Probability & Statistics

Consider a random process which has a limited number of out comes

tossing a coin $n=2$
rolling a die $n=6$
answering a SAT question $n=4$

$$P_j = \lim_{N\to\infty} \frac{N_j}{N}$$

N_j ← number of trials with outcome j

N ← total number of trials

P_j : probability of out come j

Rules on probabilities : $0 \le P_j \le 1$

and since $\sum_j N_j = N, \Rightarrow \sum_j P_j = 1$

Averages : Average roll of a die gives what?

$$\bar{x} = \langle x \rangle = \sum_j x_j P_j$$

P_j ← probability of outcome j

x_j : value of x in outcome j

$$= 1\left(\tfrac{1}{6}\right) + 2\left(\tfrac{1}{6}\right) + 3\left(\tfrac{1}{6}\right) + 4\left(\tfrac{1}{6}\right) + 5\left(\tfrac{1}{6}\right) + 6\left(\tfrac{1}{6}\right)$$

$$= \frac{1+2+3+4+5+6}{6} = \frac{21}{6} = 3.5$$

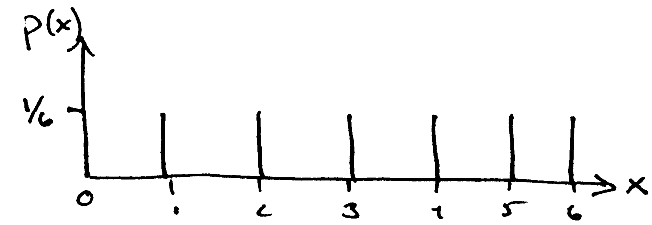
not one of the outcomes!

Loaded dice give very different means.
(let's construct a die that gives 6 more often)

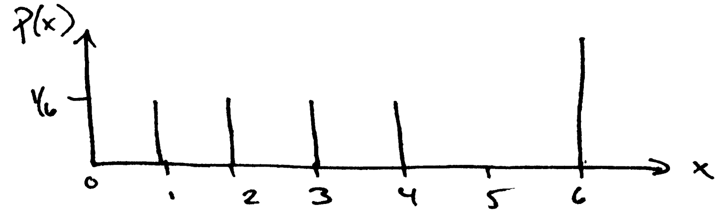
$$\langle x \rangle_{\text{cheater}} = 1\left(\tfrac{1}{6}\right) + 2\left(\tfrac{1}{6}\right) + 3\left(\tfrac{1}{6}\right) + 4\left(\tfrac{1}{6}\right) + 5(0) + 6\left(\tfrac{1}{3}\right)$$

$$= \frac{10}{6} + 2 = \frac{22}{6} = 3\tfrac{2}{3}$$

We can plot $p(x)$ ← the probability of an outcome
vs. x ← the outcome



← normal die



← cheater die

The second moment

$$\langle x^2 \rangle = \sum_j x_j^2 P_j$$

The average value of the square of the outcome.

Examples:

Normal die : $\langle x^2 \rangle = \dfrac{1+4+9+16+25+36}{6} = 15.16\overline{6}$

Cheater die: $\langle x^2 \rangle = \dfrac{1+4+9+16}{6} + \dfrac{36}{3} = 17$

The Standard Deviation:

σ_x ← sometimes called the uncertainty in x

Variance

$$\sigma_x^2 = \langle (x-\bar{x})^2 \rangle = \sum_j (x_j - \bar{x})^2 P_j$$

The average square deviation from the average

$$= \sum_j (x_j - \bar{x})(x_j - \bar{x}) P_j = \sum_j (x_j^2 - 2x_j\bar{x} + \bar{x}^2) P_j$$

$$\sigma_x^2 = \sum_j x_j^2 p_j - 2\sum_j x_j \bar{x} p_j + \sum_j \bar{x}^2 p_j$$

For a given process, $\bar{x}$ is an average quantity, and is constant.
Since $\bar{x}$ doesn't depend on j (outcome), it can come out of the sums here and:

$$\sigma_x^2 = \underbrace{\sum_j x_j^2 p_j}_{= \langle x^2 \rangle} - 2\bar{x} \underbrace{\sum_j x_j p_j}_{= \bar{x}} + \bar{x}^2 \underbrace{\sum_j p_j}_{= 1}$$

$$\sigma_x^2 = \langle x^2 \rangle - 2\langle x \rangle^2 + \langle x \rangle^2$$

$$= \langle x^2 \rangle - \langle x \rangle^2$$

$$\sigma_x = \sqrt{\sigma_x^2} = \left(\langle x^2 \rangle - \langle x \rangle^2\right)^{1/2}$$

Examples:

Normal dice: $\sigma_x = \sqrt{15.16\bar{6} - (3.5)^2} = 1.707$

Cheater dice: $\sigma_x = \sqrt{17 - (3.6\bar{6})^2} = 1.8856$

One interesting property of σ_x^2

$$\sigma_x^2 = \sum_j \underbrace{(x_j - \bar{x})^2}_{\text{square, always } \geq 0} p_j$$ ← Probability ≥ 0

$\therefore \sigma_x^2 \geq 0$

Continuous distributions

Last time we defined some important probability concepts for discrete outcomes:

Boundedness : $0 \le P_j \le 1$

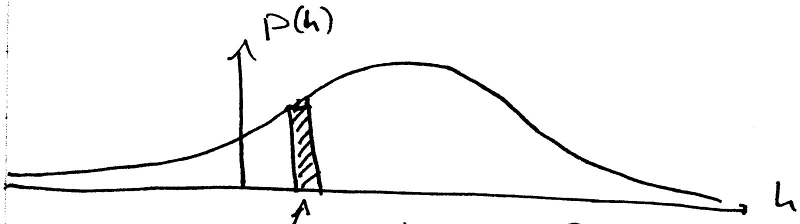
Conservation : $\sum_{j=1}^{n} P_j = 1$

means : $\langle x \rangle = \sum_{j=1}^{n} x_j P_j$

2nd moments : $\langle x^2 \rangle = \sum_{j=1}^{n} x_j^2 P_j$

Std. Dev. : $\sigma_x^2 = \sum_{j=1}^{n} (x_j - \langle x \rangle)^2 P_j$

Now, Consider the probability of finding someone with a height between 5'3" & 5'4" $= P(h) \underbrace{dh}_{\text{width of measurement} = 1}$



p(h) dh = fraction of people with heights between 5'3" & 5'4"

