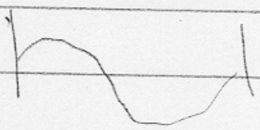
Last Time

① Review - electrons are waves $\lambda = h/p$ or $p = \hbar k$

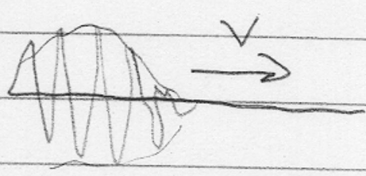
② • Standing waves:



only for discrete frequencies will an integral number of wavelengths fit in the confining region

Explains qualitatively why electron orbiting proton emitts discrete light

③ • Traveling Waves



Showed that a wave packet, e.g.

$$\psi = \cos(k_1 x - \omega_1 t) + \cos(k_2 x - \omega_2 t) + \cos(k_3 x - \omega_3 t)$$

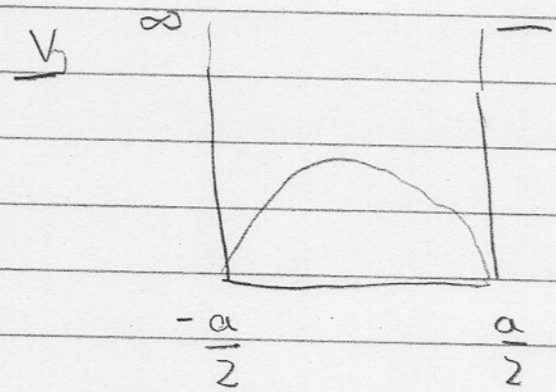
moves with speed $\omega_1 = p_1^2/2m$ $\omega_2 = p_2^2/2m$

$$V = \frac{\hbar \bar{k}}{m} \qquad \text{where } \bar{k} = \frac{k_1 + k_2 + k_3}{2}$$

good thing

(4) Then we interpretted this wave probabilistically

Ex: Suppose you put an electron inside a box of Length a



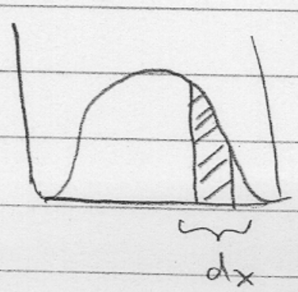
- Kind of a model for an atom

- Electron wave fcn must be inside box, No probability to be outside the box

We will show by solving that the wave fcn is

$$\psi(x) = \begin{cases} C\cos(\pi x/a) & |x| < a/2 \\ 0 & |x| > a/2 \end{cases}$$

What does it mean:



$P(x) = |\psi(x)|^2$ is the probabilty per unit length

probability density

Or

$$d\mathcal{P} = |\psi(x)|^2 \, dx = P(x)\, dx$$

probability of finding the electron in a bin centered at x
of width dx

Then

$$1 = \sum_{\text{bins}} dP = \int_{-\infty}^{\infty} dx \, |\psi(x)|^2$$ = electron must be some where

$$\overline{X} = \sum_{x} x \, dP = \int_{-\infty}^{\infty} dx \; x \, |\psi(x)|^2$$

the average position i.e. the x weighted by the chance that you will find the electron at x, $|\psi(x)|^2 dx$

$$\overline{X^2} = \int_{-\infty}^{\infty} dx \; x^2 \, |\psi(x)|^2$$

$$\overline{3} = \int_{-\infty}^{\infty} dx \; 3 \, |\psi|^2 = 3 \int_{-\infty}^{\infty} |\psi|^2 = 3$$ so $\overline{\overline{X}} = \overline{X}$

