21.09.2011

Quantum Mechanics I :-

Full energy eigenfunctions in a central potential

$V(r)$ is

$$f(r)\, Y_{lm}(\theta, \phi)$$

$\downarrow$ satisfies the ODE

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{df}{dr}\right) - \frac{l(l+1)}{r^2} f + \frac{2m}{\hbar^2}\left(E - V(r)\right) f = 0$$

$$\frac{2m}{\hbar^2}\left(E - V(r) - \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)$$

centrifugal potential

2nd order diff. eq. $\Rightarrow$ 2 linearly independent solutions

Introduce a new function. (To get rid of $\frac{df}{dr}$ term.)

$$g(r) = r f(r) \Rightarrow f(r) = \frac{1}{r} g(r)$$

$$\frac{df}{dr} = -\frac{g}{r^2} + \frac{1}{r}\frac{dg}{dr}$$

So, $$r^2 \frac{df}{dr} = -g + r\frac{dg}{dr}$$

$$\therefore \frac{d}{dr}\left(r^2 \frac{df}{dr}\right) = \cancel{-\frac{dg}{dr}} + \cancel{\frac{dg}{dr}} + r\frac{d^2 g}{dr^2}$$

$$= r\frac{d^2 g}{dr^2}$$

$$\frac{1}{r}\frac{d^2 g}{dr^2} - \frac{l(l+1)}{r^2} g/r + \frac{2m}{\hbar^2}\left(E - V(r)\right)\frac{g}{r} = 0$$

$$\Rightarrow \frac{d^2 g}{dr^2} - \frac{l(l+1)}{r^2} g + \frac{2m}{\hbar^2}\left(E - V(r)\right) g = 0$$

Potential (effective) becomes singular at $r = 0$.

$0 < r < \infty$.

(*) One can again prove Oscillation Theorem here.

Study the equation near $r = 0$. Assume that $V(r)$ grows slower than $1/r^2$ as $r \to 0$.

For small r, the equation reduces to

$$\frac{d^2 g}{dr^2} \approx \frac{l(l+1)}{r^2} g.$$

Trial solution $g(r) = C r^{\alpha}$.

We obtain, $C\alpha(\alpha-1) r^{\alpha-2} = l(l+1) C \cancel{\alpha} r^{\alpha-2}$

$$\Rightarrow \alpha(\alpha-1) = l(l+1)$$

$$\Rightarrow \alpha = l+1, \; -l.$$

[Two linearly independent solutions r^{l+1}, r^{-l}.]

~~General~~ $f \overset{\alpha}{\Longrightarrow} \boxed{r^{l}, \; \cancel{r^{-l-1}}}$ (singular)

Study the solution for $r \to \infty$ assuming that $V \to V_0$ (constant) as $r \to \infty$.

$$\frac{d^2 g}{dr^2} + \frac{2m}{\hbar^2}(E - V_0) g = 0.$$

<u>Case I</u> :- $E - V_0 > 0$. Define $k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$

$$\frac{d^2 g}{dr^2} + k^2 g = 0$$

$$\therefore g(r) = A e^{ikr} + B e^{-ikr}.$$

$\left\{ \frac{A}{B} \text{ is a fixed function of } E. \right\}$

There is one solution for every E & l.

{These solutions are scattering solutions}

Now, if $E < V_0$,

<u>Case II</u>: $\frac{d^2 g}{dr^2} + \kappa^2 g = 0$. $\left[\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}\,.\right]$

$$\frac{d^2 g}{dr^2} - \kappa^2 g = 0.$$

$\frac{1}{r}$ is not going to help

$$g = \cancel{A e^{\kappa r}} + B e^{-\kappa r}.$$

(non-normalizable)

Again, $\frac{A}{B}$ is a fixed function of E for given l.

Solutions to $\frac{A}{B} = 0$ gives the energy eigenvalues. $(E_1, E_2, \dots)$ (discrete spectrum)

$\therefore$ For bound states, energy is discrete. Also, the wavefunction falls off exponentially as $r \to \infty$.

$$\frac{d^2 g}{dr^2} - \frac{l(l+1)}{r^2} g + \frac{2m}{\hbar^2}\left(E - V(r)\right) g = 0$$

$$r = \frac{\rho}{1 + \rho e^{-\alpha\rho}} \quad \begin{array}{l} \to \rho \quad \text{as } \rho \to \infty \\ \to e^{\alpha\rho} \quad \text{as } \rho \to -\infty \end{array}$$

$\boxed{\rho \underset{\wedge}{\overset{\text{like}}{\sim}} \ln r}$

{Regularization $\leftrightarrow$ Boundary Conditions

MAPPING OF THE PROBLEM IN ρ SHOWS EVEN MORE EXPLICITLY THE CONNECTION WITH 1-D BOUNDARY CONDITIONS.

