3D Quantum Mechanics

- 3D States + Schrödinger Equation

We've looked at this a little before

- States are a "tensor product" of 1D states, or at least states for different "parts" of the state. How to build a basis for Hilbert space in 3D using 1D physics
  - For example + $|\vec{x}\rangle$ the 3D position eigenstate

$$|\vec{x}\rangle = |x\rangle|y\rangle|z\rangle = (x \text{ eigenstate})(y\text{-eigenstate})(z \text{ eigenstate})$$

$$\hat{x}|\vec{x}\rangle = x|\vec{x}\rangle, \quad \hat{y}|\vec{x}\rangle = y|\vec{x}\rangle, \quad \hat{z}|\vec{x}\rangle = z|\vec{x}\rangle$$

Or + Momentum eigenstate

$$|\vec{p}\rangle = |p_x\rangle|p_y\rangle|p_z\rangle \leftarrow \text{you see the factorization}$$

with $\langle\vec{x}|\vec{p}\rangle = \langle x|p_x\rangle\langle y|p_y\rangle\langle z|p_z\rangle = \dfrac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{x}/\hbar}$

+ As you see, the wavefunction becomes a product too

- Energy eigenstates can be degenerate (which is not possible in 1D): More than one can have same energy eigenvalue
  + Will need more than one "quantum number" to distinguish states
  + These are eigenvalues of operators that commute with H
- We will soon see an alternate decomposition (radial)(angular) in position + momentum space

- The Hamiltonian in spherical coordinates
  - Recall that $\vec{p} = -i\hbar\vec{\nabla}$ so (in the position basis)

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})$$

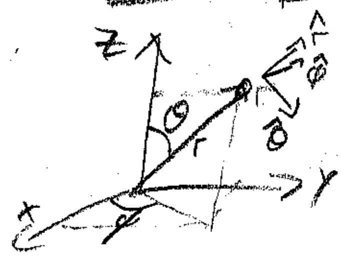
+ In Cartesian coordinates

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

+ In some cases we can use separation of variables into split the wavefunction $\psi(\vec{x}) = X(x)\, Y(y)\, Z(z)$

- Often, the potential is central $V(\vec{x}) = V(r)$
  Then it is usually convenient to use spherical polar coordinates

+ $r = \sqrt{x^2+y^2+z^2}$ | $z = r\cos\theta$
  $\cos\theta = z/r$ | $x = r\sin\theta\cos\phi$
  $\tan\phi = y/x$ | $y = r\sin\theta\sin\phi$



$d^3\vec{x} = r^2\sin\theta\, d\theta\, d\phi$

+ The Laplacian becomes

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

+ Now separate variables $\psi = R(r)Y(\theta,\phi)$

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

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

A priori, l can be any number. We will see later it is a non-negative integer

+ Normalization:
  If $Y(\theta,\phi)$ is nonsingular, we can normalize it separately b/c it is a function on a finite space (θ,ϕ make a sphere)
  So normalization requires

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta\, |Y|^2 = 1, \quad \int_0^{\infty} dr\, r^2 |R|^2 = 1$$

— The Radial Equation + Behavior

- Normalization is a bit simpler for the function

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

$$\int_0^{\infty} dr\, |u|^2 = 1 \quad \text{Almost 1D}$$

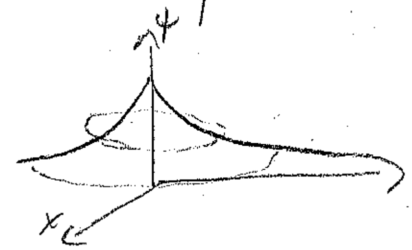
- Let's try u in the radial equation.
  + $R = \frac{u}{r}$, $\frac{dR}{dr} = \frac{1}{r^2}\left(r\frac{du}{dr} - u\right)$, $\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = r\frac{d^2u}{dr^2} + \left(\frac{du}{dr} - \frac{du}{dr}\right)$
  + The radial equation is

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

  + This looks like 1D Schrödinger with an <u>effective potential</u> including a <u>centrifugal term</u>
- Near the origin $(r \to 0)$, the centrifugal term often dominates.
  + Then $\frac{d^2u}{dr^2} \simeq \frac{l(l+1)}{r^2} \Rightarrow u \simeq A r^{l+1} + B r^{-l}$
  + Only the r^{l+1} term is normalizable. We'll use this later
- Example: Infinite Spherical Well

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

  + boundary conditions: $R(a) = 0$ from the infinite potential
    At the origin, we need $dR/dr = 0$ to keep the wavefunction smooth
    Consider the 2D example. If $dR/dr \neq 0$, the wavefunction has a kink (discontinuity in $d\psi/dx$ and $d\psi/dy$). And it must be normalizable.



  + Inside, $d^2u/dr^2 = \left[\frac{l(l+1)}{r^2} - k^2\right]u$, $k = \sqrt{2mE}/\hbar$
    For $l=0$, $u = A\sin(kr) + B\cos(kr)$. For $R = u/r$, need $B = 0$
    then $ka = n\pi \Rightarrow E_{n,0} = \frac{\pi^2\hbar^2 n^2}{2ma^2}$
  + The general solution for $l \neq 0$ is $R_l(r) = A j_l(kr) + B n_l(kr)$
    j_l and n_l are <u>spherical Bessel functions</u> (see text)
    The n_l functions are not normalizable near the origin.
    Energies determined by $j_l(ka) = 0$