Then we can use this:

$$1 = \int_{-\infty}^{\infty} dx \; |\psi(x)|^2 = \int_{-a/2}^{a/2} dx \; C^2 \cos^2\left(\frac{\pi x}{a}\right)$$

$$= C^2 a \int_{-a/2}^{a/2} \frac{dx}{a} \cos^2\left(\frac{\pi x}{a}\right)$$

$u = x/a$

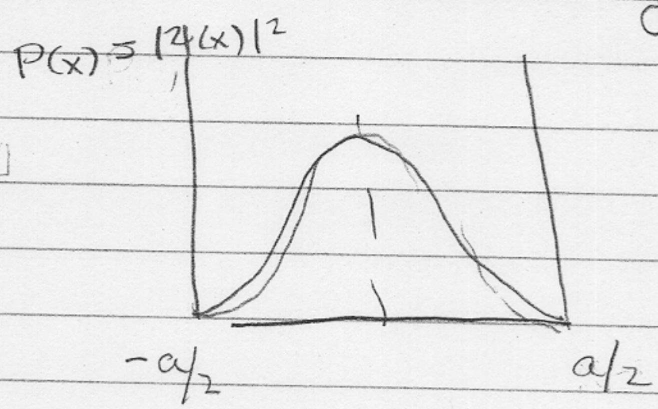
$$1 = C^2 a \int_{-1/2}^{1/2} du \; \cos^2(\pi u)$$

I explained how to do this integral in recitation

$$1 = C^2 a \, \frac{1}{2}$$

$$\sqrt{\frac{2}{a}} = C$$

Now whats the average position:



- Whats the most likely position?

$x = 0$ found by maximizing $P(x)$

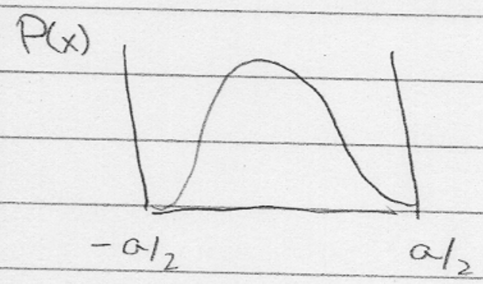
What is the average position?

$$\bar{x} = \int_{-\infty}^{\infty} dx \quad x \quad |\psi(x)|^2 \quad = 0$$

$\uparrow$

we will show this

- it is "intuitively obvious"



$$\bar{x} = \int_{-\infty}^{\infty} dx \quad \underbrace{x}_{\text{odd}} \quad \underbrace{\frac{2}{a} \cos^2\left(\frac{\pi x}{a}\right)}_{\text{even}} = 0$$

Now what is the spread or stanard deviation in the average?

Want to measure

$$x - \bar{x}$$

But $\quad \overline{x - \bar{x}} = \bar{x} - \bar{\bar{x}} = \bar{x} - \bar{x} = 0$

Could take

$$|x - \bar{x}|$$

but integrals are hard usually
So take

$$\sigma^2 \equiv \Delta x^2 \equiv \overline{(x-\bar{x})^2} = \overline{(x-\bar{x})(x-\bar{x})}$$

$$= \overline{x^2 - 2x\bar{x} + \bar{x}^2}$$

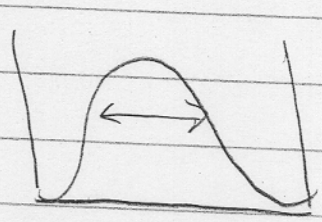
$$= \overline{x^2} - 2\bar{x}\bar{x} + \bar{x}^2$$

$$\sigma^2 = \overline{x^2} - (\bar{x})^2$$

Then the "root mean square" deviation

$$(\Delta x)^2 \equiv \left[\overline{(x-\bar{x})^2}\right]^{1/2}$$

Example: Compute the standard deviation for the particle in the box



First estimate $\Delta x \sim \frac{a}{2}$

Solution

$$\Delta x^2 \equiv \overline{x^2} - \cancelto{0}{\bar{x}}^2$$

$$(\Delta x)^2 = \int_{-\infty}^{\infty} dx \quad x^2 \; |\psi(x)|^2$$

$$(\Delta x)^2 = \int_{-a/2}^{a/2} dx \quad x^2 \; \frac{2}{a} \cos^2\left(\frac{\pi x}{a}\right)$$

$$(\Delta x)^2 = 2a^2 \int_{-a/2}^{a/2} \frac{dx}{a} \left(\frac{x}{a}\right)^2 \cos^2\left(\frac{\pi x}{a}\right)$$

