We will use:

Capital Ψ: for state functions which depend on x AND t

Little ψ: for state " only on (x).

Ψ: $\Psi(x,t)$

ψ: $\psi(x)$. ← The wavefunction at one moment in time
A snapshot of

__Question:__ Suppose we know Ψ at $t=\emptyset$:

$$\Psi(x,t=\emptyset) = \psi(x) = \text{a known function}$$

Then how does Ψ evolve in time?

__Answer:__ If we can write $\psi(x)$ as a sum of the energy eigenfunctions $\{\phi_n(x)\}$, then the time evolution is simple:

__If__
$$\psi(x) \overset{?}{=} a_1\phi_1(x) + a_2\phi_2(x) + a_3\phi_3(x) + \ldots$$
$$\overset{?}{=} \sum_{\text{all } n} a_n\phi_n(x)$$

For some set of coefficients $\{a_n\}$.

__Then__
$$\Psi(x,t) = a_1\phi_1(x)e^{-i\frac{E_1}{\hbar}t} + a_2\phi_2(x)e^{-i\frac{E_2}{\hbar}t} + \ldots$$
$$= \sum_{\text{all } n} a_n\phi_n(x)e^{-i\frac{E_n}{\hbar}t}$$

$$\text{or } = \sum_{\text{all } n} a_n\phi_n(x)e^{-i\omega_n t} \quad \text{where } \omega_n \equiv \frac{E_n}{\hbar}.$$

__So the question is__: Can we find a set of coefficients $\{a_n\}$ such that $\Psi(x,t=\emptyset) = \psi(x) \overset{?}{=} \sum_{\text{all } n} a_n\phi_n(x)$

The following is one of the most important results in QM:

> Any physical state Ψ can always be written as a sum – or "linear combination" – of energy eigenstates: $\psi(x) = \sum_{\text{all } n} a_n \phi_n(x)$ for some set of $\{a_n\}$.

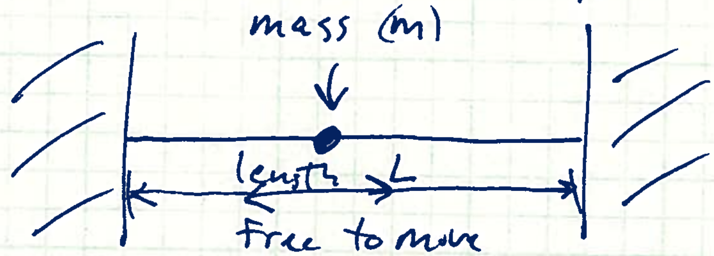
We will not prove this right now.

We say that:

- "The energy eigenfunctions are complete."
  - → Meaning: any valid state Ψ can be written in terms of the energy e.f..

Particle-in-a-box – Simplest bound state system.

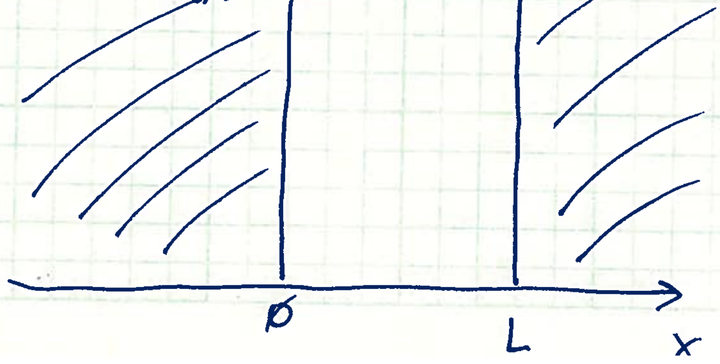
Imagine a particle on a wire trapped between 2 walls:



Like a gas molecule in a 1D container or an electron in a wire.

The potential function is

$$V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$



To study the time evolution of this system, we'll need to know the energy eigenfunctions and eigenvalues: $\{\varphi_n(x)\}$ and $\{E_n\}$.

