CHAPTER - III

ELASTIC SCATTERING OF ELECTRONS BY NEON ATOM USING THE HHOB THEORY.

INTRODUCTION :

In this chapter we discuss the HHOB theory to study the elastic scattering of electron by - Ne atom. A number of fairly accurate measurements of the aboslute differential cross sections for the elastic scattering of electron by neon atom at low, intermediate and high energies have become avaliable (Bromberg 1964, Fink and Yates 197Ø, Crooks 1972, Oda et al 1972, Furness and McCarthy 1973, M.Inokuti and M R C McDowells 1974, Byron and Joachain 1974a, 1976, 1977, Bromberg, 1974, 1975 as quoted by Jansen et al 1976, Gupta and Rees 1975, Williams and Crowe 1975, Kurepa and Vuskovic 1975, Jansen et al 1976, D P Dewangan and H R J Walters 1976, Du Bois and Rudd 1976, Jhanwer and Khare 1976, Riley and Truhlar 1975, 1976, Bransden et al 1976, F J de Heer et al 1978, Bonham and Konaka 1978, B L Jhanwer et al 1978, R W Wagenaar and F J de Heer 198Ø, W C Fon and K A Berrington 198Ø, Kaupilla et al 1981, D.A.Kohl and M.M. Arvedson 1981, D F C Brewer et al 1981, D.Thirumalai and D.G.Truhlar 1982, Y D Kaushik et al 1982, G. Staszewska et al 1983, R P Mc Eachran and A D Stauffer

1983, Coffman and Fink 1985 ,S Y Uousif and J A D Matthew 1986); hence its theoretical study is of interest.

Calculation of the phaseshift using the partial wave analysis method using the static interaction is also reported by many.

The methods for the measurements of the differential cross section were based on, static -exchange -plus -polarization -and -absorption model potentials, use of Hartree -Fock results for static potentials, use of semiclassical exchange approximation, and the absorption potentials applied especially for low angle scattering in the energy range 3Ø -1ØØ eV, variational matrix -effective potential (MEP) method, energy -dependent polarization potential and dispersion relation, localized central potential method applied for the energies between 1ØØ -1ØØØ eV, where the results are in satisfactory agreement with the experiment results for E ≥ 2ØØ eV. Optical potential from quasifree -scattering model where the absorption potential is made localized and energy dependent and is a function of the electron density of the target applied at 3Ø -3ØØØ eV, where reasonably good agreement with experimental data is found. R -Matrix calculation at 5 -2ØØ eV. Distorted -wave second Born approximation applied in the energy range 1ØØ eV to 3 KeV, where the agreement is not remarkable. Considering the effects of polarization and exchange in low -energy elastic scattering are also reported at 5 -5Ø eV in the angular range $Ø^{o}$ - $18Ø^{o}$. Polarized orbital method , where the polarization potential is obtained using the Hartree -Fock -Slater

(HFS) approximations is applied in the energy range Ø-1 Ryd. Modified Born approximation is studied in the energy range 45 - 75Ø eV, where the results obtained is quite different from those obtained by the partial wave method. Local density approximations to the exchange and coorelation potentials using the Hara exchange coupled with a Hedin -Lundqvist correlation at high electron density is also studied. Use of Born approximation using the form factor to calculate the elastic differential cross section in the energy range 1ØØ -7ØØ eV in the angular range 2 -5^{o} , indicating the situation is not clear for neon atom and concluded that neon atom behaves anamalouly where the data obtained through this are in poor agreement with the others. Charge cloud polarization effects is applied in the energy range 1ØØ -5ØØ eV for the angular range 5 -16Ø^{o}. Eikonal -Born series method for the optical -model formalism and static interaction which accounts for polarization, absorption and exchange effects and ab initio optical -model theory is studied at 1ØØ - 7ØØ eV , where the agreement is found excellent with the absolute experimental data. Byron and Joachain in their manuscript (1977) did not account for the absorption effect. These absorption effect were taken into account by Jhanwer et al (1978).

Jhanwer and Khare (1975) have obtained Δ by demanding that the total inelastic cross section in the Born approximation correct upto k^{-4} is equal to that given by the sum rule of Inokuti et al (1967). Such a procedure has yielded,

$\Delta = -\frac{1}{2} \exp [L(-1) / S(-1)]$

where L(-1) and S(-1) are the properties of the target and require the oscillator -strength distribution for their determination. L(-1) and S(-1) for neon atoms have been computed by M Inokuti (1975, in their private communication) and are equal to 2.394 and 1.94 respectively. Thus, Δ for the neon is equals to 1.717 a.u.. Jhanwer and Khare obtained the DCS and TCS for energies varying from 100 eV to 1 keV are in three different approximation viz., the static -field (SF), static field Polarization (SFP) and static field -polarization -exchange (SFPE) approximations. For energies $E \geq 200$ eV and 300 eV, inclusion of polarization effects considerably improves the results at low scattering angles. The inclusion of exchange further increases the cross section by a small amount at small angles. In general the results are in satisfatory agreement except for large scattering angles. The agreement between the theory and experiments is expected to improve further if a better ground state wave function is taken and the absorption effects are taken into account.

However for large -angle electron -(positron-) atom elastic scattering eikonal methods may lead to serious inaccuracies in the intermediate -energy -region. Since the large angle scattering is dominated by the short range static potential. The static potentials obtained in this way are very simple and behave like $\frac{ZQ}{r}$ at small distances, and fall off exponentially outside a distance of order of the size of the atom. Because of the strong Coulomb

potential,it will play a very important role in large -angle scattering. With this type of calculation it was clear that agreement is better at small angles than at large angles. First Born approximation does very poorly at all angles. Inside about 20° the lack of a polarization term and omission of absorption effects are very serious. A likely reason for this is the absorption and exchange, tend to cancel each other at large angles and have to be handled very carefully in order to achieve excellent agreement with the experiment. Further absorption potential is treated using the Glauber approximation. Another source of error is in inaccuracy for the ground state wave function for the atom also leads to a discrepancy in the results. Dewangan and Walters (1977) applied a distorted -wave second -Born approximation to calculate the σ_{el} and σ_{tot} at incident energies of 200 eV and higher. Their elastic cross sections are systematically too high by 30 -40 %. Jhanwer etal (1978) applied a real effective potential of the SEP type. Since they neglect the absorption potential for their method yields zero for σ_{abs} . This probably also explains why their calculations overestimate σ_{el} in at 200 eV and 400 eV. Fon and Berrington (1981) performed R -matrix calculations in which the ground state wave function is coupled to a ^1P pseudostate. These calculations are in excellent agreement with the experimental differential and integral elastic cross sections at both 150 and 200 eV. Devarajan Thirumalai and D.G. Truhlar (1982) applied MEP model which was very succesful

at predicting the integral and differential cross sections for elastic scattering and absorption cross section for electron -Ne collision at 15Ø - 7ØØ eV.

Having reviewed the work reported and the methods used to study the electron -Ne elastic scattering, we report here the same process but using the High Energy Higher Order Born approximation (HHOB theory). We report here the calculation of differential cross section and total cross section in the wide energy range 1ØØ to 7ØØ eV for almost the netire angular range.

Hence motivated through the limitation in the calculation involved in the above stated methods and overcoming the shortcomings in the methods used earliar. We report here the calculation of DCS and TCS using the HHOB approximation.

Having reviewd the HHOB theory in detail (Chapter II) and its complete study, we extend the HHOB theory for the elastic scattering of electrons by neon atom. We use the Hartree -Fock wave method and use of Clementti and Roettie tables for the orbital calculation. The interaction potential between the target neon atom and the incident electron is given as

$$V_d = -\frac{ZQ}{r_Ø} + \sum_{i=1}^{1Ø} \frac{1}{|\underline{r}_Ø - \underline{r}_i|} \qquad (z = 1Ø \text{ for neon}) \qquad (1),$$

where the symbols have their usual meaninigs. The full interaction is considered where,we have not neglect the cross term arising in the calculation. Hence the whole configuration is taken care. We

also calculate the third term of GES (Gkauber Eikonal Series) method and instead of third Born term we replace the third GES term. Hence the consistent picture of the scattering amplitude through $O(k_i^{-2})$ in the HHOB theory is written as discussed in the chapter II. To calculate the wave function more accurately we use the Hartree -Roothan -Fock wave method, where we used the Clementii -Roetii tables for the orbital calculation. Wave function obtained through this method for neon atom is more accurate. We treat neon atom as ten electron system and we include all the cross terms arising in the calculation. Further, while performing the calculation of the terms of the HHOB theory i.e. $f^{(1)}_{i-->f}$ (first Born term); Re1 $f^{(2)}_{HKA}$ (first real part of the real term through $O(k_i^{-1})$ and Re2 $f^{(2)}_{HKA}$ (second term of the real term through $O(K_i^{-2})$). The wave function using the Hartree -Fock wave method is just the sum of contributions from each Hartree -Fock orbital. The orbits for the neon atom is written as,

$$\phi_{1s}(r_1) = \frac{1}{(4\pi)}2 \left[\sum_{i=1}^{2} A_i \exp(-\lambda_i r_1) + \sum_{i=3}^{6} A_i r_1 \exp(-\lambda_i r_i) \right] \quad (2a),$$

$$\phi_{1s}(r_2) = \frac{1}{(4\pi)}2 \left[\sum_{i=1}^{2} A_i \exp(-\lambda_i r_2) + \sum_{i=3}^{6} A_i r_2 \exp(-\lambda_i r_2) \right] \quad (2b),$$