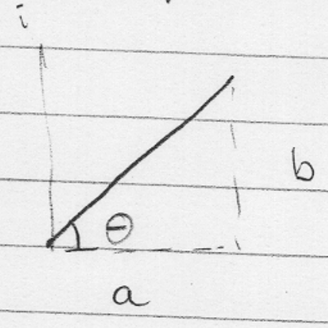
$$(\Delta x)^2 = 2a^2 \underbrace{\int_{-1/2}^{1/2} du \quad u^2 \cos^2(\pi u)}$$

$$u = \frac{x}{a}$$

$$(\Delta x)^2 = 2a^2 \left(\frac{-8 + \pi^2}{2\pi^3}\right) = a^2 \,(0.06)$$

$$\Delta x = \sqrt{a^2 (0.06)} \simeq a\,(0.25)$$

Reviewed Complex #'s



$z = a + bi$

$z = r\cos\theta + ir\sin\theta$ $\quad r = \sqrt{a^2+b^2}$ $\quad \theta = \tan^{-1}\left(\frac{b}{a}\right)$

Then

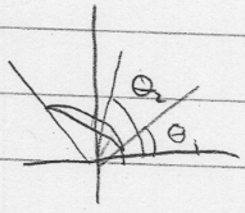
$e^{i\theta} = \cos\theta + i\sin\theta$

So

$z = re^{i\theta}$

Multiply Complex #'s

$z_1 z_2 = r_1 e^{i\theta_1} r_2 e^{i\theta_2} = r_1 r_2 e^{i(\theta_1+\theta_2)}$

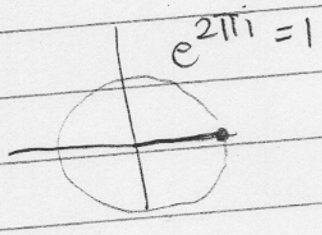


Also $\sqrt{z} = \sqrt{re^{i\theta}} = \sqrt{r}\, e^{i\theta/2}$

So Example

$$\sqrt{1} = \pm 1$$

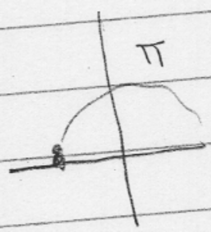
$1 = e^0$ and $1 = e^{2\pi i}$



So

$\sqrt{1} = e^{0/2}$ and $\sqrt{1} = e^{(2\pi i)/2}$

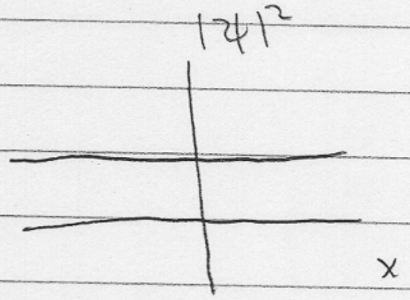
$\sqrt{1} = e^{i\pi} = -1$



Then we talked about the purest wave:

$\psi = Ce^{ikx}$ ← wavelength is precisely known

$\psi^* \psi = C^2 e^{-ikx} e^{ikx} = C^2$



But then the electron is equally likely to be anywhere

Superposition of two waves (Complex)

