10/~~28~~ 30/98

Lecture #25 Radial Equation

$$\psi_n(r,\theta,\phi) = Y_\ell^m(\theta,\phi)\, R(r)$$

Last time

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

and radial equation

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

let $U = rR \Rightarrow R = U/r \qquad R' = \frac{U'}{r} - \frac{U}{r^2}$

$\frac{\partial}{\partial r}\, r^2 R' = \frac{\partial}{\partial r}(rU' - U) = U''$ here prime $= \frac{\partial}{\partial r}$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 U}{\partial r^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]U(r) = E\,U(r)$$

This looks like one dim schrodinger eq. with an effective pot.

$$V_{eff}(r) = V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$$

(the extra piece is called the centrifugal pot.

Note also that r is allways positive while x ran from $-\infty$ to ∞

Normalization

$$\int d^3r\, \psi_n^* \psi_n = 1$$

$$1 = \left[\int_0^\infty r^2 dr \; R(r)^2 \right] \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi \; Y_l^{m*} Y_l^m$$

$$\Rightarrow \int_0^\infty r^2 dr \left(\frac{u}{r}\right)^2 \Rightarrow \boxed{\int_0^\infty dr\; u(r)^2 = 1}$$

Final difference between 1 dim and 3-dim
In 3 dim want

$$u(r=0) = 0$$

To continue we need to specify $V(r)$

Example: infinite spherical well

$$V(r) = \begin{cases} 0 & r < a \\ \infty & r > a \end{cases}$$

$$u(r) = 0 \qquad r > a$$

Inside $V = 0$

$$\frac{d^2u}{dr^2} = \left[\frac{l(l+1)}{r^2} - k^2\right] u$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

For $l=0$ this has simple solution

$l=0$: $\quad u = A \sin kr + B \cos kr$

$$R(r) = \frac{u}{r} = \frac{B}{r} + A\frac{\sin kr}{r} \quad \text{as } r \to 0$$

B term blows up. We will drop this term. [Full argument is more subtle]

In three dim. have b. condition

$$\boxed{u(r\to 0) = 0}$$

Thus $\quad u(r) = A \sin kr$

and

$$u(a) = 0 = \sin ka$$

$$\Rightarrow \quad E_{l=0} = \frac{n^2 \pi^2 \hbar^2}{2 m a^2} \qquad n = 1, 2 \ldots$$

Note no $n=0$ state

$$\psi_{n00}(r) = \frac{\sqrt{\frac{2}{a}}\,\sin\frac{n\pi r}{a}}{r}\, Y_0^0(\theta,\phi) = \frac{u(r)}{r} Y_l^m$$

$l = 0 = m$

$$u(r) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi r}{a}\right), \qquad \int_0^a u^2\,dr = 1$$

From last time $Y_0^0 = \sqrt{\frac{1}{4\pi}}$

$$\psi_{n00}(r) = \left(\frac{1}{2\pi a}\right)^{1/2} \frac{\sin \frac{n\pi r}{a}}{r}$$

The general solution to

$$\frac{\partial^2 u}{\partial r^2} = \left[\frac{\ell(\ell+1)}{r^2} - k^2\right] u$$

For $\ell \neq 0$ is

$$u(r) = A r\, j_\ell(kr) + B r\, n_\ell(kr)$$

Here $j_\ell(kr)$ is spherical Bessel function and $n_\ell(kr)$ is spherical Neumann function

$$j_\ell(x) = (-x)^\ell \left(\frac{1}{x}\frac{\partial}{\partial x}\right)^\ell \left(\frac{\sin x}{x}\right)$$

$$n_\ell(x) = -(-x)^\ell \left(\frac{1}{x}\frac{\partial}{\partial x}\right)^\ell \frac{\cos x}{x}$$

For example

$$j_0(x) = \frac{\sin x}{x} \qquad n_0(x) = -\frac{\cos x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

For small $x << 1$

$$j_\ell(x) \rightarrow \frac{x^\ell}{(2\ell+1)!!} \qquad n_\ell(x) \rightarrow -\frac{(2\ell-1)!!}{x^{\ell+1}}$$

$a!! = a(a-2)(a-4)\ldots 1$ for a odd

$n_\ell(x)$ blows up as $x \rightarrow 0$ therefore

$U_\ell(r) = A\, r\, j_\ell(kr)$ "Free particle" in 3 dim.

b. condition

$$U_\ell(a) = 0 \Rightarrow \boxed{j_\ell(ka) = 0}$$

$$k = \frac{1}{a}\beta_{n\ell}$$

Where $\beta_{n\ell}$ is n^{th} zero of $j_\ell(x)$

$$E_{n\ell} = \frac{\hbar^2}{2ma^2}\beta^2_{n\ell}$$

In general have to find $\beta_{n\ell}$ numerically

$$\psi_{n\ell m}(r,\theta,\phi) = A_{n\ell}\, j_\ell(\beta_{n\ell} r/a)\, Y_\ell^m(\theta,\phi)$$

In 3 dim. state characterized by 3 quantum #s n, l, m.

The energy only depends on n, l. Thus each ~~state~~ energy level is $(2l+1)$ fold degenerate since m can run from $-l$ to l without changing the energy or the radial wave function.

Note, the radial equation is independent of m so we expect this $2l+1$ fold "m" degeneracy to be a general feature so long as V only depends on r (and not θ, ϕ).

Example $$\psi_{\underset{n\ l\ m}{110}} = A_{11}\, j_1\!\left(\frac{\beta_{11} r}{a}\right) Y_1^0(\theta,\phi)$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

$$u \propto x\, j_1(x) = \frac{\sin x}{x} - \cos x$$

$$\frac{d^2 u}{dr^2} = k^2 \frac{d^2 u}{dx^2} \qquad \text{with } x = kr$$

$$\frac{du}{dx} = \frac{\cos x}{x} - \frac{\sin x}{x^2} + \sin x$$

$$\frac{d^2 U}{dx^2} = -\frac{\sin x}{x} - \frac{\cos x}{x^2} + 2\frac{\sin x}{x^3} - \frac{\cos x}{x^2} + \cos x$$

$$= \sin x\left(\frac{2}{x^3} - \frac{1}{x}\right) + \cos x\left(1 - \frac{2}{x^2}\right)$$

radial eq.

$$\frac{d^2 U}{dr^2} = \left[\frac{l(l+1)}{r^2} - k^2\right] U$$

divide by k^2 $\qquad$ $l = 1$

$$\frac{d^2 U}{dx^2} = \left(\frac{2}{x^2} - 1\right) U \qquad U \propto x\, j_1(x)$$

$$\sin x\left(\frac{2}{x^3} - \frac{1}{x}\right) + \cos x\left(1 - \frac{2}{x^2}\right) \stackrel{?}{=} \left(\frac{2}{x^2} - 1\right) x\left(\frac{\sin x}{x^2} - \frac{\cos x}{x}\right) \checkmark$$