412-1, Week 1, Day 1

- Welcome
- QM is one reason I pursued physics
- QM is what I do

Logistics

- Syllabus
  - Book + notes posted
  - Problem sets due ~~Mondays~~ ~~Thursdays~~ Tuesdays, here @ 9:30 or in grader box
  - P.S. #1 posted today. Math: get comfortable so you can enjoy this strange new world.
  - ~~Foundations, 1D potentials, symmetries~~
- Grading: 50% problem sets, 50% final
- Anyone not see Dirac notation $\psi(x,y,z,t) \Leftrightarrow |\psi\rangle$?
- This quarter: ① Wavefunctions + wavepackets (Intuition)/(Mostly quick review) ② Formal structure ③ Symmetries ④ Angular momentum

Intro - the back story

- Greeks recognized math surprisingly effective
- Galileo + Newton built up framework to describe particles
- Abstract points moving in invariable space + time, as described by simple diff. eqs.

- This formulation very powerful

- But also, it turned out very primitive.
- "Primitive" here not "fundamental" - but rather like primates
- Describes how monkeys can jump from tree to tree to get food.
- But for outside of dynamic range of monkeys' experience, there are problems

- 20th century physics is dominated by 2 ways this turned out to be important
  a) Einstein: space + time bound together in single
  not completely distinct +
  ~~framework~~ structure with unfamiliar geometry +
  this geometry gets curves by presence of mass
  b) 2nd revolution arguably more profound
    a) Very notion of point particle on trajectory no longer makes sense on atomic scale
    b) Once ~~these~~ understood - we realized that mysteries of atoms, solids, + radiation suddenly became unlocked

Wave - particle duality

- ~~Waves discovered that~~ Scatter e^- off surface.
- They arrive @ detector, e.g. scintillating film, in clicks. Of course - "particles" w/ well defined mass + ~~position~~ charge.
- But pattern of flashes is that of wave diffraction
- Somehow e^- either ① ~~spreads~~ is either out over surface as it hits, or ② the particle location is guided by a wave to final destination.
- Conversely, light, with macroscopic wave character, when $I\downarrow$, detected by PMT ~~as~~ in discrete elements
- Alternatively, 2-slit or 2 sources. Makes sense for light at high intensity. But Aspect experiment - turn 2 laser ~~do~~ powers down. Interp: each photon goes ~~...~~ Photon comes from both lasers interferes with itself here, not with other photons.

DeBroglie → Schr.

- In thesis, deBr. proposed that all objects with $E + p$ are simult. part. + waves
- Waves somehow guide particles + reflect particle properties
- Specifically, $\lambda + f(t)$ relate to $p + E$

Canonical wave:

when wave amp is measureable, directly like $\vec{E}$ $\Rightarrow$ $Re\left[e^{-i\omega t} e^{ikx}\right]$ or $e^{-i\omega t} e^{i\vec{k}\cdot\vec{x}}$ in 3D

or just $e^{-i\omega t} e^{ikx}$ (Allows much simpler QM formulation)

$\omega = \frac{2\pi}{T}$ is freq

$k = \frac{2\pi}{\lambda}$ is wave number

DeBr relations:

$k = P/\hbar$

$\omega = E/\hbar$, $\hbar = h/2\pi$ ← New constant of nature,

~~units of~~

in SI: $h = 6.6 \times 10^{-34}\, J \cdot s$

- It is obvious how deBr matter waves might address problems like how e^- ~~scatter~~ end up diffracting off of periodic potentials.

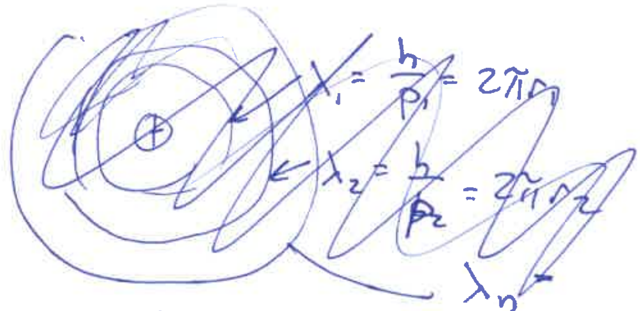
- But another mystery of early 20th century was discrete spectra.
  why does radiation from atoms comes at discrete freq,
  with
  $\Delta E = \hbar\omega$ (or $\Delta E = h\nu$) ?

