$\boxed{\text{Eigenfunctions of Schroedinger Eqn in an } \infty \text{ 3D spherical well}}$

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

We used separation of variables to get ordinary differential Eqns for $R(r)\,\Theta(\theta)\,\Phi(\phi)$

Φ : $\quad \frac{1}{\Phi} \frac{d^2\Phi}{d\phi^2} = -m^2 \qquad \Phi(\phi) = e^{im\phi} \qquad$ ϕ integer for single-valuedness

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

$$\Theta(\theta) = P_\ell^m(\cos\theta)$$

Together $A P_\ell^m(\theta) e^{im\phi} = Y_{\ell m}(\theta, \phi)$

$$P_\ell^m(x) = (1-x^2)^{|m|/2} \left(\frac{d}{dx}\right)^{|m|} P_\ell(x) \qquad \text{Associated Legendre Functions}$$

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell \qquad \text{Legendre polynomials}$$

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

Note: If we put $\ell(\ell+1)$ on lhs we get an extra term in $V(r)$ of $\hbar^2 \ell(\ell+1)/2mr^2$.

$\ell = |\vec{L}|$ length of ANY vector

This looks rather like our classical $V_{eff}(r) = V(r) + \frac{\ell^2}{2mr^2}$

which suggests $\hbar^2 \ell(\ell+1)$ might be angular momentum.

We have not dealt at all with $R(r)$.

The first step simplifies the radial eqn a bit by defining

$u(r) = r R(r)$ whence

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

Again the extra piece in "V_{eff}" is evident.

For spherical well $V = 0$ for $r < a$

$$\frac{d^2u}{dr^2} = \left[\frac{l(l+1)}{r^2} - k^2\right]u \quad \text{with} \quad \frac{\hbar^2k^2}{2m} \equiv E$$

The $l = 0$ case is simple $\therefore$ $u = A\sin kr + B\cos kr$

Note this means $R = \frac{u}{r} = \frac{A\sin kr + B\cos kr}{r}$

If R well defined at $r=0$ require $B=0$

$R = (A\sin kr)/r$ But $ka = n\pi$ since $R(r=a)=0$

$R = \frac{A}{r}\sin\frac{n\pi r}{a}$ $E_{n0} = \hbar^2\pi^2n^2/a^2 2m$ ← same as 1d?

$l=0$

$Y_{00}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$

$\int_0^\infty |u|^2 dr = \int_0^\infty R^2 r^2 dr = 1$ ← Convention is $R(r)$ and $Y_{lm}(\theta,\phi)$ separately normalized to unity

$u = \sqrt{\frac{2}{a}}\sin kr$

$$\psi_{n00}(r,\theta,\phi) = \sqrt{\frac{2}{a}}\ \frac{1}{r} \sin\frac{n\pi r}{a}\ \frac{1}{\sqrt{4\pi}}$$

$l \neq 0$ The eqn is that of "spherical Bessel functions"

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

Bessel Neumann

Can think of these as sort of like sines and cosines in sense of oscillating + and −, but distance between zeroes is not uniform (π in case of sine and cosine) and also amplitude decreases.] pictures on p 143

$$j_l(x) = (-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\sin x}{x} = 2^n x^l \sum_{s=0}^{\infty} \frac{(-1)^s (s+l)!}{s!\,(2s+2l+1)!}\, x^{2s}$$

$$n_l(x) = -(-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\cos x}{x} = \frac{(-1)^{l+1}}{2^l x^{l+1}} \sum_0^{\infty} \frac{(-1)^s (s-l)!\, x^{2s}}{s!\,(2s-2l)!}$$ as before when we set $l=0$

Examples $\quad j_0(x) = \dfrac{\sin x}{x} \qquad n_0(x) = \dfrac{\cos x}{x}$

$$j_1(x) = -x\,\frac{1}{x}\frac{d}{dx}\,\frac{\sin x}{x} = -\left[\frac{\cos x}{x} - \frac{\sin x}{x^2}\right] = \frac{\sin x - x\cos x}{x^2}$$

$$n_1(x) = -(-x)\,\frac{1}{x}\frac{d}{dx}\,\frac{\cos x}{x} = -\left[\frac{-\sin x}{x} - \frac{\cos x}{x^2}\right] = \frac{\cos x + x\sin x}{x^2}$$