$$\psi_1 = e^{ik_1x} + e^{ik_2x} = e^{i15x} + e^{i16x}$$

$$\psi = (\cos(k_1x) + i\sin(k_1x)) + (\cos(k_2x) + i\sin(k_2x))$$

$$\psi = [\cos(k_1x) + \cos(k_2x)] + i[\sin(k_1x) + \sin(k_2x)]$$

$Re\,\psi$ = super position of two cos's
$Im\,\psi$ = super position of two sins

$$\bar{k}_0 = \frac{k_1+k_2}{2} = 15.5 \qquad \Delta k = k_2 - k_1 = 16-15 = 1$$

$$k_1 = \bar{k} - \frac{\Delta k}{2} \qquad k_2 = \bar{k} + \frac{\Delta k}{2}$$

So

$$\psi = e^{i(\bar{k}-\Delta k/2)x} + e^{i(\bar{k}+\Delta k/2)x} = e^{i\bar{k}x}\left(e^{i\frac{\Delta k x}{2}} + e^{-i\frac{\Delta k x}{2}}\right)$$

$$\psi = \underbrace{e^{ikx}}_{\text{Carrier wave}}\ \underbrace{2\cos\frac{\Delta k x}{2}}_{\text{envelope}} = 2(\cos\bar{k}x + i\sin(\bar{k}x))\cos\frac{\Delta k x}{2}$$

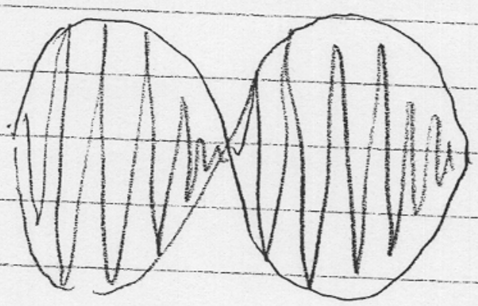
$$Im\,\psi = \underbrace{\sin(\bar{k}x)}_{\text{carrier wave}}\ \overbrace{2\cos\left(\frac{\Delta x}{2}\right)}^{\text{envelope}}$$

Summary

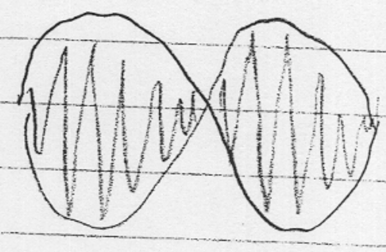
$$\psi_1 = e^{+ik_1x} + e^{ik_2x} = \overbrace{e^{i\bar{k}x}}^{\text{carrier}} \underbrace{2\cos(\Delta k\, x)}_{A(x) = \text{envelope funct}} = A(x)\, e^{i\bar{k}x}$$

Picture

Re ψ



Im ψ



$$|\psi|^2 = (A^*(x)\, e^{-i\bar{k}x})(A(x)\, e^{+i\bar{k}x}) = A^*(x)\, A(x)\, e^0$$

① $|\psi|^2 = |A(x)|^2$

The probability is determined by the envelope

② But $\psi = e^{i\bar{k}x} A(x)$

So the momentu / wavelength / wave number is determined by the rapidly fluctuating phase

$$\bar{p} = \hbar \bar{k}$$

Computing the average momentum (see handout)

$$\bar{p} = \sum_{\text{bins}} \hbar \bar{k}_{\text{bin}} \; P_{\text{bin}}$$

prob to be in bin

momentum in bin

$$\bar{p} = \sum_{\text{bins}} \hbar \bar{k} \; \psi^*(x)\, \psi(x)\, dx$$

$$= \sum_{\text{bin}} \underbrace{A^* e^{-ik\cdot x}}_{\psi^*} \; p \; \underbrace{e^{+ik\cdot x} A}_{\psi} \; dx$$

Watch:

$$p = -i\hbar \frac{d}{dx} e^{+ik\cdot x} = -i\hbar e^{+ikx} \, +ik = \hbar k \, e^{+ikx} = p e^{+ikx}$$

$$\boxed{-i\hbar \frac{d}{dx} e^{+ik\cdot x} = p \, e^{+ikx}}$$

$$\bar{p} = \sum \psi^* \quad p \quad \psi$$

$$\bar{p} = \sum_{bin} \underbrace{A^* e^{-ik\cdot x}}_{\psi^*} \; -i\hbar \frac{d}{dx} \underbrace{e^{+i\bar{k}x} A}_{\psi}$$

$$\boxed{\bar{p} = \int_{-\infty}^{\infty} dx \; \psi^* \, -i\hbar \frac{\partial}{\partial x} \, \psi}$$

