Ch. 9 Scalar ($j=0$) particles in 3d

$|\vec{r}\rangle = |x,y,z\rangle = |x_1\, x_2\, x_3\rangle$ (not'n)

$\hat{X}_i\, |\vec{r}\rangle = x_i |\vec{r}\rangle$, or $\boxed{\hat{\vec{X}}|\vec{r}\rangle = \vec{r}\,|\vec{r}\rangle}$

$\Leftrightarrow \mathcal{H}_{3d} = \mathcal{H}_x \otimes \mathcal{H}_y \otimes \mathcal{H}_z$

$[\hat{X}_i, \hat{X}_j] = 0$

on basis
$$\begin{cases} \langle \vec{r}\,|\,\vec{r}\,'\rangle = \delta^3(\vec{r}-\vec{r}\,') = \delta(x_1-x_1')\,\delta(x_2-x_2')\,\delta(x_3-x_3') \\ 1 = \int d^3r\, |\vec{r}\rangle\langle\vec{r}| \end{cases}$$

Wavefnc:
&
$$\begin{cases} \psi(\vec{r}) \equiv \langle \vec{r}|\psi\rangle \\ |\psi\rangle = \int d^3r\, \psi(\vec{r})\,|\vec{r}\rangle \end{cases}$$

$\langle\psi|\psi\rangle = 1$

$\Leftrightarrow \int d^3r\, |\psi(\vec{r})|^2 = 1$

$\Rightarrow \text{Prob}(\vec{r}, \vec{r}+d\vec{r}) = d^3r\, |\psi(\vec{r})|^2$

$\hat{P}_j\, |\vec{r}\rangle = i\hbar \frac{\partial}{\partial x_j} |\vec{r}\rangle$ or $\boxed{\hat{\vec{P}}|\vec{r}\rangle = i\hbar \vec{\nabla}_{\vec{r}}\, |\vec{r}\rangle}$

Mom. basis

$|\vec{p}\rangle = |p_x, p_y, p_z\rangle = |p_1, p_2, p_3\rangle$

$\hat{P}_i |\vec{p}\rangle = p_i |\vec{p}\rangle$ or $\hat{\vec{P}}|\vec{p}\rangle = \vec{p}\,|\vec{p}\rangle$ etc...

$\langle \vec{r}\,|\,\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\, e^{i\vec{p}\cdot\vec{r}/\hbar}$.

$\boxed{[\hat{X}_i, \hat{P}_j] = i\hbar\,\delta_{ij}}$

Particle in 3d in B-field & E-field

$\hat{H}_0 = \frac{1}{2m}\left(\hat{\vec{P}} - \frac{q}{c}\vec{A}(\hat{\vec{x}},t)\right)^2 + q\,V(\hat{\vec{x}},t)$

where: $\vec{B}(\vec{x},t) = \vec{\nabla}\times\vec{A}$, $\vec{E}(\vec{x},t) = -\vec{\nabla}V - \frac{\partial}{\partial t}\vec{A}$.

t-indep't B-fld only : $\vec{A} = \vec{A}(\vec{x})$, $V=0$ $\Rightarrow$

$\hat{H}_0 = \frac{1}{2m}\left(\hat{\vec{P}} - \frac{q}{c}\vec{A}(\hat{\vec{x}})\right)^2 = \frac{1}{2m}\,\hat{\vec{P}}\cdot\hat{\vec{P}} - \frac{q}{2mc}\left(\hat{\vec{P}}\cdot\vec{A}(\hat{\vec{x}}) + \vec{A}(\hat{\vec{x}})\cdot\hat{\vec{P}}\right) + \frac{q^2}{2mc^2}\vec{A}(\hat{\vec{x}})\cdot\vec{A}(\hat{\vec{x}})$

