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NAAC ACCREDITED ‘A’ GRADE

Topic: Partial wave analysis.

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(*) Partial wave analysis

$$\psi(\vec{r}_1, \vec{r}_2, t) = \psi(\vec{r}_1, \vec{r}_2) \cdot e^{-iEt/\hbar} \quad \text{—— (1)}$$

with $H\psi(\vec{r}_1, \vec{r}_2) = E\,\psi(\vec{r}_1, \vec{r}_2)$

where $$H = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\vec{r}_1, \vec{r}_2) \quad \text{— (2)}$$

If $V(\vec{r}_1, \vec{r}_2) = V(|\vec{r}_2 - \vec{r}_1|)$ then we can use new coordinate system in CM frame as – $\vec{r} = \vec{r}_2 - \vec{r}_1$ & $\vec{R} = \dfrac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}$

So $V(\vec{r}_1, \vec{r}_2) = V(\vec{r})$ [central potential]

And $$-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 = -\frac{\hbar^2}{2M}\cdot\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 \quad \text{—— (3)}$$

where $M = m_1 + m_2$ and $\mu = \dfrac{m_1 m_2}{m_1 + m_2}$

So Schrodinger equation in CM frame is

$$\left[-\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(r)\right]\psi(\vec{r}, \vec{R}) = E\,\psi(\vec{r}, \vec{R})$$

Let $$\psi(\vec{r}, \vec{R}) = \chi(\vec{R})\,\psi(\vec{r}) \quad \text{—— (4)}$$

Using separation of variable we can write

$$-\frac{\hbar^2}{2M}\nabla_R^2\chi - E_R\chi = 0 \quad \text{and}$$

$$-\frac{\hbar^2}{2\mu}\nabla_r^2\psi + V(r)\psi = E_r\psi \qquad [E = E_R + E_r]$$

Putting $\nabla_r \equiv \nabla$ & $E_r \equiv \varepsilon$ we have

$$\boxed{-\frac{\hbar^2}{2\mu}\nabla^2\psi + V\psi = \varepsilon\psi} \quad \text{—— (5)}$$

In spherical polar coordinate system - Let us take a recap - - -.

$$H = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)\right] + V(r)$$

$$= -\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}\right] + V(r) \quad \text{— (6)}$$

where $L^2 = (i\hbar)^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)\right]$

~~As $[H,L] = [H,L^2] = 0$ and~~

Let us consider $\psi(r,\theta,\phi) = R(r)\,Y_{lm}(\theta,\phi)$

then $-\frac{\hbar^2}{2M}\left[Y_{lm}\cdot\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - R\cdot\frac{L^2}{\hbar^2 r^2}Y_{lm}\right] + VRY_{lm} = ERY_{lm}$ — (7)

$$\Rightarrow -\frac{\hbar^2}{2M}\left[\frac{1}{Rr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{1}{Y_{lm}}\frac{L^2}{\hbar^2 r^2}Y_{lm}\right] + V = E \quad \text{— (8)}$$

as $[H,L] = [H,L^2] = 0$ so $Y_{lm}(\theta\phi)$ is ~~also~~ a simultaneous eigenfunction of L^2.

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

putting the value in the previous equation -

$$-\frac{\hbar^2}{2M}\left[\frac{1}{Rr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{l(l+1)\cancel{\hbar^2}\,\cancel{Y_{lm}(\theta\phi)}}{\cancel{Y_{lm}}\,\cancel{\hbar^2}\,r^2}\right] + V = E$$

$$\Rightarrow \cancel{-\frac{\hbar^2}{2M}\left[\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - R(l+1)l\right] = (V-E)\frac{r^2}{\hbar^2} = 0}$$

$$\Rightarrow \left[\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - R(l+1)l\right] - (V-E)\cdot\frac{2M}{\hbar^2}Rr^2 = 0 \quad \text{— (9)}$$

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2\mu r^2}{\hbar^2}(V-E)R = l(l+1)R \quad \text{— (10)}$$

if we put $u(r) = R(r) \cdot r$ then the equation (10) simplifies to —

$$\frac{d^2u}{dr^2} - \frac{2\mu}{\hbar^2}(V-E)u = l(l+1)\frac{u}{r^2} \quad \text{— (11)}$$

putting $\frac{2\mu}{\hbar^2}(E-V) = k^2$ (11) become —

$$\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2} u = -k^2 u \quad \text{— (12)}$$

