CHAPTER - IV

TWO POTENTIAL FORMULATION TO STUDY THE ELASTIC SCATTERING OF ELECTRONS BY NEON ATOM.

INTRODUCTION :

The search for an improvement over the HHOB approximation (Yates, 1979) due to the main short comings of the approximation is the appriciable over -estimation of the cross sections in the large angle region. As the scattering angle increases the differential cross sections deviate more and more from the corresponding experimental values. It is well known fact that the Born approximation gives better results for the weaker interaction potentials. Keeping this in mind, the present two -potential method is decribed.

In this chapter a brief discription of the HHOB and optical potential model and the two potential method is described. After constructing the potential (comprising of static, exchange, polarization and absorption interactions), we have carried out the partial wave analysis to study the elastic scattering cross section of electrons by neon atom. In the two potential method difference of the direct potential over the static potential is treated in the HHOB approximation, and the remaining part of the

static potential is treated using the partial wave analysis. We use our results of the elastic scattering of electrons by neon atoms calculated using the HHOB approximation for the direct interaction potential which is described in detail in chapter III. We describe here the basic theory of partial wave analysis and the calculation of the phase shift to study the elastic scattering of electrons by neon atom.

PARTIAL WAVE ANALYSIS AND CALCULATION OF PHASESHIFT :

The Schrodinger equation,

$$\left[-\frac{\hbar^2}{2m} \nabla_r^2 + V(r) \right] \psi(r) = E\,\psi(r) \qquad (1),$$

may be separated in spherical polar coordinates, and a simple connection between the radial solutions and asymptotic form of the stationary scattering wave function may be found.

This procedure, which is called the method of partial wave. Two important results, the optical theorem and the unitary relation yields from such analysis.

The copmutation of phaseshifts, which play a key role in the method of partial waves.

The Hamiltonian operator $H = -\frac{\hbar^2}{2m} \nabla_r^2 + V$, now reads in spherical polar coordinate as,

$$H = -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2} (\mathrm{Sin}^2\theta)^{-1} \frac{\partial^2}{\partial \phi^2} \right] + V(r) \qquad (2),$$

and the Schrodinger time independent equation (1) for the stationary scattering wave function ψ^{+}_{ki} can be written as,

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2}(\sin^2\theta)^{-1}\frac{\partial^2}{\partial\phi^2}\right]\psi^{(+)}_{ki}(r)+V(r)\,\psi^{(+)}_{ki}(r)=E\,\psi^{(+)}_{ki}(r) \quad (3),$$

where the operator "square of the orbital angular momentim " given by,

$$L^2=L_x^2+L_y^2+L_z^2=-\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+(\sin^2\theta)^{-1}\frac{\partial^2}{\partial\phi^2}\right. \quad (4),$$

and using

$$[L^2, L_x]=[L^2, L_y]=[L^2, L_z]=\emptyset \quad (5).$$

From (5) we deduce that one can find eigenfunctions which are common to the operators L^2 and one of the components of L.

These are the spherical harmonics $Y_{lm}(\theta,\phi)$ such that,

$$L^2\,Y_{lm}(\theta,\phi)=l(l+1)\hbar^2\,Y_{lm}(\theta,\phi) \quad (6),$$

and

$$L_z Y_{lm}(\theta,\phi)=m\hbar\,Y_{lm}(\theta,\phi) \quad (7).$$

We now return to the Hamiltonian (2) which we rewrite with the help of (4) as,

$$H=-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{L^2}{r\hbar}\right]+V(r) \quad (8),$$

so that

$$[H,L^2]=[H, L_z]=\emptyset \quad (9).$$

Expanding the scattering wave function $\psi^{(+)}_{ki}$ in partial wave

correponding to given values of the quantum numbers l and m as,

$$\psi_{ki}^{(+)}(k,r) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} C_{lm}(k)\, R_{lm}(k,r)\, Y_{lm}(\theta,\phi) \qquad (10).$$

The central problem of the method of partial wave is to take the advantage of the expansion (10) in order to obtain a convenient expression of the scattering amplitude.

Using the expansion (10) in the Schrodinger equations (6) and (8), we obtain every radial function of the equation.

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{l(l+1)}{r^2}\right] R_l(k,r) + V(r)\, R_l(k,r) = E\, R_l(k,r) \qquad (11),$$

$R_l(k,r)$ is written instead of $R_{lm}(k,r)$ since there is no dependence on magnetic quantum number m in the equation (11).

Using the new convenient unknown function

$$r\, R_l(k,r) = u_l(k,r) \qquad (12),$$

and introducing the reduced potential $U = \frac{2m}{\hbar^2} V$.

The new radial equation which are obtain from equation (11) is then,

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U(r)\right] u_l(k,r) = 0 \qquad (13).$$

There is no loss of generality in assuming that $u_l(k,r)$ is real. Since both the real and imaginary parts of a complex u_l would seperately satisfy the equation (13).

RADIAL EQUATION FOR FREE PARTICLE :

In order to solve (13) for the radial wave functions u_l it is necessary to specify the boundary conditions which must be satisfied by these equations.

Let us examine equation (13) for $u(\underline{r}) = \emptyset$, viz.,

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} \right] y_l(k,r) = \emptyset \qquad (14),$$

equation (14) is a radial equation for free particles. Changing variables to $\rho = kr$ and defining

$$f_l(\rho) = \frac{y}{\rho} \qquad (15),$$

equation (2)without interaction potential reads

$$\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} + \left(1 - \frac{l(l+1)}{r^2} \right) \right] f_l(\rho) = \emptyset \qquad (16),$$

equation (16) is known as "Spherical Bessel differential equation"

Particular solution of this equation which are often used in scattering theory are the spherical Bessel function j_l, the spherical Neumann function n_l and the spherical Hankel function $h_l^{(1)}$ and $h_l^{(2)}$.