2 particles in central potential

$$\hat{H} = \frac{1}{2m_1}\hat{p}_1^2 + \frac{1}{2m_2}\hat{p}_2^2 + V(|\hat{\vec{r}}_1 - \hat{\vec{r}}_2|)$$

$$\hat{p}^2 \doteq \hat{\vec{p}}\cdot\hat{\vec{p}}$$

$$|\hat{\vec{r}}| \doteq (\hat{\vec{r}}\cdot\hat{\vec{r}})^{1/2}$$

- Define: C.O.M. & relative coordinates (operators)

$$\vec{P} \doteq \vec{p}_1 + \vec{p}_2 \qquad \vec{p} \doteq \frac{m_2\vec{p}_1 - m_1\vec{p}_2}{m_1+m_2}$$

$$\vec{R} \doteq \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2} \qquad \vec{r} \doteq \vec{r}_1 - \vec{r}_2$$

- Check: $[\hat{\vec{R}}, \hat{\vec{p}}] = 0$

$$[\hat{R}_i, \hat{P}_j] = i\hbar\delta_{ij} \qquad [\hat{\vec{r}}, \hat{\vec{P}}] = 0 \qquad [\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

& $$\hat{H} = \underbrace{\frac{1}{2M}\hat{P}^2}_{\hat{H}_{CM}} + \underbrace{\frac{1}{2\mu}\hat{p}^2 + V(\hat{r})}_{\hat{H}_{rel}} \qquad \begin{cases} \hat{r} \equiv \sqrt{\hat{r}^2} = \sqrt{\hat{\vec{r}}\cdot\hat{\vec{r}}} \\ M \equiv m_1 + m_2 \\ \mu \equiv \dfrac{m_1 m_2}{m_1+m_2} \end{cases}$$

- $\mathcal{H}_1 \otimes \mathcal{H}_2 \simeq \mathcal{H}_{cm} \otimes \mathcal{H}_{rel}$ (*)

$$\{|\vec{r}_1, \vec{r}_2\rangle\} \xrightarrow{\text{c.o.b.}} \{|\vec{R}, \vec{r}\rangle\}$$

$$\left(|\vec{r}_1, \vec{r}_2\rangle_{12} = \left|\frac{m_1\vec{r}_1 + m_2\vec{r}_2}{M}, \vec{r}_1 - \vec{r}_2\right\rangle_{CM}\right)$$

- Check: $[\hat{H}_{cm}, \hat{H}_{rel}] = 0$

$\Rightarrow$ $\mathcal{H}_{cm}$ & $\mathcal{H}_{rel}$ "decouple".

$\hat{H}_{cm}|E_{cm}\rangle = E_{cm}|E_{cm}\rangle$ & $\hat{H}_{rel}|E_{rel}\rangle = E_{rel}|E_{rel}\rangle$

$\Rightarrow |E\rangle = |E_{cm}\rangle \otimes |E_{rel}\rangle \Rightarrow \hat{H}|E\rangle = E|E\rangle$ w/ $E = E_{cm} + E_{rel}$

"Separation of variables". $\longleftrightarrow$ factorize: $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ (*)

- $\mathcal{H}_{cm}$ part: $\hat{H}_{cm} = \frac{1}{2M}\hat{P}^2 \Rightarrow$ free 'particle' of mass $M = m_1 + m_2$

  $\Rightarrow$ eigenstates all "scattering" states of overall momentum: $|\vec{P}\rangle$

- F.N.O.: ignore! Only interested in relative motion:

- $\hat{H}_{rel} \equiv \hat{H} = \frac{1}{2\mu}\hat{p}^2 + V(\hat{r})$

  $\approx$ 'particle' of mass μ in 3d central pot'l $V(r)$.

$\mathcal{H}_{rel} \doteq \mathcal{H}$ Hilb. space.

- $\hat{H}$ has rotational symmetry around origin ($\vec{r} = 0$)

$\therefore$ (1) work in spherical coordinates

(2) angular momentum $\vec{L} \doteq \vec{r} \times \vec{p}$ is conserved.