Notice as $x \to 0$ $\quad j_0(x) \to 1$

$$j_1(x) \approx \frac{x - x^3/6 - x(1 - x^2/2)}{x^2} = \frac{x}{3}$$

But as $x \to 0$ $\quad n_0(x) \to 1/x$

$$n_1(x) \to 1/x^2$$

So j_l finite @ $x=0$ and n_l blow up @ $x=0$.

For the 3D spherical well, the conversions $R \to u$ and $u \to j$ undo each other

$$R(r) = u(r)/r \qquad u(r) = A r j_\ell(kr)$$

so that $R(r) = A j_\ell(kr)$, so the definition $R \equiv u/r$ seems unnecessary. In general, however, it __is__ useful.

We already considered the case $\ell = 0$ and saw $R = \frac{\sin kr}{kr}$ gave correct soln of radial eqn.

Let's also do $\ell = 1$ just for fun... Griffiths problem 4-8

$$\frac{d^2}{dr^2} u(r) \Rightarrow \frac{d^2}{dr^2} r j_1(kr) = \frac{d^2}{dr^2}\left(\frac{\sin kr - kr\cos kr}{k^2 r}\right)$$

$$= \frac{d}{dr}\left(\frac{k\cos kr - k\cos kr + \cancel{k^2 r\sin kr} + k^2 r \sin kr}{k^2 r} - \frac{\sin kr - kr\cos kr}{k^2 r^2}\right)$$

$$= \frac{d}{dr}\left(\frac{k^2 r^2 \sin kr - \sin kr + kr\cos kr}{k^2 r^2}\right)$$

Ⓐ 2 ✓ ✓ term Ⓐ

$$= \frac{2k^2 r\sin kr + k^3 r^2 \cos kr - k\cos kr + k\cos kr - k^2 r \sin kr}{k^2 r^2}$$

$$- 2\frac{1}{k^2 r^3}\left(k^2 r^2 \sin kr - \sin kr + kr\cos kr\right)$$

$$= \frac{1}{k^2 r^3}\left\{ \begin{array}{l} 3k^2 r^2 \sin kr + k^3 r^3 \cos kr - \\ -2k^2 r^2 \sin kr \qquad + 2\sin kr - 2kr\cos kr \end{array}\right\}$$

$$= \frac{1}{k^2 r^3}\left[\left\{-k^2 r^2 + 2\right\}\sin kr + \left\{k^2 r^2 - 2\right\} kr\cos kr\right]$$

$$= \frac{1}{k^3 r^3}\left(2 - k^2 r^2\right)\left(\sin kr - kr\cos kr\right) = \left(\frac{2}{r^2} - k^2\right)\frac{\sin kr - kr\cos kr}{k^2 r}$$

$$\left(\ell(\ell+1)/r^2 - k^2\right) \qquad u_1(r) \quad ✓$$

Require also $R(r=a)=0$ since $V \to \infty$ there.

In $\ell=0$ case since $R = j_0(kr) = \frac{\sin kr}{kr}$

We needed $\sin ka = 0$ or $k_n = n\pi/a$.

In $\ell \neq 0$ case, one needs $j_\ell(ka)=0$. If we denote by $\beta_{n\ell}$ the values where $j_\ell(\beta_{n\ell})=0$ then k is discretized to $k_{n\ell} = \beta_{n\ell}/a$ and the energy levels are

$$E_{n\ell} = \frac{\hbar^2}{2ma^2}\beta_{n\ell}^2$$ ← indep of m but not ℓ

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

<u>Numerical HW problem</u> ??

Code up Newton's method to find roots.

Then use it for roots of j_1, first spherical Bessel function

Try out before assigning

Vibrating string

Vibrating drumhead ...