Classical & Quantum Waves

Lecture 19-1

Quantum Waves & the Schrödinger equation

Brief timeline of important events:

~450 BC: Ancient Greeks' hypothesized that all matter is made up of tiny particles called atoms

↓ Many years, many discoveries...

~1800s: Light behaves as a wave (e.g., Young's double slit, Maxwell's eqs.)

1897: JJ Thomson discovers the electron, which acted as a particle

1900: Max Planck explains blackbody radiation, showing that the energy of light is proportional to its frequency $E = h\nu$ h: Plancks' constant

→ A stream of light consists of a stream of particles $E_{tot} = n h\nu$ "energy quanta" packet of energy

n: # particles

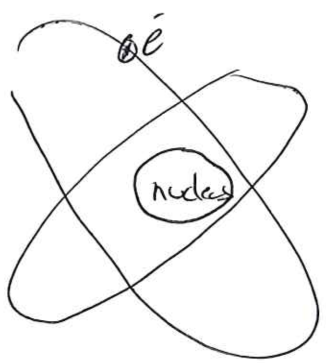
1905: Einstein explains photoelectric effect

→ only light w/ frequency above a certain value can free electrons from a material

→ Cemented the idea that the energy of light is related to its frequency $\underbrace{E = h\nu}_{\text{quanta of light}}$

→ Wave/particle duality of light now becoming accepted (but still strange...)

1911: Rutherford model of the atom



· Atoms consist of dense nucleus, electrons orbit around it

→ Problem: accelerating electrons emit light → means electrons should eventually crash into nucleus and universe implodes...

1913: Bohr model of the atom

· Borrowing quanta ideas, proposed that only certain electron orbits (energies) allowed, which brings stability to atom

· Also explains spectral lines in emission experiments

→

→ shine white light on atoms, only certain discrete colors absorbed. The energy of these colors, as given by $E=h\nu$, is the energy spacing b/t different electron orbits

→ agreed perfectly w/ Rydberg ~~times from~~ emission spectra from Hydrogen

1924: de Broglie hypothesis

- Up until this point, accepted that light can act as a particle or wave

→ postulated that electrons also act as waves. "matter waves"

quasi- Explains Bohr orbits in atom, b/c only certain wavelengths fit in orbit as standing wave (but not perfect)

- Electrons (and everything else) have an associated wavelength → de Broglie wavelength

wave concepts

$$\lambda = \frac{h}{p} \qquad \nu = \frac{E}{h}$$

particle concepts

h: Planck's constant

p: momentum of particle/wave

E: energy

→ Idea borrowed from Einstein's description of wave/particle duality for light/photons

$$E = h\nu = mc^2 \qquad \nu\lambda = c$$

← speed of light

$$\rightarrow h\cancel{\nu} = mc\cancel{\nu}\lambda \Rightarrow \lambda = \frac{h}{\underbrace{mc}_{\text{momentum of light}}} = \frac{h}{p}$$

1923-27: Davisson-Germer experiments (Bell labs)

-> showed electrons behave as waves through diffraction experiments from crystal surfaces

-> wavelength depends on energy

-> Even for single electrons, could eventually detect through averaging many events electron waves interfering with themselves!

-> strong evidence for wave/particle duality for electrons

-> ~~implanted~~ supported idea of superposition b/t quantum states (via self-interference)

-> probabilistic nature of quantum physics

· Double slit experiment ~~also~~ for electrons also performed around this time w/ similar results

1925: Heisenberg Matrix mechanics formulation of quantum mechanics

-> abandoned deterministic nature of classical physics and adopted statistical/probalistic approach

-> instead of precise positions & velocities, replace with probabilistic distributions & energy transitions

-> succeeded in calculating atomic spectra in agreement w/ experiment

- Striking aspect that product of physical quantities is generally non-commutative: $A \times B \neq B \times A$

  → challenged fundamental principles of classical physics, showing how different physics is at the sub-atomic scale

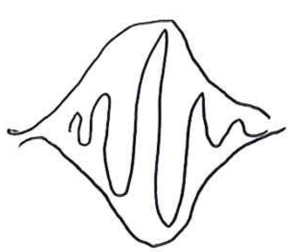
- Heisenberg also formulated the uncertainty principle (1927)

$$\underset{\substack{\uparrow \\ \text{uncertainty} \\ x}}{\Delta x} \; \underset{\substack{\uparrow \\ '' \\ p}}{\Delta p} \geq \frac{\hbar}{2} \qquad \underset{\substack{\uparrow \\ \text{"reduced Planck's constant"}}}{\hbar} = \frac{h}{2\pi}$$

