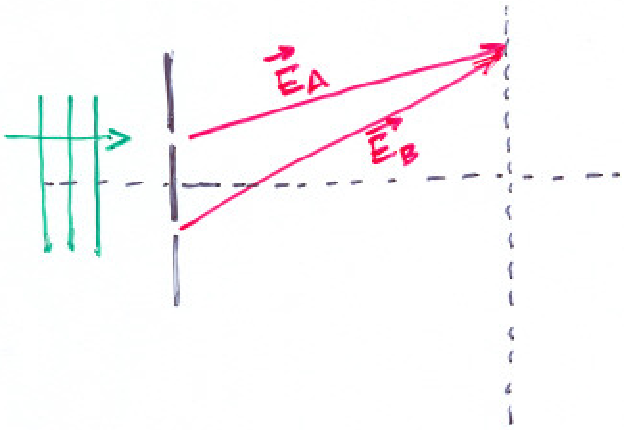
CHAPTER 6 QUANTUM MECHANICS

Recap... optics



The actual BRIGHTNESS is the INTENSITY of the combined waves

$$I = c\varepsilon_0 E_T^2$$

$$E_T = E_A + E_B \qquad \text{so} \qquad E_T^2 = (E_A + E_B)^2$$

$$= \underbrace{E_A^2}_{\text{result for one slit}} + \underbrace{E_B^2}_{\text{result for one slit}} + \underbrace{2E_AE_B}_{\text{interference term}}$$

$$I = c\varepsilon_0 E_T^2 = Nhf$$

for large "photon flux" .. large N... can measure E^2 as a measure of N

Averaging E^2 over time $\rightarrow$ N

or

$E^2 dv$ $\propto$ probability of finding a photon inside dv

volume

Our problem is with electrons...

what's the analog to E for matter waves?

It's called THE WAVE FUNCTION, $\Psi(x,t)$

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:

$$Ae^{ix} = A\cos x + iA\sin x$$

for a general wave

$$\Psi(x,t) = Ae^{2\pi i\left(\frac{x}{\lambda} - ft\right)} = Ae^{i(p_x x - Et)/\hbar}$$

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

$$\Psi(x,t) = A e^{i(p_x x - Et)/\hbar}$$

has a particle-like relationship to E and p:

$$\underset{\substack{\uparrow \\ \text{kinetic} \\ \text{energy}}}{\frac{p^2}{2m}} + \underset{\substack{\uparrow \\ \text{potential} \\ \text{energy}}}{V} = \underset{\substack{\uparrow \\ \text{total energy.}}}{E}$$

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:

$$\frac{\partial \Psi}{\partial x} = \frac{i}{\hbar} p_x \Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{1}{\hbar^2} p_x^2 \Psi \qquad \Psi(x,t) = A e^{i(p_x x - Et)/\hbar}$$

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} E \Psi$$

Take the energy equation and multiply it by Ψ

$$\frac{p_x^2}{2m} \Psi(x,t) + V \Psi(x,t) = E \Psi(x,t)$$

and look above:

$$p_x^2 \Psi = -\hbar \frac{\partial^2 \Psi}{\partial x^2}$$

$$E \Psi = -\frac{\hbar}{i} \frac{\partial \Psi}{\partial t}$$

use this:

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

TIME-DEPENDENT SCHRÖDINGER 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

$$E \Psi = -\frac{\hbar}{i} \frac{\partial \Psi}{\partial t}$$

.. the energy operator

$$\hat{E} \equiv -\frac{\hbar}{i} \frac{\partial}{\partial t}$$

$\Rightarrow$ take classical momentum & energies and replace

$$p_{x,y,z} \rightarrow \hat{p}_{x,y,z} \quad \text{to "quantize"}$$

$$E \rightarrow \hat{E}$$

"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 Ψ :

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

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

Ψ often called the probability amplitude...

The imaginary nature of Ψ is critical

... making Ψ not a directly observable entity. unlike $\vec{E}(x,t)$

Ψ has to be somewhere _ the particle has to be somewhere

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

and the Ψ functions are "normalized" to insure this.

The probability for the particle to be between x_A and x_B:

$$P = \int_{x_A}^{x_B} \Psi^*(x,t)\,\Psi(x,t)\,dx$$

Suppose there is no potential .. $V=0$

then $\quad E = \dfrac{p^2}{2m}$

$$\Psi(x,t) = A e^{i(p_x x - Et)/\hbar}$$

cannot be a wave function

Because $\quad \displaystyle\int_{-\infty}^{\infty} \Psi^* \Psi \, dx = \infty$

but... this is not unexpected because

$$e^{i(p_x x - Et)/\hbar}$$

implies a particular p_x and x

which cannot be.