Equation (16) is then a linear combination of two linearly independent particular solutions.

Since the pairs of functions (j_l, n_l) and $(h_l^{(1)}, h_l^{(2)})$ are linearly independent solutions of equation (16). We may write the general solution y_l of equation (16) as

$$y_l(k,r) = kr \left[C_l^{(1)}(k)\, j_l(kr) + C_l^{(2)}(k)\, n_l(kr) \right] \qquad (17),$$

or

$$y_l(k,r) = kr \left[D_l^{(1)}(k)\, h_l^{(1)}(kr) + D_l^{(2)}(k)\, h_l^{(2)}(kr) \right] \qquad (18),$$

where two pairs of "integration constants " $(C_l^{(1)}, C_l^{(2)})$ and $(D_l^{(1)}, D_l^{(2)})$ may still of course depends on k.

BOUNDARY CONDITION :

The radial equation (13) to be examined using the boundary conditions which we must impose upon the radial functions $u_l(k,r)$. Outside the "range" of the potential we may use equation (17) to express $u_l(k,r)$ as,

$$u_l(k,r) = kr \left[C_l^{(1)}(k)\, j_l(kr) + C_l^{(2)}(k)\, n_l(kr) \right], \; r >> a \qquad (19).$$

Assuming r so large that the terms u(r) and $l(l+1)/r^2$ may be neglected in equation (13).

An asymptotic solution is then obeviously of the form $\exp(\pm ikr)$. We may write for large r

$$u_l(k,r) = F_l(k,r) \exp(\pm ikr) \qquad (2\emptyset),$$

$F_l(k,r)$ is slowly varying function of r to be determined. Substitution of (2Ø) in (13), we find

$$\frac{F_l''}{F_l} \pm 2ik \frac{F_l'}{F_l} = W_l(r) \qquad (21),$$

where we have set

$$W_l(r) = u(r) + l(l+1)/r^2 \qquad (22),$$

we have

$$F_l' = \frac{dF_l}{dr} \quad , \quad F_l'' = \frac{d^2F_l}{dr^2}$$

since F_l'' is a slowly varying function we may drop F_l''/F_l in equation (21) and write

$$\pm 2ik \frac{F_l'}{F_l} = W_l(r) \qquad (23),$$

for large r

$$F_l(k,r) = \exp\left[\pm \frac{1}{2ik} \int_0^r W_l(r')\, dr' \right] \qquad (24),$$

therefore, if

$$\lim_{r\to\infty} | u(r) | < m/r^{l+1} \qquad (25),$$

where m is some constant greater then zero. We deduce (24) that the function F_l is independent of r for $r \to \infty$. Thus if the condition (25) satisfied the gengeral solution of equation (24) for large r given by,

$$u_l(k,r) = B_l^{(1)}(k)\ e^{ikr} + B_l^{(2)}\ e^{-ikr} \qquad (26),$$

where $B_l^{(1)}(k)$ and $B_l^{(2)}(k)$ are independent of r. using the facts

$$j_l(x) \xrightarrow[x\to\infty]{} -\frac{1}{x} \sin\left(x - \frac{l\pi}{2} \right) \qquad (27a),$$

$$n_l(x) \xrightarrow[x\to\infty]{} -\frac{1}{x} \cos\left(x - \frac{l\pi}{2} \right) \qquad (27b),$$

$$h_l^{(1)}(x) \xrightarrow[x\to\infty]{} -i\,\frac{\exp\{i(x-l\pi/2)\}}{x} \qquad (27c),$$

$$h_l^{(2)}(x) \xrightarrow[x\to\infty]{} i\,\frac{\exp\{i(x-l\pi/2)\}}{x} \qquad (27d).$$

We may use equation (26) in the form of equations (17) or (18). Thus we have, inaccordance with the equation (19),

$$u_l(k,r) \xrightarrow[x\to\infty]{} kr\,[\,C_l^{(1)}(k)\,j_l(kr) + C_l^{(2)}(k)\,n_l(kr)] \qquad (28),$$

or

$$u_l(k,r) \xrightarrow[x\to\infty]{} kr\,[\,D_l^{(1)}(k)\,h_l^{(1)}(kr) + D_l^{(2)}(k)\,h_l^{(2)}(kr)] \qquad (29).$$

Coulomb field which falls off like r^{-1} as $r \to\infty$ does not satisfy the condition (25), so that equations (28) - (29) are not valid for coulomb interaction.

We may use equation (27) to express boundary condition (28) or (29) in slightly different manners. For example, from equations (27a) and (27b), we obtain

$$u_l(k,r) \xrightarrow[x\to\infty]{} A_l(k)\sin\left[\,kr - \frac{l\pi}{2} + \delta_l(k)\,\right] \qquad (30),$$

with

$$A_l(k) = \{\,[C_l^{(1)}(k)\,]^2 + [\,C_l^{(2)}(k)\,]^2\,\}^{1/2} \qquad (31a),$$

and

$$\tan\delta_l(k) = -\,C_l^{(2)}(k)/\,C_l^{(1)}(k) \qquad (31b).$$

We note that equations (12), (28) and (31b) also imply that

$$R_l(k,r) \xrightarrow[r\to\infty]{} \tilde{A}_l(k)\,[\,j_l(kr) - \tan\delta_l(k)\,n_l(kr)\,] \qquad (32),$$

where $\hat{A}_l(k)$, is independent of r. Quantities δ_l ,which are called the phase shifts, display the influence of interaction.