$$\phi_{2s}(r_3) = \frac{1}{(4\pi)}2 \left[\sum_{i=1}^{3} B_i \exp(-\lambda_i r_3) + \sum_{i=3}^{6} B_i r_3 \exp(-\lambda_i r_3) \right] \quad (2c),$$

$$\phi_{2s}(r_4) = \frac{1}{(4\pi)}2 \left[\sum_{i=1}^{2} B_i \exp(-\lambda_i r_4) + \sum_{i=3}^{6} B_i r_4 \exp(-\lambda_i r_4) \right] \quad (2d)$$

$$\phi_{2Px}(r_5) = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{i\phi} \left[\sum_{i=7}^{10} \sum_{m=7}^{10} C_i r_5 \exp(-\lambda_m r_5) \right] \quad (2e),$$

$$\phi_{2Px}(r_6) = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{i\phi} \left[\sum_{i=7}^{10} \sum_{m=7}^{10} C_i r_6 \exp(-\lambda_m r_6) \right] \quad (2f),$$

$$\phi_{2Py}(r_7) = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta \left[\sum_{i=7}^{10} \sum_{m=7}^{10} C_i r_7 \exp(-\lambda_m r_7) \right] \quad (2g),$$

$$\phi_{2Py}(r_8) = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta \left[\sum_{i=7}^{10} \sum_{m=7}^{10} C_i r_8 \exp(-\lambda_m r_8) \right] \quad (2h),$$

$$\phi_{2Pz}(r_9) = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{i\phi} \left[\sum_{i=7}^{10} \sum_{m=7}^{10} C_i r_9 \exp(-\lambda_m r_9) \right] \quad (2i),$$

$$\phi_{2Pz}(r_{10}) = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{i\phi} \left[\sum_{i=7}^{10} \sum_{m=7}^{10} C_i r_{10} \exp(-\lambda_m r_{10}) \right] \quad (2j),$$

where the exponents A's , B's, C's and λ's are defined as follows:

$A_1 = 55.7513411$; $A_2 = 1.1182599$; $A_3 = 3.6104\ E\text{-}04$

$A_4 = -0.0102605$; $A_5 = 0.3254106$; $A_6 = 3.9125783$

$\lambda_1 = 9.98486$; $\lambda_2 = 15.5659$; $\lambda_3 = 1.96184$

$\lambda_4 = 2.86423$; $\lambda_5 = 4.8253$; $\lambda_6 = 7.79242$

$B_1 = -13.47907$; $B_2 = -0.1449469$; $B_3 = 1.1590656$

$B_4 = 10.677485$; $B_5 = 18.25468$; $B_6 = -27.149262$

$C_1 = 0.6395614$; $C_2 = 5.3915624$

$C_3 = 16.198531$; $C_4 = 5.4513467$

$\lambda_7 = 1.45208$; $\lambda_8 = 2.38168$

$\lambda_9 = 4.48489$; $\lambda_{10} = 9.13464.$

We then calculate the complex form of ϕ's i.e. ϕ^* , and then we take the product with the ϕ's which is total charge density of the target atom. This is nothing but the ground state wave function for the target atom. The product $\phi^*\phi$ is used to evaluate the terms of the scattering amplitude in the HHOB approximation.

The cross terms arising in the product $\phi^*\phi$ are all considered as well as the target atom i.e. neon is considered as ten electron system.

We then perform the calculation of the terms in the HHOB scattering amplitude for the energy of incidence from 100 eV to 700 eV for the wide angular region. We then compare our results with experimental and theoretical results in the tabular form as well as through graphs also. And in the last we have discussed the results produced by this method with the others.

We now directly write the terms of the HHOB theory and then evaluate them to a simpler form. We also use the Static potential i.e. V_{st} and the use of Cox -Bonham parameters is also made to evaluate the term which is used in the chapter IV. We first took the fourier transform of the interaction potential as we took in the cahpter II for the various target atom. Since it is concluded that the first Born term does very poor at all energies and at all angle for the neon atom we use the static potential expression and we use the Cox -Bonham parameters and we write directly the expression for the first Born term using the following equation for neon atom as,

$$f^{(1)}_{i\text{-->}f} = -\frac{1}{2\Pi}\int dr_{\emptyset}\, \exp(i\,(q\cdot r_{o}))\, V_{fi}(r_{\emptyset}) \qquad (2),$$

$$= 2\emptyset \sum_{j=1}^{6} \gamma_j \frac{1}{q^2 + \lambda_j^2} \qquad (3),$$

where the γ 's and λ 's are defined as follows:

$\gamma_1 = 1.2524$, $\gamma_2 = -\emptyset.2408$, $\gamma_3 = 3.5572$, $\gamma_4 = 1.7522$;

$\gamma_5 = -3.5758$, $\gamma_6 = -1.74\emptyset1$ and

$\lambda_1 = 2.7495$, $\lambda_2 = 22.8979$, $\lambda_3 = 9.5848$, $\lambda_4 = 15.89\emptyset1$;

$\lambda_6 = 14.8774$.

The imaginary term in the HHOB theory for the neon atom can be written as,

$$\mathrm{Im}\, f^{(2)}_{HKA} = \frac{4\Pi^3}{k_i}\int dp\, U_{Im}(\, q - p - \beta_i\hat{y}\, ;\, p + \beta_i\hat{y};\, r_1 \ldots . r_{1\emptyset}) \qquad (4),$$

The term $U_{Im}(\ .....;.....;\ .....)$ defined as,

$$U_{Im}(\, q - p - \beta_i\hat{y};\, p + \beta_i\hat{y};\, r_1 \ldots . r_{1\emptyset}) = \int\int\int\int\int\int\int\int\int\int dv_1 \cdot$$

$$\ldots . dv_{1\emptyset}\, \psi^{*}_{f}\,(r_1 \ldots . r_{1\emptyset})\, \psi_i(r_1 \ldots . r_{1\emptyset})\, \{ [\sum_{i=1}^{1\emptyset} e^{i|q\,-p|\cdot b_i - i\beta_i z_i}$$

$$- 1\emptyset\ ] \ * \ [\sum_{j=1}^{1\emptyset} e^{ip\cdot b_j} + i\,\beta_i z_j \ - 1\emptyset\ ] \} \qquad (5),$$

where the product of the $\phi^{*}\phi$ gives the total charge density of the target atom, which is nothing but the ground state wave function

of the target atom. This can be obtain from the set of equations (2a to 2j). Where we write the individual terms and the compound product of the $\phi^{*}\phi$. After substitution of ϕ $\overset{*}{\phi}$ and using the Fourier transform of the interaction potential we solve the above equation to get the final form of the imaginary term through $O(k_i^{-4})$ as,

$$\text{Im } f^{(2)}_{\text{HEA}} = \frac{2}{k}- \{ 2 \sum_{i=1}^{2} A_i^2 \; I_1(q^2, \beta_i^2) \; [-D(\lambda_i)*(q^2+ \lambda_i^2)^{-1}+ \frac{32\emptyset}{\lambda_i}_3] + \sum_{i=3}^{6} A_i^2$$

$$I_1(q^2,\beta_i^2) \; [\; -2 \; D^3(\lambda_i)*(q^2+ \lambda_i^2)^{-1} - \frac{53\emptyset}{\lambda_i}_5] \; + \; 2A_1A_2 \quad I_1(q^2,\beta_i^2)$$

$$[-2D(\lambda_{12})*(q^2 + \lambda_{12}^2)^{-1} + \frac{32\emptyset}{\lambda_{12}}_3] + \sum_{\substack{i=1,2 \\ j=3..6 \\ i\neq j}} 2A_iA_j \; I_1(q^2,\beta_i^2) \quad [\; D^2(\lambda_{ij})$$

$$(q^2+ \lambda_{ij}^2)^{-1}+ \frac{96\emptyset}{\lambda_{ij}}_4] \quad + \sum_{\substack{i=1,4,5 \\ j=4,5,6 \\ i\neq j}} 2A_iA_j \; I_1(q^2,\beta_i^2)[-2D^3(\lambda_{ij}) \; (q^2+\lambda_{ij})^{-1}$$

$$\frac{384\emptyset}{\lambda_{ij}}_5] \; - \; 4\emptyset \; \sum_{i=1}^{2} A_i^2 \; \frac{D(\lambda_i)}{\lambda_i}_2 \; I_1(q^2,\beta_i^2, \lambda_i^2) \; - \; 4\emptyset \; \sum_{i=3}^{6} A_i^2 \quad \frac{D(\lambda_i)}{\lambda_i}_2$$

$$I_1(q^2,\beta_i^2,\lambda_i^2) \; - \; 8\emptyset \; A_1A_2 \; \frac{D(\lambda_{12})}{\lambda_{12}}_2 \; I_1(q^2,\beta_i^2,\lambda_{12}^2) + 8\emptyset \sum_{\substack{i=1,2 \\ j=3,..,6 \\ i\neq j}} A_iA_j$$

$$\frac{D^2(\lambda_{ij})}{\lambda_{ij}}_2 \; I_1(q^2,\beta_i^2,\lambda_{ij}^2) \; - \; 8\emptyset \sum_{\substack{i=3,4,5 \\ j=4,5,6 \\ i\neq j}} A_iA_j \; \frac{D(\lambda_{ij})}{\lambda_{ij}}_2 \; I_1(q^2,\beta_i^2,\lambda_{ij}^2) \}$$