Goal: further separation of variables $\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_{\theta,\varphi}$

radial angular

& $\mathcal{H}_{\theta,\varphi} = \bigoplus_{j=0}^{\infty} \mathcal{H}_j$ ang. mom. H.S. $\{|j,m\rangle, |m| \leq j\}$

- **Summary:**

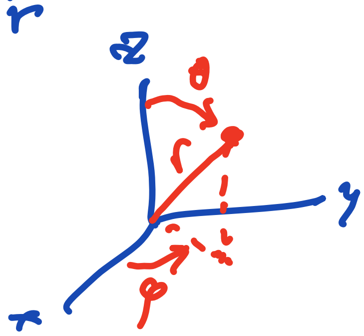
$$\mathcal{H}_{2\text{-particle}} = \mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H}_{1x} \otimes \mathcal{H}_{1y} \otimes \mathcal{H}_{1z} \otimes \mathcal{H}_{2x} \otimes \mathcal{H}_{2y} \otimes \mathcal{H}_{2z}$$

$$= \mathcal{H}_{rel} \otimes \mathcal{H}_{cm}$$

$$= \mathcal{H}_r \otimes \left(\bigoplus_{j=0}^{\infty} \mathcal{H}_j \right) \otimes \mathcal{H}_{cm}$$

(I) Spherical Coordinates (review)

$$(x, y, z) \longleftrightarrow (r, \theta, \varphi) \equiv \vec{r}$$



$$\begin{cases} x = r \sin\theta \cos\varphi \\ y = r \sin\theta \sin\varphi \\ z = r \cos\theta \end{cases}$$

$$\begin{cases} r = \sqrt{x^2 + y^2 + z^2} \\ \theta = \cdots \\ \varphi = \cdots \end{cases}$$

$0 \leq \theta \leq \pi$ not periodic!

$0 \leq \varphi < 2\pi$ periodic!

$$\vec{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) = \text{? in sph. coords?}$$

Chain rule: $\frac{\partial}{\partial r} = \frac{\partial x}{\partial r}\frac{\partial}{\partial x} + \frac{\partial y}{\partial r}\frac{\partial}{\partial y} + \frac{\partial z}{\partial r}\frac{\partial}{\partial z}$

$$\frac{\partial}{\partial \theta} = \ldots$$

$$\frac{\partial}{\partial \varphi} = \ldots$$

$\frac{\partial x}{\partial r} = \frac{x}{r}, \ldots \Rightarrow \boxed{r\frac{\partial}{\partial r} = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z} = \vec{r}\cdot\vec{\nabla}}$

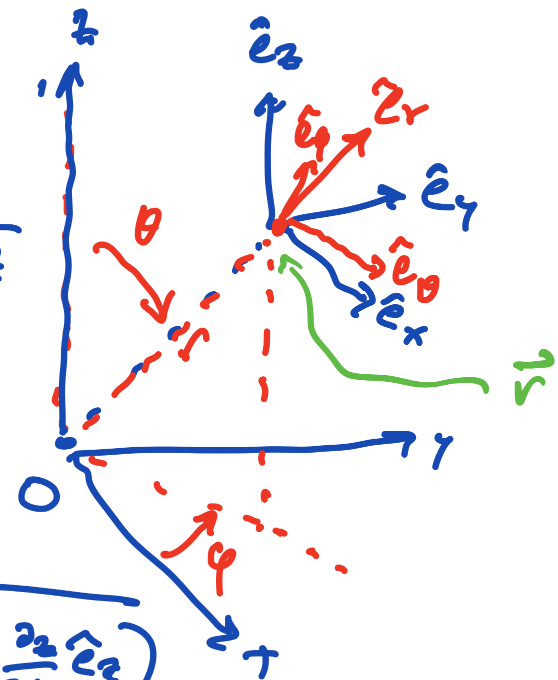
$\frac{\partial x}{\partial \varphi} = -y, \frac{\partial y}{\partial \varphi} = x, \frac{\partial z}{\partial \varphi} = 0$

$\therefore \boxed{\frac{\partial}{\partial \varphi} = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} = \hat{e}_z\cdot(\vec{r}\times\vec{\nabla})}$