THE PHASE SHIFTS :

Knowledge of phase shifts allows one to obtain the scattering amplitude by means of the important relation

$$f(k,\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [\exp\{2i\delta_l(k)\} - 1] P_l(\cos\theta) \qquad (33),$$

we may write

$$f(k,\theta) = \sum_{l=0}^{\infty} (2l+1) a_l(k) P_l(\cos\theta) \qquad (34),$$

where the partial wave amplitudes $a_l(k)$ are such that

$$a_l(k) = \frac{1}{2ik} [\exp\{ 2i\delta_l(k)\} - 1] = \frac{1}{2ik} [S_l(k) - 1] \qquad (35),$$

rewritting equation (33) again as

$$f(k,\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp\{ i\delta_l(k)\} \sin\delta_l(k) P_l(\cos\theta) \qquad (36),$$

while (35) becomes

$$a_l(k) = \frac{1}{k} \exp\{ i\delta_l(k) \} \sin\delta_l(k) \qquad (37).$$

Now let us deduce the relation between the phase shift and the interaction potential. For that let us consider the scattering

by two reduced potential u(r) and $\bar{u}(r)$, with respective radial equations as,

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - u(r) \right] u_l(r) = \emptyset \qquad (38a),$$

and

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \bar{u}(r) \right] \bar{u}_l(r) = \emptyset \qquad (38b),$$

u_l and $\bar{u}_l$ are normalized. Hence,

$$u_l(r) \xrightarrow[r \to \infty]{} \frac{1}{k} \left[\sin\left(kr - \frac{l}{2}\pi\right) + \cos\left(kr - \frac{l}{2}\pi\right) \tan\delta_l \right] \qquad (39a),$$

and

$$\bar{u}_l(r) \xrightarrow[r \to \infty]{} \frac{1}{k} \left[\sin\left(kr - \frac{l}{2}\pi\right) + \cos\left(kr - \frac{l}{2}\pi\right) \tan\bar{\delta}_l \right] \qquad (39b).$$

The Wronskian of the two solutions u_l and $\bar{u}_l$ is defined as,

$$W(u_l, \bar{u}_l) = u_l \bar{u}_l' - u_l' \bar{u}_l \qquad (4\emptyset),$$

where the prime denotes the derivatives with respect to variable r. Multiplying equation (38a) by $\bar{u}_l$, equation (38b) by u_l and substracting the terms we have

$\bar{u}_l u_l'' - u_l \bar{u}_l'' - (u - u') u_l \bar{u}_l = \emptyset$ or

$$\frac{d}{dr} W(u_l, \bar{u}_l) = -(u - u') u_l \bar{u}_l \qquad (41),$$

upon integration over variable r in the interval [a,b]. We deduce that,

$$[\ W(u_l,\bar{u}_l)\ ]_a^b = -\int_a^b \bar{u}_l(r)\ [u(r) - \bar{u}(r)]\ u_l(r)\ dr \qquad (42),$$

choosing a = Ø and b = α and using $u_l(Ø) = \bar{u}_l(Ø) = Ø$ and with the help of equation (39) that,

$$\tan\delta_l - \tan\bar{\delta}_l = - k \int_Ø^\infty \bar{u}_l(r)\ [u(r) - \bar{u}(r)]\ u_l(r)\ dr \qquad (43),$$

provided that u(r) and $\bar{u}(r)$ tend to zero faster then r^{-1} when r--->∞ . Also it is must that the potential u(r) and $\bar{u}(r)$ should not be more singular than r^{-2} at origin.

Since $u_Ø(r) \sim r$ as r -->Ø for $\bar{u}$ = Ø, equation (43) reduces to an important integral representation,

$$\tan\delta_l = - k \int_Ø^\infty j_l(kr)\ u(r)\ R_l(r)\ r^2\ dr \qquad (44),$$

where $R_l(r)$ the radial function is normalized. Equation (43) provides the dependence of the phase shifts on the potential.

CALCULATION OF PHASE SHIFT :

Phase shift expression can be obtained if one solves the radial equations (11) and (13) numerically.

Solution obtained inside the range of the potential must go over smoothly to the "asymptotic " solution, valid outside the range of the interaction.

When the potential has a strict finite range, i.e. vanishes for r > a, one can devide the domain of the variable r into an

interval region (r <a) and an external region (r>a).

The boundary condition at r = a are then that both R_l and $\frac{dR_l}{dr}$ [or u_l and $\frac{du_l}{dr}$] be continous at r=a.

Now exterior solution can be written as,

$$R_l(k,r) = \hat{A}_l(k) [j_l(kr) - \tan\delta_l \, n_l(kr)] \qquad (45).$$

Thus, if we denote by

$$\gamma_l = [R_l^{-1} (\frac{dR_l}{dr})]_{r=a} \qquad (46),$$

value of logarithmic derivative of the interior solution $R_l(k,r)$ at r = a, we find that

$$\gamma_l(k) = \frac{k [j_l'(ka) - \tan\delta_l(k) \, n_l'(ka)]}{j_l(ka) - \tan\delta_l(k) \, n_l(ka)} \qquad (47),$$

where we have defined

$$j_l'(ka) = [\frac{dj_l(x)}{dx}]_{x = ka} \quad \text{and} \quad n_l'(ka) = [\frac{dn_l(x)}{dx}]_{x = ka}.$$

Hence,

$$\tan\delta_l(k) = \frac{k \, j_l'(ka) - \gamma_l(k) \, j_l(ka)}{k \, n_l'(ka) - \gamma_l(k) \, n_l(ka)} \qquad (48).$$

If the potential does not vanish identically beyond a certain value of r, but has nevertheless a " range ", one can choose a distance d ≥ a at which the influence of the potential is negligible.