For free particle $V=0$ then $k^2 = \frac{2\mu E}{\hbar^2}$

equation (12) can be written as — (~~putting~~

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \cdot \frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right] R_{El}(r) = 0 \quad \text{— (13)}$$

if we change the veriable $\rho = kr$ then the equation (13) become —

$$\boxed{\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho}\left(1 - \frac{l(l+1)}{\rho^2}\right)\right] R_l(\rho) = 0} \quad \text{— (14)}$$

The equation (14) is the actual Spherical Bessel ~~functio~~ equation and it has a particular solution known as spherical Bessel functions — $j_l(\rho)$ and spherical Neumann function $n_l(\rho)$ $\quad | \; \rho = (kr) |$

$$j_l(kr) = \left(\frac{\pi}{2kr}\right)^{\frac{1}{2}} J_{(l+\frac{1}{2})}(kr) = (-\rho)^l \left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right) \frac{\sin\rho}{\rho} \text{ and}$$

$$n_l(\rho) = (-1)^{l+1}\left(\frac{\pi}{2\rho}\right)^{\frac{1}{2}} J_{-l-\frac{1}{2}}(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right) \frac{\cos\rho}{\rho}$$

(4)

~~Every l give two~~

For every l the two functions $[j_l(kr) \& n_l(kr)]$ provides a pair of linearly independent solutions of the spherical Bessel differential equation.

So general solution can be written as a linear combination of these two functions.

Another pair of linearly independent solution of spherical Bessel equation ~~is~~ can be written as Spherical Hankel function of 1st and 2nd kind —

$$\left.\begin{aligned} h_l^1(\rho) &= j_l(\rho) + i n_l(\rho) \quad \text{and} \\ h_l^2(\rho) &= j_l(\rho) - i n_l(\rho) = [h_l^1(\rho)]^* \end{aligned}\right\} \quad (15)$$

$$h_l^1(\rho) = \frac{(-i)^l}{\rho} \cdot e^{(i(\rho - l\pi/2))} = \frac{(-i)^{l+1}}{\rho} e^{i\rho} \quad \text{for } \rho \to \infty \quad e^{-il\pi/2} = (-i)^l \quad (16)$$

Some Bessel, Neumann and Hankel functions

$$j_0(kr) = \frac{\sin(kr)}{(kr)} \qquad n_0(\rho) = -\frac{\cos(\rho)}{\rho}$$

$$j_1(kr) = \frac{\sin(kr)}{(kr)^2} - \frac{\cos(kr)}{kr} \qquad n_1(\rho) = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho}$$

$$j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin(\rho) - \frac{3}{\rho^2}\cdot\cos(\rho) \qquad n_2(\rho) = -\left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\cos\rho - \frac{3}{\rho^2}\sin\rho$$

In Asymptotic region $\left(\rho \to \infty \ \& \ \rho > \frac{l(l+1)}{2}\right)$

$$j_l(\rho) \xrightarrow[\rho\to\infty]{} \frac{1}{\rho}\sin\left(\rho - \frac{l\pi}{2}\right) \quad (17) \qquad n_l(\rho) \xrightarrow[\rho\to\infty]{} \frac{1}{\rho}\cos(\rho - l\pi/2) \quad (18)$$

$$h_0^{(1)}(\rho) = -i \cdot \frac{e^{i\rho}}{\rho} \ ; \ h_1^{(1)}(\rho) = -\left(\frac{1}{\rho} + \frac{i}{\rho^2}\right) \cdot e^{i\rho}$$

$$h_l^{(1)}(\rho) \xrightarrow[\rho\to\infty]{} -\frac{i}{\rho} \exp[i(\rho - l\pi/2)] \quad (19)$$

The eigenfunction of the free particle in ~~spheri~~ spherical polar coordinates:-

The spherical Neumann function —

$$n_l(\rho) = \frac{1\cdot1\cdot3\cdot5\cdots(2l+1)}{\rho^{l+1}} \quad \text{for}(\rho\to0)$$

has a pole of order $(l+1)$ at origin, and is therefore an irregular solution of Bessel differential equation (13).

The complete solution of (13) is spherical Hankel function as

$$R_{El}(\rho) = C\cdot H_l'(\rho) = C[j_l(\rho) + i n_l(\rho)] \quad \text{— (20)}$$

But $j_l(\rho)$ at $\rho\to0$ have finite values and give a regular solution at the origin.

