Lecture 9a : Partial Waves

Review: Stationary states for spherically symmetric V

For Hamiltonians of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r})$$

where $\frac{\hat{p}^2}{2m} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2m\hat{r}^2}$: kinetic energy

$V(\hat{r})$ = Central potential (spherically symmetric)

We can find solutions to the T.I.S.E. of the form

$$\hat{H}\,\psi_{l,m,E}(r,\theta,\phi) = E\,\psi_{l,m,E}(r,\theta,\phi)$$

where $\psi_{l,m,E}(r,\theta,\phi) = R_{l,E}(r)\,Y_l^m(\theta,\phi)$

Where $\hat{L}^2\,Y_l^m(\theta,\phi) = \hbar^2 l(l+1)\,Y_l^m(\theta,\phi)$

$$\hat{L}_z\,Y_l^m(\theta,\phi) = \hbar m\,Y_l^m(\theta,\phi)$$

The Stationary state is thus a common eigenstate of the mutually commuting set

$$\{\hat{H},\ \hat{L}^2,\ \hat{L}_z\}$$

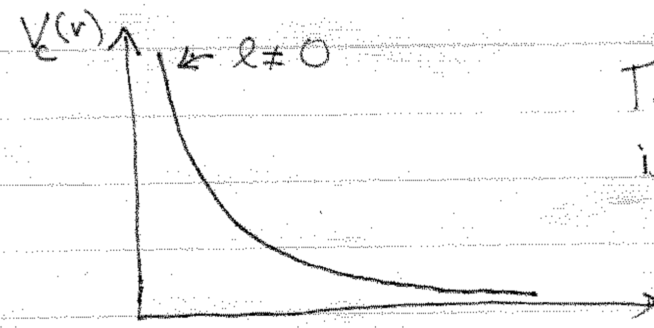
Note: Although $\hat{H}$ does not depend on $\hat{L}_z$ alone, it is necessary necessary to specify ~~m~~ to find ψ

The radial equation

Given a value for the angular momentum magnitude $\hat{L}^2$, l, we need to find the Radial wave function

$$\left[\frac{\hat{P}_r^2}{2m} + \underbrace{\frac{\hbar^2 l(l+1)}{2m\hat{r}^2} + V(\hat{r})}_{V_{eff}^{(l)}(\hat{r})} \right] R_{l,E}(r) = E\, R_{l,E}(r)$$

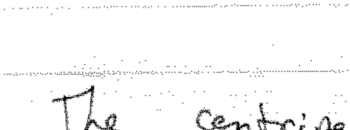
The effective potential $V_{eff}(\hat{r})$ is the sum of the true potential plus the "centripetal potential" $\frac{\hbar^2 l(l+1)}{2mr^2} = V_c(r)$



The centripetal potential is sometimes known as the "angular momentum barrier"

The angular momentum barrier means that a particle with high angular momentum cannot penetrate to the origin. This is a familiar concept in classical trajectories

e.g. Keppler motion



$$r_{min} = \frac{L}{P}$$

The "reduced" radial wave function

Let us express the radial equation as a O.D.E. using $\hat{p}_r^2 \doteq \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\ )$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{d^2}{dr^2}(r R_\ell(r))\right) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} R_\ell(r) + V(r) R_\ell(r) = E R_\ell(r)$$

Multiply both sides by r, and let

$$u_\ell(r) \equiv r R_\ell(r) = \text{"reduced radial wave function"}$$

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u_\ell(r) + V_{eff}^{(\ell)}(r)\, u_\ell(r) = E\, u_\ell(r)}$$

The equation of motion for the reduced radial wave function is <u>exactly</u> the form of the 1D T.~~I~~.S.E., with effective potential

$$V_{eff}^{(\ell)}(r) = V(r) + \frac{\hbar^2 \ell(\ell+1)}{r^2}$$

As before, unless $V(r)$ has singularities, we must have $u(r)$ continuous and $\frac{du(r)}{dr}$ continuous

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Important: The Radial wave function is defined only on the half-line

$$0 \le r \le \infty$$

there are no negative radii

Normalization $\int_0^\infty r^2 dr \, |R(r)|^2 = 1$

$$\Rightarrow \int_0^\infty dr \, |r R(r)|^2 = \int_0^\infty dr \, |u(r)|^2 = 1$$

For a normalizable state we must have $u(r) \to 0$ as $r \to \infty$ ($\Rightarrow \lim_{r \to \infty} R(r) \to 0$ faster than $\frac{1}{r}$)

What about the boundary condition at $r = 0$?

