CHAPTER III

THE STUDY OF PHASE SHIFT

In the previous two chapters historical backgrounds of the experimental and theoretical studies were described in order to make the thesis consistent. Inspite of many successful attempts made in studing the polar molecules by the scattering of slow electrons the controversy over understanding of certain phenomena still exist.

From the study of the problem of following points for further investigations emerged. These are enlisted below:-

(1) Most of the work done for slow electron polar molecule scattering was based on considering a molecule as a rigid rotator. The application of symmetrical top model

was also made by some of the authors. One could have considered the non rigidity of the rotator and also the torsional motion of molecules.

(2) In the scattering problem a very important factor was the scattering amplitude. Ofcourse the scattering amplitude is dependent on molecular potential. The accuracy in the determination of this factor is of great importance. So far the author has not come across the literature which compared the accuracy of various methods of determining the amplitude factor for a point dipole field.

(3) The numerical calculations of the amplitude factor could be made to a fair accuracy by the calculations of phase shift. The nature of the potential and scattering cross section could be well studied by the knowledge of phase shift. The accuracy of the amplitude factor depends on the quantum number :l:. The phase shift δ_l could be calculated by using various methods. The accuracy of the methods can be compared and the amplitude factor can be found.

(4) The various modifications and even the overall change in potential was possible. Various modifications in the potential field e.g. point dipole field, finite dipole field; screen dipole field, spin dipole field at various stages were also possible. In place of a dipole model, quadrupole,

octupole models could have been imagined and consideration of different model led to the change in scattering cross section and hence momentum transfer cross section.

(5) Over and above the dipole field the superimposition of some another field was also possible. It was confirmed that the predominating term in slow electron polar molecule interaction was the dipole interaction, yet pure dipole field did not give the perfect agreement with the experiments and led to some theoretical difficulties. In this circumstances some short range potentials over and above the dipole field was thought also.

(6) There were also chances of resonance effect in the slow electron polar molecule interaction. The study of resonance required the knowledge of the wave function on initial and final states of rotations. The study of formation of negative ion its life time and capture cross section gave the detail understanding of the molecular structure.

(7) In certain cases the anomalous behaviour of cross section around D_{min} was observed. Three factors were mainly effective for this (a) The additional short range attractive potential due to the induced moments. Such a situation would cause same effect as an increased in dipole moment. The effect also depended on the total potential well and would have affected the magnitude of the cross section very

critically around D_{min}. (b) Change in a dipole length "a" :- It was observed that, in the range just above D_{min} (1.8 to 2.0 Debye) for a fixed atomic number Z, the binding energy of the electron to the dipole was an extremely stron function of dipole length "a". Thus change in Z, a or short range effect were contributing to the spreading of the data, especially around D_{min}. (c) Possible effect of rotational state:- In this type of effect the another constant introduced was the moment of inertia. It might have affected the cross section.

In the present work an attempt is made to study various points at various stages. Concentration is made on points 2, 3,4, 5 and 6.

3.1 SCATTERING PHASE SHIFT.

Consider the potential V(r) as spherically symmetrical. In this case the wave function must have cylindri-cal symmetry about the direction of motion of the incident particals; choosen as the polar axis of a spherical polar system of coordinates r, θ, ϕ. We expand $\Psi(r)$ in Legendre polynomials according to the formula

$$(r) = \sum_{l=0}^{\infty} A_l R_l (r) P_l (\cos \theta) \quad .....(3.1)$$

which is commonly referred to as an expansion in partial waves.

Substituting in to the Schrodinger's equation, this gives

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_l}{dr}\right)+\left\{K^2 - U(r) - \frac{l(l+1)}{r^2}\right\} R_l = 0 \qquad (3.2)$$

On setting $R_l(r) = u_l(r)/r$, we obtain the radial equation =

$$\frac{d^2 u_l}{dr^2} + \left\{ K^2 - U(r) - \frac{l(l+1)}{r^2} \right\} u_l = 0 \quad \ldots\ldots \quad (3.3)$$

where $u_l(r)$ must vanish at the origin r=0, since $R_l(r)$ is necessarily finite at all points. Suppose that V(r) falls off more rapidly than r^{-2} as $r \longrightarrow \infty$ we find for larger r

$$u_l(r) \sim r \left\{ a_l j_l(kr) + b_l n_l(kr) \right\}$$

where j_l and n_l are the spherical Bessel and Newmann functions. Hence we may choose a_l and b_l so that

$$u_l(r) \sim K^{-l} \operatorname{Sin}\left(Kr - \frac{l}{2} + \delta_l\right) \qquad (3.4)$$

as $r \to \infty$ $\quad \tan \delta_l = -b_l/a \qquad (3.5)$

known as the scattering phase shift for the l th partial waves it vanishes for the case of a null potential.

Now we know that the plane wave $e^{i\, k\cdot r}$ can be expanded as

$$e^{ik\cdot r} = \sum_{l=0}^{\infty} i^{l} (2l+1)\, j_{l}(kr)\, P_{l}(\cos\theta) \qquad (3.6)$$

and so putting

$$f(\theta) = \sum_{l=0}^{\infty} c_{l} P_{l}(\cos\theta) \qquad (3.7)$$

we see that for large r

$$A_{l}\, u_{l}(r) \sim i^{l}(2l+1)\, k^{-1} \sin\left(kr - \frac{1}{2} l\pi\right) + C_{l}\, e^{ikr} \qquad (3.8)$$

on equating the coefficients of e^{ikr} and e^{-ikr} we get

$$A_{l} = i^{l} (2l+1)\, e^{i\delta_{l}} \quad \ldots\ldots \qquad (3.9)$$

and $$C_{l} = \frac{1}{2ik} (2l+1)\, (e^{2i\delta_{l}} - 1) \quad \ldots\ldots \qquad (3.10)$$

hence the scattering amplitude can be expressed in the form

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)\, e^{i\delta_{l}} \sin\delta_{l}\, P_{l}(\cos\theta) \qquad (3.11)$$

For considering molecule as a rigid rotator and averaging over the entire dipole range the total cross section becomes

$$\sigma_{t} = \frac{2\pi}{k^{2}} \int_{0}^{\pi} \left| y_{lm}(\mu,\nu)\, f(\theta,\phi) \right|^{2} \sin\mu\, d\mu\, d\nu \qquad (3.12)$$

which finally leads to the expression for momentum transfer cross section

$$Q_{D} = 2\pi \int_{0}^{\pi} (1-\cos\theta)\, \sigma_{t} \sin\theta\, d\theta \qquad (3.13)$$

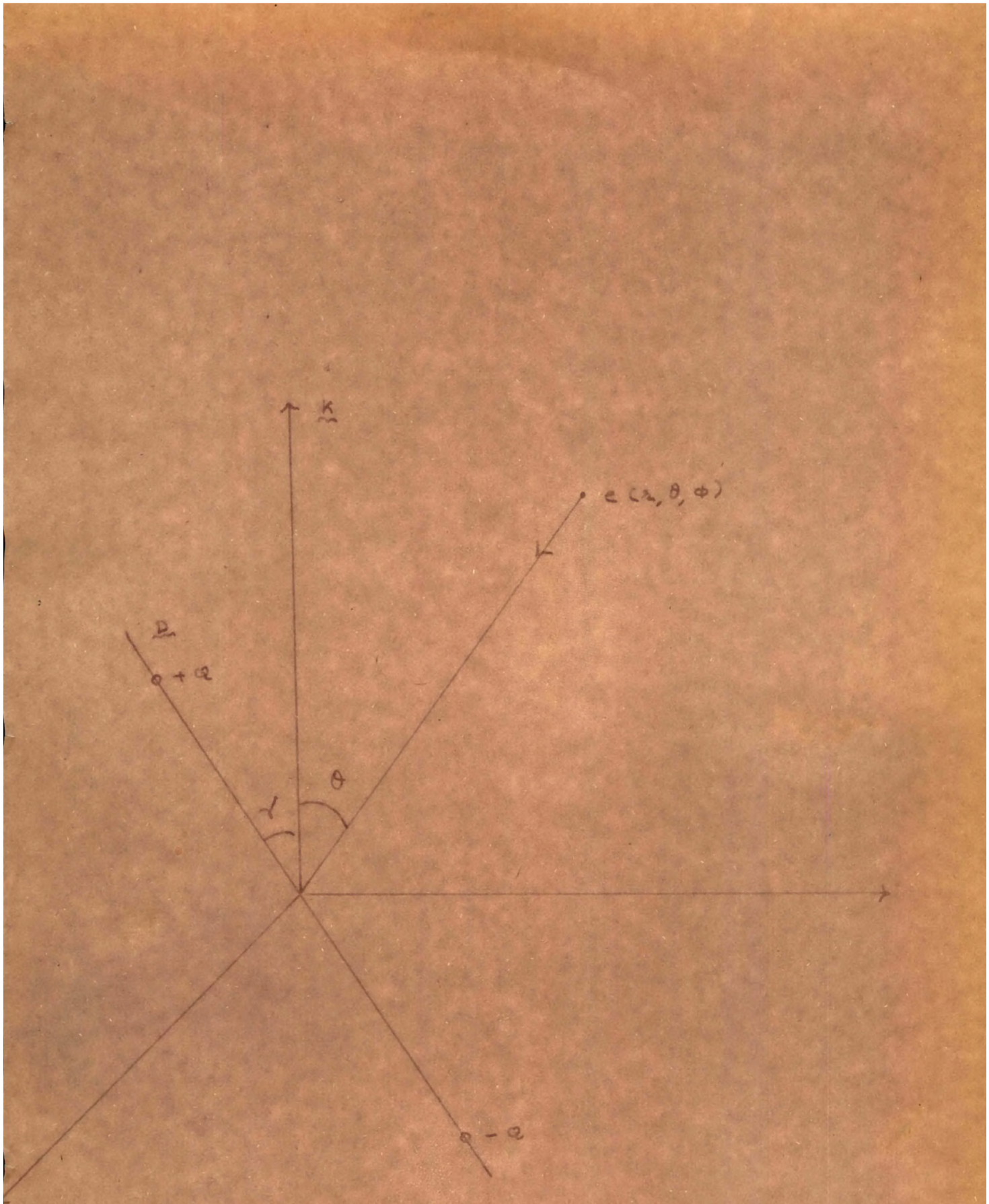


Fig. 3.1. Geometry of the problem.

