Phys 137A

Quantum Mechanics

Preliminaries:

- Website: bcourses.berkeley.edu
- Poll on office hrs:
  * Thursday 2-3
  * Tuesday 11-12
- Grades

  HW: 30%

  Midterm: 30%

  Final: 40%

Midterm

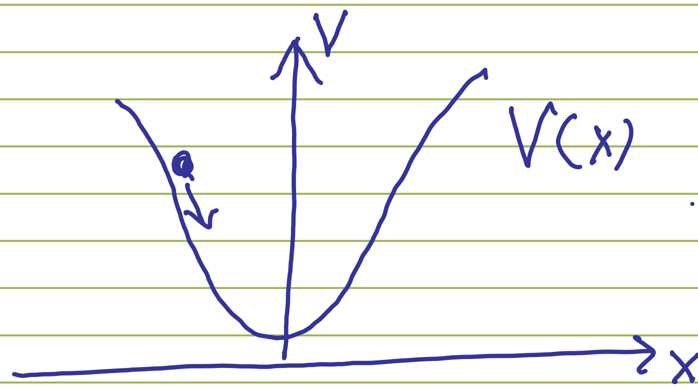
Thursday, Oct 18, in class

Final

Tuesday, Dec 12, TBA

Classical Mechanics

Particle of mass m in potential



Experiences a force:

$$F = -\frac{dV}{dx}$$

Newton's 2nd Law

$$ma = F,$$

with

$$a = \frac{dv}{dt}, \quad v = \frac{dx}{dt}$$

$$\Rightarrow \qquad m\frac{d^2}{dt^2}x + \frac{d}{dx}V = 0$$

Second order equation for

$$x = x(t)$$

$\Rightarrow$ Unique solution, given initial conditions

$$x(t_0) = x_0$$
$$v(t_0) = v_0$$

Classically:

motion in a given potential is completely determined, given

$$x_0, v_0$$

"Obviously" the particle has a definite, precisely determined

position: $x = x(t)$

velocity $v = \frac{d}{dt} x(t)$

for all time.

Several discoveries, at the end of 19'th century lead to realization that this description is only approximate.

There is a fundamental constant in nature, the Planck constant,

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

with units of

Energy × time:

In terms of everyday units of Joules and seconds the planck's constant is very small:

$$\boxed{\hbar = 1.054572 \times 10^{-34}\ J\cdot s}$$

Because it is so small, we do not notice it is not zero. But, the fact it isn't actualy zero, Becomes realy im portant for

microscopic objects

electrons, atoms, molecules.

This is analogous to modifications of classical physics which come from finite value of

$$c = 3 \times 10^{8}\ m/s$$

This is to a good approximation infinite, for velocities we ordinarily experience.

The discoveries were:

* Planck's explanation of black-Body radiation:

A Black Body emits EM radiation in chunks of energy

$$E = h\nu = \hbar\omega$$

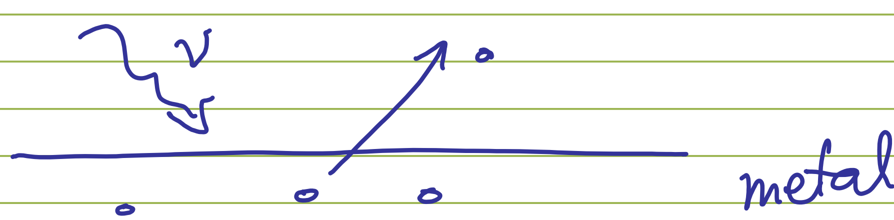
ν = frequency

angular frequency

* Photo-electric effect; Einstein 1905

$$E = h\nu$$

not only for emmission of EM waves, but for absorbtion too



Energy of knocked out electrons independent of Intensity of EM radiation - depends only on frequency :

$$E_{kin} = h\nu - E_{Binding}$$

- Atomic Spectra
  with quantized energy levels, and spacing $\to 0$ as $\hbar \to 0$.

Quantum mechanics

position $x(t)$ $\longrightarrow$ complex wave function $\psi(x,t)$

$\psi(x,t) \leftarrow$ complete information about the state system is in. "state"

Eqns of motion for $x(t)$ $\longrightarrow$ Eqn for wave function: $\psi(x,t)$

Schroedinger Eqn

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

Initial condition

$x_0 = x(0)$

$v_0 = v(0)$

$\longrightarrow$

Initial condition

$\Psi(x,0)$

Given $\Psi(x,0)$, can find

$\Psi(x,t)$ for all other times

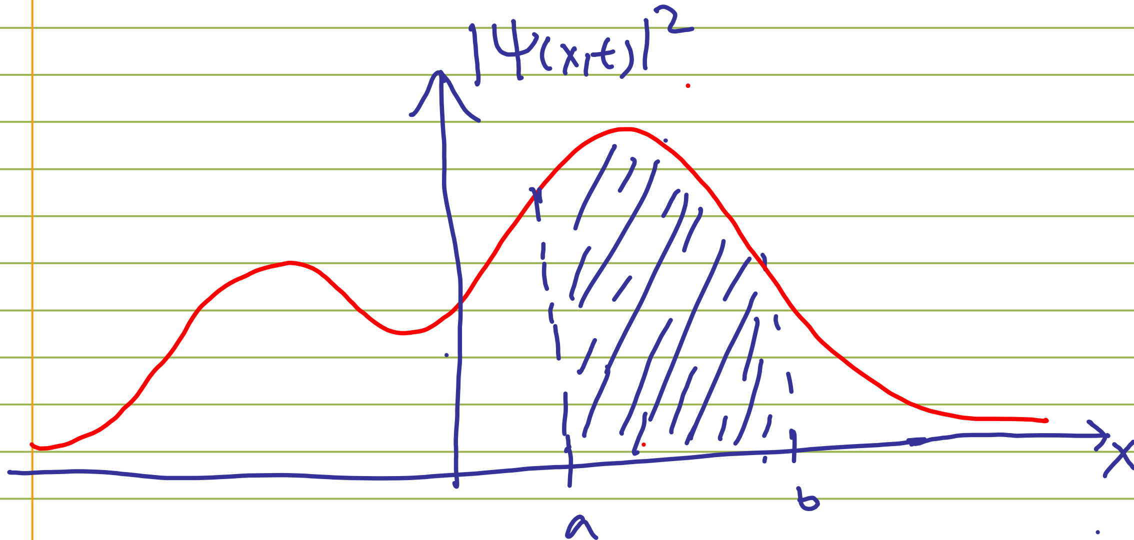
Quantum mechanics is just as deterministic as classical physics, just what can be determined is different!

all info is in $\Psi(x,t)$

Statistical interpretation

$$\int_a^b |\Psi(x,t)|^2 \, dx$$

= probability of finding a particle between a and B



Higher $|\Psi(x,t)|$ → higher prob.