Find them by solving the energy eigenvalue equation:

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

where $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ for $0 < x < L$

In this region:

$$\cancel{\hat{H}\varphi_n = E_n\varphi_n} \quad \hat{H}\varphi = E\varphi \quad \text{is}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} = E\varphi(x)$$

$$\boxed{\varphi''(x) + \frac{2mE}{\hbar^2}\varphi(x) = 0}$$

General Solution is

$$\varphi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}$$

But we have boundary conditions which restrict the solution further:

① $\varphi(x)$ must be zero outside the box. (No probability to find the particle where $V \to \infty$.)

② $\varphi(x)$ must be continuous.

Putting these together we have

$$\phi(x=0) = \emptyset \quad ①$$

and $$\phi(x=L) = \emptyset. \quad ②$$

Then from ① we have

$$A + B = \emptyset \qquad -A = B$$

and from ② we have

$$A e^{ikL} + \underset{-A}{B} e^{-ikL} = \emptyset$$

$$A\left(e^{ikL} - e^{-ikL}\right) = \emptyset$$

$$2iA \sin(kL) = \emptyset$$

$$\boxed{\sin(kL) = \emptyset} \leftarrow k \text{ must satisfy this.}$$

$$kL = n\pi, \quad n = \emptyset, \pm 1, \pm 2, \pm 3, \ldots$$

$$k_n = \frac{n\pi}{L} \Rightarrow \boxed{E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}} \leftarrow \text{Energy eigenvalue}$$

The eigenfunctions are

$$\phi_n(x) = Ae^{ik_n x} + Be^{-ik_n x}, \text{ where } B = -A \text{ and } k_n = \frac{n\pi}{L}$$

$$= \underbrace{2iA}_{\equiv C} \sin(k_n x)$$

$$\phi_n(x) = C \sin\left(\frac{n\pi x}{L}\right) \leftarrow \text{The energy eigenfunctions}$$

<u>However</u>: the $n = 0$ solution is phony:

$$\psi_0(x) = C\sin\left(\frac{0\pi x}{L}\right) = 0 \quad \text{? particle is nowhere ?}$$

Also, the $(-n)$ solutions are not unique:

$$\psi_{-n}(x) = C\sin\left(\frac{-n\pi x}{L}\right) = \underbrace{-C}_{\equiv D}\sin\left(\frac{n\pi x}{L}\right)$$

$$= \underbrace{D\sin\left(\frac{n\pi x}{L}\right)}_{\text{same as } \psi_{+n}(x).}$$

~~So the solutions e.f.'s and e.v.'s are~~

What about the constant C? It is determined by the normalization condition:

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

$$C^2 \underbrace{\int_0^L \sin^2 \frac{n\pi x}{L} \, dx}_{\frac{L}{2}} = 1$$

$$\therefore \quad C = \sqrt{\frac{2}{L}}$$

So the normalized energy eigenfunctions and eigenvalues are

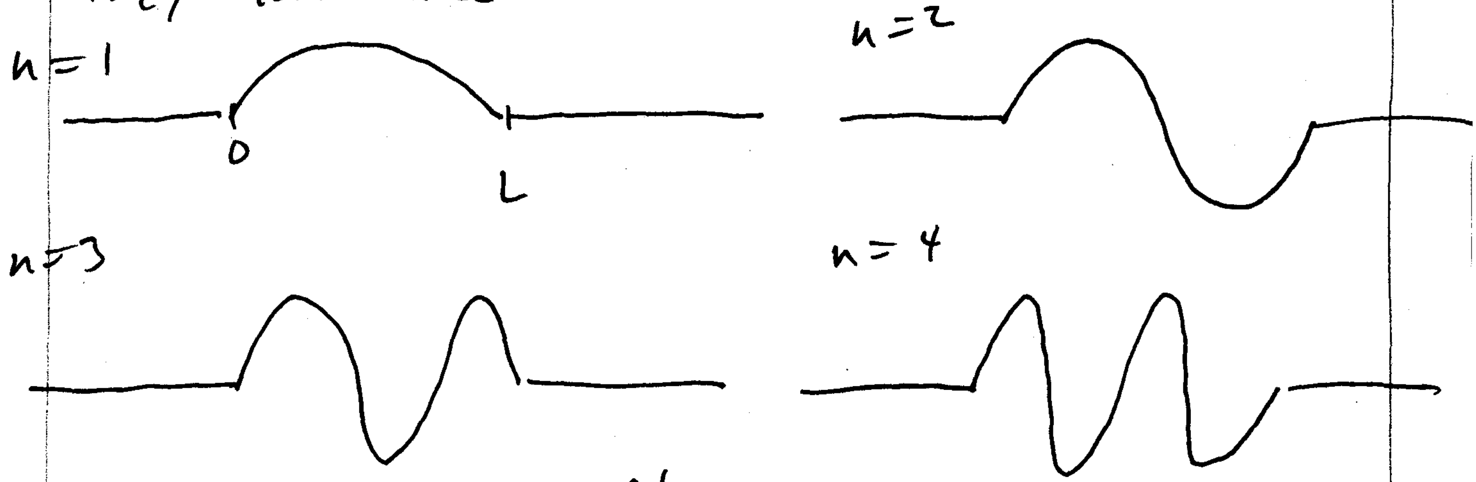
$$\boxed{\begin{aligned} &\phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), & 0 < x < L \\ 0, & \text{otherwise} \end{cases} \\ &\text{and} \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \\ &\text{where } n = 1, 2, 3, 4, \ldots \end{aligned}}$$