$$* -\frac{2}{k} \{ \sum_{i=1}^{2} B_i^2 I_1(q^2,\beta_i^2) [-D(\lambda_i) * (q^2+\lambda_i^2)^{-1} + \frac{32\emptyset}{\lambda_i^3}] + \sum_{i=3}^{6} B_i^2$$

$$I_1(q^2,\beta_i^2) [-2 D^3(\lambda_i) * (q^2+\lambda_i^2)^{-1} - \frac{36\emptyset}{\lambda_i^5}] + 2 B_1B_2 I_1(q^2, \beta_i^2) [$$

$$- 2D(\lambda_{12}) * (q^2+\lambda_{12})^{-1} + \frac{32\emptyset}{\lambda_{12}^3}] + \sum_{\substack{i=1,2 \\ j=3,..6 \\ i\neq j}} 2 B_iB_j I_1(q^2,\beta_i^2) [2D^2(\lambda_{ij}) *$$

$$(q^2+\lambda_{ij}^2)^{-1} + \frac{96\emptyset}{\lambda_{ij}^4}] + \sum_{\substack{i=3,4,5 \\ j=4,5,6 \\ i\neq j}} 2 B_iB_j I_1(q^2,\beta_i^2) [-2D^3(\lambda_{ij}) * (q^2+\lambda_{ij}^2)^{-1}$$

$$[-2D^3(\lambda_{ij}) * (q^2+\lambda_{ij}^2)^{-1} + \frac{384\emptyset}{\lambda_{ij}^5}] - 4\emptyset \sum_{i=3}^{6} B_i^2 I_1(q^2,\beta_i^2,\lambda_i^2) \frac{D(\lambda_i)}{\lambda_i^2} -$$

$$8\emptyset B_1B_2 \frac{D(\lambda_{12})}{\lambda_{12}^2} I_1(q^2,\beta_i^2,\lambda_{12}^2) + 8\emptyset \sum_{\substack{i=1,2 \\ j=3,..,6 \\ i\neq j}} B_iB_j \frac{D^2(\lambda_{ij})}{\lambda_{ij}^2} I_1(q^2,\beta_i^2,\lambda_{ij}^2)$$

$$- 8\emptyset \sum_{\substack{i=3,4,5 \\ j=4,5,6 \\ i\neq j}} B_iB_j \frac{D^3(\lambda_{ij})}{\lambda_{ij}^2} I_1(q^2,\beta_i^2,\lambda_{ij}^2) \} + -\frac{2}{k_i} \{ \sum_{i=1}^{4} \sum_{m=7}^{10} C_i^2 [I_1(q^2, \beta_i^2)$$

$$\{ (- \frac{6}{q^2}) [D^2(\lambda_m)\lambda_m * (q^2+\lambda_m^2)^{-1} + D(\lambda_m) * (q^2+\lambda_m^2)^{-1}] + \frac{384\emptyset}{\lambda_m^5} \} + \frac{96\emptyset}{\lambda_m^5}$$

$$I_1(q^2,\beta_i^2,\lambda_m^2)] + \sum_{\substack{i=1,2,3 \\ j=2,3,4 \\ i\neq j}} \sum_{\substack{m=7,8,9 \\ n=8,9,10 \\ m\neq n}} C_iC_j [I_1(q^2,\beta_i^2) \{ (- \frac{12}{q^2}) [D^2(\lambda_{mn})$$

$$\lambda_{mn} * (q^2+\lambda_{mn}^2)^{-1} + D(\lambda_{mn}) * (q^2+\lambda_{mn}^2)^{-1}] + \frac{768\emptyset}{\lambda_{mn}^5} \} + \frac{192\emptyset}{\lambda_{mn}^5}$$

$$I_1(q^2,\beta_i^2,\lambda_{mn}^2)] \} + \text{the other cross term of different combination}$$

(6),

integration. In addition to the above terms of the equation (6) we have so many cross terms of the product of the $\phi^*\phi$. We are very sorry to mention at this stage that we have not written all the cross terms but while preparing the computer program we use arrays in such a manner that it does the calculation for all the terms appearing. These terms are too long and also it consumes lot of space. But we have prepared a program with arrays properly defined, which take care of all these cross terms. We also do the same for the real part thorugh $O(K_i^{-1})$ and for $O(k_i^{-2})$ of the HHOB approximation. Hence here due to limited intention of text we have not shown the cross terms. But one can go through our computer program and coding we have done which take care of the terms. Then we use the first term of the real part in the second Born term through $O(k_i^{-1})$ is written as,

$$\text{Re } 1\, f^{(2)}_{\text{HKA}} = -\frac{4\Pi^2}{k}\, \mathcal{P} \int dp \int_{-\infty}^{+\infty} \frac{dp_z}{(P_z - \beta_i)}\; U^{(2)}_{fi}(q - p - p_z\hat{y};\; p + p_z\hat{y}) \tag{7},$$

where the general form of $U^{(2)}_{fi}(\ldots\ldots;\ldots\ldots)$ is,

$$U^{(2)}_{fi}(x, X; y, Y) = \langle \psi_f \mid \bar{V}(x,X)\, \bar{V}(y,Y) \mid \psi_i \rangle \tag{8}.$$

The evaluation of the above integral can be done in the same manner as we did it in the chapter II (for the case of hydrogen, helium and lithium atom). The only difference between the imaginary term and the real term is that, instead of β_i in imaginary one has to replace it by p_z part only.

We write $U^{(2)}_{fi}(q - p - p_z\hat{y};\; p + p_z\hat{y})$ is equal to,

$$= \langle \psi_f \mid \bar{V}(q - p - p_z\hat{y} ; r_1,\ldots,r_{10})\ \bar{V}(p + p_z\hat{y};\ r_1,\ldots r_{10}) \mid \psi_i \rangle$$

Substituting the fourier form of the potential $\bar{V}$'s from the set of equations (9 and 10, chapter II.) and substituting in equation (7), we get

$$\mathrm{Re1}\ f^{(2)}_{HKA} = -\frac{4\pi^2}{k_i}\frac{1}{4\pi}4\,\mathcal{P}\int dp_{-\infty}\int^{+\infty}\frac{dp_z}{(p_z - \beta_i)}\ \frac{1}{(|q-p|^2+p_z^2)\ (p^2+p_z^2)}$$

$$\psi_f^*\,\psi_i\ \{\sum_{j=1}^{10} e^{i|q-p|.b_j - ip_z z_j - 10}\}\ \{\sum_{j=1}^{10} e^{ip\ .b_j + ip_z z_j - 10}\} \qquad (9).$$

We use the same method of Yates (1979) of evaluating the real terms through $O(K_i^{-2})$, which is discussed in detail in chapter II. Hence we write the straight forward solution of the above real term of the HHOB scattering amplitude in terms of the integrals term like $I_2(\ldots)$, $I_2'(\ldots.)$ and $I_3(\ldots)$ as follows:

$$\mathrm{Re2}\ f^{(2)}_{HKA} = -(2\pi^2 k_i)^{-1}\ \{\ [\ -\sum_{i=1}^{2} A_i^2\ \frac{D(\lambda_i)}{q^2+\lambda_i^2} - \sum_{i=3}^{6} A_i^2\ \frac{D^3(\lambda_i)}{q^2+\lambda_i^2}$$

$$- A_1A_2\ \frac{D(\lambda_{12})}{q^2+\lambda_{12}^2} + \sum_{\substack{i=1,2\\ j=3,..6\\ i\neq j}} A_iA_j\ \frac{D^2(\lambda_{ij})}{q^2+\lambda_{ij}^2} - \sum_{\substack{i=3,4,5\\ j=4,5,6\\ i\neq j}} A_iA_j$$

$$\frac{D^3(\lambda_{ij})}{q^2+\lambda_{ij}^2}\ ]\ \ I_2(q^2,\beta_i^2,\emptyset) + [\ -\sum_{i=1}^{2} B_i^2\ \frac{D(\lambda_i)}{q^2+\lambda_i^2} - \sum_{i=3}^{6} B_i^2$$

$$\frac{D^3(\lambda_i)}{q^2+\lambda_i^2} - B_1B_2\ \frac{D(\lambda_{12})}{q^2+\lambda_{12}^2} + \sum_{\substack{i=1,2\\ j=3,..6\\ i\neq j}} B_iB_j\ \frac{D^2(\lambda_{ij})}{q^2+\lambda_{ij}^2} -$$

$$\sum_{\substack{i=3,4,5\\ j=4,5,6\\ i\neq j}} B_i B_j \left[\frac{D^3(\lambda_{ij})}{q^2+\lambda_{ij}^2} \right] I_2(q^2,\beta_i^2,\emptyset) + \left[(-12) \sum_{i=1}^{4} \sum_{m=7}^{10} C_i^2 \right.$$

$$\left(\frac{D^2(\lambda_m)\lambda_m}{q^2+\lambda_m^2} + \frac{D(\lambda_m)}{q^2+\lambda_m^2} \right) I_2(q^2,\beta_i^2,\emptyset) - 24 \sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}} \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_i C_j$$

$$\left(\frac{D^2(\lambda_{mn})\lambda_{mn}}{q^2+\lambda_{mn}^2} + \frac{D(\lambda_{mn})}{q^2+\lambda_{mn}^2} \right) I_2(q^2,\beta_i^2,\emptyset) - 240 \sum_{i=1}^{4} \sum_{m=7}^{10} C_i^2 \left[\frac{D^2(\lambda_m)}{\lambda_m} \right.$$