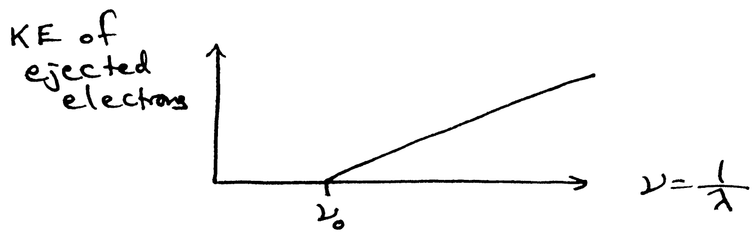
Some analogies between discrete outcomes (dice) & continuous outcomes (height)

	Discrete	Continuous
Boundedness :	$0 \le P_j \le 1$	$\cancel{0 \le p(h) \le 1}$ ← not alway true!
Conservation :	$\sum_{j=1}^{n} P_j = 1$	$\int_{-\infty}^{\infty} p(h)\,dh = 1$
Mean :	$\langle x \rangle = \sum_{j=1}^{n} x_j P_j$	$\langle h \rangle = \int_{-\infty}^{\infty} h\, p(h)\,dh$
2nd Moment :	$\langle x^2 \rangle = \sum_{j=1}^{n} x_j^2 P_j$	$\langle h^2 \rangle = \int_{-\infty}^{\infty} h^2\, p(h)\,dh$
Variance ~~Std. Dev.~~ :	$\sigma_x^2 = \sum_{j=1}^{n} (x_j - \langle x \rangle)^2 P_j$	$\sigma_h^2 = \int_{-\infty}^{\infty} (h - \langle h \rangle)^2 p(h)\,dh$
Std. Dev. :	$\sigma_x = \sqrt{\sigma_x^2}$	$\sigma_h = \sqrt{\sigma_h^2}$

De Broglie's wavelength

- Some experiments show light to have wave-like properties (eg. refraction from a prism or 2-slit experiments)

- Some experiments show light to have particle-like properties (e.g. the photoelectric effect and low-fluence 2-slit experiments)



De Broglie hypothesized that there was a wave/particle duality for light, and using the photoelectric effect he argued that high frequency (small wavelength) light has more momentum than low frequency light

$$\text{wavelength} \rightarrow \lambda = \frac{h}{p} \begin{array}{l} \leftarrow \text{constant (Planck's constant)} \\ \leftarrow \text{momentum } (p = mv) \end{array}$$

Why not reverse this and find λ for particles?

Baseballs: 5 oz = 0.14 kg @ 90 mph (40 m s^{-1})

$$p = mv = 5.6 \text{ kg m s}^{-1}$$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34} \text{ J}\cdot\text{s}}{5.6 \text{ kg m s}^{-1}} = 1.2 \times 10^{-34} \text{ m}$$

much smaller than a baseball

Electron in a 100V field:

$$\lambda = \frac{6.626 \times 10^{-34} \text{ J}\cdot\text{s}}{9.11 \times 10^{-31} \text{ kg} \;\; 5.9 \times 10^{6} \frac{\text{m}}{\text{s}}} = 1.2 \text{ Å}$$

larger than the size of an electron

Last time we talked a bit about

De Broglie's wavelength:

$$\lambda = \frac{h}{p}$$

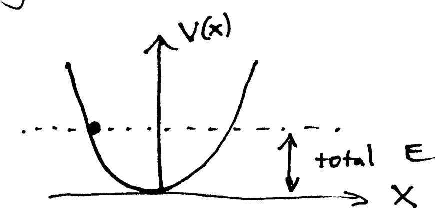
h ← Planck's constant

p ← equivalent momentum

λ ↖ wavelength of light

This connects wavelike behavior to a particle-like concept (momentum = mass * velocity)

Now let's briefly consider a particle (or a ball) rolling around on a potential energy surface



As the ball rolls, the potential energy $V(x)$ is converted into kinetic energy, but the sum is always constant.

$$E = KE + V(x)$$

Kinetic energy in 1D $= \frac{1}{2}mv^2 = \frac{1}{2m}(mv)^2 = \frac{p^2}{2m}$

$$E = \frac{p^2}{2m} + V(x)$$ ← let's solve this for p

∴

$$p^2 = 2m\,(E - V(x))$$

$$p = \sqrt{2m(E - V(x))}$$

← momentum can be a function of position.

If you are keeping track,:

$$\boxed{\lambda = \frac{h}{\sqrt{2m(E - V(x))}}}$$

← Use De Broglie's wavelength to connect a wave-like property to the potential energy

Now to Schrodinger:

1) Suppose particles <u>do</u> have a wavefunction
$\Psi(x,t)$

and suppose they <u>do</u> follow the classical wave equation:

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \Psi(x,t)}{\partial t^2}$$

- If we approach this like any other CWE problem, we'd try to separate the variables:

$$\Psi(x,t) = \psi(x)\,T(t)$$

And we'd guess that the time function $T(t)$ is a textbook solution to a 2^{nd} order ordinary differential equation:

$$T(t) = A\cos(\omega t) + B\sin(\omega t)$$

with some frequency <u>ω</u>

Putting this back in the wave equation, we get:

$$T(t)\frac{\partial^2 \psi(x)}{\partial x^2} = \psi(x)\frac{1}{v^2}\frac{\partial^2}{\partial t^2}\left[A\cos(\omega t) + B\sin(\omega t)\right]$$

$$= -\frac{\omega^2}{v^2}\psi(x)\,T(t)$$

Divide by $T(t)$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{\omega^2}{v^2}\psi(x) = 0$$

Details about <u>waves</u>: $\omega = 2\pi\nu \leftarrow$ frequency (s^{-1})

angular frequency (radians s^{-1})

$\nu\lambda = v \leftarrow$ <u>velocity</u> of the wave

<u>wavelength</u>

we have this in the wave equation

$$\frac{\omega}{v} = \frac{2\pi\nu}{\nu\lambda} = \frac{2\pi}{\lambda}$$

we've gotten rid of a wave property!

$$\frac{\omega^2}{v^2} = \frac{4\pi^2}{\lambda^2}$$

So:

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{4\pi^2}{\lambda^2}\psi(x) = 0$$

Now, we've reduced this to only <u>one</u> property of the wave, the <u>wavelength</u>,

and if we go back to our discussion of the ball rolling around, we found: $\lambda = \frac{h}{\sqrt{2m(E-V(x))}}$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m(E-V(x))\,4\pi^2}{h^2}\psi(x) = 0$$

$$-\frac{h^2}{4\pi^2(2m)}\frac{\partial^2 \psi}{\partial x^2} - E\psi(x) + V(x)\psi(x) = 0$$

$$\boxed{\hbar = \frac{h}{2\pi}}$$

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

$$\underbrace{\left[-\hbar^2\frac{\partial^2}{\partial x^2} + V(x)\right]}\psi(x) = E\psi(x)$$

This thing is called the <u>Hamiltonian</u> operator and what Schrodinger discovered is an <u>eigenvalue</u> equation that gives the <u>energies</u> of particular wavefunctions

$$\boxed{\hat{H}\,\psi(x) = E\psi(x)}$$

2 <u>big</u> ideas: <u>Particles have wavefunctions</u>, <u>Wavelength</u> is connected to <u>momentum</u>

The Rules

1) The State of a system is completely specified by the wavefunction $\psi(x)$

The Schrödinger equation is a lot like the classical wavefunction in that it sets down rules governing what kinds of wavefunctions we can have.

