Solving the 3-d Schrödinger Equation

Certain problems look like 3 1-d solutions multiplied together:

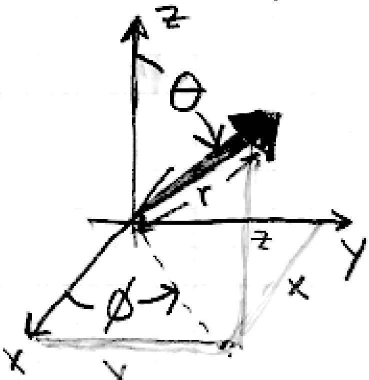
1) 3-d square well
2) 3-d simple harmonic oscillator.

Many important problems involve motion in a spherically symmetric potentials.

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

3-d vector magnitude $\equiv r$

For these problems it is natural to use spherical polar coordinates:



$$r = \sqrt{x^2+y^2+z^2} \qquad z = r\cos\theta$$

$$\cos\theta = \frac{z}{r} \qquad y = r\sin\theta\sin\phi$$

$$\tan\phi = \frac{y}{x} \qquad x = r\sin\theta\cos\phi$$

To find the energy eigenstates of the Hamiltonian

$$\underset{\sim}{H}|\Psi\rangle = E|\Psi\rangle$$

μ = mass $$\left(\frac{\vec{P}^2}{2\mu} + V(\underset{\sim}{\vec{x}})\right)|\Psi\rangle = E|\Psi\rangle$$

represent this in co-ordinate space:

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{x})\right)\Psi(\vec{x}) = E\Psi(\vec{x})$$

rectilinear: $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$; $dV = dx\,dy\,dz$

spherical polar: $V(\vec{x}) \to V(r)$ assume spherical symmetry.

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

why so complicated? Because the volume element $dV = r^2 \sin\theta \, dr\, d\theta\, d\phi$, not simply $dr\,d\theta\,d\phi$. In other words, the Jacobian.

The θ, ϕ dependence looks ferocious. When $V(r)$ is independent of $\theta + \phi$, however, there is a significant simplification...

$$-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \doteq \underset{\sim}{L}^2$$

its representation

orbital angular momentum operator

Do I have a proof? Your text just says it on page 335, 12.5.36. The real proof is not much fun.. I will skip it, and review the solution to the eigenvalue problem for $\underset{\sim}{L}^2$ alone.

abstract	coordinate space
$\underset{\sim}{L}^2 \lvert l\, m\rangle = l(l+1)\hbar^2 \lvert l\, m\rangle$ $l = 0, 1, 2, \ldots \infty$	$-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] Y_l^m(\theta,\phi) = l(l+1)\hbar^2 Y_l^m(\theta,\phi)$

there are $2l+1$ degenerate states, enumerated by there eigenvalue of $\underset{\sim}{L}_z$:

$\underset{\sim}{L}_z \lvert l m\rangle = m\hbar \lvert l m\rangle$ $-l \le m \le l$	$-i\hbar\frac{\partial}{\partial\phi} Y_l^m = m\hbar Y_l^m$

The $Y_\ell^m(\theta,\phi)$ are fundamental functions for describing angular distributions. They are used throughout physics.

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12.5.39

$\ell=0$ $(m=0)$ $\quad Y_0^0 = 1/\sqrt{4\pi}$

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

$m=\pm1$ $\quad Y_1^{\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$

$\ell=2$ $m=0$ $\quad Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1)$

$m=\pm1$ $\quad Y_2^{\pm1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}$

$m=\pm2$ $\quad Y_2^{\pm2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}$

Qualitative Points:
- $e^{\pm im\phi}$
- power of $\sin^x\theta\cos^y\theta$ satisfies $x+y=\ell$

Orthonormal: $\int d\Omega\, Y_{\ell'}^{m'*}(\theta,\phi)\, Y_\ell^m(\theta,\phi) = \delta_{\ell'\ell}\,\delta_{m'm}$

Complete: $f(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} C_\ell^m\, Y_\ell^m(\theta,\phi)$

