Lecture 11: **02/11/09**

- Approach to the Schrödinger equation
- Hamiltonian Operator
- Physical meaning of the <u>Wave Function</u>
  - Statistical Interpretation
  - Probability
  - Normalization

Recap:

II$_1$ *Schrödinger's Theory of Quantum Mechanics*

particle wave equation (differential equation) tells how Ψ changes with position and time $\longrightarrow$ Solution: wave function $\Psi(x,t)$ ("particle wave")

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

1) Consitent with $p = \hbar k \quad E = \hbar\omega$
2) Superposition principle $\Rightarrow$ linear in Ψ
3) $E = \frac{p^2}{2m} + V \Rightarrow \omega = \frac{\hbar k^2}{2m} + \frac{V}{\hbar}$

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

free particle ($V = $ const) with constant $E = \hbar\omega$ and $p = \hbar k$

$\Rightarrow$ Postulate particle wave equation: $\alpha \frac{\partial \Psi}{\partial t} = \beta \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$

1st try: Associated particle wave/wave function:

$\Psi(x,t) \stackrel{?}{=} \cos(kx - \omega t)$: plane wave $\Rightarrow$ **Doesn't work!**

Why is it so important for the particle wave equation (the Schrödinger Equation) to be linear in the wave function?

A. To get the right units

B. To be consistent with the classical energy relation of a non-relativistic particle

C. To be able to explain interference of particle waves

sum of waves → still a wave

2^{nd} try:

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

- But: Try different wave function for free particle with constant E, p

(1b) $\Psi(x,t) \stackrel{?}{=} \cos(kx - \omega t) + \eta \sin(kx - \omega t)$ ← eta

– will pick η later

– still a traveling wave with $\lambda = 2\pi/k$, $\nu = \omega/2\pi$

- Insert (1b) into (2)

$$\frac{\partial \Psi}{\partial t} = \omega \sin(kx - \omega t) - \eta\,\omega \cos(kx - \omega t)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 \cos(kx - \omega t) - \eta\, k^2 \sin(kx - \omega t)$$

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

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

$\Rightarrow$ (a) $\alpha\omega + \eta k^2\beta - \eta V \overset{!}{=} 0 \Rightarrow \dfrac{\alpha\omega}{\eta} + k^2\beta - V = 0$

(b) $\alpha\eta\omega - k^2\beta + V \overset{!}{=} 0$

(a)+(b): $\dfrac{\alpha\omega}{\eta} + \alpha\eta\omega = 0 \Rightarrow \dfrac{1}{\eta} + \eta = 0 \Rightarrow \eta = -\dfrac{1}{\eta}$

$\Rightarrow \eta^2 = -1 \Rightarrow \underline{\eta} = \pm\sqrt{-1} = \underline{\pm i}$

<u>Note:</u> - imaginary number!

- $\underline{\Psi \text{ is complex!}}$

$\Rightarrow$ choose $\eta = +i$ (sign has no physical consequences) substitude $\eta = +i$ into (a)

$$\Rightarrow \alpha\omega = i(-k^2\beta + V)$$

needs to be in agreement with energy relation.

$$E = \frac{p^2}{2m} + V \quad \text{or} \quad \omega = \frac{\hbar k^2}{2m} + \frac{V}{\hbar}$$

$$\Rightarrow \alpha\left\{\frac{\hbar k^2}{2m} + \frac{V}{\hbar}\right\} = i\left(-k^2\beta + V\right)$$

$$\Rightarrow \left(\alpha\frac{\hbar}{2m} + i\beta\right)k^2 = \left\{i - \frac{\alpha}{\hbar}\right\}V \quad \text{for any } V_{\text{const}}=$$

$\Rightarrow$ satisfied if:

$$\underline{\alpha = \hbar i} \qquad \underline{\beta = -\frac{\hbar^2}{2m}}$$

Result: with $\eta = +i$; $\alpha = i\hbar$; $\beta = -\hbar^2/2m$

$\Rightarrow$ wave function for free particle with const E, p

$$\underline{\Psi(x,t)} = \cos(kx - \omega t) + i\sin(kx - \omega t) = \underline{e^{i(kx-\omega t)}}$$

complex wave!

is solution of wave equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

⇒ generalize: for $V = V(x,t)$, i.e. time, position dependent potential energy

<u>Postulate</u> for wave equation

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

time-dependent Schrödinger equation for <u>non</u>-relativistic particles

<u>Note:</u>

- no proof that this must be true!
- experimentally confirmed
- includes complex factor $i = \sqrt{-1}$
- solve for given $V(x,t) \rightarrow \Psi(x,t)$
- first order in time:

recall: for particle: $\omega \propto k^2$

$\partial/\partial t$ $\partial^2/\partial x^2$

compare to EM waves:

$\omega = ck$

$\partial^2/\partial t^2$ $\partial^2/\partial x^2$

- <u>Hamiltonian Operator</u>:

define: $\hat{H} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$ "energy operator"

$\Rightarrow$ short form of <u>time-dep.</u> Schrödinger Equ:

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\, \Psi(x,t)}$$

<u>Operator</u>: "Instruction to do something to the function that follows"

The wave function is a complex function. This means that…

A. The wave function can not directly represent something that can be measured, so it itself has no physical existence

B. This theory must still be wrong

C. Something else

$II_{1,4}$ Physical Significance of the Wave Function $\Psi(x,t)$:

$\Psi(x,t)$:
- function of position and time
- complex function
- computational device, no physical existance!
- but: contains all the information about the particle!

