Recap -- optics

\[ I = c E_0 E_T^2 \]

\[ E_T = E_A + E_B \quad \Rightarrow \quad E_T^2 = (E_A + E_B)^2 \]

\[ = E_A^2 + E_B^2 + 2E_A E_B \]

\[ \uparrow \] \quad \text{result for one slit} \quad \text{for one slit} \quad \text{interference term} \]

\[ I = c E_0 E_T^2 = N hf \]

for large "photon flux" -- large \( N \) -- can measure \( E_T^2 \) as a measure of \( N \)
Averaging $E^2$ over time $\rightarrow N$

or

$E^2 dv \propto \text{probability of finding a photon inside } dv$ volume

Our problem is with electrons...

What’s the analog to $E$ in matter waves?

It’s called THE WAVE FUNCTION, $\Phi(x,t)$

At first you might imagine it to be optics-like and you would be right, except a more general treatment is not just sines and cosines alone.

Use Euler’s relation:

$$e^{ix} = A \cos x + i A \sin x$$

for a general wave

$$\Phi(x,t) = A e^{i(\frac{px - Et}{\hbar} - ft)} = A e^{i}px - Et)/\hbar$$
It is the square of this object that will somehow be related to actual electrons ... we'll see.

actual derivation of the basic equation — "beyond this course" ... as they say.

can sneak up on it.

Keeping in mind that our electron

\[ \Psi(x, t) = Ae \]

has a particle-like relationship to \( E \) and \( p \):

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

\[ \uparrow \quad \uparrow \quad \uparrow \]

kinetic energy \hspace{1cm} potential energy \hspace{1cm} total energy.

Obviously... non-relativistic (there's a story here)

Whatever results... the particle's \( p, V, \) and \( E \)

must be related like this.
Take some "arbitrary" derivatives:

\[
\frac{\partial \Phi}{\partial x} = \frac{i}{\hbar} P_x \Phi
\]

\[
\frac{\partial^2 \Phi}{\partial x^2} = -\frac{i}{\hbar^2} P_x^2 \Phi
\]

\[
\frac{\partial \Phi}{\partial t} = -\frac{i}{\hbar} E \Phi
\]

\[
\Phi(x,t) = Ae^{i(\frac{P_x x - E x}{\hbar})} t
\]

Take the energy equation and multiply it by \( \Phi \)

\[
\frac{P_x^2}{2m} \Phi(x,t) + V \Phi(x,t) = E \Phi(x,t)
\]

and look above:

\[
P_x \Phi = -\frac{i}{\hbar} \frac{\partial \Phi}{\partial x}
\]

\[
E \Phi = -\frac{i}{\hbar} \frac{\partial \Phi}{\partial t}
\]

Use this:

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \Phi(x,t)}{\partial x^2} + V \Phi(x,t) = -\frac{i}{\hbar} \frac{\partial \Phi(x,t)}{\partial t}
\]

**TIME-DEPENDENT SCHRODINGER EQUATION**
This leads to a prescription on how to go from classical physics to quantum mechanics called "First Quantization."

Go back to the derivatives...

\[ P_x \psi = \frac{\hbar}{i} \frac{\partial \psi}{\partial x} \]

Define the "momentum operator"

\[ \hat{P}_x \equiv \frac{\hbar}{i} \frac{\partial}{\partial x} \]

and

\[ \hat{E} \psi = \frac{-\hbar}{2} \frac{\partial^2 \psi}{\partial x^2} \]

"the energy operator"

\[ \hat{E} = \frac{-\hbar}{2} \frac{\partial^2}{\partial x^2} \]

Take classical momentum & energies and replace

\[ P_{x,q,3} \rightarrow \hat{P}_{x,q,3} \]

\[ E \rightarrow \hat{E} \]
"I am now convinced that theoretical physics is actually philosophy."

Max Born

Sandy: Oh Danny, is this the end? Danny: No Sandy. It's only the beginning.

Max Born's granddaughter
Properties of $\Psi$:

1) $\Phi^*(x,t)\Phi(x,t)dx = |\Phi(x,t)|^2dx = P(x)dx$

$P(x)$ is the probability density of finding the particle represented by $\Psi$ at $x$ to $x+dx$.

$\Psi$ is often called the probability amplitude...

The imaginary nature of $\Psi$ is critical in making $\Psi$ not a directly observable entity, unlike $E(x,t)$.

$\Psi$ has to be somewhere—the particle has to be somewhere.

$$P = \int_{-\infty}^{\infty} \Phi^* \Phi dx = 1$$

and the $\Psi$ functions are "normalized" to ensure this.

The probability for the particle to be between $x_a$ and $x_b$:

$$P = \int_{x_a}^{x_b} \Phi^*(x,t)\Phi(x,t)dx$$
Suppose there is no potential \( V = 0 \)

Then \( \mathcal{E} = \frac{p^2}{2m} \)

\[ \Psi(x,t) = Ae^{i(\mathcal{E}x - \mathcal{E}t)/\hbar} \]

\( \text{cannot be a wave function} \)

Because \( \int_{-\infty}^{\infty} \Psi^* \Psi \, dx = \infty \)

but... This is not unexpected because

\( e^{i(\mathcal{E}x - \mathcal{E}t)/\hbar} \)

implies a particular \( \mathcal{E}x \) and \( \mathcal{E} \)

which cannot be.