So the general solution for $V=0$ & $k=\sqrt{\frac{2ME}{\hbar^2}}$ is of the form —

$$R_{El}(r) = C\cdot j_l(\rho) \quad \left[j_l(\rho) = \frac{\rho^l}{1\cdot3\cdot5\cdots(2l+1)} \text{ at } \rho\to0\right]$$

(21)

So free particle wave eigenfunction in spherical polar system be written as

$$\boxed{\psi_{Elm}(r) = C.j_l(kr)\,Y_{lm}(\theta,\phi)} \rightarrow (22)$$

⑥

Expansion of Plane wave in terms of Spherical Harmonics :—

TISE → $-\frac{\hbar^2}{2\mu}\nabla^2\psi(\vec{r}) = E\psi(\vec{r})$

In Cartetian coordinate - let $\psi(\vec{r}) = X(x)\,Y(y)\,Z(z)$

Then using separation of veriable we have -

$$-\frac{\hbar^2}{2\mu}\frac{d^2X(x)}{dx^2} = E_x X(x)$$

The solution $X(x) = \underbrace{A e^{i|k_x|x}}_{\text{incident}} + \underbrace{B e^{-i|k_x|x}}_{\text{reflected}}$

where $k_x = \sqrt{\frac{2\mu E_x}{\hbar^2}}$

$$\therefore \psi_{k}(\vec{r}) = c\exp(ik_x x + ik_y y + ik_z z)$$

$$= c\exp[i\vec{k}\cdot\vec{r}] \quad -㉓ \qquad E = E_x + E_y + E_z$$

$$E = \frac{\hbar^2}{2\mu}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2 k^2}{2\mu} = \frac{p^2}{2\mu} \qquad [p = \hbar k]$$

The free particle Hamiltonian $H = -\frac{\hbar^2}{2\mu}\nabla^2$ and the linear momentum operator $\vec{P}_{op} = -i\hbar\vec{\nabla}$ are characterised by the three well-defined Cartesian components $p_x = \hbar k_x$; $p_y = \hbar k_y$ and $p_z = \hbar k_z$ & energy $E = \frac{p^2}{2\mu}$ but they does not commute with L^2 & L_z, so they have no simultaneous eigenfunctions.

So the plane wave state ㉓ can not be labelled by the quantum number (l, m), so that the orbital angular momentum is poorly defined in those states.

On the other hand the spherical wave states (22) are states of well-defined orbital angular momentum, which are characterised by the quantum numbers (l, m), and for which the linear momentum is poorly defined.

Since both the plane-wave states (23) & spherical wave states (22) form a complete set, an arbitrary state can be written as a superposition of either of them.

In particular, a plane wave $e^{i\vec{k}\cdot\vec{r}}$ can be expressed in terms of spherical waves, so that we may write

$$e^{i\vec{k}\cdot\vec{r}} = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} C_{lm}\, j_l(kr)\, Y_{lm}(\theta,\phi) \quad \text{— (24)}$$

where C_{lm} (with is independent of r) must be determine.

In order to do that, we first consider the special case in which the vector $\vec{k}$ lies along z-axis. So $e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\theta}$ which is independent of ϕ and $Y_{lm}(\theta,\phi)$ will reduce to Legendre polynomials $P_l(\cos\theta)$ and $e^{i\vec{k}\cdot\vec{r}}$ may be expressed as

$$\text{So } e^{i\vec{k}\cdot\vec{r}} = \sum_{l=0}^{\infty} a_l\, j_l(kr)\, P_l(\cos\theta) \quad \text{— (25)}$$

where a_l can be determined in the following way — Orthogonality of L-polynomial

$$\int_{-1}^{+1} P_l(\omega) P_{l'}(\omega)\, d\omega = \frac{2}{2l+1}\delta_{ll'} \quad (\omega = \cos\theta) \quad \text{— (26)}$$

$$\therefore \int_{-1}^{+1} P_{l'}(\omega)\, e^{i(kr\omega)}\, d\omega = \sum_{l=0}^{\infty}\int_{-1}^{+1} a_l\, j_l(kr)\, P_l(\omega) P_{l'}(\omega)\, d\omega$$

$$\int_{-1}^{+1} P_l(\omega)\, e^{i(\omega kr)}\, d\omega = \frac{2}{(2l+1)}\cdot a_l\, j_l(kr) \quad [l = l'] \quad \text{— (27)}$$

$$\therefore \frac{2}{2l+1} a_l\, j_l(kr) = \left[\frac{e^{i(\omega kr)}}{ikr} P_l(\omega)\right]_{-1}^{1} - \int_{-1}^{1} \frac{e^{i(k\omega r)}}{ikr}\left[\frac{d}{d\omega}P_l(\omega)\right] d\omega$$

