Particle-in-a-box in Dirac Notation:

energy eigen states: $\{|n\rangle\}$ and/or $\{\langle n|\}$ ← Dirac bra vector

↑ Dirac ket vectors

Explicitly,

$$|n\rangle = \text{column vector} = \begin{pmatrix} \vdots \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \leftarrow n^{th} \text{ position}$$

$$\langle n| = \text{row vector} = (\ldots 0\,0, 1, 0\,0, 0\,0)$$

Then $\langle n|n\rangle = 1$ ~~and~~ $= (\ldots, 0, 0, 1, 0, 0 \ldots)\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

$\langle m|n\rangle = \delta_{mn}$ ← orthonormality statement in Dirac notation

An arbitrary state is written

$$|\text{arbitrary}\rangle = \langle a| = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \\ \vdots \end{pmatrix}$$ where $\{a_n\}$ are the expansion coefficients.

and $\langle \text{arbitrary}| = \langle a| = (a_1^*, a_2^*, a_3^*, \ldots)$

$$\langle a|a\rangle = \sum_n a_n^* a_n = \sum_n |a_n|^2 = 1.$$

We can also write

~~$\langle$arbitrary$|$~~ $|\text{arbitrary}\rangle = |a\rangle = a_1|1\rangle + a_2|2\rangle + a_3|3\rangle + a_4|4\rangle + \ldots$

We used to write this as $\psi(x) = a_1\varphi_1(x) + a_2\varphi_2(x) + a_3\varphi_3(x) + a_4\varphi_4(x) + \ldots$

If we multiply an arbitrary state vector by $\langle n|$, then we get

$$\langle n|\text{arbitrary}\rangle = \langle n|a\rangle = (\ldots 0, 0, 1, 0, 0, \ldots)\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \\ \vdots \end{pmatrix}$$

$$= a_n \leftarrow \text{a complex \#}$$

$$\therefore \boxed{a_n = \langle n|a\rangle} \longleftarrow \text{a complex \#}$$

We used to write this as $a_n = \int_{-\infty}^{\infty} \psi(x)\, \varphi_n^*(x)\, dx$

Now we can write

$$|\text{arbitrary}\rangle = |a\rangle = a_1|1\rangle + a_2|2\rangle + a_3|3\rangle + \ldots$$

$$= |1\rangle \underset{\langle 1|a\rangle}{a_1} + |2\rangle \underset{\langle 2|a\rangle}{a_2} + |3\rangle \underset{\langle 3|a|}{a_3} + \ldots$$

$$= |1\rangle\langle 1|a\rangle + |2\rangle\langle 2|a\rangle + |3\rangle\langle 3|a\rangle + \ldots$$

$$|a\rangle = \sum_n |n\rangle\langle n|a\rangle$$

In ordinary vectors this is

$$\vec{a} = \hat{x}\underset{\hat{x}\cdot\vec{a}}{a_x} + \hat{y}\underset{\hat{y}\cdot\vec{a}}{a_y} + \hat{z}\underset{\hat{z}\cdot\vec{a}}{a_z}$$

$$\vec{a} = \hat{x}(\hat{x}\cdot\vec{a}) + \hat{y}(\hat{y}\cdot\vec{a}) + \hat{z}(\hat{z}\cdot\vec{a})$$

Let $\hat{x}_1 = \hat{x}$
$\hat{x}_2 = \hat{y}$
$\hat{x}_3 = \hat{z}$.

Then $\vec{a} = \sum_{n=1}^{3} \hat{x}_n (\hat{x}_n \cdot \vec{a})$

Just like $|a\rangle = \sum_n |n\rangle\langle n|a\rangle$

But notice $|a\rangle = \left[\sum_n |n\rangle\langle n|\right] |a\rangle$ ← Factor out $|a\rangle$ from every term

This says $|a\rangle = \left[\text{thing in brackets}\right] |a\rangle$

$\therefore \left[\text{thing in brackets}\right] = \hat{I}$ = Identity operator

$$\therefore \boxed{\hat{I} = \sum_n |n\rangle\langle n|}$$

Mathematical statement of completeness for the $\{|n\rangle\}$.

