q^2} N^2 \sum_{i=1}^{6} \frac{\gamma_i \lambda_i}{(\lambda_i^2 + q^2)^2}] \qquad (3.2.8)$$

Equation (3.2.8) is the generalized first Born approximation for the elastic scattering from ground state of $[He \quad or \quad Li^{+1}, Be^{+2}, B^{+3}, \ldots]$ process.

3.3 IMAGINARY PART OF SECOND BORN AMPLITUDE :

The systematic development of scattering amplitude of the order (k_i^{-1}) is carried out with HHOB approximation for He like ions. First beginning with the case of He-atom then it is applied to the He-like +ve ions due to the symmetry of electronic structure.

Now the imaginary part of the second Born amplitude in HHOB approximation equation (1.6.14) can be written as

$$\text{Im } f_{HEA}^{(2)} = \frac{4\pi^3}{k_i}\int d\underline{p}\; U_{fi}^{(2)}(\underline{q}-\underline{p}-\beta_i\hat{\xi};\underline{p}+\beta_i\hat{\xi}),$$

where $U_{fi}^{(2)} = \left\langle \psi_f \left| \overline{V}(\underline{q}-\underline{p}-\beta_i\hat{\xi};\underline{r}_1,\underline{r}_2)\overline{V}(\underline{p}+\beta_i\hat{\xi};\underline{r}_1,\underline{r}_2) \right| \psi_i \right\rangle$

$$= \int\int \psi_f \overline{V}\overline{V}' \psi_i^* d\underline{r}_1 d\underline{r}_2; \quad \psi_i = \psi_f = \phi_{1s}^{He}(r_1)\phi_{1s}^{He}(r_2)\,. \tag{3.2.1}$$

Considering Fourier form of the interaction potential, $\overline{V}(\,)$ has the following form

$$\overline{V}(\underline{p}+\beta_i\hat{\xi};\underline{r}_1,\underline{r}_2) = \frac{1}{2\pi^2(p^2+\beta_i^2)}\sum_{j=1}^{2}(e^{i\underline{p}\,\underline{b}j}\, e^{i\beta_i z_j} - 1) \qquad \text{and}$$

$$\overline{V}(|\,\underline{q}-\underline{p}\,|-\beta_i\hat{\xi};\underline{r}_1,\underline{r}_2) = \frac{1}{2\pi^2(|\,\underline{q}-\underline{p}\,|^2+\beta_i^2)}\sum_{j=1}^{2}(e^{i(\underline{q}-\underline{p})\,\underline{b}j}\, e^{-i\beta_i z_j} - 1). \tag{3.3.2}$$

$$\therefore \overline{V}\overline{V}' = \frac{1}{4\pi^2(|\,\underline{q}-\underline{p}\,|^2+\beta_i^2)(p^2+\beta_i^2)}\sum_{j=1}^{2}(e^{i(\underline{q}-\underline{p})\,\underline{b}j}\, e^{-i\beta_i z_j} - 1)\sum_{k=1}^{2}(e^{i\underline{p}\,\underline{b}_k}\, e^{i\beta_i z_k} - 1)$$

$$= \frac{1}{4\pi^2(|\,\underline{q}-\underline{p}\,|^2+\beta_i^2)(p^2+\beta_i^2)}\left[\sum_{j=1}^{2}e^{i\underline{q}\,\underline{b}j} + \sum_{j=1}^{2}\sum_{k\neq j}^{2}e^{i[(\underline{q}-\underline{p})\,\underline{b}j-\beta_i z_j]}\, e^{i(\underline{p}\,\underline{b}_k+\beta_i z_k)}\right.$$

$$\left. -2\sum_{j=1}^{2}e^{i(p\,b_j+\beta_i z_j)} - 2\sum_{j=1}^{2}e^{i(|q-p|\,b_j-\beta_i z_j)} + (2)^2\right] \tag{3.3.3}$$

Considering the individual terms of the square bracket .

Square terms :

$$U_{f_i}^{(2)}\Big|_{Square\ terms} = \frac{1}{4\pi^2(|\,\underline{q}-\underline{p}\,|^2+\beta_i^2)(p^2+\beta_i^2)}\left\langle \psi_f \left| \sum_{j=1}^{2}e^{i\underline{q}\,\underline{b}j} \right| \psi_f \right\rangle \tag{3.3.4}$$

For one square term

$$\left\langle \psi_f \,|\, e^{iq\,b_1} \,|\, \psi_i \right\rangle = \int e^{iq\,b_1}\,|\,\phi_{1s}^{He}(r_1)\,|^2\, d\underline{r}_1 \times \int |\,\phi_{1s}^{He}(r_2)\,|^2\, d\underline{r}_2$$

$$= \frac{N^2}{4\pi}\int e^{iq\,b_1}[\sum_{i=1}^{6}\gamma_i\, e^{-\lambda_i r_1}]\, d\underline{r}_1 \times 1 = \frac{N^2}{4\pi}\sum_{i=1}^{6}\gamma_i \int e^{iq\,b_1} e^{-\lambda_i r_1}\, d\underline{r}_1$$

$$= \frac{N^2}{4\pi}\sum_{i=1}^{6}\gamma_i[4\pi\frac{2\lambda_i}{(\lambda_i^2+q^2)^2}]$$

Both the square terms gives the same results, thus

$$U_{f_i}^{(2)}\Big|_{Square\ terms} = \frac{1}{4\pi^2(|\,\underline{q}-\underline{p}\,|^2+\beta_i^2)(p^2+\beta_i^2)}\left[2\times N^2\sum_{i=1}^{6}\gamma_i[\frac{2\lambda_i}{(\lambda_i^2+q^2)^2}]\right]. \tag{3..3..5}$$

Similarly following the above procedure for ***Cross terms :***

$$U_{f_i}^{(2)}\Big|_{Cross\ terms} = \frac{1}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\left\langle \psi_f \left| \sum_{j=1}^{2}\sum_{k\neq j}^{2} e^{i[(\underline{q}-\underline{p})\underline{b}j-\beta_i z_j]}\, e^{i(\underline{p}\,\underline{b}_k+\beta_i z_k)} \right| \psi_i \right\rangle$$

(3..3.6)

For one cross term

$$\left\langle \psi_f \left| e^{i[(\underline{q}-\underline{p})\,\underline{b}j-\beta_i z_j]}\, e^{i(\underline{p}\,\underline{b}_k+\beta_i z_k)} \right| \psi_i \right\rangle$$

$$= \int e^{i[(\underline{q}-\underline{p})\,\underline{b}j-\beta_i z_j]}\, |\phi_{1s}^{He}(r_1)|^2\, d\underline{r}_1 \int e^{i(\underline{p}\,\underline{b}_k+\beta_i z_k)}\, |\phi_{1s}^{He}(r_2)|^2\, d\underline{r}_2$$

$$= \frac{N^2}{4\pi}\int e^{i[(\underline{q}-\underline{p})\,\underline{b}j-\beta_i z_j]} \sum_{i=1}^{6}\gamma_i e^{-\lambda_i r_1}\, d\underline{r}_1 \times \frac{N^2}{4\pi}\int e^{i(\underline{p}\,\underline{b}_k+\beta_i z_k)} \sum_{j=1}^{6}\gamma_j e^{-\lambda_j r_2}]d\underline{r}_2$$

$$= \frac{N^2}{4\pi}\sum_{i=1}^{6}\gamma_i[4\pi\frac{2\lambda_i}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)^2}]\times\frac{N^2}{4\pi}\sum_{j=1}^{6}\gamma_j[4\pi\frac{2\lambda_j}{(\lambda_j^2+p^2+\beta_i^2)^2}]$$

$$= N^4\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j[\frac{2\lambda_i}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)^2}]\times[\frac{2\lambda_j}{(\lambda_j^2+p^2+\beta_i^2)^2}]$$

Both the cross terms gives the same results due to symmetric integrals.

Thus $U_{f_i}^{(2)}\Big|_{Cross\ terms}$

$$= \frac{2N^4}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\left[\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j\frac{2\lambda_i}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)^2}\frac{2\lambda_j}{(\lambda_j^2+p^2+\beta_i^2)^2}\right]$$

(3.3.7)

Similarly for ***Single term1 :***

$$U_{f_i}^{(2)}\Big|_{Single\ term1} = \frac{1}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\left\langle \psi_f \left| \sum_{j=1}^{2} e^{i(p\,b_j+\beta_i z_j)} \right| \psi_f \right\rangle \qquad (3.3.8)$$

For one single term1

$$\left\langle \psi_f \left| e^{i(p\,b_1+\beta_i z_1)} \right| \psi_f \right\rangle = \int e^{i(p\,b_1+\beta_i z_1)}\, |\phi_{1s}^{He}(r_1)|^2\, d\underline{r}_1 \times \int |\phi_{1s}^{He}(r_2)|^2\, d\underline{r}_2$$

$$= \frac{N^2}{4\pi}\int e^{i(p\,b_1+\beta_i Z_1)}[\sum_{i=1}^{6}\gamma_i e^{-\lambda_i r_1}]d\underline{r}_1 \times 1 = \frac{N^2}{4\pi}\sum_{i=1}^{6}\gamma_i\int e^{i(p\,b_1+\beta_i Z_1)}e^{-\lambda_i r_1}\, d\underline{r}_1$$

$$= \frac{N^2}{4\pi}\sum_{i=1}^{6}\gamma_i[4\pi\frac{2\lambda_i}{(\lambda_i^2+p^2+\beta_i^2)^2}].$$

Both the terms gives the same results, thus

$$U_{f_i}^{(2)}\Big|_{Single\ term1} = \frac{2N^2}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\sum_{i=1}^{6}\gamma_i[\frac{2\lambda_i}{(\lambda_i^2+p^2+\beta_i^2)^2}. \qquad (3.3.9)$$

Similarly for ***Single term2 :***

$$U_{f_i}^{(2)}\Big|_{Single\ term2} = \frac{1}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\left\langle \psi_f \left| \sum_{j=1}^{2} e^{i(|q-p|b_j-\beta_i z_j)} \right| \psi_f \right\rangle$$

(3.3.10)

For one single term2 :

$$\left\langle \psi_f \left| e^{i(|q-p|b_1-\beta_i z_1)} \right| \psi_f \right\rangle = \int e^{i(|q-p|.b_1-\beta_i z_1)} \, |\phi_{1s}^{He}(r_1)|^2 \, d\underline{r}_1 \times \int |\phi_{1s}^{He}(r_2)|^2 \, d\underline{r}_2$$

$$= \frac{N^2}{4\pi}\sum_{i=1}^{6}\gamma_i[4\pi\frac{2\lambda_i}{(\lambda_i^2+|q-p|^2+\beta_i^2)^2}]$$

Both the terms gives the same results, thus

$$U_{f_i}^{(2)}\Big|_{Single\ term2} = \frac{2N^2}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\sum_{i=1}^{6}\gamma_i[4\pi\frac{2\lambda_i}{(\lambda_i^2+|q-p|^2+\beta_i^2)^2}. \qquad (3.3.11)$$

Now ***Constant trem :***

$$U_{f_i}^{(2)}\Big|_{Const\ term} = \frac{1}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\left\langle \psi_f \left| (2)^2 \right| \psi_f \right\rangle$$

$$= \frac{(2)^2}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}. \qquad (3.3.12)$$

$$\Rightarrow U_{f_i}^{(2)}(\underline{q}-\underline{p}-\beta_i\hat{\xi};\underline{p}+\beta_i\hat{\xi})$$

$$= U_{f_i}^{(2)}\Big|_{\substack{Single\\term}} + U_{f_i}^{(2)}\Big|_{\substack{Gross\\term}} - 2\times U_{f_i}^{(2)}\Big|_{\substack{Single\\term1}} - 2\times U_{f_i}^{(2)}\Big|_{\substack{Single\\term2}} + U_{f_i}^{(2)}\Big|_{\substack{Const\\term}}$$

$$= \frac{1}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\Bigg[2N^2\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{\lambda_i^2+q^2}$$

$$+2N^4\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)}\frac{1}{(\lambda_j^2+p^2+\beta_i^2)}$$

$$-2\times 2N^2\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+p^2+\beta_i^2)} - 2\times 2N^2\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)} + (2)^2\Bigg]$$

(3.3.13)

Evaluation of $\int d\underline{p}$ ***integral :***

Now different integral terms of $\int U_{f_i}^{(2)}(\underline{q}-\underline{p}-\beta_i\hat{\xi};\underline{p}+\beta_i\hat{\xi})\,d\underline{p}$ are evaluated in the closed form by taking individual terms of equation (3.3.13).

Square terms :

$$\int \frac{2N^2}{4\pi^4(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{\lambda_i^2+q^2}\,d\underline{p}$$

$$=\frac{2N^2}{4\pi^4}\int\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\frac{1}{(\lambda_i^2+q^2)}\,d\underline{p}$$

$$=\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+q^2)}\int\frac{d\underline{p}}{(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}$$

$$=\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ip[1]}. \qquad (3.3.14)$$

Where $\mathbf{Ip[1]}=\frac{1}{(\lambda_i^2+q^2)}\int\frac{d\underline{p}}{(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}=\frac{1}{(\lambda_i^2+q^2)}I_1(\beta_i^2,0)$,

where $I_1(\beta_i^2,0)=I_1(\beta_i^2,\lambda^2)\big|_{\lambda=0}$ is defined in appendix [A1].

Cross terms :

$$\int\frac{2N^4}{4\pi^4(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)}\frac{1}{(\lambda_j^2+p^2+\beta_i^2)}\,d\underline{p}$$

$$=\frac{2N^4}{4\pi^4}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\int\frac{d\underline{p}}{(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)(\lambda_j^2+p^2+\beta_i^2)}$$

$$=\frac{2N^4}{4\pi^4}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\,\mathbf{Ip[2]}. \qquad (3.3.15)$$

Where $\mathbf{Ip[2]}=\frac{1}{\lambda_i^2}(\frac{1}{\lambda_j^2})\left[I_1(\beta_i^2,0)-I_1(\beta_i^2,\lambda_i^2)-I_1(\beta_i^2,\lambda_j^2)+I_4(\beta_i^2,\lambda_i^2,\lambda_j^2)\right]$,

Integral in the above equation is derived in the form of integral I_1 and I_4 using the method of partial fraction. Integral $I_4(\beta_i^2,\lambda_i^2,\lambda_j^2)$ is defined in appendix [A2].

Single term1 :

$$\int\frac{-2\times2N^2}{4\pi^4(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+p^2+\beta_i^2)}\,d\underline{p}$$

$$=\frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\int\frac{d\underline{p}}{(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)(\lambda_i^2+p^2+\beta_i^2)}$$

$$=\frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ip[3]} \qquad (3.3.16)$$

Partial fraction is used for the above integral to obtain it in the form of I_1 .

Where $\mathbf{Ip[3]}=\frac{1}{\lambda_i^2}\left[I_1(\beta_i^2,0)-I_1(\beta_i^2,\lambda_i^2)\right]$.

Single term2 :

$$\int\frac{-2\times 2N^2}{4\pi^4(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)}d\underline{p}$$

$$=\frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\int\frac{d\underline{p}}{(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)}$$

$$=\frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ip[4]} \qquad (3.3.17)$$

Where $\mathbf{Ip[4]}=\mathbf{Ip[3]}=\frac{1}{\lambda_i^2}\left[I_1(\beta_i^2,0)-I_1(\beta_i^2,\lambda_i^2)\right]$.

Because the $\int d\underline{p}$ integrals in single term1 & single term2 are symmetric.

Constant term :

$$\int\frac{2^2}{4\pi^4(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}d\underline{p}\;=\frac{2^2}{4\pi^4}\int\frac{d\underline{p}}{(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}$$

$$=\frac{2^2}{4\pi^4}\,\mathbf{Ip[5]} \qquad (3.3.18)$$

Where $\mathbf{Ip[5]}=I_1(\beta_i^2,0)$.

Finally from the equations (3.2.) to (3.2.)

$$\mathrm{Im}\,f_{HEA}^{(2)}=\frac{4\pi^3}{k_i}\int U_{f_i}^{(2)}(\underline{q}-\underline{p}-\beta_i\hat{\xi};\underline{p}+\beta_i\hat{\xi})\,d\underline{p}$$

$$=\frac{4\pi^3}{k_i}\left[\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ip[1]}+\frac{2N^4}{4\pi^4}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\,\mathbf{Ip[2]}\right.$$

$$\left.+\frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ip[3]}+\frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ip[4]}+\frac{2^2}{4\pi^4}\,\mathbf{Ip[5]}\right] \qquad (3.3.19)$$

Thus the final form of the imaginary part is obtained as

Thus the final form of the imaginary part is obtained as

$$\mathrm{Im}\, f^{(2)}_{HEA} = \frac{2N^2}{\pi k_i}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ip[1]},\lambda_i)] + \frac{2N^4}{\pi k_i}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j D(\mathbf{Ip[2]},\lambda_i,\lambda_j)$$

$$-2\frac{2\times 2N^2}{\pi k_i}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ip[3]},\lambda_i)] + (2)^2\frac{1}{\pi k_k}\mathbf{Ip[5]} \qquad (3.3.20)$$

Here $D(\mathbf{Ip[\,]},\lambda_i)$ represents the first order partial derivative with respect to λ_i and accordingly $D(\mathbf{Ip[\,]},\lambda_i,\lambda_j)$ represents partial derivative with respect to λ_i and λ_j.