3.2 DETERMINATION OF PHASE SHIFT FOR THE CRITICAL DIPOLE MOMENT.

In the last section the definition of the phase shift and its relation with the cross section was given. In this study the dipole field was important. Dipole field is not the spherically symmetric field, but dependent on $\cos\theta$. Due to this $\cos\theta$ dependence characteristic of the dipole field very few attempts were made for the phase shift determination (Mittleman et al 1968; Takayanagi and Itikawa 1965, Garrett 1971). Mittleman et al and Garrett calculated the phase shift for restricted circumstances. Mittleman et al have calculated the phase shift for the point dipole field in case of dipole moment greater than critical dipole moment. Garrett has calculated phase shift for finite dipole field for very large l. Takayanagi et al have calculated phase shift for finite dipole field in little more detailed manner. Calculations of phase shift for point dipole potential by various methods are reported in this chapter.

3.2 PHASE SHIFT FOR THE DIPOLE FIELD.

The geometry of the problem is as represented in figure 3.1. Our starting point is the wave equation,

$$\left[-\frac{\hbar^2}{2m} \nabla^2 - \frac{D e \cos(\bar{D} \hat{\ } \bar{r})}{r^2} \right] \psi = E \psi \quad \ldots \quad (3.14)$$

which can be represented in atomic units as

$$\left[\nabla^2 + k^2 + \frac{\alpha' \cdot \bar{r}}{r^3} \right] \varphi = 0 \qquad (3.15)$$

where $\alpha' = 2 D \cos \gamma / e a_0$ (3.16)

this equation is separable in the usual spherical coordinates

$$\therefore \varphi = R(r) \Theta(\theta) e^{im\Phi} \qquad (3.17)$$

The separated equations are

$$-\frac{d}{d\mu}(1-\mu^2)\frac{d\Theta}{d\mu} + \left\{ \alpha'\mu - \frac{m^2}{1-\mu^2} + L_n^m (L_n^m + 1) \right\} \Theta = 0 \qquad (3.18)$$

where $\mu = \cos\theta$

and

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial R}{\partial r}\right) + \left[K^2 - \frac{l(l+1)}{r^2} - \frac{U(r)}{r^2} \right] R = 0 \qquad (3.19)$$

where the condition that be single valued required that m be an integer. The separation constant is denoted by $L_n^m (L_n^m + 1)$. The condition that $\Theta(\pm 1)$ be finite is a restriction upon L_n^m to certain allowed values. The integer n will denumerate these eigen values. A solution of equation 3.18 may be expanding in the complete set P^m.

$$\Theta = \sum_{q=0}^{\infty} \Delta^m_{n,q} P^m_{q+|m|}(\mu) \times \left[\frac{2q+2|m|+1}{2} \frac{q!}{(q+2|m|)!} \right]^{1/2} \qquad (3.20)$$

where the coefficients and eigen values are determined from three term recurrence relation,

$$\left[L_n^m \quad (L_n^m + 1) - (q + |m|)(q + |m| + 1) \right] \Delta^m_{n,q} +$$

$$\propto \gamma' \left[\Delta^m_{n,q+1} \left\{ \frac{(q+1)\ (q+2|m|+1)}{(2q+2|m|+1)(2q+2|m|+3)} \right\}^{1/2} + \right.$$

$$\left. \Delta^m_{n,q-1} \left\{ \frac{q\ (q+2m)}{(2q+2|m|+1)\ (2q+2|m|-1)} \right\}^{1/2} \right] = 0 \qquad (3.21)$$

The solution of radial equation 3.19 which is finite at the origin is the spherical Bessel function $J_{L_n^m}(kr)$ The condition that this function be finite at the origin places a bound upon the eigen values

$$L_n^m > -1/2 \qquad \ldots \qquad (3.22)$$

which results in an upper bound on the magnitude of the dipole moment

$$\propto < \frac{1.279}{\gamma'} \qquad (3.23)$$

($\gamma' = \cos\gamma$, $\gamma = 1$ leads us to the Mittleman et al results) Otherwise the potential is too attractive and no solution exist.

In order to make estimate of phase shift let us take

$$L_n^m = -l(l+1) \qquad \ldots \qquad \ldots \qquad (3.24)$$

such that for $l = 0, 1, 2 \ldots$ etc. the value of L_n^m is always less than 1/2

$$R_l = j L_n^m (kr)$$
$$= -j - (l+1)^{(kr)} \quad \ldots\ldots \quad \ldots\ldots \quad (3.25)$$

we know that

$$j_{-(l+1)}(kr) = n_l (kr) (-i)^{-l+1}$$

where

$n_1 (kr)$ = Spherical Newmann function. The asymptotic behaviour of this function at large r is

$$(-1)^{-(l+1)} \frac{1}{kr} \text{ Sin } \left\{ kr - 1/2 \pi (l+1) \right\} \quad \ldots (3.26)$$

By comparision with fundamental equation it can be say that, the phase shift δ_o if given by

$$\delta_o = - \frac{\pi}{2} \quad \ldots\ldots \quad \ldots (3.27)$$

Here we have taken $L_n^m = -(1+1)$, which is always smaller than - 1/2 hence the condition 3.22 is fulfill completely. But even substituting $1=0$, $L_n^m = -1$, so this assumption do not gives the value of phase shift exactly for $L_n^m = - 1/2$. Only thing which we can presume is for a critical dipole moment $\alpha = 1.279/\gamma'$, $\delta_l < -\frac{\pi}{2}$. The negative sign of the phase shift suggests that in certain direction the radial wave function is pushed out in comparision with the force free wave function or

in certain direction potential behave as the repulsive potential.

3.4 APPLICATION OF THE BORN APPROXIMATION TO THE POINT DIPOLE POTENTIAL.

For determination of the phase shift for a point dipole field it was observed that the quantity L_n^m ($L_n^m + 1$) was very important. It could be observed that the relation of L_n^m (L_n^m+1) with U(r) could given by the following equation

$$\frac{L_n^m (L_n^m + 1)}{r^2} = \frac{l(l + 1)}{r^2} + U(r) \qquad (3.28)$$

The expression for Born approximation for l dependent phase shift is

$$\delta_l = - \int_0^\infty k\, r^2\, j_l^2 (kr)\, U(r)\, dr. \qquad .. (3.29)$$

For the point dipole field this expression turns out to be

$$\delta_l = - \int_0^\infty k\, r^2\, j_1^2 (kr) \left\{ \frac{L_n^m (L_n^m + 1)}{r^2} - \frac{l(l+1)}{r^2} \right\} dr. \quad (3.30)$$

By the help of equation 3.30, the Born approximation for the phase shift for a point dipole field for any value of l can evaluated. For effective electron scattering the important

phase shift is δ_0 . We have estimated δ_0 , δ_1 , for Born approximation. It was necessary to determine the value of $\frac{L_n^m (L_n^m + 1)}{r^2}$ for every value of l, This was determined by the expression 3·21, substituting n = 0, m = 0, q = 1, expression for 1 = 0 can be obtain as

$$\frac{L_n^m (L_n^m + 1)}{r^2} = \frac{L_0^0 (L_0^0 + 1)}{r^2} \quad \ldots\ldots \quad (3\cdot31)$$

which on substituting in 3·30 and performing elementary integration gave the δ_0 as

$$\delta_0 = - L_0^0 (L_0^0 + 1) \pi /2 \quad \ldots\ldots \quad (3\cdot32)$$

For $\lambda=1$, U(r) was determined as $\lambda = 0$. The form of U(r) in this case is given by,

$$U(r) = \frac{1}{r^2} \left[\frac{\alpha^2 \gamma'^2}{3 L_0(L_0+1)} - L_0^0 (L_0^0 + 1) \right] \quad (3\cdot33)$$

using 3·30 and 3·33 the δ_1 is obtain as

$$\delta_1 = \left[\frac{\alpha^2 \gamma'^2}{3 y} - y \right] (k_0 - \frac{2k_0^2}{3}) \quad \ldots\ldots \quad (3\cdot34)$$

where $y = L_0^0 (L_0^0 + 1)$

It can be observed that δ_0 is independent of energy while δ_1 is dependent on k.