& $\frac{\partial x}{\partial \theta} = z\cos\varphi, \frac{\partial y}{\partial \theta} = z\sin\varphi, \frac{\partial z}{\partial \theta} = -r\sin\theta$

$\therefore \left[\frac{\partial}{\partial \theta} = \ldots \text{ messy}\right]$

$$\vec{\nabla} = \hat{e}_x\frac{\partial}{\partial x} + \hat{e}_y\frac{\partial}{\partial y} + \hat{e}_z\frac{\partial}{\partial z}$$



Geometry ⇒

$$\hat{e}_r = \frac{\vec{r}}{r} = \frac{x\hat{e}_x + y\hat{e}_y + z\hat{e}_z}{r}$$

$$\hat{e}_\theta = \widehat{\frac{\partial \vec{r}}{\partial \theta}} = \overbrace{\frac{1}{r}\left(\frac{\partial x}{\partial \theta}\hat{e}_x + \frac{\partial y}{\partial \theta}\hat{e}_y + \frac{\partial z}{\partial \theta}\hat{e}_z\right)}$$

$$\hat{e}_\varphi = \widehat{\frac{\partial \vec{r}}{\partial \varphi}} = \ldots$$

Cartesian $\longleftrightarrow$ Spherical

$$d\vec{r} = dx\,\hat{e}_x + dy\,\hat{e}_y + dz\,\hat{e}_z = dr\,\hat{e}_r + r\,d\theta\,\hat{e}_\theta + r\sin\theta\,d\varphi\,\hat{e}_\varphi$$

$$\vec{r} = x\,\hat{e}_x + y\,\hat{e}_y + z\,\hat{e}_z = r\,\hat{e}_r \qquad d^3r = r^2 dr \sin\theta\, d\theta\, d\varphi$$

$$\begin{aligned}
\hat{e}_x &= \sin\theta\cos\varphi\,\hat{e}_r + \cos\theta\cos\varphi\,\hat{e}_\theta - \sin\varphi\,\hat{e}_\varphi \\
\hat{e}_y &= \sin\theta\sin\varphi\,\hat{e}_r + \cos\theta\sin\varphi\,\hat{e}_\theta + \cos\varphi\,\hat{e}_\varphi \\
\hat{e}_z &= \cos\theta\,\hat{e}_r - \sin\theta\,\hat{e}_\theta
\end{aligned}
\qquad\Bigg|\qquad
\begin{aligned}
\hat{e}_r &= \sin\theta\cos\varphi\,\hat{e}_x + \sin\theta\sin\varphi\,\hat{e}_y + \cos\theta\,\hat{e}_z \\
\hat{e}_\theta &= \cos\theta\cos\varphi\,\hat{e}_x + \cos\theta\sin\varphi\,\hat{e}_y - \sin\theta\,\hat{e}_z \\
\hat{e}_\varphi &= -\sin\varphi\,\hat{e}_x + \cos\varphi\,\hat{e}_y
\end{aligned}$$

$$\vec{\nabla} = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta} + \hat{e}_\varphi \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial r}(\hat{e}_r, \hat{e}_\theta, \hat{e}_\varphi) = 0, \text{ but } \left(\frac{\partial}{\partial\theta}, \frac{\partial}{\partial\varphi}\right)(\hat{e}_r, \hat{e}_\theta, \hat{e}_\varphi) \neq 0 \,! \Rightarrow \cdots$$

$$\vec{\nabla}\cdot\vec{A} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 A_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\theta) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}(A_\varphi)$$

$$\vec{\nabla}\times\vec{A} = \cdots$$

w/ $\vec{A} = A_r\,\hat{e}_r + A_\theta\,\hat{e}_\theta + A_\varphi\,\hat{e}_\varphi$.

$$\boxed{\nabla^2 f = \vec{\nabla}\cdot\vec{\nabla} f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\varphi^2}}$$

(2) Angular momentum ("Orbital")

$$\vec{L} = \vec{r}\times\vec{p} \quad\Leftrightarrow\quad L_i = \sum_{j,k=1}^{3} \epsilon_{ijk}\, r_j\, p_k$$