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Before going to perform integration by parts for another time let us make some assumptions – the 2nd terms in 28 will vary as r^{-2} for another integration and for large value of r $(r \to \infty)$ the 2nd term will go to zero more rapidly than the 1st term and also for $r \to \infty$

$$j_l(kr) \to \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right)$$

So finally we have

$$\frac{2}{(2l+1)} \cdot a_l \frac{1}{(kr)} \sin\left(kr - \frac{l\pi}{2}\right) = \frac{1}{ikr}\left[e^{ikr} P_l(1) - e^{-ikr} P_l(-1)\right]$$

$$\frac{2}{2l+1} a_l \cdot \frac{1}{kr} \left[\frac{e^{ikr} \cdot e^{-il\pi/2} - e^{-ikr} \cdot e^{il\pi/2}}{2ikr}\right] = \frac{1}{ikr}\left[e^{ikr} - (-1)^l \cdot e^{-ikr}\right]$$

$$e^{i\pi/2} = i \quad \therefore \quad e^{il\pi/2} = (i)^l \quad \& \quad e^{-il\pi/2} = (-i)^l = (i)^{-l}$$

$$\Rightarrow \frac{1}{2l+1} \cdot a_l \left[\frac{e^{ikr}(-i)^l - e^{-ikr}(i)^l}{ikr}\right] = \frac{1}{ikr}\left[e^{ikr} - (-1)^l e^{-ikr}\right]$$

$$\Rightarrow \frac{a_l (i)^{-l}}{2l+1}\left[e^{ikr} - e^{-ikr}(i)^{2l}\right] = \left[e^{ikr} - e^{-ikr}(i)^{2l}\right]$$

$$\therefore \boxed{a_l = (2l+1) \cdot (i)^l} \quad \text{— (29)}$$

$$\therefore \boxed{e^{i\vec{k}\cdot\vec{r}} = \sum_{l=0}^{\infty} (2l+1)\, i^l\, j_l(kr)\, P_l(\cos\theta)} \quad \text{— (30)}$$

This equation is known as Rayleigh's formula.

To find out the C_{lm} in equation 24 we have to use the addition formula of $P_l(\cos\theta)$

$$P_l(\cos\theta) = \frac{4\pi}{2l+1}\sum_{m=-l}^{+l} Y^*_{lm}(\theta_1,\phi_1)\, Y_{lm}(\theta_2,\phi_2)$$

where θ_1, ϕ_1 & θ_2, ϕ_2 are polar angles of $\vec{r}_1$ & $\vec{r}_2$

$$\therefore e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} i^l j_l(kr)\, Y^*_{lm}(\hat{k})\, Y_{lm}(\hat{r})$$

where $\hat{k}$ & $\hat{r}$ represent the polar angle of $\vec{k}$ & $\vec{r}$.

$$\therefore C_{lm}(\hat{k}) = 4\pi\, i^l\, Y^*_{lm}(\hat{k}). \quad — (31)$$

Schrodinger equation for spherically symmetric potential $V(r)$ admits the separable solution $\psi(r,\theta,\phi) = R(r)\, Y_l^m(\theta,\phi)$

putting $u(r) = rR(r)$, the SE radial equation become $-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{2}\right]u = Eu$

Now ~~for~~ at a large distance where the effect of potential is practically zero and for s-wave condition $(l=0)$ the above equation reduce to $\frac{d^2u}{dr^2} + k^2u = 0 \quad k^2 = \left(\frac{2\mu E}{\hbar^2}\right)$

which has a solution $u = Ce^{ikr} + De^{-ikr}$

For scattered wave the 1st term ~~representing~~ representing outgoing wave have validity but the 2nd term, representing reflected wave have no validity.

So $u_{sc} = Ce^{ikr}$

$$\boxed{R(r) \propto \frac{e^{ikr}}{r}}$$

So we have radial part for the scatterd wave have the form $\frac{e^{i\vec{k}\cdot\vec{r}}}{r}$ ~~but fo~~ not only for $l=0$ but for all value of l the nature must not change.

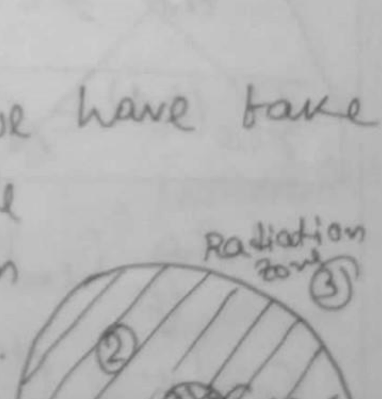
That is why we can choose the radial wave function for incident and scattered wave as -

$$\psi(r,\theta,\phi) = A\left\{ e^{ikz} + f(\theta,\phi)\cdot\frac{e^{i\vec{k}\cdot\vec{r}}}{r} \right\}$$

Finally we are rady to go with partial wave analysis

① Region of application

In partial wave analysis we have take the effect of potential is negligible due to the large distance from Scattering centre i.e $kr \gg 1$. This condition is known as radiation zone in optics, where there is no effect of potential and Centrifugal term.