3·5 W. K. B. APPROXIMATION.

For the ℓ th partial wave shift WKB method gave the expression as

$$\delta_\ell = \int_{r=\frac{(\ell+\frac{1}{2})}{K}}^{\infty} \frac{U(r)\,dr}{2\left\{k^2 - \frac{(\ell+1)^2}{r}\right\}^{\frac{1}{2}}} \quad \ldots\ldots \quad (3\cdot35)$$

for the dipole field use of equation 3·28 for l=0 gave the value of δ_o as

$$\delta_o = - \; L_o^o \; (L_o^o + 1)\; \pi/2 \quad \ldots\ldots \quad (3\cdot36)$$

It was interesting to note that δ_o for Born approximation and WKB approximation were equal. Using the value of U(r) of 3·33 and substituting it to 3·35 δ_1 for WKB could be obtained

$$\delta_1 = - 1/3 \left[\alpha^2 \gamma^2 / 3y_0 - y_0 \right] \pi/2 \quad (3\cdot37)$$

it can be observed from equation 3·36 and 3·37 that WKB phase shift for l=0, 1 are independent of energy.

3·6 VARIATIONAL APPROACH TO PHASE SHIFT.

Variational approach to the point dipole was also applied. A variational integral is given in the -

form

$$I_t = \int_0^\infty G_t \left\{ \frac{d^2}{dr^2} + K^2 - U(r) \right\} G_t \; dr \; \ldots \qquad (3.38)$$

where G_t is the trial wave function. $G_t = G_t(c_1, c_2 \ldots c_n, \lambda)$ containing n adjustable parameter, which satiesfy the boundary conditions $G_t(0) = 0$, $G_t \sim \text{Sin}kr + \lambda \text{Cos } kr$. We have tried the wave function of the form

$$G_t = \text{Sin} kr + \lambda(1-e^{-2/a}) \text{Cos } kr \ldots \qquad (3.39)$$

for the derivation of considering U(r) from equation 3.28 and taking wave function 3.39, lengthy but straight forward solution of 3.38 gives

$$I_t = \frac{4 a \lambda k}{1 + 4 a^2} - \frac{\lambda^2(2a^2 + 1)}{4 a^2 + 1)} + \frac{\lambda^2(a^2+2)}{4(a^2+1)} - L_n^m (L_n^m + 1)$$

$$\left\{ \frac{k\pi}{2} - \frac{2a \lambda^2(2a^2+1)}{4a^2 + 1} + \frac{a \lambda^2 (a^2 + 2)}{4(a^2 + 1)} \right\} \qquad \ldots\ldots \quad (3.40)$$

Applying Kohn's variation method the phase shift for a dipole field was obtained as

$$\delta_o = \left[\frac{4 a k}{1+4a^2} + K \right] \Big/ \frac{2(2a^2+1)}{4a^2+1} - \frac{2(a^2+2)}{4(a^2+1)} + \lambda \left\{ \frac{-4a(2a^2+1)}{4a^2 + 1} + \frac{2a (a^2 + 2)}{4 (a^2 + 1)} \right\} \qquad .. \quad (3.41)$$

where "a" is taken as the mean molecular diameter. In the case of a dipole field a can be taken as the length of the dipole i.e. distance between two charges. Then for the same function Hulthan's variational principle was also applied to the phase shift which gave

$$\tan \delta_o = \left[-\frac{4ak}{1+4a^2} \pm \left\{ \frac{16a^2k^2}{(1+4a^2)2} - \frac{4yk}{2} \left(\frac{a^2+2}{4(a^2+1)} - \frac{2a^2+1}{4a^2+1} + \frac{2ya(2a^2+1)}{4a^2+1} - \frac{ay(a^2+2)}{4(a^2+1)} \right) \right\}^{\frac{1}{2}} \right] \Big/ Y \qquad (3.42)$$

Here $y = L_n^m \ (L_n^m + 1)$

$$Y = \frac{a^2+2}{4(a^2+1)} - \frac{2a^2+1}{4a^2+1} + \frac{2ya(2a^2+1)}{4a^2+1} - \frac{ay(a^2+2)}{4(a^2+1)}$$

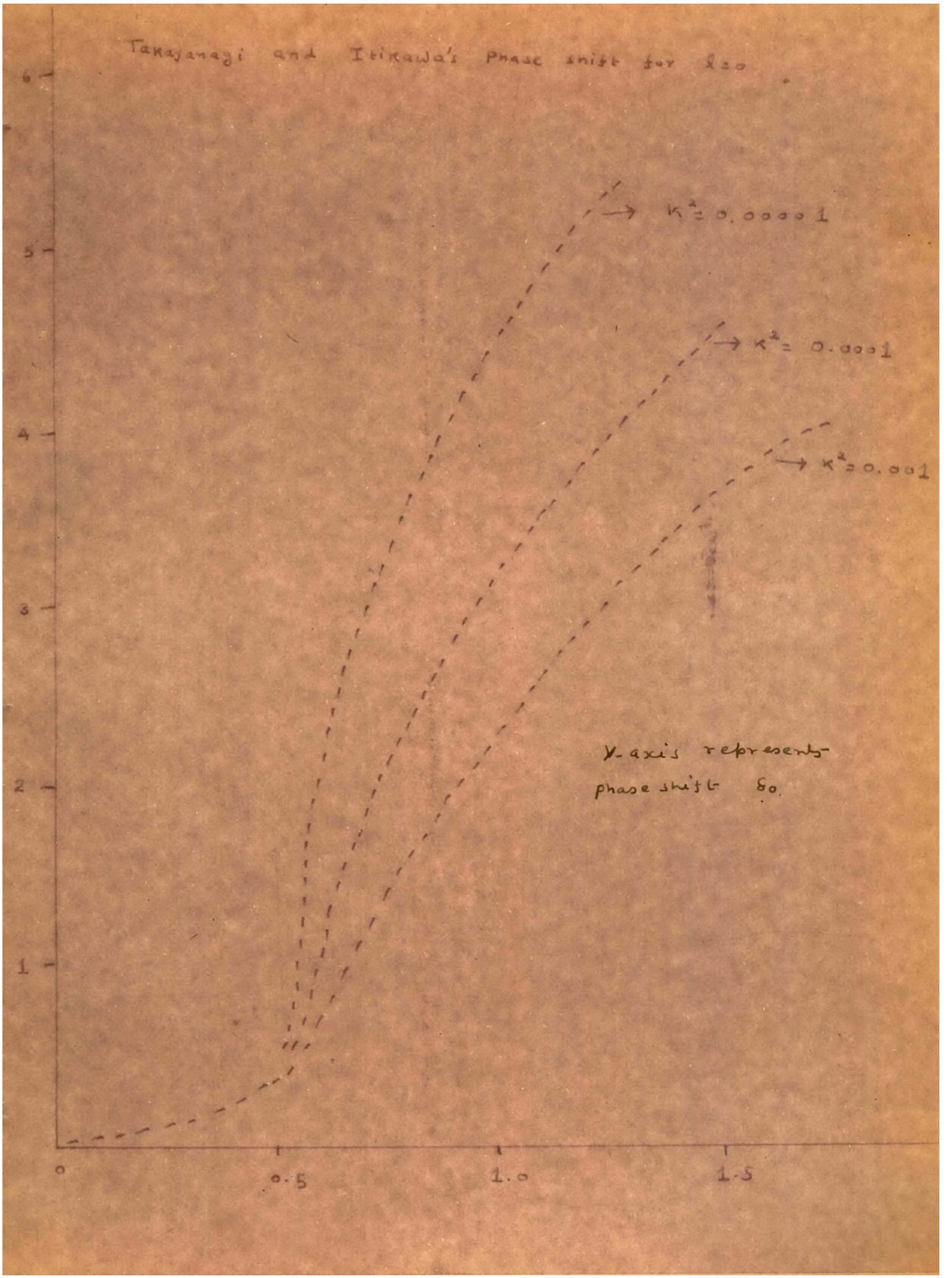
3.8 NUMERICAL CALCULATIONS.

For the numerical calculations the first important thing was to calculate the value of $L_o^o \ (L_o^o + 1)$. In every methods used to determine the phase shift the value of $L_o^o \ (L_o^o + 1)$ was required. The numerical estimation of this quantity was determined by the help of equation 3.21. Taking $n=m=0$ and $q=1$ the secular equation gave different elements of

the matrix for different value of ℓ (i.e. ℓ=0,1,2,3....etc). The form of this matrix upto ℓ = 9 is as shown in appendix I. In this matrix $y = L_o^o (L_o^o + 1)$. It was observed that the roots of y depended on α, γ'. α is a dimensionless dipole moment given by $\alpha = 2D/ea_o$. While $\gamma' (= \cos\gamma)$, is the direction cosine of the dipole axis with respect to the direction of K. K is a wave vector. We have selected the value of α = 0.2, 0.4, 0.6, 0.8, 1.0, 1.2 while $\gamma = 0^o, 25^o, 50^o, 75^o$, which means that for the different combination of $\alpha\gamma'$, for determining the roots of y, 24 matrices are to be diagonalized. The diagonaliza-tion of matrices were made by the help of IBM 360/44 computor. The method used for diagonalization was Jacobi's method. While the programming was made in Fortran IV language. The Jacobi's method is described in appendix II.