Suppose $V(r) = V_0$.

$$\frac{d^2 g}{dr^2} - \frac{l(l+1)}{r^2}\, g + \frac{2m}{\hbar^2}(E - V_0) = 0.$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{df}{dr}\right) - \frac{l(l+1)}{r^2} f + \frac{2m}{\hbar^2}(E - V_0) f = 0.$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V_0\psi = E\psi$$

Solution $\Rightarrow$ $\psi = e^{i\vec{k}\cdot\vec{r}}$ $\qquad k^2 = \frac{2m}{\cancel{K}\hbar^2}(E - V_0)$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{df}{dr}\right) - \frac{l(l+1)}{r^2} + k^2 f = 0$$

Define $\boxed{\rho = kr}$

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2 \frac{df}{d\rho}\right) - \frac{l(l+1)}{\rho^2} f + \cancel{k} f = 0.$$

Spherical Bessel equation

Solutions are $j_l(\rho),\ n_l(\rho)$.

Linearly independent solutions as $\rho \to \infty$ are $\frac{e^{\pm i\rho}}{\rho}$.

$$\left.\begin{aligned} \text{As } \rho \to \infty,\ j_l &\to \frac{1}{\rho}\sin\left(\rho - \frac{1}{2} l\pi\right). \\ n_l &\to -\frac{1}{\rho}\cos\left(\rho - \frac{1}{2} l\pi\right). \end{aligned}\right\}$$

As $\rho \to 0$,

$j_l(\rho) \sim \rho^{l}$, $n_l(\rho) \sim \rho^{-l-1}$.

Only j_l's are allowed for free particle...

If $\rho = 0$ is ~~th~~ within the region of potential, $n_l(\rho)$'s are not allowed.

What if $E < V_0$?

$$\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} = i\kappa .$$

General solution is a linear combination of

$$\cancel{j_\ell(i\kappa\rho) + n_\ell(i\kappa\rho)}$$

$$j_\ell(i\kappa r) + n_\ell(i\kappa r)$$

Why there is no bound state ?

For regular solutions, we must pick j_ℓ's.

But j_ℓ's are blowing up! (for $r \to 0$).

Suppose $V = V_0$ for $r \geq a$ & we are solving the equation for $r \geq a$.

Solution

We have to pick ~~such~~ a solution (linear combination) which damps out for $\to \infty$.

$$a\, j_\ell(ikr) + b\, n_\ell(ikr)$$

$$\underline{n_\ell - i j_\ell}$$

$$e^{i\rho} \xrightarrow[\rho = ikr]{} e^{-\kappa r} \; (\checkmark) \qquad \underline{(-i)(j_\ell + i n_\ell)}$$

$$e^{-i\rho} \xrightarrow[\rho = i\kappa r]{} e^{\kappa r} \; (\times)$$

This solution blows up for $r \to$

No bound state for free particle. ($V \to V_0$ everywhere)

$V = V_0$ everywhere $\quad (E > V_0)$

$$E = V_0 + \frac{\hbar^2 k^2}{2m} \qquad k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

The eigenfunctions are

$$j_\ell(kr)\, Y_{\ell m}(\theta, \phi)$$

→ arbitrary ℓ, m

→ controls the energy

linear combinations

$$e^{i\vec{k}\cdot\vec{r}} \rightarrow \text{Cartesian}$$

$\vec{k}$ can point in arbitrary direction

infinite no. of eigenfunction

Take $\vec{k}$ along z-direction

$$e^{ikz} = e^{ikr\cos\theta} \qquad m = 0$$

$$= \sum_\ell C_\ell\, j_\ell(kr)\, P_\ell(\cos\theta)$$

constants

$$C_\ell = (2\ell+1)\, i^\ell \rightarrow \text{it turns out !}$$

$$e^{ikr\cos\theta} = \sum_\ell i^\ell (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta)$$

Mathematical identity (Crucial in scattering theory)

22.09.2011 Quantum Mechanics :-

Scattering in a central potential

$V(r) \rightarrow V_0$ as $r \rightarrow \infty$.

$$k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} \qquad (E > V_0)$$

$$E = V_0 + \frac{\hbar^2 k^2}{2m}.$$

Eigenfunctions are of the form

$$f_\ell(r)\, Y^\ell_m(\theta, \phi).$$

$$f_\ell \xrightarrow{\text{satisfies}} \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{df}{dr}\right) + \frac{\ell(\ell+1)}{r^2} f + \dots = 0.$$

General solution has the form

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_{lm} f_l(r) P_l^m(\cos\theta) e^{im\phi} \quad \text{--- (S)}$$

As $r \to \infty$, $f_l(r)$ is a linear combination of

$$\frac{e^{ikr}}{r} \text{ and } \frac{e^{-ikr}}{r}:$$

$$f_l(r) \xrightarrow[r\to\infty]{} \frac{1}{r}\sin\left(kr - \frac{1}{2}l\pi + \underset{\substack{\uparrow \\ \text{constant (real)}}}{\delta_l}\right)$$

Solutions can always be taken as real.

(*) δ_l is determined by $V(r)$ and it's a function of energy E. (Consider $\rho \to 0$.)

(*) For any constant potential V_0, $\delta_l = 0$.