The value of the logarithmic derivative of the interior solution is then matched at r=d with that of the exterior solution (free), in that case

$$\tan\delta_l(k) = \frac{k\, j_l'(kd) - \gamma_l(k)\, j_l(kd)}{k\, n_l'(kd) - \gamma_l(k)\, n_l(kd)} \qquad (49).$$

Phase shift so obtained are insensitive (within the accuracy required) to any increase in the quantity d.

The potentials having a strict finite range and those having a " range " will then be treated on the same footing.

Let us discuss the behavior of the phase shift at low , high and at intermediate energies with the scattering length. We also discuss here the behavior of the phase shift with the partial wave.

Scattering at low energies is isotropic.

$l = 0$ and $ka << 1$,

$$\tan\delta_0(k) = ka\, \frac{q_0(k) - 1}{1 - 3(ka)^{-2} q_0(k)} \qquad (50),$$

where k tend to zero , the quantity $\tan\delta_l$ behaves as k^{-1}. So that the phase shift δ_0 reaches the value $\frac{\pi}{2}$ (modulo π) in this case S -matrix element S_0 and S wave amplitude $a_0(k)$ are such that,

$$S_0(k) \underset{k \to 0}{\sim} -1 \quad ; \quad a_0(k) \underset{k \to 0}{\sim} \frac{i}{k} \qquad (51).$$

BEHAVIOR OF THE PHASE SHIFT FOR LARGE l :

Increase in the value of the l (for fixed k) tends to diminish the importance of a given potential of finite range because of the centrifugal barrier term $l(l+1)/r^2$ appearing in the radial equation (13).

We expect that the phase shifts $\delta_l(k)$ will tend to zero (modulo π) as $l \longrightarrow \infty$ (for fixed k).

For a potential of finite " range ", we have already shown that the radial function R_l will differ little from the corresponding free wave j_l when $l >> ka$. Hence we may write,

$$\tan\delta_l = (\tan\delta_l)_{Bl} = - k \int_0^\infty [\, j_l(kr)\,]^2 U(r)\, r^2\, dr \quad (l>>ka) \quad (52),$$

where $(\tan\delta_l)_{Bl}$ - first Born approximation to $\tan\delta_l$. If the potential has a strict finite range, we may use the approximate formula fof j_l to obtain simple estimate as

$$\tan\delta_l \underset{l>>ka}{\sim} \frac{-k^{2l+1}}{[(2l+1)!!]^2} \int_0^\infty r^{2l+2}\, u(r)\, dr \qquad (53),$$

in case of the square well (reduced) potential u(r) such that

$$u(r) = \begin{cases} -u_0, & r < a \\ 0, & r > a \end{cases} \qquad (54).$$

We deduce (53) that

$$\tan\delta_l \underset{l>>ka}{\sim} u_0\, a^2\, \frac{ka^{2l+1}}{[(2l+1)!!]^2(2l+3)} \qquad (55),$$

for $l >> ka$ (for fixed k) quantities $\tan\delta_l$ falls off rapidly as l increases. In fact, we have

$$\frac{\delta_{l+1}}{\delta_l} = \left(\frac{k}{2}\frac{a}{l}\right)^2 \qquad l >> ka, \qquad (56).$$

It worth watching that simple formula (53) can not be used for interaction potential which have a sizeable "tail", since the major contribution to the integral (52) comes from the region near the point $r_\emptyset = -\frac{l}{k}$, where the function $j_l(kr)$ takes as significant values. Hence in the case in particular for the Yukawa potential

$$U(r) = U_\emptyset \frac{e^{-r/a}}{r} \qquad (57),$$

for the potential having the form $U_\emptyset/r^2$ for large r.

PHASE SHIFT AT HIGH ENERGIES :

i.e. for a case where l is fixed and $k \longrightarrow \infty$.

Importance of the potential will become vanishingly small so that the radial function R_l will again be very close to the corresponding free wave.

Using equation (52) (large x) and with the asmptotic form. We deduce

$$\tan\delta_l \underset{k\to\infty}{\sim} -\frac{1}{2} k^{-1} \int_\emptyset^\infty U(r)\, dr + O(k^{-2}) \qquad (58).$$

Phase shift $\delta_l(k) \longrightarrow \emptyset$ (modulo π) as $k \to \infty$. This suggest that

a reasonable absolute definitions of phase shift may be requiring that,

$$\lim_{k\to\infty} \delta_l(k) = \emptyset \qquad (59).$$

We require that $\delta_l = \emptyset$ when particle is effectively free.

We can separate out the terms of equation (36) in the real and imaginary parts of the f(k,θ). We also obtain for the total elastic cross section given by,

$$\sigma_{tot}^{el} = \frac{4\pi}{k^2} \text{ Im } f(\theta = \emptyset) \qquad (60),$$

known as the optical theorem.

Having dicussed the method of the partial wave analysis and how the calculation of the phase shift is to be carried out and the behavior of the phase shift for large l (fixed k) and for high k (fixed l), we apply this method to study the elastic scattering of electron by neon atom in the two potential method.