2) To every observable in classical mechanics, there corresponds a linear operator in QM.

The energy observable corresponds to $\hat{H}$, the Hamiltonian operator in Quantum Mechanics.

3) In any measurement of an observable, with operator $\hat{A}$, the only values we can measure are given by eigenvalue equations

$$\hat{A}\,\psi_n = a_n\,\psi_n$$

each n represents a "state" of the system

How is this different from classical rules?

$\psi(x) \longrightarrow x, v \longleftarrow$ position & velocity tell us about the current state of the system

only some things are observable $\longrightarrow$ all variables are observable

only some values can be measured $\longrightarrow$ all values can be measured

A brief reminder about eigenvalue equations:

$$\hat{A}\,\phi(x) = a\,\phi(x)$$

a: the eigenvalue

Suppose

$$\hat{A} = \frac{d^2}{dx^2} + 2\frac{d}{dx} + 3 \quad \text{and} \quad \phi(x) = e^{\alpha x}$$

$$\hat{A}\,\phi(x) = \frac{d^2}{dx^2} e^{\alpha x} + 2\frac{d}{dx} e^{\alpha x} + 3e^{\alpha x}$$

$$= \alpha^2 e^{\alpha x} + 2\alpha e^{\alpha x} + 3e^{\alpha x}$$

$$= (\alpha^2 + 2\alpha + 3)\,e^{\alpha x}$$

So, $e^{\alpha x}$ is an eigenfunction of $\frac{d^2}{dx^2} + 2\frac{d}{dx} + 3$

with eigenvalue $a = (\alpha^2 + 2\alpha + 3)$

The Schrodinger equation is also formulated as an eigenvalue equation

$$\underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]}_{\hat{H}} \psi(x) = E\,\psi(x)$$

$$\hat{H}\,\psi(x) = E\,\psi(x)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$\leftarrow$ the definition of the Hamiltonian in 1-D

This is the QM operator that "measures" energy.

One interesting consequence of identifying $\hat{H}$ with E:

$$\underset{\text{total Energy}}{E} = \underset{\text{kinetic}}{T} + \underset{\text{potential}}{V}$$

This means that

$$\hat{T}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad \left(\text{classically } T_x = \frac{1}{2}mv^2 = \frac{p^2}{2m}\right)$$

$$\frac{\hat{p}_x^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$\hat{p}_x^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

square of an operator: $\hat{p}_x^2 f \equiv \hat{p}_x(\hat{p}_x f)$

If $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$,

$$\hat{p}_x^2 f = \hat{p}_x\left(-i\hbar\frac{\partial f}{\partial x}\right) = (-i\hbar)^2\frac{\partial^2 f}{\partial x^2} = -\hbar^2\frac{\partial^2}{\partial x^2}f$$

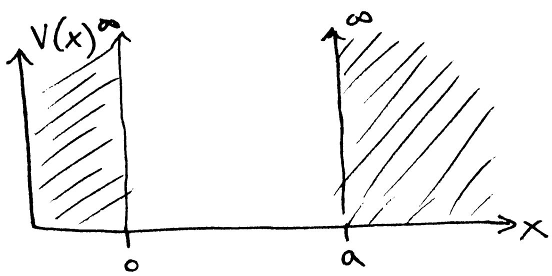
$$\therefore \quad \boxed{\hat{p}_x = -i\hbar\frac{\partial}{\partial x}}$$

What is $\psi(x)$?

ψ is interpreted as a measure of probability.

The probability of finding the particle between x & $x+dx$ $= |\psi(x)|^2 dx = \psi^*(x)\,\psi(x)\,dx$

Consider a particle-in-a-box:



The particle is restricted to the line (along the x axis). It can never go outside the range $0 \le x \le a$ because there are walls (infinitely high) of potential energy outside this.

Inside the box, there is no potential.

Start with the underlying physics providing guidance of ψ:

$$\hat{H}\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x) \qquad 0 \le x \le a$$

Since $|\psi(x)|^2$ is a measure of probability

$$\left.\begin{array}{ll} |\psi(x)|^2 = 0 & \text{when } x > a \\ |\psi(x)|^2 = 0 & \text{when } x < 0 \end{array}\right\} \Rightarrow \psi(x) = 0 \;\left\{\begin{array}{l} x > a \\ x < 0 \end{array}\right.$$

These are the Boundary Condition

Also, the partcle must be in the box

$$\underbrace{\int_{-\infty}^{\infty} p(x)\,dx = 1}_{\text{This is a normalization condition}} = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)\,dx = \int_0^a \psi^*(x)\psi(x)\,dx$$

Solving the particle-in-a-box:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad 0 < x < a$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \qquad \text{set } k = \frac{\sqrt{2mE}}{\hbar}$$

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

We've seen this exact differential equation a hundred times already! By now we should be able to write down the general solution without thinking:

$$\psi(x) = A\cos(kx) + B\sin(kx)$$

Verify:

$$\frac{d}{dx}\psi(x) = -kA\sin kx + kB\cos(kx)$$

$$\frac{d^2}{dx^2}\psi(x) = -k^2A\cos kx - k^2 B\sin kx \qquad = -k^2\psi(x)$$

$$-k^2\psi(x) + k^2\psi(x) = 0 \qquad \checkmark \qquad \text{great!}$$

So

$$\psi(x) = A\cos kx + B\sin kx \qquad \text{is a solution.}$$

Boundary conditions:

$$\psi(0) = 0 \implies A = 0 \implies \psi(x) = B\sin kx$$

$$\psi(a) = 0 \implies \psi(x) = B\sin\left(\frac{n\pi x}{a}\right) \qquad n = 1, 2, \ldots$$

and $k = \frac{n\pi}{a}$

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{a}$$

$$2mE = \frac{\hbar^2 n^2 \pi^2}{a^2}$$

$$E = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \longrightarrow \boxed{E = \frac{h^2 n^2}{8ma^2}}$$

Energy is Quantized only some energies are allowed!

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

$$\boxed{\psi_n(x) = B \sin \frac{n\pi x}{a}}$$

what is B?
How can we figure it out?