2) Ψ must be finite everywhere

3) Ψ must be single-valued

4) Ψ and $\dfrac{\partial \Psi}{\partial x}$ must be continuous at any potential boundary $\Rightarrow \dfrac{\partial^2 \Psi}{\partial x^2}$ is single-valued.

5) $\Psi \rightarrow$ as $x \rightarrow \pm\infty$

These are boundary conditions to the solution of Sch. Equation.

V determines the form of Ψ ...

many times it will be independent of time.

Then, the wave function is factorized:

$$\Psi(x,t) = \psi(x)\, e^{-i\omega t} = \psi(x)\, e^{-iEt/\hbar}$$

capital psi   lower case psi

Now...

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

$$= i\hbar\, \psi(x) \frac{\partial}{\partial t} e^{-iEt/\hbar}$$

$$= i\hbar \left(-i\frac{E}{\hbar}\right) e^{-iEt/\hbar}\, \psi(x)$$

$$= E\, \Psi(x,t)$$

So,

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

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)e^{-iEt/\hbar} + V(x)\,\psi(x)e^{-iEt/\hbar} = i\hbar\frac{\partial}{\partial t}\psi(x)e^{-iEt/\hbar}$$

$$e^{-iEt/\hbar}\,\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + e^{-iEt/\hbar}\,V(x)\,\psi(x) = E\,\psi(x)\,e^{-iEt/\hbar}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\,\psi(x)$$

TIME - INDEPENDENT Schrödinger Equation

Probabilities:

$$\int \Psi^*(x,t)\,\Psi(x,t)\,dx = \int \psi^*(x)\,\psi(x)\,e^{+iEt/\hbar}\,e^{-iEt/\hbar}\,dx$$

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

EXPECTATION VALUES

Think about averages... $\longrightarrow$ how do you calculate your gpa?

$$\langle \text{grade} \rangle = \frac{N_4\,(4.0) + N_{35}\,(3.5) + \cdots}{N_4 + N_{35} + N_{30} + \cdots}$$

$$\langle x \rangle = \frac{N_1 x_1 + N_2 x_2 + \cdots}{N_1 + N_2 + \cdots} = \frac{\sum_i N_i x_i}{\sum N_i}$$

for a continuous quantity...

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

$P(x)$: probability distribution of finding x

In quantum mechanics such averages are called

Expectation Values:

$$\langle x \rangle \equiv \frac{\int_{-\infty}^{\infty} x \, \Psi^*(x) \Psi(x) \, dx}{\int_{-\infty}^{\infty} \Psi^*(x) \Psi(x) \, dx}$$

works for any function

$$\langle f(x) \rangle = \frac{\int_{-\infty}^{\infty} \Psi^*(x,t) \, f(x) \, \Psi(x,t) \, dx}{\int_{-\infty}^{\infty} \Psi^*(x,t) \Psi(x,t) \, dx}$$

wrote it this way for a reason -- OPERATORS

have important expectation values ... and

they must "operate" in a particular "direction"

$\longrightarrow$ to the RIGHT

An important fact of quantum mechanical life

OBSERVABLES ARE ALL REPRESENTED BY OPERATORS:

$$\langle A \rangle \equiv \frac{\int_{-\infty}^{\infty} \Psi^*(x,t) \, \hat{A} \, \Psi(x,t) \, dx}{\int_{-\infty}^{\infty} \Psi^*(x,t) \, \Psi(x,t) \, dx}$$

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

BY: the expectation of observing p_x or E

$$\hat{p}_x \equiv -i\hbar \frac{\partial}{\partial x}$$

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

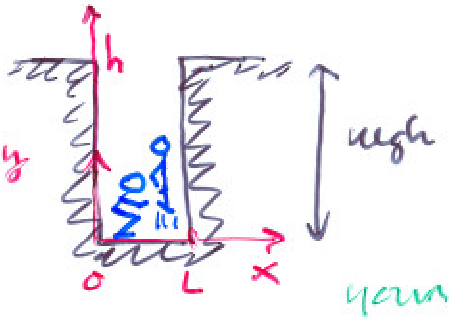
$$\langle p_x \rangle = \frac{-i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t)\, \frac{\partial}{\partial x} \Psi(x,t)\,dx}{\int_{-\infty}^{\infty} \Psi^*(x,t)\, \Psi(x,t)\,dx}$$

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

The circumstances dictate the functional form of $\Psi(x,t)$

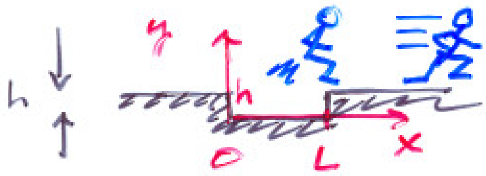
... the physics is in the form and configuration of V...

Imagine a well



your state of motion is defined by your ability to jump.

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



$V(y) = mgh$ characterizes your state of motion and possibilities...