Now taking the case of He like +ve ions equation (3.2.) will have the form as follows

$$\overline{V}\overline{V}' = \frac{1}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\left[\sum_{j=1}^{2}e^{i\underline{q}\,\underline{b}_j} + \sum_{j=1}^{2}\sum_{k\neq j}^{2}e^{i[(\underline{q}-\underline{p})\,\underline{b}_j-\beta_i z_j]}\,e^{i(\underline{p}.\underline{b}_k+\beta_i z_k)}\right.$$

$$\left. -Z\sum_{j=1}^{2}e^{i(p\,b_j+\beta_i z_j)} - Z\sum_{j=1}^{2}e^{i(|q-p|\,b_j-\beta_i z_j)} + (Z)^2\right]$$

$$\Rightarrow U^{(2)}_{f_i}(\underline{q}-\underline{p}-\beta_i\hat{\xi};\underline{p}+\beta_i\hat{\xi})$$

$$= U^{(2)}_{f_i}\Big|_{\substack{Single\\ term}} + U^{(2)}_{f_i}\Big|_{\substack{Gross\\ term}} - Z\times U^{(2)}_{f_i}\Big|_{\substack{Single\\ term1}} - Z\times U^{(2)}_{f_i}\Big|_{\substack{Single\\ term2}} + U^{(2)}_{f_i}\Big|_{\substack{Const\\ term}}$$

$$= \frac{1}{4\pi^2(|\underline{q}-\underline{p}|^2+\beta_i^2)(p^2+\beta_i^2)}\left[2N^2\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{\lambda_i^2+q^2}\right.$$

$$+2N^4\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)}\frac{1}{(\lambda_j^2+p^2+\beta_i^2)}$$

$$\left. -Z\times 2N^2\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+p^2+\beta_i^2)} - Z\times 2N^2\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+\beta_i^2)} + (Z)^2\right] \qquad (3.3.21)$$

Thus the generalised form of the imaginary part is obtained as

$$\mathrm{Im}\, f^{(2)}_{HEA} = \frac{2N^2}{\pi k_i}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ip[1]},\lambda_i)] + \frac{2N^4}{\pi k_i}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j D(\mathbf{Ip[2]},\lambda_i,\lambda_j)$$

$$-2\frac{Z\times 2N^2}{\pi k_i}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ip[3]},\lambda_i)] + (Z)^2\frac{1}{\pi k_k}\mathbf{Ip[5]} \qquad (3.3.22)$$

3.4.1 REAL PART-1 OF SECOND BORN AMPLITUDE : $O(k_i^{-1})$

Now the real part of the order (k_i^{-1}) of the second Born amplitude, equation (1.6.12) can be written as

$$\text{Re1}\ f_{HEA}^{(2)} = -\frac{4\pi^2}{k_i} \text{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{p_z - \beta_i} U_{fi}^{(2)}(\underline{q} - \underline{p} - p_z\hat{\xi}, \underline{p} + p_z\hat{\xi}) \qquad (3.4.1)$$

The basic difference between this real part and imaginary part is only the principle value integral $\int d\underline{p}$, the evaluation of volume integral $\int d\underline{r}_1$ and $\int d\underline{r}_2$ are same as imaginary part. Replacing β_i in equation (3.2.) by p_z $U_{fi}^{(2)}$ will be obtained as

$$U_{f_i}^{(2)}(\underline{q} - \underline{p} - p_z\hat{\xi}; \underline{p} + p_z\hat{\xi})$$

$$= U_{f_i}^{(2)}\Big|_{\substack{Single \\ term}} + U_{f_i}^{(2)}\Big|_{\substack{Cross \\ term}} - 2\times U_{f_i}^{(2)}\Big|_{\substack{Single \\ term1}} - 2\times U_{f_i}^{(2)}\Big|_{\substack{Single \\ term2}} + U_{f_i}^{(2)}\Big|_{\substack{Const. \\ term}}$$

$$= \frac{1}{4\pi^2(|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)} \Bigg[2N^2 \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \frac{1}{\lambda_i^2 + q^2}$$

$$+ 2N^4 \sum_{i=1}^{6} \sum_{j=1}^{6} \gamma_i \gamma_j \left(\frac{\partial}{\partial \lambda_i}\right)\left(\frac{\partial}{\partial \lambda_j}\right) \frac{1}{(\lambda_i^2 + |\underline{q} - \underline{p}|^2 + p_z^2)} \frac{1}{(\lambda_j^2 + p^2 + p_z^2)}$$

$$- 2\times 2N^2 \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \frac{1}{(\lambda_i^2 + p^2 + p_z^2)} - 2\times 2N^2 \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \frac{1}{(\lambda_i^2 + |\underline{q} - \underline{p}|^2 + p_z^2)} + (2)^2 \Bigg] \qquad (3.4.2)$$

Evaluation of $\int d\underline{p}$ ***integral :***

Now different integral terms of $\text{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{p_z - \beta_i} U_{fi}^{(2)}(\underline{q} - \underline{p} - p_z\hat{\xi}, \underline{p} + p_z\hat{\xi})$ are evaluated in the closed form by taking individual terms of equation (3.2.).

Square terms :

$$\text{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{p_z - \beta_i} \frac{2N^2}{4\pi^4(|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \frac{1}{(\lambda_i^2 + q^2)}$$

$$= \frac{2N^2}{4\pi^4} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \frac{1}{(\lambda_i^2 + q^2)} \mathrm{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{(p_z - \beta_i)(|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)}$$

$$= \frac{2N^2}{4\pi^4} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \mathbf{Ipr1[1]}. \qquad (3.4.3)$$

Where $\mathbf{Ipr1[1]} = \frac{1}{(\lambda_i^2 + q^2)} \mathrm{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{(p_z - \beta_i)(|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)}$

$$= \frac{1}{(\lambda_i^2 + q^2)} I_2(\beta_i^2, 0),$$

where $I_2(\beta_i^2, 0) = I_2(\beta_i^2, \lambda^2)\Big|_{\lambda=0}$ is defined in appendix [A3].

Cross terms :

$$\mathrm{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{p_z - \beta_i} \frac{2N^4}{4\pi^4 (|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)} \sum_{i=1}^{6} \sum_{j=1}^{6} \gamma_i \gamma_j \left(\frac{\partial}{\partial \lambda_i}\right)\left(\frac{\partial}{\partial \lambda_j}\right) \times$$

$$\left[\frac{1}{(\lambda_i^2 + |\underline{q} - \underline{p}|^2 + p_z^2)} \frac{1}{(\lambda_j^2 + p^2 + p_z^2)}\right]$$

$$= \frac{2N^4}{4\pi^4} \sum_{i=1}^{6} \sum_{j=1}^{6} \gamma_i \gamma_j \left(\frac{\partial}{\partial \lambda_i}\right)\left(\frac{\partial}{\partial \lambda_j}\right) \mathrm{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{(p_z - \beta_i)(|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)} \times$$

$$\left[\frac{1}{(\lambda_i^2 + |\underline{q} - \underline{p}|^2 + p_z^2)} \frac{1}{(\lambda_j^2 + p^2 + p_z^2)}\right]$$

$$= \frac{2N^4}{4\pi^4} \sum_{i=1}^{6} \sum_{j=1}^{6} \gamma_i \gamma_j \left(\frac{\partial}{\partial \lambda_i}\right)\left(\frac{\partial}{\partial \lambda_j}\right) \mathbf{Ipr1[2]}. \qquad (3.4.4)$$

Where $\mathbf{Ipr1[2]} = \frac{1}{\lambda_i^2}\left(\frac{1}{\lambda_j^2}\right)\left[I_2(\beta_i^2, 0) - I_2(\beta_i^2, \lambda_i^2) - I_2(\beta_i^2, \lambda_j^2) + I_5(\beta_i^2, \lambda_i^2, \lambda_j^2)\right]$, obtained using partial fraction of integral of equation (3.3.),where the integral $I_5(\beta_i^2, \lambda_i^2, \lambda_j^2)$ is defined in appendix [A4].

Single term1 :

$$\mathrm{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{p_z - \beta_i} \frac{-2 \times 2N^2}{4\pi^4 (|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \frac{1}{(\lambda_i^2 + p^2 + p_z^2)}$$

$$= -2\frac{2N^2}{4\pi^4} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \mathrm{P} \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{(p_z - \beta_i)(|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)(\lambda_i^2 + p^2 + p_z^2)}$$

$$= \frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr1[3]} \qquad (3.4.5)$$

Partial fraction is used for the above integral to obtain it in the form of I_2 .

Where $\mathbf{Ipr1[3]} = \frac{1}{\lambda_i^2}\left[I_2(\beta_i^2,0) - I_2(\beta_i^2,\lambda_i^2)\right]$.

Single term2 :

$$\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{p_z-\beta_i}\,\frac{-2\times 2N^2}{4\pi^4(|\underline{q}-\underline{p}|^2+p_z^2)(p^2+p_z^2)}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+p_z^2)}$$

$$= -2\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{(p_z-\beta_i)(|\underline{q}-\underline{p}|^2+p_z^2)(p^2+p_z^2)}\,\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+p_z^2)}$$

$$= -2\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr1[4]} \qquad (3.4.6)$$

Where $\mathbf{Ipr1[4]} = \mathbf{Ipr1[3]} = \frac{1}{\lambda_i^2}\left[I_2(\beta_i^2,0) - I_2(\beta_i^2,\lambda_i^2)\right]$.

Because the $\int d\underline{p}$ integrals in single term1 & single term2 are symmetric.

Constant term :

$$\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{p_z-\beta_i}\,\frac{2^2}{4\pi^4(|\underline{q}-\underline{p}|^2+p_z^2)(p^2+p_z^2)}$$

$$= \frac{2^2}{4\pi^4}\,\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{(p_z-\beta_i)(|\underline{q}-\underline{p}|^2+p_z^2)(p^2+p_z^2)}$$

$$= \frac{2^2}{4\pi^4}\,\mathbf{Ipr1[5]} \qquad (3.4.7)$$

Where $\mathbf{Ipr1[5]} = I_2(\beta_i^2,0)$.

Finally from the equations (3.4.3) to (3.4.7)

$$\mathrm{Re1}\;\; f_{HEA}^{(2)} = -\frac{4\pi^2}{k_i}\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{p_z-\beta_i}U_{fi}^{(2)}(\underline{q}-\underline{p}-p_z\hat{\xi},\underline{p}+p_z\hat{\xi})$$

$$= -\frac{4\pi^2}{k_i}\left[\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr1[1]} + \frac{2N^4}{4\pi^4}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\,\mathbf{Ipr1[2]}\right.$$

$$\left. + \frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr1[3]} + \frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr1[4]} + \frac{2^2}{4\pi^4}\,\mathbf{Ipr1[5]}\right] \tag{3.4.8}$$

Thus the final form of the real part-1 $O(k_i^{-1})$ is obtained as

$$\mathrm{Re}1f_{HEA}^{(2)} = -\frac{2N^2}{\pi^2 k_i}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr1[1]},\lambda_i)] - \frac{2N^4}{\pi^2 k_i}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j D(\mathbf{Ipr1[2]},\lambda_i,\lambda_j)$$

$$+2\frac{2\times 2N^2}{\pi^2 k_i}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr1[3]},\lambda_i)] - (2)^2\frac{1}{\pi^2 k_i}\mathbf{Ipr2[5]} \tag{3.4.9}$$

Here $D(\mathbf{Ipr1[\,]},\lambda_i)$ represents the first order partial derivative with respect to λ_i and accordingly $D(\mathbf{Ipr1[\,]},\lambda_i,\lambda_j)$ represents partial derivative with respect to λ_i and λ_j.

Now as we discussed in the case of imaginary part for He like +ve ions equation (3.3.22) general form of real part-1 can be obtained as

$$\mathrm{Re}1f_{HEA}^{(2)} = -\frac{2N^2}{\pi^2 k_i}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr1[1]},\lambda_i)] - \frac{2N^4}{\pi^2 k_i}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j D(\mathbf{Ipr1[2]},\lambda_i,\lambda_j)$$

$$+2\frac{Z\times 2N^2}{\pi^2 k_i}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr1[3]},\lambda_i)] - (Z)^2\frac{1}{\pi^2 k_i}\mathbf{Ipr2[5]} \tag{3.4.10}$$

3.4.2 REAL PART-2 OF SECOND BORN AMPLITUDE : $O(k_i^{-2})$

Now the real part of the order (k_i^{-2}) of the second Born amplitude, equation (1.6.13) can be written as

$$\mathrm{Re}2\ f_{HEA}^{(2)} = -\frac{2\pi^2}{k_i^2}\frac{\partial}{\partial\beta_i}\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{p_z-\beta_i}(p^2+p_z^2)U_{fi}^{(2)}(\underline{q}-\underline{p}-p_z\hat{\xi},\underline{p}+p_z\hat{\xi}) \tag{3.4.11}$$

The basic difference between this real part-1 and real part-2 is $\int dp_z$ integral with additional term $(p^2+p_z^2)$ in numerator and the whole expression is differentiated with respect to average excitation energy β_i.

Evaluation of $\int d\underline{p}$ integral :

Now different integral terms of $\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z(p^2+p_z^2)}{p_z-\beta_i}U_{fi}^{(2)}(\underline{q}-\underline{p}-p_z\hat{\xi},\underline{p}+p_z\hat{\xi})$ are evaluated in the closed form by taking individual terms of equation (3.2.).

Square terms :

$$\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z(p^2+p_z^2)}{p_z-\beta_i}\frac{2N^2}{4\pi^4(|\underline{q}-\underline{p}|^2+p_z^2)(p^2+p_z^2)}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+q^2)}$$

$$=\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\frac{1}{(\lambda_i^2+q^2)}\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{(p_z-\beta_i)(|\underline{q}-\underline{p}|^2+p_z^2)}$$

$$=\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr2[1]}. \qquad (3.4.12)$$

Where $\mathbf{Ipr2[1]}=\frac{1}{(\lambda_i^2+q^2)}\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{(p_z-\beta_i)(|\underline{q}-\underline{p}|^2+p_z^2)}$

$$=\frac{1}{(\lambda_i^2+q^2)}I_3(\beta_i^2,0),$$

where $I_3(\beta_i^2,0)=I_3(\beta_i^2,\lambda^2)\big|_{\lambda=0}$ is defined in appendix [A5].

Cross terms :

$$\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z(p^2+p_z^2)}{p_z-\beta_i}\frac{2N^4}{4\pi^4(|\underline{q}-\underline{p}|^2+p_z^2)(p^2+p_z^2)}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\times$$

$$\left[\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+p_z^2)}\frac{1}{(\lambda_j^2+p^2+p_z^2)}\right]$$

$$=\frac{2N^4}{4\pi^4}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z}{(p_z-\beta_i)(|\underline{q}-\underline{p}|^2+p_z^2)}\times$$

$$\left[\frac{1}{(\lambda_i^2+|\underline{q}-\underline{p}|^2+p_z^2)}\frac{1}{(\lambda_j^2+p^2+p_z^2)}\right]$$

$$= \frac{2N^4}{4\pi^4} \sum_{i=1}^{6} \sum_{j=1}^{6} \gamma_i \gamma_j \left(\frac{\partial}{\partial \lambda_i}\right)\left(\frac{\partial}{\partial \lambda_j}\right) \mathbf{Ipr2[2]}. \qquad (3.4.13)$$

Where $\mathbf{Ipr2[2]} = \frac{1}{\lambda_i^2}\left[I_2(\beta_i^2, \lambda_j^2) - I_5(\beta_i^2, \lambda_i^2, \lambda_j^2)\right]$, obtained using partial fraction of integral of equation (3.3.),where the integral $I_5(\beta_i^2, \lambda_i^2, \lambda_j^2)$ is defined in appendix [A4].

Single term1 :

$$\mathrm{P}\int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z (p^2 + p_z^2)}{p_z - \beta_i} \frac{-2 \times 2N^2}{4\pi^4 (|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \frac{1}{(\lambda_i^2 + p^2 + p_z^2)}$$

$$= -2\frac{2N^2}{4\pi^4} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \mathrm{P}\int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{(p_z - \beta_i)(|\underline{q} - \underline{p}|^2 + p_z^2)(\lambda_i^2 + p^2 + p_z^2)}$$

$$= \frac{-2 \times 2N^2}{4\pi^4} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \mathbf{Ipr2[3]} \qquad (3.4.14)$$

Partial fraction is used for the above integral to obtain it in the form of I_2 .

Where $\mathbf{Ipr2[3]} = I_2(\beta_i^2, \lambda_i^2)$.

Single term2 :

$$\mathrm{P}\int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z (p^2 + p_z^2)}{p_z - \beta_i} \frac{-2 \times 2N^2}{4\pi^4 (|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \frac{1}{(\lambda_i^2 + |\underline{q} - \underline{p}|^2 + p_z^2)}$$

$$= -2\frac{2N^2}{4\pi^4} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \mathrm{P}\int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{(p_z - \beta_i)(|\underline{q} - \underline{p}|^2 + p_z^2)} \frac{1}{(\lambda_i^2 + |\underline{q} - \underline{p}|^2 + p_z^2)}$$

$$= -2\frac{2N^2}{4\pi^4} \sum_{i=1}^{6} \gamma_i \left(-\frac{\partial}{\partial \lambda_i}\right) \mathbf{Ipr2[4]} \qquad (3.4.15)$$

Where $\mathbf{Ipr2[4]} = \frac{1}{\lambda_i^2}\left[I_3(\beta_i^2, 0) - I_3(\beta_i^2, \lambda_i^2)\right]$, considering partial fraction.