① Scattering zone $V \neq 0$

② Intermediate zone $V = 0$

③ Radiation zone $kr \gg 1$ $V = 0$

We have seen before that for spherical wavefront (scattered wave) the solution of radial part is ~~Han~~ Hankel function of 1st kind

$$R(r) \sim h_l^{(1)}(kr) \Rightarrow \frac{1}{kr}(-i)^{l+1} e^{ikr} \cdot \quad (kr \gg 1) \qquad (32)$$

Thus the exact wave-function outside the scattering region ($V(r)=0$) is

$$\psi(r,\theta,\phi) = A\Big\{\underbrace{e^{ikz}}_{\text{incident}} + \underbrace{\sum_{l,m} C_{lm}\, h_l^1(kr)\, Y_l^m(\theta,\phi)}_{\text{Scattered wave}}\Big\} \quad -(13)$$

we have considered that potential is symmetric and wave-function is azimuthally ~~same~~ symmetric, so there is no variation of the 'm' ~~quan~~ quantum number. So for $m=0$ we have $Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)$

and the expansion coefficient can be redefined as.

$$\cancel{C_{l,0} = i^{l+1}\sqrt{4\pi(2l+1)}\cdot a_l} \quad \left[C_{lm}(\hat{k}) = 4\pi i^l Y^*_{lm}(\hat{k})\right]$$

$$\cancel{C_{l,0}(\theta,\phi) = 4\pi i^l \cdot \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)} \quad \left[a_l = (2l+1)\, i^l\right]$$

Using $C_{lm}(\hat{k}) = 4\pi i^l Y^*_{lm}(\hat{k})$. we $a_l = (2l+1)\, i^l$

$$C_{l,0} = i^{l+1}\sqrt{4\pi(2l+1)}\cdot a_l$$

Thus $\psi(r,\theta) = A\Big\{e^{ikz} + \sum_{l=0}^{\infty} i^{l+1}(2l+1)\, a_l\, h_l^1(kr)\, P_l(\cos\theta)\Big\}$

where a_l is called the l-th partial wave amplitude.

For large value of kr $\quad h_l^1(kr) \to (-i)^{l+1}\frac{e^{ikr}}{kr}$

$$\therefore \psi(r,\theta) = A\Big\{e^{ikz} + \sum (i)^{l+1}(2l+1)\, a_l\, (-i)^{l+1}\cdot\frac{e^{ikr}}{kr}\, P_l(\cos\theta)\Big\}$$

$$= A\Big\{e^{ikz} + \frac{1}{k}\sum(2l+1)\, a_l\, \frac{e^{ikr}}{r}\, P_l(\cos\theta)\Big\} \quad -(35)$$

We have got ~~prip~~ previous part that total wave function

$$\psi(r,\theta,\phi) = A\left\{e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}\right\} \quad -(36)$$

~~eq~~ compairing (35) & (36) we have

$$\boxed{f(\theta,\phi) = \frac{1}{k}\sum_{l=0}^{\infty} a_l(2l+1)P_l(\cos\theta)} = f(l)P_l(\cos\theta) \quad -(37)$$

The differential scattering cross-section

$$D(\theta) = |f(\theta,\phi)|^2 = \frac{1}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)a_l^* a_{l'} P_l(\cos\theta)P_{l'}(\cos\theta)$$

$$\int_{-1}^{+1} P_l(\cos\theta)P_{l'}(\cos\theta)\,d(\cos\theta) = \frac{2}{(2l+1)}\delta_{ll'}$$

$$\sigma = \int \frac{d\sigma}{d\Omega}d\Omega$$

$$= \frac{1}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)a_l^* a_{l'}\int_0^{2\pi}d\phi\int_{-1}^{+1}P_l(\cos\theta)P_{l'}(\cos\theta)\,d(\cos\theta)$$

$$= \frac{1}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)|a_l^2| \cdot 2\pi \cdot \frac{2}{(2l+1)}\delta_{ll'}$$

$$\boxed{\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)|a_l|^2} \quad -(38)$$

(13)

Effect of potential in partial wave analysis - (~~Sphe~~ Phase shift):-

The spherical wave form of the incident plane wave $e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta)$

Using this wave function we have full wave function in the scattering region -

$$\psi(r,\theta) = A \sum_{l=0}^{\infty} i^l (2l+1)[j_l(kr) + i a_l h_l^1(kr)] P_l(\cos\theta) \quad (39)$$

[As at radiation zone there is only scattered wave]