$\delta_l \Rightarrow$ phase shift

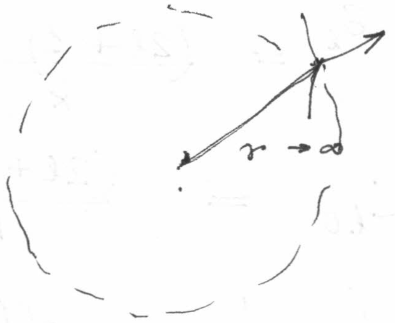
l^{th} term in the sum (S) is called the l'th partial wave.

$$\psi \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_{lm} \cdot \frac{1}{r} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) P_l^m(\cos\theta) e^{im\phi}$$

$$= \left[\frac{1}{2i}\frac{e^{ikr}}{r} \sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_{lm} e^{i(-\frac{1}{2}l\pi + \delta_l)} - \frac{1}{2i}\frac{e^{-ikr}}{r}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_{lm} e^{-i(-\frac{1}{2}l\pi + \delta_l)}\right] P_l^m(\cos\theta) e^{im\phi}. \quad \text{--- (A)}$$

$$= \frac{e^{ikr}}{r} g_1(\theta,\phi) + \frac{e^{-ikr}}{r} g_2(\theta,\phi)$$

$$p_r = \frac{\hbar}{i}\frac{\partial}{\partial r}.$$



$$-i\hbar\frac{\partial}{\partial r}\left(\frac{e^{ikr}}{r}\right)$$

$$= \hbar k\,\frac{e^{ikr}}{r} + i\hbar\,\frac{e^{ikr}}{r^2}$$

For large r, $\approx \hbar k\,\dfrac{e^{ikr}}{r}$

So, $\begin{cases} \dfrac{e^{ikr}}{r}\, g_1(\theta,\phi) \longrightarrow \text{outgoing wave} \\[2ex] \dfrac{e^{-ikr}}{r}\, g_2(\theta,\phi) \longrightarrow \text{incoming wave} \end{cases}$

$$\boxed{j_l(kr) \xrightarrow[r\to\infty]{} \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right) = \frac{1}{kr}\cdot\frac{1}{2i}\left[e^{i\left(kr-\frac{l\pi}{2}\right)} - e^{-i\left(kr-\frac{l\pi}{2}\right)}\right]}$$

Desired form

$$e^{ikz} + f(\theta,\phi)\,\frac{e^{ikr}}{r}.$$

$$= \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta) + f(\theta,\phi)\,\frac{e^{ikr}}{r}$$

$$\xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty}\left[(2l+1)\, i^l\, P_l(\cos\theta)\,\frac{1}{2i}\cdot\frac{1}{kr}\left(e^{i\left(kr-\frac{l\pi}{2}\right)} - e^{-i\left(kr-\frac{l\pi}{2}\right)}\right)\right] + f(\theta,\phi)\,\frac{e^{ikr}}{r}. \quad \text{---} \; (B)$$

$C_{lm} = 0$ for $m \neq 0$.

C_{l0}'s have to be determined.

Compare coefficients of $\dfrac{e^{-ikr}}{r}$ on both sides

[(A) & (B).]

$$C_{l0}\, e^{-i\delta_l} = \frac{(2l+1)\, i^l}{k}$$

$$\text{or,} \quad C_{l0} = \frac{(2l+1)\, i^l}{k}\, e^{i\delta_l}.$$

$e^{i\delta_l}$ → known for given potential

$f(\theta,\phi)$ (compare coefficients of $\frac{e^{ikr}}{r}$.)

$$= \sum_{l=0}^{\infty} \frac{1}{2i} \frac{(2l+1)\, i^l}{k}\, e^{2i\delta_l}\, \underbrace{e^{-\frac{i}{2} l\pi}}_{\to 1 \leftarrow}\, P_l(\cos\theta)$$

$$- \sum_{l=0}^{\infty} \frac{1}{2ik} (2l+1) \underbrace{i^l\, e^{-\frac{i}{2} l\pi}}_{1} P_l(\cos\theta)$$

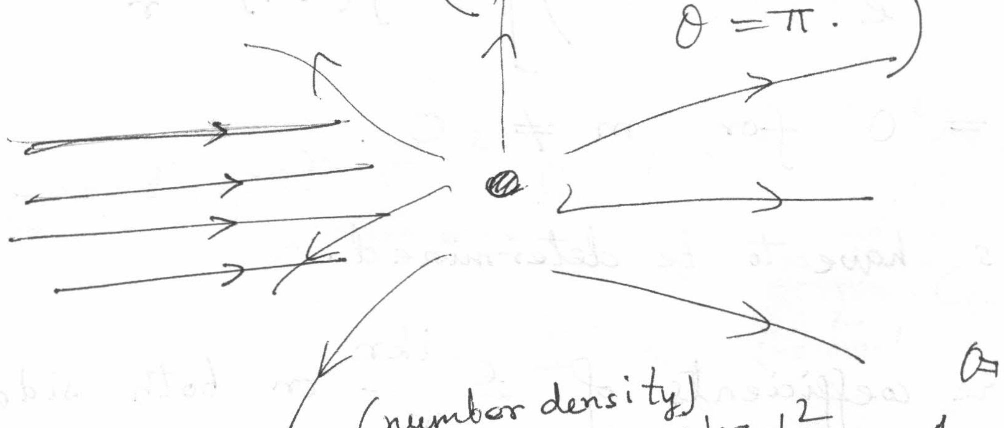
$$= \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \frac{\left(e^{2i\delta_l} - 1\right)}{(2i)} P_l(\cos\theta)$$

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

$$\psi = \underbrace{e^{ikz}}_{\text{incident wave}} + \underbrace{\frac{e^{ikr}}{r} f(\theta,\phi)}_{\text{scattered wave}}$$

$f(\theta,\phi)$: actually independent of ϕ for spherically symmetric potential

(carries back waves also $\theta = \pi$.)



