Energy Eigenstates for Rot. Invariant Hamiltonians

Spinless Non-Relativistic Particle Moving in a Central Potential:

$$\hat{H} = \frac{\hat{\vec{P}}^2}{2\mu} + \hat{V}(|\hat{\vec{r}}|),$$

μ = Particle mass (or Reduced Mass for 2-Body Problem with Central Forces only — Discussed in 301)

$$\hat{\vec{P}} = \sum_{a=1}^{3} \hat{P}_a \vec{n}_a \; ; \; \hat{\vec{r}} = \sum_{a=1}^{3} \hat{X}_a \vec{n}_a$$

$\hat{H}$ is Rotationally Invt.:

$$e^{+i\frac{\hat{\vec{L}}\cdot\vec{\theta}}{\hbar}} \hat{H} e^{-i\frac{\hat{\vec{L}}\cdot\vec{\theta}}{\hbar}} = \hat{H} \rightarrow [\hat{H}, \hat{L}_z] = [\hat{H}, \hat{\vec{L}}^2] = 0$$

$\therefore$ Can Find Simultaneous Eigenstates of $\hat{H}, \hat{\vec{L}}^2, \hat{L}_z$: $|E\ell m\rangle$; $\langle \vec{r}|E\ell m\rangle \equiv \psi_{E\ell m}(\vec{r})$

Write $\psi_{E\ell m}(r,\theta\phi) \equiv R_{E\ell}(r)\, Y_{\ell m}(\theta,\phi) \Leftarrow \langle\theta\phi|\ell m\rangle$ Spherical Harmonic

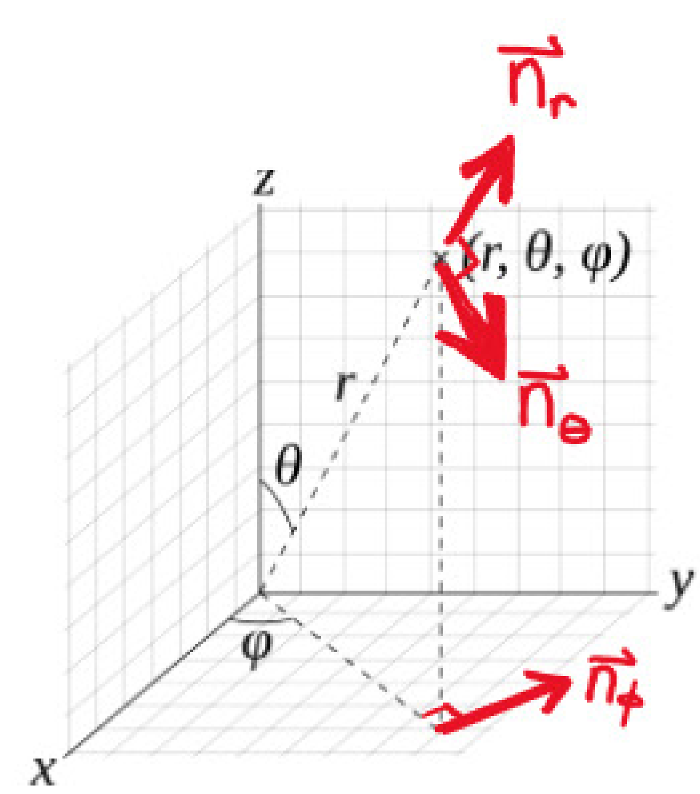
- $\hat{\vec{L}}^2|\ell m\rangle = \hbar^2\ell(\ell+1)|\ell m\rangle$
- $\hat{L}_z|\ell m\rangle = m\hbar|\ell m\rangle$

$\Uparrow$ Radial Part

- Can depend on ℓ [Total Ang. Mom. $\hat{\vec{L}}^2 = \hbar^2\ell(\ell+1)$, Part of Kinetic Energy]
- Does not change under a rotation $\Rightarrow$ Indept. of m!

$$\left[-\frac{\hbar^2}{2\mu}\vec{\nabla}^2 + V(r)\right] R_{E\ell}(r)\, Y_{\ell m}(\theta,\phi) = E\; R_{E\ell}(r)\, Y_{\ell m}(\theta,\phi)$$

