Lecture 10: 02/09/09

- From the "Old Quantum Theory" to Modern Quantum Mechanics
  - Philosophy of Quantum Theory
  - Critique of the "Old Quantum Theory"
  - Approach to the Schrödinger equation

Erwin Schrödinger (1887 – 1961): Schrödinger equation, for which he received the Nobel Prize in 1933. In 1935, he proposed the Schrödinger's cat thought experiment.

Recap: $I_{3,4}$ **Group and Phase Velocity for Particle Waves:**

$$f(x,t) = \mathrm{Re}\Big\{ \underbrace{e^{i[k_0 x - \omega(k_0)t]}}_{\text{infinite plane wave: crests move at } v_{phase} = \frac{\omega}{k} = \frac{c^2}{v}} \underbrace{\int \phi(s)\, e^{is\left(x - \left.\frac{d\omega}{dk}\right|_{k_0} t\right)} ds}_{\text{envelope function travels at group velocity}} \Big\}$$

infinite plane wave: crests move at $v_{phase} = \frac{\omega}{k} = \frac{c^2}{v}$

envelope function travels at group velocity $v_{group} = \frac{d\omega(k)}{dk} \overset{!}{=} v_{particle}$

$I_{3,5}$ **λ=h/p: Order of Magnitude Estimate**

typical: $\lambda \lesssim 1\,\text{Å}$ ⇒ crystals, atom, nucleus size

$I_{3,6}$ **Evidence for de Broglie's Particle Waves:**

Electron, neutron, atom, molecule diffraction and interference ... ⇒ used as tool for material science...

I_4 **The "Old Quantum Theory"**

1) Particle-wave duality
2) No defined trajectories
3) only probable behavior
4) probability $\propto$ (wave ampl.)^2
5) Quantized energy for bound states
6) $E = \hbar\omega \quad p = \hbar k$
7) Superposition principle
8) $E = \frac{p^2}{2m} + V$ for non-relativ. particle

I_4 The "Old Quantum Theory"

$I_{4,1}$ Key Ideas / Concepts / Postulates:

1) Photons, particles have both particle-like and wave-like properties

2) Precisely-defined trajectories do not exist at the quantum level

3) The exact behavior of a given particle cannot be predicted — only its probable behavior
   $\Rightarrow$ statistical interpretation

4) The probability that a single particle is observed in a given region is proportional to the intensity of its associated wave field. $I \propto |A|^2$

$$\Rightarrow P \propto |A|^2$$

5) If a particle is confined into a small volume, its energy is quantized ⇒ "energy levels", "energy states"

6) Broglie - Einstein postulates:

$$\boxed{\begin{array}{ll} \lambda = h/p & (p = \hbar k) \\ \nu = E/h & (E = \hbar \omega) \end{array}}$$

k: wave number

ω: angular frequency

7) Superposition principle applies to all particle waves

⇒ ***Add wave amplitudes, and not probabilities / intensities!***

⇒ if $\Psi_1(x,t)$ and $\Psi_2(x,t)$ are allowed waves, then $c_1\Psi_1(x,t) + c_2\Psi(x,t)$ is too

⇒ Localized particle ⇒ large Δk, σ_p ⇒ momentum of particle is not well defined

8) Non-relativistic particle

classical Energy: $E = \underbrace{\frac{p^2}{2m}}_{\text{kinetic energy}} + \underbrace{V}_{\text{potential energy}}$

$I_{4,2}$ Philosophy of Quantum Theory:

1. Copenhagen interpretation:
   - N. Bohr, Heisenberg, ...
   - fundamentally statistical theory
   - exact behavior of individual particles cannot be predicted
   - measurements force the particles to "take a stand"
   - But: How and why?
2. The "realist" interpretation:
   - Einstein ("God does not play dice with the universe"), de Broglie, ...
   - Quantum Theory is incomplete
   - indeterminancy is not a fact of nature
   - some additional information (hidden variable) is needed for complete description of particle

- More later (Bell's Theorem) ⇒ confirms Copenhagen interpretation ...

$I_{4,3}$ "Critique" of the "Old Quantum Theory":

"Old Quantum Theory:" New concepts, ideas; in many respects quite successful, but:

1) Mixture between classical physics, new ideas, postulates, arbitrary quantization...
2) lack of coherence
3) Bohr atom: only for 1 electron atoms; fails for 2 electrons...
4) wrong angular momentum of electron in Bohr atom
5) does not allow to calculate rate at which transitions happen → intensity of spectral lines...
6) ...

⇒ need new theory...

→ consistent with key ideas / concepts of "old Quantum T."

→ dynamics of particle wave ? ⇒ Schrödinger's equ.