Boundary conditions gave us:

$\psi(0) = 0 \implies A = 0$

$\psi(a) = 0 \implies k = \frac{n\pi}{a}$, $E_n = \frac{h^2 n^2}{8ma^2}$

B? There must be a particle somewhere!

$$\int_{-\infty}^{\infty} P(x)\, dx = 1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)\, dx$$

In our case $\psi(x) = 0$ outside the box, so

$$1 = \int_0^a \psi^*(x)\psi(x)\, dx$$

$$= \int_0^a \left(B \sin\left(\frac{n\pi x}{a}\right)\right)^* \left(B \sin\left(\frac{n\pi x}{a}\right)\right) dx$$

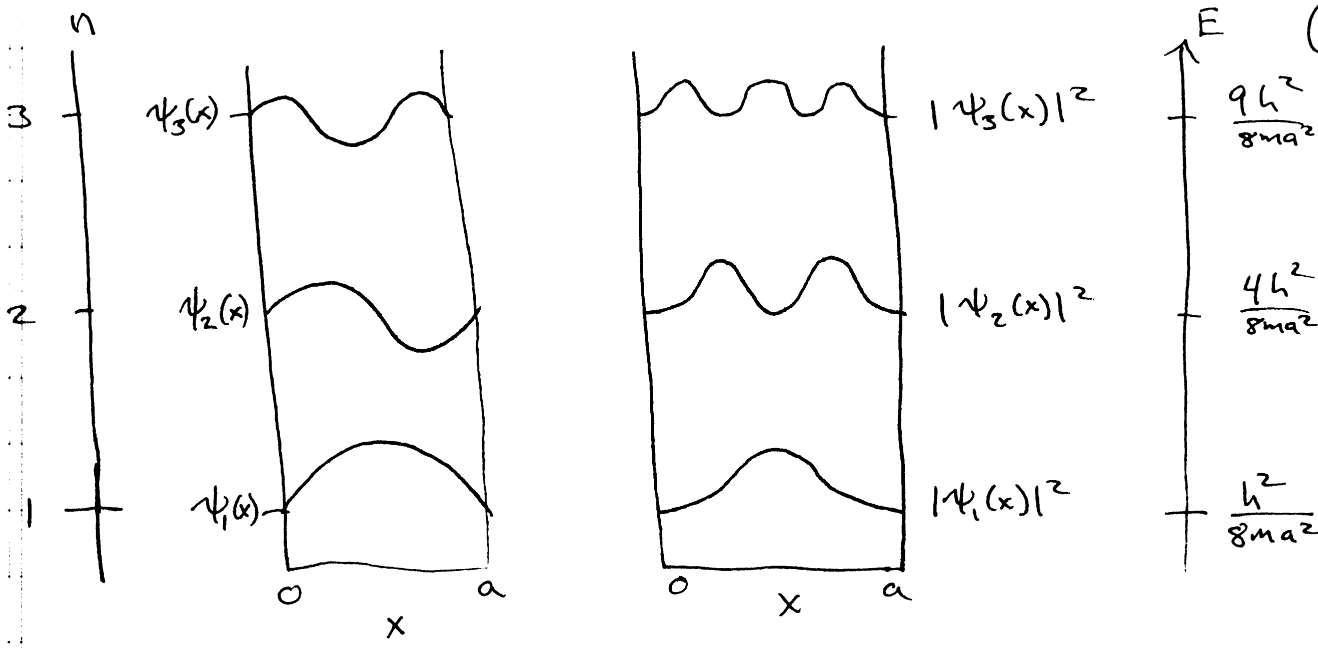
complex?

n = + integer
π = real
x = real
a = real
$\sin \frac{n\pi x}{a}$ = real

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

$$1 = B^* B \left(\frac{a}{2}\right) \implies B = \sqrt{\frac{2}{a}}$$

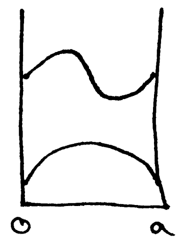
$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)}$$



\# of nodes = $n-1$

Can the particle <u>ever</u> be found at the node?
If not, how does it get to the other side?

Last time, we solved the particle-in-a-box wavefunctions:



$$\psi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \qquad E_2 = \frac{4h^2}{8ma^2}$$

$$\psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \qquad E_1 = \frac{h^2}{8ma^2}$$

General solutions:
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$
$$E_n = \frac{n^2 h^2}{8ma^2}$$

Today we'll talk about measurement, particularly: 1) where's the particle
2) where's it going?

Operators are used to make measurements:

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \quad \longleftarrow \text{Hamiltonian} \rightarrow \text{measures}$$

$$E = KE + V(x) \quad \longleftarrow \text{energy}$$

This means that

$$KE = \frac{1}{2}mv_x^2 = \underbrace{\frac{p_x^2}{2m}}_{\text{Classical}} \Rightarrow \underbrace{\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\text{quantum}}$$

The momentum $\hat{p}_x$ is what? $\quad \hat{p}_x^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$

If $\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \Rightarrow \hat{p}_x(\hat{p}_x f) = \hat{p}_x\left(-i\hbar\frac{\partial f}{\partial x}\right) = +i^2\hbar^2\frac{\partial^2}{\partial x^2}$
$= -\hbar^2\frac{\partial^2}{\partial x^2}$

$\therefore \quad \hat{p}_x = -i\hbar\frac{\partial}{\partial x} \quad \longleftarrow$ this is the operator that "measures" momentum.

Averages or Expectation values

$$\langle x \rangle_n = \int_{-\infty}^{\infty} \psi_n^*(x)\, \hat{x}\, \psi_n(x)\, dx$$

operator acts on wave function to the right.

$$\langle p_x \rangle_n = \int_{-\infty}^{\infty} \psi_n^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_n(x)\, dx$$

Let's spend a bit of time doing these:

$$\langle x \rangle_n = \int_{-\infty}^{\infty} \psi_n^*(x)\ \hat{x}\ \psi_n(x)\ dx$$

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

substitute: $\alpha = \frac{n\pi}{a}$

$$= \frac{2}{a}\left[\frac{x^2}{4} - \frac{x \sin\left(\frac{2n\pi x}{a}\right)}{4n\pi/a} - \frac{\cos\left(2n\pi x/a\right)}{8\ n^2\pi^2/a^2}\right]_0^a$$

$$= \frac{2}{a}\left[\frac{a^2}{4} - 0 - \frac{1}{8\frac{n^2\pi^2}{a^2}} - 0 + 0 + \frac{1}{8\frac{n^2\pi^2}{a^2}}\right]$$

$$\langle x \rangle_n = \frac{2}{a}\left[\frac{a^2}{4}\right] = \frac{a}{2}$$

← the average position is always in the center of the box (in <u>any</u> state)