How? ⇒ Born's statistical interpretation of the wave function:

"If, at the instant t, a measurement is made to locate the particle associated with the wave function $\Psi(x,t)$, then the probability $P(x,t)dx$ that the particle will be found at a coordinate between x and $x+dx$ is equal to:

$$P(x,t)\,dx = \Psi^*(x,t)\cdot\Psi(x,t)\,dx$$

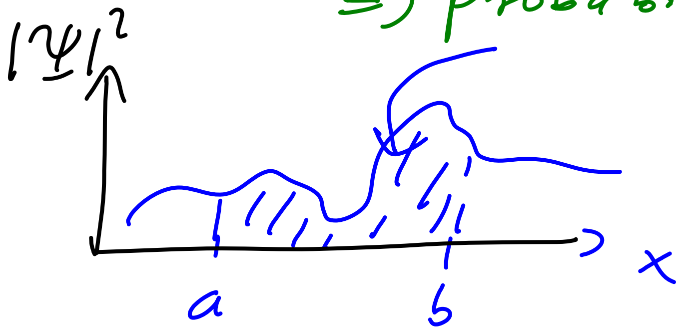
complex conjugate of Ψ

$$= |\Psi|^2\,dx$$

$P(x,t) = \Psi^*(x,t)\cdot\Psi(x,t) \geq 0$, real, probability density

$$\Rightarrow \int_a^b |\Psi(x,t)|^2 dx = \int_a^b \Psi^* \cdot \Psi \, dx = \left\{ \begin{array}{l} \text{probability of "finding"} \\ \text{the particle between} \\ \text{a and b at time t} \\ \text{if position is measured} \end{array} \right\}$$

$\Rightarrow$ probability = area under the $|\Psi|^2$ graph

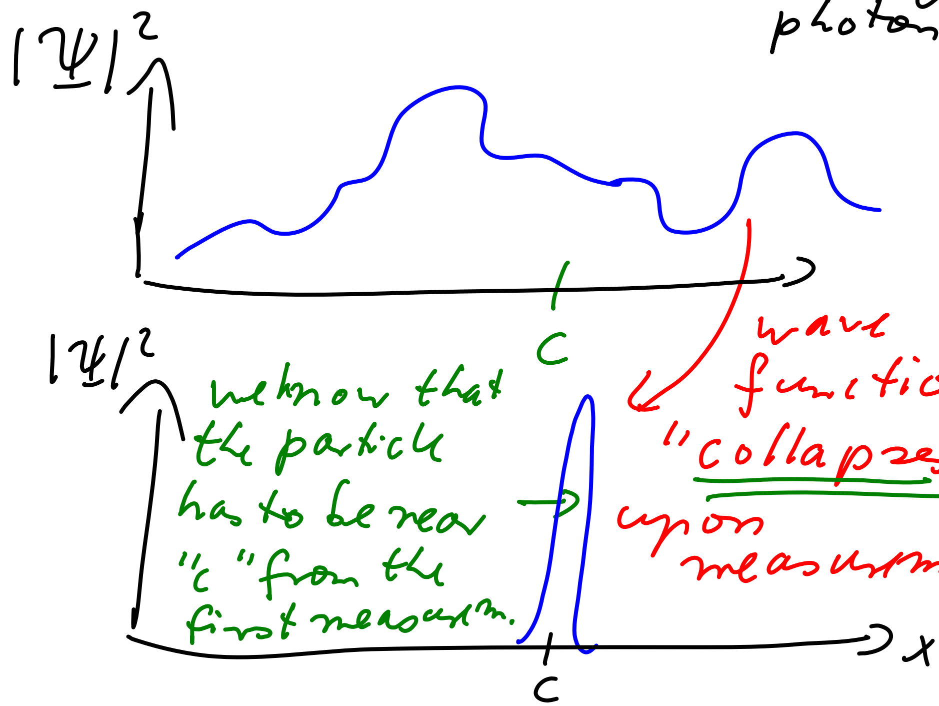


recall 2-slit exp.:

I on screen $\propto |E|^2 \propto$ probab. of finding a photon

Measurements:

- $|\Psi|^2$ just before measurement
- $|\Psi^2|$ immediately after measurement has found particle at point "c"



we know that the particle has to be near "c" from the first measurem. $\rightarrow$

wave function "collapses" upon measurement!