Constant term :

$$\mathrm{P}\int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z (p^2 + p_z^2)}{p_z - \beta_i} \frac{2^2}{4\pi^4 (|\underline{q} - \underline{p}|^2 + p_z^2)(p^2 + p_z^2)}$$

$$= \frac{2^2}{4\pi^4} \mathrm{P}\int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{(p_z - \beta_i)(|\underline{q} - \underline{p}|^2 + p_z^2)}$$

$$= \frac{2^2}{4\pi^4}\,\mathbf{Ipr2[5]} \tag{3.4.16}$$

Where $\mathbf{Ipr2[5]} = I_3(\beta_i^2, 0)$.

Finally from the equations (3.3.) to (3.3.)

$$\mathrm{Re}2\ f_{HEA}^{(2)} = -\frac{2\pi^2}{k_i^2}\frac{\partial}{\partial\beta_i}\mathrm{P}\int d\underline{p}\int_{-\infty}^{\infty}\frac{dp_z(p^2+p_z^2)}{p_z-\beta_i}\ U_{fi}^{(2)}(\underline{q}-\underline{p}-p_z\hat{\xi},\underline{p}+p_z\hat{\xi})$$

$$= -\frac{2\pi^2}{k_i^2}\frac{\partial}{\partial\beta_i}\left[\frac{2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr2[1]} + \frac{2N^4}{4\pi^4}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j(\frac{\partial}{\partial\lambda_i})(\frac{\partial}{\partial\lambda_j})\,\mathbf{Ipr2[2]}\right.$$

$$\left. + \frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr2[3]} + \frac{-2\times 2N^2}{4\pi^4}\sum_{i=1}^{6}\gamma_i(-\frac{\partial}{\partial\lambda_i})\,\mathbf{Ipr2[4]} + \frac{2^2}{4\pi^4}\,\mathbf{Ipr2[5]}\right] \tag{3.4.17}$$

Thus the final form of the real part-2 $O(k_i^{-2})$ is obtained as

$$\mathrm{Re}2f_{HEA}^{(2)} = -\frac{N^2}{\pi^2k_i^2}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr2[1]},\lambda_i,\beta_i)] - \frac{N^4}{\pi^2k_i^2}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j D(\mathbf{Ipr2[2]},\lambda_i,\lambda_j,\beta_i)$$

$$+\frac{2N^2}{\pi^2k_i^2}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr2[3]},\lambda_i,\beta_i)] + \frac{2N^2}{\pi^2k_i^2}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr2[4]},\lambda_i,\beta_i)]$$

$$-(2)^2\frac{1}{2\pi^2k_i^2}D(\mathbf{Ipr2[5]},\beta_i) \tag{3.4.18}$$

Here $D(\mathbf{Ipr1[\ ]},\lambda_i,\beta_i)$ represents the first order partial derivative with respect to λ_i and β_i. Similarly accordingly $D(\mathbf{Ipr1[\ ]},\lambda_i,\lambda_j,\beta_i)$ represents partial derivative with respect to λ_i,λ_j and β_i.

In case of He like positive ions above equation will have the generalized form as

Thus the final form of the real part-2 $O(k_i^{-2})$ is obtained as

$$\mathrm{Re}2f_{HEA}^{(2)} = -\frac{N^2}{\pi^2k_i^2}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr2[1]},\lambda_i,\beta_i)] - \frac{N^4}{\pi^2k_i^2}\sum_{i=1}^{6}\sum_{j=1}^{6}\gamma_i\gamma_j D(\mathbf{Ipr2[2]},\lambda_i,\lambda_j,\beta_i)$$

$$+Z\frac{N^2}{\pi^2k_i^2}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr2[3]},\lambda_i,\beta_i)] + Z\frac{N^2}{\pi^2k_i^2}\sum_{i=1}^{6}\gamma_i[-D(\mathbf{Ipr2[4]},\lambda_i,\beta_i)]$$

$$-(Z)^2\frac{1}{2\pi^2k_i^2}D(\mathbf{Ipr2[5]},\beta_i) \tag{3.4.19}$$

3.5 AVERAGE EXCITATION ENERGY :

In this HHOB approximation average excitation energy has an important roll in the interaction between incident electron and target electrons, which is obtained from dipole polarizibility. It is necessary to get proper normalization constant while working with wave functions and their volume integrals. It is clear that one electron orbital wave function $\phi_{1s}^{He}(r)$ must be normalized before it is used in volume integral throughout the calculations. Applying the normalization condition to the wave function we get

$\int |\phi_{1s}^{He}(r)|^2 \, d\underline{r} = 1,$

where $\phi_{1s}^{He}(r) = \frac{N}{\sqrt{4\pi}}[Ae^{-\alpha_1 r} + Be^{-\alpha_2 r} + Ce^{-\alpha_3 r}]$; $A = C_1 N_{\chi_1}$, $B = C_2 N_{\chi_2}$ $C = C_3 N_{\chi_3}$.

$$\therefore \int \frac{N^2}{4\pi}[\mathrm{A}^2 e^{-2\alpha_1 r} + \mathrm{B}^2 e^{-2\alpha_2 r} C^2 e^{-2\alpha_3 r} + 2\mathrm{AB}e^{-(\alpha_1+\alpha_2)r} + 2\mathrm{BC}e^{-(\alpha_2+\alpha_3)r} + 2\mathrm{AC}e^{-(\alpha_1+\alpha_3)r}]\, d\underline{r} = 1$$

$$\therefore \int \frac{N^2}{4\pi} \sum_{i=1}^{6} \gamma_i e^{-\lambda_i r} \, d\underline{r} = \frac{N^2}{4\pi} \sum_{i=1}^{6} \gamma_i \int e^{-\lambda_i r} \, d\underline{r} = 1 \qquad (3.5.1)$$

$$\text{Now } \int e^{-\lambda_i r} \, d\underline{r} = \int_0^{2\pi} d\varphi \int_0^{\pi} Sin\theta \, d\theta \int_0^{\infty} e^{-\lambda_i r} \, r^2 dr = 2\pi \times 2 \int_0^{\infty} e^{-\lambda_i r} \, r^2 dr$$

$$= 4\pi \frac{\Gamma(3)}{\lambda_i^3} = 4\pi \frac{2}{\lambda_i^3}$$

$$\Rightarrow \frac{N^2}{4\pi} \sum_{i=1}^{6} \gamma_i \left[4\pi \frac{2}{\lambda_i^3} \right] = 2N^2 \sum_{i=1}^{6} \frac{\gamma_i}{\lambda_i^3} = 1$$

$$\Rightarrow N = \left[2 \sum_{i=1}^{6} \frac{\gamma_i}{\lambda_i^3} \right]^{-1/2} \qquad (3.5.2)$$

Now the average excitation energy in the case of two electron system is obtained from the dipole polarizibility which is given as

$$\bar{\alpha} = 2 \sum_{n \neq 0} \frac{|\langle 0|\hat{r}.\sum_{j=1}^{2} r_j|\mathrm{n}\rangle|^2}{\omega_n - \omega_0} = \frac{2}{\bar{\omega}} \sum_n |\langle 0|\, \hat{r}.(r_1 + r_2)\,|\mathrm{n}\rangle|^2 \qquad (3.5.3)$$

where $r_1, r_2 \rightarrow$ The position vectors of target electrons,

$\hat{r} \rightarrow$ Unit vector in the direction of incident electron,

$\bar{\omega} \rightarrow$ Average excitation energy.

$|0\rangle \rightarrow$ Ground state of the target

Using the closure approximation, equation (3.5.3) is simplified to

$$\bar{\alpha} = \frac{2}{\omega}\langle 0|\,[\,\hat{r}.(r_1 + r_2)]^2\,|0\rangle = \frac{2}{\omega}\langle 0|\,(z_1 + z_2)^2\,|0\rangle$$

$$\therefore \bar{\alpha} = \frac{2}{\omega}\langle 0|\,(z_1 + z_1 z_2 + z_2)^2\,|0\rangle$$

Now $\langle 0|z_1^2|0\rangle = \int|\phi_{1s}^{He}(r_1)|^2\, z_1^2\, d\underline{r}_1 = \frac{N^2}{4\pi}\sum_{i=1}^{6}\gamma_i \int e^{-\lambda_i r}\, z_1^2 d\underline{r}_1$,

where $\int e^{-\lambda_i r}\, z_1^2 d\underline{r}_1 = 2\pi\int_0^{\infty}\int_0^{\pi}(r\,Cos\theta)^2\, Sin\theta\, d\theta\, r^2 e^{-\lambda_i r}\, dr$

$$= 2\pi\int_{-1}^{1}x^2 dx\int_0^{\pi} r^4 e^{-\lambda_i r}\, dr = 2\pi\frac{2}{3}\frac{4!}{\lambda_i^5} = \frac{32\pi}{\lambda_i^5}$$

$$\langle 0|z_1^2|0\rangle = \frac{N^2}{4\pi}32\pi\sum_{i=1}^{6}\frac{\gamma_i}{\lambda_i^5} = 8N^2\sum_{i=1}^{6}\frac{\gamma_i}{\lambda_i^5}$$

$$\Rightarrow \langle 0|z_1^2 + z_2^2|0\rangle = 16N^2\sum_{i=1}^{6}\frac{\gamma_i}{\lambda_i^5} \qquad (3.5.4)$$

Now $\langle 0|z_1 z_2|0\rangle = \int|\phi_{1s}^{He}(r_1)|^2\, z_1\, d\underline{r}_1 \int|\phi_{1s}^{He}(r_2)|^2\, z_2\, d\underline{r}_2$

$$\int|\phi_{1s}^{He}(r_1)|^2\, z_1\, d\underline{r}_1 = \sum_{i=1}^{6}\gamma_i \int e^{-\lambda_i r}\, z_1 d\underline{r}_1$$

$$= \sum_{i=1}^{6}\gamma_i 2\pi\int_0^{\infty}\int_0^{\pi} r\,Cos\theta\, Sin\theta\, d\theta\, r^2 e^{-\lambda_i r}\, dr$$

$$= \sum_{i=1}^{6}\gamma_i 2\pi\int_{-1}^{1}x\,dx\int_0^{\pi} r^3 e^{-\lambda_i r}\, dr = 0$$

$$\therefore \bar{\alpha} = \frac{2}{\omega}16N^2\sum_{i=1}^{6}\frac{\gamma_i}{\lambda_i^5}$$

$$\Rightarrow \bar{\omega} = \frac{32}{\alpha}N^2\sum_{i=1}^{6}\frac{\gamma_i}{\lambda_i^5} \qquad (3.5.5)$$

In the present calculation atomic dipole polarizibilities are obtained from the work of A Dalgarno [table 5(b)], which are more accurate theoretical values. The excitation energy for various ions in their ground state is calculated from HF-parameters given in the table-1. In the table-2 dipole polarizibility and corresponding average excitation energy for each target are given.

Table-1

Hartree-Fock parameters for He, He like +ve ions

Target	*Orbital exponents*			*Expansion Coefficients*		
	α_1	α_2	α_3	C_1	C_2	C_3
He	1.45286	2.77954	4.34600	0.82958	0.18334	0.00824
L^{+1}	2.45055	4.57259	6.67032	0.89066	0.12328	0.00088
Be^{+2}	3.43071	5.63150	7.35143	0.89855	0.09068	0.02158
B^{+3}	4.44422	7.90274	11.31380	0.930360	0.07786	0.00013
C^{+4}	5.44726	9.80425	14.61460	0.94428	0.06328	-0.00125

Table -2

Target	$\bar{\alpha}$ $(10^{-24} cm^3)$	$\bar{\omega}$ (a_0^3)
He	0.196	1.18478
Li^+	0.0286	3.07068
Be^{+2}	0.00759	6.0292
B^{+3}	0.00288	9.72251
C^{+4}	0.00132	14.3096

3.6 EXCHANGE AMPLITUDE :

Finally for the consistent picture of DCS $O(k_i^{-2})$ we have included first term of the elastic exchange amplitude , using Ochkur approximation (Joachain, 1975) given as

$$g_{el}^{och} = -(2\pi)^2 T_{el}^{och} \quad , \tag{3.6.1}$$

where $T_{el}^{och} = \frac{1}{2\pi^2 k^2} \int e^{iq\,r_1} \, |\psi_0(r_1, r_2)|^2 \, d\underline{r}_1 d\underline{r}_2$,

where $|\psi_0(r_1, r_2)|^2 = |\phi_{1s}^{He}(r_1)|^2 \, |\phi_{1s}^{He}(r_2)|^2$.

Now $I_{ex} = \int e^{iq\,r_1} \, |\phi_{1s}^{He}(r_1)|^2 \, d\underline{r}_1 \int |\phi_{1s}^{He}(r_2)|^2 \, d\underline{r}_2 = \int e^{iq\,r_1} \, |\phi_{1s}^{He}(r_1)|^2 \, d\underline{r}_1 \cdot 1$

$$= \frac{N^2}{4\pi} \sum_{i=1}^{6} \gamma_i \int e^{iq.r_1} e^{-i\lambda_i r_1} d\underline{r}_1 \quad = \frac{N^2}{4\pi} \sum_{i=1}^{6} \gamma_i \, [4\pi \frac{2\lambda_i}{(\lambda^2 + q^2)^2}]$$

$$= 2N^2 \sum_{i=1}^{6} \gamma_i \, [\frac{\lambda_i}{(\lambda^2 + q^2)^2}] . \tag{3.6.2}$$

$$\Rightarrow g_{el}^{och} = -\frac{(2\pi)^2}{2\pi^2 k^2} = 2N^2 \sum_{i=1}^{6} \gamma_i \, [\frac{\lambda_i}{(\lambda^2 + q^2)^2}]$$

$$= -\frac{4}{k^2} N^2 \sum_{i=1}^{6} \gamma_i \, [\frac{\lambda_i}{(\lambda^2 + q^2)^2}] . \tag{3.6.3}$$

The elastic differential cross section is then derived real and imaginary contributions of the second Born amplitude $f_{B2} = f_{B1} + \bar{f}_{B2}$ and the exchange amplitude. Following the equations (3.2.8), (3.3.22), (3.4.10), (3.4.19) and (3.6.3) differential cross section is calculated as

$$\frac{d\sigma}{d\Omega} = \left| f_{B1} + \mathrm{Re}\, \bar{f}_{B2} + g_{el}^{och} \right|^2 + \left| \mathrm{Im}\, \bar{f}_{B2} \right|^2$$

$$\therefore \frac{d\sigma}{d\Omega} = \left| f_{B1} + \mathrm{Re}1 f_{HEA}^{(2)} + \mathrm{Re}2 f_{HEA}^{(2)} + g_{el}^{och} \right|^2 + \left| \mathrm{Im}\, f_{HEA}^{(2)} \right|^2 \tag{3.6.4}$$

The typical calculation of the DCS is evaluated through different function programs and using two different packages developed in the latest programming language (i) *Turbo C++* and (ii) *Mathematica 2.2.*

3.7 PROGRAMS :

3.7.1 ***Programs :*** *C codes* A14.c,A15.c.

The computer codes developed in the latest programming language in Turbo C++ are presented which calculates elastic scattering cross section as a function of scattering angle for electrons colliding with He atom or He like +ve ions in ground state . It is

developed for the wave function made up of three 1S basis functions. The DCS is computed in an independent particle approach through HHOB approximation up to the order k_i^{-2} according to equation (3.6.4). The exact target potential (i.e. configuration interaction potential) is considered with the Roothaan Hartee-Fock wave function.

Apart from partial wave analysis Born approximation gives consistent results in the case of electron ion scattering which is simpler than earlier. The computations are carried out in non-relativistic limit. Atomic units ($\hbar = e = m_e = 1$) are used throughout.

Program description: A14.c

The program structure A14.c has two parts *main( )* function program and functions (i.e. subroutines) defined before it. The term f_{B1}, $\mathrm{Im}\bar{f}_{B2}$ and $\mathrm{Re}1\bar{f}_{B2}$ defined in section 3.3 and 3.4.1 are evaluated by this code. The corresponding values of these terms are displayed to the out put.

Function **main( )** : The program start execution from this function.

1. *Declaration statement*: Define variables, constants and array in double-precision for accurate calculation up to more decimal places, in static mode
2. *Input for HF parameters* : File having parameter values for the target wave function is include in function main( ) .: e.g. "I_E.He" for which the *DCS* is to be calculated.
3. *Calculation of normalization constant*: **for** loop evaluate equation (3.5.2).
4. *Input of incident energy and angle*: Incident electron energy E in eV, angular range '*ti*' and '*tf*' as well as increment '*inc*' in the angle are given as inputs for the program.
5. *Loop over angle* : Angular range for *DCS* is assigned.

   (i) ***Calculation of first Born amplitude*** f_{B1} : Evaluate the equation (3.2.8).

   (ii) ***Calculation of Imaginary part of*** $\bar{f}_{B2}$: Evaluate the equation (3.3.22). Identified by flag 'flg=0'

- Function **DH(*l*)** : compute derivative with respect to l using three point formula $f'(x) = \dfrac{-3f(x)+4f(x+h)-f(x+2h)}{2h}$

-calling function **FH(*l*)** : compute Ip[1] of equation (3.3.14).

-calling function **I1 (*l*)** : compute $I_1(\beta_i^2,0)$ of appendix [A1].

Derivative procedure is computed very carefully with proper step height in function programs computing partial derivative.