What's the average momentum?

$$\langle p_x \rangle_n = \int_{-\infty}^{\infty} \psi_n^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right) \psi_n(x)\ dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \psi_n^*(x) \frac{\partial}{\partial x} \psi_n(x)\, dx$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

$$\frac{\partial}{\partial x}\psi_n = \sqrt{\frac{2}{a}}\left(\frac{n\pi}{a}\right)\cos\frac{n\pi x}{a}$$

$$\langle p_x \rangle_n = -i\hbar\left(\frac{2}{a}\right)\left(\frac{n\pi}{a}\right)\int_0^a \sin\frac{n\pi x}{a} \cos\frac{n\pi x}{a}\, dx$$

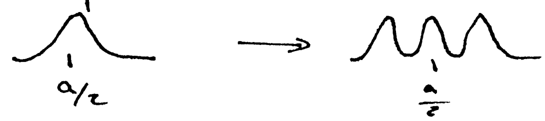
$$= \frac{-i\hbar 2\pi n}{a^2}\left[\frac{a}{2n\pi}\sin^2\frac{n\pi x}{a}\right]_0^a$$

$$= \frac{-i\hbar 2\pi n}{a^2}\left[0 - 0\right] = 0$$

$\boxed{\text{Was there an easier way?}}$

We've learned so far that in any of the <u>energy eigenstates</u>, the particle is found on average with $\langle x \rangle_n = \frac{a}{2}$ $\quad \langle p_x \rangle_n = 0$

But the <u>spread</u> in position distribution is getting larger with increasing n:



We quantify the <u>spread</u> with a std deviation of <u>uncertainty</u>:

$$\sigma_x^2 = \langle x^2 \rangle_n - \langle x \rangle_n^2$$

These are not too hard to calculate:

$$\langle x^2 \rangle_n = \int_{-\infty}^{\infty} \psi_n^*(x)\, x^2\, \psi_n(x)\, dx$$

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

$$= \frac{2}{a}\left[\frac{x^3}{6} - \left(\frac{x^2}{4n\pi/a} - \frac{1}{8\left(\frac{n\pi}{a}\right)^3}\right)\sin\frac{2n\pi x}{a} - \frac{x\cos 2n\pi x/a}{4(n\pi/a)^2}\right]_0^a$$

$$= \frac{2}{a}\left[\frac{a^3}{6} - \left(\frac{a^3}{4\pi n} - \frac{a^3}{8n^3\pi^3}\right)\cancelto{0}{\sin(2n\pi)} - \frac{a^3}{4n^2\pi^2} - 0 + 0 - 0\right]$$

$$\langle x^2 \rangle_n = \frac{2}{a}\left[\frac{a^3}{6} - \frac{a^3}{4n^2\pi^2}\right] = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}$$

$\langle x^2 \rangle$ is <u>not</u> independent of n.

$$\sigma_{x_n} = \sqrt{\langle x^2 \rangle_n - \langle x \rangle_n^2} = \sqrt{\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4}}$$

$$= a\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}} = \frac{a}{2\pi n}\left(\frac{\pi^2 n^2}{3} - 2\right)^{1/2}$$

$$\sigma_{x_1} = a\sqrt{\frac{1}{12} - \frac{1}{2\pi^2}} = 0.18\,a$$ $\longleftarrow$ minimum uncertainty when $n = 1$

$$\lim_{n\to\infty} \sigma_{x,1} = a\sqrt{\frac{1}{12}} = 0.28\overline{8} \leftarrow \text{maximum uncertainty}$$

Momentum uncertainty:

$$\langle P_x^2 \rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\, \hat{P}_x^2\, \psi_n(x)\, dx$$

$$\hat{P}_x^2 = -\hbar^2 \frac{\partial^2}{\partial x^2} \Rightarrow \hat{P}_x^2 \psi_n(x) = -\hbar^2 \left(\frac{2}{a}\right)^{1/2} \frac{\partial^2}{\partial x^2} \sin\left(\frac{n\pi x}{a}\right)$$

$$= -\hbar^2 \sqrt{\frac{2}{a}} \left(\frac{n\pi}{a}\right)^2 - \sin\left(\frac{n\pi x}{a}\right)$$

$$\langle P_x^2 \rangle_n = \hbar^2 \frac{n^2\pi^2}{a^2}\left(\frac{2}{a}\right) \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$= \frac{2\hbar^2 n^2\pi^2}{a^3}\left[\frac{x}{2} - \frac{1}{4\left(\frac{n\pi}{a}\right)} \sin\frac{2n\pi x}{a}\right]_0^a$$

$$= \frac{2\hbar^2 n^2\pi^2}{a^3}\left[\frac{a}{2}\right] = \frac{\hbar^2 n^2\pi^2}{a^2} = \frac{h^2 n^2}{4a^2}$$

$\boxed{\text{was there an easier way?}}$

$$\sigma_{p,n} = \sqrt{\langle P_x^2 \rangle_n - \langle P_x \rangle_n^2}$$

$$= \sqrt{\frac{\hbar^2 n^2 \pi^2}{a^2}} = \frac{\hbar n\pi}{a} \leftarrow \text{minimum uncertainty when } n = 1$$

$$\sigma_x \sigma_p = \frac{a}{2\pi n}\left(\frac{\pi^2 n^2}{3} - 2\right)^{1/2} \frac{\hbar n\pi}{a} = \frac{\hbar}{2}\sqrt{\frac{\pi^2 n^2}{3} - 2}$$

Minimum uncertainty: $\frac{\hbar}{2}\sqrt{\frac{\pi^2}{3} - 2} \approx \hbar \times 0.567\ldots$

Heisenberg's uncertainty principle: $\sigma_x \sigma_p \geq \frac{\hbar}{2}$

We'll derive it later, but P-I-B follows the rule!

$$\langle E \rangle_n \overset{?}{=} \int_{-\infty}^{\infty} \psi_n^*(x) \, ? \, \psi_n(x) \, dx$$

$$\hat{H}! = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$\langle E \rangle_n = \int_{-\infty}^{\infty} \psi_n^*(x) \, \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_n(x) \, dx$$

$$= \frac{1}{2m} \int_{-\infty}^{\infty} \psi_n^*(x) \, -\hbar^2 \frac{\partial^2}{\partial x^2} \psi_n(x) \, dx$$

$$= \frac{\langle p_x^2 \rangle}{2m}$$

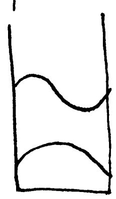
$$\langle E \rangle_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = \frac{h^2 n^2}{8ma^2}$$

The average energy in state n is exactly the same as the ~~eigenstate~~ eigenvalue of $\hat{H}$.