Particle-in-a-box

Normalized eigenfunctions and eigenvalues are

$$\boxed{\begin{gathered} \varphi_n(x) = \begin{cases} \sqrt{\dfrac{2}{L}} \sin\left(\dfrac{n\pi x}{L}\right), & 0 < x < L \\ 0, & \text{otherwise} \end{cases} \\ E_n = \dfrac{\hbar^2 \pi^2 n^2}{2mL^2} \\ n = 1, 2, 3, 4, \ldots \end{gathered}}$$

They look like:



etc.

The eigenfunction have 2 important properties:

① They are orthonormal:

$$\boxed{\int_{-\infty}^{\infty} \varphi_n^*(x)\, \varphi_m(x) = \delta_{nm}}$$

Homework #2 Problem #4

(2) They are <u>complete</u>: Any valid physical state for a particle in the box can be written as a sum of the eigenfunctions.

$$\psi(x) = \text{any valid particle-in-a-box-state}$$
$$= \sum_n a_n \varphi_n(x)$$

Just find the right set of $\{a_n\}$.

How do we know they are compute? <u>Fourier Theory</u> tells us any square-integrable function which goes to zero at $x=\emptyset$ & $x=L$ can be written as a sum of sine functions.

<u>Question</u> How do we find the right set of $\{a_n\}$ for a particular $\psi(x)$?

Answer: Fourier's Trick: (Homework #2 Problem #5)

$$a_m = \text{one particular coefficient} = \int_{-\infty}^{\infty} \psi(x)\, \varphi_m^*(x)\, dx$$

$$\boxed{a_m = \sqrt{\frac{2}{L}} \int_0^L \psi(x) \sin\left(\frac{m\pi x}{L}\right) dx.}$$

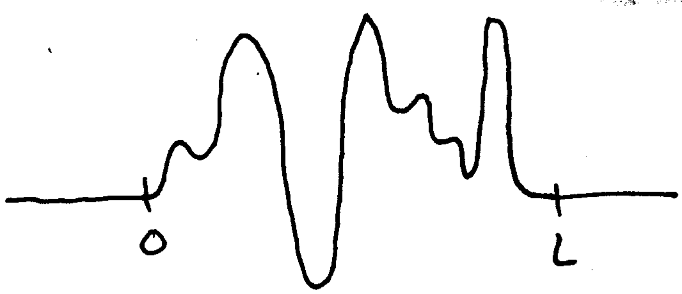
Proof: Substitute $\psi(x) = \sum_n a_n \varphi_n(x)$:

$$\int_{-\infty}^{\infty} \left[\sum_n a_n \varphi_n(x)\right] \varphi_m^*(x)\, dx =$$

$$\sum_n a_n \underbrace{\int_{-\infty}^{\infty} \varphi_n(x)\,\varphi_m^*(x)\,dx}_{\delta_{nm} \text{ by orthonormality}} = \sum_n a_n \delta_{nm} = a_m \quad \checkmark$$