- Function **D0KJ(*l1,l2*)** : compute derivative with respect to *l1* using the three point formula.

-calling function **D0J(*l1, l2*)** : compute derivative with respect to *l* 2 .

-calling function **F(*l1, l2*)** : compute Ip[2] of equation (3.3.15).

-calling function (i) **I1 (*l1*)** : compute $I_1(\beta_i^2,\lambda^2)$ of appendix [A1].

(ii) **I4 (*l1, l2*)** : compute $I_4(\beta_i^2,\lambda_i^2,\lambda_j^2)$ of appendix [A2].

- Function **DH1(*l*)** : compute derivative with respect to *l* using three point formula .

-calling function **FH1(*l*)** : compute Ip[3] of equation (3.3.16).

-calling function **I1(0),I1(*l*)** : compute $I_1(\beta_i^2,0), I_1(\beta_i^2,\lambda^2)$ of [A1].

- Addition of four terms of equation (3.3.22).

(iii) ***Calculation of Real part-1 of*** $\bar{f}_{B2}$: Evaluate the equation (3.4.10).

Identified by flag 'flg=0'.

The program structure is same as that of imaginary part. The only difference is that the function **I2 (*l*)** and **I5 (*l1,l2*)** are called in place of **I1 (*l*)** and **I4 (*l1, l2*)** respectively.

End of function **main( )**.

Program description : A15.c

The program structure of A15.c is similar to A14.c. The term $\mathrm{Re}2f_{B2}$ defined in section 3.4.2 is evaluated by this code. The main difference is partial derivative w.r. to *b* is taken in addition to partial derivative w.r.to *l1* and *l2*.

Calculation of real part-2 of $\bar{f}_{B2}$: Evaluate the equation (3.4.19).

- Function **DXB (*l*)** : compute first order derivative with respect to *l* using three point formula.

-calling function **DB(*l, b*)** : compute derivative with respect to *b* .

-calling function **FH (*l, b*)** : compute Ipr2[1] of equation (3.4.12);

compute Ipr2[3] of equation (3.4.14);

compute Ipr2[4] of equation (3.4.15);

-calling function **I3** (*l, b*) : compute $I_3(\beta_i^2,\lambda^2)$ of appendix [A5].

-calling function **I2** (*l, b*) : compute $I_2(\beta_i^2,\lambda^2)$ of appendix [A3].

- Function **DXYB(*l1,l2*)** :compute derivative with respect to *l1* and *l2* using four point formula $\frac{\partial f(x,y)}{\partial x\,\partial y} = \frac{f(x+h,y+h)-f(x+h,y-h)-f(x-h,y+h)+f(x-h,y-h)}{4h^2}$

-calling function **DB1**(*l1, l2,B*) : compute derivative with respect to b .

-calling function **FH24**(*l1, l2,b*) : compute Ipr2[2] of equation (3.4.13).

-calling function (i) **I2** (*l1,b*) : compute $I_2(\beta_i^2,\lambda^2)$ of appendix [A3].

(ii) **I5** (*l1, l2,b*) : compute $I_5(\beta_i^2,,\lambda_i^2,\lambda_j^2)$ of appendix [A4].

Accuracy in the evaluation of partial derivative is very important for these calculations. Finding the first order as well as second order derivative numerically, proper step height must be chosen, otherwise random values are evaluated some times. So more accurate mathematical procedure is needed for calculation of the partial derivative.

The latest programming language 'Mathematica' provides such mathematical tool. Enough study and exercise of 'Mathematica' code made above calculations possible. It evaluates partial derivatives of any order for the given function. Symbolic expression is the important feature of this software, which is very useful for complex calculations. Along with the Turbo C code, the Mathematica codes have been developed. It became very useful for testing the 'C' program as well as cross checking of the calculations. The useful characteristics of this programming language are listed here.

1. Each variable and their assigned values are treated in double precision by default
2. It can do symbolic computation
3. Analytical form of integration, derivative, power series etc. is obtained.
4. Individual parts of the program can be executed.

3.7.2 Programs : Mathematica codes Imfb2.ma, Refb2t1.ma, Refb2t2.ma

The Mathematica codes presented here perform partial differentiation very accurately in sophisticated manner through its built-in function. The codes evaluate second Born terms $\mathrm{Im}\,\bar{f}_{B2}$, $\mathrm{Re1}\bar{f}_{B2}$ and $\mathrm{Re2}\bar{f}_{B2}$ in the elastic scattering of electrons from He

iso-electronic series as a function of scattering angle according to equation (3.6.4) including the exchange effect.

Program description: Imfb2.ma

The window provided to edit and execute the program is called notebook in Mathematica. The program written in the notebook can be divided in to different cells for individual execution of statements grouped in a cell. The program Imfb2.ma is divided in to four- cells. Finally all the cells are merged to execute the program in single click.

First Cell : It contains input data for elastic scattering process..
Atomic number, Dipole polarizibility, Incident energy, Starting angle and HF –parameters for the target.

Second Cell : It computes Normalization constant and Average excitation energy.

Third Cell : It is a Loop over angle calculates f_{B1} and $\mathrm{Im}\,\bar{f}_{B2}$.
The angular range and increment in the angle are defined within the loop.

(i) ***Calculation of first Born amplitude*** f_{B1} : Evaluate the equation (3.2.8).

(ii) ***Calculation of Imaginary part of*** $\bar{f}_{B2}$: Evaluate the equation (3.3.22).

-Function **I1[x_]** and **I4[x_, y_]** are defined by symbolic expressions:
compute $I_1(\beta_i^2, \lambda^2)$ and $I_4(\beta_i^2, \lambda_i^2, \lambda_j^2)$ of appendix [A1,A2].

-Function **D[Ip[1], x]** : evaluate derivative of Ip[1] w.r. to x by symbolic computation, where Ip[ ] is defined in section 3.3.
D[Ip[1],x] /. x->*l* : Value of x is replaced by ***l*** in the symbolic form.

-Function **D[Ip[2], x,y]** : evaluate derivative of Ip[2] w.r. to x and y by symbolic computation.
D[Ip[2],x,y] /. { x->*l1*,y->*l2* } : Value of **x** and **y** is replaced by ***l1*** and ***l2*** in the symbolic form.

-Function **Sum [ImfB2t[i], {i,1,4}]** : Add four terms of equation (3.3.22).

Program description : Refb2t1.ma, Refb2t2.ma

The program structure of Refb2t1.ma and Imfb2.ma are the same except the use of functions **I2[x_]** and **I5[x_, y_]** in place of **I1[x_]** and **I4 [x_, y_]** respectively. It should be noted that roll of 'Signm' function is important in the evaluation of I2 [ ] and I5 [ ]. It

must be evaluated just before the use of function I2 [ ] and I5 [ ]. Because 'function calling function' algorithm is not applied in this code as in the corresponding 'C' code.

In the program Refb2t2.ma function **I3 [ ]** is used in addition to function **I2 [ ]** and **I5 [ ]** in code Refb2t1.ma. The main difference is partial derivative w.r. to ***b*** in addition to partial derivative w.r. to **x** and **y**. To evaluate these multiple partial derivative the same built-in function **D [** expr, var1,var2,.. **]** is used as earlier.

-Function **I2[x_,b_]**, **I3[x_, b_]** and **I5 [x_,y_,b_]** are defined by symbolic expressions: compute $I_2(\beta_i^2,\lambda^2)$, $I_3(\beta_i,\lambda^2)$ and $I_5(\beta_i^2,\lambda_i^2,\lambda_j^2)$.

-Function **D[Ipr2[1], x,b]** : evaluate derivative of Ipr2[ ] w.r. to x and b by symbolic computation, where Ipr2[ ] is defined in section 3.4

D[Ipr2[1],x] /. {x->*l*,*b*->β_i} : Value of **x** and **b** is replaced by ***l*** and β_i in the symbolic form.

-Function **D[Ipr2[2], x,y,b]** : evaluate derivative of Ipr2[2] w.r. to x , y and b by symbolic computation.

D[Ipr2[2],x,y,b] /. { x->*l1*,*y*->*l2*,*b*->β_i} : Value of **x** ,**y** and ***b*** is replaced by ***l1***, ***l2*** and β_i in the symbolic form.

Turbo C programs :

```
/* Calculation of Im f(2) & Re1 f(2)for ; He-Atom A14.c */

# define PI 3.1428
#include <stdio.h>
# include <math.h>
float  h1=.01,  /* h=.01Step hight for 1st derivative */
       h2=.1;   /* h=.1 Step hight for 2nd derivative */
int flg, cd=2;       /* Code no. for He-atom  */
double bi,q;

/* I1(l) and I2(l1,l2) integral         */
double I1(l)
   double l;
{  double z,q2,b2,l2,n,d,f;
   q2=q* q; b2=bi* bi; l2=l*l;
   z=sqrt(pow(l2+q2,2) + 4* q2* b2 );
   n= (q2+b2)* (z+q2+l2)+2* b2* (q2-l2);
   d= (b2+l2)* (z-q2-l2);
   f=log(n/d);
   f=PI/z * f;
   return(f);}

double I2(l)
   double l;
{  int sgn;
   double z,q2,b2,l2,A,f;
   q2=q* q; b2=bi* bi; l2=l* l;
   z=sqrt(pow(l2+q2,2) + 4* q2* b2 );
   if((l2-q2)>0) sgn=1;else sgn=-1;
   A=1-2* b2* pow(l2-q2,2)/(pow(l2+q2,2)* (b2+l2));
   f=1-sgn* ( 1/2.0-1/PI* asin(A) );
   f=-pow(PI,3)/z * f;
   return(f);}

double FH(x)
    double x;
{   double q2,l2,f;
    l2=x* x;q2=q* q;
    if(flg==0)
    f= I1((double)0)/(l2+q2);
    if(flg==1)
    f= I2((double)0)/(l2+q2);
    return(f);}

double FH1(x)
    double x;
{   double l1,l2,f;
    l1=x;l2=x* x;
    if(flg==0)
    f=(I1((double)0)-I1(l1))/l2;
    if(flg==1)
    f=(I2((double)0)-I2(l1))/l2;
    return(f);}
```

```
double DH(L)
    double L;
{   double d,h=h1;
  d=(-3* FH(L) + 4* FH(L+h) - FH(L+2* h))/(2* h);
  return(d);}
double DH1(L)
    double L;
{   double d,h=h1;
  d=(-3* FH1(L) + 4* FH1(L+h) - FH1(L+2* h))/(2* h);
  return(d);}

/* ok I4(l1,l2) and I5(l1,l2)  integrals          */
double I4(L1,L2)
   double L1,L2;
{  double z,q2,b2,l1,l2,u2,v2,n,d,f;
   q2=q* q; b2=bi* bi; l1=L1* L1; l2=L2* L2;
                  v2=b2+l1;  u2=b2+l2;
   z=sqrt( u2* u2 + pow(q2+v2,2) -2* u2* (v2-q2) );

   n=(q2+v2)* (q2+v2+z)-u2* (v2-q2);
   d= u2* (z+v2-u2-q2);
   f=log(n/d);
   f=PI/z * f;
   return(f);}

double I5(L1,L2)          /* I2(bi* bi,l* l) */
   double L1,L2;
{  int sgn1,sgn2;
   double E1,E2,q2,b2,l1,l2,L,v2,u2,A1,A2,f;
   q2=q* q; b2=bi* bi; l1=L1* L1; l2=L2* L2; L=l1-l2;
                  v2=b2+l1;  u2=b2+l2;
   if(L+q2>0) sgn1=1;else sgn1=-1;
   if(L-q2>0) sgn2=1;else sgn2=-1;
   E1=sqrt(pow(L+q2,2) + 4* q2* v2);
   E2=sqrt(pow(L-q2,2) + 4* q2* u2);
   A1=1-2* b2* pow(L+q2,2)/((pow(L+q2,2)+4* q2* l1)* v2);
   A2=1-2* b2* pow(L-q2,2)/((pow(L-q2,2)+4* q2* l2)* u2);
   f= ( sgn1* ( 1/(2* E1)-asin(A1)/(PI* E1) )
       -sgn2* ( 1/(2* E2)-asin(A2)/(PI* E2) ) );
   f=-PI* PI* f;
   return(f);}

double F(x1,x2)
    double x1,x2;
{   double l1,l2,b,f;
  l1=x1;l2=x2;
  if(flg==0)
  f =1/pow(l1* l2,2) * (I1((double)0)-I1(l1)-I1(l2)+I4(l1,l2));
  if(flg==1)
  f =1/pow(l1* l2,2) * (I2((double)0)-I2(l1)-I2(l2)+I5(l1,l2));
return(f);}

double D0J(y1,y2)
    double y1,y2;
```

```
{   double d,h=h1;
 d=(-3* F(y1,y2) + 4* F(y1,y2+h) - F(y1,y2+2* h))/(2* h);
 return(d);}
double D0KJ(y1,y2)
    double y1,y2;
{   double d,h=h1;
 d=(-3* D0J(y1,y2) + 4* D0J(y1+h,y2) - D0J(y1+2* h,y2))/(2* h);
 return(d);}

main(){
int i,j,Z=cd;
float E,t;
float ti,tf,inc;
static double ki,s,N,r[6],l[6],S1[6],S3[6];
static double c1,c2,c3,n1,n2,n3,          dE=1.187; /*  a.u. */
static double z1,z2,z3,pd,t1,t2,t3,t4,Imfb2,Relfb2;
static double fB1p,Ib0,Ib1,S,fB1e,fB1;
clrscr();
/* Input Energy and angle */
printf("\nEnergy (eV) = "); scanf("%f",&E);
printf("ti = "); scanf("%f",&ti);
printf("tf = "); scanf("%f",&tf);
printf("inc ="); scanf("%f",&inc);
#include <I_E.He>
/* Normalization Constant */
for(s=(double)0,i=1;i<=6;i++) s=s+r[i]/pow(l[i],3);
N= 1/sqrt(2* s);
printf("\nN = %f",N);
printf("\nE = %.2f",E);
ki=sqrt(2* E/27.2);
bi=dE/ki;

for(t=ti;t<=tf;t=t+inc){
    printf("\n@ = %.2f ",(float)t);
    q=2* ki* sin(t* PI/360);
    fB1p=Z* 2/(q* q); Ib0=2* PI* 2/(q* q);
    for(S=(double)0,i=1;i<=6;i++){
      S=S+r[i]* l[i]/pow(l[i]* l[i]+q* q,2);}
    Ib1=N* N* 2* S;
    fB1e=-1/(2* PI)* Ib0* Ib1;
    fB1=fB1p+2* fB1e;
    printf(" fB1 = %.4f ",fB1);

flg=0;  /* IMAGINARY PART  */
/* Squar Terms : single derivative */
           for(t1=(double)0,i=1;i<=6;i++){
           S1[i]=r[i]* (-DH(l[i]));
           t1=t1+S1[i];}
/* Cross Terms : single Two derivative */
           for(t2=(double)0,i=1;i<=6;i++){
           for(j=1;j<=6;j++){
                pd=D0KJ(l[i],l[j]);
                t2=t2+r[i]* r[j]* pd;}}

 /* Single term1 & term2 : single derivative */
```

```
            for(t3=(double)0,i=1;i<=6;i++){
            S3[i]=r[i]* (-DH1(l[i]));
            t3=t3+S3[i];}
/* Constant term : no derivative */
            t4= I1((double)0);
/* Imaginary Total */
            Imfb2=  2*N*N/(PI*ki) * t1
                   +2*pow(N,4)/(PI*ki) * t2
                   -2*Z*2*N*N/(PI*ki) * t3
                   +Z*Z/(PI*ki) * t4;
            printf("\a\nImfb2_ = %f  ",(float) Imfb2);

flg=1;  /* REAL PART  */
/*Real: Squar Terms : single derivative */
for(t1=(double)0,i=1;i<=6;i++){
      pd=DH(l[i]);
      t1=t1+r[i]* (-pd);}
/*Real: Cross Terms : single Two derivative */
for(t2=(double)0,i=1;i<=6;i++){
for(j=1;j<=6;j++){
       pd=D0KJ(l[i],l[j]);
       t2=t2+r[i]* r[j]* pd;}}
/*Real: Single term1 & term2 : single derivative */
for(t3=(double)0,i=1;i<=6;i++){
      pd=DH1(l[i]);
       t3=t3+r[i]* (-pd);}
/*Real: Constant term : no derivative */
      t4= I2((double)0);
/*Real: Total */
Re1fb2=-2*N*N/(PI* PI* ki) * t1
       -2*pow(N,4)/(PI* PI* ki) * t2
       +2*Z*2* N* N/(PI* PI* ki) * t3
       -Z*Z/(PI* PI* ki) * t4;
      printf("\a Re1fb2_ = %f  ",(float) Re1fb2);
  } getch();
}
```

```
/* Calculation of Re2 fB2 for : He-Atom
   HF-parameters, with Normalization constant N^2 A15.c */

# define PI 3.1428
# include<stdio.h>
# include <math.h>
float  h1=.01,  /* h=.01S tep hight for 1st derivative */
int flg,fflg, cd=2;       /* Code no. for He-atom  */
double bi,q;

/* I3(l) I2(l) and I5(l1,l2) integrals */
double I3(l,b)
   double l,b;
{  double f;
   f=1-2/PI * atan(l/b);
   f=-pow(PI,3) * f;return(f);}
double I2(l,b)          /* I2(bi* bi,l* l) */
   double l,b;
{  int sgn;
   double z,q2,b2,l2,A,f;
   q2=q* q; b2=b* b; l2=l* l;
   z=sqrt(pow(l2+q2,2) + 4* q2* b2 );
   if((l2-q2)>0) sgn=1;else sgn=-1;
   A=1-2* b2* pow(l2-q2,2)/(pow(l2+q2,2)* (b2+l2));
   f=1-sgn* ( 1/2.0-1/PI* asin(A) );
   f=-pow(PI,3)/z * f;
   return(f);}

double I5(L1,L2,b)
   double L1,L2,b;
{  int sgn1,sgn2;
   double E1,E2,q2,b2,l1,l2,L,v2,u2,A1,A2,f;
   q2=q* q; b2=b* b; l1=L1* L1; l2=L2* L2; L=l1-l2;
                  v2=b2+l1;  u2=b2+l2;
   if(L+q2>0) sgn1=1;else sgn1=-1;
   if(L-q2>0) sgn2=1;else sgn2=-1;
   E1=sqrt(pow(L+q2,2) + 4* q2* v2);
   E2=sqrt(pow(L-q2,2) + 4* q2* u2);
   A1=1-2* b2* pow(L+q2,2)/((pow(L+q2,2)+4* q2* l1)* v2);
   A2=1-2* b2* pow(L-q2,2)/((pow(L-q2,2)+4* q2* l2)* u2);
   f= ( sgn1* ( 1/(2* E1)-asin(A1)/(PI* E1) )
       -sgn2* ( 1/(2* E2)-asin(A2)/(PI* E2) ) );
   f=-PI* PI* f;
   return(f);}

double FH(x,fhb)
    double x,fhb;
{   double q2,l2,f;
    l2=x* x;q2=q* q;
    if(fflg==1)
    f= I3((double)0)/(l2+q2);
    if(fflg==3)
    f= I2(x,fhb);
    if(fflg==4)
```

```
    f= (I3((double)0,fhb)-I3(x,fhb))/12;
    if(fflg==5)
    f= I3((double)0,fhb); return(f);}

double DB(L)
    double L;
{   double d,b=bi,h=h1;
    d=(-3* FH(L,b) + 4* FH(L,b+h) - FH(L,b+2* h))/(2* h);
    return(d);}

double DXB(x1)
    double x1;
{   double d,          h=0.2; /*step height ok */
    d=(-3* DB(x1) + 4* DB(x1+h) - DB(x1+2* h))/(2* h);
    return(d);}

double FH24(x1,y1,b1)
    double x1,y1,b1;
{   double 12,f;
    12=x1* x1;
    f=(I2(y1,b1)-I5(y1,x1,b1))/12;
    return(f);}
double DB1(dbx1,dby1)
    double dbx1,dby1;
{   double d,b=bi,     h=0.01; /* step height ok */
    d=(-3* FH24(dbx1,dby1,b) + 4* FH24(dbx1,dby1,b+h)
                             - FH24(dbx1,dby1,b+2* h))/(2* h);
    return(d);}
double DXYB(x,y)
    double x,y;
{   double d,          h=0.01;  step height ok
    d=( DB1(x+h,y+h) - DB1(x+h,y-h) - DB1(x-h,y+h)
                                    + DB1(x-h,y-h) )/(4* h* h);
    return(d);}


main(){
int i,j,Z=cd;
float E,t;
float ti,tf,inc;
static double ki,s,N,r[6],l[6];
static double c1,c2,c3,n1,n2,n3,          dE=1.187; /*  a.u. */
static double z1,z2,z3,pd,t1,t2,t3,t4,t5,Re2fb2;
clrscr();

/* Input Energy and angle */
printf("\nEnergy (eV) = "); scanf("%f",&E);
printf("ti = "); scanf("%f",&ti);
printf("tf = "); scanf("%f",&tf);
printf("inc ="); scanf("%f",&inc);
#include "I_E.He"

/* Normalization Constant */
for(s=(double)0,i=1;i<=6;i++) s=s+r[i]/pow(l[i],3);
N= 1/sqrt(2* s);
```

```
printf("\nE = %.2f",E);
ki=sqrt(2* E/27.2);
bi=dE/ki;
printf("\nbi = %.4f",bi);

for(t=ti;t<=tf;t=t+inc){
    printf("\n@ = %.2f ",(float)t);
    q=2* ki* sin(t* PI/360);

/* REAL PART-2 */
/*Real: Squar Terms : single derivative */   fflg=1;
for(t1=(double)0,i=1;i<=6;i++){
     pd=DXB(l[i]);
     t1=t1+r[i]* (-pd);}
/*Real: Cross Terms : single Two derivative */
for(t2=(double)0,i=1;i<=6;i++){
for(j=1;j<=6;j++){
     pd=DXYB(l[i],l[j]);
     t2=t2+r[i]* r[j]* pd;}}
/*Real: Single term1 : single derivative */   fflg=3;
for(t3=(double)0,i=1;i<=6;i++){
     pd=DXB(l[i]);
     t3=t3+r[i]* (-pd);}
/*Real: Single term2 : single derivative */   fflg=4;
for(t4=(double)0,i=1;i<=6;i++){
     pd=DXB(l[i]);
     t4=t4+r[i]* (-pd);}
/*Real: Constant term : no derivative */      fflg=5;
     t5= DB((double)0);
/*Real: Total */
Re2fb2=-N* N/pow(PI* ki,2) * t1
       -pow(N,4)/pow(PI* ki,2) * t2
       +Z* N* N/pow(PI* ki,2) * (t3+t4)
       -Z*Z/pow(PI* ki,2) * t5/2;

     printf("\a Re2fb2_ = %f  \n",(float) Re2fb2);

  } getch();
}
```