Further the calculations for Born, WKB and variational phase shift were also determined by the computor together with the diagonalization.

For Born approximation δ_o, δ_1 were calculated. Here δ_1 is again energy dependent. For the calculations of δ_1 the values of K selected were 0.1, 0.01, 0.001, 0.0001. In Kohn's variation method one more constant "a" over and above the "k" appeared. The wave function of the form 3.39 used for phase shift problem of electron atom collision (Bates 1961). There


Takayanagi and Itikawa's Phase shift for l=0
6
5
4
3
2
1
0
0.5
1.0
1.5
$K^2 = 0.00001$
$K^2 = 0.0001$
$K^2 = 0.001$
Y-axis represents phase shift δ_0.

"a" is taken as mean radius of the atom. Here we have considered 'a' as dipole length. Moreover "a" was infact an adjustable parameter, we have taken the range of "a" from 1-4$\mathring{A}$ U. All the quantities were taken in atomic units.

It is physically not possible to give all the results over here. Some of the important results are exhibited in table I to V. As we have taken the value of U(r) which was dependent on minimum eigen values L_o^o, the restriction came in our calculations that we could not calculate the phase shift for $\alpha > \alpha_{crit}$. The very interesting point of our study was the dependence of α_{crit} and phase shift on the angle between dipole axis and the wave vector. It means that the phase shift is dependent on the position of molecular dipole.

In table II the phase shift for Born approximation is exhibited. As discussed in the above paragraph we could not calculate phase shift for $\alpha > \alpha_{crit}$, therefore instead of taking different polar molecules we have considered the dipole field. It was observed from the table II that as α increases, phase shift increases, while as γ increases phase shift decreases.

The phase shift δ_1 (for $\ell = 1$) is represented in table III and IV. It was observed that the δ_1, for Born approxima-tion is energy dependent values of k. the values of δ_1 for WKB

were very large in comparision of Born values. But the tendency of both the phase shift was the same and reverse of δ_o. It was observed that δ_1 decreases with increasing α.

The variational phase shift calculations are represented in table V. Here one more variable "a" is introduced. As discussed above "a" is considered as the dipole length. It was observed that with decreasing "k" phase shift decreases and with increasing "a" phase shift decreases.

3.9 COMPARISION OF THE RESULTS.

It is rather surprising to find that very few work has been reported on this particular aspect of scattering problem. Mittleman et al (1968), Garrett (1971), Takayanagi and Itikawa (1968) have calculated phase shift for very restricted situations. Mittleman et al have calculated shase shift for a point dipole for which $D > D_{crit}$. We have calculated phase shift $D < D_{crit}$. Takayanagi & Itikawa (1968) and Garrett (1971) have calculated phase shift for a finite dipole potential. The brief discussion of the work of these authors is made here.

Mittleman et al have for the point dipole potential considered the simplest case for which $\alpha > \alpha_{crit}$, so that L_o^o was complex, but all the other L_n^m are real and greater than -1/2. The radial wave equation in thise case is represented

as,

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{d}{dr} + K^2 - \frac{\Lambda_{oo}}{r^2} f(r) \right] R_{oo}(r) = 0 \qquad (3.43)$$

(R_{oo} represents that n = 0,, m = 0)

Λ_{oo} Eigen value of the radial equation. By hypothesis

$$- \Lambda_{oo} = \Lambda^1 = a^2 + 1/4 \qquad (3.44)$$

where "a" is real. The phase shift δ_o in the limit $kr_o << 1$ can be represented as

$$\text{Tan } \delta = \frac{\text{Sin } (\phi + \xi)}{\text{Sin } (\phi - \xi)} \qquad (3.45)$$

$$\phi = a \text{ Log}(kr_o/2) + \arg \left[\Gamma(1 - ia) - \text{Tan}^{-1} \; a/ \quad (s + 1/2) \right] \qquad (3.46)$$

$$S = \Lambda_{l_o} \text{Cot } \Lambda_{l_o} - 1 \qquad (3.47)$$

$$\xi = \text{Tan}^{-1} \quad (\tan h \quad (\pi a/2)) \qquad (3.48)$$

Mittleman et al have observed the effect of this phase shift on the inelastic cross section $\sigma_{l,l'}$. They have not calculated the numerical values of phase shift. Takayanagi and Itikawa have considered the dipole potential as finite dipole, this type of potential can be represented as

$$V = - Z e^2 \left(\frac{1}{r_A} - \frac{1}{r_B} \right)$$

$$= \frac{4 Z e^2}{R} \quad \frac{\eta}{\xi^2 - \eta^2}$$

Where the prolate spheroidial coordinates ξ η are given by

$$\xi = r_A + r_B / R$$

$$\eta = r_A - r_B / R$$

r_A and r_B are the distance from the position of charge +Ze (at point A) and -Ze (at point B). R is the distance between two charges. Partial wave treatment to Schrodinger equation, gives the radial wave equation of the form

$$\frac{d^2 X_{lm}}{d} + \left[\frac{1-m^2}{(\xi^2-1)^2} + \frac{k^2 \xi^2 - A_{l,m}}{\xi^2 - 1} \right] X_{lm} = 0 \qquad (3.49)$$

Then the phase shift $\delta_{l,m}$ is obtained by solving the equation, with the initial condition $X_{l,m}(l) = 0$ and comparing the solution $X_{l,m}(\xi)$ at a point ξ $(k^2\xi^2 >> 1)$ with the asymptotic form

$$X_{l,m}(\xi) \xrightarrow{\xi \to \infty} \sin \frac{(k\xi - 1/2\, l\pi + \Delta_{l,m})}{k\xi} \qquad (3.50)$$

for $\xi >> 1$ equation 3,49 becomes

$$\frac{d^2 X_{l,m}}{d\xi^2} + \left(k^2 + \frac{k^2 - A_{l,m}}{\xi^2} \right) X_{l,m} = 0 \qquad (3.51$$

This has a general solution

$$X_{l,m}(\xi) = \alpha_{l,m}\sqrt{\xi}\, J_{\nu}^{(1)}(k\xi) + \beta_{l,m}\sqrt{\xi}\, J_{\nu}^{(2)}(k\xi) \qquad \ldots(3\cdot52)$$

where $J_{\nu}^{(1)}$ and $J_{\nu}^{(2)}$ are the two independent solution to the Bessel equation of order $\nu = (A_{l,m} + 1/4 - K^2)^{1/2}$

$$\frac{d^2 J(Z)}{dZ^2} + \frac{1}{2}\frac{d J(Z)}{dZ} + \left(1 - \frac{A_{l,m} + 1/4 - k^2}{Z^2}\right) J(Z) = 0 \qquad \ldots. \quad (3\cdot53)$$

If $A_{l,m} + 1/4 - K^2 > 0$, the equation 3·53 has two roots $J_{\nu}(1) = J_{\nu}$, $J_{\nu}(2) = J_{-\nu}$ where J_{ν} and $J_{-\nu}$ are the ordinary Bessel function. On the contrary, if $A_{l,m} + 1/4 - K^2 < 0$ the equation 3·53 becomes the Bessel equation of pure imiginary order, whose solution in the form of power series is

$$J_i(Z) = \left(\frac{Z}{2}\right)^{i\lambda} \sum_{m=0}^{\infty} \frac{(-1)^n (Z/2)^{2m}}{n!\,\Gamma(i\lambda + n + 1)}$$

$$\lambda = \sqrt{|A_{l,m} + 1/4 - k^2|}$$

In this case the real part J_i and imiginary part J_i of J_i are independent, namely

$$J_{\nu}(1) = J_{i\lambda}'(Z) =$$

$$\left(\frac{\sin h\lambda\pi}{(\lambda\pi)^{\frac{1}{2}}}\right)^{1/2}\left[\cos\left(\lambda\log\frac{z}{2}-T_\lambda\right)\sum_{n=0}^{\infty}\alpha_n'\left(\frac{z}{2}\right)^{2n}-\right.$$

$$\left.\sin\left(\lambda\log\frac{z}{2}-T_\lambda\right)\sum_{n=0}^{\infty}\alpha_n''\left(\frac{z}{2}\right)^{2n}\right.$$

$$J_\nu^{(2)} = J_{i\lambda}''(z) =$$

$$\left(\frac{\sin h\lambda\pi}{(\lambda\pi)^{\frac{1}{2}}}\right)^{1/2}\left[\sin\left(\lambda\log\frac{z}{2}-T_\lambda\right)\sum_{n=0}^{\infty}\alpha_n'\left(\frac{z}{2}\right)^{2n}\right.$$

$$\left.+\cos\left(\lambda\log\frac{z}{2}-T_\lambda\right)\sum_{n=0}^{\infty}\alpha_n''\left(\frac{z}{2}\right)^{2n}\right]$$

where $\alpha_0' = 1, \quad \alpha_0'' = 0$

$$\alpha_n' = -\frac{1}{n}\,\frac{n\alpha_{n-1}' + \lambda\alpha_{n-1}''}{n^2+\lambda^2}$$

$$\alpha_n'' = -\frac{1}{n}\,\frac{n\alpha_{n-1}'' - \lambda\alpha_{n-1}'}{n^2+} \quad \text{for} \quad n \geq 1$$

and $$T_\lambda = -\lambda\gamma + \sum_{p=1}^{\infty}\left(\frac{\lambda}{p} - \tan^{-1}\lambda/p\right)$$