→ the better you know position, the less you know momentum

→ This is the quantum version of the time-bandwidth theorem of waves! (Lecture 18)

→ reflects the fact that "particles" ~~are~~ can be described as wave packets



The Schrödinger eq. (1926)

- At this point, there was clear evidence for matter waves, but no wave equation, to describe them.
- Schrödinger figured this out.
- Recall classical wave eq.

$$\frac{\partial^2 y(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y(x,t)}{\partial t^2}$$

- satisfied by plane wave solutions, e.g. $y(x,t) = A\cos(kx-\omega t)$

provided that $v = \frac{\omega}{k} = f\lambda$

- What is the equivalent wave eq. for a quantum matter wave?
- Try classical wave eq. w/ traveling wave solution

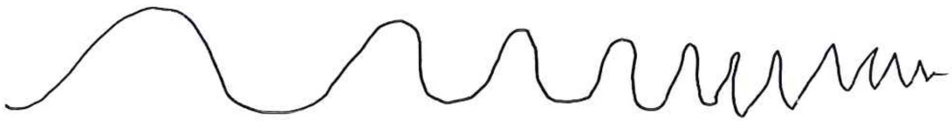
$$\Psi(x,t) = A\cos(kx-\omega t) \rightarrow \text{fixed } f \text{ and } \lambda$$

w/ $p = \frac{h}{\lambda}$ (de Broglie) and $E = hf$ (Einstein)

constant $p \leftrightarrow$ constant λ constant $E \leftrightarrow$ constant f

$\rightarrow$ works for freely moving particle w/ no forces applied

- The problem is that when a force is applied, then particle's momentum changes by Newton 2nd law



Force $\longrightarrow$ change in p $\longrightarrow$ change in λ

$F = \frac{dp}{dt}$ (Newton) $\qquad \lambda = \frac{h}{p}$ (de Broglie)

$\longrightarrow$ means that concept of wavelength not defined, since separation of adjacent maxima $\neq$ ~~adj~~ separation b/t adjacent minima

$\longrightarrow$ means that functions more complex than $\psi(x,t) = A\cos(kx - \omega t)$ are required

- Need to ~~determine~~ Find wave eq. that can determine wave function for <u>any</u> given situation provided $\underbrace{\text{information about force}}$ acting on particle

↳ do this by specifying potential energy corresponding to the force

Considerations for constructing quantum wave eq:

1) Must be consistent w/ de Broglie - Einstein postulates

$\lambda = \frac{h}{p}$ connects wavelength w/ momentum

$f = E/h$ connects frequency w/ energy

2) Must be consistent w/ energy eq. for a particle

$$E = KE + PE$$

total energy, kinetic energy, potential energy

$$KE = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$\underbrace{PE = V(x,t)}_{\text{provides info about forces acting on particle}}$$

$$F = -\frac{\partial V}{\partial x}$$

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

3) Must be linear in $\Psi(x,t)$

→ If Ψ_1 and Ψ_2 both different solutions, then linear combo must be solution $\Psi = c_1\Psi_1 + c_2\Psi_2$

4) When $V(x,t) = $ constant, must get sinusoidal traveling wave solutions w/ constant wavelength & frequency

$V(x,t) = \text{constant} \rightarrow F = -\frac{\partial V}{\partial x} = 0 \rightarrow$ constant momentum b/c $F = \frac{dp}{dt}$

· Use these considerations to arrive at a wave eq.

· Rewrite $E = \frac{p^2}{2m} + V$ using $\lambda = \frac{h}{p}$, $f = \frac{E}{h}$

$$\Rightarrow hf = \frac{h^2}{2m\lambda^2} + V(x,t)$$

· Rewrite this using $\omega = 2\pi f$, $k = \frac{2\pi}{\lambda}$, $\hbar = \frac{h}{2\pi}$
(to simplify)

$$\Rightarrow \frac{\hbar^2 k^2}{2m} + V(x,t) = \hbar\omega$$

→ notice the k^2 on left side, ω on right.

