2/28/01

Lec. 21 QM in 3 Dim.

Generalization to 3 dim is easy

$$T = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$$

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad p_y = \frac{\hbar}{i}\frac{\partial}{\partial y} \qquad p_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

$$T = -\frac{\hbar^2}{2m}\nabla^2, \qquad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Laplacian

$$i\hbar \frac{\partial}{\partial t}\Psi(x,y,z,t) = \hat{H}\,\Psi(x,y,z,t)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)$$

Commutation relations

$$\hat{x} \to x \qquad \hat{y} \to y \qquad \hat{z} \to z$$

so $[r_i, p_j] = i\hbar\,\delta_{ij}, \qquad [r_i, r_j] = [p_i, p_j] = 0$

since $y\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}(y f(x,y))$ etc.

so H.U.P.

$$\sigma_x\,\sigma_{p_x} \geq \frac{\hbar}{2} \qquad \sigma_y\,\sigma_{p_y} \geq \hbar/2 \quad \text{etc.}$$

but $\sigma_x\,\sigma_{p_y} \geq 0$

Time dep. S. eq.

$$-\frac{\hbar^2}{2m}\nabla^2\psi_n + V\psi_n = E_n\psi_n$$

$$\Psi(\vec{r},t) = \sum c_n \underbrace{\psi_n(\vec{r})}_{\psi_n(x,y,z)} e^{-iE_n t/\hbar}$$

Normalization

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \; |\Psi(\vec{r})|^2 = 1$$

$$\int d^3r \; |\Psi(\vec{r})|^2 = 1$$

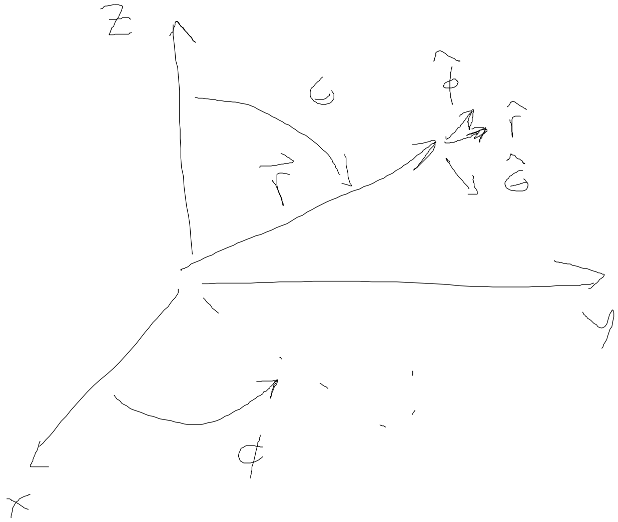
Seperation of Variables

Often $V(\vec{r}) = V(|\vec{r}|)$

then look for

$$\psi_n(\vec{r}) = R(r)\,Y(\theta,\phi)$$

and use spherical coordinates



Change of variables

$z = r\cos\theta$ θ = polar angle

$x = r\sin\theta\cos\phi$ ϕ = azimuthal angle

$y = r\sin\theta\sin\phi$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

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

$$-\frac{\hbar^2\nabla^2}{2m}R(r)Y(\theta,\phi) + V(r)R(r)Y(\theta,\phi) = E_n R(r)Y(\theta,\phi)$$

$$-\frac{\hbar^2}{2mr^2}\left[\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{1}{\sin\theta\, Y}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta\, Y}\frac{\partial^2 Y}{\partial\phi^2}\right] + V(r) = E$$

divided through by $R(r)Y(\theta,\phi)$

Now multiply by $-\frac{2m}{\hbar^2}r^2$

$$\left\{\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2m}{\hbar^2}r^2\left(V(r)-E\right)\right\}$$

$$+\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = 0$$

First { } only function of r

Second [ ] only function of θ,ϕ

let $\{ \} = \text{const.} = l(l+1)$

$$\frac{1}{Y}[\ ] = -l(l+1)$$

$l(l+1) =$ seperation constant, indep. of r, θ, ϕ.

Angular eq.

$$\sin\theta \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -l(l+1)\sin^2\theta\, Y$$

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

$$\underbrace{\left\{\frac{1}{\Theta}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\, \Theta'\right) + l(l+1)\sin^2\theta\right\}}_{\text{seperation constant } = m^2} + \underbrace{\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2}}_{-m^2} = 0$$

$$\frac{\partial^2\Phi}{\partial\phi^2} = -m^2\Phi$$

$$\Phi(\phi) = e^{im\phi}$$

m could be positive or negative

Boundary condition

$$\Phi(\phi + 2\pi) = \Phi(\phi)$$

same point in 3 space

$\Rightarrow \quad m = \text{integer} = 0, \pm 1, \pm 2, \pm 3, \ldots$

$$e^{im2\pi} = 1$$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \left[l(l+1)\sin^2\theta - m^2\right]\Theta = 0$$

$$\Theta = A\, P_l^m(\cos\theta)$$

$$P_l^m = (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} P_l(x)$$

associated Legendre Func.

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{\partial}{\partial x}\right)^\ell (x^2-1)^\ell$$

Legendre polynomials are orthogonal on -1,1

$$\int_{-1}^{1} dx \; P_\ell(x) \, P_{\ell'}(x) = \frac{2}{2\ell+1}\delta_{\ell\ell'}$$

Note $P_\ell^m \propto \left(\frac{\partial}{\partial x}\right)^{\ell+|m|} (x^2-1)^\ell$

This will be zero if $\ell + |m| > 2\ell$

Thus

$$-\ell \leq m \leq \ell$$

$2\ell+1$ possible m values for a given ℓ

example $\ell = 2$ $\quad m = -2, -1, 0, 1, 2$

Normalize

$$d^3r = dx\,dy\,dz = r^2 \sin\theta \, dr \, d\theta \, d\phi$$

$$\int_0^\infty |\Psi|^2 r^2 \, dr \, \sin\theta \, d\theta \, d\phi = 1$$

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

$$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta \, d\theta \; |Y(\theta,\phi)|^2 = 1$$

Normalized angular functions are called spherical harmonics

$$\boxed{Y_\ell^m(\theta,\phi) = \epsilon \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}} \, e^{im\phi} P_\ell^m(\cos\theta)}$$

$\epsilon = (-1)^m \quad m \geq 0 \quad$ else $1 \quad m < 0$

$$\int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi \; Y_l^{m*} \, Y_{l'}^{m'} = \delta_{ll'} \delta_{mm'}$$

Radial equation

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left(V(r) - E\right) R = l(l+1)R$$

Let $u = r R(r)$ $\qquad R = \frac{u}{r} \qquad R' = \frac{u'}{r} - \frac{u}{r^2}$

$$\frac{d}{dr}\left(r^2 \left(\frac{dR}{dr}\right)\right) = \frac{d}{dr}\left(r u' - u\right) = r u''$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2 u}{dr^2} + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right] u = E u}$$

Radial equation