$\gamma =$ Euler's constant,

knowing $\alpha_{l,m}$, $\beta_{l,m}$ in 3·52, the phase shift is given by

$$\delta_{l,m} = \tan^{-1}\left[\frac{\alpha_{l,m}+\beta_{l,m}}{\alpha_{l,m}-\beta_{l,m}}\cot\frac{\nu\pi}{2}\right] - \pi/4 + \frac{l\pi}{2}$$

for $A_{l,m} + 1/4 - k^2 > 0$ ..... (3·54)

$$\delta_{l,m} = \tan^{-1}\left[\frac{\alpha_{l,m}}{\beta_{l,m}} \operatorname{Cot} h \frac{\lambda\pi}{2}\right] - \pi/4 + \frac{l\pi}{2} \quad \cdots 3.55$$

$$\text{for } A_{lm} + 1/4 = k^2 < 0$$

The phase shift δ_0, δ_1 calculated by this method is exhibited in graph 1. In this case the incident electron was so slow that the phase shifts of the partial waves $l \geq 1$ were very small moreover the dependence of $\delta_{l,m}$ on dipole moment was not strong except in the case of $l = 0$ therefore the D dependence of the cross section was mainly due to that of δ_0.

Considering the same potential as Takayanagi and Itikawa but with a slight different method Garrett has calculated phase shift for very large l. In this method the radial equation is put up in the form

$$\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi} f_1^m - \left(\frac{m^2}{\xi^2-1} - K^2\xi^2 + \lambda_t^m + V_0\right) f_1^m = 0 \quad \cdots\cdot(3.56)$$

which for large value of ξ takes the form

$$\frac{d^2}{d\xi^2} f_1^m + \frac{2}{\xi}\frac{d}{d\xi} f_1^m - \left(K^2 - \frac{\lambda_t^m + V_0}{\xi^2}\right) f_1^m = 0 \quad (3.57)$$

This is Bessel's equation which has a solution

$$f_1^m(\xi) \sim \xi^{-\frac{1}{2}} J_{l+\frac{1}{2}}(K\xi + \delta_l) \sim$$

$$\left[\sin(K\xi - 1/2\, l\pi + \delta_l)\right]/K\xi \quad (3.58)$$

where $\ell\,(\ell+1) = \lambda_\ell^m$ and δ_ℓ phase shift due to V_o, however by the argument just given, the term $V_o f_1^m$ goes as asymptotically like a spheroidial wave with a multiplicative ℓ dependent constant, thus the solution of equation 3.57 may be written as

$$f_1^m(\xi) \sim \xi^{-\frac{1}{2}} J_{\nu+1/2}(k\xi) \sim \left\{\sin\left[K\xi - 1/2\,\ell\pi - 1/2\,\pi(\nu-\ell)\right]\right\}/k\xi \qquad \ldots(3.59)$$

For determination of "ℓ" dependent phase shift Garrett used the characteristic of eign values λ_ℓ^m for large ℓ, $\lambda_\ell^m \sim (\ell+1)$

$$\text{therefore } \nu(\nu+1) \sim \lambda_\ell^m + \nu_o$$

$$\underset{\ell\to\infty}{\sim} \ell(\ell+1) + \nu_o \qquad \ldots(3.60)$$

From 3.59 and 3.60 a result analogus to that for a spherically symmetric r^{-2} potential can be obtained as

$$\delta_{\ell,m} = 1/2\,\pi(\nu-\ell) \sim 1/2\,\pi\nu_o \Big/ 2\ell+1$$

and as $$\nu_o \sim \left\{\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}\right\} + \ldots\ldots$$

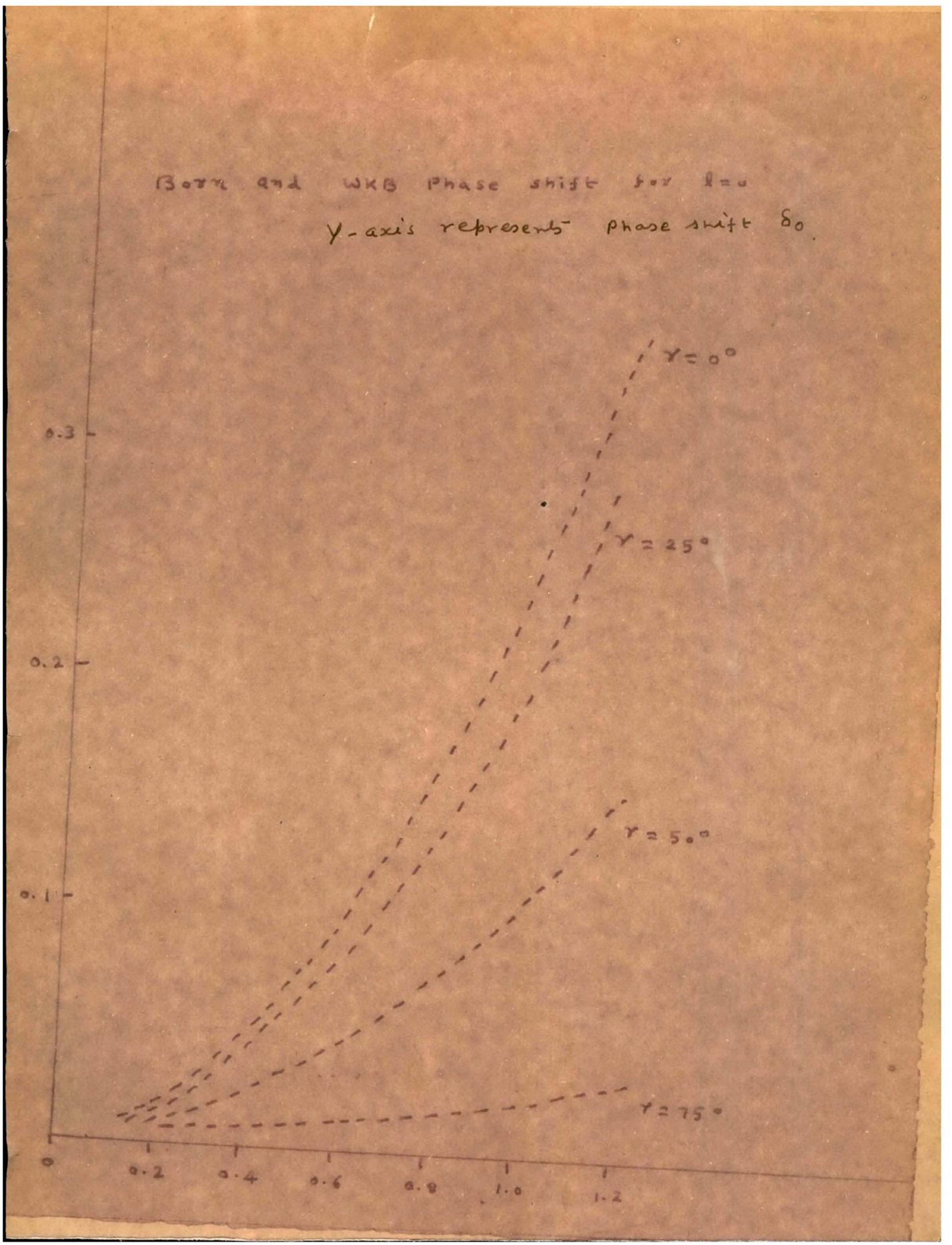
$$\delta_{\ell,m} = \frac{\pi}{2}\left\{\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)(2\ell+1)}\right\} + \ldots\ldots(3.61)$$

For $\ell = 0$, $m = 0$

$$\delta_{oo} = \pi/2 \cdot 1/3 = \pi/6 = 0.5233 \qquad \ldots(3.62)$$

Born and WKB Phase shift for $l=0$

y-axis represents phase shift δ_0.



As Garrett has not calculated the value for different dipole moment it was very difficult to compare the results.

3.10 AMPLITUDE AND SCATTERING CROSS SECTION

The knowledge of phase shift is important for the study of scattering amplitude and cross section. In section 3.1 $f(\theta)$ and total cross section Q is calculated. For the slow electron scattering the important phase shift term was . Hence cross section was calculated for $\ell = 0$. The experimental important quantity is the momentum transfer cross section. Considering Born phase shift and WKB phase shift, the expression for momentum transfer cross section in πa_o^2 units turns out to be

$$Q_D' = \frac{341.8}{E'} \delta_o^2 \quad \ldots\ldots \quad \ldots\ldots \quad (3.63)$$

where E' = Energy of electron in $\sqrt{\text{Volt}}$.