(number density)

Incident density $= |e^{ikz}|^2 = 1$.

Incident flux $= v \cdot 1 = v = \left(\frac{\hbar k}{m}\right)$

(v = velocity)

Scattered number density (Elastic scattering → real potentials)

$$= \frac{1}{r^2} \left| f(\theta, \phi) \right|^2 .$$

$$\text{Scattered flux} = \frac{1}{r^2} \left| f(\theta, \phi) \right|^2 v .$$

(Here, unlike in 1-D, velocity of scattered wave = velocity of incident wave).

Total # of scattered particles per unit time

$$\int d\theta \, d\phi \; r^2 \sin\theta \, \frac{1}{r^2} \left| f(\theta, \phi) \right|^2 v$$

$$= v \int d\theta \, d\phi \; \sin\theta \; \left| f(\theta, \phi) \right|^2$$

Define total cross-section

$$\sigma = \frac{\text{Total no. of scattered particles / time}}{\text{Total no. of incident particles / time (incident flux)}}$$

$$= \frac{\cancel{v} \int d\theta \, d\phi \; \sin\theta \left| f(\theta, \phi) \right|^2}{\cancel{v}}$$

$$= \int \underbrace{d\theta \, d\phi \; \sin\theta}_{d\Omega} \left| f(\theta, \phi) \right|^2 .$$

Differential cross section

$$= \frac{\text{\# of scattered particles / unit time / unit solid angle}}{\text{incident flux}}$$

$$= \left| f(\theta, \phi) \right|^2 . \qquad \left(\frac{d\sigma}{d\Omega} \right) .$$

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Total cross section

$$\sigma = \int \sin\theta \, d\theta \, d\phi \, |f(\theta,\phi)|^2 \cancel{\sin}$$

$$= \int \sin\theta \, d\theta \, d\phi \times \frac{1}{k^2} \sum_l \sum_{l'} (2l+1) e^{i(\delta_l - \delta_{l'})} \sin\delta_l \sin\delta_{l'} P_l(\cos\theta) P_{l'}(\cos\theta)$$

$$= \frac{2\pi}{k^2} \sum_l (2l+1)^2 \sin^2\delta_l \frac{2}{2l+1}$$

$$= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2\delta_l .$$

l^{th} term $\to$ σ_l (cross-section due to l^{th} partial wave)

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

$\parallel$

$f(\theta)$.

$$f(\theta) - f^*(\theta)$$

$$= \frac{1}{k} \sum_l (2l+1) \cdot 2i \sin^2\delta_l \, P_l(\cos\theta)$$

$$\therefore \; f(0) - f^*(0) = \frac{2i}{k} \sum_l (2l+1) \sin^2\delta_l$$

$[\because P_l(1) = 1.]$

$$= \frac{ik}{2\pi} \sigma .$$

$\Rightarrow$ Optical Theorem

(related with conservation of probability)

$$\boxed{\mathrm{Im}\, f(0) = \frac{k\sigma}{4\pi}}$$

(valid even if azimuthal symmetry not present)

Definition of δ_l

Energy eigenfunctions $\to f_l(r) \, Y_m^l(\theta,\phi)$

As $r \to \infty$, $\quad f_l(r) = \frac{1 \cdot C}{r} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$.

$$k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} \qquad \left\{ V_0 = \text{value of the potential at infinity} \right\}$$

Example

Hard sphere

$$\left\{ \begin{array}{ll} V(r) = 0 & \text{for } r \geqslant a \\ V(r) = \infty & \text{for } r < \infty \end{array} \right\}$$

$$f_l = A_l\, j_l(kr) + B_l\, n_l(kr)$$

$\to$ Bessel functions

How to express δ_l in terms of A_l and B_l?

As $r \to \infty$, $\quad f_l = A_l \cdot \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right)$

$$+ \; B_l \left(-\frac{1}{kr}\right) \cos\left(kr - \frac{l\pi}{2}\right).$$

$$= \frac{C}{r}\left\{ \sin\left(kr - \frac{l\pi}{2}\right)\cos\delta_l + \cos\left(kr - \frac{l\pi}{2}\right)\sin\delta_l \right\}$$

$\therefore \tan\delta_l = -\frac{B_l}{A_l}$. $\qquad C = \frac{1}{k}\sqrt{A_l^2 + B_l^2}$ (depends on how you normalize)

$$\Rightarrow \boxed{\delta_l = -\tan^{-1}\left(\frac{B_l}{A_l}\right)}$$

f_l must vanish at $r = a$. (Potential is ∞)

$$\Rightarrow A_l\, j_l(ka) + B_l\, n_l(ka) = 0$$

$$\Rightarrow \tan\delta_l = -\frac{B_l}{A_l} = \frac{+\,j_l(ka)}{n_l(ka)}.$$

What happens if k is small?