Note $R(r) = \frac{u(r)}{r}$, and $\psi(r, \theta, \phi) = R(r) Y_\ell^m(\theta, \phi)$

Thus if $\psi(r, \theta, \phi)$ is everywhere well behaved, $R(r)$ cannot blow up at the origin

$$\Rightarrow \boxed{u(r) \to 0 \text{ at least like } r \text{ at } r = 0}$$

New boundary condition for reduced radial wave function

<u>The free particle in spherical coordinates</u>

We have studied the solution to the T.I.S.E. for a free particle in 3D by separating coordinates in Cartesian variables

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m}$$

$$\hat{H}\psi = E\,\psi(x,y,z)$$

A Solution $\psi(x,y,z) = \left(\frac{e^{ik_x x}}{\sqrt{2\pi}}\right)\left(\frac{e^{ik_y y}}{\sqrt{2\pi}}\right)\left(\frac{e^{ik_z z}}{\sqrt{2\pi}}\right)$

$$\psi_{k_x,k_y,k_z}(x,y,z) = \frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}}$$

This state is a common eigenfunction of the mutually commuting set $\{\hat{p}_x, \hat{p}_y, \hat{p}_z\}$

Energy eigenvalue $E(k_x,k_y,k_z) = \frac{\hbar^2 k^2}{2m}$

where $k^2 = |\vec{k}|^2 = k_x^2 + k_y^2 + k_z^2$

Note: This energy level is continously degenerate. E depends only on $|\vec{k}|$ and not the direction of $\vec{k}$. This is because of <u>rotation</u> <u>symmetry</u>.

A free particle is a spherically symmetric geometry:

$\Rightarrow$ We can look for solutions by separating coordinates in r, θ, ϕ

$$\hat{H}_{free} = \frac{\hat{p}^2}{2m} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2}, \quad \hat{H}_{free}\psi = E\psi$$

Fix $\rightarrow$ Now $\psi(r, \theta, \phi) = R_{\ell,E}(r)\, Y_\ell^m(\theta, \phi)$

$$\Rightarrow \left(\frac{\hat{p}_r^2}{2m} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right) R_{\ell,E}(r) = E\, R(r)$$

These solutions are common eigenstates of $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$

Note: $[\hat{L}_z, \hat{\vec{p}}] \neq 0$: Thus these solutions are not plane waves

They are superpositions of plane waves all will the same $|\vec{k}|$. $E = \frac{(\hbar k)^2}{2m}$

Because of degeneracies, there are many different solutions with same energy.

The solutions above are spherical waves with definite angular momentum, not definite momentum.

Spherical waves of definite angular momentum are known as "partial waves" for reasons that will become clear later.

Partial wave radial wave functions

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(rR) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}R(r) = E\,R(r)$$

or $$\frac{1}{r}\frac{d^2}{dr^2}(rR) - \frac{\ell(\ell+1)}{r^2}R(r) + k^2 R(r) = 0$$

where $k^2 = \frac{2mE}{\hbar^2}$

Consider case $\underline{\ell = 0}$, $u(r) = rR(r)$

$$\Rightarrow \frac{d^2}{dr^2}u(r) + k^2 u(r) = 0$$

This is none other than the 1D T.I.S.E. for a constant potential

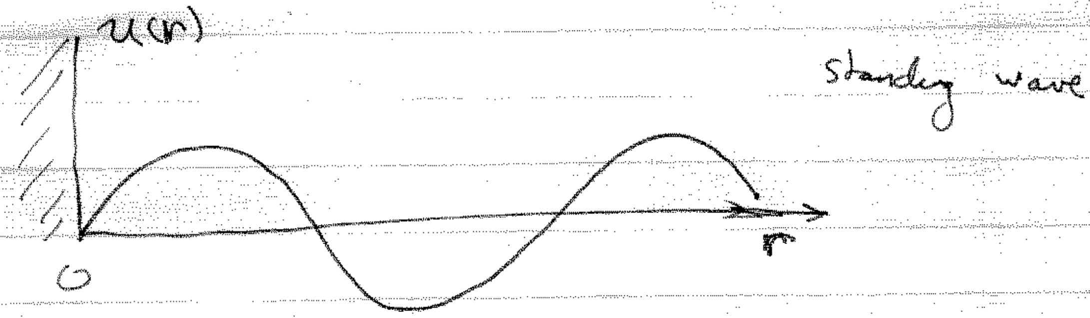
Now we have the boundary condition

$$u(r=0) = 0$$

$\Longrightarrow$ Solution for $\ell = 0$ $\quad u(r) = A\sin kr$

This is like a free particle in 1D with an ∞ wall at the origin

$l=0$, reduced radial wave function, free particle



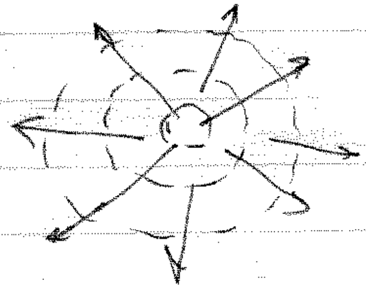
Back to the full radial wave function

$$R(r) = \frac{u(r)}{r} = A\,\frac{\sin kr}{r} = -2iA\left(\frac{e^{-ikr}}{r} - \frac{e^{+ikr}}{r}\right)$$