(See appendix IV for the detail of this calculations)

Altshuler (1957) calculated Q_D' for a point dipole potential applying Born approximation, his expression for Q_D' is

$$Q_D' = \frac{5.6 \left(D' \right)^2}{E'} \quad \ldots\ldots\ldots \quad (3.64)$$

$D^{?}$ is the dipole moment in debye.

It is difficult to compare our results with Altshuler's results because he has calculated cross section averaging over the dipole orientation. We have derived the value of phase shift for different γ. Moreover the restriction $\alpha < \alpha_{crit.}$ remains for momentum transfer cross section for our calculations, while Altshuler's results can be applied to any dipole moment.

The interesting result of phase shift is the mean scattering cross section. In recent experiments of thermal electron collision with polar molecules mean momentum transfer cross section averaging over the Maxwellian distribution of velocity was reported (N.B. The detailed discussion of the momentum transfer cross section and mean momentum transfer cross section will be made in chapter IV). The mean scattering cross section is defined as

$$\langle \sigma_m (v) \rangle = 4\pi \int_0^\infty \sigma_m(v)\, f_o (v)\, v^2\, dv \qquad (3.65)$$

where $\sigma_m(v)$ = velocity dependent momentum transfer cross section. The expression for $\langle \sigma_m(v) \rangle$ of δ_o phase shift is turns out to be

$$\langle \sigma_m (v) \rangle = \frac{32\, \pi^3\, \hbar^2}{m\, K\, T} \sin^2 \delta_o$$

where K = Boltzman constant

T * Absolute temperature

for thermal electrons $T = 300^{o}K$.

Substituting the values of $\hbar$, m, K, T and knowing that δ_o is very small we get the results as

$$\langle \sigma_m(v) \rangle = 2905 \times 10^{-14} \delta_o^2 cm^2 \qquad (3.66)$$

The Born results for the same is

$$\langle \sigma_m(v) \rangle = 3.8083 \times 10^{-14} \mu^2 cm^2 \qquad (3.67)$$

(μ in Debye)

It was observed that for $\alpha = 0.2$ expression 3.66 gave the value of $\langle \sigma_m (v) \rangle = 0.2905 \times 10^{-14}$ cm^2, while expression 3.67 gave $\langle \sigma_m (v) \rangle = 0.2546 \times 10^{-14}$ cm^2, Which means that our results for $\langle \sigma_m (v) \rangle$ is higher than Altshuler. Altshuler's calculation gives $\langle \sigma_m (v) \rangle$ lower than experimental one (Christophorou et al 1969). Our calculations modifies the Altshuler's results and gives better agreement with experimental values.

The estimation of Q_D' and $\langle \sigma_m (v) \rangle$ is not made for the variational phase shift because the variational phase shift is very small hence its effect to cross section is also very small.

TABLE 1

Minimum Eigen values $\Psi = L_o^o (L_o^o + 1)$ for different values of γ

No.	α	$\gamma' = \cos\gamma$: $\Psi = L_o^o (L_o^o + 1)$			
		$\gamma = 0^o$	$\gamma = 25^o$	$\gamma = 50^o$	$\gamma = 75^o$
1	0.2	-0.00665	-0.005465	-0.002752	-0.000447
2	0.4	-0.02641	-0.021731	-0.01097	-0.001785
3	0.6	-0.05874	-0.04843	-0.024569	-0.004013
4	0.8	-0.10282	-0.084984	-0.04338	-0.007127
5	1.0	-0.15762	-0.130698	-0.067213	-0.011119
6	1.2	-0.2222	-0.18479	-0.09582	-0.015983

TABLE 2

" δ_o " Born approximation method = $(\delta_o)_{WKB}$

No	α	Phase shift δ_o for different γ			
		0^o	25^o	50^o	75^o
1	0.2	0.01044645	0.00858436	0.00432238	0.00070136
2	0.4	0.04148683	0.03413486	0.01723761	0.00280407
3	0.6	0.09226942	0.07606888	0.03859362	0.00630396
4	0.8	0.1615011	0.13349235	0.06814754	0.01119433
5	1.0	0.24765497	0.20529968	0.10557872	0.01746572
6	1.2	0.34903371	0.29026735	0.15051329	0.02510615

TABLE 3

The value of Phase shift " δ_1 " by Born approximation, for $\gamma = 0$

K_1 represents K = 0.1 , K_2 represents K = 0.01

K_3 represents K = 0.001, K_4 represents K = 0.0001

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.18650216	0.01984916	0.0019969	0.00019981
2	0.4	0.18600619	0.01979637	0.0019959	0,00019993
3	0.6	0.18518680	0.01970916	0.0019828	0.00019840
4	0.8	0.18405271	0.01958346	0.0019707	0.00019719
5	1.0	0.18261290	0.01943522	0.00195526	0.00019564
6	1.2	0.18087939	0.01925078	0.00193671	0.00019379

T A B L E 3 Contd.

The value of Phase shift = " δ_1 " by Born Approximation for $\gamma = 25^{\circ}$

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.18653172	0.0198523	0.00199722	0.00019984
2	0.4	0.18612355	0.01980885	0.00199285	0.00019940
3	0.6	0.18544894	0.01973706	0.00198363	0.00019868
4	0.8	0.18451488	0.01963765	0.00197563	0.00019768
5	1.0	0.18332487	0.01951100	0.00196283	0.00019641
6	1.2	0.18188936	0.01935822	0.00194751	0.00019487

TABLE 3 Contd..

The value of phase shift " δ_L " by Born approximation for $\gamma = 50^0$

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.18656218	0.01985534	0.00199755	0,00019937
2	0.4	0.18639374	0.01983761	0.00199574	0.00019969
3	0.6	0.18605244	0.01980129	0.00199209	0.00019933
4	0.8	0.18557709	0.01975070	0.00198700	0.00019882
5	1.0	0.18497270	0.01968638	0.00198053	0.00019817
6	1.2	0.18423414	0.01960777	0.00197262	0.00019738

T A B L E 3 Contd...

The value of phase shift " δ_1 " by Born approximation for $\gamma = 75^{\circ}$

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.18665582	0.01986551	0.00199855	0.00019947
2	0.4	0.18662236	0.01986200	0.00199820	0.00019994
3	0.6	0.18656868	0.01985623	0.00199762	0.00019988
4	0.8	0.18649054	0.01984791	0.00199678	0.0001998
5	1.0	0.18639010	0.01983723	0.00199570	0.00019969
6	1.2	0.18626827	0.01982426	0.00199400	0.00019956

TABLE 4

The value of phase shift " δ_1 " by WKB method.

No.	α	Phase shift			
		$\gamma = 0^\circ$	$\gamma = 25^\circ$	$\gamma = 50^\circ$	$\gamma = 75^\circ$
1	0.2	1.053	1.046	1.046	1.046
2	0.4	1.043	1.043	1.044	1.046
3	0.6	1.039	1.040	1.043	1.046
4	0.8	1.034	1.035	1.040	1.045
5	1.0	1.023	1.021	1.036	1.045
6	1.2	1.014	1.020	1.032	1.045

TABLE 5

The value of phase shift " δ_o " by variational method, for $\gamma = 0^o$ and a = 1 A^o. U. (In actual calculations "a" is converted in atomic Units. (K_1, K_2 , K_3 , K_4 are as defined in Table 3.)

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.31448996	0.03144896	0.0031449	0.00031449
2	0.4	0.28089398	0.02808939	0.00280894	0.00028089
3	0.6	0.23910552	0.02391054	0.00239105	0.00023911
4	0.8	0.19878358	0.01987834	0.00198783	0.00019878
5	1.0	0.16431016	0.01643100	0.00164310	0.00016431
6	1.2	0.13646007	0.01364600	0.00136460	0.00013646

TABLE 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 25^{\circ}$ and a = 1 A°. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.31676269	0.03167625	0.00316762	0.00031676
2	0.4	0.23318572	0.02881856	0.00288185	0.00028819
3	0.6	0.25101838	0.02510183	0.00251019	0.00025102
4	0.8	0.21334147	0.02133413	0.00213341	0.00021334
5	1.0	0.17962641	0.01796263	0.00179626	0,00017963
6	1.2	0.15132350	0.01513284	0.00153283	0.00015133

T A B L E 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 50^\circ$ and $a = 1\ A^\circ$. U,

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.32209027	0.03220901	0.00322090	0.00032209
2	0.4	0.30647039	0.03064720	0.00306471	0.00030647
3	0.6	0.28371900	0.02837189	0.0028379	0.00028372
4	0.8	0.25728697	0.02572868	0.00257287	0.000257287
5	1.0	0.23013264	0.02301325	0.00230132	0.00023013
6	1.2	0.20425409	0.02042540	0.00204254	0.00020425

T A B L E 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 75^{\circ}$ and a = 1° A°. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.32675952	0.03267594	0.00326759	0.00032676
2	0.4	0.32403177	0.03240316	0.00324032	0.00032403
3	0.6	0.3195911	0.03195909	0.00319591	0.00031959
4	0.8	0.31358629	0.03135861	0.00313586	0.00031395
5	1.0	0.30620807	0.03062079	0.00306210	0.00030621
6	1.2	0.29767537	0.02976752	0.00297675	0.00029767

TABLE 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 8$ and $a = 2$ A°. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.24125388	0.02412529	0.00241253	0.00023125
2	0.4	0.19859135	0.01985914	0.00198591	0.00019859
3	0.6	0.15403003	0.01540299	0.00154030	0.00015403
4	0.8	0.11794519	0.01179451	0.00117945	0.00011795
5	1.0	0.09132659	0.00913265	0.00091326	0.00009133
6	1.2	0.07216090	0.00721609	0.00072161	0.00007216

TABLE 5 Contd.

