3/2/01

Lec. 22 Radial Equation

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

Angular eq.

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

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

$$Y(\theta,\phi) = A\, P_l^m(\cos\theta)\, e^{im\phi}$$

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

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

Note $P_l^m \propto \left(\frac{d}{dx}\right)^{l+|m|} (x^2-1)^l$

thus $P_l^m = 0$ for $|m| > l$

$\Rightarrow$ $2l+1$ possible m values between $-l, \ldots l-1, l$

$$-l \le m \le l$$

Normalize

$$\int |\psi|^2 d^3r = \int |\psi|^2 r^2\, dr \sin\theta\, d\theta\, d\phi = 1$$

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

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

$$\boxed{Y_l^m(\theta,\phi) = \epsilon \sqrt{\left(\frac{2l+1}{4\pi}\right)\frac{(l-|m|)!}{(l+|m|)!}}\; e^{im\phi}\, P_l^m(\cos\theta)}$$

ϵ = phase = $\begin{cases} (-1)^m & m \geq 0 \\ 1 & m < 0 \end{cases}$

Spherical Harmonics are orthogonal

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

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

$-l \leq m \leq l$

Radial Equation

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

Seperation constant

let $u = r R(r)$ $\quad R = u/r \quad R' = \frac{u'}{r} - \frac{u}{r^2}$

$$\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial R}{\partial r} = \frac{1}{r^2}\frac{\partial}{\partial r}(r u' - u) = \frac{u''}{r}$$

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

$$\psi(r, \theta, \phi) = \frac{u(r)}{r} Y_l^m(\theta, \phi)$$

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

Centrifugal term

$$\int_0^{\infty} |u|^2 \, dr = 1$$

Only one angular wave function for all central pot.

Example $Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$ $\quad l=m=0$

$$\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi \;\frac{1}{\sqrt{4\pi}}\frac{1}{\sqrt{4\pi}} = 1$$

Need to specify radial form of pot.

<u>Example</u> infinite spherical well

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

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

Inside $V=0$

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

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

Solutions spherical Bessel and spherical Neumann functions

$$u(r) = A r\, j_l(kr) + B r\, n_l(kr)$$

$$j_l(x) \equiv (-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \left(\frac{\sin x}{x}\right)$$

$$n_l(x) \equiv -(-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \left(\frac{\cos x}{x}\right)$$

$j_0(x) = \frac{\sin x}{x}$ $\qquad$ $j_1 = -x \frac{1}{x}\frac{d}{dx}\frac{\sin x}{x} = \frac{\sin x}{x^2} - \frac{\cos x}{x}$

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

Note $\frac{\cos x}{x} \to \infty$ as $x \to 0$

but $\frac{\sin x}{x} \to 1$

Therefore $n_\ell(kr)$ is singular as $r \to 0$

chose $B = 0$

$u = Ar\, j_\ell(kr)$

Boundary condition at $r = a$

$u(a) = 0 = j_\ell(ka)$

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

$\beta_{n\ell}$ is n^{th} zero of ℓ^{th} spherical Bessel Function

$$\boxed{E_{n\ell} = \frac{\hbar^2}{2ma^2}\beta_{n\ell}^2}$$ indep. of m

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

$A_{n\ell}$ from normalization

Finite spherical well (Prob. 4.9)

$$V = \begin{cases} 0 & r \geq a \\ -V_0 & r < a \end{cases}$$

Look for $l=0$ solutions (lowest energy)

$$\frac{\partial^2 u}{\partial r^2} = -k^2 u \qquad r < a$$

$$k = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

Looks just like section 2.6 finite square well

outside $r > a$

$$\frac{\partial^2 u}{\partial r^2} = \kappa^2 u \qquad \kappa = \frac{\sqrt{-2mE}}{\hbar}$$

bound state $E < 0$ but $-V_0 < E < 0$

Only difference in 3 dim is b.c. at $r = 0$

$$\psi = \frac{u}{r} Y_{0m}^{0}$$

so $u \to 0$ as $r \to 0$

$$\psi = A \sin kr \qquad r < a$$

$$B e^{-\kappa r} \qquad r > a$$

match ψ and ψ' at $r = a$

$$\frac{\psi'}{\psi} = k \frac{\cos kr}{\sin kr}\bigg|_{r=a} = -\kappa$$

$$k \cot ka = -\kappa$$

In limit of very weakly bound state $E \to 0$ from below.

$$\cot ka \simeq 0 \quad \text{or} \quad ka \doteq \pi/2$$

$$\frac{\hbar^2 k^2}{2m} = E + V_0 \simeq V_0$$

$$V_0 \geq \frac{\hbar^2}{2ma^2}\left(\frac{\pi^2}{4}\right) = \frac{\hbar^2 \pi^2}{8 m a^2}$$

If V_0 is less than this $\Rightarrow$ no bound state in 3 dim.

<u>Example</u> proton + neutron has one bound state deuteron $E \simeq 0$ while pot. for two protons or two neutrons is slightly weaker and di-proton or di-neutron does not ~~b~~ exist.

Not in 1 dim always a bound state for any attractive pot.

If $p+p$ did bind to form ^2He Sun would burn in seconds instead of 10 billion years.