Why is this useful? Suppose we want to multiply:

$\langle \text{arbitrary } a | \text{arbitrary } b\rangle = \langle a|b\rangle$
$= \langle a|\hat{I}|b\rangle$ ← insert Identity operator

$= \cancel{\ldots}$

$$= \langle a | \left[\sum_n |n\rangle\langle n| \right] |b\rangle$$

$$= \sum_n \underbrace{\langle a|n\rangle}_{(\langle n|a\rangle)^* \;\to\; \{a_n^*\}} \underbrace{\langle n|b\rangle}_{\{b_n\}}$$

$\cancel{= \sum_n}$

$(\langle n|a\rangle)^*$ ← Homework #5

$$= \sum_n a_n^* b_n$$

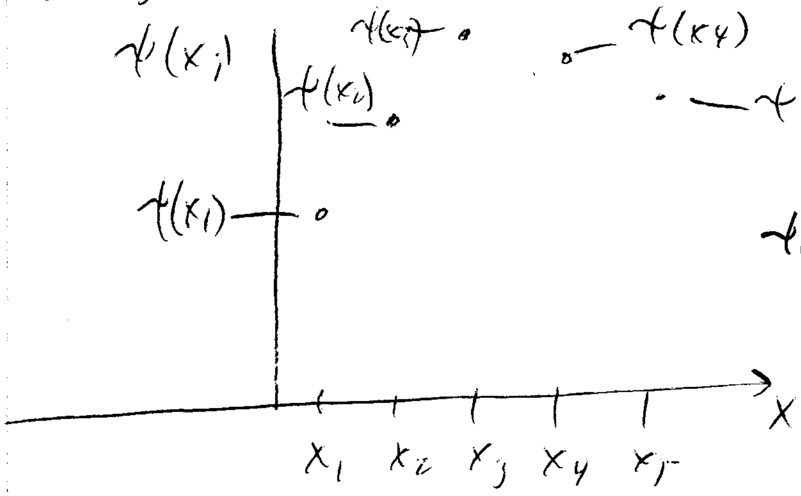
$$= (a_1^*, a_2^*, a_3^*, \dots) \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ \vdots \end{pmatrix}$$

<u>Position basis.</u>

a_n = QM amplitude to observe ~~E_n~~ E_n $= \langle n|a\rangle$

$\psi(x)$ = QM amplitude to observe x $\stackrel{?}{=}$ $\langle ?|a\rangle$

Imagine that x is discrete:



Then $\psi(x)$ is like a vector:

$$\psi(x) \sim \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \end{pmatrix} \sim |\psi\rangle$$

where $\psi_1 = \psi(x_1)$

$\psi_2 = \psi(x_2)$

$\dots$

and $\psi^*(x) \overset{\sim\langle\psi|}{\sim} (\psi_1^*, \psi_2^*, \psi_3^*, \dots)$

Then $\langle\psi|\psi\rangle = \psi_1^*\psi_1 + \psi_2^*\psi_2 + \psi_3^*\psi_3 + \dots$

$$= \sum_n \psi_n^*\psi_n$$

In the continuum limit this is

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

Now $\langle n|a\rangle \overset{=a_n}{}$ picks out the amplitude to observe E_n.

What picks out the amplitude to observe x?

$$\langle ?|a\rangle \overset{?}{=} \psi(x)$$

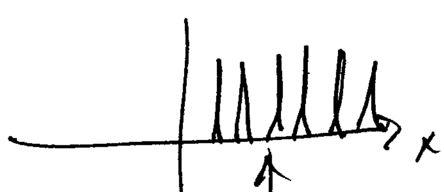
↑
what is this

Well, to get a_n, we multiplied by an energy eigenstate. To get $\psi(x)$, we must multiply by an eigenstate of x: $\langle x|$

↑ an eigenstate of position in bra vector form.

$\therefore$ $\boxed{\langle x|a\rangle = \psi(x)}$

What do the $|x\rangle$ look like?