Let us apply the partial wave process to hard sphere scattering where $V(r) = \begin{cases} \infty & \text{for } r \leq a \\ 0 & \text{for } r > a \end{cases}$

The boundary condition $\psi(a,\theta) = 0$ [on the surface of scatterer wave function should be zero]

$$A \sum i^l (2l+1) [j_l(kr) + i a_l h_l^1(kr)] P_l(\cos\theta) = 0 \quad \text{at } r = a$$

$$\therefore j_l(ka) + i a_l h_l^1(ka) = 0$$

$$a_l = \frac{j_l(ka)}{i h_l^1(ka)}$$

$$\therefore \sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left| \frac{j_l(ka)}{h_l^1(ka)} \right|^2 \qquad \boxed{k^2 \propto E}$$

for low energy scattering $k.a \ll 1$ & we have

$$j_l(x) = \frac{2^l . l!}{(2l+1)!} x^l \quad (x \ll 1)$$

$$n_l(x) = -\frac{(2l)!}{2^l . l!} \cdot \frac{1}{x^{l+1}} \quad \therefore n_l(x) \gg j_l(x)$$

$$\therefore h_l(x) = j_l(x) + i n_l(x) \approx i n_l(x) \quad x \ll 1$$

$$\therefore \frac{j_l(ka)}{h_l^1(ka)} \approx -i \cdot \frac{j_l(ka)}{n_l(ka)}$$

$$\therefore \frac{j_l(ka)}{h_l(ka)} = (-i)\left[\frac{2^l l!}{(2l+1)!}(ka)^l \times (-1)\frac{2^l \cdot l!}{(2l)!}\cdot(ka)^{l+1}\right]$$

$$= \frac{i}{(2l+1)}\left(\frac{2^l l!}{(2l)!}\right)^2 (ka)^{2l+1}.$$

$$\therefore \sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\left[\frac{1}{(2l+1)}\cdot\left\{\frac{2^l \cdot l!}{(2l)!}\right\}^2 (ka)^{2l+1}\right]^2$$

for low energy approximation we can write $l=0$

$$\therefore \sigma = \frac{4\pi}{k^2}\left[\frac{2^0 \cdot 0!}{0!}\cdot(ka)\right]^2 = \frac{4\pi}{k^2}\cdot k^2a^2$$

$= 4\pi a^2$ [comparable with classical result]

So what is the effect of potential?

if $V \to 0$ $R(r) \to j_l(kr)$ or $n_l(kr)$ or the linear combination of $j_l(kr)$ & $n_l(kr)$

But due to the effect of potential the spherical Bessel and Neumann function get distorted by ~~some am~~ its amplitude.

So let the solution of spherical wave ~~for~~ modified by the effect of potential is

$$R(r) = A_l j_l(kr) + B_l n_l(kr)$$

(*) at $r \to 0$ $n_l(kr) \to \infty$ so we can drope ~~$B_l = 0$~~ 2nd term by $B_l = 0$ for $V \to 0$ but due to $V(r) \neq 0$ we can not make $B_l = 0$.

So ~~A_l~~ the existance of A_l & B_l is the effect of $V(r)$ in the solution which will satisfy at $r \to 0$ & at $r \to \infty$ both region.

at $r \to \infty$ $\quad j_l(kr) \to \frac{1}{kr} \sin(kr - l\pi/2)$

$\quad n_l(kr) \to -\frac{1}{kr} \cos(kr - l\pi/2)$

$$\therefore R(r) = \frac{A_l}{kr} \sin(kr - l\pi/2) - \frac{B_l}{(kr)} \cdot \cos(kr - l\pi/2)$$

Let $A_l = C_l \cos\delta_l$ & $B_l = -C_l \sin\delta_l$

$$\therefore R(r) = \frac{1}{kr} C_l \cos\delta_l \sin(kr - l\pi/2) + C_l \sin\delta_l \cos(kr - l\pi/2)$$

$$\boxed{R(r) = \frac{C_l}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)} \quad \text{—— (40)}$$

where $C_l = \sqrt{A_l^2 + B_l^2}$ and $\tan\delta_l = \left(-\frac{B_l}{A_l}\right)$

it shows that at $B_l = 0$ $\delta_l \to 0$ and it will satisfy the result for $V(r) = 0$. ~~So~~

At that moment the effet of $V(r)$ convert in the form of C_l (amplitude) and δ_l (called phase shift).

But our aim is to find out σ_{tot}.