$$\left. + \frac{D(\lambda_m)}{\lambda_m} - 2 \right] I_2(q^2,\beta_i^2,\lambda_m^2) - 480 \sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}} \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_i C_j \left[\frac{D^2(\lambda_{mn})}{\lambda_{mn}} \right.$$

$$\left. + \frac{D(\lambda_{mn})}{\lambda_{mn}} - 2 \right] I_2(q^2,\beta_i^2,\lambda_{mn}^2) - 150 \sum_{i=1}^{4} \sum_{m=7}^{10} C_i^2 \frac{1}{\lambda_m} 5 \; I_2(q^2,\beta_i^2) -$$

$$9600 \sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}} \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_i C_j \frac{1}{\lambda_{mn}} 5 \; I_2(q^2,\beta_i^2) \Big] + 3 \sum_{i=1}^{4} \sum_{m=7}^{10} C_i^2$$

$$\left(- \frac{2D^3(\lambda_m)}{q^2+\lambda_m^2} + \frac{4}{q^2} \left[\frac{D^2(\lambda_m)\lambda_m}{q^2+\lambda_m^2} + \frac{D(\lambda_m)}{q^2+\lambda_m^2} \right] \right) I_2(q^2,\beta_i^2) + 6$$

$$\sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}} \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_i C_j \left(- \frac{2D^3(\lambda_{mn})}{q^2+\lambda_{mn}^2} + \frac{4}{q^2} \left[\frac{D^2(\lambda_{mn})\lambda_{mn}}{q^2+\lambda_{mn}^2} + \frac{D(\lambda_{mn})}{q^2+\lambda_{mn}^2} \right] \right)$$

$$I_2(q^2,\beta_i^2) + 60 \sum_{i=1}^{4} \sum_{m=7}^{10} C_i^2 \left(- \frac{2D^3(\lambda_{mn})}{\lambda_{mn}} 2 \; I_2(q^2,\beta_i^2,\lambda_m^2) + 4 \frac{D^2(\lambda_m)}{\lambda_m} \right.$$

$$\left. I_2(q^2,\beta_i^2,\lambda_m^2) + 4 \frac{D(\lambda_m)}{\lambda_m} 2 \; I_2(q^2,\beta_i^2,\lambda_m^2) \right) - 120 \sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}} \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_i C_j$$

$$\left(- \frac{2D^3(\lambda_{mn})}{\lambda_{mn}^2} I_2(q^2,\beta_i^2,\lambda_{mn}^2) + 4 \frac{D^2(\lambda_{mn})}{\lambda_{mn}} I_2(q^2,\beta_i^2,\lambda_{mn}^2) + \frac{D(\lambda_{mn})}{\lambda_{mn}^2} \right.$$

$$\left. I_2(q^2,\beta_i^2,\lambda_{mn}^2) \right) + \left\{ 2 \sum_{i=1}^{2} \sum_{j=1}^{2} A_i^2 \frac{D(\lambda_i)}{\lambda_i^2} \frac{D(\lambda_j)}{\lambda_j^2} I_3(q^2,\beta_i^2,\lambda_{ij}^2) + \right.$$

---------plus the other cross terms for different combintation.

(1Ø).

Similarly for the second part of the real term of the HHOB approximation through $O(k_i^{-2})$ is written as,

$$\text{Re2 } f_{HHA}^{(2)} = - \frac{2\Pi^2}{K_i^2} \frac{\partial}{\partial \beta_i} \mathcal{P} \int dp \int_{-\infty}^{+\infty} \frac{dp_z}{(p_z^2 - \beta_i^2)} (p^2 + p_z^2) U_{fi}^{(2)}(....;..)$$

(11).

Where we have not neglected the cross terms eventhough their contribution is not very large. This is because we consider the target atom i.e. neon atom as ten electron system. Hence we get so many cross terms in the expression. Besides to write all these cross terms within the limted text is really a difficult task, hence we have not shown the cross terms for the second part of the real term i.e. through $O(k_i^{-2})$. But one can check our computer program and its array defined where the cross terms are being included in the final expression for all the terms i.e. imaginary part, the first part of the real term through $O(k_i^{-})$ and second part of the real term through $O(k_i^{-2})$. We also follow the same technique to reduce the above equation (11) to a simpler form like equation (1Ø).

We write the equation (11) as,

$$\mathrm{Re}2\, f^{(2)}_{HKA} = -(\Pi^2 k_i^2)^{-1} \frac{\partial}{\partial \beta_i} \mathcal{P} \int d\underline{p} \int_{-\infty}^{+\infty} \frac{dp_z}{(p_z - \beta_i)} \frac{1}{(|\underline{q} - \underline{p}|^2 + p_z^2)}$$

$$\psi_f^* \psi_i \{ (\sum_{i=1}^{10} e^{i|\underline{q} - \underline{p}| . b_i} - ip_z z_j - 10) * (\sum_{i=1}^{10} e^{i\underline{p} . \underline{b}_j} + ip_z z_j - 10) \} \qquad (12).$$

We then use the product of $\psi^* \psi$ using the set of equations (2.0a to 2.0j) in the above equation. We here write the straight forward solution of the above equation as,

$$= -(\Pi^2 k_i^2)^{-1} \{ [-2 \sum_{i=1}^{2} A_i^2 \frac{D(\lambda_i)}{q^2 + \lambda_i^2} I_3'(\beta_i, 0) + 40 \sum_{i=1}^{2} A_i^2 \frac{D(\lambda_i)}{\lambda_i} 2$$

$$(I_3'(\beta_i, 0) - \frac{1}{\lambda} 2_i I_3(\beta_i^2, \lambda_i^2)) + 25 \sum_{i=1}^{2} A_i^2 \frac{1}{\lambda} -3_i I_3'(\beta_i, 0)] + [-2 \sum_{i=3}^{6}$$

$$A_i^2 \frac{D^3(\lambda_i)}{q^2 + \lambda_i^2} I_3'(\beta_i, 0) + 40 \sum_{i=3}^{6} A_i^2 \frac{D^3(\lambda_i)}{\lambda_i} -2 (I_3'(\beta_i, 0) - \frac{1}{\lambda} 2_i$$

$$I_3(\beta_i^2, \lambda_i^2)) + \sum_{i=3}^{6} A_i^2 \frac{75}{\lambda} 5_i I_3'(\beta_i, 0)] + 2A_1 A_2 [- \frac{2D(\lambda_{12})}{q^2 + \lambda_{12}^2}$$

$$I_3(\beta_i, 0) + 40 \frac{D(\lambda_{12})}{\lambda} (I_3'(\beta_i, 0) - \frac{1}{\lambda} - I_3(\beta_i^2, \lambda_i^2)) + \frac{400}{\lambda} 3 I_3(\beta_i, 0)]$$

$$+ 2 \sum_{\substack{i=1,2 \\ j=3,..6 \\ i \neq j}} A_i A_j [\frac{2D^2(\lambda_{ij})}{q^2 + \lambda_{ij}^2} I_3'(\beta_i, 0) - 40 \frac{D^2(\lambda_{ij})}{\lambda_{ij}} 2 (I_3'(\beta_i, 0) -$$

$$\frac{1}{\lambda} -2 I_3(\beta_i^2, \lambda_i^2)) + \frac{1200}{\lambda} 4 I_3'(\beta_i, 0) + 2 \sum_{\substack{i=3,4,5 \\ j=4,5,6 \\ i \neq j}} A_i A_j [$$

$$- \frac{2D^3(\lambda_{ij})}{q^2 + \lambda_{ij}^2} I_3'(\beta_i,0) + 40 \frac{D^3(\lambda_{ij})}{\lambda_{ij}^2} (I_3'(\beta_i,0) - \frac{1}{\lambda}{}^2_{ij} I_3(\beta_i^2,\lambda_{ij}^2))$$

$$+ \frac{4800}{\lambda}{}^5 I_3'(\beta_i,0)] + [-2 \sum_{i=1}^{2} B_i^2 \frac{D(\lambda_i)}{q^2 + \lambda_i^2} I_3'(\beta_i,0) +$$

$$40 \sum_{i=1}^{2} \frac{D(\lambda_i)}{\lambda}{}^2_i B_i^2 (I_3'(\beta_i,0) - \frac{1}{\lambda}{}^2_i I_3(\beta_i^2, \lambda_i^2) + 25 \sum_{i=1}^{2} B_i^2 \frac{1}{\lambda}{}^3_i$$

$$I_3(\beta_i,0)] + [-2 \sum_{i=3}^{6} B_i^2 \frac{D^3(\lambda_i)}{q^2 + \lambda_i^2} I_3'(\beta_i,0) + 40 \sum_{i=3}^{6} \frac{D^3(\lambda_i)}{\lambda}{}^2_i$$

$$(I_3'(\beta_i,0) - \frac{1}{\lambda}{}^2_i I_3(\beta_i^2,\lambda_i^2)) + \sum_{i=3}^{6} A_i^2 \frac{75}{\lambda}{}^5_i I_3'(\beta_i,0)] + 2B_1B_2$$

$$[- \frac{2D(\lambda_{12})}{q^2 + \lambda_{12}^2} I_3'(\beta_i,0) + 40 \frac{D(\lambda_{12})}{\lambda_{12}^2} (I_3'(\beta_i,0) - \frac{1}{\lambda}{}^2_i I_3(\beta_i^2,\lambda_i^2))$$