While $\Psi(x,t)$ is complex probability density is always real.

What does probability mean?

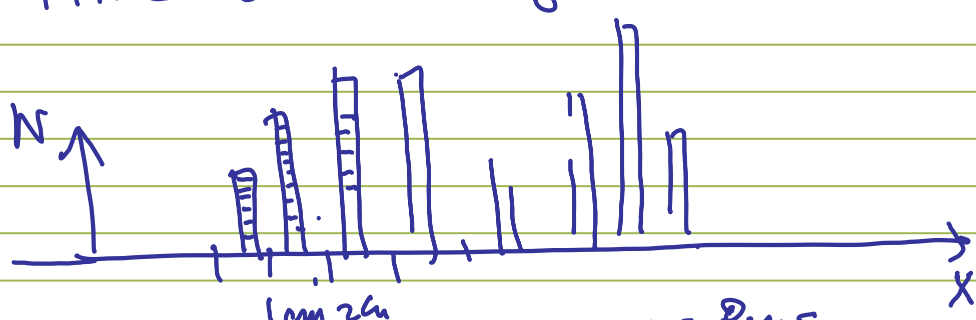
Suppose you have a very large number of particles,

10^6

and prepare each to be in same state

$\psi(x,t)$

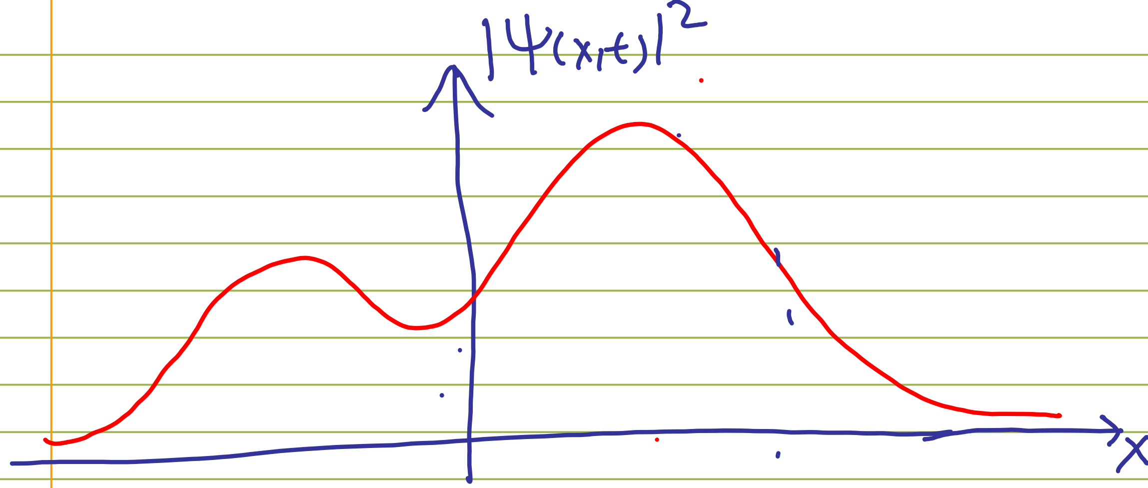
Measure their positions at time t (using 10^6 experimentalists)



sum over bins

$$\sum_i N_i = N = 10^6$$

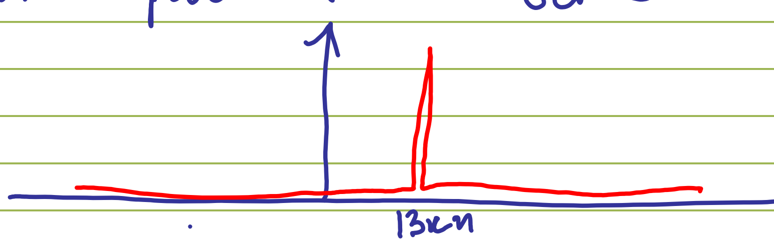
Move to smaller bins



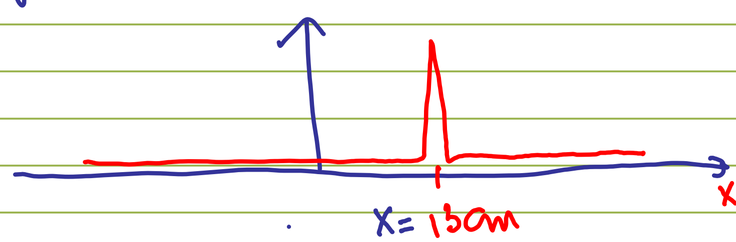
Suppose you instead have 1 experimentalist perform 10^6 measurements

$|\Psi(x,t)|^2$ "collapses" to a single spike, where particle was detected

Measure again the position of same particle: Get same state.



Every time, one detects a single whole particle, and distribution of outcomes is encoded by $|\Psi(x,t)|^2$. Interaction with apparatus disturbs $|\Psi(x,t)|^2$ to produce a different state



with definite position for electron.

