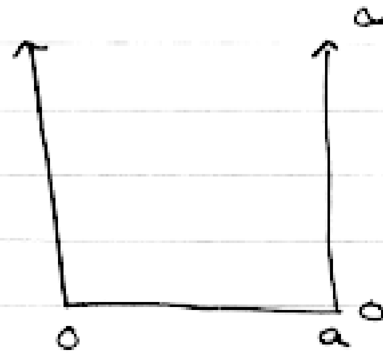
Inside the box



$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} = E_n\psi_n$$

FROM BEFORE

$$\psi_n = A\sin\left(\frac{n\pi}{a}x\right)$$

$n = 1, 2, 3, \ldots$

$\psi_n^2(x)$ tells us probability of finding the particle at x

$$\int_0^a \psi_n^2(x)\,dx = 1$$ the particle has to be in the box!

$$\int_0^a A^2\sin^2\left(\frac{n\pi}{a}x\right)dx = 1$$

Table of Integrals

$$A = \sqrt{\frac{2}{a}} \quad \therefore \quad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

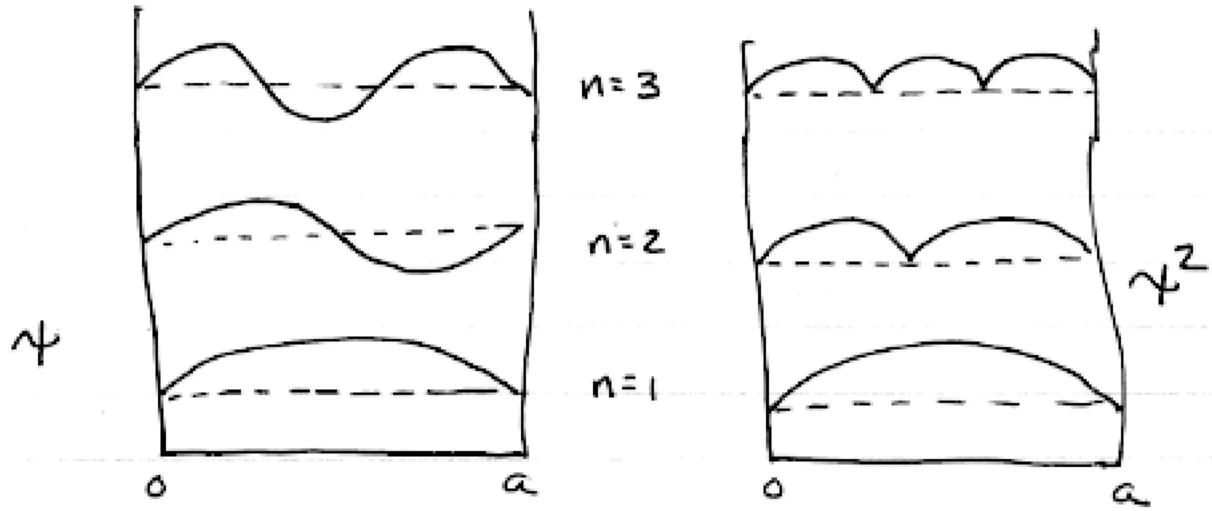
What about "n"?

It tells us that
$$\psi_1 = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)$$
$$\psi_2 = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)$$
$$\psi_3 = \sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right)$$
$$\vdots$$

Are all valid wavefunctions

HOMEWORK

Verify that $$\int_0^a \left[\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\right]^2 dx = 1$$



The picture at right says that for $n=2$, there is one position $\left(\frac{a}{2}\right)$ at which the probability of finding the electron is <u>ZERO</u>.

This a <u>wave</u> property, not intuitive for <u>particles</u>

Think <u>orbitals</u>: $\underbrace{2s \text{ or } 2p}_{n=2 \quad 1 \text{ node}}$ <u>vs.</u> $\underbrace{1s}_{n=1 \quad 0 \text{ nodes}}$

FINALLY $\mathcal{H}\psi_n = E_n\psi_n$

Calculate $E_n \Rightarrow$ $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\right) = E_n\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$

p.457

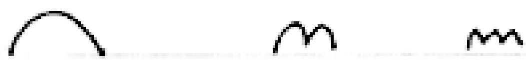
Solving $\Rightarrow$

$$E_n = \frac{\hbar^2\pi^2n^2}{2ma^2} = \frac{h^2n^2}{8ma^2}$$

$E_1 < E_2 < E_3 \ldots$

BIG CONCLUSION: <u>NATURE IS QUANTIZED</u>

The electron can exist
with the following probability distributions



but not  etc...

Also the electron can only have discrete (quantized)
~~values~~ energy values. <u>NOT INTUITIVE</u>!

For a 9.11×10^{-31} kg $e^{\ominus}$ in a 2.0 Å box,
allowed lowest energies are:

See Ex 9.1
p. 458-9

$E_1 = 1.5 \times 10^{-18}$ J $\qquad E_2 = 6.0 \times 10^{-18}$ J

BUT <u>NOT</u> 3.0×10^{-18} J

~~For a 0.2 kg billiard~~

1) Only certain energies allowed

2) Lowest energy is <u>not</u> 0 (!).

Q: Is a billiard ball quantized?

A 0.1 kg biliard ball in a 1 meter box

$$E_n = \left[\frac{(6.6\times10^{-34}\,J\cdot s)^2 (kg\cdot m^2\cdot s^{-2}\cdot J^{-1})}{8(0.1\,kg)(1m)^2} \right] n^2$$

$$\approx (5\times10^{-34}\,J)(n^2)$$

2) (Lowest) Zero point energy is much closer to 0, less than we can measure

Our measurements yield 0 "exactly"

1 ~~2~~) Spacing between allowed levels ~~is~~ is also on that order — too small to discriminate.
We measure a continuum of allowed levels.

Answer: Yes, but we would never know it.

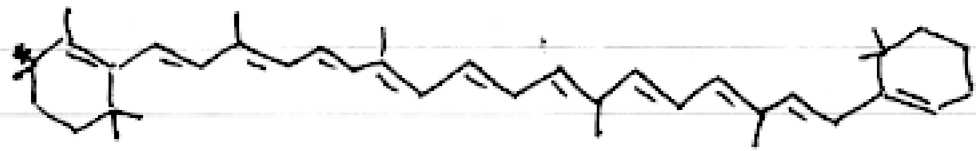
Implications of particle in a box

$$E_n = \frac{h^2 n^2}{8ma^2}$$

$$\underbrace{E_{n_2} - E_{n_1} = \frac{h}{8ma^2}(n_2^2 - n_1^2)}_{\text{energy of a transition}}$$

Example of a "box" from text/nature

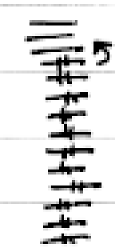
a



$\lambda_{MAX} = 452nm$ β - carotene

22π electrons
11 lowest E orbitals are therefore filled.

$$E_{N+1} - E_N = \frac{h^2}{8ma^2}\left[(N+1)^2 - N^2\right]$$



$$\Delta E = \frac{h^2}{8ma^2}(2N+1)$$

$$\Delta E = \frac{hc}{\lambda} \quad \text{light excitation}$$

$$\frac{hc}{\lambda} = \frac{h^2}{8ma^2}(2N+1)$$

$$\lambda_{N \to N+1} = \frac{8mca^2}{h(2N+1)}$$

$\lambda = 175nm$	$\lambda = 217nm$	$\lambda = 258nm$
		
$N=2$	$N=4$	$N=6$
a	bigger a	biggest a

a^2 gets big faster than $\frac{1}{2N+1}$ gets small

Bigger Box → longer wavelength