& $[\hat{L}_i, \hat{L}_j] = i\hbar \sum_k \epsilon_{ijk}\hat{L}_k$ (follows fr $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$)

& $\Rightarrow \quad [\hat{L}_i, \hat{p}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{p}_k \quad \Rightarrow [\hat{L}_i, \hat{p}^2] = 0$

$$[\hat{L}_i, \hat{r}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{r}_k \quad \Rightarrow [\hat{L}_i, \hat{r}^2] = 0 \quad \Rightarrow [\hat{L}_i, \hat{r}] = 0.$$

$$\therefore \quad [\hat{L}_i, \hat{H}] = 0 \quad \checkmark$$

- Choose max. commuting subset of $\hat{L}_i, \hat{L}^2, \hat{p}_i, \hat{p}^2, \hat{r}_i, \hat{r}^2, \hat{H}$

$\Rightarrow \quad \hat{H}, \hat{L}^2, \hat{L}_z \quad \Rightarrow$ common eigenstates $|n, l, m\rangle$

$\hat{H}|n, l, m\rangle = E_n |n, l, m\rangle \qquad n = 1, 2, 3, \ldots \quad E_n = ??$

$\hat{L}^2|n, l, m\rangle = \hbar^2 l(l+1) |n, l, m\rangle \qquad l = ?? \quad \in \{0, \cancel{\tfrac{1}{2}}, 1, \cancel{\tfrac{3}{2}}, \ldots\}$

$\hat{L}_z|n, l, m\rangle = \hbar m |n, l, m\rangle \qquad m \in \{-l, -l+1, \ldots, l-1, l\}$

- $\underline{l \in \{0, 1, 2, 3, \ldots\} \text{ only!}}$

$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$ on w. fncs

$= -i\hbar \frac{\partial}{\partial \varphi}$

Say have eigenstate w/ wvfnc $\psi(r, \theta, \varphi)$ & $\hat{L}_z$ eigenvalue $\hbar m$:

$$\Rightarrow \quad -i\hbar \frac{\partial \psi}{\partial \varphi} = \hbar m \psi$$

$$\Rightarrow \quad \frac{\partial \psi}{\partial \varphi} = i m \psi \quad \Rightarrow \quad \psi = \alpha e^{i m \varphi}$$

But periodic $\varphi \simeq \varphi + 2\pi \quad \Rightarrow \quad m \in \mathbb{Z}$

$\Rightarrow \quad l$ integer. $\checkmark$ $\qquad e^{2\pi i m} = 1$

- $$\boxed{\langle \vec{r}|\hat{p}^2|\psi\rangle = -\hbar^2\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)\psi(r,\theta,\varphi) + \frac{1}{r^2}\langle \vec{r}|\hat{L}^2|\psi\rangle}$$

$\hat{H} = \frac{1}{2\mu}\hat{p}^2 + \cdots \Rightarrow$ What is $\hat{p}^2$ in $\vec{r}$-basis?

$\hat{\vec{p}}\,|\vec{r}\rangle = i\hbar\vec{\nabla}|\vec{r}\rangle$ ----> change variables...

Alternative derivation:

$$\hat{L}^2 = (\hat{\vec{r}}\times\hat{\vec{p}})\cdot(\hat{\vec{r}}\times\hat{\vec{p}}) = \sum_i\left(\sum_{jk}\epsilon_{ijk}\hat{x}_j\hat{p}_k\right)\left(\sum_{lm}\epsilon_{ilm}\hat{x}_l\hat{p}_m\right)$$

$$= \sum_{jklm}\left(\sum_i \epsilon_{ijk}\epsilon_{ilm}\right)\hat{x}_j\hat{p}_k\hat{x}_l\hat{p}_m \qquad \text{(keep order!)}$$

$$= \sum_{jklm}(\delta_{jl}\delta_{km}-\delta_{jm}\delta_{kl})\hat{x}_j\hat{p}_k\hat{x}_l\hat{p}_m$$