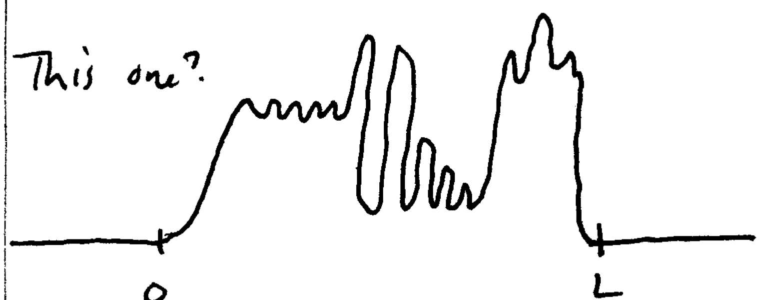
δ_{nm} kills all terms except a_m

Question: Is this a valid particle-in-a-box state?



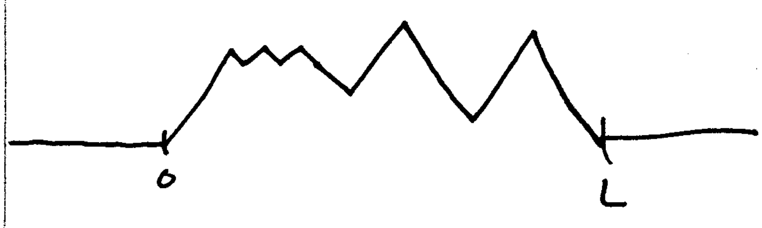
Yes! Just find the right set of $\{a_n\}$.

This one?



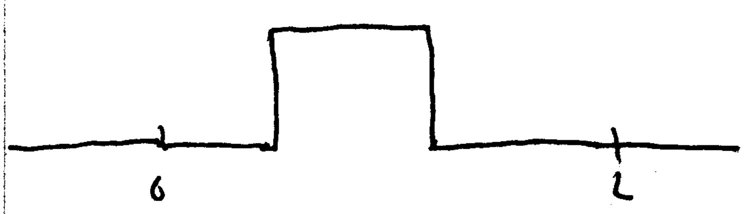
Yes! Just find the right set of $\{a_n\}$.

This one?



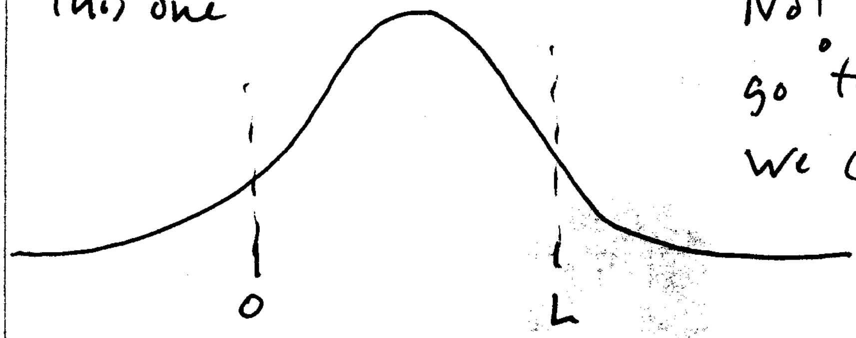
Yes!

This one?



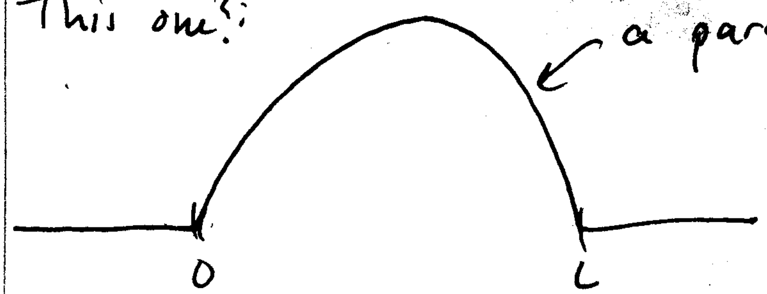
Yes!

This one?



