

• 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

• For example + $|\vec{x}\rangle$ the 3D position eigenstate

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

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

Or + momentum eigenstate

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

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

+ 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

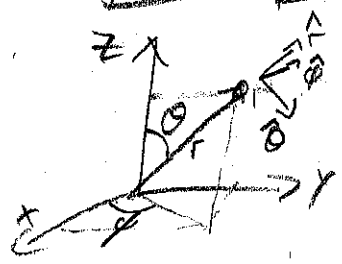
$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

+ In some cases we can use separation of variables,
w/o 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

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



$d^3x = r^2 \sin \theta dr d\theta d\phi$

+ The Laplacian becomes

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

+ Nonseparate 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.

+ $R = \frac{u}{r}$, $\frac{dR}{dr} = \frac{1}{r^2}(r \frac{du}{dr} - u)$, $\frac{d}{dr}(r^2 \frac{dR}{dr}) = r \frac{d^2u}{dr^2} + (\frac{du}{dr} - \frac{du}{dr})$

+ 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 effective potential including a centrifugal term

• Near the origin ($r \rightarrow 0$), the centrifugal term often dominates.

+ Then $\frac{d^2u}{dr^2} \approx \frac{l(l+1)}{r^2} \Rightarrow u \approx A r^{l+1} + B r^{-l}$

+ Only the r^{l+1} term is normalizable. We'll use this later.

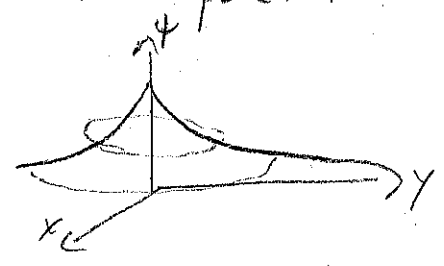
• Example: Infinite Spherical Well

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

+ 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 $d\psi/dr \neq 0$, the wavefunction has a kink



(discontinuity in $d\psi/dx$ and $d\psi/dy$). And it must be normalizable.

+ Inside, $\frac{d^2u}{dr^2} = \left[\frac{l(l+1)}{r^2} - k^2 \right] u$, $k = \sqrt{2mE}/\hbar$

For $l=0$, $u = A \sin(kr) + B \cos(kr)$. For $R = u/r$, need $B=0$

then $ka = n\pi \Rightarrow E_{n,0} = \frac{\hbar^2 k^2}{2ma^2} = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$

+ 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 spherical Bessel functions (see text)
 The n_l functions are not normalizable near the origin.
 Energies determined by $j_l(ka) = 0$