$$= \sum_{jk}(\hat{x}_j\hat{p}_k\hat{x}_j\hat{p}_k - \hat{x}_j\hat{p}_k\hat{x}_k\hat{p}_j)$$

$$= \sum_{jk}(\hat{x}_j\hat{x}_j\hat{p}_k\hat{p}_k - i\hbar\delta_{jk}\hat{x}_j\hat{p}_k \qquad [\hat{x}_j,\hat{p}_k]=i\hbar\delta_{jk}$$

$$- \hat{x}_j\hat{p}_j\hat{x}_k\hat{p}_k - i\hbar\delta_{jk}\hat{x}_j\hat{p}_k + \hat{x}_j\hat{p}_j i\hbar\delta_{kk}) \qquad (\vec{r}\cdot\vec{p}\neq\vec{p}\cdot\vec{r}\ !)$$

$$= \hat{r}^2\hat{p}^2 - (\hat{\vec{r}}\cdot\hat{\vec{p}})^2 + i\hbar(\hat{\vec{r}}\cdot\hat{\vec{p}}).$$

Use: $\langle\vec{r}|\hat{\vec{r}} = \vec{r}\langle\vec{r}|$ & $\langle\vec{r}|\hat{\vec{p}} = -i\hbar\vec{\nabla}\langle\vec{r}| \Rightarrow$

$$\langle\vec{r}|\hat{L}^2 = r^2\langle\vec{r}|\hat{p}^2 + \hbar^2(\vec{r}\cdot\vec{\nabla})^2\langle\vec{r}| + \hbar^2(\vec{r}\cdot\vec{\nabla})\langle\vec{r}|$$

$$\therefore \langle\vec{r}|\hat{p}^2|\psi\rangle = \frac{1}{r^2}\left[\langle\vec{r}|\hat{L}^2|\psi\rangle - \hbar^2\left(r\frac{\partial}{\partial r}\right)^2\psi - \hbar^2\left(r\frac{\partial}{\partial r}\right)\psi\right] \quad \checkmark$$

Since $\hat{p}^2 \sim -\hbar^2\nabla^2$, also written

"$$\boxed{\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{1}{\hbar^2}\frac{\hat{L}^2}{r^2}}$$"

- $\langle \vec{r} | \hat{H} | \psi \rangle = \frac{1}{2\mu} \langle \vec{r} | \hat{p}^2 | \psi \rangle + \langle \vec{r} | V(\hat{r}) | \psi \rangle$

$$= -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\psi + \frac{1}{2\mu r^2}\langle \vec{r} | \hat{L}^2 | \psi \rangle + V(r)\psi$$

Choose $|\psi\rangle = |n, l, m\rangle \Rightarrow \hat{L}^2 |\psi\rangle = \hbar^2 l(l+1)|\psi\rangle \Rightarrow$

$$\langle \vec{r} | \hat{H} | \psi \rangle = \underbrace{-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\psi}_{\text{"radial KE"}} + \underbrace{\Bigg[\underbrace{\frac{\hbar^2 l(l+1)}{2\mu r^2}}_{\text{"centrifugal barrier"}} + \underbrace{V(r)}_{\text{P.E.}}\Bigg]}_{\text{"effective" radial P.E.}}\psi$$

$\psi(r, \theta, \varphi) \doteq \langle \vec{r} | n, l, m \rangle$, then $\hat{H}|n l m\rangle = E_n |n l m\rangle$

gives P.D.E. for ψ, depends only on r ! :

$$\underbrace{-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\psi + \left(\frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right)\psi}_{= D_l(r)\psi} = E_n \psi$$

Solved by $\psi(r, \theta, \varphi) = R(r)\, Y(\theta, \varphi)$ (any Y)

s.t. $D_l(r) R(r) = E_n R(r) \leftarrow$ ODE = "radial Schrö. eqn."

