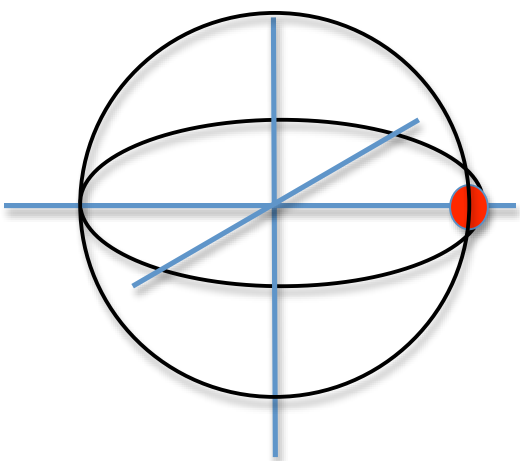
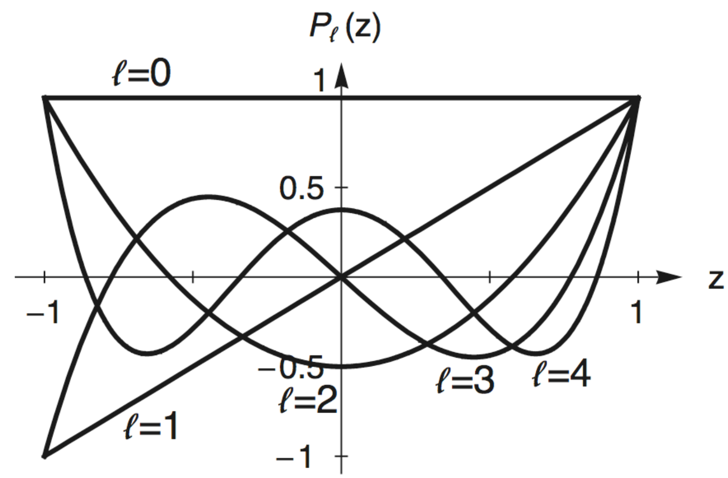
The Rigid Rotor Problem: A quantum particle confined to a sphere

Reading: McIntyre 7.6





Summary

- So far:

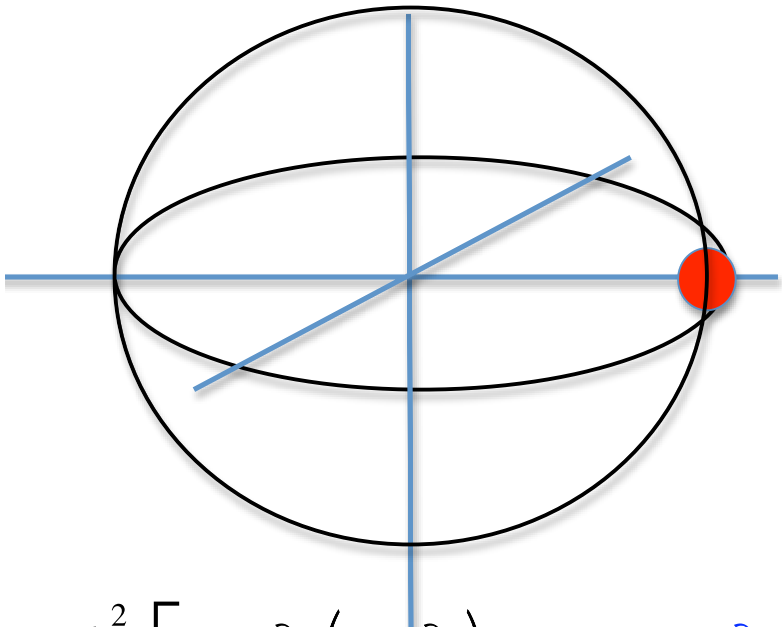
$$\frac{d^2\Phi(\phi)}{d\phi^2} = -m^2\Phi(\phi) \qquad \Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}$$

$$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right) - m^2\frac{1}{\sin^2\theta}\right]\Theta(\theta) = -A\Theta(\theta)$$

$$\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) - \frac{2\mu}{\hbar^2}(E - V(r))r^2R(r) \equiv AR(r)$$

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\Theta_\ell^m(\theta)\Phi_m(\phi)$$