No! It does not go to zero at $x=0$ & $x=L$. We cannot write it as a sum of $\sin\left(\frac{n\pi x}{L}\right)$ functions.

This one?:



Answer: Yes: From Griffiths: If $\psi(x) = \sqrt{\frac{30}{L^5}}\, x(L-x)$,

Then

$$a_n = \begin{cases} 0, & n \text{ even} \\ \frac{8\sqrt{15}}{(n\pi)^3}, & n \text{ odd} \end{cases}$$

$$\therefore\ \psi(x) = \sum_{n\ \text{odd}} \left(\frac{8\sqrt{15}}{(n\pi)^3}\right) \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L$$

How does this state evolve in time?

Answer: $$\Psi(x,t) = \sum_{n\ \text{odd}} \left(\frac{8\sqrt{15}}{(n\pi)^3}\right) \sin\left(\frac{n\pi x}{L}\right) e^{-i\omega_n t}$$

where $\omega_n \equiv \frac{E_n}{\hbar} = \frac{\hbar^2\pi^2 n^2}{2mL^2\hbar}$

Physical Interpretation of the $\{a_n\}$

In QM, we use the word "amplitude" to mean

$$\boxed{\text{"amplitude"} = \text{a complex number whose square is the probability to make some particular measurement.}}$$

Each coefficient a_n is an amplitude to measure energy eigenvalue E_n:

$$\boxed{|a_n|^2 = P(E_n) = \text{Prob. to measure } E_n}$$

Proof: From Postulate II:

$$\langle E \rangle = \int \psi^* \hat{H} \psi \, dx = \int \underbrace{\left(\sum_n a_n^* e_n^*\right)}_{\psi^*} \hat{H} \underbrace{\left(\sum_m a_m e_m\right)}_{\psi} dx$$

$$= \sum_n \sum_m a_n^* a_m \int e_n^* \underbrace{\hat{H} e_m}_{E_m e_m} dx$$

$$= \sum_n \sum_m a_n^* a_m E_m \underbrace{\int e_n^* e_m \, dx}_{\delta_{nm} \text{ by orthonormality.}}$$

$$= \sum_n \sum_m a_n^* a_m E_m \delta_{nm}$$

$$\langle E \rangle = \sum_n a_n a_n^* E_n = \sum_n |a_n|^2 E_n$$

But from statistics we know that

$$\langle E \rangle = \sum_n P(E_n) E_n$$

$$\therefore \boxed{|a_n|^2 = P(E_n)}$$

Example Suppose that $\psi(x) = \frac{1}{\sqrt{2}} \phi_3 + \frac{1}{\sqrt{2}} \phi_7$.

What is the probability to measure $E = E_3$?

Answer: $a_3 = \frac{1}{\sqrt{2}}$ so $P(E_3) = \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$.

What about E_7?

Answer: $a_7 = \frac{1}{\sqrt{2}}$ so $P(E_7) = \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$.

Note: $\psi(x)$ is also an amplitude, just like a_n.

continuous $\rightarrow$ $|\psi(x)|^2 dx$ = Probability to measure x between x & $x+dx$

"amplitude density"

discrete $\rightarrow$ $|a_n|^2$ = Prob to measure E_n.

Phys 401 - Lecture 10 - Fall 2011

Amplitudes in QM

QM is the study of "amplitudes" $\Rightarrow$ complex numbers whose square gives the probability to make a particular measurement.

Example 1 $\{a_n\}$

When we write $\psi(x) = \sum_n a_n \phi_n(x)$, and $\{\phi_n(x)\}$ are the stationary states (energy eigenfunctions) Then each a_n is "the amplitude to measure energy eigenvalue E_n:

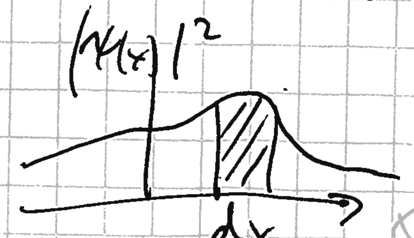
$$|a_n|^2 = \text{Prob}(E_n)$$

We proved this using postulate III: $\langle E \rangle = \int \psi^* \hat{H} \psi \, dx$

Example 2 The wavefunction $\psi(x)$

If we square $\psi(x)$ and multiply by a small interval (dx) we get the Probability to measure the position of the particle between x and $x + dx$:

$$|\psi(x)|^2 dx = P(x)\, dx$$



Strictly speaking

$\psi(x)$ is an "amplitude density" $\Rightarrow$ Multiply by a small interval to get a prob. This is because x is a

Continuous variable.