$$+ \frac{400}{\lambda}{}^3 I_3'(\beta_i,0)] + 2 \sum_{\substack{i=1,2 \\ j=3,6 \\ i\neq j}} B_iB_j [2 \frac{D^2(\lambda_{ij})}{q^2 + \lambda_{ij}^2} I_3'(\beta_i,0) - 40$$

$$\frac{D^2(\lambda_{ij})}{\lambda}{}^2_{ij} (I_3'(\beta_i,0) - \frac{1}{\lambda}{}^2_{ij} I_3(\beta_i^2,\lambda_{ij}^2)) + \frac{1200}{\lambda}{}^4_{ij} I_3'(\beta_i,0)] +$$

$$2 \sum_{\substack{i=3,4,5 \\ j=4,5,6 \\ i\neq j}} B_iB_j [-2 \frac{D^3(\lambda_{ij})}{q^2 + \lambda_{ij}^2} I_3'(\beta_i,0) + 40 \frac{D^3(\lambda_{ij})}{\lambda}{}^2_{ij} (I_3'(\beta_i,0) - \frac{1}{\lambda}{}^2_{ij}$$

$$I_3(\beta_i^2,\lambda_{ij}^2)) + \frac{4800}{\lambda}{}^5_{ij} I_3'(\beta_i,0)] + [-12 \sum_{i=1}^{4} \sum_{m=7}^{10} C_i^2 (\frac{D^2(\lambda_m)\lambda_m}{q^2 + \lambda_m^2}$$

$$+ \frac{D(\lambda_m)}{q^2 + \lambda_m^2}) I_3'(\beta_i,0) - 24 \sum_{\substack{i=1,2,3 \\ j=2,3,4 \\ i\neq j}} \sum_{\substack{m=7,8,9 \\ n=8,9,10 \\ m\neq n}} C_iC_j (\frac{D^2(\lambda_{mn})\lambda_{mn}}{q^2 + \lambda_{mn}^2} +$$

$$\frac{D(\lambda_{mn})}{q^2+\lambda_{mn}^2}\Big)\, I_3'(\beta_i,0) - 240 \sum_{i=1}^{4}\sum_{m=7}^{10} C_i^2 \Big(\frac{D^2(\lambda_{mn})}{\lambda_{mn}} [\, I_3'(\beta_i,0) -$$

$$I_3(\beta_i^2,\lambda_{mn}^2)\,] + \frac{D(\lambda_{mn})}{\lambda_{mn}^2}\,[\, I_3'(\beta_i,0) - I_3(\beta_i^2,\lambda_{mn}^2)\,]\Big) - 480$$

$$\sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}}\ \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_iC_j \Big(\frac{D^2(\lambda_{mn})}{\lambda_{mn}} [\, I_3'(\beta_i,0) - I_3(\beta_i^2,\lambda_{mn}^2)\,] + \frac{D(\lambda_{mn})}{\lambda_{mn}^2}$$

$$[\, I_3'(\beta_i,0) - I_3(\beta_i^2,\lambda_{mn}^2)\,]\Big) + \frac{1200}{8} \sum_{i=1}^{4}\sum_{m=7}^{10} C_i^2\, \frac{1}{\lambda_m^5}\, I_3'(\beta_i,0)$$

$$- 9600 \sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}}\ \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_iC_j\, \frac{1}{\lambda_{mn}^5}\, I_3'(\beta_i,0) + \Big[\sum_{i=1}^{4}\sum_{m=7}^{10} C_i^2$$

$$\Big(-2\, \frac{D^3(\lambda_m)}{q^2+\lambda_m^2} + \frac{4}{q^2}\Big[\frac{D^2(\lambda_m)\,\lambda_m}{q^2+\lambda_m^2} + \frac{D(\lambda_m)}{q^2+\lambda_m^2}\Big]\, I_3'(\beta_i,0) + 6$$

$$\sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}}\ \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_iC_j \Big(-2\, \frac{D^3(\lambda_{mn})}{q^2+\lambda_{mn}^2} + \frac{4}{q^2}\Big[\frac{D^2(\lambda_{mn})\lambda_{mn}}{q^2+\lambda_{mn}^2} + \frac{D(\lambda_{mn})}{q^2+\lambda_{mn}^2}\Big]$$

$$I_3'(\beta_i,0)\Big) - 30 \sum_{i=1}^{4}\sum_{m=7}^{10} C_i^2 \Big(-2\, \frac{D(\lambda_{mn}^3)}{\lambda_{mn}^2}\,[\, I_3'(\beta_i,0) - I_3(\beta_i^2,\lambda_{mn}^2)$$

$$+ 4\, \frac{D^2(\lambda_m)}{\lambda_m}\{\, I_3'(\beta_i,0) - \frac{1}{\lambda_m^2} I_3(\beta_i^2,\lambda_m^2)\} + 4\, \frac{D(\lambda_m)}{\lambda_m^2}\{\, I_3'(\beta_i,0) - \frac{1}{\lambda_m^2}$$

$$I_3(\beta_i^2,\lambda_m^2)\}\Big) - 120 \sum_{\substack{i=1,2,3\\ j=2,3,4\\ i\neq j}}\ \sum_{\substack{m=7,8,9\\ n=8,9,10\\ m\neq n}} C_iC_j \Big([\, -2\, \frac{D^3(\lambda_{mn})}{\lambda_{mn}^2}$$

$$\{I_3'(\beta_i,\emptyset) - \frac{1}{\lambda_m^2} I_3(\beta_i,\emptyset)\}] - 24\emptyset \sum_{\substack{i=1,2,3\\ j=2,3,4\\ i=j}} \sum_{\substack{m=7,8,9\\ n=8,9,1\emptyset\\ m=n}} C_i C_j \Big(4$$

$$\frac{D^2(\lambda_m)}{\lambda_m^2}\{ I_3'(\beta_i,\emptyset) - I_3(\beta_i^2,\lambda_m^2)\} + 4 \frac{D(\lambda_m)}{\lambda_m^2} \{I_3(\beta_i,\emptyset) - I_3(\beta_i^2,\lambda_m^2)\}\Big)\Big]$$

$$+ 2 \sum_{i=1}^{2} A_i^2 \sum_{j=1}^{2} B_j^2 \left(\frac{D(\lambda_i)}{\lambda_i^2} \frac{D(\lambda_j)}{\lambda_j^2}\right) I_4(q^2,\beta_i^2,\lambda_i^2,\lambda_j^2) + \text{-------}$$

plus the other compound cross term (12).

Here also we have not written all other compound cross term to reduce the text. Our program show that it calculates all other compound cross term.

We then use the set of equations (6,1Ø and 12) to evaluate the scattering amplitude in the HHOB theory. Instead of the third Born term we evaluate the third Glauber term, so that a consistent picture of scattering amplitude through $O(k_i^{-2})$ is obtained. Further, if one looks at the expression of the second Born term for the case of neon atom, is too cumbersome and too long. Hence to avoid all this discrepany and computational flexibility we replace third Born term by third Glauber term. We have not included the exchange for the case of neon atom. But one can always include the effect of exchange or the higher order exchange wdterms in the calculation. We use the equation (2Ø,21 of chapter -II) to calculate the differential cross section. We report here the calculation of the process of elastic scattering of electrons by neon atom for 1ØØ to 4ØØ eV energy range in the angular range Ø to 18Ø deg. The third Gluber term is calculated as follows:

THE GLAUBER APPROXIMATION :

The Glauber approximation is a many body generalization of the Eikonal approximation for a direct collision leading from initial state $| \emptyset >$ to a final state $| n >$. The Glauber scattering amplitude is given by

$$f_G = \frac{k}{2\pi i} \int d^2\underline{b} \; e^{i\underline{q}\cdot\underline{b}} < m | \{ e^{i\chi_G(\underline{b},\underline{x})} - 1 \} | \emptyset > \qquad (13),$$

where the Glauber phase shift function is given in terms of V_d as,

$$\chi_G(\underline{b}, \underline{x}) = -\frac{1}{k} \int_{-\infty}^{+\infty} V_d(\underline{b}, z, \underline{x}) \, dz \qquad (14),$$

where integration is being performed along z - axis perpendicular to $\underline{q}$. Where V_d is written as

$$V_d = -\frac{z}{r} + \sum_{i=1}^{z} \frac{1}{|\underline{r}_i - \underline{r}|} \qquad (15).$$

Now expanding the bracket exponent terms in the equation (13). We have

$$\{ e^{i\chi_G(\underline{b}, \underline{x})} - 1 \} = 1 + i\chi_G + \frac{1}{2!} i^2\chi_G^2 + \frac{1}{3!} i^3 \chi_G^3 + \ldots.$$

negelcting the higher order terms after third term we have,

$$i\chi_G + \frac{1}{2!} i^2\chi_G^2 + \frac{1}{3!} i^3 \chi_G^3$$

Now, to have $< \emptyset | V_d | \emptyset >$; when we take from $| n >$ to $| \emptyset >$. We can have a sum over all n state, hence the above term can be written as

$\sum_n < \emptyset | V_d | \emptyset > < n | V_d | \emptyset >$ and this is nothing but,

$$< \emptyset | V_d | \emptyset > \; < \emptyset | V_d | \emptyset >$$

which is nothing but the form of the static potential. Hence, V_d can be replaced by V_{st}. Hence, equation (14) can be rewritten as,

$$\chi_G = -\frac{1}{k} \int_{-\infty}^{+\infty} V_{st}(b, z)\, dz$$

Hence, we write the expression of the Glauber scattering amplitude as,

$$f_G = \frac{k}{2\pi i} \frac{i}{k} 3 \int e^{iq\cdot b}\, db \left\{ \int_{-\infty}^{+\infty} V_{st}(b, z)\, dz \right\}^3$$

Now we have choosen $r = b + z\,\hat{n}$, such that b is always perpendicular to z.