There is a nice pedagogical setup that illustrates the difference between quantum and classical probabilities, and interplay of wave and particle natures

Probability & QM

Probability of an outcome A

$$P(A) = \frac{N_A}{N}$$

N = total # of possible outcomes

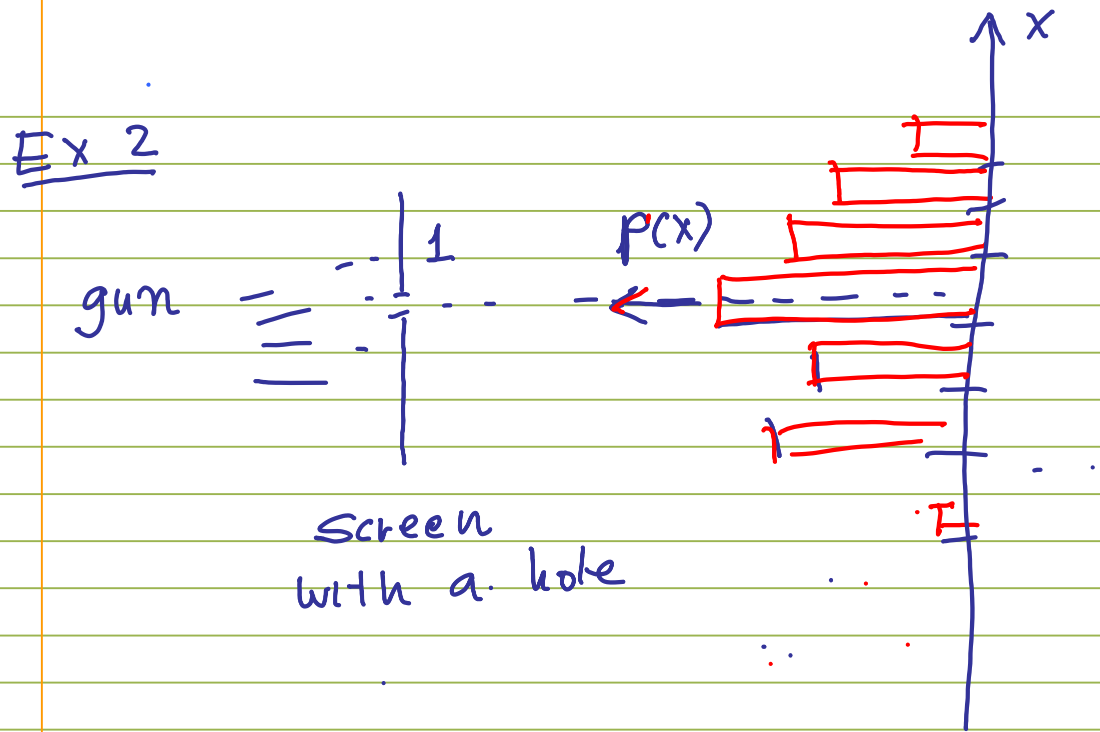
N_A = # of times A occurs

Ex 1 Throw a dice

$$N = 6$$

$$\sum_A P(A) = \frac{1}{6} + \quad + \frac{1}{6} = 1$$

Ex 2



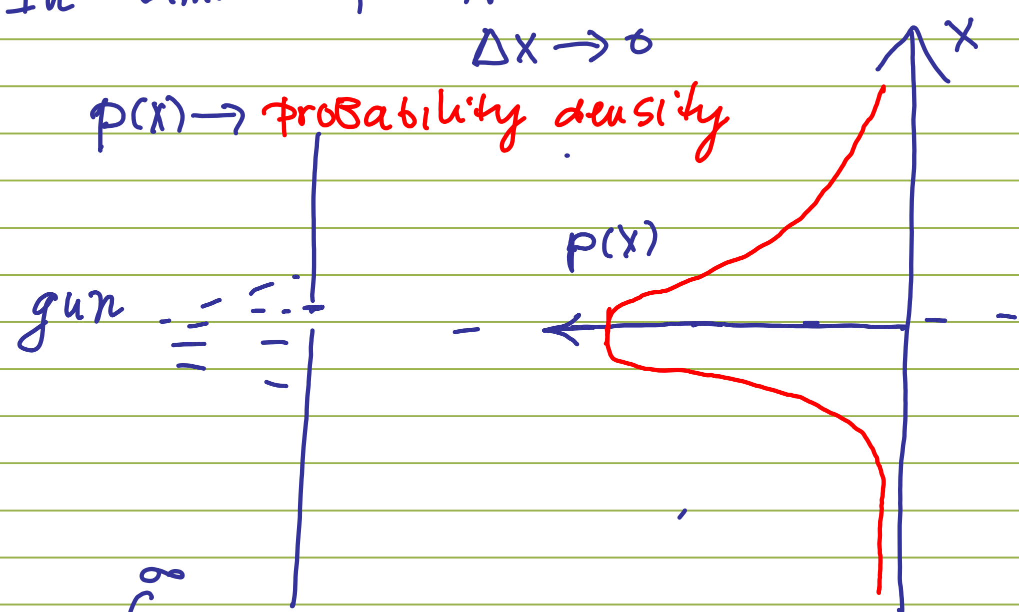
$$p(x) = \frac{\Delta N(x)}{N\,\Delta x}$$

