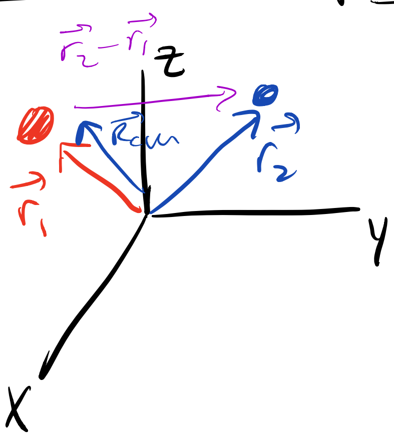
3D QM w/ 2 particles



$V(\vec{r}_1, \vec{r}_2)$

Central Potential

$V(|\vec{r}_2 - \vec{r}_1|)$

$V(r)$

$\vec{r} = \vec{r}_2 - \vec{r}_1$

$$\vec{R}_{cm} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}$$

electron/nuclei

$m_1 >> m_2$

nucleus mass >> electron mass

$\vec{R}_{cm} \simeq \vec{r}_1$

$\vec{r}$ electron relative to nucleus

$$H_{sys}|E_{sys}\rangle = E_{sys}|E_{sys}\rangle$$

$$\Downarrow$$

$$\boxed{H_{cm}|E_{cm}\rangle = E_{cm}|E_{cm}\rangle}$$

$$H_{rel}|E_{rel}\rangle = E_{rel}|E_{rel}\rangle$$

free particle → no V

$$H_{rel} |E_{rel}\rangle = E_{rel} |E_{rel}\rangle , \; V(r)$$

$$\left[\frac{p_{rel}^2}{2\mu} + V(r) \right] \psi = E_{rel} \psi$$

electron Hydrogen atom

$$V(r) \Rightarrow \text{spherical sym.}$$

$$\Downarrow$$

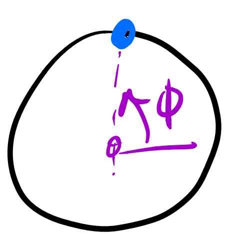
$$H_{sys}(r,\theta,\phi) \Leftarrow \text{spherical coords.}$$

Hydrogen atom

$$\psi(r,\theta,\phi) = R(r)\, \Theta(\theta)\, \Phi(\phi)$$

Sep Coeffs. A & B

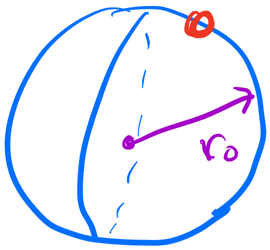
focus on this first



$$\frac{d^2\Phi}{d\phi^2} = -B\Phi$$

$$\Phi = Ne^{im\phi} \qquad m = \pm 1, 2, 3 \ldots, 0$$

Particle on a Sphere



ϕ, θ are free

$r = r_0$ is fixed.

$$-\frac{\hbar^2}{2\mu r_0^2}\left(\underbrace{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\left(\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}}\right)\psi$$

$$+V(r_0)\psi = E\psi$$

$$H_{sphere}|E_{sphere}\rangle = E_{sphere}|E_{sphere}\rangle$$

Simplification

(1) $\psi(r_0, \theta, \phi) = Y(\theta, \phi)$

(2) set $V(r_0) = 0$

$I = \mu r_0^2$ particle of mass μ

$$\boxed{\frac{-\hbar^2}{2I}\left(\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)}Y=EY$$

L^2 operator position rep in spherical coords

$$\boxed{\frac{L^2}{2I}Y(\theta,\phi)=EY(\theta,\phi)}$$

Remember:

eigenstate $|lm\rangle$ of L_z, L^2 $\rightarrow L_z|lm\rangle = m\hbar|lm\rangle$

evalues $\rightarrow \underline{L^2|lm\rangle = l(l+1)\hbar^2|lm\rangle}$

$$L^2Y(\theta,\phi)=l(l+1)\hbar^2Y(\theta,\phi)$$

$$E=\frac{l(l+1)\hbar^2}{2I}$$ energy quantized

$$L^2Y(\theta,\phi)=A\hbar^2Y(\theta,\phi)$$

sep. constant $= l(l+1)$

Separate Variables again

$$Y(\theta,\phi) = \Theta(\theta)\,\Phi(\phi)$$

$$\left(\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta} - B\frac{1}{\sin\theta}\right)\Theta = -A\Theta \quad (1)$$

$$\frac{d^2\Phi}{d\phi^2} = -B\Phi \quad (2)$$

☆ $Y_\ell^m(\theta,\phi) \Leftarrow$ these solutions can be used and how we use them

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particle on ring $\quad B = m^2$

$m = 0, \pm1, \pm2, \pm3, \ldots$

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)-\frac{m^2}{\sin\theta}\right)\Theta(\theta) = -A\,\Theta(\theta)$$

① exchange of variable $\Theta(\theta) = P(z)$

$z = \cos\theta \qquad \sin\theta = \sqrt{1-z^2}$

② new Diffy Q

$$\left((1-z^2)\frac{d^2}{dz^2} - 2z\frac{d}{dz} + A - \frac{m^2}{(1-z^2)}\right)P(z) = 0$$

"associated Legendre eqn."