Summary

- $\{a_n\}$: discrete amplitudes for discrete energy eigenvalues $\{E_n\}$.

both are complex numbers

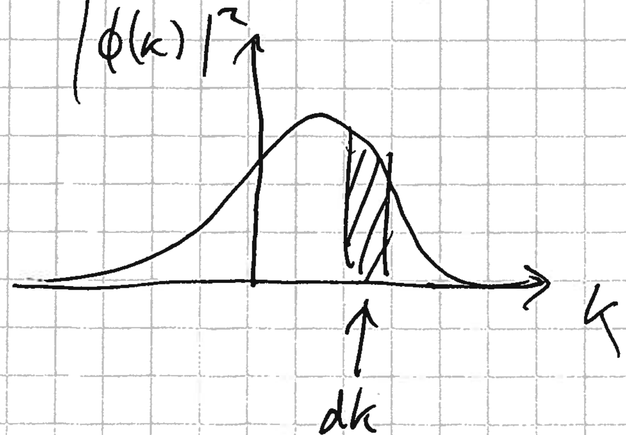
- $\psi(x)$: a continuum of amplitudes for the continuous variable (x).

Example 3 The "momentum space" wavefunction.

Let $\phi(k)$ stand for the continuum of amplitudes whose square gives the probability to make ~~particular~~ momentum measurements:

$$|\phi(k)|^2 dk = P(k)\,dk.$$

= Probability to observe momentum between $\hbar k$ and $\hbar(k+dk)$.

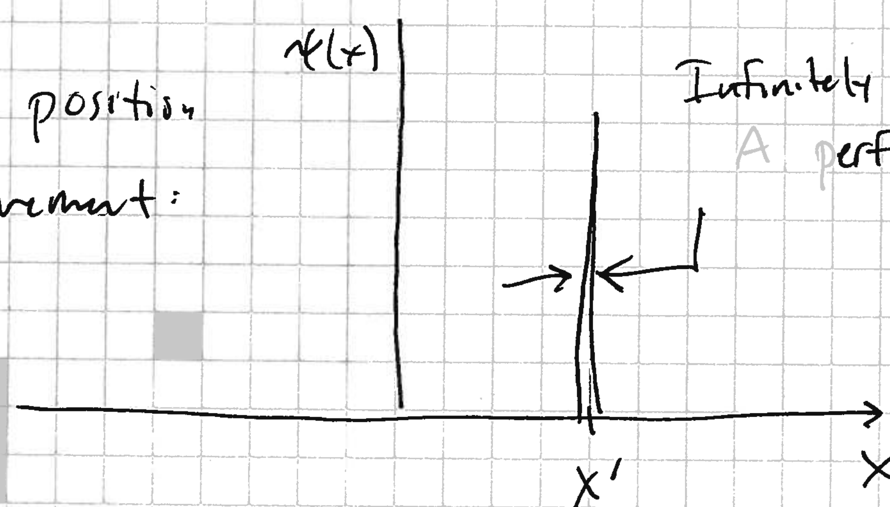


Since $\phi(k)$ = "momentum-space wavefunction"
we should call $\psi(x)$ = "position-space wavefunction".

Measurement of Position (x)

In the 2-slit experiment, the screen measures the location of the particle after it passes through the 2-slit barrier. Each particle shows up as a point-like object on the screen. According to postulate III, the screen ~~causes~~ measures position, and causes the wavefunction to collapse to an eigenstate of position. The eigenstate function for position must be infinitely narrow and localized, if the screen is extremely accurate and precise.

After a position measurement:



Infinitely narrow! A perfect spike.

We call this function a Dirac Delta Function, $\delta(x)$.

Actually, $\delta(x)$ is not really a function because it is only defined inside an integral.