The Postulates of Quantum Mechanics

Today I want to put this on a more formal footing. QM operates with 5 postulates or rules for using and interpreting the quantities & functions.

We'll use (as a sample problem) the energy eigenstates of the particle in a box

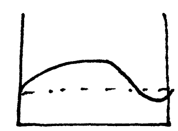


$$\left.\begin{aligned}\psi_2(x) &= \sqrt{\tfrac{2}{a}}\sin\frac{2\pi x}{a}\\ \psi_1(x) &= \sqrt{\tfrac{2}{a}}\sin\frac{\pi x}{a}\end{aligned}\right\}$$ These are energy eigenstates

$$\hat{H}\psi_n = E_n\psi_n$$

Last time, I asked you to consider what would happen if we prepared the system in a "mixed" state:

$$\psi = c\left[\psi_1(x) + \psi_2(x)\right] =$$



On to the postulates:

P1: The state of a system is completely described by $\psi(x)$, a well-behaved function of the position of the particle coordinates. $\psi^*\psi\,dx$ is a measure of probability:

"well-behaved" means:
1) single-valued
2) continuous
3) finite
4) normalizable
5) 1^{st} derivative is also single valued, continuous, and finite ← why?

3 & 5 are sometimes relaxed, but only ~~[illegible]~~ when $V(x)$ does something strange.

So, is our mixed state a well-behaved function?

continuous ✓ normalizable? if so: $\int_{\text{all space}} |\psi|^2 dx = 1$

single-valued ✓

finite ✓

$$\int_0^a \psi^* \psi \, dx = \int_0^a c^* \left(\psi_1^*(x) + \psi_2^*(x)\right) c\left(\psi_1(x) + \psi_2(x)\right) dx$$

$$= c^*c\left[\int_0^a (\psi_1^*\psi_1 + \psi_1^*\psi_2 + \psi_2^*\psi_1 + \psi_2^*\psi_2)\,dx\right]$$

$$= c^*c\left[\int_0^a \psi_1^*\psi_1\,dx + \int_0^a \psi_1^*\psi_2\,dx + \int_0^a \psi_2^*\psi_1\,dx + \int_0^a \psi_2^*\psi_2\,dx\right]$$

$$= c^*c\left[\frac{2}{a}\int_0^a \sin^2\frac{\pi x}{a}\,dx + \underbrace{\frac{2}{a}\int_0^a \sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx + \frac{2}{a}\int_0^a \sin\frac{2\pi x}{a}\sin\frac{\pi x}{a}\,dx}_{\text{These are on your next Homework.}} + \frac{2}{a}\int_0^a \sin^2\frac{2\pi}{a}\right.$$

$$= c^*c\left[\frac{2}{a}\left(\frac{a}{2}\right) + \frac{2}{a}(0) + \frac{2}{a}(0) + \frac{2}{a}\left(\frac{a}{2}\right)\right]$$

$$= c^*c\,2$$

If the function is normalizable

$$\int |\psi|^2 dx = c^*c\,2 = 1$$

$$c^*c = \frac{1}{2}$$

$$c = \frac{1}{\sqrt{2}} \Rightarrow \psi(x) = \frac{1}{\sqrt{2}}\left[\psi_1(x) + \psi_2(x)\right]$$

Postulate 2: To every observable in classical M there corresponds a linear operator in QM.

Postulate 3: $\hat{O}\psi_n = o_n\psi_n$ ← measured values will always be <u>eigenvalues</u> of the operator doing the measurement.

Back to our example wave function:

What **energies** will we measure with our particle in the mixed state?

$$\hat{H}\psi = \frac{1}{\sqrt{2}}\left(\hat{H}\psi_1 + \hat{H}\psi_2\right)$$

$$= \frac{1}{\sqrt{2}}\left(\frac{h^2}{8ma^2}\psi_1 + \frac{4h^2}{8ma^2}\psi_2\right) \leftarrow \psi \text{ is } \underline{\text{not}} \text{ an eigenfunction of } \hat{H}.$$

We measure energies of $\frac{h^2}{8ma^2}$ sometimes and $\frac{4h^2}{8ma^2}$ sometimes but we don't know when!

Postulate 4: If ψ is normalized, the average or expectation value of a measurement is

$$\langle A \rangle = \int_{\text{all space}} \psi^* \hat{A} \psi \, dx$$

So what's the average energy of our mixed state:

$$\langle E \rangle = \int_{\text{allspace}} \psi^* \hat{H} \psi \, dx$$

$$= \int_0^a \frac{1}{\sqrt{2}}\left(\psi_1^*(x) + \psi_2^*(x)\right) \hat{H} \frac{1}{\sqrt{2}}\left(\psi_1(x) + \psi_2(x)\right) dx$$

$$= \frac{1}{2}\int_0^a \left(\psi_1^* + \psi_2^*\right)\left(\hat{H}\psi_1 + \hat{H}\psi_2\right) dx$$

$$= \frac{1}{2}\int_0^a \left(\psi_1^* + \psi_2^*\right)\left(\frac{h^2}{8ma^2}\psi_1 + \frac{4h^2}{8ma^2}\psi_2\right) dx$$

$$= \frac{1}{2}\left(\frac{h^2}{8ma^2}\right)\int_0^a \left(\psi_1^* + \psi_2^*\right)\left(\psi_1 + 4\psi_2\right) dx$$

$$= \frac{1}{2}\left(\frac{h^2}{8ma^2}\right)\left[\int_0^a \psi_1^*\psi_1 \, dx + 4\int_0^a \psi_1^*\psi_2 \, dx + \int_0^a \psi_2^*\psi_1 \, dx + 4\int_0^a \psi_2^*\psi_2 \, dx\right]$$

$$\langle E \rangle = \frac{h^2}{8ma^2}\left(\frac{1}{2}\right)\left[1 + 4(0) + 0 + 4(1)\right]$$

$$\langle E \rangle = \frac{5}{2}\frac{h^2}{8ma^2} = \frac{1}{2}\left(\frac{h^2}{8ma^2} + \frac{4h^2}{8ma^2}\right)$$

($\frac{1}{2}$ of the times we measure $\frac{h^2}{8ma^2}$
$\frac{1}{2}$ of the times we measure $\frac{4h^2}{8ma^2}$)

Something to ponder:
whats $\langle p_x \rangle$ of $\langle x \rangle$ for this mixed state?