(Low energies)

$$C\,\frac{(ka)^{l}}{(ka)^{-l-1}} \approx (ka)^{2l+1} \quad \left(\frac{j_l(ka)}{n_l(ka)} \text{ for low energies} \right)$$

$$\approx 0 \quad (\text{for small } k \ldots)$$

$\therefore$ Total cross section σ [Only $l = 0$ contributes substantially (δ_0 remains).]

$$= \frac{1 \cdot 4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l$$

$$\xrightarrow[k \to 0]{} \boxed{\frac{4\pi}{k^2} \sin^2 \delta_0} \longrightarrow \frac{4\pi}{\cancel{k^2}} \cancel{k^2} a^2 \longrightarrow 4\pi a^2 \Rightarrow a^2$$

$$\begin{pmatrix} \tan \delta_0 \propto k \\ \sin \delta_0 \propto k \end{pmatrix} \quad \text{small } k$$

$$C \to \frac{1}{(2l+1)!!\,(2l-1)!!}$$

$$= 1 \text{ for } l = 0$$

Classical expectation

$$\{ \sigma = \cancel{4}\pi a^2 \} \xrightarrow{QM} \text{~~Double~~ 4 times}$$

High energy $\dashrightarrow$ Classical result (!!)

$V(r) = K\delta(r-a)$. For $r > a$,

f_l can be taken as $A_l j_l(kr) + B_l n_l(kr)$

$$\tan \delta_l = -\frac{B_l}{A_l} \quad \checkmark$$

$\boxed{\text{For } r < a}$: $f_l = C_l j_l(kr)$

Wavefunction at $r = a$ is continuous

$$\Rightarrow \quad A_l j_l(ka) + B_l n_l(ka) = C_l j_l(ka)$$

Derivatives ?? $\longrightarrow$ Integrate the Schrödinger equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{df_l}{dr}\right) - \frac{l(l+1)}{r^2} f_l + \frac{2m}{\hbar^2}\left(E - K\delta(r-a)\right) f_l = 0$$

$$\frac{d}{dr}$$

$$\int_{a-\epsilon}^{a+\epsilon} \frac{d}{dr}$$

Tak

$$\frac{d}{dr}\left(r^2 \frac{df_l}{dr}\right) - l(l+1) f_l + \frac{2m}{\hbar^2}\left(E - K\,\delta(r-a)\right) r^2 f_l = 0.$$

$$\int_{a-\epsilon}^{a+\epsilon} \frac{d}{dr}\left(r^2 \frac{df_l}{dr}\right) dr \;:-\; \cancel{l(l+1)}\; a^2 \left\{ \left.\frac{df_l}{dr}\right|_{a+\epsilon} - \left.\frac{df_l}{dr}\right|_{a-\epsilon} \right\}$$

$$- \frac{2mK}{\hbar^2} a^2 f_l(a) = 0$$

$$\Rightarrow a^2 \left\{ k A_l j_l'(ka) + k B_l n_l'(ka) - k C_l j_l'(ka) \right\}$$

$$- \frac{2mK}{\hbar^2} a^2 C_l j_l(ka).$$

One can now get B_l in terms of C_l

A_l " " "

Take the ratio $\longrightarrow$ $\boxed{\delta_l = \xi(B_l, A_l).}$

In one dimension,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dq^2} + V(q)\psi = E\psi$$

$$\Rightarrow \frac{d}{dq}\left(\psi^* \frac{d\psi}{dq} - \psi \frac{d\psi^*}{dq}\right) = 0$$

{ independent of q }

$\rightarrow$ Derive an analogous relation in 3D (!!)

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{df_l}{dr}\right) - \frac{l(l+1)}{r^2} f_l + \frac{2m}{\hbar^2}\left(E - V(r)\right) f_l = 0$$

$\boxed{g_l = r f_l}$ satisfies the following –

$$\frac{d^2 g_l}{dr^2} - \frac{l(l+1)}{r^2} g_l + \frac{2m}{\hbar^2}\left(E - V(r)\right) g_l = 0.$$

Check $\frac{d}{dr}\left(g_l^* \frac{dg_l}{dr} - g_l \frac{dg_l^*}{dr}\right) = 0$

$$\Rightarrow \frac{d}{dr}\left(rf_l^* \frac{d}{dr}(rf_l) - rf_l \frac{d}{dr}(rf_l^*)\right) = 0.$$

<u>This is not the whole story (!)</u>

$$\Rightarrow \frac{d}{dr}\left\{\underbrace{r^2\left(f_l^* \frac{df_l}{dr} - f_l \frac{df_l^*}{dr}\right)}_{\text{constant}}\right\} = 0$$

$$r^2\left(f_l^* \frac{df_l}{dr} - f_l \frac{df_l^*}{dr}\right) = \text{constant.}$$