~~Conservation of energy tells~~ (If $E_\gamma = \hbar\omega$) $\Rightarrow$

- Particles of light evidently come out at definite energies corresponding to definite atomic ΔE (by cons. of energy)

- Why would that be?

- deBr showed in 1924 that he could reproduce levels of Bohr atom by insisting e^- only occupied whole # wavelength orbits



- But ~~not~~ wave eqn, no predictive power for other bound systems, other inconsistencies.
- Laughlin anecdote (over Christmas vacation)
- In 1925-26, Schr found his wave eqn.
- Not first. Heisenberg "matrix mechanics" contained some physics, but Schr couldn't understand.
- Schr ~~picture~~ mechanics is concrete & pictorial & has become favorite conceptual framework

Schr eqn

- He tried to write a wave eq which would lead to

deBr ~~de~~ wave deR Exp with $\to e^{-i\omega t} e^{i\vec{k}\cdot\vec{x}}$ (cannot derive Schr from deBr, but can go in reverse)

$$E = \hbar\omega = i\hbar\frac{\partial}{\partial t}$$, since $i\hbar\frac{\partial}{\partial t}e^{-i\omega t} = (i\hbar)(-i\omega)e^{-i\omega t} = \hbar\omega e^{-i\omega t}$

energy operator. Acting on ~~state~~ fn of def. energy returns $E * fn$

Similarly $p_x = -i\hbar\frac{\partial}{\partial x}$

$+$

$$\vec{p} = \hbar\vec{k} = -i\hbar\frac{\partial}{\partial\vec{x}} = -i\hbar\vec{\nabla}$$ ~~where~~ $\cancel{\frac{\partial}{\partial\vec{x}} = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z}}$

Then

$$E = \frac{p^2}{2m} + V(x)$$

$\Downarrow$

$$\left(i\hbar\frac{\partial}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)$$ acting on wave

Two dif ways of extracting E from wave

Energy = energy. Also applies when state doesn't have definite E

Call wave $\psi(\vec{x},t)$, schr. w.f.

whatever it is. we know it's like deBr waves, but still fuzzy. That's fine - Already, some things will clearly work.

$\Downarrow$

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t) = \frac{-\hbar^2}{2m}\nabla^2\psi(\vec{x},t) + V(x)\,\psi(\vec{x},t)}$$

- We have ~~so~~ guessed at it in free space, where deBr also worked pretty well.

- But let's see if Schr. takes us further than deBr could when imagining bound systems.
- will work in 1D
- Particle in a box

$$V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{outside this interval} \end{cases}$$

- Specify $\psi(x,t) = 0$ outside box, which makes $V(x)\psi(x)$ smooth. (will discuss more later)
- Schr is 2nd order in $x \Rightarrow 2$ b.c.'s required to ~~find unique~~ ~~soln.~~ — ~~2 Done~~. specify a unique solution. Done.

- 1st-order in time $\Rightarrow 1$ b.c. needed

$$\psi(x, t=0) = \psi_0(x)$$

- With these 3 B.C.s we can specify unique ψ for all x,t
- Can "integrate forward" in time, to find unique soln. ~~&~~ space arising from ~~these~~ those I.C. / B.C.

- Let's find most general soln.