Note The $j_l(kr)$ part ~~shows the~~ represent the incident wave on the condition where no scattering occur or no effect of potential. But the main term representing the effect of $V(r)$ is the ~~Aeller~~ coefficient of $n_l(kr)$.

$$e^{-\frac{l\pi}{2}} = (-i)^l$$

$$\sin\left(kr - \frac{l\pi}{2} + \delta_l\right) = \frac{1}{2i}\left[(-i)^l \cdot e^{ikr} \cdot e^{i\delta_l} - (i)^l \cdot e^{-ikr} e^{-i\delta_l}\right]$$

putting the form in scattering part of ~~ϕ~~ $\psi(r,\theta)$

$$\psi_{sc}(r,\theta) = \sum_l a_l\, h_l^1(kr)\, P_l(\cos\theta)$$

$$= \sum_l a_l P_l(\cos\theta)\, \frac{\sin\left(kr - \frac{l\pi}{2} + \delta_l\right)}{(kr)}$$

$$\boxed{C Y_l(\theta) \to a_l P_l(\cos\theta)}$$

$$\therefore \psi_{sc}(r,\theta) = \sum_l a_l P_l(\cos\theta)\, \frac{1}{2ikr}\left[(-i)^l\, e^{ikr}\, e^{i\delta_l} - (i)^l\, e^{-ikr}\, e^{-i\delta_l}\right] \quad \text{— (41)}$$

ψ equation (41) is ~~the~~ ~~at~~ also the total wave function ψ/z at $r\to\infty$ because there is no incident wave at $r\to\infty$.
We have to equate the (41) with the wave function at scattering zone.
for r is small [scattering zone)

$$\psi_{tot} = \psi_{in} + \psi_{sc} = e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \quad \text{[for unit amplitude } A=1]$$

using Rayleigh formula $e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta)$

$$\therefore \psi_{tot}(r,\theta) = \sum_{l=0}^{\infty}\left[i^l(2l+1)\, j_l(kr)\, P_l(\cos\theta)\right] + f(\theta)\frac{e^{ikr}}{r} \quad \text{— (42)}$$

$$j_l(kr) \to \frac{\sin\left(kr - \frac{l\pi}{2}\right)}{kr} = \frac{1}{2ikr}\left(e^{ikr}\cdot e^{-\frac{l\pi}{2}} - e^{-ikr}\cdot e^{l\pi/2}\right)$$

$$= \frac{1}{2ikr}\left[e^{+ikr}\cdot(-i)^l - e^{-ikr}\,(i)^l\right]$$

$$\cancel{\therefore \psi_{tot} = \sum_{l=0}^{\infty} i^l(2l+1)(-1)\frac{e^{-ikr}}{2ikr}(i)^l P_l(\cos\theta) + \sum_{l=0}^{\infty} i} $$
$$\cancel{+ \sum_{l=0}^{\infty} i^l (2l+1)\frac{e^{ikr}}{r}\left[f(\theta) + \frac{(-i)^l P_l(\cos)}{2ik}\right]}$$

$$\therefore \psi_{tot} = \sum_{l=0}^{\infty} i^l(2l+1)(-1)\, i^l\, \frac{e^{-ikr}}{2ikr} P_l(\cos\theta) + \frac{e^{ikr}}{r}\left(f(\theta) + \sum_{l=0}^{\infty} i^l(2l+1)\cdot\frac{(-i)^l P_l(\cos\theta)}{2ik}\right) \quad \text{— (43)}$$

from — 41

$$\psi_{tot\ compare} = \sum_{l=0}^{l} a_l P_l(\cos\theta)\, \frac{(-i)^l\cdot e^{ikr}\, e^{i\delta_l}}{2ikr} - \frac{a_l P_l(\cos\theta)\, i^l\cdot e^{-ikr}\cdot e^{-i\delta_l}}{2ikr}$$

Comparing the coefficient of e^{-ikr} for both the wave ψ_{tot} at $r \to 0$ & ψ_{tot} at $r \to \infty$

$$\frac{(-1) a_l P_l(\cos\theta) \cdot i^l \cdot e^{-i\delta_l}}{2ikr} = \frac{i^l \cdot (2l+1)(-1)(i)^l \cdot}{2ikr} P_l(\cos\theta)$$

$$\therefore a_l = \frac{i^l (2l+1)}{2ikr} \cdot \frac{e^{i\delta_l}}{P_l(\cos\theta)}$$

$$\therefore \boxed{a_l = i^l (2l+1) \cdot e^{i\delta_l}} \quad \text{— (44)}$$

$\therefore$ equation — (41) will get the form —

$$\psi_{sc}(r\theta) = \sum_{l=0}^{\infty} a_l P_l(\cos\theta) \left[\frac{(-i)^l e^{ikr} \cdot e^{i\delta_l}}{2ikr} - \frac{(i)^l e^{-ikr} e^{-i\delta_l}}{2ikr} \right]$$