Now, writing the expression for the static potential using Cox -Bonham parameters for neon atom as,

$$V_{st}(r) = -\frac{z}{r} \frac{z_p(r)}{z} \quad \text{and,} \quad \frac{z_p(r)}{z} = \sum_{i=1}^{n} \gamma_i \exp(-\lambda_i r)$$

Hence,

$$V_{st}(r) = -\frac{z}{r} \sum_{i=1}^{n} \gamma_i \exp(-\lambda_i r)$$

Substitution of the above equation in (') we have,

$$f_G = \frac{1}{2\pi k^2} \int e^{iq\cdot b}\, db \left\{ -z \sum \gamma_i \int_{-\infty}^{+\infty} \frac{\exp(-\lambda_i r)}{r}\, dz \right\}^3$$

We simplify the above equation further to get the simple analytical form. We then compute it using the numerical technique of Gauss quadrature rule to calculate the Glauber term appearing in the expression of the scattering amplitude. Where the values of the Cox -Bonham parameter i.e. γ 's and λ 's are given as follows:

$\lambda_1 = 2.7495$, $\lambda_2 = 22.8979$, $\lambda_3 = 9.5848$, $\lambda_4 = 15.8901$, $\lambda_5 = 8.5939$ and $\lambda_6 = 14.8774$;

$\gamma_1 = 1.2524$, $\gamma_2 = -0.2468$, $\gamma_3 = 3.5527$, $\gamma_4 = 1.7522$, $\gamma_5 = -3.5758$ and $\gamma_6 = -1.7401$.

RESULTS AND DISCUSSION :

We perform the calculation for the differential cross section in the energy range 100 - 400 eV with the angular range 5 - 180 deg. We compare our results calculated using the HHOB theory with the other theoretical and experimental methods available. We compare our results in the tabular form as well as in a graphical mode also. We compare our results with methods described in the beginning of this chapter.

As concluded by many workers that the accuracy in the wave function is seeking and the full interaction should be considered. Where the effect of polarization, absorption are to be handled very carefully.

We calculated the ground state wave function for the neon atom accurately using the Roothan - Hartrre -Fock wave method, where we used the Clementii -Roetii tables for the orbital calculation. After having the accurate wave function we considered the elastic scattering of electrons by neon atom through the interaction potential. We also use the Fourier transform of the inter action potential. We calculate the integrand involving dp , dp_z accurately.

The terms appeared in the expression of the scattering amplitude in the HHOB theory are calculated accurately. Each terms are calculated individually and then at last the final sum is performed to get the scattering amplitude for the calculation of the differential cross section.

The differential cross sections and total collisional cross sections are calculated for e^--Ne atom scattering for a variety of incident energies and a wide range of scattering angle using above discussed HHOB theory. 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 convergent due to the presence of β_i term. If we put $\beta_i = 0$ in the present HHOB terms we will get the corresponding terms in the GES (Glauber eikonal series). The imaginary part of the second HHOB term will not diverge for forward elastic scattering due to β_i.

We did not neglect any of the cross term contribution in the calculation. We discuss the calculation of the differential cross section calculated in detail for the 100 eV first.

It is quite unfortunate that the experimental data and theoretical data for the given range are not available for the complete angular range i.e. 0 - 180 deg. Although there are some methods which calculates for all angular range for a particular value of the incident energy and they are compared. Hence we compare and discuss our results for that angular range and energy range.

It is well known fact that the EBS results over estimate the experimental results for all energies. This being due to the fact that the Glauber series converge slowly.

As expected at low scattering angles agreement is better

compared to the high scattering angles. This is due to the mutual cancellation of absorption and polarization effects. The agreement can be improved further if the absorption and polarization effects are handled carefully and large scattering angles. Here k_i^{-1} part of the real term partly corresponds to distortion. Where it is to understood that the distortion is not complete one. This term where partly the distortion of incoming wave and target wave is taken care off.

To have the complete account for the distortion we have to design a separate model or we can use the DWBA (distorted wave Born approximation).

Table III.I and III.II compares the present DCS value with the theoretical and experimental results at a incidence energy 100 eV and 200 eV respectively. The results are compared up to 50 deg. with the other results. It can be seen that the present results are in better agreement with the experimental results at small angle of scattering. Afterwards the discrepancy is observed when it is compared with the experimental results but this discrepancy observed is within the error limit. The results are still comparable compare to the other results available. At large angle this discrepancy increase further, but still one can compare the results at large scattering angle with the other theory. We find that for both energies i.e. 100 eV and 200 eV results are close to the results of Byron and Joachain (1974b,76).

Table III.III also compares the differential cross section

for energy of incidence 400 eV with the theoretical and experimental results for 10 to 180 deg. We find that our results are close to the results of Devrajan Thirumalai et al and also very close the results of Byron and Joachains (optical model calculation). We find our results also agrees well with the experimental results of Gupta and Rees within the error limit.

Table III.IV gives the present differential cross section value for the energy of incidence starting from 100 eV to 400 eV in the angular range 5 to 180 deg. Results are expressed in a_0^2/sr.

We also compare our results graphically also. We find that at large scattering angle the discrepancies between the results obtained increases further. This is due to the fact that HHOB approximation is found to give better results at high energy and for small angle of scattering. In figure III.I, III.II and III.III shows the present differential cross sections for the energy of incidence 100 eV, 200 eV and 400 eV respectively. As energy of incidence increases further the discrepancies at small angle of scattering is negligible but at large angle of scattering i.e. for $\theta \geq 60$ deg, results found to deviate from the experimental results. Still one can observe that the results are still comparable with the other methods.

The results improves for $E \geq 200$ eV. The first Born term calculation, where no approximation is made, does very poorly at all energies and angles.

The contribution due to exchange is not included for energy

100 tv. Because at large angle the absorption cross sections overestimates at this low energy. Hence exchange effects may not be appreciable at 100 eV for neon like target. At large scattering angles with high incident energy one can include the first order or even higher order exchange terms in the calculation.

Here Hartree-Roothan -Fock wave function with all completed correlated terms to remove the inaccuracy in the wave function used here for neon atom. Though all speak of non negligible contributions of polarization effects, particularly for dipole allowed transitions, Mohr predicted behavior of cross section could be explained through investigation of higher Born terms.

The results can improve further at large scattering angles if the absorption and polarization effects are handled carefully. Neglecting distortion of incident electron wave function which can not be satisfied further for the strong scattering potential. Polarization effects should decrease as the interaction time decreases. For the energy $E \geq 200$ eV results improves further and the results are quite comparable with theoretical and experimental methods.

TABLE III.I

Comparison of differential cross section for elastic scattering of electrons by neon atom with the experimental and theoretical results for the energy of incidence 100 eV. [expressed in a_0^2/sr].

theta deg.	THEORETICAL				EXPERIMENTAL		
	Present results	Fink & Yates (1970)	Walker (1974)	Byron & Joachain (1974b,76)	Hughs McMillan (1933)	Williams et al (1975)	Jansen et al (1976)
5.0	13.8	2.98	4.40	14.3	10.3	---	10.4
10.0	8.98	2.80	4.06	10.1	7 33	9.33	7.75
20.0	4.28	2.21	3.02	4.37	3.28	4.28	4.15
30.0	1.76	1.56	1.94	1.70	1.75	2.16	2.11
40.0	6.65(-1)	1.03	1.15	6.23(-1)	1.12	1.36	1.10
50.0	2.43(-1)	6.45(-1)	6.75(-1)	2.40(-1)	5.30(-1)	6.79(-1)	6.33(-1)

TABLE III.II

Comparaision of differential cross section for elastic scattering of electrons by neon atom with the experimental and theoretical results for the energy of incidence 200 eV. [expressed in a_o^2 /sr].

theta deg.	THEORETICAL				EXPERIMENTAL	
	Present results	Walker	Byron & Joachain	Bromberg	Hughs McMillan	Jansen et al
5.0	10.9	4.96	11.2	9.75	----	9.44
10.0	7.89	4.35	7.07	6.42	6.68	6.20
20.0	2.45	2.67	2.68	2.82	2.64	2.75
30.0	8.97(-1)	1.35	9.92(-1)	1.17	9.83(-1)	1.20
40.0	3.46(-1)	6.39(-1)	3.84(-1)	5.48(-1)	4.47(-1)	5.33(-1)
50.0	1.45(-1)	3.24(-1)	1.77(-1)	2.73(-1)	2.20(-1)	2.73(-1)

TABLE III.III

Comparison of differential cross section for elastic scattering of electrons by neon atom with experimental and theoretical results for the energy of incidence 400 eV. [expressed in a_o^2 /sr].

theta deg.	THEORETICAL				EXPERIMENTAL		
	Present results	Devrajan thirumalai	Byron & Joachain OM BJ	Bromberg	Hughs McMillan	Gupta & Rees	Jansen et al
10.0	5.87	7.16	5.04	5.16	6.51	---	4.97
20.0	1.78	4.63	1.69	1.86	1.84	5.39	5.38(-1)
30.0	5.45(-1)	5.38(-1)	5.76(-1)	6.85(-1)	6.58(-1)	7.29(-1)	6.93(-1)
40.0	2.42(-1)	1.97(-1)	2.38(-1)	3.07(-1)	3.09(-1)	2.51(-1)	3.07(-1)
50.0	1.21(-1)	9.84(-2)	1.31(-1)	1.85(-1)	1.53(-1)	1.69(-1)	1.66(-1)
60.0	8.76(-2)	6.38(-2)	8.84(-2)	---	---	1.03(-1)	---
90.0	4.17(-2)	3.38(-2)	4.72(-2)	---	---	5.07(-2)	---
120.0	3.98(-2)	2.78(-2)	4.33(-2)	---	---	4.80(-2)	---
180.0	5.12(-2)	2.69(-2)	5.09(-2)	---	---	---	---