Use orthonormality: $\int d\Omega\, f(\theta,\phi)\, Y_{\ell'}^{*m'}(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} C_\ell^m \underbrace{\int d\Omega\, Y_{\ell'}^{m*}\, Y_\ell^m}_{\delta_{\ell'\ell}\,\delta_{m'm}}$

so $\quad C_{\ell'}^{m'} = \int d\Omega\, f(\theta,\phi)\, Y_{\ell'}^{*m'}(\theta,\phi)$

in other words

$$f(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\int d\Omega' f(\theta',\phi') Y_{l'}^{m'*}(\theta',\phi')\right\} Y_l^m(\theta,\phi)$$

rearrange this:

$$f(\theta,\phi) = \int d\Omega' \underbrace{\left[\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{l'}^{m'*}(\theta',\phi') Y_l^m(\theta,\phi)\right]}_{\text{must be a } \delta\text{-function!}} f(\theta',\phi')$$

$$d(\cos\theta)\,d\phi \qquad \delta(\cos\theta' - \cos\theta)\,\delta(\phi'-\phi)$$

$$\boxed{\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{l'}^{m'*}(\theta',\phi') Y_l^m(\theta,\phi) = \delta(\cos\theta'-\cos\theta)\,\delta(\phi'-\phi) \quad \text{means } \boxed{\text{completeness}}}$$

<u>Parity</u>: $\underset{\sim}{\Pi}\, Y_l^m = (-1)^l\, Y_l^m$

Back to solving the Schrödinger Equation.

let $\quad \psi(\vec{x}) = R_{Elm}(r)\, Y_l^m(\theta,\phi) \quad$ (try)

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

ignores Y_l^m ignores R_{Elm}, Y_l^m is eigenfunction

$$= Y_l^m(\theta,\phi)\left\{\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right\} R_{Elm}(r)$$

the whole Schrödinger equation is then

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right)\psi(\vec{x}) = E\psi(\vec{x})$$

$$Y_l^m(\theta,\phi)\left(\frac{\hbar^2}{2\mu}\left[-\frac{1}{r^2}\frac{\partial}{\partial r} r^2\frac{\partial}{\partial r} + \frac{l(l+1)}{r^2}\right] + V(r)\right) R_{Elm}(r) = E R_{Elm}(r)\, Y_l^m(\theta,\phi)$$

→ $Y_\ell^m(\theta,\phi)$ cancels out

→ $\ell(\ell+1)$ now in the radial equation, but m is not: $R_{E\ell m}(r) \rightarrow R_{E\ell}(r)$

We arrive at the

RADIAL EQUATION

$$\boxed{\left(\frac{\hbar^2}{2\mu}\left[-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{\ell(\ell+1)}{r^2}\right]+V(r)\right)R_{E\ell}(r)=ER_{E\ell}(r)}$$

p.340 (12.6.3)

this is beginning to resemble the 1-d Schrödinger; the most glaring difference is the complicated radial derivative. This can be simplified by expressing $R_{E\ell}(r)$ as a product of:

$$R_{E\ell}(r)=\frac{U_{E\ell}(r)}{r}, \quad U_{E\ell}(r)=rR_{E\ell}(r)$$

so $$\frac{\partial R_{E\ell}(r)}{\partial r}=-\frac{U_{E\ell}(r)}{r^2}+\frac{1}{r}\frac{\partial U_{E\ell}(r)}{\partial r}$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R_{E\ell}(r)}{\partial r}\right)=\frac{\partial}{\partial r}\left(-U_{E\ell}(r)+r\frac{\partial U_{E\ell}(r)}{\partial r}\right)$$

$$=\cancel{-\frac{\partial U_{E\ell}(r)}{\partial r}}+\cancel{\frac{\partial U_{E\ell}(r)}{\partial r}}+r\frac{\partial^2 U_{E\ell}(r)}{\partial r^2}$$

$$\therefore -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R_{E\ell}(r)}{\partial r}\right)=\frac{1}{r}\frac{\partial^2 U_{E\ell}(r)}{\partial r^2}=\frac{1}{r}\frac{d^2U_{E\ell}(r)}{dr^2}$$

since $U_{E\ell}(r)$ depends only on r.

substituting:

$$\left(\frac{\hbar^2}{2\mu}\cancel{\frac{1}{r}}\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}\right]+V(r)\right)U_{E\ell}(r)=E\frac{U_{E\ell}(r)}{\cancel{r}}$$