$$= \sum_{l=0}^{\infty} i^l (2l+1) \cdot e^{i\delta_l} \left[\frac{(-i)^l \cdot e^{ikr} e^{i\delta_l}}{2ikr} - \frac{e^{-ikr} \cdot e^{-i\delta_l} (i)^l}{2ikr} \right] P_l(\cos\theta)$$

$$= \sum_{l=0}^{\infty} \left[\frac{(+1)^l (2l+1) e^{2i\delta_l} \cdot e^{ikr}}{2ikr} - \frac{(-1)^l (2l+1) \cdot e^{-ikr}}{2ikr} \right] P_l(\cos\theta) \quad \text{— (45)}$$

Compairing the coefficient of $\frac{e^{ikr}}{r}$ in (43) & (45)

$$\boxed{\cancel{f(\theta) + \sum_{l=0}^{\infty} \frac{i^l (2l+1)(-i)^l P_l(\cos\theta)}{2ik} = \sum_{l=0}^{\infty} \frac{(2l+1) e^{2i\delta_l}}{2ik} P_l(\cos\theta)}}$$

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

$$f(\theta) = \sum_{l=0}^{\infty} \frac{(2l+1) P_l(\cos\theta)}{2ik} \left(e^{2i\delta_l} - 1 \right) \quad \text{— (46)}$$

$$= \sum_{l=0}^{\infty} \frac{(2l+1) P_l(\cos\theta)}{k} \cdot e^{+i\delta_l} \left[\frac{e^{i\delta_l} - e^{-i\delta_l}}{2i} \right]$$

$$= \sum_{l=0}^{\infty} \frac{(2l+1) P_l(\cos\theta) e^{i\delta_l}}{k} \sin\delta_l \quad \text{— (47)}$$

$$\therefore \frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{1}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)\,P_l(\cos\theta)\cdot P_{l'}(\cos\theta)\cdot e^{i(\delta_l-\delta_{l'})}\cdot\sin\delta_l)\cdot\sin\delta_{l'}$$

$$\sigma_{tot} = \int\frac{d\sigma}{d\Omega}d\Omega = \frac{2\pi}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)\cdot\frac{2}{(2l+1)}\delta_{ll'}\cdot e^{i(\delta_l-\delta_{l'})}\cdot\sin(\delta_l)\cdot\sin\delta_{l'}$$

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l)$$

$$\therefore \sigma = 2\pi\int_0^{\pi}|f(\theta)|^2\sin\theta\,d\theta \qquad |f(\theta)|^2 = \frac{1}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

$\therefore$ total scattering cross-section $\qquad \frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{\sigma}{4\pi}$

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l)$$

Optical theorem

for low energy scattering k is small or the wave length is large $\left(k = \frac{2\pi}{\lambda}\right)$ and we can consider $l = 0$

$$\therefore f_0 = \frac{1}{k}(2l+1)P_l(\cos\theta)\cdot e^{i\delta_l}\cdot\sin\delta_l\Big|_{l=0}$$

$$= \frac{1}{k}\cdot e^{i\delta_0}\cdot\sin\delta_0 \quad [P_0(\cos\theta) = 1]$$

$$\therefore \frac{d\sigma}{d\Omega} = \frac{1}{k^2}\cdot\sin^2\delta_0$$

Now for forward scattering $(\theta\to 0)$ $\cos\theta = 1$ $\quad P_l(1) = 1$

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

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

$$f(0) = \frac{1}{k}\sum(2l+1)(\underbrace{\cos\delta_l \cdot \sin\delta_l}_{\text{real}} + \underbrace{i\sin^2\delta_l}_{\text{imag}})$$

$$\therefore \sigma = \frac{4\pi}{k^2}|f(0)|^2$$

$$= \cancel{\frac{1}{k}\sum(2l+1)\cdot\cos\delta_l}$$

$$Im\, f(0) = \frac{1}{k}\sum(2l+1)\sin^2\delta_l$$

$$\therefore \cancel{\sigma_{tot} = 4\pi}$$

$$\therefore \frac{4\pi}{k}\cdot Im\, f(0) = \frac{4\pi}{k^2}\cdot\sum(2l+1)\sin^2\delta_l = \sigma_{tot}$$

$$\therefore \sigma_{tot} = \frac{4\pi}{k}\cdot Im\, f(0)$$ where

$f(0)$ is known as forward scattering amplitude.

This is relation between the total scattering cross-section and forward scattering amplitude is known as optical theorem.