$\Delta N(x)$ = Number of Bullets in Bin at x, width Δx

$$\sum_{\text{Bins}} p(x)\,\Delta x = 1$$

In Limit of $N \to \infty$
$\Delta x \to 0$

$p(x) \to$ probability density



$$\int_{-\infty}^{\infty} p(x)\,dx = 1$$

Probability of a Bullet
between $x=a$, $x=b$

$$\int_{+a}^{b} p(x)\,dx = P_{ab}$$

Ex 3

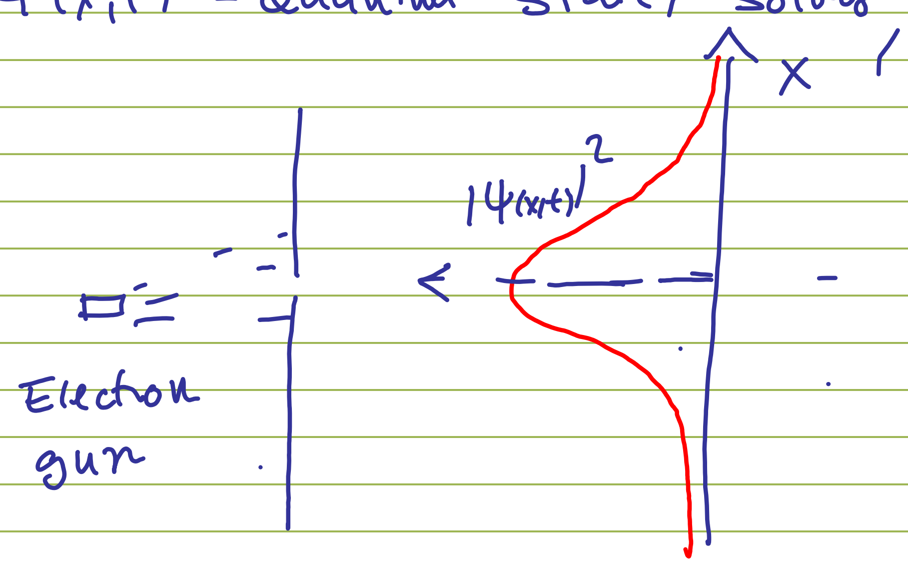
In Quantum mechanics

$$p(x,t) = |\Psi(x,t)|^2$$

probability can depend on time

$$= \Psi^*(x,t) \cdot \Psi(x,t)$$

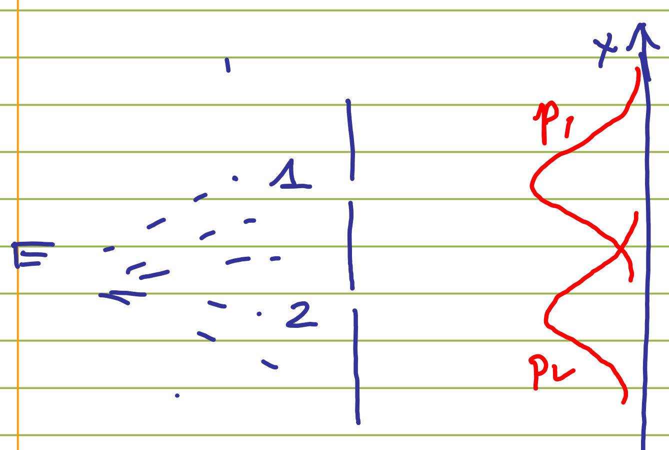
$\Psi(x,t)$ = quantum state, solving S.E.



(Refers to repeated experiments on particles in identically prepared state, not to state of particle after measurement.)

Important difference between electrons and Bullets,

Described in Feynman, Ch 1.



- Run experiment with Bullets

- Run experiment w/ electrons (in identically prepared state)

Pick a point on screen

$P_1(x)$ = probability for Bullet to pass through hole 1 and hit screen at x

$P_2(x)$ = same with hole 2

$P_{12}(x)$ = probability for Bullet to pass through either hole 1 or hole 2 and land at x

$$P_{12}(x) = P_1(x) + P_2(x)$$

classical probabilities add

$$P_{12}(x) = \frac{\Delta N_{12}(x)}{N\,\Delta x} = \frac{\Delta N_1(x) + \Delta N_2(x)}{N\,\Delta x}$$

$$= P_1(x) + P_2(x)$$

Run with electrons:

$$P_{12}(x) \neq P_1(x) + P_2(x)$$

Probabilities do not add!

What does add are the wave functions

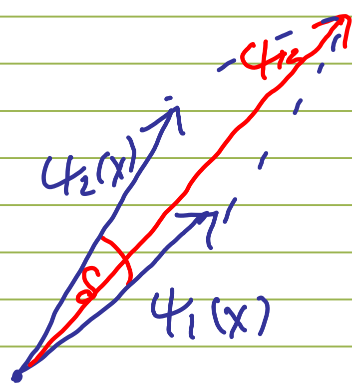
$$\psi_{12}(x) = \psi_1(x) + \psi_2(x)$$

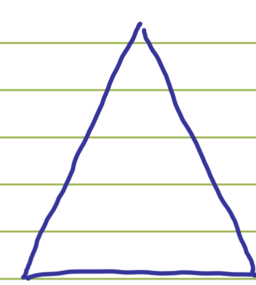
and $\quad P_{12}(x) = |\psi_{12}(x)|^2$

$$P_1(x) = |\psi_1(x)|^2, \quad P_2(x) = |\psi_2(x)|^2$$

The reason probabilities do not add are interference effects.

vectors in complex plane





$|\psi|$ = length of vector

$\delta =$ phase difference between ψ_1 and ψ_2

$$|\psi_1|^2 + |\psi_2|^2 \neq |\psi_1 + \psi_2|^2 = |\psi_{12}|^2$$

$$P_1 + P_2 \neq P_{12}$$

- "=" only if $\delta = \frac{\pi}{2}$

$\delta \neq \frac{\pi}{2}$ there are interference effects

For electrons, unlike for bullets probability or more precisely

$\psi(x,t)$

is <u>fundamental</u>.

For bullets, we can remove prob. aspects by keeping better track of data. Not so with electrons.

If we replace electrons by photons the wave aspect is familiar

$$\psi(x,t) \propto \text{EM wave } E(x,t)$$

$$p(x,t) = |\psi(x,t)|^2 \propto$$

Intensity of EM wave (photon flux)

Normalization

For $|\Psi(x,t)|^2$ to describe probability density, it has to be normalized:

$$\int_a^b |\psi(x,t)|^2 dx = $$ probability to find particle between a and b

Require: $$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$$

"Particle has to be somewhere with probability 1."

To require

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dt = 1 \qquad (*)$$

is to fix normalization of wave function.

A-priori (*) seems like a different equation for $\psi(x,t)$ for every separate t. Can we satisfy this?

Claim:
$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx$$
is independent of time, so if
$$\int_{-\infty}^{\infty} |\psi(x,0)|^2 dx = 1$$
at one time, it is true at all times.