The waves $\frac{e^{-ikr}}{r}$ and $\frac{e^{ikr}}{r}$ represent

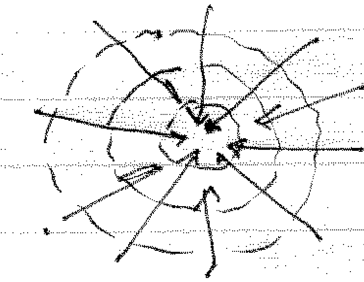
incomming $(\vec{k} = -k\vec{e}_r)$ and outgoing $(\vec{k} = +k\vec{e}_r)$ spherical waves. The wave fronts are surfaces of constant phase (r = constant = sphere).

The "intensity" falls off as $|R(r)|^2 = \frac{1}{r^2}$



$$\frac{e^{i(kr-\omega t)}}{r}$$

outgoing



$$\frac{e^{-i(kr+\omega t)}}{r}$$

incomming

Solutions for arbitrary l

Radial equation: $\frac{1}{r}\frac{d^2}{dr^2}(rR_l) - \frac{l(l+1)}{r^2}R_l(r) + k^2 R_l(r) = 0$

Make dimensionless: Characteristic length $\frac{1}{k}$

$\Rightarrow$ Let $x = kr$

$$\Rightarrow \boxed{\frac{d^2}{dx^2}R_l(x) + \frac{2}{x}\frac{dR_l}{dx} + \left(1 - \frac{l(l+1)}{x^2}\right)R_l(x) = 0}$$

This is a well ~~k~~nown O.D.E. it's solution are the "spherical Bessel Functions"

For a given l

$$R_l(x) = A_l\, j_l(x) + B_l\, \eta_l(x)$$

$j_l(x)$ = Spherical Bessel function first kind $= \sqrt{\frac{\pi}{2x}}\, J_{l+\frac{1}{2}}(x)$

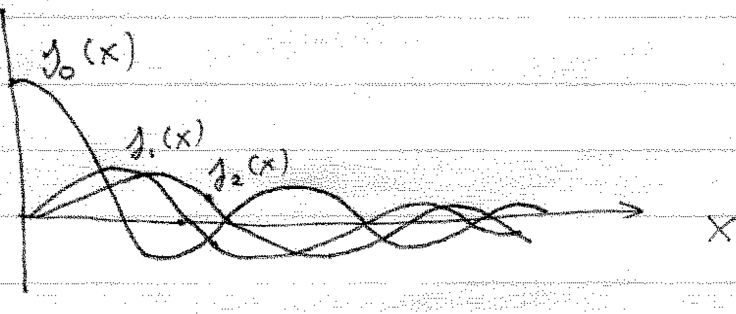
$\eta_l(x)$ = Spherical Bessel function second kind $= \sqrt{\frac{\pi}{2x}}\, N_{l+\frac{1}{2}}(x)$

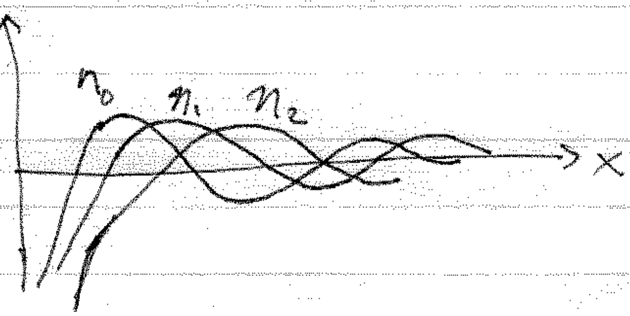
$$j_0(x) = \frac{\sin x}{x} \qquad \eta_0(x) = -\frac{\cos x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad \eta_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$\vdots$ $\qquad$ $\vdots$

Sketch





Note the spherical Neumann functions blow up at the origin. $\Rightarrow$ Not allowed free particle solutions.

Putting it altogether the partial wave free particle solutions:

$$\boxed{\begin{aligned}
|k, l, m\rangle &\doteq A\, j_l(kr)\, Y_l^m(\theta, \phi) \\
\hat{H}\, |k, l, m\rangle &= \frac{(\hbar k)^2}{2m}\, |k, l, m\rangle \\
\hat{L}^2\, |k, l, m\rangle &= \hbar^2\, l(l+1)\, |k, l, m\rangle \\
\hat{L}_z\, |k, l, m\rangle &= \hbar m\, |k, l, m\rangle
\end{aligned}}$$