If we look at the interaction potentials expression and if such interaction is studied then we can say that the interaction is strong enough. We also know that when the interaction is too strong and if one applies the HHOB theory then still one concludes that there may not be a accuracy at large angle. To study the scattering at large angle we have to make the total potential weak enough so that we can rely upon the accuracy in the measurements of the cross sections. Hence we write the total potential in the two potential method as follows.

$$V = \{ V_d - V_{st1} \} + V_{st2} \qquad (61).$$

Here we have already done the calculation considering the V_d part which is reported in the chapter III. Here we calculate the V_{st1} part using the static potential of the simple form in the HHOB approximation, where we use the Cox -Bonhamm parameters. Hence from the full interaction the contribution due to the static part is substracted. This makes the interaction weak. The remaining part of the potential i.e. V_{st2} we treat this through the partial wave analysis. Which is found to give more accurate information about the scattering. Hence using this picture of the two potential method we again calculate the differential cross section and using optical theorem we calculate the total cross section.

The static potential given by Bonham and Strand (1963) is chosen and is of the form for neon atom as,

$$V_{st}(r) = -10 \sum_{j=1}^{6} \gamma_j \frac{e^{-\lambda_j r}}{r} \qquad (62),$$

which is simple in view of the analytical purposes and same formulation can be extended to different atoms with changes in γ_j and λ_j . The γ_j's and λ_j's for neon atom is given below.

$\lambda_1 = 2.7495$; $\lambda_2 = 22.8979$; $\lambda_3 = 9.5848$; $\lambda_4 = 15.8901$;
$\lambda_5 = 8.5939$; $\lambda_6 = 14.8774$ and
$\gamma_1 = 1.2524$; $\gamma_2 = -0.2468$; $\gamma_3 = 3.5572$; $\gamma_4 = 1.7522$;
$\gamma_5 = -3.5758$; $\gamma_6 = -1.7401$.

Now the scattering amplitude in the HHOB approximation id given by,

$$f_{HHOB} = f^{(1)}_{i-->f} + \text{Re}1\ f^{(2)}_{HEA} + \text{Re}\ 2\ f^{(2)}_{HEA} + i\ \text{Im}\ f^{(2)}_{HEA} + f^{(3)}_{GES} \qquad (63).$$

We have to evaluate various terms using the static potential of the form (62).

First we evluate the first Born term appearing in expression of the scattering amplitude in the HHOB approximation. We write

$$f_{B1} = -\frac{1}{2\pi} \int e^{iq\cdot r} \quad V(r)\ dr \qquad (64),$$

where we substitute $V(r)$ by the static potential of the form given by (61).

$$f_{B1} = \frac{10}{2\pi} \sum_{j=1}^{6} \gamma_j \int e^{iq\cdot r} \quad \frac{e^{-\lambda_j r}}{r}\ dr \qquad (65),$$

further simplifying the above as,

$$f_{B1} = 10 \sum_{j=1}^{6} \gamma_j \int_0^{\infty} e^{-\lambda_j r} \sin qr\ dr \qquad (66),$$

reduces to

$$f_{B1} = 20 \sum_{j=1}^{6} \gamma_j \frac{1}{q^2+\lambda_j^2} \qquad (67).$$

Now the imaginary part of the 2nd Born term in the HHOB theory is given by,

$$\text{Im}\ f^{(2)}_{HEA} = \frac{4\pi}{k_i^3} \int dp\ U^{(2)}_{fi}\ (\ldots\ ;\ \ldots\ldots) \qquad (68),$$

where the term $U^{(2)}_{fi}$ is given by,

$$U_{fi}^{(2)} = \bar{V}_1 (\underline{p} + p_z \hat{y}) \; \bar{V}_2 (| \underline{q} - \underline{p} | - p_z \hat{y}) \qquad (69).$$

For the given potential we have,

$$U_{fi}^{(2)} = \frac{1}{4\Pi^4} \sum_i \sum_j \frac{\gamma_i \gamma_j}{(p^2 + p_z^2 + \lambda_i^2)\; (|\underline{q} - \underline{p}|^2 + p_z^2 + \lambda_j^2)}$$

so that

$$\text{Im } f_{HEA}^{(2)} = \frac{4\Pi^3}{k} \int d\underline{p} \; \bar{V}_1 \; \bar{V}_2$$

reduces to a form

$$= \frac{10}{\Pi k} \sum_i \sum_j \gamma_i \gamma_j \; \frac{\Pi}{\zeta} \ln \left[\frac{2\zeta^2 + b(\beta^2 + \lambda_i^2) + 2\zeta y}{(\beta^2 + \lambda_i^2)\; (b + 2\zeta)} \right] \qquad (70),$$

where,

$$\zeta^2 = (q^2 - \lambda_i^2 + \lambda_j^2)^2 + 4q^2(\beta^2 + \lambda_i^2) \quad ; \quad b = -2q^2 - \lambda_i^2 + \lambda_j^2$$

and

$$y = [\; (\beta^2 + \lambda_i^2)^2 + (\beta^2 + \lambda_i^2) b + \zeta^2 \;]^{1/2}.$$

For the term $O(k_i^{-1})$ real part of the second Born term given as

$$\text{Re1 } f_{HEA}^{(2)} = - \frac{4\pi^3}{k} \mathcal{P} \int d\underline{p} \int_{-\alpha}^{+\alpha} \frac{dp_z}{(p_z - \beta)} \frac{1}{(p^2 + p_z^2 + \lambda_i^2)\; (|\underline{q} - \underline{p}|^2 + p_z^2 + \lambda_j^2)} \qquad (71),$$

where $\bar{V}_1 \bar{V}_2$ given by (62) and $\mathcal{P}$ stands for the principal value of integral.