Postulate 5: The time-dependence of Ψ is governed by the time dependent Schrödinger Equation

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

Let's consider what this means for energy eigenstates $\psi_n(x)$

$$\Psi(x,t) = \psi_n(x)\, f_n(t) \quad \leftarrow \text{separation of variables}$$

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

$$\frac{1}{\psi_n(x)}\,\hat{H}\,\psi_n(x) = \frac{i\hbar}{f_n(t)}\,\frac{\partial f_n(t)}{\partial t}$$

since $\psi_n(x)$ is an eigenfunction of $\hat{H}$

$$\frac{E_n\,\psi_n(x)}{\psi_n(x)} = \frac{i\hbar}{f_n(t)}\,\frac{\partial f_n(t)}{\partial t}$$

$$\frac{d f_n(t)}{dt} = \frac{-iE_n}{\hbar}\,f_n(t)$$

$$\frac{d f_n(t)}{f_n(t)} = \frac{-iE_n}{\hbar}\,dt$$

$$\ln f_n(t) = \frac{-iE_n t}{\hbar} \implies f_n(t) = e^{-iE_n t/\hbar}$$

So, when ψ is an eigenfunction of $\hat{H}$:

$$\Psi_n(x,t) = \psi_n(x) e^{-iE_n t/\hbar}$$

Is $\Psi_n(x,t)$ normalized?

$$1 = \int_{\substack{\text{all}\\ \text{space}}} \Psi^*(x,t)\, \Psi(x,t)\, dx$$

$$= \int \psi_n^*(x) e^{+iE_n t/\hbar} \psi_n(x) e^{-iE_n t/\hbar} dx.$$

time dependence drops out!

$$1 = \int \psi_n^*(x)\, \psi_n(x)\, dx$$

So if $\psi_n(x)$ was normalized $\psi_n(x) e^{-iE_n t/\hbar}$ is also!

What about mixed states:

$$\psi(x) = \frac{1}{\sqrt{2}}\left(\psi_1(x) + \psi_2(x)\right)$$

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\Psi_1(x,t) + \Psi_2(x,t)\right)$$

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_1(x) e^{-iE_1 t/\hbar} + \psi_2(x) e^{-iE_2 t/\hbar}\right)$$

24.5

Now, what's $\langle x(t) \rangle$

$$\langle x(t) \rangle = \int_{\substack{\text{all}\\ \text{space}}} \Psi^*(x,t)\, \hat{x}\, \Psi(x,t)\, dx$$

$$= \frac{1}{2}\left[\int \left(\psi_1^* e^{iE_1 t/\hbar} + \psi_2^* e^{iE_2 t/\hbar}\right) x \left(\psi_1 e^{-iE_1 t/\hbar} + \psi_2 e^{-iE_2 t/\hbar}\right) dx\right.$$

$$= \frac{1}{2}\left[\int \psi_1^* x \psi_1\, dx + \int \psi_2^* x\, \psi_2\, dx + e^{-i(E_2 - E_1)t/\hbar} \int \psi_1^* x\, \psi_2\, dx \right.$$
$$\left. + e^{-i(E_1 - E_2)t/\hbar} \int \psi_2^* x\, \psi_1\, dx \right]$$

24.5

$$\langle E(t)\rangle = \int \Psi(x,t)^* \hat{H} \Psi(x,t)\, dx$$

$$= \int \left(\frac{1}{\sqrt{2}}\right)^2 \left(\psi_1^*(x) e^{+iE_1 t/\hbar} + \psi_2^*(x) e^{+iE_2 t/\hbar}\right) \hat{H} \left(\psi_1(x) e^{-iE_1 t/\hbar} + \psi_2(x) e^{-iE_2 t/\hbar}\right)$$

$$= \frac{1}{2}\Big[\int \psi_1^* \hat{H} \psi_1\, dx\, e^{+iE_1 t/\hbar} e^{-iE_1 t/\hbar} + \int \psi_1^* \hat{H} \psi_2\, e^{+i(E_1-E_2)t/\hbar}$$

$$+ \int \psi_2^* \hat{H} \psi_1\, e^{+i(E_2-E_1)t/\hbar} + \int \psi_2^* \hat{H} \psi_2\, e^{+(E_2-E_2)t/\hbar}$$

$$= \frac{1}{2}\Big[E_1 \cancel{\int \psi_1^* \psi_1}^{\,1} + E_2 \cancel{\int \psi_1^* \psi_2}^{\,0} e^{+i(E_1-E_2)t/\hbar} + E_1 \cancel{\int \psi_2^* \psi_1}^{\,0} e^{+i(E_2-E_1)t/\hbar} + E_2 \cancel{\int \psi_2^* \psi_2}^{\,1} \Big]$$

$$= \frac{1}{2}\left(E_1 + E_2\right]$$

Side-effects of the postulates

1) Eigenvalues of Quantum operators correspond to real measurable quantities (positions, energies, etc.) and since the wavefunctions can be complex, this places some formal limits on the kind of operators we can use:

Hermitian operators

A Definition:
$\hat{A}$ is Hermitian if it has this property for all functions f & g.

3-identical forms:

$$\int f^* (\hat{A} g)\, dx = \int (\hat{A} f)^* g\, dx$$

$$\langle f \mid \hat{A} g \rangle = \langle \hat{A} f \mid g \rangle$$

$$\langle f \mid \overrightarrow{\hat{A}} \mid g \rangle = \langle f \mid \overleftarrow{\hat{A}} \mid g \rangle$$

Suppose we try this out with a single eigenfunction of $\hat{A}$: $\quad \hat{A} f = a_f f$

$$\int f^* (\hat{A} f)\, dx = \int f^* a_f f\, dx = a_f \int f^* f\, dx$$

$$\int (\hat{A} f)^* f\, dx = \int (a_f f)^* f\, dx = \int a_f^* f^* f\, dx$$
$$= a_f^* \int f^* f\, dx$$

If $\hat{A}$ is Hermitian:

$$a_f \int f^* f\, dx = a_f^* \int f^* f\, dx$$

$$a_f = a_f^* \quad \text{so } a_f \text{ is } \underline{\text{Real}}$$

P2′: All QM operators are linear Hermitian operators.

So, the eigenvalues (what we can measure) of QM operators are <u>real</u>.