'Mathematica' programs :

```
(*Calculation of w,fB1,ImfB2_ for He like +ve ions :
  using HF-3 parameter w.f                    Imfb2.ma*)

Z=2;
Dpol=0.196 10^-24; (* He atom *)
Energy=200;
Theta=1;
"HF -parameters for the Target"

(*Normalization constant*)
Nm=1/Sqrt[2 Sum[r[i]/l[i]^3,{i,1,6}]]; PI=22.0/7;
dp=Dpol/Power[(.529 10^-8),3];
Iw=Nm^2 16 Sum[r[i]/l[i]^5,{i,1,6}];
w=2 Iw/dp
E0=Energy;k=Sqrt[2 E0/27.2];
b=w/k;
t=Theta;
Print["Energy = ",E0," eV"];Print[" "];
Print["t    fB1       ImfB2"];

For[i0=1,t<=40,If[t<=9,t=t+1,t=t+10];i0++,
      q=2 k Sin[t 3.14/(180 2)];

      (*First Born Calculation*)
      fB1p[i0]=Z 2/q^2;
      Ib0=2PI 2/q^2;
      Ib1=Nm^2 2Sum[r[i] l[i]/(l[i]^2+q^2)^2,{i,1,6}];
      fB1e[i0]=-1/(2PI) Ib0 Ib1;
      fB1[i0]=fB1p[i0]+2 fB1e[i0];

      (*function I1[],I4[]; for 2nd Born Calculation*)
      zt[x_]:=Sqrt[(x^2+q^2)^2+4q^2 b^2];
      Clear[n,d];n[x_]:=(q^2+b^2)(zt[x]+q^2+x^2)+2b^2(q^2-x^2);
                        d[x_]:=(b^2+x^2)(zt[x]-q^2-x^2);
      ln1[x_]:=Log[n[x]/d[x]];
      I1[x_]:=PI/zt[x] ln1[x];
      Clear[V,U,E1,n4,d4];
      V[x_]:=(b^2+x^2)^(1/2);
      U[y_]:=(b^2+y^2)^(1/2);
  E1[x_,y_]:=Sqrt[U[y]^4+(q^2+V[x]^2)^2-2 U[y]^2(V[x]^2-q^2)];
  n4[x_,y_]:=(q^2+V[x]^2)(q^2+V[x]^2+E1[x,y])-U[y]^2(V[x]^2-q^2);
      d4[x_,y_]:=U[y]^2(E1[x,y]+V[x]^2-U[y]^2-q^2);
      Clear[ln2,I4];
      ln2[x_,y_]:=Log[n4[x,y]/d4[x,y]];(*0.900726*)
      I4[x_,y_]:=PI/E1[x,y] ln2[x,y];

      Ip[1]=1/(x^2+q^2);
    • S1=Sum[r[i](-D[Ip[1],x]/.x->l[i]),{i,1,6}]I1[0];
      Ip[2]=1/x^2 1/y^2 (I1[0]-I1[x]-I1[y]+I4[x,y]);
      (*Nested sum & Multiple derivative*)
      S2=Sum[r[i]r[j](D[Ip[2],x,y]/.{x->l[i],y->l[j]}),
                                        {i,1,6},{j,1,6}];
```

```
      Ip[3]=1/l1^2 (I1[0]-I1[l1]);
      S3=Sum[r[i](-D[Ip[3],l1]/.l1->l[i]),{i,1,6}];

      Ip[4]=I1[0];

      Imfb2t[1]=2 Nm^2/(PI k) S1;
      Imfb2t[2]=2 Nm^4/(PI k) S2;
      Imfb2t[3]=-2Z 2Nm^2/(PI k) S3;
      Imfb2t[4]=Z^2/(PI k)Ip[4];
      S=Sum[Imfb2t[i],{i,1,4}];
      Print[" "]; Print[t,"  ",fB1[i0],"  ",S];

];

(*Calculation of w,fB1,RefB2_1 HF-3 parameter w.f;
  for He-atom/He like Ions                Refb2t1.ma *)

Z=2;
Dpol=0.196 10^-24;
Energy=200;
Theta=1;
"HF -parameters for the Target"

Nm=1/Sqrt[2 Sum[r[i]/l[i]^3,{i,1,6}]];
PI=22.0/7;
dp=Dpol/Power[(.529 10^-8),3];
Iw=Nm^2 16 Sum[r[i]/l[i]^5,{i,1,6}];
w=2 Iw/dp;
E0=Energy;k=Sqrt[2 E0/27.2];
b=w/k;
t=Theta;
Print["Energy= ",E0," eV"];Print[" "];
Print["t    RefB2_1"];

For[i0=1,t<=40,If[t<=9,t=t+1,t=t+10];i0++,
      q=2 k Sin[t PI/(180 2)];

      (*function I2[],I5[];2nd Born Calculation*)
      Clear[zt,n,n1,n2,d,d1,d2,AS,E1,E2,A1,A2];
      zt[x_]:=Sqrt[(x^2+q^2)^2+4q^2 b^2];
       n[x_]:=2b^2(x^2-q^2)^2;
       d[x_]:=(x^2+q^2)^2(b^2+x^2);
       AS[x_]:=ArcSin[1-n[x]/d[x]];
       I2[x_]:=-PI^3/zt[x](1+(1/2-1/PI AS[x]));
       E1[x_,y_]:=Sqrt[(x^2-y^2+q^2)^2+4q^2(b^2+x^2)];
       E2[x_,y_]:=Sqrt[(x^2-y^2-q^2)^2+4q^2(b^2+y^2)];
       n1[x_,y_]:=2b^2(x^2-y^2+q^2)^2;
       d1[x_,y_]:=((x^2-y^2+q^2)^2+4q^2x^2)(b^2+x^2);
       A1[x_,y_]:=1-n1[x,y]/d1[x,y];
       n2[x_,y_]:=2b^2(x^2-y^2-q^2)^2;
       d2[x_,y_]:=((x^2-y^2-q^2)^2+4q^2y^2)(b^2+y^2);
       A2[x_,y_]:=1-n2[x,y]/d2[x,y];

      Clear[I2,Ipr1];
      For[S1=0;S3=0;i=1,i<=6,i++,
```

```
            sgn=If[(l[i]^2-q^2)>0,1,-1];
            I2[x_]:=-PI^3/zt[x](1- sgn(1/2-1/PI AS[x]));
            Ipr1[1]=1/(x^2+q^2)I2c;
            S1=S1+r[i](-D[Ipr1[1],x]/.x->l[i]);
            Ipr1[3]=1/x^2(I2c-I2[x]);
            S3=S3+r[i](-D[Ipr1[3],x]/.x->l[i]);
          ];

      Clear[I2x,I2y,I5];
      (*Nested sum & Multiple derivative*)

      For[S2=0;i=1,i<=6,i++,
            sgnx=If[l[i]^2-q^2>0,1,-1];
            I2x[x_]:=-PI^3/zt[x](1- sgnx(1/2-1/PI AS[x]));
            For[j=1,j<=6,j++,
                  sgny=If[l[j]^2-q^2>0,1,-1];
                  I2y[x_]:=-PI^3/zt[x](1- sgny(1/2-1/PI AS[x]));
                  sgn1=If[(l[i]^2-l[j]^2+q^2)>0,1,-1];
                  sgn2=If[(l[i]^2-l[j]^2-q^2)>0,1,-1];
         I5[x_,y_]:=-PI^2( sgn1/E1[x,y](1/2-ArcSin[A1[x,y]]/PI)
                        -sgn2/E2[x,y](1/2-ArcSin[A2[x,y]]/PI));
         Ipr1[2]=1/x^2 1/y^2 (I2c-I2x[x]-I2y[y]+I5[x,y]);
         S2=S2+r[i]r[j](D[Ipr1[2],x,y]/.{x->l[i],y->l[j]});
                  ];
            ];

      Ipr1[4]=I2[0];
      Clear[S,Refb2t];
      Refb2t[1]=-2 Nm^2/(PI^2 k) S1;
      Refb2t[2]=-2 Nm^4/(PI^2 k) S2;
      Refb2t[3]=+2Z 2Nm^2/(PI^2 k) S3;
      Refb2t[4]=-Z^2/(PI^2 k)Ipr1[4];
      S=Sum[Refb2t[i],{i,1,4}];
      Print[" "]; Print[t,"  ",fB1[i0],"  ",S];

    ];
```

```
(*Calculation of w,Re2 fB2 for He like +ve ions atom;
  HF-3 parameter w.f:                          Refb2t2.ma*)

Z=2;
Dpol=0.196 10^-24; (* He-atom*)
Energy=200;
Theta=1;
"HF -parameters for the Target"

Nm=1/Sqrt[2 Sum[r[i]/l[i]^3,{i,1,6}]];
PI=22.0/7;
dp=Dpol/Power[(.529 10^-8),3];
Iw=Nm^2 16 Sum[r[i]/l[i]^5,{i,1,6}];w=2 Iw/dp;
E0=Energy;k=Sqrt[2 E0/27.2];t=Theta;
Print["Energy= ",E0," eV"];Print[" "];
Print["t     RefB2_2"];
```

```
For[i0=1,t<=40,If[t<10,t=t+1,t=t+10];i0++,
      q=2 k Sin[t 3.14/(180 2)];
      (*function I2[],I3[],I4[] for 2nd Born Calculation*)
      Clear[b,zt,n,n1,n2,d,d1,d2,AS,E1,E2,A1,A2];
      zt[b_,x_]:=Sqrt[(x^2+q^2)^2+4q^2 b^2];
       n[b_,x_]:=2b^2(x^2-q^2)^2;
       d[b_,x_]:=(x^2+q^2)^2(b^2+x^2);
      AS[b_,x_]:=ArcSin[1-n[b,x]/d[b,x]];
      E1[b_,x_,y_]:=Sqrt[(x^2-y^2+q^2)^2+4q^2(b^2+x^2)];
      E2[b_,x_,y_]:=Sqrt[(x^2-y^2-q^2)^2+4q^2(b^2+y^2)];
       n1[b_,x_,y_]:=2b^2(x^2-y^2+q^2)^2;
       d1[b_,x_,y_]:=((x^2-y^2+q^2)^2+4q^2x^2)(b^2+x^2);
       A1[b_,x_,y_]:=1-n1[b,x,y]/d1[b,x,y];
       n2[b_,x_,y_]:=2b^2(x^2-y^2-q^2)^2;
       d2[b_,x_,y_]:=((x^2-y^2-q^2)^2+4q^2y^2)(b^2+y^2);
       A2[b_,x_,y_]:=1-n2[b,x,y]/d2[b,x,y];
       Clear[I3,Ipr1];
       I3[x_,b_]:=-PI^3(1-2/PI ArcTan[x/b]);
       Ipr2[1]=1/(x^2+q^2)I3[0,b];
       Ipr2[4]=(I3[0,b]-I3[x,b])/x^2;
       Clear[I2];
       For[S1=0;S3=0;S4=0;i=1,i<=6,i++,
              sgn=If[(l[i]^2-q^2)>0,1,-1];
              I2[x_,b_]:=-PI^3/zt[b,x](1- sgn(1/2-1/PI AS[b,x]));
              Ipr2[3]=I2[x,b];
              S1=S1+r[i](-D[Ipr2[1],x,b]/.{x->l[i],b->w/k});
              S3=S3+r[i](-D[Ipr2[3],x,b]/.{b->w/k,x->l[i]});
              S4=S4+r[i](-D[Ipr2[4],x,b]/.{b->w/k,x->l[i]});
            ];
      Clear[I2y,I5];
      (*Nested sum & Multiple derivative*)
      For[S2=0;i=1,i<=6,i++,
          For[j=1,j<=6,j++,
            sgny=If[(l[j]^2-q^2)>0,1,-1];
            I2y[b_,y_]:=-PI^3/zt[b,y](1- sgny(1/2-1/PI AS[b,y]));
            sgn1=If[(l[j]^2-l[i]^2+q^2)>0,1,-1];
            sgn2=If[(l[j]^2-l[i]^2-q^2)>0,1,-1];
   I5[b,x_,y_]:=-PI^2( sgn1/E1[b,x,y](1/2-ArcSin[A1[b,x,y]]/PI)
                      -sgn2/E2[b,x,y](1/2-ArcSin[A2[b,x,y]]/PI));
   Ipr2[2]=1/x^2 (I2y[b,y]-I5[b,x,y]);
   S2=S2+r[i]r[j](D[Ipr2[2],b,x,y]/.{b->w/k,x->l[i],y->l[j]});

          ];
        ];
      Ipr2[5]=D[I3[0,b],b]/.b->w/k;

      Refb2t[1]=-Nm^2/(PI^2 k^2) S1;
      Refb2t[2]=-Nm^4/(PI^2 k^2) S2;
      Refb2t[3]=Z Nm^2/(PI^2 k^2)(S3+S4);
      Refb2t[4]=-Z^2/(PI^2 k^2)Ipr2[5]/2;
      S=Sum[Refb2t[i],{i,1,4}];
      Print[" "];
      Print[t,"  ",S];

];
```

3.8 TABLES :

Table 3.1 : He-atom

Behavior of the Born scattering amplitudes: [eq. 3.2.8 ,3.4.10, 3.4.19, 3.6.3, 3.3.22, 3.6.4]
In ESGSHe process with: Hartree-Fock.wave functions.