Hence,

$$\text{Re1 } f_{HEA}^{(2)} = - \frac{1}{k} \frac{1}{\pi} 2 \sum_i \sum_j \gamma_i \gamma_j \; I_{st} \qquad (72),$$

where,

$$I_{st} = \mathcal{P} \int d\underline{p} \int_{-\infty}^{+\infty} \frac{dP_z}{(p_z - \beta_i)} \frac{1}{(p^2 + p_z^2 + \lambda_i^2)\ (|\underline{q} - \underline{p}|^2 + p_z^2 + \lambda_j^2)} \tag{73}$$

The derivation of which is given in appendix. Now, the term through $O(k_i^{-2})$ real part of the second Born term is written as,

$$\mathrm{Re2}\ f_{HEA}^{(2)} = -\frac{2\pi^2}{k_i^2} \frac{\partial}{\partial \beta_i} \mathcal{P} \int d\underline{p} \int_{-\infty}^{+\infty} \frac{dP_z}{(p_z - \beta_i)} (p^2 + p_z^2)\ \bar{V}_1\ \bar{V}_2 \tag{74},$$

$$= -\frac{1}{2\pi^2 k_i^2} \sum_i \sum_j \mathcal{P} \frac{\partial}{\partial \beta_i} \int d\underline{p} \int_{-\infty}^{+\infty} \frac{dP_z}{(p_z - \beta_i)} \frac{1}{(p^2 + p_z^2 + \lambda_i^2)\ (|\underline{q} - \underline{p}|^2 + p_z^2 + \lambda_j^2)}$$

$$\mathrm{Re2}\ f_{HEA}^{(2)} = -\frac{1}{2\pi^2 k_i^2} \sum_i \sum_j \gamma_i \gamma_j \frac{\partial}{\partial \beta_i} \{ \mathcal{P} \int d\underline{p} \int_{-\infty}^{+\infty} \frac{dP_z}{(p_z - \beta_i)}$$

$$\frac{1}{|\underline{q} - \underline{p}|^2 + p_z^2 + \lambda_j^2} - \lambda_i^2 \mathcal{P} \int d\underline{p} \int_{-\infty}^{+\infty} \frac{dP_z}{(p_z - \beta_i)}$$

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

$$= -\frac{1}{2\pi^2 k_i^2} \sum_i \sum_j \gamma_i \gamma_j \frac{\partial}{\partial \beta_i} [\ I_3(\beta, \lambda_j^2) - \lambda_i^2 I_{st}\ ] \tag{75},$$

where $I_3(\beta, \lambda_j^2)$ is the same as I_3 integral which is already defined in chapter III and I_{st} is defined as above and the method of evaluating such integrals is described in detail in the appendix.

We write the scattering amplitude for the static potential using the HHOB theory as,

$$f_{HHOB} = f^{(1)}_{i-->f} + i\ Im\ f^{(2)}_{HEA} + Re1\ f^{(2)}_{HEA} + Re2\ f^{(2)}_{HEA} + f^{(3)}_{QES} \qquad (76).$$

Now to evaluate the V_{st2} part which we treat using the partial wave analysis. Having discussed the partial wave analysis and the behavior of the phase shift for large l (fixed k) and for high k (fixed l). We write the scattering amplitude as,

$$f = -\frac{1}{k} \sum_{l} (2l + 1)\ P_l(\cos\theta)\ e^{i\delta l}\ \sin\delta_l \qquad (77),$$

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

$$f = -\frac{1}{k} \sum_{l=\emptyset}^{N} (2l + 1)\ P_l(\cos\theta)\ e^{i\delta l}\ \sin\delta_l + f^{(1)}_B - -\frac{1}{k} \sum_{l=\emptyset}^{N}$$

$$(2l+1)\ P_l(\cos\theta)\ \delta^{(B)}_l \qquad (78),$$

through which we are considering the partial wave analysis for l=Ø to ∞ . Here, $f^{(1)}_B$ is the Ist Born amplitude for V_{st} and δ_l and $\delta^{(B)}_l$ are the exact and Born phase shift respectively.

The N -value is obtained by matching the two phase shift values. The Born phase shift $\delta^{(B)}_l$ for the static potential (62) is given by

$$\delta_l^{(B)} = \frac{10}{k} \sum_{j=1}^{6} \gamma_j \; Q_l \left(\frac{2k_i^2 + \lambda_j^2}{2k_i^2} \right) \qquad (79).$$

For the evaluation of the exact phase shift δ_l correspondingly, the value of V(x) is ,

$F(x) = \frac{l(l+1)}{x^2} - k_i^2 + 2\,V(x)$ has to be taken as

$$V(x) = -10 \sum_j \gamma_j \frac{e^{-\lambda_j x}}{x} \; . \qquad (80).$$

There after same procedure has to be followed for the solution of the differential equation and evaluation of the phase shift. After obtaining the two phase shifts $\delta_l^{(B)}$ and δ_l ; their values may be matched to fix value of N suitably. To calculate the phase shift one has to solve the second order differential equation. We use the Numerov method for the evaluation with the predictor -corrector method, where the step height is calculated automatically.