↑ delta functions in position space

In vector form,

$$|x\rangle \sim \begin{pmatrix} \vdots \\ 0, \\ 0, \\ 0, \\ 1, \\ 0, \\ 0, \\ 0, \\ \vdots \end{pmatrix} \begin{array}{l} \\ \\ \\ \leftarrow \text{the } x^{th} \text{ position} \\ \\ \\ \\ \\ \end{array}$$

but x is actually continuous, so I can't really write it this way

Nevertheless, $\langle x|a\rangle = \psi(x) \leftarrow$ amplitude to observe x

$\langle n|a\rangle = a_n \leftarrow$ amplitude to observe E_n.

For $|n\rangle$ we had $\sum_n |n\rangle\langle n| = \hat{I} \leftarrow$ completeness

$|x\rangle$ are also complete, so

$$\int_{-\infty}^{\infty} |x\rangle\langle x|\, dx = \hat{I}$$

$|x\rangle$ are continuous! must integrate rather than sum

We can use $\hat{I}$ to calculate dot-products.

$$\langle a|b\rangle = \langle a|\hat{I}|b\rangle = \langle a|\left[\int |x\rangle\langle x|\, dx\right]|b\rangle$$

$$= \int \underbrace{\langle a|x\rangle}_{\psi_a^*(x)} \underbrace{\langle x|b\rangle}_{\psi_b(x)} dx$$

$\therefore \quad \langle a|b\rangle = \int_{-\infty}^{\infty} \psi_a^*(x)\, \psi_b(x)\, dx \leftarrow$ How to calculate $\langle a|b\rangle$ in position space

$\uparrow$

Continuous sum

just like $\langle a|b\rangle = \sum_n a_n^* b_n \leftarrow$ How to calculate $\langle a|b\rangle =$ energy space

$\uparrow$

discrete sum in energy space

The momentum basis

For free particles, the energy eigenstates form a continuum. In practice, we use the momentum eigenstates, because they are complete & are also energy eigenstates.

We write the momentum eigenstates in Dirac Notation as $\{|k\rangle\}$.

What do these states look like? Well, in the position basis they are plane waves:

$$|k\rangle \underset{\text{like}}{\overset{\text{look}}{\sim}} \underbrace{\frac{1}{\sqrt{2\pi}} e^{ikx}}_{\text{a continuum of QM amplitudes.}} \text{ in the position basis}$$

We can use an equals sign if we project $|k\rangle$ onto $|x\rangle$:

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

The $|k\rangle$ are complete for free particles.

$$\hat{I} = \int |k\rangle\langle k|\, dk$$

So we can write an arbitrary state $|\psi\rangle$ as

$$|\psi\rangle = \hat{I}\,|\psi\rangle = \left(\int |k\rangle\langle k|\, dk\right)|\psi\rangle$$

$$= \int |k\rangle\langle k|\psi\rangle\, dk.$$

What is $\langle k|\psi\rangle$? It is the arbitrary state as it appears in momentum space. In other words, it is the momentum space wavefunction $\phi(k)$.

arbitrary state

$$\langle k|\psi\rangle = \phi(k) \quad \text{just like} \quad \langle x|\psi\rangle = \psi(x).$$

$$\therefore \; |\psi\rangle = \int |k\rangle\langle k|\psi\rangle\, dk = \int |k\rangle\, \phi(k)\, dk \quad \text{for continuous } |k\rangle.$$

(This is ~~the~~ analogous to

$$|\psi\rangle = \sum_n a_n |n\rangle \quad \text{for discrete } |n\rangle \text{)}$$

We can make this statement more concrete, and easier to understand by projecting it into the position basis:

$$\langle x|\psi\rangle = \langle x|\left(\int |k\rangle\, \phi(k)\, dk\right)$$

$$= \int \underbrace{\langle x|k\rangle}_{\frac{1}{\sqrt{2\pi}}e^{ikx}}\, \phi(k)\, dk$$

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int \phi(k)\, e^{ikx}\, dk \quad \leftarrow \text{Fourier Transform}$$

By projecting into the position basis, we recover the expression for the wavefunction as the Fourier Transform of $\phi(k)$.