· Recall 4th consideration is that when $V(x,t) = 0$, we should get plane wave solutions: e.g., $\psi(x,t) = A\cos(kx - \omega t)$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \cos(kx-\omega t) = -k^2\psi(x,t)$$ → gives k^2 term

$$\frac{\partial \psi}{\partial t} = \omega \sin(kx - \omega t)$$ → gives ω

⇒ suggests that the differential eq. we seek should have $\frac{\partial^2\psi}{\partial x^2}$ and $\frac{\partial\psi}{\partial t}$ involved,

→ should also have a $V(x,t)$ term that is proportional to $\psi(x,t)$
[required to preserve linearity, condition #3)

- Putting all this together, we are left w/ a differential eq of the following form:

$$\alpha \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) = \beta \frac{\partial \Psi(x,t)}{\partial t}$$

α, β to be determined

- Assume to start $V(x,t) = V_0$ (constant), so $\psi(x,t) = \cos(kx - \omega t)$

$$\Rightarrow -\alpha k^2 \cos(kx-\omega t) + V_0 \cos(kx - \omega t) = \beta \omega \sin(kx - \omega t)$$

rewrite $\longrightarrow$ $(\alpha k^2 - V_0)\cos(kx - \omega t) + \beta\omega \sin(kx-\omega t) = 0$

$\rightarrow$ This can only be true if $\beta = 0$

and $\alpha k^2 - V_0 = 0$, b/c mix of sine & cosine

$\rightarrow$ does not satisfy $\frac{\hbar^2 k^2}{2m} + V(x,t) = \hbar\omega$

$\times$

- What went wrong? Part of difficulty is that differentiating changes sine $\longleftrightarrow$ cosine, which gave us mixture of the two.

- This is b/c borrowed result from classical physics

- Try instead $\psi(x,t) = \cos(kx - \omega t) + \gamma \sin(kx - \omega t)$

$\longrightarrow$

- Take $\frac{\partial \psi^2}{\partial x^2} = -k^2 \cos(kx-\omega t) - k^2 \gamma \sin(kx-\omega t)$

k^2 terms

- Take $\frac{\partial \psi}{\partial t} = \omega \sin(kx-\omega t) - \omega \gamma \cos(kx-\omega t)$

$\rightarrow k^2, \omega$ & mix of sine, cosine

- Plug into wave eq. ansatz

$$\alpha \frac{\partial^2 \psi}{\partial x^2} + V \psi = \beta \frac{\partial \psi}{\partial t}$$

[skipped algebra]

$$\Rightarrow -\alpha k^2 \left[\underline{\cos(kx-\omega t) + \gamma \sin(kx-\omega t)}\right]$$

same form as ψ

(*) $$+V_0 \left[\underline{\cos(kx-\omega t) + \gamma \sin(kx-\omega t)}\right]$$

$$= \frac{\beta \omega}{\gamma}\left[\underline{-\gamma^2 \cos(kx-\omega t) + \gamma \sin(kx-\omega t)}\right]$$

almost same form as ψ

$-\gamma^2$ term prevents right side

From being same as left terms in [ ]

- If we could choose γ appropriately, could drastically simplify eq b/c terms in [ ] would cancel

$\longrightarrow$

- That is, we want:

$$-\gamma^2 \cos(kx-\omega t) + \gamma \sin(kx-\omega t) = \cos(kx-\omega t) + \gamma \sin(kx-\omega t)$$

$\rightarrow$ requires $-\gamma^2 = 1 \Rightarrow \gamma = \pm\sqrt{-1} = \pm i$

- Let's set $\gamma = +i$, then terms in [ ] in eq (*) cancel out

$$\Rightarrow -\alpha k^2 + V_0 = \frac{\beta\omega}{\gamma}$$

- compare w/ energy-momentum relationship (condition #1-2)

$$\frac{\hbar^2 k^2}{2m} + V_0 = \hbar\omega$$

$\rightarrow$ This matches our criterion if $\alpha = -\frac{\hbar^2}{2m}$

$\beta = \gamma\hbar = i\hbar$

- Substitute back into our wave eq. ansatz

$$\alpha \frac{\partial^2 \psi}{\partial x^2} + V\psi = \beta \frac{\partial \psi}{\partial t}$$

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

1D Schrödinger eq.

- This eq. satisfies all 4 of our initial requirements
- We derived assuming $V(x,t) = V_0$ (a constant), but we postulate that ~~the solutions obtained~~ this will also work for the general case of $V(x,t)$

  → "postulate" means we cannot prove it, but we can compare w/ experiments to check its validity

//

How to use Schrödinger eq?