Laplacian in Sph. Polar Coordinates



$$\vec{\nabla} = \vec{n}_r \frac{\partial}{\partial r} + \vec{n}_\theta \frac{1}{r}\frac{\partial}{\partial\theta} + \vec{n}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\vec{n}_r = \frac{\vec{r}}{r} = \cos\phi\sin\theta\,\vec{n}_x + \sin\phi\sin\theta\,\vec{n}_y + \cos\theta\,\vec{n}_z$$

$$\vec{n}_\theta = \cos\phi\cos\theta\,\vec{n}_x + \sin\phi\cos\theta\,\vec{n}_y - \sin\theta\,\vec{n}_z$$

$$\vec{n}_\phi = -\sin\phi\,\vec{n}_x + \cos\phi\,\vec{n}_y$$

$$\vec{n}_\alpha\cdot\vec{n}_\beta = \delta_{\alpha,\beta}$$

$$\alpha,\beta \in \{r,\theta,\phi\}$$

$$\therefore\ \vec{\nabla}^2 = \vec{\nabla}\cdot\vec{\nabla} = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \left\{\begin{array}{l}\text{TERMS THAT ARISE FROM}\\ \text{DERIVATIVES OF BASIS VEC.S}\end{array}\right\}$$

- SEE LEC 15, p.4 FOR 2D EXAMPLE (∇^2 IN 2D POLAR COORDS)
- 3D SPHERICAL POLAR RESULT:

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]$$

- CLAIM (HW!): $\hat{\vec{L}}^2 \Rightarrow -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

$$\therefore\ \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(r)\right]R_{E\ell}(r)Y_{\ell m}(\theta,\phi)$$

$$= \left\{\frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{\vec{L}}^2}{\hbar^2 r^2}\right] + V(r)\right\}R_{E\ell}(r)Y_{\ell m}(\theta,\phi)$$

$$= \left\{\frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\ell(\ell+1)}{r^2}\right] + V(r)\right\}R_{E\ell}(r)Y_{\ell m}(\theta,\phi)$$

THE SCHRÖDINGER EQN. REDUCES TO THE EFFECTIVE RADIAL EQUATION

$$\left\{\frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{\ell(\ell+1)}{r^2}\right] + V(r)\right\}R_{E\ell}(r) = E\,R_{E\ell}(r)$$

NORMALIZATION INTEGRAL:

$$\langle E\ell m|E\ell m\rangle = \int d^3\vec{r}\ \psi^*_{E\ell m}(\vec{r})\,\psi_{E\ell m}(\vec{r})$$

$$= \int_0^\infty r^2dr\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\ \sin\theta\ |R_{E\ell}(r)|^2\,|Y_{\ell m}(\theta,\phi)|^2$$

$$= \int_0^\infty r^2dr\ |R_{E\ell}(r)|^2$$

$\Rightarrow$ WE CAN MAKE THIS LOOK LIKE A NORM. INTEGRAL IN 1D IF WE DEFINE

$$\boxed{r\,R_{E\ell}(r) \equiv u_{E\ell}(r)}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R_{E\ell}(r) = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\left[\frac{u_{E\ell}}{r}\right]\right) = \frac{1}{r^2}\frac{d}{dr}\left(r u_{E\ell}' - u_{E\ell}\right)$$

$$= \frac{1}{r^2}\left(\cancel{u_{E\ell}'} + r u_{E\ell}'' - \cancel{u_{E\ell}'}\right)$$

$$= \frac{1}{r}\frac{d^2}{dr^2} u_{E\ell}$$

$$\therefore \quad \left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{eff}(r)\right]u_{E\ell}(r) = E\,u_{E\ell}(r) \; ; \quad V_{eff}(r) = \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r)$$

3D ROT. INVT. PROBLEM ⟹ EFFECTIVE 1D SCHRÖDINGER EQ.