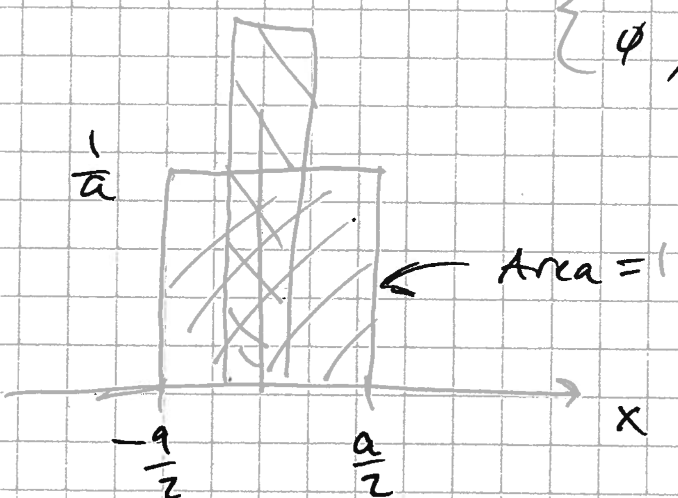
Definition of $\delta(x)$: ① $\displaystyle\int_{-\infty}^{\infty} f(x)\,\delta(x-x')\,dx = f(x')$

picks out one value $f(x')$

② $\delta(x) = 0$ for all $x \neq 0$.

We can picture $\delta(x)$ like this, Let

$$g(x) = \begin{cases} \frac{1}{a}, & -\frac{a}{2} < x < \frac{a}{2} \\ 0, & \text{otherwise} \end{cases}$$



: $\displaystyle\int_{-\infty}^{\infty} g(x)\,dx = 1.$

Then $\delta(x) = \lim_{a \to 0} g(x).$

Although $\delta(x)$ is not really a function (it's called a "functional") nevertheless it is the eigenstates of position, and a perfect position measurement will cause the wavefunction to collapse: $\psi(x) = \delta(x)$ after a perfect x measurement.

Free Particle

What are the energy eigenstates of a free particle?

$V(x) = \phi$ for all x, so $\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$

energy eigenvalue equation: $\frac{-\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} = E\varphi(x).$

$$\boxed{\varphi''(x) + \frac{2mE}{\hbar^2}\varphi(x) = \phi}$$

Solution: $\varphi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$

We got the same result for the particle-in-a-box, but in that case only certain, quantized values of k were allowed due to the boundary conditions. ($k = n\pi/L$ for the particle in a box.). Here, there are no boundary conditions so k is a continuous variable (not quantized).

We can simplify $\varphi(x)$ by noting that k could be positive or negative. Thus

$\varphi(x) = Ae^{ikx}$ ← where k could be $(+k)$ or $(-k)$.

Note that this is a momentum eigenstate also! For a free particle, all momentum eigenstates are also energy eigenstates.

As before, we will expand our wavefunctions $\psi(x)$ as a sum of energy eigenstates e^{ikx}.

Before (particle-in-a-box): We had a discrete set eigenfunctions $\{\varphi_n(x)\} \Rightarrow$ Discrete sum $\psi(x) = \sum_n a_n \varphi_n$

Now (free particle): We have a continuum of eigenfunctions $\{e^{ikx}\}$

k is continuous, so we have a continuous set of eigenfunctions:

$$\{\ldots, e^{i(2.2)x}, e^{i(2.21)x}, e^{i(2.22)x}, \ldots\}$$

for example

So $\psi(x)$ will be a continuous sum of the e^{ikx}, or an integral:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \; \phi(k) \, e^{ikx}$$

a continuous sum over k!

a continuum of coefficients!

And since the $\{a_n\}$ are a <u>discrete</u> set of amplitudes to measure the discrete energy eigenvalues $\{E_n\}$, the continuum amplitudes $\phi(k)$ must be a continuum of amplitudes to measure the various values of momentum:

$$|\phi(k)|^2 dk = P(k)\, dk$$

$\phi(k)$ = "momentum space wavefunction"

Similar to

$\psi(x)$ = "position space wavefunction"