- Not obvious now ~~the~~ it will work, but let's first try periodic in time : $\psi(x,t) = \varphi_E(x)e^{-i\omega t}$

– Which needs to correspond to deBr's

$E = \hbar\omega$ (Energy we get by extracting info from time part must match what we get from spatial part)

– Inserting into Schr, we find "time-ind." Schr:

$$\underbrace{\hbar\omega}_{E}\, \varphi(x)\cancel{e^{-i\omega t}} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi_E(x)\cancel{e^{-i\omega t}}$$

– Easy to solve. Rewrite as familiar wave eqn w/ wavenumber k:

$$\frac{\partial^2}{\partial x^2}\varphi_E(x) + k^2\varphi_E(x) = 0$$

(since $E = \frac{p^2}{2m}$ for $V=0$)

where $k^2 = \frac{2mE}{\hbar^2} = \frac{p^2}{\hbar^2}$

which once again, like in free space, corresponds to deBr's $k = p/\hbar$

~~Reason we have simple correspondence where $E=\frac{p^2}{2m}$ is that potential is flat. Of course~~

– Soln's to that are $\sin(kx)$ & $\cos(kx)$

~~Much like in~~

meets bc's for $\left\{ k = \frac{2\pi}{\lambda},\ \frac{n\lambda}{2} = a \right.$

Set $\varphi_E(x) = \left\{ \sin\left(\frac{\pi n}{a}x\right) \right\}$ $n = 1,2,3\ldots$

Corresponding def energies are

$$E_n = \frac{p_n^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi n}{a}\right)^2$$

Teaser: What is p_n? Positive or negative? Both? Well-defined momentum going both ways at once? (No)

Success 1

Quantized! ← wave eqn for matter leads here

+ Schr also matches deBr expr.

(Note: quantization we get from Schr. is robust. DeBroglie quant. of Bohr atom was rather ad hoc & limited in predictive power)

Success 2

- Note that $E_1 > 0$.
- Zero-point energy

$$E_1 \propto \frac{1}{a^2}$$

- Box smaller ⇒ lowest energy state ↑
- This is in fact ultimate explanation for chemical bond. Bring 2 atoms together & let e^- spread out & range over both nuclei

is making box bigger ⇒ $E\downarrow$ ⇒ chemical bond

So without specifying exactly what ψ means, we already see that Schr qualitatively predicts some features of matter we were at a loss to explain before

Back to math

Soln's are of form

$$\sin\left(\frac{\pi n}{a}x\right)e^{-i\omega_n t} \qquad \text{where} \quad \hbar\omega_n = \frac{\hbar^2}{2m}\left(\frac{\pi n}{a}\right)^2$$

Since Schr eqn is linear

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{\pi n}{a}x\right)e^{-i\omega_n t} \quad , \; c_n \text{ arb compl \#s}$$

is also a soln.

In fact, this represents most general soln

For that to be true, (plugging in $t=0$)

$$\Psi_0(x) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{\pi n}{a}x\right) \quad \text{must}$$

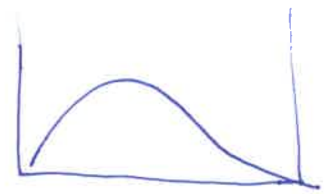
represent most general I.C. (~~Note~~ Recall that specifying that $\Psi_0(x)$ allows us to $\int$ up to ~~unique~~ $\Psi(x,t)$ arising from there)

– Statement that $\Psi_0(x)$ is indeed completely general is statement of Fourier's theorem: any fn on $x=(-a,a)$ can be approx'd by series of this fn's on that interval

Motion

Math + P.S. 1 : Get comfortable so you can enjoy this strange new world.

How does a particle move?

