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 = \( r \)

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

\[ r = \sqrt{x^2 + y^2 + z^2} \]
\[ z = r \cos \theta \]
\[ \cos \theta = \frac{z}{r} \]
\[ \frac{\tan \phi}{x} = \frac{y}{r} \]
\[ x = r \sin \theta \cos \phi \]

To find the energy eigenstates of the Hamiltonian

\[ \hat{H} |\psi\rangle = E |\psi\rangle \]

\( \chi = \text{mass} \left( \frac{\hat{r}^2}{2\mu} + V(\vec{x}) \right) |\psi\rangle = E |\psi\rangle \)

represent this in coordinate space:

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

rectilinear:
\[ \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \]

\[ dV = \lambda dx dy dz \]
spherical polar: \( V(x) \rightarrow V(r) \) 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 \( dr \, d\theta \). In other words, the Jacobian.

The \( \Theta, \Phi \) dependence looks ferocious. When \( V(r) \) is independent of \( \Theta + \Phi \), however, there is a significant simplification...

\[
-\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \equiv \frac{l^2}{r}
\]

orbital angular momentum operator

\( \uparrow \rightarrow \) its representation

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 \( L^2 \) alone.

abstract

\[
L^2 |lm\rangle = (l(l+1)\hbar^2 |lm\rangle
\]

\( l = 0, 1, 2, \ldots \infty \)

coordinate space

\[
-\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y^m_l(\Theta, \Phi) = (l(l+1)\hbar^2) Y^m_l(\Theta, \Phi)
\]

- there are \( 2l+1 \) degenerate states, enumerated by the eigenvalue of \( L^2 \):

\[
L^2 |lm\rangle = m \hbar |lm\rangle
\]

\(-l \leq m \leq l \)
The $Y^m_l(\theta, \phi)$ are fundamental functions for describing angular distributions. They are used throughout physics.

\[
\begin{align*}
  l = 0 \quad (m = 0) & \quad Y^0_0 = \frac{1}{\sqrt{4\pi}} \\
  l = 1 \quad m = 0 & \quad Y^0_1 = \sqrt{\frac{3}{4\pi}} \cos \theta \\
  m = \pm 1 & \quad Y^1_1 = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi} \\
  l = 2 \quad m = 0 & \quad Y^0_2 = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1) \\
  m = \pm 1 & \quad Y^1_2 = \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\phi} \\
  m = \pm 2 & \quad Y^2_2 = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi}
\end{align*}
\]

**Qualitative Points:**

- $e^{\pm i\phi}$
- Power of $\sin^2 \theta \cos^2 \theta$ satisfies $x + y = l$

**Orthonormal:**

\[
\int d\Omega \, Y^m_1(\theta, \phi) Y^{\ast m}_1(\theta, \phi) = \delta_{e e'} \delta_{mm'}
\]

**Complete:**

\[
f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c^m_l Y^m_l(\theta, \phi)
\]

**Use orthonormality:**

\[
\int d\Omega f(\theta, \phi) Y^{\ast m'}_{l'}(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c^m_l \int d\Omega Y^m_l(\theta, \phi) Y^{\ast m'}_{l'}(\theta, \phi) \delta_{e e'} \delta_{m m'}
\]

so

\[
c^m_{l'} = \int d\Omega f(\theta, \phi) Y^{\ast m'}_{l'}(\theta, \phi)
\]
in other words
\[ f(\theta', \phi') = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \{ \delta_{l,l'} \delta_{m,m'} Y_{le}^m(\theta, \phi) \} Y_{le}^m(\theta, \phi) \]

rearrange this:
\[ f(\theta', \phi') = \int d\omega \left[ \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{le}^m(\theta, \phi) \delta_{l,l'} \delta_{m,m'} Y_{le}^m(\theta, \phi) \right] f(\theta', \phi') \]

must be a \( \delta \)-function!
\[ \delta(\cos \theta - \cos \theta') \delta(\phi - \phi') \]

means \textbf{completeness}

\[ \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{le}^m(\theta', \phi') Y_{le}^m(\theta, \phi) = \delta(\cos \theta - \cos \theta') \delta(\phi - \phi') \]

Parity: \( \Pi Y_{le}^m = (-1)^l Y_{le}^m \)

Back to solving the Schrödinger Equation.

let \( \Psi(x) = R_{Elm}(r) Y_{le}^m(\theta, \phi) \) (try)

then \( \nabla^2 \Psi(x) = \left\{ \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial}{\partial r} \right] + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial}{\partial \theta} \right] + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right\} \Psi(x) \)

ignores \( Y_{le}^m \)

\( Y_{le}^m \) is eigenfunction

\[ \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \{ \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial}{\partial r} \right] - \frac{l(l+1)}{r^2} \} R_{Elm}(r) \]

The whole Schrödinger equation is then
\[ \left( -\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right) \Psi(x) = E \Psi(x) \]

\[ Y_{le}^m(\theta, \phi) \left( \frac{\hbar^2}{2\mu} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial}{\partial r} \right] + \frac{l(l+1)}{r^2} \right] + V(r) \right) R_{Elm}(r) = E R_{Elm}(r) Y_{le}^m(\theta, \phi) \]
\[ y_\ell^m(\theta, \phi) \text{ cancels out} \]

\[ l(l+1) \text{ now in the radial equation, but } m \text{ is not: } R_{E\ell m}(r) \rightarrow R_{E\ell}(r) \]

We arrive at the RADIAL EQUATION

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

p. 240 (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:

\[ R_{E\ell}(r) = \frac{U_{E\ell}(r)}{r}, \quad U_{E\ell}(r) = r R_{E\ell}(r) \]

so

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

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

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

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

Since \( U_{E\ell}(r) \) depends only on \( r \),

\[
\left( \frac{\hbar^2}{2\mu} \frac{1}{r} \left[ -\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{r^2} \right] + V(r) \right) U_{E\ell}(r) = E \frac{U_{E\ell}(r)}{r}
\]