We need to show
$$\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 0$$
Independent of time

Use
$$\frac{d}{dt}\int |\psi(x,t)|^2 dx = \int \psi^* \frac{\partial}{\partial t}\psi(x,t)\, dx$$
$$+ \int \frac{\partial}{\partial t}\psi^*(x,t)\,\psi(x,t)\, dx$$
and use Schrodinger eqn for ψ and ψ^*:

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

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

It follows

$$i\hbar \int \left(\psi^* \frac{\partial}{\partial t}\psi + \frac{\partial}{\partial t}\psi^* \psi\right) dx =$$

$$= -\frac{\hbar^2}{2m}\int \left(\psi^* \frac{\partial^2}{\partial x^2}\psi - \frac{\partial^2}{\partial x^2}\psi^* \psi\right) dx$$

$$= -\frac{\hbar^2}{2m}\int \frac{\partial}{\partial x}\left(\psi^* \frac{\partial}{\partial x}\psi - \frac{\partial}{\partial x}\psi^* \psi\right) dx$$

$$= -\frac{\hbar^2}{2m}\left[\underbrace{\psi^* \frac{\partial}{\partial x}\psi}_{0} - \underbrace{\frac{\partial}{\partial x}\psi^* \psi}_{0}\right]\Bigg|_{-\infty}^{\infty}$$

Since for

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx < \infty$$

$$\psi(x,t) \longrightarrow 0 \quad \text{at} \quad x \to \pm\infty$$

So

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 0$$

✓

Lecture 3

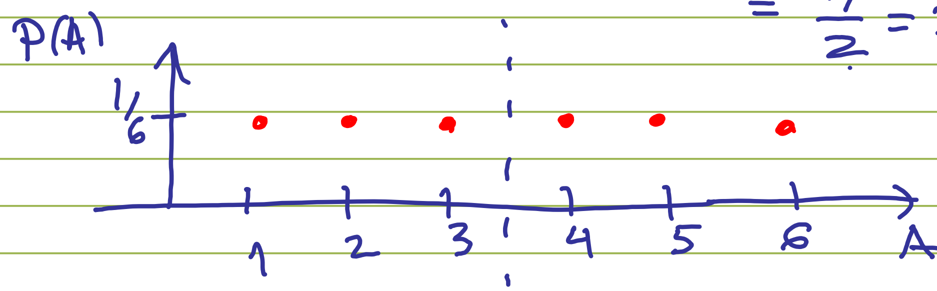
Expectation values

Ex 1 Throw a dice

$A = 1, 2, 3, \quad , 6$

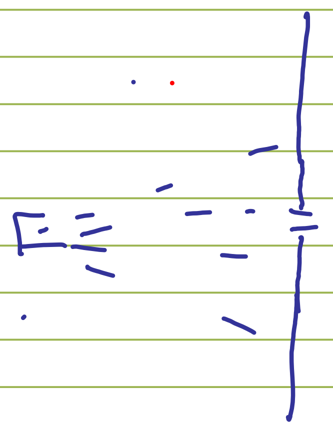
$$\langle A \rangle = \sum_A A \cdot P(A) = \frac{1}{6} + \frac{2}{6} + \quad + \frac{6}{6}$$

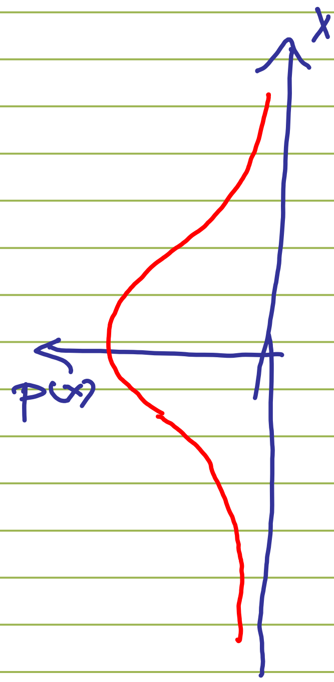
$$= \frac{7}{2} = 3.5$$



Note: $\langle A \rangle$ is not necessarily a likely, or even a possible outcome.

Ex 2 Bullets





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

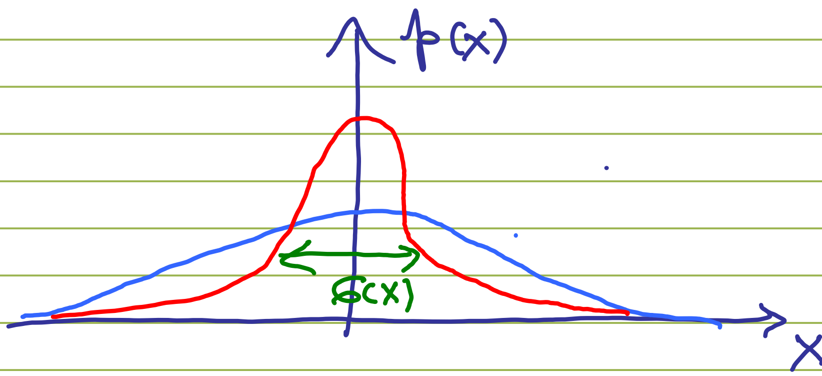
Ex 3 Electrons

$$p(x) = |\Psi(x,t)|^2$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x \, |\Psi(x,t)|^2 \, dx$$

$\langle x \rangle$ can be the same for

two very different distributions



For this reason one wants

"standard deviation in x".

$$\sigma(x) = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \, p(x) \, dx$$

Note

$$\langle x^2 \rangle - \langle x \rangle^2 = \langle (x - \bar{x})^2 \rangle \geq 0$$

where $\bar{x} = \langle x \rangle$

This is because

$$\langle (x-\bar{x})^2 \rangle =$$

$$= \langle x^2 - 2x\cdot\bar{x} + \bar{x}^2 \rangle$$

since $\bar{x} = \langle x \rangle$ is a number

$$= \langle x^2 \rangle - 2\cdot\bar{x}\cdot\langle x \rangle + \bar{x}^2\cdot\langle 1 \rangle$$

$$= \langle x^2 \rangle - 2\cdot\bar{x}\cdot\bar{x} + \bar{x}^2$$

$$= \langle x^2 \rangle - \bar{x}^2 = \langle x^2 \rangle - \langle x \rangle^2$$

We get to treat

$$|\psi(x,t)|^2$$

as any probability distribution.

So... why do we need $\psi(x,t)$,
why not just $|\psi|^2 = p(x,t)$?

We need it to compute expectation values of quantities involving momentum

p.

Momentum

Momentum of a classical particle:

$$p = m \cdot v = m \cdot \frac{d}{dt} x \qquad (*)$$

A quantum particle has

no well defined trajectory,
such as

$$x = x(t)$$

so formula like does <u>not</u> make sense.

It turns out that quantum particle <u>follows</u> <u>classical</u> trajectory <u>on average</u>.