θ (deg.)	E=200 eV f_{B1}	Re1$\bar{f}_{B2}$	Re2$\bar{f}_{B2}$	g_{och}	Im$\bar{f}_{B2}$	***Rao & Desai*** ***DCS***	Present work : *DCS (a.u)* 200 eV	1000 eV	2000 eV
2	0.7821	1.9989	-5.6311	-0.1355	0.9370		9.7919	0.6464	0.6143
4	0.7753	0.7155	-1.2675	-0.1341	0.8836		0.7888	0.6227	0.5153
6	0.7644	0.4057	-0.4609	-0.1318	0.8115		0.9920	0.5275	0.3983
8	0.7496	0.2601	-0.1820	-0.1287	0.7341		1.0275	0.4356	0.2944
10	0.7313	0.1750	-0.0571	-0.1249	0.6597	1.3113	0.9599	0.3541	0.2123
15	0.6741	0.0714	0.0542	-0.1131	0.5063		0.7278	0.2039	0.0911
20	0.6073	0.0324	0.0864	-0.0994	0.4003	0.6093	0.5529	0.1167	0.0426
25	0.5386	0.0179	0.1017	-0.0856	0.3294		0.4363	0.0679	0.0222
30	0.4731	0.0133	0.1118	-0.0727	0.2816	0.3126	0.3555	0.0429	0.0128
35	0.4138	0.0122	0.1182	-0.0612	0.2486		0.2951	0.0285	0.0081
40	0.3618	0.0122	0.1213	-0.0514	0.2247	0.1863	0.2475	0.0201	0.0054

Table 3.2 : He-atom

Behavior of the Born scattering amplitudes:
In ESGSHe process with: Hartree-Fock.wave functions.

θ (deg.)	E=400 eV f_{B1}	Re1$\bar{f}_{B2}$	Re2$\bar{f}_{B2}$	g_{och}	Im$\bar{f}_{B2}$	***Rao & Desai*** ***DCS***	Present work : *DCS (a.u)* 400 eV	4000 eV	10,000 eV
2	0.7798	0.6360	-1.3979	-0.0675	0.7258		0.5293	0.5622	0.4714
4	0.7666	0.2250	-0.2792	-0.0661	0.6213		0.8037	0.4101	0.2434
6	0.7454	0.1090	-0.0749	-0.0639	0.5193		0.7817	0.2664	0.1111
8	0.7176	0.0581	-0.0073	-0.0610	0.4359		0.6904	0.1645	0.0517
10	0.6846	0.0324	0.0209	-0.0576	0.3706	0.6760	0.6001	0.1009	0.0260
15	0.5897	0.0090	0.0446	-0.0479	0.2639		0.4241	0.0327	0.0065
20	0.4931	0.0048	0.0537	-0.0383	0.2057	0.2899	0.3058	0.0131	0.0023
25	0.4066	0.0050	0.0588	-0.0299	0.1720		0.2236	0.0062	0.0010
30	0.3346	0.0055	0.0607	-0.0232	0.1506	0.1319	0.1653	0.0034	0.0006
35	0.2767	0.0058	0.0524	-0.0180	0.1353		0.1187	0.0021	0.0003
40	0.2308	0.0056	0.0536	-0.0140	0.1233	0.0660	0.0914	0.0014	0.0002

Table 3.3 : Li^{+1} – *Ion*

Behavior of the Born scattering amplitudes: [eq. 3.2.8 ,3.4.10, 3.4.19, 3.6.3, 3.3.22, 3.6.4]
In ESGS Li^{+1} process with: Hartree-Fock.wave functions.

θ	$E=200$ eV					Present work : *DCS (a.u)*				
(deg.)	f_{B1}	Re1$\bar{f}_{B2}$	Re2$\bar{f}_{B2}$	g_{och}	Im$\bar{f}_{B2}$	200 eV	400 eV	1000 eV	4000 eV	10,000 eV
2	112.04	10.900	-10.449	-0.1358	0.9472	12,624	3,566	657.63	46.959	8.0359
4	28.239	4.8688	-2.4717	-0.1353	0.9377	931.17	276.12	53.426	4.0561	0.8437
6	12.720	3.1527	-0.9943	-0.1344	0.9226	218.22	67.151	13.307	1.1411	0.2674
8	7.2861	2.3355	-0.4780	-0.1332	0.9026	82.003	25.914	5.2525	0.5035	0.1200
10	4.7695	1.8513	-0.2402	-0.1316	0.8788	39.822	12.825	2.6666	0.2744	0.0627
15	2.2777	1.2008	-0.0102	-0.1265	0.8091	11.823	3.9143	0.8635	0.0899	0.0173
20	1.3971	0.8695	0.0638	-0.1198	0.7355	5.4273	1.8217	0.4132	0.0383	0.0065
25	0.9813	0.6702	0.0930	-0.1122	0.6660	3.1081	1.0494	0.2362	0.0191	0.0030
30	0.7481	0.5394	0.1056	-0.1039	0.6041	2.0270	0.6837	0.1489	0.0107	0.0016
35	0.6011	0.4484	0.1115	-0.0954	0.5504	1.4383	0.4812	0.0991	0.0065	0.0009
40	0.5003	0.3822	0.1143	-0.0871	0.5043	1.0820	0.3566	0.0698	0.0042	0.0006

Table 3.4 : ***Be^{+2} – Ion***

Behavior of the Born scattering amplitudes:
In ESGS Be^{+2} process with: Hartree-Fock.wave functions.

θ (deg.)	E=200 eV f_{B1}	Re1$\bar{f}_{B2}$	Re2$\bar{f}_{B2}$	g_{och}	Im$\bar{f}_{B2}$	Present work : DCS (a.u) 200 eV	400 eV	1000 eV	4000 eV	10,000 eV
2	223.63	19.826	-12.8889	-0.1359	0.7556	53,101	14,502	2,637.2	198.43	32.202
4	56.041	9.0452	-3.0886	-0.1356	0.7534	3,827.5	1,096.1	213.14	15.751	2.5569
6	25.005	5.8837	-1.2720	-0.1352	0.7498	869.73	259.12	52.210	3.7701	0.6491
8	14.142	4.3765	-0.6362	-0.1345	0.7449	315.54	97.056	19.838	1.4341	0.2595
10	9.1135	3.4914	-0.3425	-0.1337	0.7387	147.65	46.558	9.5424	0.7008	0.1297
15	4.1453	2.3228	-0.0554	-0.1309	0.7184	39.978	13.087	2.6596	0.2029	0.0362
20	2.4041	1.7343	0.0408	-0.1272	0.6927	16.898	5.6107	1.1303	0.0854	0.0141
25	1.5956	1.3751	0.0820	-0.1227	0.6636	9.0259	3.0029	0.5995	0.0432	0.0066
30	1.1541	1.1317	0.1024	-0.1175	0.6327	5.5564	1.8402	0.3624	0.0245	0.0035
35	0.8857	0.9559	0.1134	-0.1120	0.6015	3.7585	1.2338	0.2384	0.0151	0.0021
40	0.7095	0.8233	0.1196	-0.1062	0.5710	2.7169	0.8813	0.1664	0.0099	0.0013

Table 3.5 : B^{+3} – *Ion*

Behavior of the Born scattering amplitudes:
In ESGS B^{+3} process with: Hartree-Fock.wave functions.

θ (deg.)	E=200 eV f_{B1}	Re1$\bar{f}_{B2}$	Re2$\bar{f}_{B2}$	g_{och}	Im$\bar{f}_{B2}$	Present work : DCS (a.u) 200 eV	400 eV	1000 eV	4000 eV	10,000 eV
2	335.32	27.323	-16.307	-0.1359	0.5914	119,852	32,259	5,810.7	450.20	77.200
4	83.925	12.421	-3.9527	-0.1358	0.5908	8,511.8	2,395.6	463.77	37.147	5.9073
6	37.371	8.0499	-1.6606	-0.1355	0.5896	1,903.5	556.85	113.34	8.8182	1.3840
8	21.077	5.9720	-0.8579	-0.1351	0.5880	679.27	205.42	43.163	3.2394	0.5158
10	13.535	4.7575	-0.4865	-0.1346	0.5860	312.63	97.245	20.798	1.5178	0.2460
15	6.0859	3.1698	-0.1206	-0.1328	0.5792	81.375	26.652	5.7378	0.4039	0.0661
20	3.4777	0.5700	-0.1305	2.3839	0.0058	33.236	11.220	2.3736	0.1638	0.0259
25	2.2695	1.9109	0.0625	-0.1276	0.5589	17.248	5.9099	1.2213	0.0821	0.0123
30	1.6124	0.5463	-0.1242	1.5929	0.0915	10.364	3.5665	0.7197	0.0466	0.0067
35	1.2153	1.3634	0.1074	-0.1204	0.5326	6.8662	2.3569	0.4648	0.0289	0.0040
40	0.9567	1.1896	0.1165	-0.1164	0.5182	4.8753	1.6618	0.3204	0.0190	0.0025

Table 3.6 : C^{+4} – ***Ion***

Behavior of the Born scattering amplitudes:
In ESGS C^{+4} process with: Hartree-Fock.wave functions.

θ (deg.)	E=200 eV f_{B1}	Re1$\bar{f}_{B2}$	Re2$\bar{f}_{B2}$	g_{och}	Im$\bar{f}_{B2}$	Present work : DCS (a.u) 200 eV	400 eV	1000 eV	4000 eV	10,000 eV
2	447.02	32.874	-17.318	-0.1360	0.4607	213,855	56,676	10,084	781.81	141.12
4	111.84	14.908	-4.2180	-0.1358	0.4605	14,980	4,137.9	789.87	66.349	11.111
6	49.766	9.6397	-1.7842	-0.1357	0.4600	3,304.9	946.99	190.93	16.130	2.5569
8	28.041	7.1382	-0.9315	-0.1354	0.4594	1,163.9	344.49	72.369	5.9631	0.9244
10	17.985	5.6785	-0.5367	-0.1350	0.4587	528.85	161.08	34.854	2.7779	0.4284
15	8.0537	3.7774	-0.1472	-0.1339	0.4561	133.61	43.090	9.6714	0.7156	0.1105
20	4.5772	2.8434	-0.0117	-0.1322	0.4525	53.154	17.847	4.0174	0.2823	0.0429
25	2.9677	2.2860	0.0500	-0.1302	0.4481	26.967	9.3030	2.0650	0.1394	0.0206
30	2.0931	1.9145	0.0825	-0.1279	0.4429	15.895	5.5772	1.2116	0.0789	0.0112
35	1.5654	1.6483	0.1011	-0.1252	0.4370	10.364	3.6699	0.7781	0.0488	0.0067
40	1.2225	1.4478	0.1122	-0.1223	0.4306	7.2625	2.5799	0.5336	0.0323	0.0043

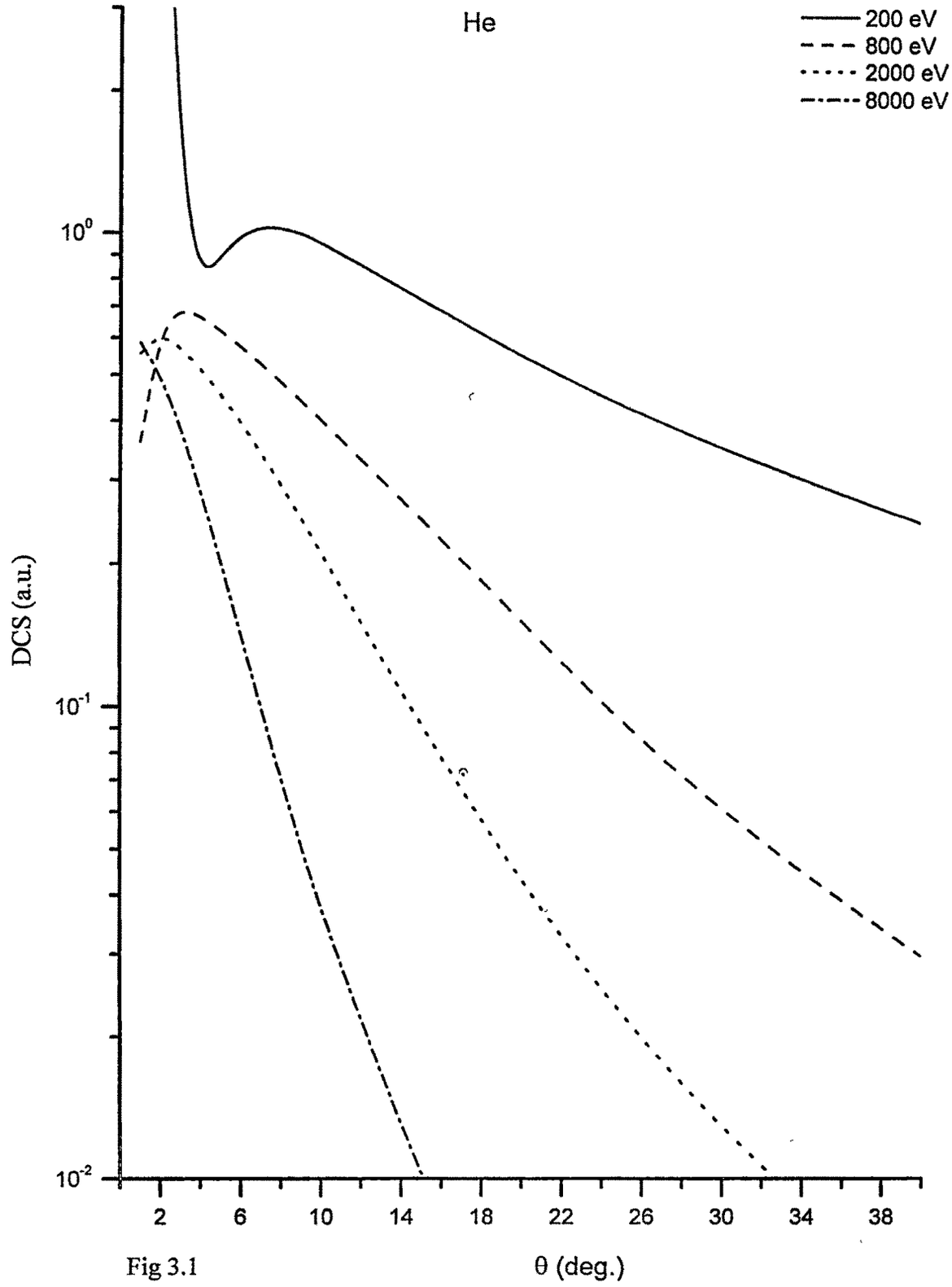
He
200 eV
800 eV
2000 eV
8000 eV
DCS (a.u.)
10^0
10^{-1}
10^{-2}
2
6
10
14
18
22
26
30
34
38
θ (deg.)