(independent of r)

Near $r = 0$, $f_l \propto r^l$

$$r^{(2l-1)} \cdot r^2 = r^{2l+1} \longrightarrow 0 \text{ as } r \to 0.$$

This constant must vanish.

$$\therefore \boxed{f_l^* \frac{df_l}{dr} - f_l \frac{df_l^*}{dr} = 0}$$

$$\Psi = \sum C_{lm} f_l(r) Y^l_m(\theta, \phi)$$

$$\therefore \overbrace{r^2\left(\Psi^* \frac{d\Psi}{dr} - \Psi^* \frac{d\Psi}{dr}\right)}^{\text{radial probability current}}$$

$$= \boxed{\sum_{l,m} \sum_{l',m'} C^*_{lm} C_{l'm'} Y^{l\,*}_m(\theta,\phi) Y^{l'}_{m'}(\theta,\phi)\, r^2\left[f_l^* \frac{df_{l'}}{dr} - f_{l'} \frac{df_l^*}{dr}\right]}$$

$$\int \sin\theta\, d\theta\, d\phi \left(\Psi^* \frac{d\Psi}{dr} - \Psi \frac{d\Psi^*}{dr}\right)$$

$$= 0. \quad \underbrace{(Y^l_m\text{'s are orthonormal})}_{\delta_{ll'}\,\delta_{mm'} \text{ comes in}}.$$

$$\oint_S \vec{j} \cdot d\vec{A} = 0$$

Take $\psi = e^{ikr\cos\theta} + \frac{e^{ikr}}{r} f(\theta,\phi)$ and substitute in the above equation.

$$r^2 \int \sin\theta\, d\theta\, d\phi \Big[\Big\{ e^{-ikr\cos\theta} + \frac{e^{-ikr}}{r} f^* \Big\} \Big\{ ik\cos\theta\, e^{ikr\cos\theta} + \frac{ik}{r} e^{ikr} f(\theta,\phi) - \frac{e^{ikr}}{r^2} f(\theta,\phi) \Big\} - c.c. \Big]$$

$$= 0.$$

(for all values of r.)

{Study the equation for large r} ....

$$r^2 \int \sin\theta\, d\theta\, d\phi \Big[2ik\cos\theta + \frac{2ik}{r^2} f^* f - \cancel{\frac{1}{r^3} f^* f} \quad \rightarrow 0 \text{ as } r\to\infty$$

$$+ \frac{ik}{r} e^{ikr(1-\cos\theta)} f$$

$$- \frac{e^{ikr(1-\cos\theta)}}{r^2} f + \cancel{\frac{ik\cos\theta}{} e^{ikr}}$$

$$+ \frac{ik\cos\theta}{r} e^{-ikr(1-\cos\theta)} f^*$$

$$+ \frac{ik}{r} e^{-ikr(1-\cos\theta)} f^* + \frac{e^{-ikr(1-\cos\theta)}}{r^2} f^*$$

$$+ \frac{ik\cos\theta}{r} e^{ikr(1-\cos\theta)} f \Big] = 0$$

$$\Rightarrow \quad 2ik\sigma + \int \sin\theta\, d\theta\, d\phi \Big[ikr(1+\cos\theta)\, e^{ikr(1-\cos\theta)} f(\theta,\phi)$$

$$+ ikr(1+\cos\theta)\, e^{-ikr(1-\cos\theta)} f^*(\theta)$$

$$- e^{ikr(1-\cos\theta)} f + e^{-ikr(1-\cos\theta)} f^* \Big]$$

$$= 0.$$

{ Write $u = \cos\theta$. $\therefore du = -\sin\theta\, d\theta$

$$\int_0^{\pi} \sin\theta\, d\theta = -\int_1^{-1} du = \int_{-1}^{1} du. \Big\}$$

So, $$0 = 2ik\sigma + 2\pi \int_{-1}^{1} du \Big[ikr(1+u)\, e^{ikr(1-u)} f(0) + ikr(1+u)\, e^{-ikr(1-u)} f^* \underbrace{- e^{+ikr(1-u)} f + e^{-ikr(1-u)} f^*}_{\text{Integrate to zero}} \Big]$$

[For $r \to \infty$, the integral simplifies.]