Consider starting from $\psi(t=0) =$ 

$$\psi(t=0) \approx \sin\frac{\pi x}{a} + \frac{1}{2}\sin\frac{2\pi x}{a}$$

$$i\hbar\frac{\partial}{\partial t}\psi \neq E\psi \quad \text{, but} \quad i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + \underset{\downarrow \atop 0}{V\psi} \neq E\psi$$

for all x, t

$$\Rightarrow \psi(x,t) = \sin\frac{\pi x}{a}\, e^{-\frac{i\hbar}{2m}\left(\frac{\pi}{a}\right)^2 t} + \frac{1}{2}\sin\frac{2\pi x}{a}\, e^{-\frac{i\hbar}{2m}\left(\frac{2\pi}{a}\right)^2 t}$$

Phase of 2nd term winds 4x faster than 1st

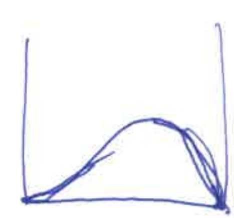
In a time given by t_π

$$\Delta\phi = \Delta\omega\, t_\pi = \pi$$

(phase difference is π at this time)

$$= \frac{\hbar}{2m}\left(\frac{\pi}{a}\right)\cdot 3 \cdot t_\pi$$

$$\psi(t=t_\pi) = \begin{pmatrix}\text{phase}\\ \text{factor}\end{pmatrix}\cdot\left(\sin\frac{\pi x}{a} - \frac{1}{2}\sin\frac{2\pi x}{a}\right)$$



B

- Tempting to say particle has moved to RHS

- But what exactly is relation between ψ & particle position?

- We can get a clue by considering Sch. properties

In 1D

$$i\hbar \frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi \Leftrightarrow -i\hbar\frac{\partial}{\partial t}\psi^* = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi^* + V(x)\psi^*$$

Let's compute $\left(|\psi(x)|^2 = \psi^*\psi \right)$

$$\frac{\partial}{\partial t}\int dx\, |\psi(x)|^2 = \int dx \left\{ \left(\frac{\partial}{\partial t}\psi^*\right)\psi + \psi^*\left(\frac{\partial}{\partial t}\psi\right)\right\}$$

$$= \int dx \left\{ \frac{1}{-i\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi^* + V(x)\psi^*\right]\psi + \frac{\psi^*}{i\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi\right]\right\}$$

$$= \int dx \left\{\left(\frac{-i\hbar}{2m}\right)\left[\left(\frac{\partial^2}{\partial x^2}\psi^*\right)\psi - \psi^*\left(\frac{\partial^2}{\partial x^2}\psi\right)\right]\right.$$

$\int u\,dv = \overset{0}{uv|} - \int v\,du$

If ~~uv~~ ~~boundary~~

$\Downarrow$

$\Rightarrow \int u \frac{dv}{dx}dx = -\int v \frac{du}{dx} dx$

$\int u\,dv = uv\Big| - \int v\,du$

we ~~can~~ have a way to ~~slide~~ get that derivative over ~~~~ to operate on ψ & ~~the ψ^*~~ & make ~~it~~ 1st term look like 2nd term.

- Boundary term is 0 b/c $\psi = 0$ at $x = 0, a$
- Pick up one ~~2~~ minus sign for each $\frac{d}{dx}$

$\int \psi \frac{\partial}{\partial x}\psi^* dx$

$= -\int \psi^* \frac{\partial}{\partial x}\psi\, dx$

$$\Rightarrow \frac{\partial}{\partial t}\int dx\, |\psi(x)|^2 = 0$$

Convenient to work w/ normalized wave fns s.t. $\int dx\, |\psi_0(x)|^2 = 1$

$\Rightarrow$ $\int dx\, |\psi(x,t)|^2 = 1$ for all time.

This is an invariant in time.

$\Rightarrow$ Particle moves, but this

$\Rightarrow$ Suggests interpretation that $|\psi(x)|^2 dx$ is prob of finding particle between x & $x+dx$ ~~at some position~~ &

particle never disappears. ~~Just moves around~~.

- But we are left with idea that maybe not at well defined place.
- Prob dist. sloshes, but inst. pos. ~~never~~ generally not well defined
- This is hardest part of QM to accept after being used to thinking like monkeys.

~~Determinism~~

- Some claim that position is real, because common conception of definite reality must exist
- But experiments keep putting the squeeze on related interps like that & it appears that Schr. w.f. is "real" & something is wrong with monkey-headed question "where is particle?"