What determines $Y(\theta, \varphi)$? Other eigenvalue eqns:

$$\left.\begin{aligned} \hat{L}^2 |n l m\rangle &= \hbar^2 l(l+1) |n l m\rangle \\ \hat{L}_z |n l m\rangle &= \hbar m |n l m\rangle \end{aligned}\right\} \rightarrow \text{only involves } \theta, \varphi \ldots$$

• Angular part $\quad \psi = R(r)\, Y(\theta,\varphi)$

& $\begin{cases} \hat{L}^2|\psi\rangle = \hbar^2 \ell(\ell+1)|\psi\rangle \\ \hat{L}_z|\psi\rangle = \hbar m|\psi\rangle \end{cases} \Rightarrow$ eqns for Y ...

∴ Need $\langle \vec{r}|\hat{L}^2|\psi\rangle$ & $\langle \vec{r}|\hat{L}_z|\psi\rangle$ in sph. coords.

∴ Use c.o.v. ...

$$\langle \vec{r}|\hat{L}^2|\psi\rangle = -\hbar^2 r^2\left(\nabla^2 - \frac{\partial^2}{\partial r^2} - \frac{2}{r}\frac{\partial}{\partial r}\right)\psi$$

& $\nabla^2 = \dfrac{\partial^2}{\partial r^2} + \dfrac{2}{r}\dfrac{\partial}{\partial r} + \dfrac{1}{r^2\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial}{\partial\theta}\right) + \dfrac{1}{r^2\sin^2\theta}\dfrac{\partial^2}{\partial\varphi^2}$

$$\Rightarrow \boxed{\langle \vec{r}|\hat{L}^2|\psi\rangle = -\frac{\hbar^2}{\sin\theta}\left(\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right)}$$

& calc. $\boxed{\langle \vec{r}|\hat{L}_z|\psi\rangle = -i\hbar\dfrac{\partial\psi}{\partial\varphi}}$

Only depend on (θ,φ), so plug in $\psi = R(r)\,Y(\theta,\varphi)$

$\Rightarrow$ $R(r)$'s cancel & get for $Y_{\ell m}(\theta,\varphi)$:

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)Y_{\ell m} = -\ell(\ell+1)Y_{\ell m} \qquad (*\theta)$$

$$\frac{\partial}{\partial\varphi}Y_{\ell m} = im\,Y_{\ell m} \qquad (*\varphi)$$

& normalization: $\displaystyle\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\varphi\, |Y_{\ell m}|^2 = 1$

Solve by sep. of vars.: $Y_{\ell m}(\theta,\varphi) = P(\theta)Q(\varphi)$

$(*\varphi) \Rightarrow \dfrac{dQ}{d\varphi} = imQ \rightarrow Q = e^{im\varphi}$ & per. $\Rightarrow m\in\mathbb{Z}$.

$\therefore\ Y_{\ell m}(\theta,\varphi) = P_{\ell m}(\theta)e^{im\varphi}$ & $P_{\ell m}$ satisfies

norm: $\displaystyle 1 = 2\pi\int_0^\pi \sin\theta\, d\theta\, |P_{\ell m}|^2$

eqn: $$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\right]P_{\ell m} = -\ell(\ell+1)P_{\ell m} \qquad (**)$$

- How to solve? • Chang vars $\theta \to a \equiv \cos\theta \ldots$

Better: Know from angular mom. algebra: $\hat{L}_+|\ell,\ell\rangle = 0$

& $\hat{L}_+ = \hat{L}_x + i\hat{L}_y = \cdots$ (in sph. coord). $\Rightarrow$ 1^{st} order ODE

Result: $P_{\ell\ell}(\theta) \propto \sin^\ell\theta$. Then rest $P_{\ell m}$ by

$\hat{L}_-|\ell,\ell\rangle \propto |\ell,\ell-1\rangle$, etc.