- To determine structure of wavefunction associated w/ a particle of mass m, you need to:

  1) Specify $V(x,t)$ that encodes information about forces acting on the particle

  2) Solve S.E. to find $\Psi(x,t)$

- But what does $\Psi(x,t)$ actually represent?
- How does it relate to the particle that it is associated with?

- Let's return to our solution for $\Psi(x,t)$ when we assumed $V(x,t) = V_0$ (constant)

$$\Rightarrow \Psi(x,t) = \cos(kx - \omega t) + \gamma \sin(kx - \omega t) \qquad \gamma = i$$

$$= \underbrace{\cos(kx - \omega t) + i \sin(kx - \omega t)}_{\text{complex \#, required by de Broglie-Einstein postulates}}$$

- Important point: The Schrödinger eq. and $\Psi(x,t)$ are fundamentally complex, in that they involve complex numbers
  - This differs from classical waves, where the ~~in that the~~ wave eq. & solutions are real
    (sometimes we used the complex representation to simplify the math, but the eq. & solutions were always real quantities)

- But complex ~~we~~ quantities cannot be measured by any actual physical instruments. So $\Psi(x,t)$ not measurable.

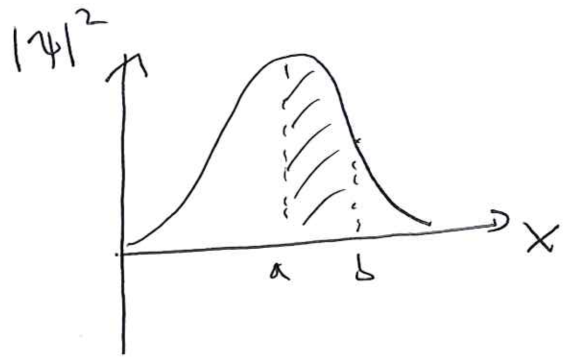
- But, $|\Psi(x,t)|^2 = \Psi^* \Psi$ <u>is</u>

- Perhaps $|\Psi(x,t)|^2$ corresponds to something real that can be determined experimentally

1926: Max Born suggested that $|\Psi(x,t)|^2$ represents the probability ~~that~~ of finding a particle between x and $x+dx$

$$\Rightarrow P(x,t)\,dx = |\Psi(x,t)|^2 dx$$

- To find probability of particle b/t points a and b



$$P(x,t) = \int_a^b |\psi(x,t)|^2 dx$$

Justification:

- Wave & particle entities must be associated in space

↓

- Particle must be at some location where the waves have appreciable amplitude

↓

- Probability density $P(x,t)$ is a measurable quantity

↓

- It should be a real, positive #

↓

- $\psi^* \psi$ is always real, positive

- Implications
  - Born's interpretation introduces indeterminacy into quantum mechanics

    ↓

  - Cannot predict w/ certainty the outcome of an experiment, even if you know all relevant parameters

    ↓

  - Quantum mechanics offers statistical information about the possible results
- This interpretation laid foundation for ~~is known as~~ the "Copenhagen interpretation" which also states that the act of "observing" or "measuring" a particle collapses the wavefunction into a definite position
- Schrödinger did not like this indeterministic interpretation. He thought wavefunctions should represent real physical waves w/ definite energy & momentum, much like classical waves.

  → "Schrödinger's cat" gedanken experiment

  to show absurdity of the idea in the influence of macroscopic objects

- Einstein also didn't like this indeterminate interpretation of quantum mechanics
- "Einstein - Podolsk - Rosen (EPR) Paradox"
- Take two particles that are prepared in an entangled quantum state. This means that the quantum state of each particle cannot be described independently of the quantum state of the others, even at large distances
- Move particles ∞ far apart. Measure one particle, which collapses wavefunction into a definite probability amplitude. This, via the entanglement, will immediately determine the state of the other instantly, faster than speed of light...
- "spooky action at a distance"
- Yet, there is plenty of experimental data suggesting this is the case, so ...?

- Alternative interpretation given by Everett (1957)
- There is a "universal wavefunction" through which all particles in the universe are entangled, which is real and contains all possible realities
- When a measurement is made, the universe branches off into separate worlds, each containing a different outcome
- These worlds are parallel to our own, and hidden from our existence
- This interpretation means everything is definite and gets around the measurement/indeterminacy problem
- This is the "Many worlds interpretation"