$e^{ikr(1-u)} \rightsquigarrow$ oscillates very rapidly

Integrals cancel

$\int_a^b e^{i\Lambda u} f(u)\, du$ (ends contribute)

If $u \to \phi(u)$, the extrema points contribute.

$$0 = 2ik\sigma - 2\pi \times 2 f(0) + 4\pi f^*(0).$$

$$\Rightarrow \quad 2ik\sigma = 4\pi \left(f(0) - f^*(0) \right)$$

$$\Rightarrow \quad f(0) - f^*(0) = \frac{2ik\sigma}{4\pi} = \frac{ik\sigma}{2\pi}.$$

$$\int_a^b e^{i\Lambda u} f(u)\, du$$

$$= \int_a^b \frac{1}{i\Lambda} \frac{d}{du}\left(e^{i\Lambda u}\right) f(u)$$

$$= \frac{1}{i\Lambda} e^{i\Lambda u} f(u) \Big|_a^b - \frac{1}{i\Lambda} \int_a^b e^{i\Lambda u} \frac{df}{du}$$

$$= \frac{1}{i\Lambda} \left(e^{i\Lambda b} f(b) - e^{i\Lambda a} f(a) \right) - \frac{1}{i\Lambda} \int_a^b \frac{1}{i\Lambda} \frac{d}{du}\left(e^{i\Lambda u}\right) \frac{d}{du}$$

If we have $\int_a^b e^{i\Lambda g(u)} f(u)\, du$

$$= \frac{1}{g'(u)} \frac{d}{du} e^{i\Lambda g(u)}$$

? $g'(u) = 0$

$$g(u) = g(u_0) + a(u - u_0)^2 + \cdots$$

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$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{df}{dr}\right) - \frac{l(l+1)}{r^2}f + \frac{2m}{\hbar^2}\big(E - V(r)\big)f = 0$$

Take $V(r) = -\dfrac{\alpha}{r}$ (α = constant)

$\Rightarrow$ Attractive Coulomb potential

Near $r = 0$: $f \sim r^{l}$ ✓ , $\cancel{r^{-l-1}}$

Introduce new variable ρ by the relation

$$r = \beta\rho.$$

Multiply by r^2

$$\Rightarrow \frac{d}{dr}\left(r^2\frac{df}{dr}\right) - l(l+1)f + \frac{2m}{\hbar^2}\big(E - V(r)\big)r^2 f = 0$$

$$\Rightarrow \frac{d}{d\rho}\left(\rho^2\frac{df}{d\rho}\right) - l(l+1)f + \left(\frac{2mE}{\hbar^2}\beta^2\rho^2 + \frac{2m\alpha}{\hbar^2}\beta\rho\right) = 0$$

(Using $V = -\dfrac{\alpha}{r}$).

Choose β as $\dfrac{\hbar^2}{m\alpha}$. $\dfrac{2mE}{\hbar^2}\beta^2 = -\kappa^2$. ($E < 0$).

$$E = -\frac{\hbar^2}{2m}\kappa^2 * \frac{m^2\alpha^2}{\hbar^4} = -\frac{m\alpha^2}{2\hbar^2}\kappa^2$$

$$\frac{d}{d\rho}\left(\rho^2\frac{df}{d\rho}\right) - l(l+1)f + \left(-\kappa^2\rho^2 + 2\rho\right)f = 0.$$

(Rescaling variables)

$f \sim \rho^{l}$ as $\rho \to 0$.

Let's look near $\rho \to \infty$. (!)

$$\rho^2 \frac{d^2 f}{d\rho^2} + 2\rho \frac{df}{d\rho} - l(l+1) f + (-\kappa^2 \rho^2 + 2\rho) f = 0$$

$$\Rightarrow \frac{d^2 f}{d\rho^2} + \frac{2}{\rho}\frac{df}{d\rho} - \overset{\times}{\frac{l(l+1)}{\rho^2}} f + (-\overset{\checkmark}{\kappa^2} + \overset{\times}{\frac{2}{\rho}}) f = 0$$

if we ignore this,

$$\frac{d^2 f}{d\rho^2} = \kappa^2 f \qquad \text{(we can't choose } A = 0 \text{ for all E)}$$

$$f \to \cancel{Ae^{\kappa\rho}} + Be^{-\kappa\rho} \checkmark$$

$\rho \to \infty$

fix κ (or energy), because $\rho \to 0$ behaviour is fixed. (specific values of κ are allowed).

$$\frac{d^2 f}{d\rho^2} \sim \kappa^2 e^{-\kappa\rho} \checkmark \qquad \frac{df}{d\rho} \sim -\kappa e^{-\kappa\rho}.$$

So $\frac{2}{\rho}\frac{df}{d\rho}$ is ignorable w.r.t. $\frac{d^2 f}{d\rho^2}$. ($\checkmark$)

Correct form is $f = \rho^{\gamma} e^{-\kappa\rho}$

$$= e^{-\kappa\rho + \gamma \ln \rho}$$

$$\frac{d}{d\rho}\left(\rho^2 \frac{df}{d\rho}\right) - l(l+1) f + (-\kappa^2\rho^2 + 2\rho) f = 0$$