So, what <u>is</u> true is that

$$\langle p \rangle = m \frac{d}{dt} \langle x \rangle$$

To make sense of this equation it turns out we need not just

$$\rho(x,t) = |\psi(x,t)|^2$$

But

$\psi(x,t)$

itself:

$$\langle x \rangle = \int dx\, x\, |\psi(x,t)|^2$$

$$\langle p \rangle = \int dx\, \psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x} \psi(x,t)\right)$$

Proof:

$$\frac{d}{dt}\langle x \rangle = \frac{d}{dt} \int dx\, x\, |\psi(x,t)|^2$$

$$= \int dx \cdot x \left[\left(\frac{\partial}{\partial t}\psi^*\right) \cdot \psi + \psi^* \frac{\partial}{\partial t}\psi\right]$$

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

So

$$\frac{d}{dt}\langle x \rangle = \int dx \cdot \frac{i\hbar}{2m} x \cdot \frac{\partial}{\partial x}\left[\psi^* \frac{\partial}{\partial x}\psi - \frac{\partial}{\partial x}\psi^* \psi\right]$$

$$\overset{\text{I.P.}}{=} \int dx\, \frac{-i\hbar}{2m}\left[\psi^* \frac{\partial}{\partial x}\psi - \frac{\partial}{\partial x}\psi^* \psi\right]$$

after integrating by parts (I.P

$$\int_a^b f \frac{d}{dx} g = f \cdot g \Big|_a^b - \int g \frac{d}{dx} f$$

$$\overset{I.P}{=} \int dx \, \frac{-i\hbar}{m} \psi^* \frac{\partial}{\partial x} \psi$$

$$= \langle p \rangle / m \quad \checkmark$$

One can write the expressions more symmetrically as

$$\langle x \rangle = \int dx \, \psi^*(x,t) \, x \, \psi(x,t)$$

$$\langle p \rangle = \int dx \, \psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x}\right) \psi(x,t)$$

We think of

$$-i\hbar\frac{\partial}{\partial x} \equiv \text{"momentum operator"}$$

$$x = \text{"position operator"}$$

where an operator $\mathcal{O}$

takes any wave function and maps it to another one

$$\mathcal{O} : \underbrace{\psi(x,t)}_{\text{original wave fn}} \longrightarrow \underbrace{\mathcal{O}\psi(x,t)}_{\text{result of acting on } \psi \text{ by operator}}$$

$$x : \psi(x,t) \longrightarrow x\,\psi(x,t)$$

$$p : \psi(x,t) \longrightarrow -i\hbar\frac{\partial}{\partial x}\psi(x,t)$$

More generally

Classical	QM
$Q(x,p) \rightarrow$	operator
	$Q\left(x, -i\hbar\frac{\partial}{\partial x}\right)$
	$+\mathcal{O}(\hbar)$

E.g

$$\underbrace{\frac{p^2}{2m}}_{\text{kinetic energy}} \rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$\left\langle \frac{p^2}{2m} \right\rangle = \int_{-\infty}^{\infty} \psi^*_{(x,t)} \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \right) \psi$$

in state ψ

$$\underbrace{L_z}_{\text{z-component of momentum.}} = x \cdot p_y \rightarrow x \cdot \left(-i\hbar\frac{\partial}{\partial y} \right)$$

"Ehrenfest's Theorem"

$$\frac{d}{dt}\langle x\rangle = \langle p\rangle/m .$$

$$\frac{d}{dt}\langle p\rangle = -\left\langle \frac{d}{dx}V(x)\right\rangle$$

In any quantum state Ψ, expectation values of x and p obey classical equations of motion, as functions of time.

$\boxed{\text{Lecture 4}}$

<u>Uncertainty principle:</u>

Schroedinger equation

implies

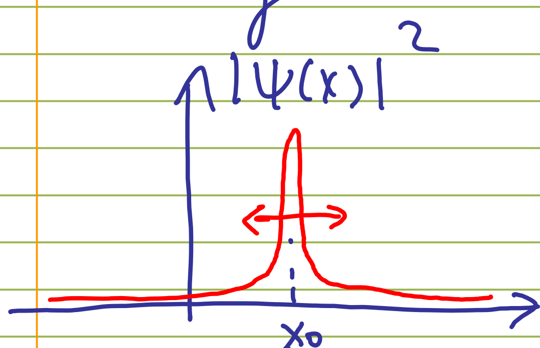
(we will prove it later, in greater generality)

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

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

$$\sigma_p = \langle p^2 \rangle - \langle p \rangle^2$$

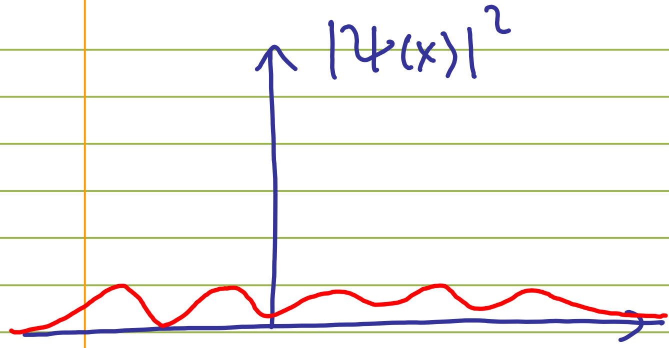
Position and momentum of a particle cannot both be known to arbitrary accuracy



σ_x small $\Longleftrightarrow$ little uncertainty in position

$\Downarrow$ $\qquad\qquad$ $\Downarrow$

σ_p large $\qquad$ huge uncertainty in momentum.



σ_x Large $\Longleftrightarrow$ Little uncertainty in momentum

The fact

$$\sigma_x \cdot \sigma_p \geq \hbar/2$$

means that quantum ($\hbar \neq 0$) effects prevent us from having

$$\sigma_x = 0 = \sigma_p$$

simultaneously. Consequently, we cannot know both position and momentum with arbitrary accuracy: prevents existance of meaningful particle path