Fig 3.1

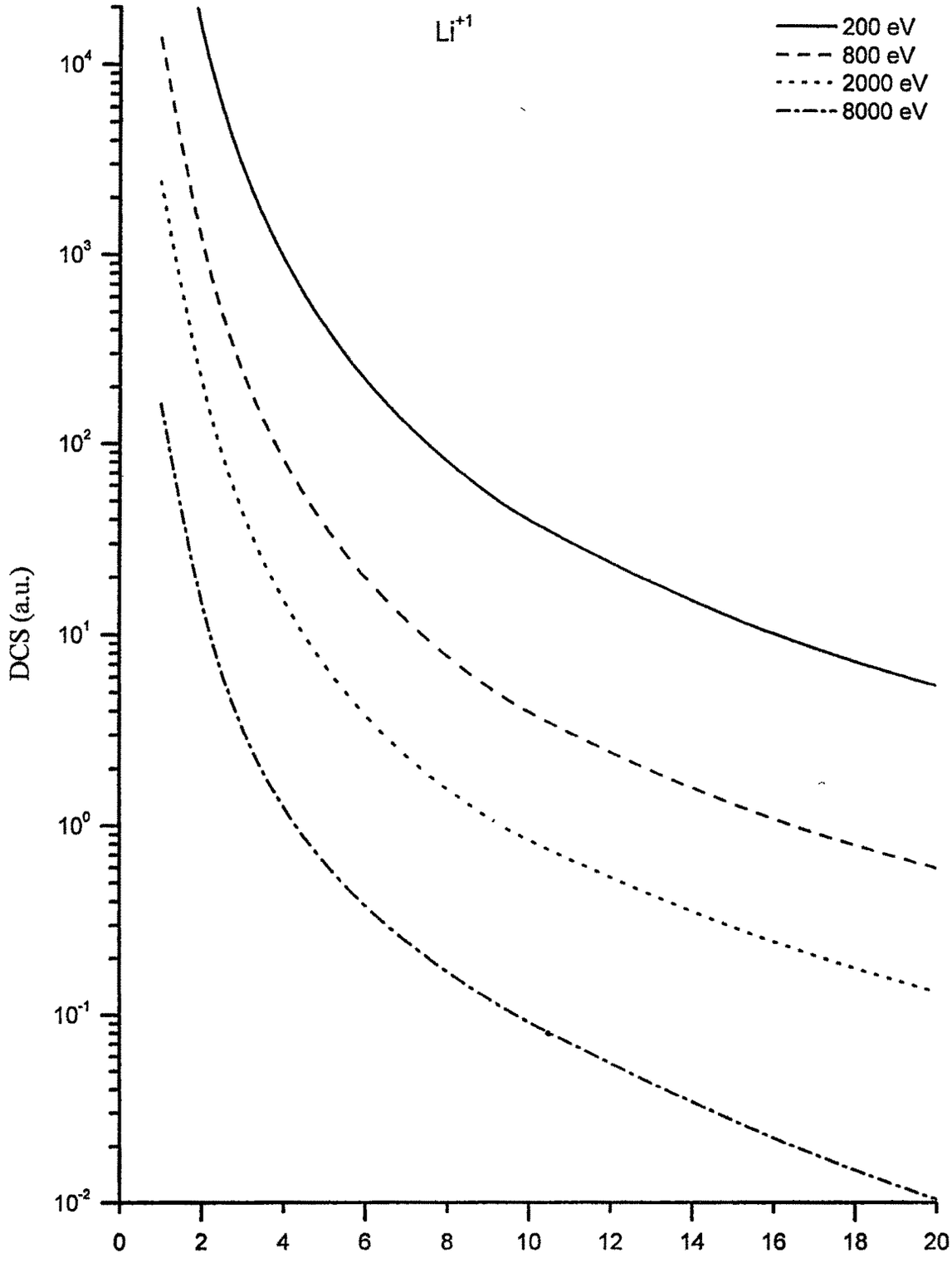
Li+1
200 eV
800 eV
2000 eV
8000 eV
DCS (a.u.)
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
0
2
4
6
8
10
12
14
16
18
20
θ (deg.)

Fig 3.2

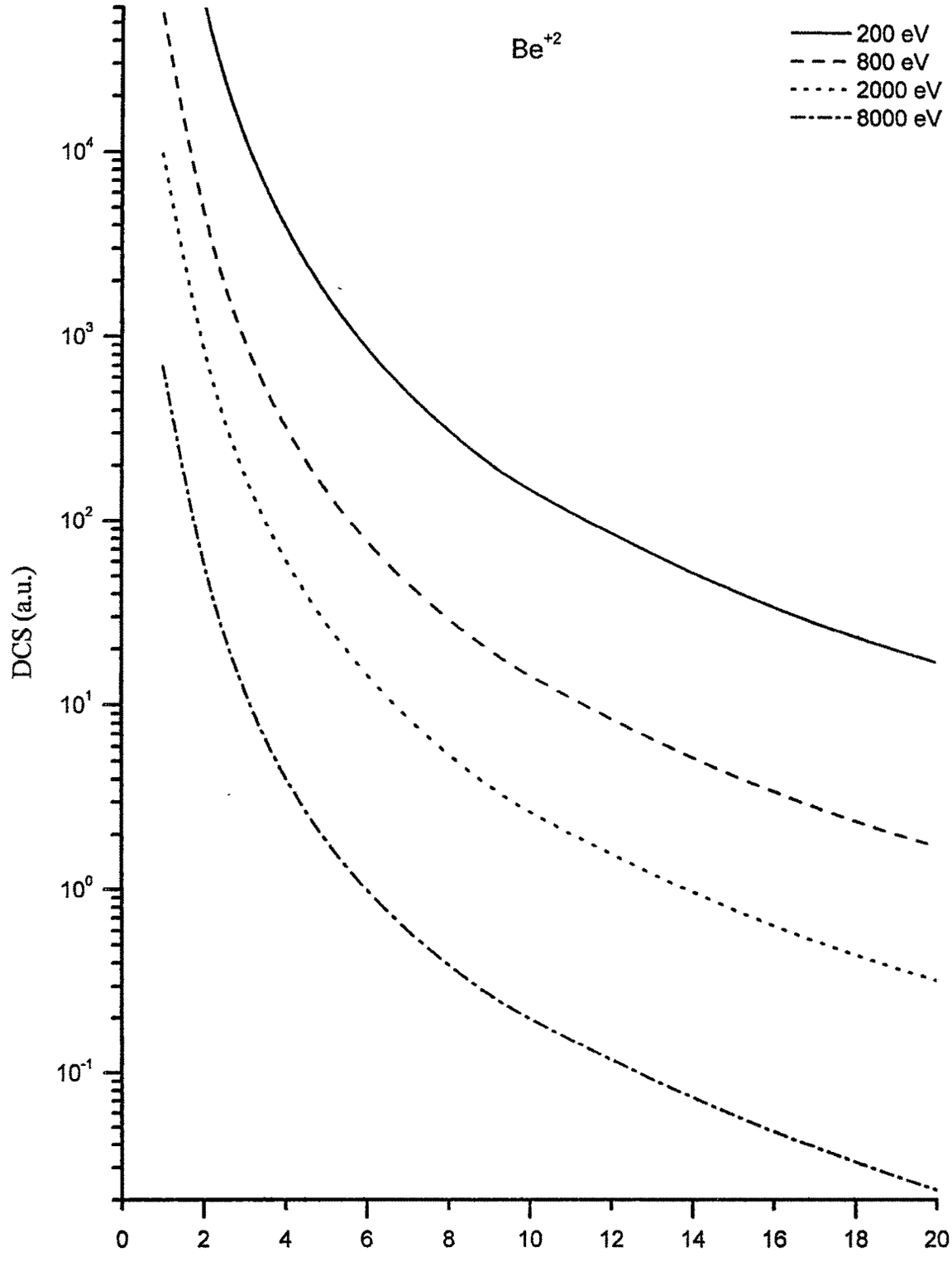
Be+2
200 eV
800 eV
2000 eV
8000 eV
DCS (a.u.)
10^4
10^3
10^2
10^1
10^0
10^-1
0
2
4
6
8
10
12
14
16
18
20
θ (deg.)

Fig 3.3

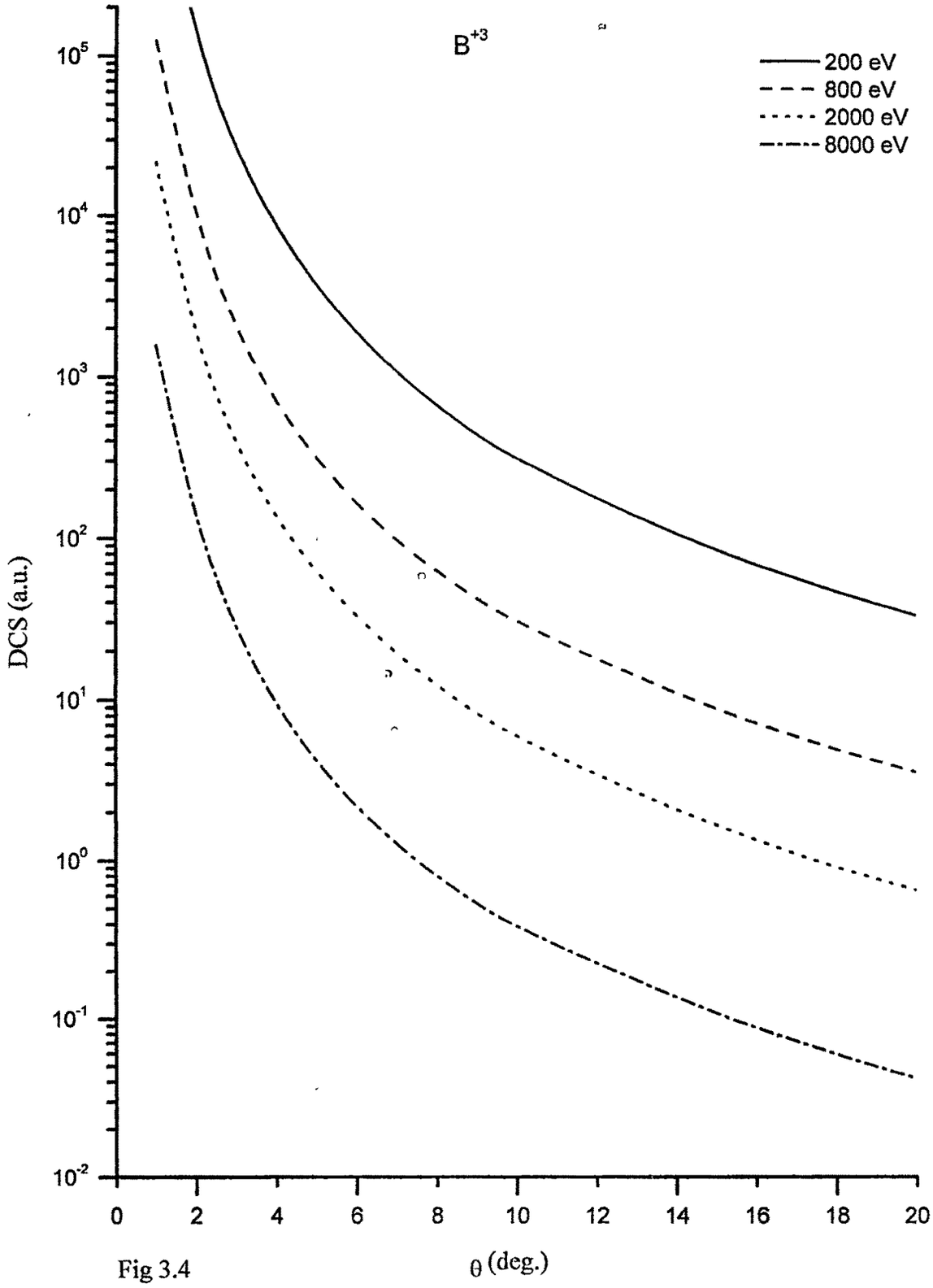
B+3
200 eV
800 eV
2000 eV
8000 eV
DCS (a.u.)
10^5
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
0
2
4
6
8
10
12
14
16
18
20
θ (deg.)

Fig 3.4

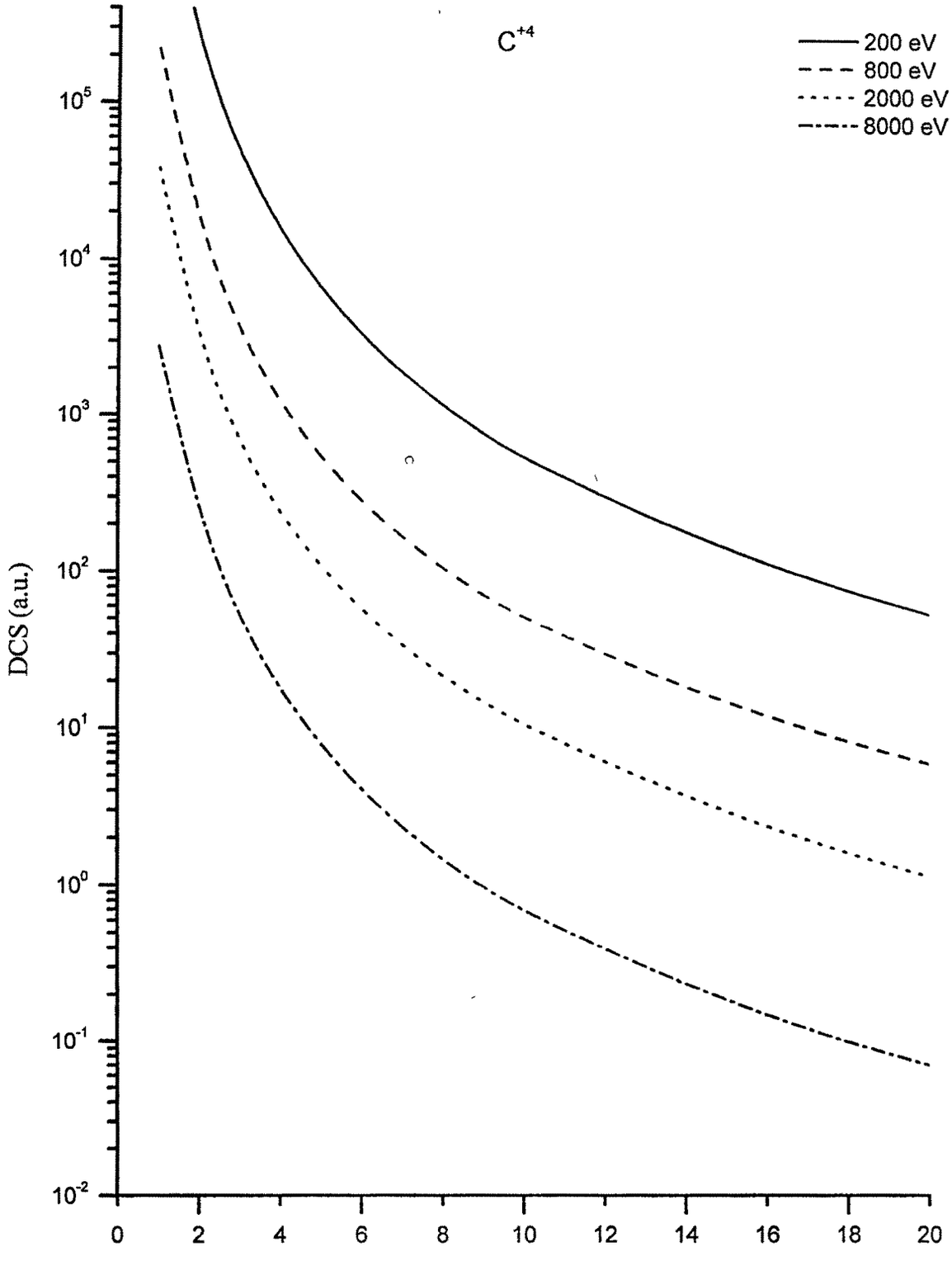
C+4
200 eV
800 eV
2000 eV
8000 eV
DCS (a.u.)
10^5
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
0
2
4
6
8
10
12
14
16
18
20
θ (deg.)

Fig 3.5

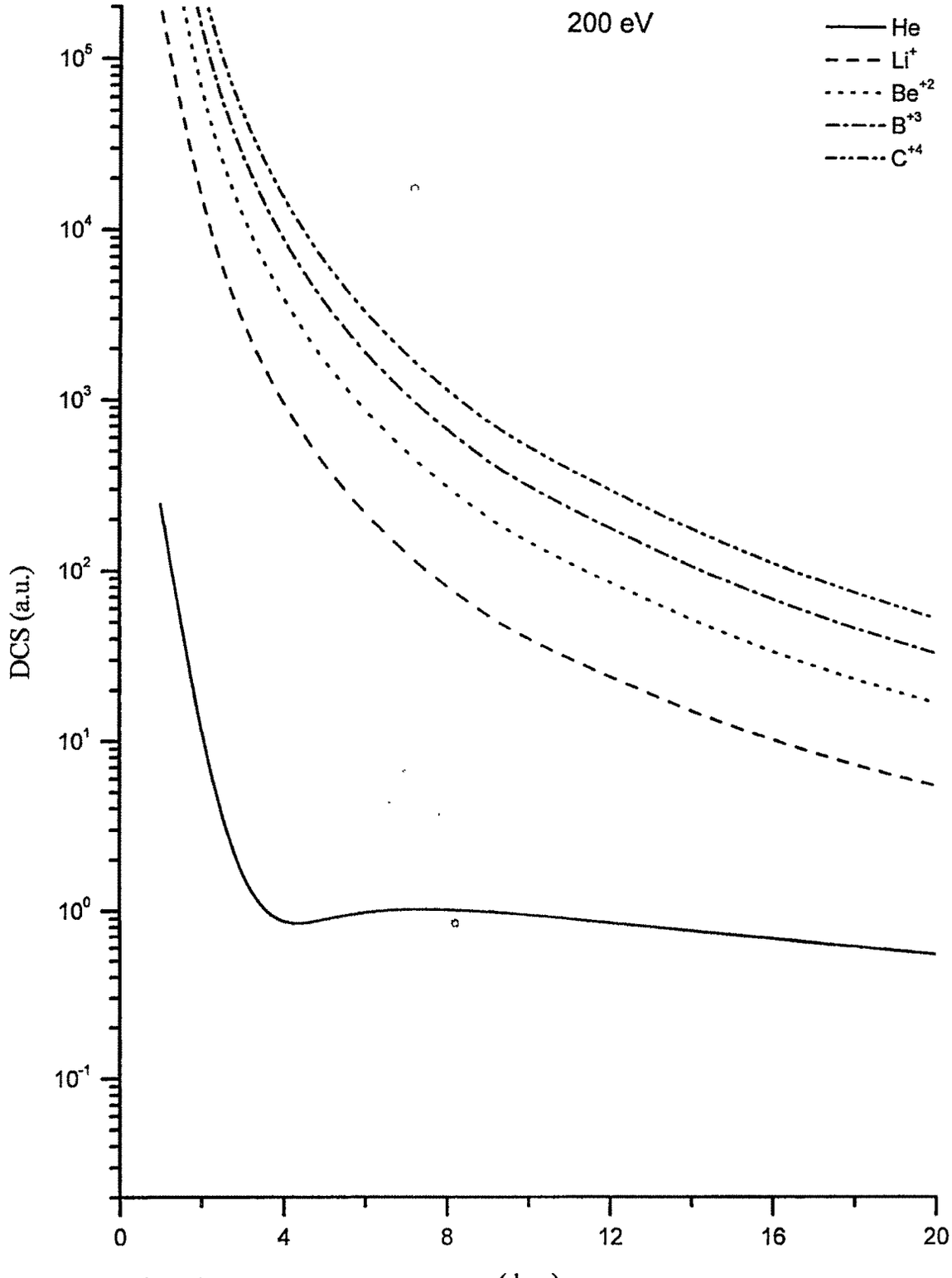
200 eV
He
Li+
Be+2
B+3
C+4
DCS (a.u.)
10^6
10^4
10^3
10^2
10^1
10^0
10^-1
0
4
8
12
16
20
θ (deg.)