→ physical meaning of particle wave ⇒ wave function Ψ

II Introduction to Wave Mechanics

II_1 *Schrödinger's Theory of Quantum Mechanics*

$II_{1,1}$ Preliminary Remarks:

start 1-D

- Particle wave: wave function $\Psi(x,t)$
  function of position and time
- Dynamics of particle wave? ⇒ wave equation!

$\underbrace{\text{particle wave equation, differential equation (tells how } \Psi \text{ changes with time and position)}}$ $\longrightarrow$ solution: wave function $\Psi(x,t)$

indep. variables

⇒ contains partial derivatives wrt. position, time

$$\frac{\partial \Psi}{\partial x}, \quad \frac{\partial \Psi}{\partial t}, \quad \frac{\partial^2 \Psi^2}{\partial x^2}, \quad \frac{\partial^2 \Psi}{\partial t^2}, \ldots$$

Partial derivatives: $\dfrac{\partial \Psi(x,t)}{\partial x} = \left[\dfrac{d\Psi(x,t)}{dx} \right]$ evaluate by treating t as a constant

- Examples of other wave equations:

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

2) Electromagnetic wave in empty space:

$$\frac{\partial^2 \vec{E}}{\partial t^2} = c^2 \underbrace{\nabla^2}_{\frac{\partial^2}{\partial x^2} \text{ in 1-D}} \vec{E}$$

check: Energy of photon: $E = pc \Rightarrow \hbar\omega = \hbar k c \Rightarrow \omega = ck$ for light

Plane light wave: $\psi = \cos(kx - \omega t)$

$\frac{\partial \psi}{\partial t} = \omega \sin(kx - \omega t)$ $\qquad$ $\frac{\partial \psi}{\partial x} = -k \sin(kx - \omega t)$

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

$\Rightarrow -\omega^2 \cos(kx - \omega t) = c^2 (-k^2 \cos(kx - \omega t))$

$\Rightarrow \omega^2 = c^2 k^2 \Rightarrow \omega = ck$ or $E = pc$ ✓

$\Rightarrow$ plane wave satisfies EM wave equation

$II_{1,2}$ Constrains for the Particle Wave Equation:

from before:

1) Need to be consistent with

$$\lambda = h/p \quad (p = \hbar k) \quad \text{and} \quad \nu = \frac{E}{h} \quad (E = \hbar\omega)$$

2) Superposition principle for particle waves:

⇒ if $\Psi_1(x,t)$ and $\Psi_2(x,t)$ are solutions of wave equation, then $\Psi(x,t) = c_1\Psi_1 + c_2\Psi_2$ is too!

⇒ need linear differential equation in Ψ

3) Must be consistent with energy relation

$$E = \frac{p^2}{2m} + V$$ for non-relativistic particles

Note: ⇒ Schrödinger's wave equation is for non-relativistic particles only!

⇒ not for photons!

$II_{1,3}$ Plausibility Argument leading to Schrödinger's Equation:

Note: Postulate, not proof!

1st: Consider free particle (no external forces, i.e. $V = \text{const}$) with constant $E = \hbar\omega$, $p = \hbar k$

$\Rightarrow$ postulate wave function and wave equation for this particle

(1a) Associated particle wave / wave function of free particle $\Psi(x,t) \overset{?}{=} \cos(kx - \omega t)$ plane wave

- wave equation needs to be consistent with energy equation: $E = \frac{p^2}{2m} + V$ ← const here or $E\Psi = \frac{p^2}{2m}\Psi + V\Psi$

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

$\Rightarrow$ Need wave equ. consistent with $\omega = \frac{\hbar k^2}{2m} + \frac{V}{\hbar}$ and has (1a) as solution

$\frac{\partial \Psi}{\partial t}$ gives ω-term

$\left(\frac{\partial \Psi}{\partial x}\right)^2$? $\Rightarrow$ not linear in Ψ $\Rightarrow$ doesn't work

try $\frac{\partial^2 \Psi}{\partial x^2}$ $\Rightarrow$ gives term $\propto k^2$

$\Rightarrow$ <u>postulate</u> particle wave equation:

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

<u>Note:</u> – α, β need to be determined

– linear in Ψ $\Rightarrow$ superposition principle applies! $\rightarrow$ <u>good</u>

$\Rightarrow$ let's see if simple wave function (1a) for <u>free</u> particle with constant E, p satisfies this wave equation (2)

$\rightarrow$ substitute $\Psi(x,t) = \cos(kx - \omega t)$ into

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

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

$$\Rightarrow \alpha \omega \underline{\sin}(kx - \omega t) = [-\beta k^2 + V]\, \underline{\cos}(kx - \omega t)$$

$\Rightarrow$ needs to be true for all t, x!

$\Rightarrow$ doesn't work ....