$$x = x(t), \quad p = p(t)$$

Ex Consider following quantum state

$$\Psi(x,t) = A\, e^{-\frac{m\omega}{2\hbar}x^2}\, e^{-\frac{i\omega t}{2}}$$

Solves

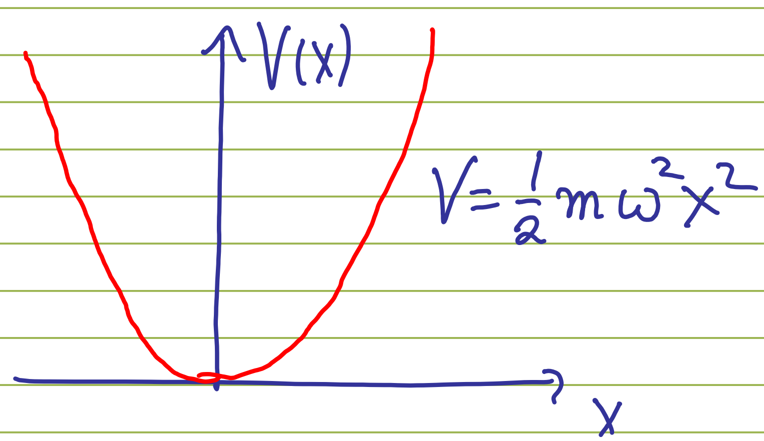
$$i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + V(x)\,\Psi(x)$$

with $V(x) = \frac{m\omega^2}{2} x^2$

Particle in lowest energy state

$$E = \hbar\omega/2$$

of harmonic oscillator potential



Fix normalization:

$$\int_{-\infty}^{\infty} |\Psi|^2 dx = 1 \quad \text{for}$$

$$A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

Since $$\int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} dx = \sqrt{\frac{2\pi}{\alpha}}$$

or $$\Psi(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} e^{-\frac{i\omega t}{2}}$$

Some basic operators acting on Ψ

$$\underbrace{i\hbar\frac{\partial}{\partial t}}_{\text{energy operator } E}\Psi = \frac{1}{2}\hbar\omega\,\Psi$$

$$\underbrace{-i\hbar\frac{\partial}{\partial x}}_{\text{momentum operator } p}\Psi = i m\omega x\,\Psi$$

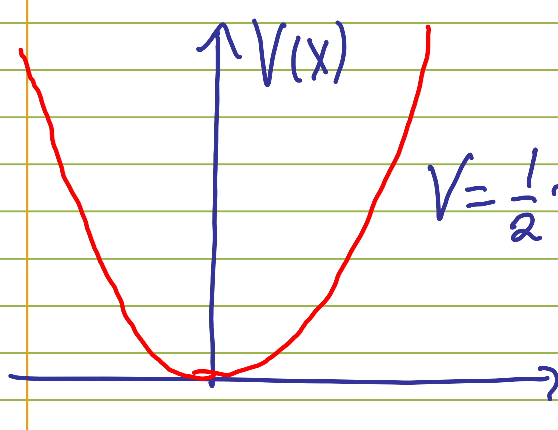
$$\underbrace{-\hbar^2\frac{\partial^2}{\partial x^2}\psi}_{p^2\text{ operator}} = \left(i\hbar\frac{\partial}{\partial x}\right)\left(im\omega x\,\psi\right)$$

$$= m\omega\hbar\,\psi - (m\omega x)^2\,\psi$$

NB: not a momentum eigenstate since coeff. is not constant

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi}_{\frac{p^2}{2m}\text{ operator}} + \underbrace{\frac{m\omega^2}{2}x^2\psi}_{V(x)\text{ operator}} = \underbrace{\frac{\omega\hbar}{2}\psi}_{\text{Energy operator}}$$

Show uncertainty principle holds:



$V=\frac{1}{2}m\omega^2x^2$

Expect: as ω grows, steeper pot'l, more localized particle;

σ_x decreases, σ_p increases with ω

As ω grows $\Leftrightarrow$ steeper potential

$\Leftrightarrow$ more localized packet

$\Leftrightarrow$ smaller σ_x

uncertainty principle:

$\Longrightarrow$ larger σ_p, $\sigma_p \geq \frac{\hbar}{2\sigma_x}$

Use:

$$\int_{-\infty}^{\infty} x e^{-\alpha x^2/2} dx = 0$$

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2/2} dx = -2 \frac{\partial}{\partial \alpha} \int_{-\infty}^{\infty} e^{-\alpha x^2/2} dx$$

$$= -2 \frac{\partial}{\partial \alpha} \sqrt{\frac{2\pi}{\alpha}} = \sqrt{\frac{2\pi}{\alpha^3}}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x\,|\psi|^2\,dx = 0$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2\,|\psi|^2\,dx = \frac{\hbar}{2\omega m}$$

$$\Rightarrow \quad \sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{\hbar}{2m\omega}}$$

decreases as ω increases

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x} \psi\right) dx$$

$$= \int_{-\infty}^{\infty} \psi^* (i m \omega x) \psi \, dx$$

$$= 0$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \psi^* \left[(m\omega\hbar)\, \psi - (m\omega x)^2 \psi \right]$$

$$= m\omega\hbar - (m\omega)^2 \langle x^2 \rangle$$

$$= m\omega\hbar - (m\omega)^2 \cdot \frac{\hbar}{2\omega m}$$

$$= \frac{1}{2} m\omega\hbar$$ ← increases w/ ω

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\tfrac{1}{2} m\omega\hbar}$$

$$\sigma_x \cdot \sigma_p = \sqrt{\frac{\hbar}{2m\omega}} \cdot \sqrt{\frac{m\omega\hbar}{2}} = \frac{\hbar}{2}$$

↑ saturates uncertainty bound

Lecture 5

Ch 2

Time-Independent S.E

To find allowed states

$\Psi(x,t)$

$V(x,\cancel{t})$

need to solve:

$\downarrow$

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

"SEPARATION OF VARIBLES"

Try $\Psi(x,t) = \psi(x)\varphi(t)$

$\uparrow$ restrictive, but hang on...

$$\Rightarrow \frac{\partial}{\partial t}\Psi(x,t) = \psi(x)\frac{d}{dt}\varphi(t)$$

$$\frac{\partial^2}{\partial x^2}\Psi(x,t) = \frac{d^2}{dx^2}\psi \cdot \varphi(t)$$

S.E Becomes

$$\underbrace{i\hbar\frac{\frac{d}{dt}\varphi}{\varphi}}_{\text{fn of t but not of x}} = \underbrace{-\frac{\hbar^2}{2m}\frac{\frac{d^2}{dx^2}\psi}{\psi} + V(x)}_{\text{fn of x but not of t}}$$

$\Rightarrow$ two sides are equal and constant:

$$\frac{i\hbar \frac{d}{dt}\varphi}{\varphi} = \underset{\substack{\uparrow \\ \text{const}}}{E} = \frac{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V}{\psi}$$

Get two equations:

$\varphi(t)$ solves:

$$i\hbar \frac{d}{dt}\varphi = E\varphi$$

which has solution:

$$\underline{\varphi(t) = e^{-iEt/\hbar}}$$

$\psi(x)$ solves:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V\psi = E\psi}$$

TIME INDEPENDENT SCHROEDINGER EQN

So, there are special solutions

of S.E

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

of the form

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

where $\psi(x)$ solves

T.I. S.E

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

Q: what makes these solutions special?