Fig 3.6

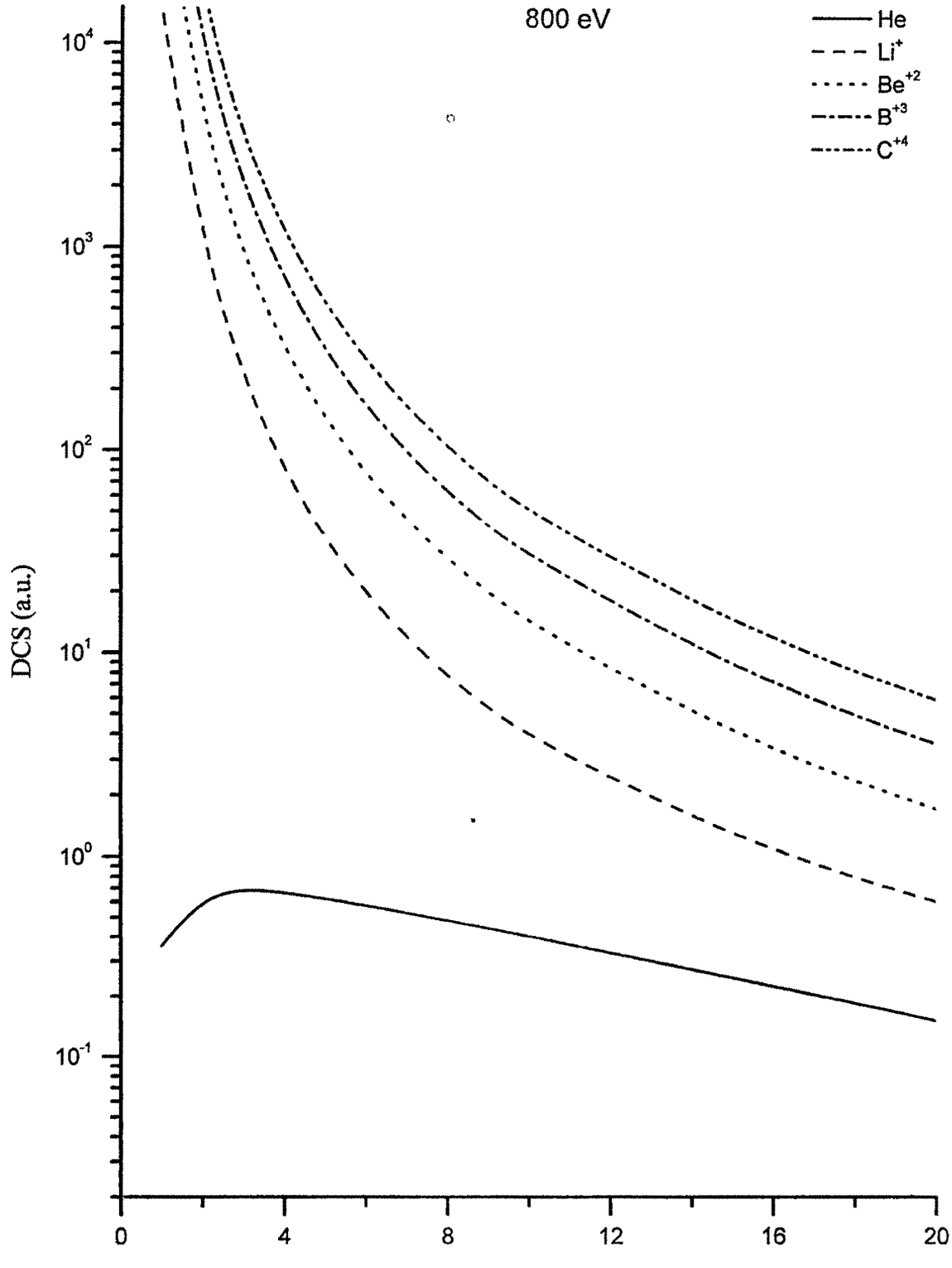
800 eV
He
Li+
Be+2
B+3
C+4
DCS (a.u.)
10^4
10^3
10^2
10^1
10^0
10^-1
0
4
8
12
16
20
θ (deg.)

Fig 3.7

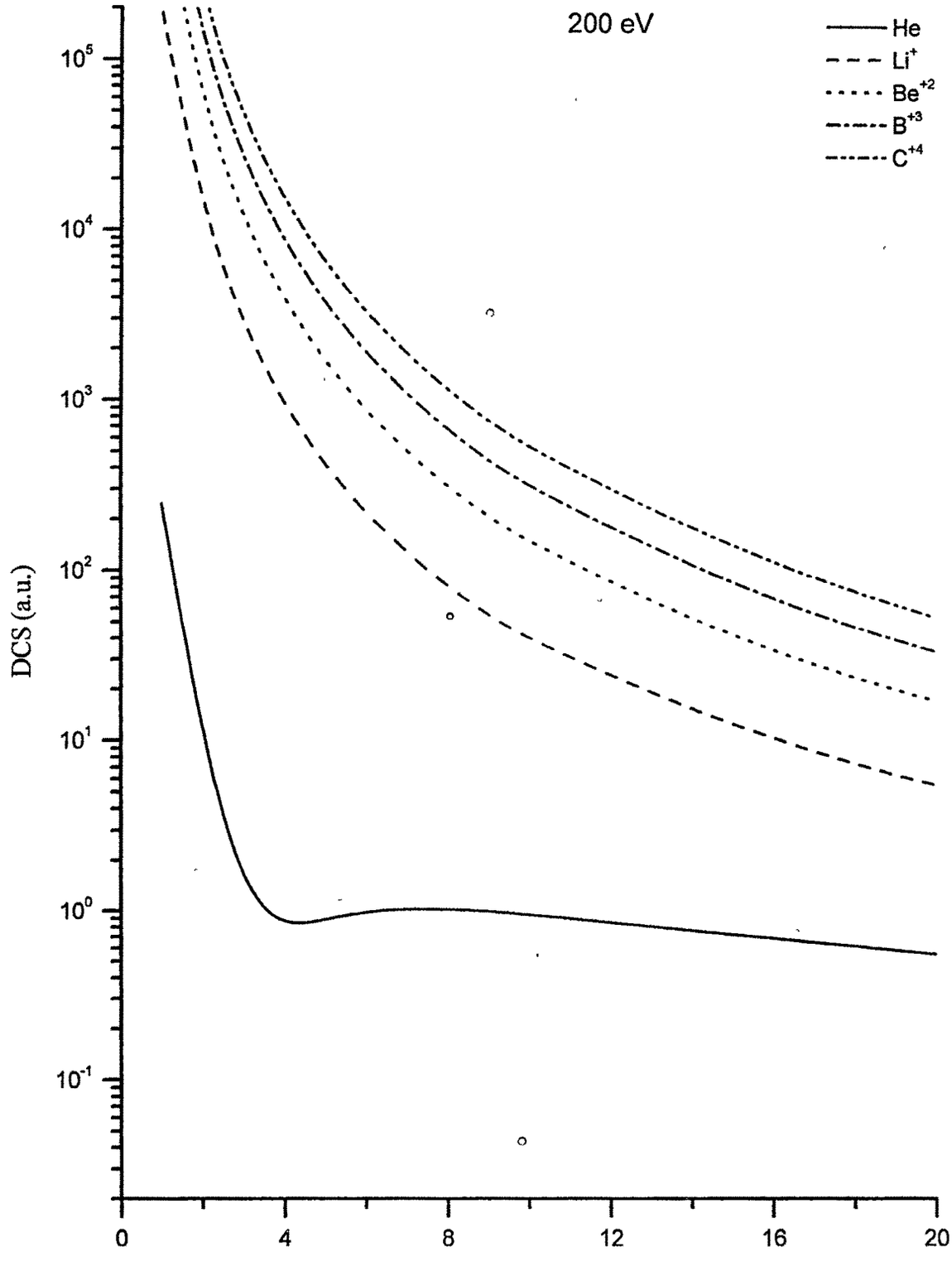
200 eV
He
Li+
Be+2
B+3
C+4
DCS (a.u.)
10^5
10^4
10^3
10^2
10^1
10^0
10^-1
0
4
8
12
16
20
θ (deg.)

Fig 3.8

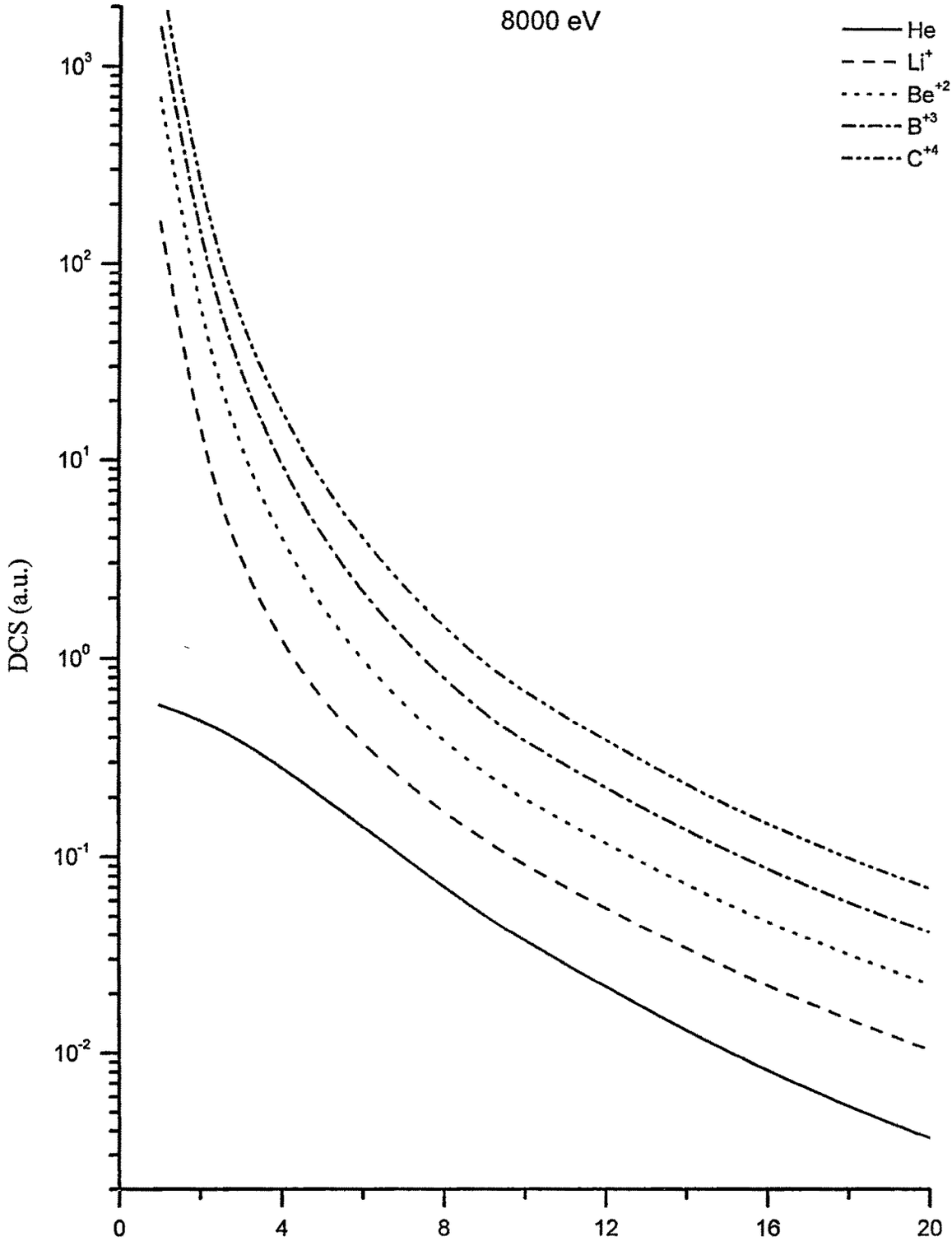
8000 eV
He
Li+
Be+2
B+3
C+4
DCS (a.u.)
10^3
10^2
10^1
10^0
10^-1
10^-2
0
4
8
12
16
20
θ(deg.)

Fig 3.9

3.10 RESULTS AND DISCUSSIONS :

Using the scattering amplitudes equation (3.2.8, 3.4.10, 3.4.19, 3.6.3, 3.3.22) the DCS (3.6.4) have been calculated at incident energies E=200, 400,800,1000 ,2000, 4000,8000 and 10,000 eV. Average excitation energy needed for second Born terms is obtained by the exact calculation (3.5.5) based on the target wave functions [58] and accurate experimental & theoretical values of polarizibility [59]. It is given in table-2 in atomic unit. The results calculated at 200eV and 400eV for ESGHe process are presented in tables (3.1,3.2) along with the theoretical data given by N.S.Rao [19]. Rao has compared his data with experimental results of Crooks et al & Register et al. [51-52]. Our results are found in good agreement with the compared data as well as these experimental data. Present DCS can be compared at different energies from the table up to 40°, indicate change in the behavior of DCS with respect to angle and energy. Similarly the results for ESGHe like +ve ions are presented in the following tables 3-3 to 3.6 are in agreement with ionic behavior to DCS. The results given in the tables are also displayed graphically in fig. 3.1 to 3.8. for different targets and energies. The details of our comparisons are as follows.

The present results in table 3.1 & 3.2 are slightly more than that of Rao, but it matches with the experimental data of Croors et al. These agreement verifies our HHOB results for He atom. Thus the HHOB theory so far applied in the case of Li^{+1}, Be^{+2}, B^{+3} and C^{+4} ions is found to be valid. In the other way more general formulation done for scattering amplitudes in the present work is correct. The general characteristics of DCS for He (atom) and He like ions (ion) are maintained properly. Final checking of present results is the marching of each term of column two to column six with those given by Rao. Accuracy of last three columns depends on the HHOB approximation, which is well applied at higher energies.

In the case of *He atom*: Contribution of real part is maximum at lower angle up to 3° then it decreases faster than first Born. The special behavior of the DCS is observed within 10° at 200 eV and 6° at 400 eV with a small peak. It is also clear from fig. 3.1, that the peak is shifting towards 0° angle as energy increases. Finally the peak is disappeared nearly at 8 keV incident energy. The peak in the lower angular range is due to fluctuations in $\mathrm{Re}\,2\bar{f}_{B2}$ within the region. At 200 eV for He atom DCS first decreases than increases

and again decreases, which is quite different from ionic behavior. At 5° onwards rate of decrease in DCS increases with energy (fig.3.1)

In case of the *ions* : For a given angle and energy DCS for He like ion is more than He atom. Exchange effect is higher than the He atom.(table 3.3-3.6). As energy increases DCS decreases faster. At 0° angle DCS is large but finite. Fluctuation in $\mathrm{Re}\,\bar{f}_{B2}$ is observed as in case of He atom but it is not effective to DCS because of higher value of f_{B1}. Within 5° DCS decrease suddenly, then after it decreases slowly (fig. 3.2 to 3.5). Table 3.3 – 3.6 indicates that DCS increases with increasing nuclear charge. The results can be compared at different energies for each ion from fig. 3.2 - 3.5. (i) For a particular ion DCS increases rapidly as incident angle decreases. (ii) Parallel behaviour of graphs after 8° angle show that rate of decreases in DCS is same for all energies and ions.

Behaviour of DCS for He atom with its iso electronic series is interesting within 0° - 3° at different energies. At 200 eV there exist sharp decrease in DCS, which is similar to that of ion. At 800 eV DCS first increases and then decreases which is dissimilar to the ionic case. At 2000 eV DCS increase by very small value, which start decreasing then onwards. At 8000 eV DCS decreases from the fixed small value. It is cleared from the figures that the variation in DCS is more in small angle region.

Table 3.1 – 3.6 exhibit the individual terms of the present HHOB scattering amplitude at 200 eV. Where the real part of second Born term account for polarization effect and absorption effects are taken care of by the imaginary term. Thus tables and Figures give the complete analysis of behaviour of DCS with different angle and energies except the experimental results, which are not currently available.