Answer: "Spherical Harmonics"

$$Y_{00} = \sqrt{\frac{1}{4\pi}} \qquad \left(\text{b/c } \int \sin\theta \, d\theta \, d\varphi = 4\pi\right)$$

$$Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}} \underbrace{e^{\pm i\varphi}\sin\theta}_{=\frac{x\pm iy}{r}}, \qquad Y_{1,0} = \sqrt{\frac{3}{4\pi}} \underbrace{\cos\theta}_{=\frac{z}{r}}$$

$$Y_{2,\pm2} = \cdots, \quad Y_{2,\pm1} = \cdots \quad Y_{2,0} = \cdots \quad \text{etc.}$$

- Useful properties:

order ℓ

$$Y_{\ell,m} = \text{Polynomial}(\sin\theta, \cos\theta)\, e^{im\varphi} = \frac{\text{Poly}(z, x\pm iy)^{\ell}}{r^{\ell}}$$

$$Y_{\ell,-m} = (-)^m \left(Y_{\ell,m}\right)^*$$

- Orthonormal:

$$\int d\Omega \, Y^*_{\ell m} Y_{\ell' m'} = \delta_{\ell\ell'}\delta_{mm'} = \langle \ell, m | \ell', m' \rangle$$

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta,\varphi)\, Y^*_{\ell m}(\theta',\varphi') = \delta^2_{\Omega}(\theta-\theta', \varphi-\varphi')$$

$\leftrightarrow \sum_{\ell m} |\ell m\rangle\langle \ell m| = \mathbb{1}$ in $\mathcal{H}_{\theta,\varphi}$

where
$$\boxed{\begin{cases} \int d\Omega \equiv \int d\varphi \int \sin\theta \, d\theta \\ \delta^2_{\Omega} \equiv \frac{1}{\sin\theta}\,\delta(\theta-\theta')\,\delta(\varphi-\varphi'). \end{cases}}$$

$$Y_{\ell,m}(\theta,\varphi) = \langle \theta, \varphi | \ell, m \rangle$$

$$\mathcal{H}_{\vec{r}} = \mathcal{H}_r \otimes \mathcal{H}_{\theta,\varphi}$$
$$\{|r\rangle\} \otimes \{|\theta,\varphi\rangle\}$$

Ortho-normality of $\{|\theta,\varphi\rangle\}$:

$$\begin{cases} \langle \theta,\varphi | \theta',\varphi' \rangle = \delta^2_\Omega(\theta-\theta',\varphi-\varphi') \\ \int d\Omega\, |\theta,\varphi\rangle\langle\theta,\varphi| = \hat{1} \end{cases}$$

$$\langle \theta,\varphi | Y \rangle = \int d\Omega' \langle \theta,\varphi | \theta',\varphi' \rangle \langle \theta',\varphi' | Y \rangle$$

$$= \int d\Omega' \; \delta^2_\Omega(\theta-\theta',\varphi-\varphi') \; \langle \theta',\varphi' | Y \rangle$$

$$= \int (\sin\theta') d\theta' d\varphi' \; \delta^2_\Omega(\theta-\theta',\varphi-\varphi') \langle \theta',\varphi' | Y \rangle$$

$$\therefore \quad \delta^2_\Omega(\theta-\theta',\varphi-\varphi') = \frac{1}{\sin\theta} \delta(\theta-\theta')\delta(\varphi-\varphi')$$

$$\delta_{\ell\ell'}\delta_{mm'} = \langle \ell,m | \ell',m' \rangle = \int d\Omega \, \langle \ell,m | \theta,\varphi \rangle \langle \theta,\varphi | \ell',m' \rangle$$
$$= \int d\Omega \; Y^*_{\ell m}(\theta,\varphi) \; Y_{\ell' m'}(\theta,\varphi)$$

$$\langle \theta,\varphi | \left(\hat{1} = \sum_{\ell,m} |\ell,m\rangle\langle \ell,m| \right) | \theta',\varphi' \rangle$$

$$\Rightarrow \quad \langle \theta,\varphi | \theta',\varphi' \rangle = \sum_{\ell,m} \langle \theta,\varphi | \ell,m \rangle \langle \ell,m | \theta',\varphi' \rangle$$

$$\delta^2_\Omega(\theta-\theta',\varphi-\varphi') \qquad \sum_{\ell,m} Y_{\ell m}(\theta,\varphi)\, Y^*_{\ell m}(\theta',\varphi')$$