The value of phase shift " δ_0 " by variational method, for $\gamma = 25^\circ$ and a = 2 A°. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.24440265	0.02444026	0.0024440_2	0.00024440
2	0.4	0.20727259	0.02072725	0.00207272	0.00020727
3	0.6	0.16590613	0.01659061	0.00165906	0.00016591
4	0.8	0.13029683	0.01302967	0.00130297	0.00013030
5	1.0	0.10272545	0.01027254	0.00102725	0.00010273
6	1.2	0.08215499	0.00821549	0.00082155	0.00008215

TABLE 5 Contd.

The value of phase shift " δ_0 " by variational method, for $\gamma = 50^\circ$ and a = 2 Å. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.25193059	0.02519305	0.00251930	0.00025193
2	0.4	0.2304237	0.02304231	0.00230423	0.00023042
3	0.6	0.20191944	0.02019193	0.00201919	0.00020192
4	0.8	0.17240578	0.01724057	0.00172406	0.00017241
5	1.0	0.14547485	0.01454748	0.00145475	0.00014547
6	1.2	0.12250316	0.01225031	0.00122503	0.00012250

TABLE 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 75^\circ$ and a = 2 A°. U.

No.	α	Phase shift			
		K_{111}	K_2	K_3	K_4
1	0.2	0.25870061	0.02587005	0.00258700	0.0002587
2	0.4	0.25472569	0.02547256	0.00254725	0.0002547_3
3	0.6	0.24837369	0.02483736	0.00248373	0.00024837
4	0.8	0.24001080	0.02400107	0.00240011	0.00024001
5	1.0	0.23007631	0.02300762	0.00230076	0.00023008
6	1.2	0.21903116	0.02190311	0.00219031	0.00021903

TABLE 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 0^o$ and a = 3 A°. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.21393436	0.02139343	0.00213934	0.00021393
2	0.4	0.16379154	0.01637914	0.0016379	0.00016379
3	0.6	0.11839306	0.01183930	0.00118393	0.00011839
4	0.8	0.03592170	0.00359217	0.00035922	0.00003592
5	1.0	0.06406212	0.00640621	0.00064062	0.00006406
6	1.2	0.04930117	0.00493011	0.00049301	0.00004930

T A B L E 5 Contd.

The value of phase shift "δ_o" by a variational method, for $\gamma = 25^o$ and a = 3 A.U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.2179366	0.0217936	0.00217937	0.00021794
2	0.4	0.17341876	0.01734187	0.00173419	0.00017342
3	0.6	0.12987715	0.01298771	0.00129877	0.00012988
4	0.8	0.09664774	0.00966477	0.00096648	0.00009665
5	1.0	0.07322127	0.00732213	0.00073221	0.00007322
6	1.2	0.05690122	0.00569012	0.00056901	0.00005690

TABLE 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 50^{\circ}$ and a = 3 A°. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.22768641	0.02276863	0.00227686	0.00022769
2	0.4	0.20050490	0.02005048	0.00200505	0.00020050
3	0.6	0.16744977	0.01674496	0.00167450	0.00016745
4	0.8	0.13634372	0.01363437	0.00136344	0.00013634
5	1.0	0.11037511	0.01103750	0.00110375	0.00011037
6	1.2	0.08983487	0.00898348	0.00089835	0.00008983

T A B L E 5 Contd.

The value of phase shift " δ_o" by variational method, for $\gamma = 75^o$ and a = 3 A°. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.23668230	0.02366821	0.00236682	0.00023668
2	0.4	0.23137385	0.02313737	0.00231374	0.00023137
3	0.6	0.22304714	0.02230470	0.00223047	0.00022305
4	0.8	0.21236795	0.02123673	0.00212368	0.00021237
5	1.0	0.20008292	0.02000829	0.00200080	0.00020008
6	1.2	0.13691045	0.01369103	0.00136910	0.00013691

T A B L E 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 0^\circ$ and $a = 4$ A.$^\circ$ U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.19812441	0.01981243	0.00198124	0.00019812
2	0.4	0.14228779	0.01422878	0.00142288	0.00014229
3	0.6	0.09738600	0.00973860	0.00097386	0.00009739
4	0.8	0.06808907	0.00680891	0.00068089	0.00006809
5	1.0	0.04954540	0.00495454	0.00049545	0.00004955
6	1.2	0.03752002	0.00375200	0.00037520	0.00003752

TABLE 5 contd.

The value of phase shift " δ_0 " by variational method, for $\gamma = 25^{\circ}$ and a = 4 A.U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.20290083	0.02029008	0.00202901	0.00020290
2	0.4	0.15246493	0.01524649	0.00152465	0.00015246
3	0.6	0.1082875	0.01082875	0.00108287	0.00010829
4	0.8	0.07752633	0.00775263	0.00077526	0.00007753
5	1.0	0.05720552	0.00572055	0.00057205	0.00005721
6	1.2	0.0436632	0.00436632	0.00043663	0.00004366

Table 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 50^\circ$ and a = 4 A.° U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.21475077	0.02147507	0.00214751	0.00021475
2	0.4	0.13245924	0.01324592	0.00132459	0.00013246
3	0.6	0.14612627	0.01461263	0.00146126	0.00014613
4	0.8	0.11455780	0.01145577	0.00114558	0.00011456
5	1.0	0.08994675	0.00899468	0.00089947	0.00008995
6	1.2	0.07150549	0.00715055	0.00071505	0.00007151

TABLE 5 Contd.

The value of phase shift " δ_o " by variational method, for $\gamma = 75^o$ and a = 4 A^o. U.

No.	α	Phase shift			
		K_1	K_2	K_3	K_4
1	0.2	0.22596294	0.02259629	0.00225963	0.00022596
2	0.4	0.21931380	0.02193137	0.00219314	0.00021931
3	0.6	0.2090736	0.02090736	0.00209073	0.00020907
4	0.8	0.19626368	0.01962686	0.00196269	0.00019627
5	1.0	0.18197596	0.01819759	0.00181976	0.00018197
6	1.2	0.16714680	0.0167147	0.00167147	0.00016715

APPENDIX I

Matrix derived from equation 3.21, for different values of here $n = m = 0$, $\ell = l$.

l	$\Delta^{\circ}_{0,0}$	$\Delta^{\circ}_{0,1}$	$\Delta^{\circ}_{0,2}$	$\Delta^{\circ}_{0,3}$	$\Delta^{\circ}_{0,4}$	$\Delta^{\circ}_{0,5}$	$\Delta^{\circ}_{0,6}$	$\Delta^{\circ}_{0,7}$	$\Delta^{\circ}_{0,8}$	$\Delta^{\circ}_{0,9}$
0	Y	$\frac{\alpha\gamma'}{\sqrt{3}}$	0	0	0	0	0	0	0	0
1	$\frac{\alpha\gamma'}{\sqrt{3}}$	y-2	$\frac{2\alpha\gamma'}{\sqrt{15}}$	0	0	0	0	0	0	0
2	0	$\frac{2\alpha\gamma'}{\sqrt{15}}$	y-6	$\frac{3\alpha\gamma'}{\sqrt{35}}$	0	0	0	0	0	0
3	0	0	$\frac{3\alpha\gamma'}{\sqrt{35}}$	y-12	$\frac{4\alpha\gamma'}{\sqrt{63}}$	0	0	0	0	0
4	0	0	0	$\frac{4\alpha\gamma'}{\sqrt{63}}$	y-20	$\frac{5\alpha\gamma'}{\sqrt{99}}$	0	0	0	0
5	0	0	0	0	$\frac{5\alpha\gamma'}{\sqrt{99}}$	y-30	$\frac{6\alpha\gamma'}{\sqrt{13\cdot11}}$	0	0	0
6	0	0	0	0	0	$\frac{6\alpha\gamma'}{\sqrt{13\cdot11}}$	y-42	$\frac{7\alpha\gamma'}{\sqrt{13\cdot15}}$	0	0
7	0	0	0	0	0	0	$\frac{7\alpha\gamma'}{\sqrt{13\cdot15}}$	y-56	$\frac{8\alpha\gamma'}{\sqrt{15\cdot17}}$	0
8	0	0	0	0	0	0	0	$\frac{8\alpha\gamma'}{\sqrt{15\cdot17}}$	y-72	$\frac{9\alpha\gamma'}{\sqrt{17\cdot19}}$
9	0	0	0	0	0	0	0	0	$\frac{9\alpha\gamma'}{\sqrt{17\cdot19}}$	y-90

APPENDIX II

Jacobi's method of diagonalization of matrix.