TABLE III.IV

Value of differential cross section for the process of elastic scattering of electrons by by neon atom. [expressed in a_0^2 /sr].

theta deg.	ENERGY IN eV 100	200	300	400
5.0	13.8	10.9	9.63	8.64
10.0	8.98	7.89	5.43	4.87
20.0	4.28	2.45	1.87	1.78
30.0	1.76	3.97(-1)	6.87(-1)	5.45(-1)
40.0	6.65(-1)	3.46(-1)	2.54(-1)	2.42(-1)
50.0	2.43(-1)	1.45(-1)	1.32(-1)	1.21(-1)
60.0	1.18(-1)	3.98(-2)	8.87(-2)	8.76(-2)
70.0	8.61(-2)	6.54(-2)	6.87(-2)	6.63(-2)
80.0	6.86(-2)	5.40(-2)	5.65(-2)	5.32(-2)
90.0	4.43(-2)	5.10(-2)	5.23(-2)	4.76(-2)
100.0	2.92(-2)	5.21(-2)	5.10(-2)	4.19(-2)
120.0	4.43(-2)	7.64(-2)	5.87(-2)	4.12(-2)
140.0	1.42(-1)	1.10(-1)	7.10(-1)	4.32(-2)
160.0	3.87(-1)	1.89(-1)	8.82(-1)	4.65(-2)
180.0	5.10(-1)	2.01(-1)	9.34(-1)	5.21(-2)

Fig III-1

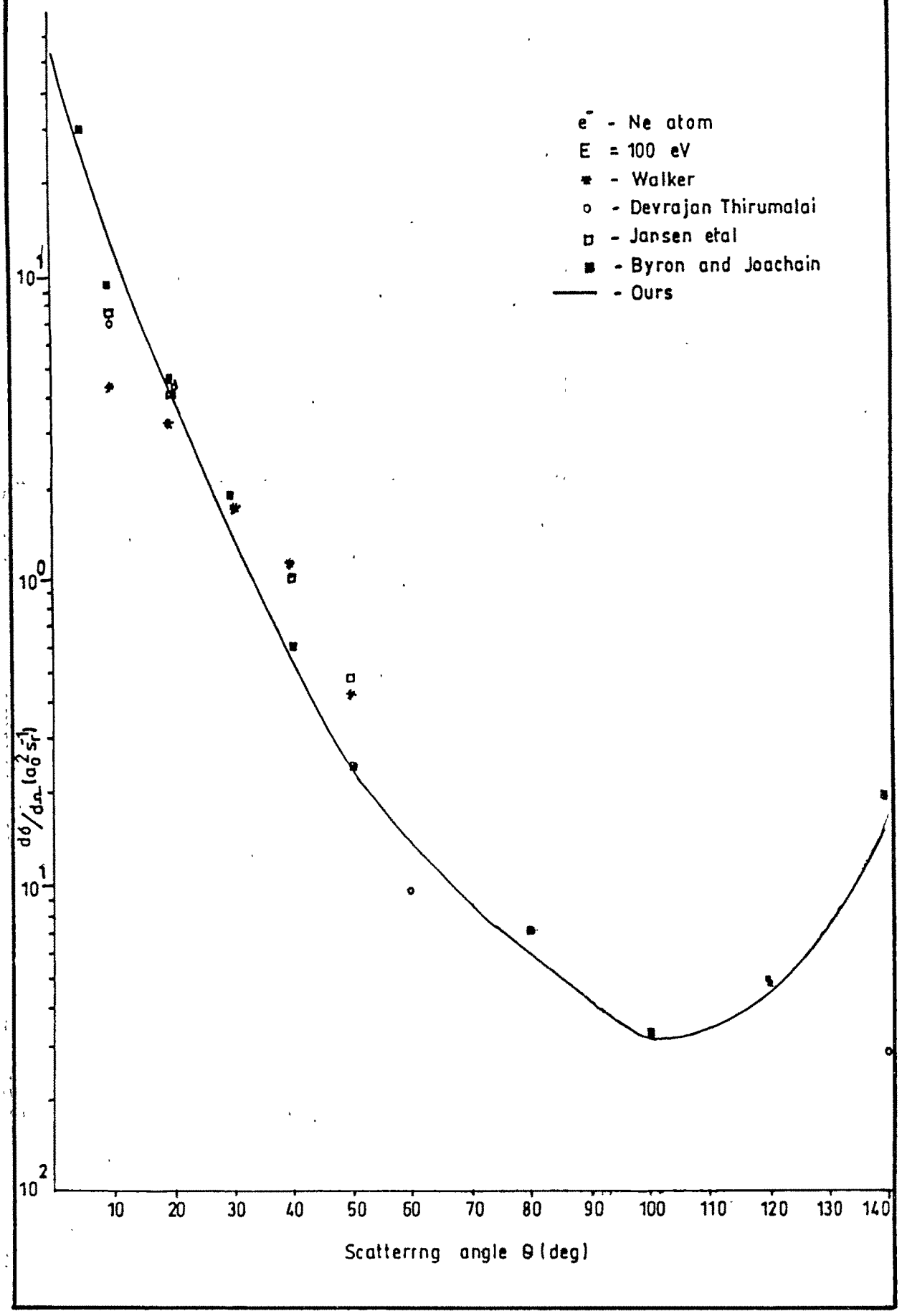

e⁻ - Ne atom
E = 100 eV
* - Walker
o - Devrajan Thirumalai
□ - Jansen etal
■ - Byron and Joachain
— - Ours
10⁻¹
10⁰
10⁻¹
10⁻²
dσ/dΩ (a₀² sr⁻¹)
10
20
30
40
50
60
70
80
90
100
110
120
130
140
Scatterrng angle θ (deg)

Fig III-II

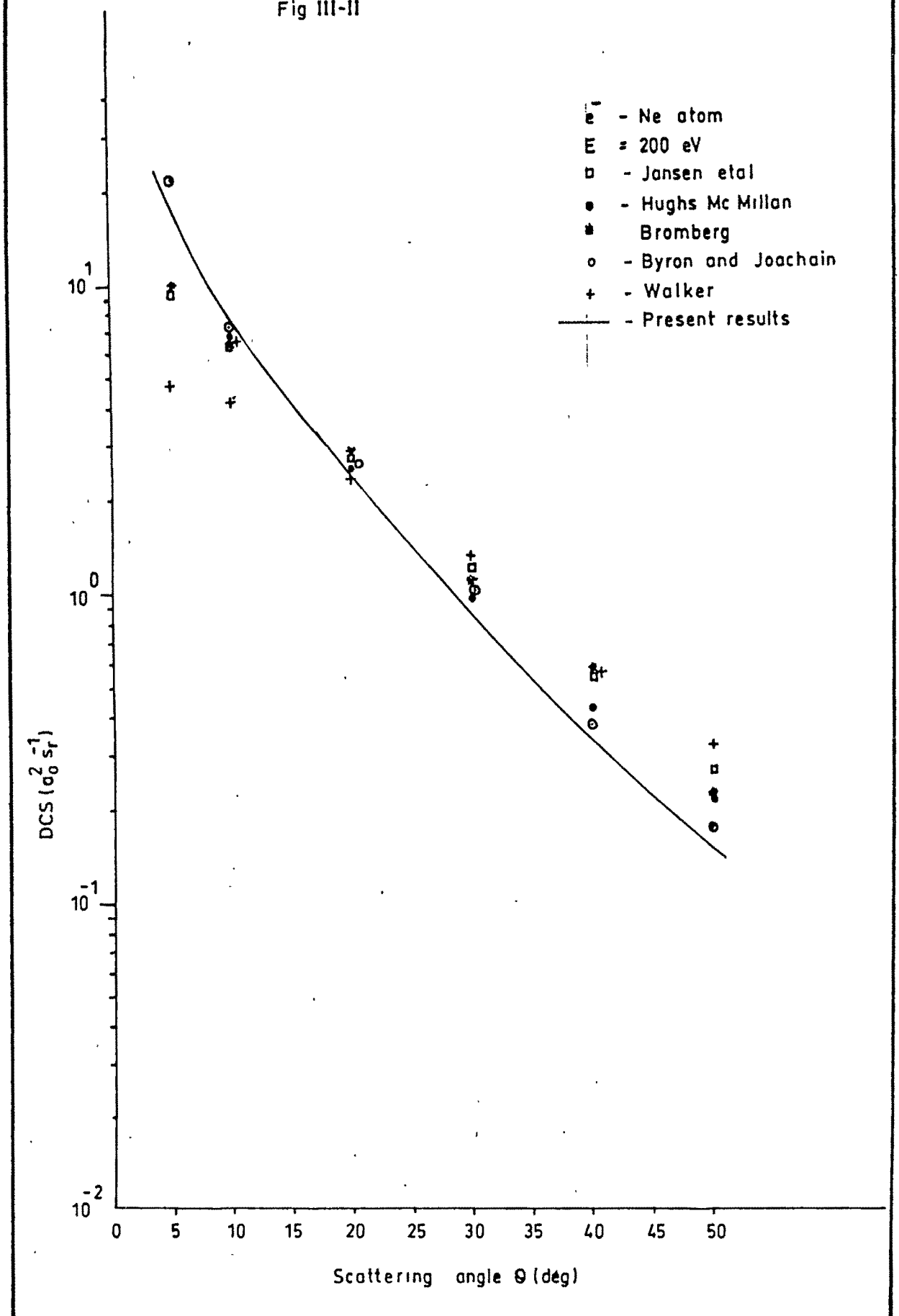

e⁻ - Ne atom
E = 200 eV
- Jansen etal
- Hughs Mc Millan
Bromberg
- Byron and Joachain
- Walker
- Present results
DCS (a_0^2 sr^{-1})
10^{1}
10^{0}
10^{-1}
10^{-2}
0 5 10 15 20 25 30 35 40 45 50
Scattering angle θ (deg)