Hermitian operators have another useful property — their eigenfunctions are orthogonal:

Suppose $\hat{A}$ is Hermitian and we have 2 eigenfunctions

$$\hat{A} f_n = a_n f_n \qquad \hat{A} f_m = a_m f_m$$

Also: $\quad f_n \neq f_m \qquad a_n \neq a_m$

$$\hat{A} f_n = a_n f_n \qquad \hat{A} f_m = a_m f_m$$

$$(\hat{A} f_m)^* = a_m^* f_m^*$$

$$\int f_m^* \hat{A} f_n \, dx = \int (\hat{A} f_m) f_n \, dx$$

$$a_n \int f_m^* f_n \, dx = a_m^* \int f_m^* f_n \, dx$$

$$(a_n - a_m^*) \int f_m^* f_n \, dx = 0$$

Since $a_n \neq a_m$ this means $\quad \int f_m^* f_n \, dx = 0$

So whenever we have eigenstates of a Quantum operator, we can assume:

1) The eigenvalues are real
2) The eigenstates are orthogonal

Uncertainty and the ~~Schwartz~~ inequality

Schwartz inequality:

$$\left(\int f^* f\,dx\right)\left(\int g^* g\,dx\right) \geq \left|\int f^* g\,dx\right|^2$$

One oddity of this general rule is that we can take 2 arbitrary operators multiplying ψ as these functions

$$f = (\hat{A} - \langle A \rangle)\psi$$
$$g = (\hat{B} - \langle B \rangle)\psi$$

and get this very bizarre result:

$$\sigma_A \sigma_B \geq \frac{1}{2}\left|\int \psi^* [\hat{A}, \hat{B}] \psi\,dx\right|$$

(the proof of this is not hard, but is tedious)

Remember that $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

← the "commutator"

So rather than going through the work of calculating $\langle A^2 \rangle$, $\langle A \rangle$, $\langle B^2 \rangle$, $\langle B \rangle$, we can calculate the <u>expectation value</u> of the <u>commutator</u> to find an uncertainty relation.

Suppose:

$$\hat{A} = x$$
$$\hat{B} = \hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

$$\hat{A}\hat{B}f = \hat{x}\left(-i\hbar \frac{\partial f}{\partial x}\right) = -i\hbar x \frac{\partial f}{\partial x}$$
$$\hat{B}\hat{A}f = -i\hbar \frac{\partial}{\partial x}(\hat{x}f) = -i\hbar\left(x\frac{\partial f}{\partial x} + f\frac{\partial x}{\partial x}\right) = -i\hbar\left(x\frac{\partial f}{\partial x} + f\right)$$

$$[\hat{A}, \hat{B}]f = \hat{A}\hat{B}f - \hat{B}\hat{A}f = -i\hbar x\frac{\partial f}{\partial x} + i\hbar x\frac{\partial f}{\partial x} + i\hbar f = i\hbar f$$

$$\therefore \quad [\hat{A}, \hat{B}] = i\hbar$$

Or: $[\hat{x}, \hat{p}_x] = +i\hbar$

$$\sigma_x \sigma_p \geq \frac{1}{2} \left| \int \psi^* [\hat{x}, \hat{p}_x] \psi \, dx \right|$$

$$\geq \frac{1}{2} \left| \int \psi^* \; i\hbar \; \psi \, dx \right|$$

$$\geq \frac{1}{2} \left| i\hbar \int \psi^* \psi \, dx \right|$$

If ψ is normalized

$$\geq \frac{1}{2} |i\hbar|$$

$$\geq \frac{1}{2} \sqrt{(-i\hbar)(i\hbar)}$$

$$\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$$

Heisenberg's Uncertainty principle!

One Last "Foundational" topic: Hilbert Spaces

Let's start with a vector space

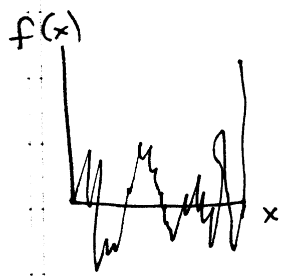
In cartesian coordinates, a vector is a set of components (v_x, v_y, v_z). Any vector can be written in terms of the 3 unit vectors or the basis set for this space

$$\vec{V} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = v_x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + v_y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + v_z \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

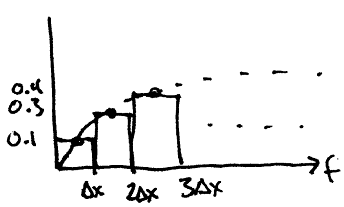
$$= v_x \hat{i} + v_y \hat{j} + v_z \hat{k}$$

$\hat{i}, \hat{j}$, and $\hat{k}$ form a complete basis for 3d space, i.e. they span the vector space.

Hilbert Spaces can have many dimensions. Consider the particle-in-a-box world with some arbitrary function $f(x)$.



We could describe $f(x)$ as a vector where each element was a small chunk of the line along x:



$$f(x) = 0.1 \times \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + 0.3 \times \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} + 0.4 \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}$$

$$+ \dots$$

This is not very efficient or sensible because we'd need to know Δx to describe a function and if we decide to change Δx (ie for a rapidly-varying function) we have to change all of our coefficients.

However, we could also write $f(x)$ in terms of other functions:

$$f(x) = 0.1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + 0.2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + 0.1 \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} + \ldots$$

represents $\sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}$ — represents $\sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}$ — represents $\sqrt{\frac{2}{a}} \sin \frac{3\pi x}{a}$

A Hilbert space is a functionspace where each function is treated as an independent vector.

$$\left.\begin{aligned} f(x) &= \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \\ &= \sum_{n=1}^{\infty} c_n \psi_n(x) \\ &= \sum_{n=1}^{\infty} c_n |n\rangle \end{aligned}\right]$$

← expansion of $f(x)$ in the energy eigenstates for the particle in a box

3 equivalent forms

In this case the Hilbert space has an infinite number of dimensions.

Consider a vector dot product:

$$\vec{v} \cdot \vec{u} = v_x u_x + v_y u_y + v_z u_z$$

← multiply the coefficients

In a Hilbert space we do something similar

$$\int f^*(x)\, g(x)\, dx$$

← Is this like a dot product? How?

$$f^*(x) = \sum_{n=1}^{\infty} c_n^* \psi_n^*(x)$$

$$g(x) = \sum_{n'=1}^{\infty} g_{n'} \psi_{n'}(x)$$

f & g have unique expansions in the same set of functions

$$\int f^*(x)\, g(x)\, dx = \int \left(\sum_{n=1}^{\infty} c_n^* \psi_n^*(x)\right)\left(\sum_{n'=1}^{\infty} g_{n'} \psi_{n'}(x)\right) dx$$

$$= \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \int c_n^* \psi_n^*(x)\, g_{n'} \psi_{n'}(x)\, dx$$

$$= \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} c_n^* g_{n'} \underbrace{\int \psi_n^*(x)\, \psi_{n'}(x)\, dx}$$

we <u>know</u> the states of the particle in a box are orthonormal, so

$$\int \psi_n^*(x) \psi_{n'}(x) dx = \delta_{nn'}$$

0 when n, n' are not the same

1 when $n = n'$

$$\int f^*(x)\, g(x)\, dx = \sum_{n=1}^{\infty} c_n^* g_n$$

massively complicated integral

<u>just like</u> a dot product (and very simple)

We're going to be using this as we move on into real problems.