A1: They are

"stationary states"

No time dependence of ordinary

physical quantities

$$|\Psi(x,t)|^2 = |\psi(x)|^2$$

and also of expectation values

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

$$= \int dx\, \psi^*(x)\, \hat{Q}\, \psi(x)$$

$$\Rightarrow \quad \frac{d}{dt}\langle Q(x,p)\rangle = 0$$

A2: They are states of definite total energy:

Energy operator
a.k.a Hamiltonian

$$\hat{H}(p,x) = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

$\downarrow$

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

Time dependent S.E

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

Time Independent S.E (TISE)

$$\hat{H}\Psi(x) = E\Psi(x)$$

"Solution of TISE is an eigenstate (eigenvector) of $\hat{H}$ with eigen-value E"

The state has definite energy since

$$\hat{H}\Psi = E\Psi \Rightarrow \hat{H}^2\Psi = E^2\Psi$$

$$\langle H \rangle = \int_{-\infty}^{\infty} dx \, \Psi^* \hat{H} \Psi$$

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

$$\langle H^2 \rangle = \int_{-\infty}^{\infty} dx \, \Psi^* \hat{H}^2 \Psi$$

$$= E^2 \int_{-\infty}^{\infty} dx \, \Psi^* \Psi = E^2$$

$$\sigma_H = \sqrt{\langle H^2 \rangle - \langle H \rangle^2} = \sqrt{E^2 - E^2} = 0$$

Every measurement of energy in state

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

gives energy E with no spread or uncertainty.

A3.

An arbitrary solution of S.E can be written as an arbitrary linear combination of solutions with definite energies.

Assume energy spectrum is discrete (more later),

soln's of TISE with corresponding energies.

$$\left\{\begin{array}{l} \psi_1(x), \quad \psi_2(x), \quad \ldots \quad \psi_n(x), \ldots \\ E_1, \quad E_2, \quad \ldots \quad E_n, \ldots \end{array}\right.$$

- An linear combination

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$

is a solution

- Every solution of SE can be written in this way for some (complex) constants c_n.

Strategy

1. Solve TISE, finding

$\psi_1(x), \psi_2(x), \ldots, \psi_n(x), \ldots$

$E_1, E_2, \ldots, E_n, \ldots$

2. Any initial condition for S.E

$\Psi(x,0)$

can be written as

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

(one has to find the appropriate constants c_n. More on this later.)

3. The corresponding solution for arbitrary t is

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_n t/\hbar}$$

(check solves S.E and agrees w/ $\psi(x,0)$ at $t=0$).

4. How to find c_n:

Assume $E_n \neq E_m$ if $n \neq m$

"non-degenerate spectrum".

Then

$$\int_{-\infty}^{\infty} \psi_n^*(x)\, \psi_m(x)\, dx = 0 \qquad n \neq m$$

"orthogonality"

and

$$\int_{-\infty}^{\infty} \psi_n^*(x)\, \psi_n(x)\, dx = 1$$

In short

$$\int_{-\infty}^{\infty} \psi_n^*(x)\, \psi_m(x)\, dx = \delta_{nm}$$

$$\delta_{nm} = \begin{cases} 1 & , n = m \\ 0 & , n \neq m \end{cases}$$

Then:

$$c_n = \int_{-\infty}^{\infty} dx\, \psi_n^*(x)\, \Psi(x,0)$$

Found By integrating.

Proof.

Let

$$\Psi(x,0) = \sum_{m=1}^{\infty} c_m \psi_n(x)$$

Multiply Both sides By

$\psi_n^*(x)$

and integrate. Left side

$$\int_{-\infty}^{\infty} \psi_n^*(x)\, \Psi(x,0)\, dx \quad \checkmark$$

Right hand side :

$$\int_{-\infty}^{\infty} \psi_n^*(x) \sum_{m=1}^{\infty} c_m \psi_m(x)\, dx$$

$$= \sum_{m=1}^{\infty} c_m \int_{-\infty}^{\infty} \underbrace{\psi_n^*(x)\, \psi_m(x)\, dx}_{\substack{=1 \text{ if } n=m \\ 0 \text{ otherwise}}}$$

$$= c_n$$

5. Solutions w/ more than one c_n non-vanishing give time dependent states

$$|\psi(x,t)|^2$$

$$= \psi^*(x,t) \cdot \psi(x,t)$$

E.g

$$\psi(x,t) = c_1 e^{-iE_1 t/\hbar} \psi_1(x) + c_2 e^{-iE_2 t/\hbar} \psi_2(x)$$

(assume $\psi_{1,2}$ and $c_{1,2}$ are real)

$$|\Psi(x,t)|^2 = \Psi^*(x,t) \cdot \Psi(x,t)$$

$$= \left(c_1 \psi_1 e^{+iE_1 t/\hbar} + c_2 \psi_2 e^{+iE_2 t/\hbar}\right)$$
$$\left(c_1 \psi_1 e^{-iE_1 t/\hbar} + c_2 \psi_2 e^{-iE_2 t/\hbar}\right)$$

$$= c_1^2 \psi_1^2 + c_2^2 \psi_2^2 + c_1 c_2 \psi_1 \psi_2 \cdot$$
$$\cdot \left(e^{i(E_1 - E_2)t/\hbar} + e^{-i(E_1 - E_2)t/\hbar}\right)$$

$$= c_1^2 \psi_1^2 + c_2^2 \psi_2^2 + 2 c_1 c_2 \psi_1 \psi_2 \cos\left((E_1 - E_2) t/\hbar\right)$$

depends on time for

$c_1 c_2 \neq 0$