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Lecture #24 Three dimensions

- Start reading chapter 4 sections 4.1, 4.2
- No class Wend. Oct 28

Generalization of past work to 3-dim. is easy

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

$$\hat{H} = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V(x,y,z)$$

So $p_x \to \frac{\hbar}{i}\frac{\partial}{\partial x}$ $\quad p_y = \frac{\hbar}{i}\frac{\partial}{\partial y}$ $\quad p_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$

$$\vec{p} \to \frac{\hbar}{i}\vec{\nabla}$$

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

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

Laplacian

Normalization $\int |\Psi|^2 \, d^3r = 1$

$$\Psi_n(\vec{r},t) = \psi_n(\vec{r})\, e^{-iE_n t/\hbar}$$

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

Seperation of variables

If V is only a function of $|\vec{r}| = r$ and independent of angles

[Example: electrostatic pot. for H atom

$$V(\vec{r}) = -\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{r}$$ indep. of angle.

adopt spherical coordinates (r, θ, ϕ)

$$z = r\cos\theta$$
$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$

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

Look for solutions

$$\psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi)$$

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right)+\frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{d\theta}\right)\right.$$

$$\left.+\frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]+VRY=ERY$$

Divide by YR and multiply by $-\frac{2mr^2}{\hbar^2}$

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

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

First term only func. of r, second only θ,ϕ. Each must be a constant.

Radial eq. [depends on form of $V(r)$]

$$\boxed{\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}\left[V(r)-E\right]=\text{const.}=l(l+1)}$$

Will see why $l(l+1)$ in a while

Angular eq. (true for any central pot.)

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

We can solve angular equation once for all problems

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

Cont. with seperation of variables

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

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

and $\frac{1}{\Phi}\frac{\partial^2 \Phi}{\cancel{\partial}\phi^2} = -m^2$

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi \Rightarrow \boxed{\Phi(\phi) = e^{im\phi}}$$

note could have $e^{-im\phi}$ but we will let m run negative

If we go once around, expect

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

so $m = 0, \pm 1, \pm 2, \pm 3 \ldots$
(integers)

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

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

associated Legendre function

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

$P_l(x) = l$ th Legendre polynomial (of degree x^l)

$$P_l \equiv \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l$$

$$P_0 = 1 \qquad P_1 = \frac{1}{2}\frac{d}{dx}(x^2-1) = x$$

$$P_2 = \frac{1}{2}(3x^2-1) \quad \ldots$$

Note if $|m| > l$ then $P_l^m \equiv 0$

$$\frac{d^m}{dx^m} x^l \equiv 0 \quad \text{for} \quad m > l$$

l must be nonnegative integer

Thus $\ell = 0, 1, 2, 3 \ldots$

For a given ℓ there are $2\ell+1$ allowed m values

$$m = -\ell, -\ell+1, -\ell+2 \ldots \ell-1, \ell$$

Normalize the solution

$$\int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi \; Y_\ell^m(\theta,\phi)^* \, Y_\ell^m(\theta,\phi) = 1$$

We have labeled Y by its quantum #s

$\ell =$ total angular momentum

$m =$ projection of ang. momentum on z axis (will see this later)

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

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

Examples $Y_0^0 = \sqrt{\frac{1}{4\pi}}$ $\quad Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$

$$Y_1^{\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{\pm i\phi}$$

Note Y_ℓ^m are orthonormal

$$\int d\theta \sin\theta \int d\phi \; Y_\ell^{m*} \, Y_{\ell'}^{m'} = \delta_{\ell\ell'} \, \delta_{mm'}$$