For a real symmetric matrix A; all eigen values are real, and that there exists a real orthogonal matrix O such that $O^{-1} A O$ is diagonal. We shall now try to produce the desired orthogonal matrix as a product of very special orthogonal matrices. Among the off diagonal elements we choose the numerically largest element $|a_{ik}| = \max$. The elements a_{ii}, a_{ik}, a_{ki} $(=a_{ik})$ and a_{kk} form a (2, 2) - submatrix which can easily transformed to diagonal form, we put

$$O = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}$$

and get

$$D = O^{-1} A O = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} a_{ii} & a_{ik} \\ a_{ik} & a_{kk} \end{pmatrix} \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \quad \ldots\ldots\ldots 1.$$

$$d_{ii} = a_{ii} \cos^2\phi + 2 a_{ik} \sin\phi \cos\phi + a_{kk} \sin^2\phi$$

$$d_{ik} = d_{ki} = -(a_{ii} - a_{kk}) \sin\phi \cos\phi + a_{ik}(\cos^2\phi - \sin^2\phi)$$

$$d_{kk} = a_{ii} \sin^2\phi - 2a_{ik} \sin\phi \cos\phi + a_{kk} \cos^2\phi$$

Now choose Φ such that $d_{ik} = d_{ki} = 0$, that is

$\tan 2\Phi = 2a_{ik} / (a_{ii} - a_{kk})$. We put

$$R^2 = (a_{ii} - a_{kk})^2 + 4a_{ik}^2$$ and after some simple computations we get

$$d_{ii} = 1/2 \ (a_{ii} + a_{kk} + R)$$

$$d_{kk} = 1/2 \ (a_{ii} + a_{kk} - R) \qquad \ldots\ldots 2.$$

$$d_{ik} = d_{ki} = 0$$

(Note that $d_{ii} + d_{kk} = a_{ii} + a_{kk}$ and $d_{ii}\, d_{kk} = a_{ii}\, a_{kk} - a_{ik}^2$)

We perform z series of such two dimentional totations, the transformation matrices have the form given above in the elements (i, i) (i, k) (k, i) and (k,k) and are identical with the unit matrix elsewhere. Each time we choose such values, i and k that a_{ik} = max. Then it can be proved that with $O = o_1\, o_2 \cdots o_r$, the matrix $B = o^{-1} A o$ comes closer and closer to a diagonal matrix when r increases, and further that the columns of o converges to the eigen vectors.

If $\sum_{k \neq i} |a_{ik}|$ is denoted by ε_i, we know that $|(a_{ii} - \lambda)| < \varepsilon_i$ for some value of i, and if the process has been brought

sufficiently far, every circle defined in this was contains exactly one eigen value. Thus it is easy to see when sufficient accuracy has been attained and the procedure can be discontinued.

The convergence of the method has been examined by Von Newmanu and Goldstine in the following way. We put $T^2(A) = \sum_i \sum_{k \neq i} a_{ik}^2 = N^2(A) - \sum_i a_{ii}^2$ and, as before $B = O^{-1} A O$. The orthogonal transfermation effects only the ith row and column and the Kth row and column. Taking only off diagonal elements a_{ik}, a_{ki}, that is

$$T^2(A') = T^2(A) - 2\, a_{ik}^2$$

since a_{ik} was the absolutely largest of all n (n-1) off diagonal elements we have

$$a_{ik}^2 \geq \frac{T^2(A)}{n(n-1)}$$

and

$$T^2(A') \leq T^2(A) \cdot \left(1 - \frac{2}{n(n-1)}\right) <$$

$$T^2(A) \cdot \exp\left\{-\frac{2}{n(n-1)}\right\}$$

Hence we get the final estimate

$$T(A') < T(A) \cdot \exp\left\{-\frac{1}{n(n-1)}\right\}$$

After N intertions, T (A) has decreased with at least the factor exp (- N/n (n-1)) and for a sufficiently large N we come arbitrarily close to the diagonal matrix containing the eigen value.

In a slightly different modifications, we go through the matrix row by row, performing a rotation as soon as $|a_{ik}| > \varepsilon$. Here ε is a prescribed tolarance which, of course, has to be changed each time the whole matrix passed. The method was first suggested by Jacobi. It has the advantage that the computations usually can be performed without resorting to a floting representation.

APPENDIX III

Scattering phase shift for spherically symmetric field :-

Let the potential energy at distance r from the nucleus be γr^{-2}. Then the wave equation to determine L is

$$\frac{d^2L}{dr^2} + \frac{2}{r}\frac{dL}{dr} + \left\{ K^2 - \frac{\ell(\ell+1) + \beta}{r^2} \right\} L = 0$$

$$(\beta = 2m\gamma/\hbar^2) \qquad \ldots\ldots\ldots \quad (1)$$

The solutions of this equation are

$$r^{-1/2} J_{\nu+1/2}(Kr) \qquad \ldots\ldots\ldots \quad (2)$$

Where ν is either root of

$$\nu(\nu+1) = \ell(\ell+1) + \beta$$

i.e. $$\nu = 1/2 \left[-1 \pm (1 + 4\ell + 4\ell^2 + 4\beta)^{1/2} \right] \ldots \quad (3)$$

Now the wave function L (r) must be finite at the origin. That is to say, since $r^{-1/2} J_{\nu \pm 1/2}(Kr)$ behaves like r^{ν} at the origin we must have

$$\nu \geq 0 \quad (\text{all } \ell)$$

If β is positive (repulsive field), then this condition is satisfied for one root and not the other. Thus

the bounded solution is unique, as it is a field with a lower singularity. If β is negative (attractive force) there are then two possibilities, if $-1/4 < \beta < 0$ then for $\ell = 0$, both solutions are unbounded at the origin, but there is one solution for which the singularity is of a lower order then for any other solution. If we choose to take this as our solution a formula for the scattered intensity may be obtained. If on the other hand, $\beta < -1/4$, both solutions behave like $r^{-1/2} \exp(\pm i \alpha \log r)$ near the origin. There is therefore no solution of the scattering problem for this case. It is not merely that a signularity of this type at the origin is objectionable. There is no solution because there is no criterian as to which solution of equation 1 ought to be taken, and thus the phase δ_0 can not be defined.

Returning to the case of repulsive field we see from the asymptotic form of equation 2 that

$$\delta_\ell = 1/2\,\pi(\nu - \ell)$$

where ν is the positive root of equation 3. For large this reduces to

$$1/2\,\pi\beta/(2\ell + 1)$$

APPENDIX IV

Calculations of scattering amplitude and diffusion cross section.

As derived in the section 3.1 the scattering amplitude is given by

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

$$\sigma_t = 2\pi \int_0^{\pi} y_{lm}(\mu\nu)\, |f(\theta)|^2 \cdot y^*_{lm}(\mu\nu) \sin\mu\, d\mu$$

since we have two values of δ, e.g. δ_0 and δ_1

$$|f(\theta)|^2 = \frac{1}{k^2}\Big[\Big\{e^{i\delta_0}\sin\delta_0 P_0(\cos\theta) + 3\, e^{i\delta_1}\sin\delta_1 P_1(\cos\theta)\Big\} \times \Big\{e^{-i\delta_0}\sin\delta_0 P_0(\cos\theta) + 3\, e^{-i\delta_1}\sin\delta_1 P_1(\cos\theta)\Big\}\Big]$$

$$\therefore |f(\theta)|^2 = \frac{1}{k^2}\Big[\sin^2\delta_0 + 9\sin^2\delta_1\cos^2\theta + 6\sin\delta_0\sin\delta_1(\cos(\delta_0-\delta_1)\cos\theta\Big]$$

Since δ_0 and δ_1 are small

$$|f(\theta)|^2 = \frac{1}{k^2}\Big[\delta_0^2 + 9\,\delta_1^2\cos^2\theta + 6\,\delta_0\delta_1\cos\theta\Big]$$

$$\sigma_t = \frac{2\pi}{k^2}\left[\int_0^{\pi} \delta_0^2 \left| y_{lm}(\mu\nu)\right|^2 \sin\mu\, d\mu + 9\cos^2\theta \int_0^{\pi} \delta_1^2 \left| y_{lm}(\mu\nu)\right|^2 \sin\mu\, d\mu + 6\cos\theta \int_0^{\pi} \delta_0\delta_1 \left| y_{lm}'(\mu\nu)\right|^2 \sin\mu\, d\mu\right.$$

which leads to the expression for Q_D as

$$Q_D = \frac{\pi}{k_0^2}\left[8\pi \sin^2\delta_0 + 24\pi \sin^2\delta_1 (1+\delta_1^2)\right.$$

Converting energy in to $\sqrt{\text{Volt}}$ units, the expression observed was

$$Q_D' = \frac{Q_D}{\pi a_0^2} = \left[8\pi \sin^2\delta_0 + 24\pi \sin^2\delta_1 (1+\delta_1^2)\right]\frac{13.61}{E'}$$

The important phase shift for slow electron scattering is δ_0. The effect of second term is neglected. The δ_0 dependent for $\gamma' = 0$ turns out to be

$$Q_D' = \frac{341.8\ \delta_0^2}{E'}$$