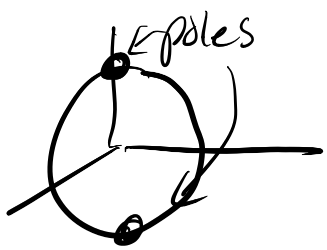
$m=0$ special case

$$\left[(1-z^2)\frac{d^2}{dz^2} - 2z\frac{d}{dz} + A\right]P(z) = 0$$

"Legendre eqn."

expect issues when $z = \pm 1$

$\Rightarrow \theta = 0, \pi$



Build a Series Solution

propose $P(z) = \sum_{n=0}^{\infty} a_n z^n$

plug it in.

$$\frac{dP}{dz} = \sum_{n=0}^{\infty} n a_n z^{n-1}$$

$$\frac{d^2P}{dz^2} = \sum_{n=0}^{\infty} n(n-1) a_n z^{n-2}$$

$$\sum_{n=0}^{\infty} n(n-1) a_n z^{n-2} - \sum_{n=0}^{\infty} n(n-1) a_n z^n - 2\sum_{n=0}^{\infty} n a_n z^n + A\sum_{n=0}^{\infty} a_n z^n = 0$$

$$\underbrace{0(-1)a_0 z^{-2}}_{0} + \underbrace{(1)(0)a_1 z^{-1}}_{0} + 2(1)a_2 z + \ldots$$

$$\sum_{n=0}^{\infty} n(n-1)\, a_n z^{n-2} = \sum_{n=-2}^{\infty} (n+2)(n+1)\, a_{n+2} z^n$$

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

$$\sum_{n=0}^{\infty} \Big((n+2)(n+1)\, a_{n+2} - n(n-1)a_n - 2na_n + Aa_n \Big) z^n = 0$$

every z^n this holds

either $z^n = 0$ for all n $\times$ $P(z)=0$

arg. ( ) $= 0$ for all n

$$(n+2)(n+1)\, a_{n+2} - n(n-1)a_n - 2na_n + Aa_n = 0$$

$$\boxed{a_{n+2} = \frac{n(n+1) - A}{(n+2)(n+1)}\, a_n}$$

$$a_0 \to a_2, a_4, a_6 \dots$$
$$a_1 \to a_3, a_5, a_7 \dots$$

$$P(z) = a_0 z^0 + a_1 z^1 + a_2 z^2 + a_3 z^3 + \dots$$

$$a_2 \uparrow a_0 \qquad a_3 \uparrow a_1$$

$$f(a_0) \qquad g(a_1)$$

Properties $\sum_{n=0}^{\infty} \to$ converge?

$$\lim_{n\to\infty}\left(\frac{a_{n+2}}{a_n}\right) \simeq 1 \quad \text{problem}$$

$$a_{n+2} = \frac{\boxed{n(n+1) - A}}{(n+2)(n+1)} a_n \qquad \boxed{n(n+1) - A} \to 0$$

$L^2 Y = A\hbar^2 Y \qquad L^2|lm\rangle = l(l+1)\hbar^2|lm\rangle$

$A = n_{max}(n_{max}+1) = l(l+1)$

$n_{max} = l$

$l = 0, 1, 2, 3, \ldots$

$\Rightarrow$ dictating total number of terms

$\Rightarrow$ ensures convergence, l

Legendre Polynomials

$A = l(l+1) \Leftarrow$ separation const.

$m = 0$

$$P_l(z) = \frac{1}{2^l l!} \frac{d^l}{dz^l} (z^2-1)^l$$ Rodrigues formula

$P_0(z) = 1$

$P_1(z) = z$

$P_2(z) = \frac{1}{2}(3z^2 - 1)$

etc

tabulated

Orthogonal

$$\int_{-1}^{+1} P_k^*(z) P_\ell(z) dz = \frac{2}{2\ell+1} \delta_{k\ell}$$

$m \neq 0$

$$\left((1-z^2)\frac{d^2}{dz^2} - 2z\frac{d}{dz} + \ell(\ell+1) - \frac{m^2}{(1-z^2)}\right) P(z) = 0$$

"associated Legendre functions"

$$P_\ell^m(z) = P_\ell^{-m}(z) = (1-z^2)^{m/2} \frac{d^m}{dz^m} P_\ell(z)$$

$$= \frac{1}{2^\ell \ell!}(1-z^2)^{m/2} \frac{d^{m+\ell}}{dz^{m+\ell}} (z^2-1)^\ell$$

$m > \ell \qquad \dfrac{d^{m+\ell}}{dz^{m+\ell}}(z^2-1)^\ell = 0$

$\Rightarrow \quad m = -\ell, -\ell+1, \ldots, 0, \ldots, \ell-1, \ell$

$|m| \le \ell$

<u>Orthogonal</u>

$$\int_{-1}^{+1} P_\ell^m(z)\, P_q^m(z)\, dz = \frac{2}{2\ell+1} \frac{(\ell+m)!}{(\ell-m)!} \delta_{\ell q}$$

Translate to Solution $\Theta(\theta)$

$z = \cos\theta$

$$\boxed{\Theta_\ell^m(\theta) = (-1)^m \frac{(2\ell+1)}{2} \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(\cos\theta), \quad m \ge 0}$$

$$\int_0^\pi \Theta_\ell^m(\theta)\, \Theta_q^m \sin\theta\, d\theta = \delta_{\ell q}$$

$P_\ell^m(\cos\theta)$

$P_0^0 = 1$

etc.

$P_1^0 = \cos\theta$

tabulated

$P_1^1 = \sin\theta$