- **SOLUTION TO 3D PROBLEM:** $\psi_{E\ell m}(r,\theta,\phi) = \dfrac{u_{E\ell}(r)}{r} \times Y_{\ell m}(\theta,\phi)$

- **EFFECTIVE 1D (RADIAL) ENERGY EIGENVALUE PROBLEM:**

(1.) NORMALIZATION IS OVER HALF-LINE $r \geq 0$:

$$\langle u_{E\ell} | u_{E\ell} \rangle = \int_0^\infty dr \; |u_{E\ell}(r)|^2$$

(2.) EFFECTIVE POTENTIAL INCLUDES CENTRIFUGAL BARRIER TERM

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

COMPARE TO CLASSICAL MECHANICS: CENTRAL-FORCE MOTION REDUCES TO RADIAL ODE WITH EFFECTIVE POTENTIAL

PHYS 301 $\Longrightarrow$ $V_{eff}(r) = V(r) + \dfrac{L^2}{2\mu r^2}$ ✓

(3.) BOUNDARY CONDITIONS FOR $u_{E\ell}(r)$ AT $r=0$, $r\to\infty$

WE WANT THE EFFECTIVE RADIAL HAMILTONIAN $\hat{H}_u^{(\ell)}$ TO BE HERMITIAN FOR SQUARE-NORMALIZABLE (AND DIRAC-δ NORMALIZABLE) WAVE FUNCTIONS OVER $0 \leq r < \infty$

$$\hat{H}_u^{(\ell)\dagger} = \hat{H}_u^{(\ell)} \; ; \quad \hat{H}_u^{(\ell)} \Rightarrow -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{eff}(r)$$

$$\langle u_1|\hat{H}_u^{(\ell)}|u_2\rangle^* = \langle u_2|\hat{H}_u^{(\ell)\dagger}|u_1\rangle = \int_0^\infty dr\; u_1(r)\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{eff}(r)\right]u_2^*(r)$$

$\Downarrow$ INTEGRATE BY PARTS TWICE

$$= \int_0^\infty dr\; u_2^*(r)\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{eff}(r)\right]u_1(r) \;-\frac{\hbar^2}{2\mu}\left[u_1(r)\frac{du_2^*}{dr} - u_2^*(r)\frac{du_1}{dr}\right]\Bigg|_0^\infty$$

$$\therefore\; \langle u_2|\hat{H}_u^{(\ell)\dagger}|u_1\rangle = \langle u_2|\hat{H}_u^{(\ell)}|u_1\rangle \quad \text{IF} \quad \underbrace{\left[u_1(r)\frac{du_2^*}{dr} - u_2^*(r)\frac{du_1}{dr}\right]\Bigg|_0^\infty}_{\text{BOUNDARY TERM}} = 0$$

CF. LEC. 7, p. 2-3

(A) $r \to \infty$ BEHAVIOR

CAN IGNORE BOUNDARY TERM FOR ① $\lim_{r\to\infty} u(r) = 0$, EXPECTED FOR BOUND STATES

② $\lim_{r\to\infty} u(r) = e^{\pm ikr}$, EXPECTED FOR CONTINUUM STATES

? WHY DOES THIS NOT CONTRIBUTE TO THE BOUNDARY TERM ABOVE ?

- OSCILLATIONS IN kr "CANCEL OUT" AS $r \to \infty$
- MORE RIGOROUS ARGUMENT: SEC. 1.10 IN SHANKAR

NOTE: $R_{E\ell}(r) = \dfrac{u_{E\ell}(r)}{r} \simeq \dfrac{e^{\pm ikr}}{r}$ } OUTGOING (+) OR INCOMING (−) SPHERICAL WAVE !

PROBABILITY TO FIND PARTICLE BETWEEN RADII r AND $r+dr$: $|R_{E\ell}(r)|^2 r^2 dr \simeq dr$, INDEPT. OF r

- THIS IS A STATEMENT OF **PROBABILITY CONSERVATION** FOR AN INCOMING OR OUTGOING WAVE ; IMPORTANT FOR 3D SCATTERING THEORY (CF. LEC. 18)

(B) $r \to 0$ BEHAVIOR

$\hat{H}_u^{(\ell)\dagger} = \hat{H}_u^{(\ell)}$ IF WE RESTRICT TO ① $\lim_{r\to 0} u_{E\ell}(r) = 0$

OR

② $\lim_{r\to 0} \dfrac{du_{E\ell}}{dr} = 0 \Rightarrow \lim_{r\to 0} u_{E\ell}(r) = c$ (CONST.)