The first Born amplitude f_{B1} for the static potential (62) is,

$$f_{B1} = -\frac{1}{2\pi} \int dv \; e^{iq\cdot r} \; V_{st}(r) \qquad (81),$$

which can be evaluated using the standard integration techniques as,

$$f_{B1} = 20 \sum_{j=1}^{1} \frac{\gamma_j}{(q^2 + \lambda_j^2)} \qquad (82).$$

Hence, knowing all the quantities in the scattering amplitude, the Differential cross section for the e Ne process can be calculated as,

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

This method which is formulated here, is an attempt to check the feasibility of the two -potential method within the framework of the recent HHOB approximation. This formulation was aimed at the improvement of the HHOB approximation, particularly in the large scatterinig angle region. The value of DCS and TCS are calculated and it is observed that the results through this method is better than their HHOB approximation. The partial wave summation was taken with a view to account for the infinite number of partial waves. For this purpose, the method suggested by Jhanwer et al (1978) was used, which involves the exact Born phase shifts and their comparison . The phase shifts was generated with the aid of computer. The present method can be extended to other atom also.

RESULTS AND DISCUSSION :

Here we neglect the third Born term because of the following reason.

It is found that even for the whole interaction V_d the contribution due to this term is very small. Hence in the present

case where the interaction is $V_d - V_{st}$, the contribution will be still less.

It is observed during the process of evaluation of the various terms in the scattering amplitude in the HHOB theory that the contribution due to the Re2 term in the Born approximation is spuriously large. Hence, the inclusion or exclusion of the less significant third Born term does not make much of a difference because Re 2 and fB_3 are of the same order.

The evaluation of the third Born term, further increses the computation complexity.

In order to have a comparison of the present two -potential method results with the simple HHOB results, the two -potential results excluding the third Born term may be compared with the HHOB results excluding the contribution of the same term. Hence the comparison is justified.

The differential cross section and the total cross sections are calculated for the elastic scattering of electrons by a neon atom process in the two -potential HHOB formulation as discussed above for a variety of incident energies and wide range of scattering angle. The present two potential method results are shown at incident energies for 100, 200 and 500 eV along with the other theoretical (Byron and Joachain (1975)and etc.) and experimental results (Jansen et al (1976), R D Du Bois and Rudd (1975), Gupta and Rees (1975), Williams and Crowe (1975)) and others.

We also compare our own results of the HHOB theory with the direct interaction potential which is discussed in detail in chapter III. We conclude at the end of the chapter III, that since the HHOB theory is basically a good approximation for high energy and small scattering anlge. It may not give a very good results at the large scattering angle. We found that at small scattering angle the results are in better agreement as compare to the large scattering angle also. This is due to the strong interaction potential.

With the two -potential method we make the interaction weak enough so that we can expect more accurate information and differential cross section at large scattering angle. As expected and since the rest part of the potential where the partial wave analysis is employed accurately, we find that there has been a considerable amount of improvement in the results at the large scattering angle.

Hence we conclude that the present method gives better agreement over the entire angular region.

Since the two -potential method discussed here was basically an attempt to improve upon the HHOB method of Yates (1979), the real comparison should be made between the results produced in the chapter III and the present method of approach. They are compared graphically by the curve A and B, and they are also compared with the other theoretical and experimental results as discussed in the chapter III.

However, this type of reasonable comparison between the curves asserts that the improvements whatsoever obtained are due to the approximation introduced and not due to the inclusion or exclusion of any particular term. Thus avoiding the laborious third Born evaluation finds enough justification.

In the HHOB approximation Re $f_{HEA}^{(3)} = f_1^{(3)} + f_2^{(3)}$ and if $\beta = \emptyset$, then only $f_1^{(3)}$ remains such that Re $f_{HEA}^{(3)}(\beta=\emptyset) = f_1^{(3)}(\beta=\emptyset) = f_{GES}^{(3)}$. In the high energy approximation, $\beta = \Delta E/k_i$ being very small, it can be approximated as zero in practical situations for the sake of simplicity. The contribution of β in the scattering amplitudes is small, when compared to the important part played by it in saving some of the integrals from the divergence problem (comparison between GES and HHOB integrals), hence the significane of the β factor. Keeping all this in mind, third Born term can be approximated to the third GES term within a certain accuracy. Thus the present study and the HHOB calculations were done incorporating the third GES term. The detail calculation and the basic formulaes of the GES method (approximation) is given in chapter II. The calculation of the third GES term for the elastic scattering of electrons by neon atom is discussed and given in detail in the chapter III.

The main attraction of the present two -potential method in the HHOB approximation is that it gives reasonably good agreements even at low energies, for the entire angular range. This is due to the reason that, since the total interaction

potential V_d is replaced by a reduced interaction i.e. $V_d - V_{st1}$ in the two -potential method, the lower limit of E can be pulled down slightly such that $\frac{V}{E} < < 1$. Hence the approximation should give better results than in the simple HHOB approximation in the case of low enregy of incidence also. From the comparison one can readily observed that as expected the results improve with higher incident energies. But the most covatable feature of the present two -potential method results is the very satisfactory cross sections in the large scattering angle region. The general experience is that many a theory which gives quite good results at small angle, gives poorer results at large scattering angles. Same is the case with the HHOB approximation of Yates (1979). Hence, the improvement of the present two -potential method is the most significant in the large scattering region. At all incident energies, the two -potential method results are far better than the simple HHOB approximation at large scattering angles.

In light of the above discussion, the conclusion can be drawn that the two -potential method in the HHOB approximation as derived in this chapter, improves the basic HHOB approximation of Yates (1979). We report here the calculation of the differential cross section and total cross section for the elastic scattering of electrons by neon atom. The comparison is made with the same experimental and theoretical methods compared in the chapter III.