2) \( \Psi \) must be finite everywhere
3) \( \Psi \) must be single-valued
4) \( \Psi \) and \( \frac{\partial \Psi}{\partial x} \) must be continuous at any potential boundary \( \Rightarrow \frac{\partial \Psi}{\partial x} \) is single-valued.
5) \( \Psi \to 0 \) as \( x \to \pm \infty \)

These are boundary conditions to the solution of Schrödinger equation.
\[ \psi(x,t) \] determines the form of \( \psi \) many times it will be independent of time.

Then, the wave function is factorized:

\[
\psi(x,t) = \psi(x) e^{-i\omega t} = \psi(x) e^{-iE\tau / \hbar}
\]

\( \psi \) capital psi \( \psi \) lowercase psi

Now...

\[
\hat{H} \psi(x,t) = \frac{i\hbar}{\hbar} \frac{\partial \psi}{\partial t} \psi(x,t)
\]

\[
= \frac{i\hbar}{\hbar} \psi(x) \left( \frac{1}{\hbar} \frac{\partial}{\partial x} \right) e^{-iE\tau / \hbar}
\]

\[
= \frac{i\hbar}{\hbar} (-iE) \psi(x) e^{-iE\tau / \hbar}
\]

\[
= E \psi(x,t)
\]

So,

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x) \psi(x) = \frac{i\hbar}{\hbar} \frac{\partial \psi(x,t)}{\partial t}
\]

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} e^{-iE\tau / \hbar} + V(x) \psi(x) e^{-iE\tau / \hbar} = \frac{i\hbar}{\hbar} \frac{\partial \psi(x)}{\partial t} e^{-iE\tau / \hbar}
\]

\[
e^{-iE\tau / \hbar} \frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + e^{-iE\tau / \hbar} V(x) \psi(x) = E \psi(x) e^{-iE\tau / \hbar}
\]
\[-\frac{k}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x)\]

**TIME-INDEPENDENT** Schrödinger Equation

**Probabilities:**

\[
\int \overline{\psi(x,t)} \psi(x,t) \, dx = \int \psi^*(x) \psi(x) e^{\frac{-iE\tau}{\hbar}} \, dx
\]

\[
= \int \psi^*(x) \psi(x) \, dx \neq f(t)
\]

**EXPECTATION VALUES**

Think about averages... → How do you calculate your GPA?

\[ \langle \text{grade} \rangle = \frac{N_4 \cdot 4.0 + N_{35} \cdot 3.5}{N_4 + N_{35}} \]

\[ \langle x \rangle = \frac{N_1 \cdot x_1 + N_2 \cdot x_2 + \cdots}{N_1 + N_2 + \cdots} = \frac{\sum N_i \cdot x_i}{\sum N_i} \]

for a continuous quantity...

\[ \langle x \rangle = \frac{\int_{-\infty}^{\infty} x \, P(x) \, dx}{\int_{-\infty}^{\infty} P(x) \, dx} \]

\[ P(x) : \text{probability distribution of finding } x \]
In quantum mechanics such averages are called expectation values:

\[
\langle x \rangle = \frac{\int_{-\infty}^{\infty} x \psi^*(x) \psi(x) \, dx}{\int_{-\infty}^{\infty} \psi^*(x) \psi(x) \, dx}
\]

works for any function

\[
\langle f(x) \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,t) f(x) \psi(x,t) \, dx}{\int_{-\infty}^{\infty} \psi^d(x,t) \psi(x,t) \, dx}
\]

write it this way for a reason... OPERATORS have important expectation values... and they must "operate" in a particular direction

→ to the RIGHT

An important fact of quantum mechanical life

OBSERVABLES ARE ALL REPRESENTED BY OPERATORS:

\[
\langle A \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,t) A \psi(x,t) \, dx}{\int_{-\infty}^{\infty} \psi^*(x,t) \psi(x,t) \, dx}
\]
we have seen two operators \( \hat{p}_x \) and \( \hat{E} \) and they are connected to things that can be actually measured:

- a particle's momentum in the \( x \) direction
- a particle's energy

\[ \langle p_x \rangle = -\frac{i \hbar}{\partial x} \]

\[ \langle p_x \rangle = \frac{\int_{-\infty}^{\infty} \Psi^*(x,t) \hat{p}_x \Psi(x,t) \, dx}{\int_{-\infty}^{\infty} \Psi^*(x,t) \Psi(x,t) \, dx} \]

\[ \langle p_x \rangle = -i \hbar \int_{-\infty}^{\infty} \Psi^*(x,t) \frac{\partial}{\partial x} \Psi(x,t) \, dx \frac{\int_{-\infty}^{\infty} \Psi^*(x,t) \Psi(x,t) \, dx}{\int_{-\infty}^{\infty} \Psi^*(x,t) \Psi(x,t) \, dx} \]

\[ \langle E \rangle = \frac{i \hbar}{\partial x} \int_{-\infty}^{\infty} \Psi^*(x,t) \frac{\partial}{\partial x} \Psi(x,t) \, dx \]

\[ \langle E \rangle = \frac{i \hbar}{\partial x} \int_{-\infty}^{\infty} \Psi^*(x,t) \Psi(x,t) \, dx \]

The circumstances dictate the functional form of \( \Psi(x,t) \).
... the physics is in the form and configuration of $V$... 

Imagine a well

You're confined to $0 < x < L$ due to your inability — or ability — to overcome the potential barrier, ugh.

$V(y) = \text{ugh}$ characterizes your state of motion and possibilities...