Majic formula

$$-i\hbar \frac{d}{dx} e^{+ikx} = p \, e^{+ikx}$$

$$-i\hbar \frac{d}{dx}\left(-i\hbar \frac{d}{dx} e^{ikx}\right) = -i\hbar \frac{d}{dx} p \, e^{+ikx} = p^2 e^{+ikx}$$

<u>So</u>

$$\overline{p^2} = \sum_b \psi^* \; p^2 \; \psi$$

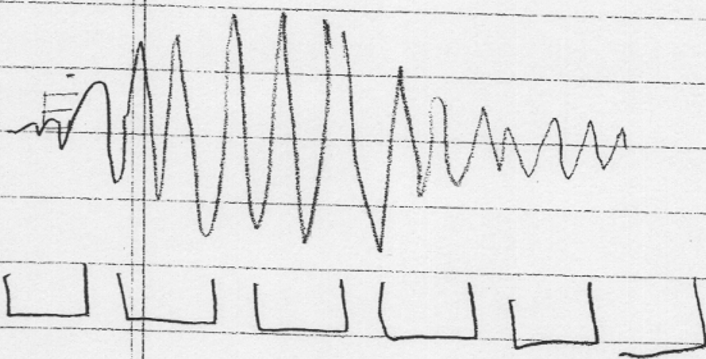
$$= \sum \psi^* \left(-i\hbar \frac{d}{dx}\right)^2 \psi$$

$$\overline{p^2} = \sum \psi^* \; -\hbar^2 \frac{d^2}{dx^2} \psi$$

$$KE = \frac{p^2}{2m} \quad \text{so.....}$$

$$\overline{KE} = \int_{-\infty}^{\infty} dx \; \psi^* \; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \; \psi \qquad KE \sim \frac{\hbar^2}{2mL^2}$$

So Far we've been discussing space what about time? and energy



$$\overline{E} = \sum_{bins} E_{bin} \cdot P_{bin}$$

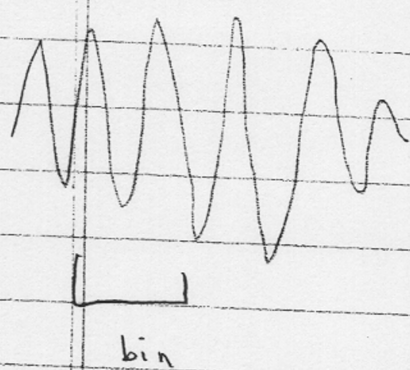
$$\overline{E} = \sum_{bins} E_{bin} \, |A|^2_{bin} \, dx = \sum_{bins} \underbrace{A^* e^{+i\omega t + ikx}}_{\psi^*} \; E_b \; \underbrace{A e^{-i\omega t +}}_{\psi}$$

Watch

$$+i\hbar \frac{d}{dt} e^{-i\omega t} = +i\hbar \, -i\omega \, e^{-i\omega t} = \hbar\omega \, e^{-i\omega t} = E \, e^{-i\omega t}$$

$$\boxed{\overline{E} = \int_{-\infty}^{\infty} dx \; \psi^* \; +i\hbar \frac{\partial}{\partial t} \; \psi}$$

The Schrödinger Equation



In a single bin we have two expressions for the energy

$$\psi^* \left[\frac{p^2}{2m} + V(x) \right] \psi(x) = \psi^* \left[E \right] \psi$$

$$\psi^* \left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = \psi^* \left[+i\hbar \frac{\partial}{\partial t} \right] \psi$$

So Find:

$$\boxed{\left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = +i\hbar \frac{\partial \psi}{\partial t}}$$