First we study the process described for the incident energy of 100 eV. We have compared the results in the tabular form

One can observe that the discrepancy observed in the results produced in the chapter III at the large scattering angle has reduced a lot. Hence for the whole angular range the results are comparable and are found in better agreement.

We also find that as the energy of incidence increases further the accuracy also increases. This one can observe for the incident energy 200 eV. The results improves further. We have given the comparison of the results at this incident energy in the tabular form.

We have done the calculation for the energy range varying from 100 to 700 eV . We find that the results are getting closer and closer for the high energy of incidence. We also find that with the present method of approach the agreement is better at the large scattering angle. The results are much better in agreement at the small angular region.

We also compare the results produced by us, by taking the ratio of the previous absolute experimental measurements and theoretical calculations with the present data. A comparision of the type by means of ratio is given in the table IV.III. We conclude by this comparasion that the present method of approach and the results are in better agreement as compare to other methods described above. We find that as the energy of incidence increases the discrepancy reduces faster in comparasion with the other methods described. Also the results produced for the large

scattering angle match well compare to the methods described earlier.

Hence, looking at the simplicity in the method used and the method of calculation of the two -potential in the HHOB approximation gives very good comparasion for the wide variety of enrgies and for wide angular range. Further, the avoiding the computational complexity in the calculation and the numerical techniques used for the calculation of the phase shifts is self starting. Where the computer programm is so prepared that it can generates the phase shifts for very large number of partial wave, but the main problem is the computer machine used takes lot of time for the calculation. We also know that for fixed incident energy when we increase the number of partial wave to a large value then it becomes less significant. Hence the calculation is preformed her for few partial wave only. Hence we hope that the present approach is very useful for the calculation of the differential cross section and the total cross section, because it gives better results than the results of simple HHOB approximation given by Yates (1979). The method described here is such that, the divergence probelm gets eliminated automatically due to the presence of the term β i.e. the average excitation energy transferred during the course of collision. And above all the wave function used for evaluating the scattering amplitude in the HHOB approximation is calculated accurately. We have used the Roothan -Hartree -Fock wave method for the calculation of the wave

function and we use the Clementii - Roetii tables for the orbital calculation for the neon atom. Hence the present method where the scattering amplitude is calculated for the direct interaction potential where we have not neglected any of the cross terms arising in the expression. Hence we conclude that the results produced here are in much better agreement as compare to any other method described earlier.

TABLE IV.II

Value and comparison of the total cross section for the elastic scattering of electron by a target neon atom, with theoretical and experimental results. expressed in $a_{\emptyset}^2$]. For different incident energy.

ENERGY eV	EXPERIMENTA RW FJ	K	N	THEORETICAL OM BJ	First Born IMcD	DWBSA DW	Present results
100	11.03	10.3	9.4	14.2	29.5	---	13.8
200	8.45	7.98	7.0	9.64	16.8	9.77	9.87
300	6.80	6.38	5.4	7.53	11.9	7.63	7.85
400	5.76	5.47	4.5	6.29	9.27	6.35	6.86
500	5.02	4.78	---	5.45	7.57	5.47	5.69
700	4.03	3.90	---	4.40	5.66	4.37	4.56

RW FJ - R W wagner and F J de Heer (1980)

K - Kaupilla et al (1980)

N - Normand (1930)

IMcD - Inokuti and Mc Dowell (1974).

DW - Dewangan and Walters (1977)

BJ - Byron and Joachain (1977).

TABLE IV.III

Ratio of previous absolute measurements and theoretical calculations to present data for neon. Exptal.: J, Jansen et al (1976); B, Bromberg (1974); GR, Gupta and Rees (1975) ; WC, Williams and Crowe (1975). Theoretical : FY, Fink and Yates (1970); BJ, Byron and Joachain (1975). PR - present results.

Theta deg.	100 eV WC/PR	GR/PR	J/PR	BJ/PR	FY/PR	200 eV WC/PR	GR/PR	J/PR	B/PR	BJ/PR	FY/PR
5			0.75	1.03	0.21			0.86	0.89	1.02	
10		1.48	0.86	1.12	0.31		1.00	0.78	0.81	0.89	0.15
20	1.00	1.38	0.96	1.02	0.51	0.94	0.82	1.12	1.15	1.09	0.19
30	1.22	1.27	1.19	0.96	0.88	0.94	0.89	1.33	1.30	1.10	0.24
40	1.29	1.31	1.65	0.93	1.54	0.94	0.85	1.54	1.58	1.10	0.26
50	2.65	1.29	2.60	0.98	0.34	0.99	0.95	1.88	1.88	1.22	0.28
60	1.28	1.22		0.93	0.33	1.00	0.92			1.14	0.22
70	1.23	1.16		0.88	0.28	1.03	0.94			0.87	0.27
80	1.14	1.17		0.69	0.18	1.09	0.87			0.92	0.27
90	0.95	1.14		0.67	0.08	1.24	1.01			0.89	0.27
100	0.76	1.30		0.50	0.18	1.29	1.05			0.73	0.32
110	0.90	0.85		0.44	0.30	1.27	0.98			0.74	0.34
120	1.10	0.67		0.38	0.31	1.26	0.93			0.77	0.35
130	0.96	0.61		0.53	0.29	1.30	0.84			0.77	0.39
140	0.99	0.63		0.43	0.27	1.23	0.82			0.79	0.35
150	0.96	0.67		0.36	0.25	1.21	0.85			0.78	0.35