- CONSIDER CASE ②; $R_{E\ell}(r) \underset{r\to 0}{\simeq} \dfrac{c}{r}$ BLOWS UP. NOT NECESSARILY A PROBLEM, $\int_0^\infty r^2 dr\, |R_{E\ell}(r)|^2$ DOES NOT DIVERGE AT $r \to 0$.

$$\psi_{E\ell m}(r,\theta,\phi) = R_{E\ell}(r)\, Y_{\ell m}(\theta,\phi) \;;\quad \lim_{r\to 0} \psi_{E\ell m} \simeq \frac{c}{r}$$

FULL S.E. (p.1):

$$\left[-\frac{\hbar^2}{2\mu}\vec{\nabla}^2 + V(r)\right]\psi = E\psi \;;\quad \textbf{PROBLEM:}\; -\vec{\nabla}^2 \frac{1}{r} = 4\pi\,\delta^{(3)}(\vec{r})$$

$$\Downarrow r\to 0$$

$$\frac{\hbar^2}{2\mu} 4\pi c\, \delta^{(3)}(\vec{r}) + V(r)\,\psi(r) = E\,\psi(r)$$

$\therefore$ **V(r) MUST CONTAIN TERM $\sim -c\,\delta^{(3)}(\vec{r})$**

I.E., $1/r$ IS THE GREEN'S FUNCTION FOR THE COULOMB POTENTIAL IN 3D.

GAUSS'S LAW: $-\nabla^2 \Phi = 4\pi\rho$

ELECTRIC POTENTIAL (Φ), CHARGE DENSITY (ρ)

$$\Phi(r) = \frac{q}{r} \Rightarrow -\frac{\nabla^2}{4\pi}\Phi = q\,\delta^{(3)}(\vec{r}) = \rho \checkmark$$

→ IF V(r) DOES **NOT** CONTAIN A δ-FCN PIECE AT THE ORIGIN (AND IT USUALLY WON'T),

MUST SET $c \to 0$. $\therefore \lim_{r\to 0} U_{E\ell}(r) = 0.$

SUMMARY: EIGENENERGY SPECTRUM FOR ROT. INVARIANT HAMILTONIAN

- $\hat{H}|E\ell m\rangle = E|E\ell m\rangle$
- $\hat{L}^2|E\ell m\rangle = \hbar^2 \ell(\ell+1)|E\ell m\rangle$
- $\hat{L}_z|E\ell m\rangle = \hbar m|E\ell m\rangle$

  $0 \le |m| \le \ell$

$$\langle \vec{r}|E\ell m\rangle = \psi_{E\ell m}(r,\theta,\phi) \equiv \frac{U_{E\ell}(r)}{r} Y_{\ell m}(\theta,\phi)$$

EFFECTIVE RADIAL S.E.:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{eff}(r)\right] U_{E\ell}(r) = E\, U_{E\ell}(r)$$

$$V_{eff}(r) = \underbrace{\frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}}_{\text{CENTRIFUGAL BARRIER}} + \underbrace{V(r)}_{\text{ACTUAL POTENTIAL ENERGY}}$$

① NORMALIZATION

$$\langle u_1|u_2\rangle = \int_0^\infty dr\; U_1^*(r)\, U_2(r)$$

② BOUNDARY CONDITIONS

Ⓐ $\lim_{r\to\infty} U_{E\ell}(r) \Rightarrow \begin{cases} 0, & \text{BOUND STATES} \\ e^{\pm ikr}, & \text{CONTINUUM STATES (Sph. WAVES)} \end{cases}$

Ⓑ $\lim_{r\to 0} U_{E\ell}(r) = 0.$