Particle on a sphere



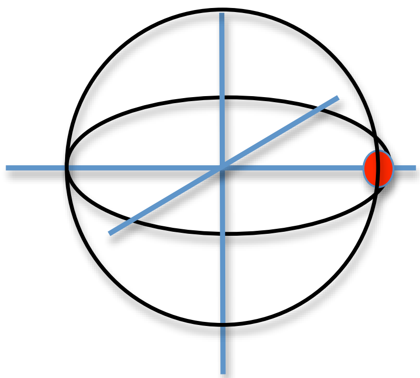
$$\mathbf{r} = r_0 \sin\theta\cos\phi\mathbf{i} + r_0 \sin\theta\sin\phi\mathbf{j} + \cos\theta\mathbf{k}$$

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

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(r,\theta,\phi)$$

$$+V(r)\psi(r,\theta,\phi) = E_{sphere}\psi(r,\theta,\phi)$$

$$-\frac{\hbar^2}{2\mu r_0^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(\theta,\phi) + \underbrace{V(r_0)}_{assume\ =\ 0}\psi(\theta,\phi) = E_{sphere}\psi(\theta,\phi)$$



Particle on a sphere

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

$$\frac{-\hbar^2}{2I}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]Y(\theta,\phi) = E_{sphere}Y(\theta,\phi)$$

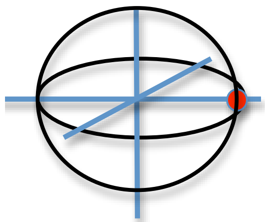
Looks like

$$\frac{1}{\hbar^2}\mathbf{L}^2 Y(\theta,\phi) = AY(\theta,\phi) \qquad A = \frac{2I}{\hbar^2}E_{sphere}$$

$$H = \frac{L^2}{2I}$$

← L^2 not Lz^2

$$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right) - m^2\frac{1}{\sin^2\theta}\right]\Theta(\theta) = -A\Theta(\theta)$$



Legendre's equation (m = 0)

$$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)-m^2\frac{1}{\sin^2\theta}\right]\Theta(\theta)=-A\Theta(\theta)$$

- Change variables: $z = \cos\theta$, $P(z)=\Theta(\theta)$ (see text)

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)=\frac{d}{dz}\left(\left(1-z^2\right)\frac{d}{dz}\right)$$

$$=\left(1-z^2\right)\frac{d^2}{dz^2}-2z\frac{d}{dz}$$

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

Series Solution of Legendre's equation (m = 0)

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

- Try an infinite series: $P(z)=\sum_{n=0}^{\infty}a_n z^n$
- Perform derivatives and plug in:

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

- Write out the first few terms of the first sum

Series Solution of Legendre's equation (m = 0)

$$\sum_{n=0}^{\infty} a_n n(n-1)z^{n-2} = a_0 0(-1)z^{-2} + a_1(1)(-1)z^{-1} + a_2 2(1)z^0 + a_3 3(2)z + \ldots$$

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

- Let p = n - 2 ; n = p + 2

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

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

Legendre's equation (m = 0) Recurrence relation

- Magic part!

$$\sum_{n=0}^{\infty}\left[a_{n+2}(n+2)(n+1)-a_n n(n-1)-2a_n n+Aa_n\right]z^n=0$$

- Each coefficient of z^n is zero => recurrence relation

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

- All evens related; all odds related

$$P(z)=a_0\left[z^0-\left(\frac{A}{2}\right)z^2+\ldots\right]+a_1\left[z^1+\left(\frac{2-A}{6}\right)z^3+\ldots\right]$$

Legendre's equation ($m = 0$)
The series must be finite!

- If the series is not finite, the polynomial blows up (check ratio for large *n*)

$$A = n_{\max}\left(n_{\max}+1\right)$$

$$A = \ell\left(\ell+1\right)$$

← Anticipated this!

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

- These special values of *A* give Legendre polynomials.

$$P_0(z) = 1$$

$$P_1(z) = z$$

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

$$P_3(z) = \frac{1}{2}(5z^3-3z)$$

$$P_4(z) = \frac{1}{8}(35z^4-30z^2+3)$$

$$P_5(z) = \frac{1}{8}(63z^5-70z^3+15z)$$