Introduce a new function $g(\rho)$ such that

$$f(\rho) = \rho^{l} e^{-\kappa\rho} g(\rho).$$

$$\frac{d}{d\rho}\left(\rho^2 \frac{d}{d\rho}\left(\rho^l e^{-\kappa\rho} g(\rho)\right)\right) - l(l+1)\rho^l e^{-\kappa\rho} g$$

$$+ (-\kappa^2\rho^2 + 2\rho)\rho^l e^{-\kappa\rho} g = 0$$

$$\Rightarrow \frac{d}{d\rho}\left(l\rho^{l+1} e^{-\kappa\rho} g - \kappa\rho^{l+2} e^{-\kappa\rho} g + \rho^{l+2} e^{-\kappa\rho} g'\right)$$

$$= \Big[\cancel{l(l+1)\rho^l e^{-\kappa\rho}} g - \kappa l \rho^{l+1} e^{-\kappa\rho} g + l\rho^{l+1} e^{-\kappa\rho} g'$$

$$- \kappa(l+2)\rho^{l+1} e^{-\kappa\rho} g + \cancel{\kappa^2 \rho^{l+2} e^{-\kappa\rho}} g$$

$$- \kappa\rho^{l+2} e^{-\kappa\rho} g' + (l+2)\rho^{l+1} e^{-\kappa\rho} g' - \kappa\rho^{l+2} e^{-\kappa\rho} g'$$

$$+ \rho^{l+2} e^{-\kappa\rho} g''\Big] - \cancel{l(l+1)\rho^l e^{-\kappa\rho}} g$$

$$\cancel{-\kappa^2 \rho^{l+2} e^{-\kappa\rho}} g + 2\rho^{l+1} e^{-\kappa\rho} g$$

$$= \rho^l e^{-\kappa\rho}\Big[\rho^2 g'' + g'\left(l\rho + (l+2)\rho - 2\kappa\rho^2\right) + g\left(-\kappa l\rho - \kappa(l+2)\rho + 2\rho\right)\Big] = 0.$$

$$= \rho^{l+1} e^{-\kappa\rho}\underbrace{\Big[\rho g'' + 2(l+1-\kappa\rho) g' + 2\left(1 - \kappa(l+1)\right) g\Big] = 0}.$$

Generalized Laguerre polynomials → solutions

Look for solutions

$$g = \sum_n a_n \rho^n$$

$$g' = \sum_{n=0}^{\infty} n a_n \rho^{n-1} \qquad g'' = \sum_{n=0}^{\infty} n(n-1) a_n \rho^{n-2}$$

$$\Rightarrow \sum n(n-1) a_n \rho^{n-1} + 2(l+1) \sum_n n a_n \rho^{n-1}$$

$$- 2k \sum_n n a_n \rho^n + 2(1 - k(l+1)) \times \sum_n a_n \rho^n = 0$$

$n \longrightarrow n+1$ in first two terms

$$\sum_{n=0}^{\infty} a_{n+1}(n+1) n \rho^n + 2(l+1) \sum_{n=0}^{\infty} (n+1) a_{n+1} \rho^n$$

$$- 2k \sum_{n=0}^{\infty} n a_n \rho^n + 2(1 - k(l+1)) \times \sum_n a_n \rho^n$$

$$= 0.$$

$\rho^n \longrightarrow$ coeff$\underline{\underline{n}}$ goes to zero

$$\frac{a_{n+1}}{a_n} = \frac{2kn - 2(1 - k(\rho + 1))}{(n+1)n + 2(l+1)(n+1)}$$

$$\frac{a_{n+1}}{a_n} = 2' \frac{k(n+l+1) - 1}{(n+1)\{n + 2(l+1)\}}$$

$$\kappa = \frac{1}{n+l+1} \quad \text{for some integer } n.$$

$\longleftrightarrow$

($\exists$ κ for every integer n)

$g(\rho) \sim \rho^n$ for large ρ

$$f \sim \rho^{n+l} e^{-\kappa \rho} \quad \text{for large } \rho$$

$$= \rho^{1/\kappa - 1} e^{-\kappa \rho}$$

$$E = -\frac{m\alpha^2}{2\hbar^2} \kappa^2$$

$$E_{nl} = -\frac{m\alpha^2}{2\hbar^2 \underbrace{(n+l+1)^2}_{\text{principal q. no.}}}$$

1 state

Ground state : $n = l = 0$ $\quad E_0 = -\dfrac{m\alpha^2}{2\hbar^2}$

1st excited state : $n=1,\ l=0$; $n=0,\ l=1$ $\quad \rightarrow E_1 = -\dfrac{m\alpha^2}{8\hbar^2}$.

4 states

Coulomb scattering :-

Usual case : $\dfrac{e^{ikr}}{r}$, $\dfrac{e^{-ikr}}{r}$ $\longrightarrow$ NOT SOLUTIONS FOR COULOMB PROBLEM

$\dfrac{1}{r} \rightarrow$ related to $\left(\dfrac{2}{r}\dfrac{df}{dr}\right)$ term

$$\frac{d^2f}{dr^2} + \frac{2}{r}\frac{df}{dr} - \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}\left(E - V(r)\right) = 0.$$

$$f = r^{\gamma} e^{ikr} \quad \text{for large } r.$$

exercise Check that if we ignore $V(r)$, we shall get $\gamma = -1$.

$$\frac{2}{r}\frac{df}{dr} \sim \frac{2}{r}\, ik\, r^{\gamma} e^{ikr}.$$

$$-\frac{2m}{\hbar^2} V f \sim \frac{2m}{\hbar^2}\frac{\alpha}{r}\, r^{\gamma} e^{ikr}$$

for large r