Fig III-11

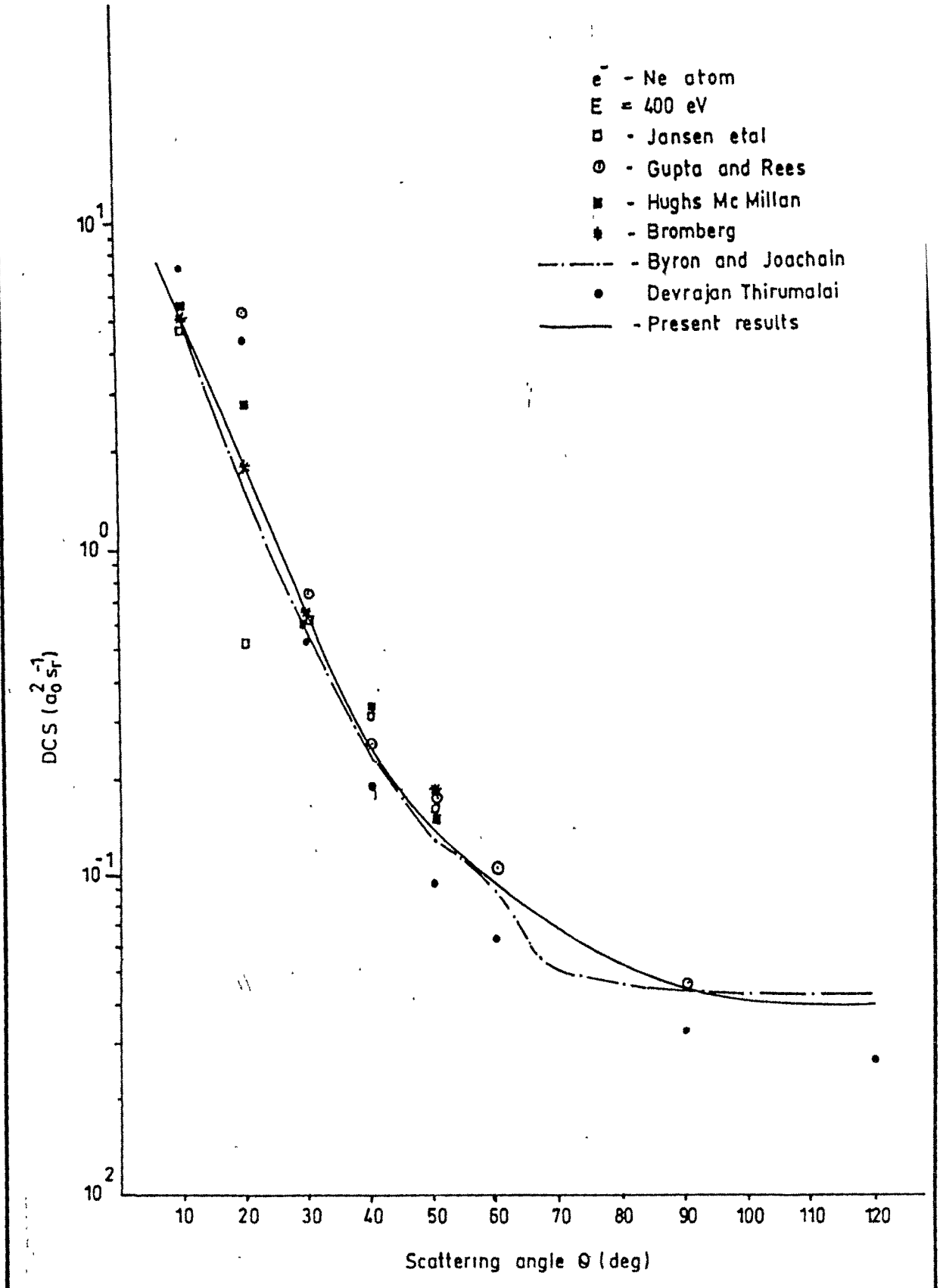
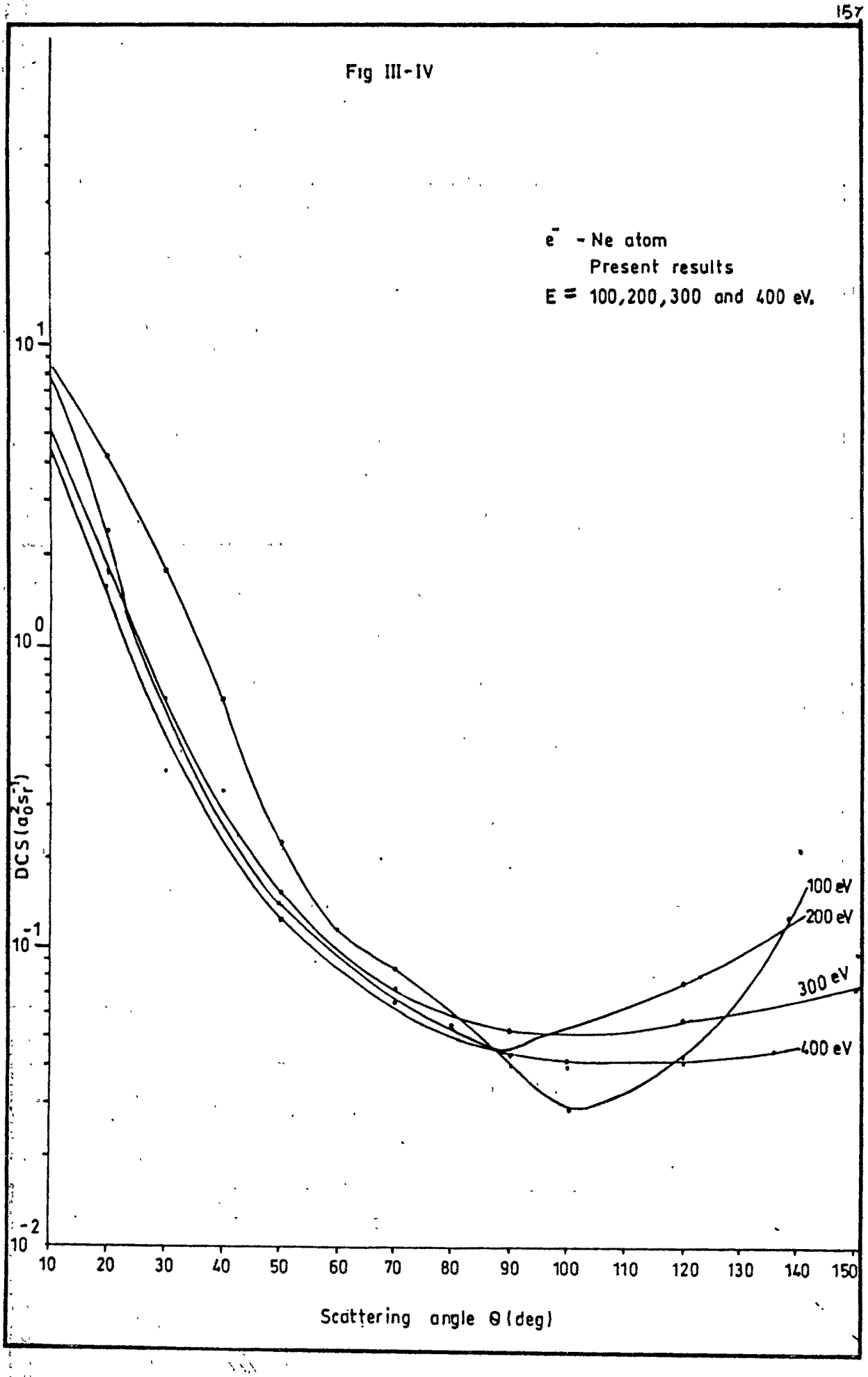

e⁻ - Ne atom
E = 400 eV
□ - Jansen etal
⊙ - Gupta and Rees
■ - Hughs Mc Millan
✱ - Bromberg
—·—·— - Byron and Joachain
● Devrajan Thirumalai
——— - Present results
DCS (a_0^2 sr^{-1})
10^1
10^0
10^{-1}
10^{-2}
10 20 30 40 50 60 70 80 90 100 110 120
Scattering angle θ (deg)

Fig III-IV


e⁻ - Ne atom
Present results
E = 100,200,300 and 400 eV.
100 eV
200 eV
300 eV
400 eV
DCS (a₀² sr⁻¹)
10 1
10 0
10 -1
10 -2
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150
Scattering angle θ (deg)