The $\{|k\rangle\}$ are also orthonormal:

$$\langle k|k\rangle = \delta(k-k') \quad \leftarrow \text{Dirac delta function}$$

How can we demonstrate this? Use the position basis to calculate $\langle k|k'\rangle$:

$$\langle k|k'\rangle = \langle k|\hat{I}|k'\rangle = \langle k|\left(\int |x\rangle\langle x|\,dx\right)|k'\rangle$$

$$= \int \underbrace{\langle k|x\rangle}_{\frac{1}{\sqrt{2\pi}}e^{-ikx}}\underbrace{\langle x|k'\rangle}_{\frac{1}{\sqrt{2\pi}}e^{ik'x}}\,dx$$

$$= \underbrace{\frac{1}{2\pi}\int e^{i(k'-k)x}\,dx}_{\text{this is the delta function}} = \delta(k'-k).$$

Similarly, for the position basis we have

$$\int |x\rangle\langle x|\,dx = \hat{I} \quad \text{completeness}$$

$$\langle x|x'\rangle = \delta(x-x') \quad \text{orthonormality}$$

Hermitian Operators

In QM we use three types of mathematical objects.

(1) complex numbers : c
(2) state vectors (kets) : $|arb\rangle$
(3) Operators : $\hat{A}$

For (1) & (2), we have "partner" or "dual" objects :
(1) $c \rightarrow c^*$ complex conjugation
(2) bra vectors : $\langle arb|$

There is also a "partner" object for operators. It is called the "Hermitian Conjugate Operator", and written as $\hat{A}^+$. So we have

	Mathematical object	"partner"
number:	c	c^*
vector:	$\|arb\rangle$	$\langle arb\|$
operator:	$\hat{A}$	$\hat{A}^+$

these are the objects we use in QM.

We can write the laws of QM in terms of the "objects" or their "partners". They both describe the same thing. For example, the TDSE is

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

but we could also write

$$-i\hbar \frac{\partial \Psi^{+}(x,t)}{\partial t} = \hat{H}^{\dagger} \Psi^{*}(x,t)$$ ← this describes the same physics.

~~We will define the meaning of $\hat{A}^{+}$ in a minute, but first let's discuss why it is important. Basically,~~

When an operator is equal to it's Hermitian conjugate, we say that the operator is "Hermitian".

$\boxed{\text{If } \hat{A} = \hat{A}^{+} \text{, we say "}\hat{A}\text{ is Hermitian".}}$

This situation is the moral equivalent of a real number, except for the case of an operator.

"Hermitian Operators" are important ~~because 2 things~~ for two reasons.

(1) They always have real eigenvalues. Since observable quantities must be real, we modify Postulate I:

> Postulate I For every observable A, there is a Hermitian operator $\hat{A}$ for which $\underbrace{\hat{A}|n\rangle = a_n|n\rangle}_{\text{Eigenvalue Eq. in Dirac Notation}}$

(2) Hermitian Operators have eigenfunctions which are orthogonal. ⇒ If $\{|n\rangle\}$ are eigenvectors of $\hat{A}$, and $\hat{A} = \hat{A}^{+}$, then $\langle m|n\rangle = \delta_{mn}$.

The meaning of $A^\dagger$

Loosely speaking, if $\hat{A}$ is an operator which can be applied to a |ket vector⟩, then $A^\dagger$ is the equivalent operator which should be applied to the partner ⟨bra vector| :

$$\underbrace{\hat{A}\,|arb\rangle}_{\text{applied to the right}} \overset{\text{partners}}{\Longleftrightarrow} \underbrace{\langle arb|\,\hat{A}^\dagger}_{\text{applied to the left}}$$

Strict definition: if ~~$|\alpha\rangle$ and $|\beta\rangle$ are two ket vectors, ~~and $\hat{A}$ can operate on them,~~ ~~then~~ $\hat{A}^\dagger$ is the operator which satisfies

$$\left(\langle\alpha|\hat{A}^\dagger\right)|\beta\rangle \overset{\text{definition}}{\equiv} \langle\alpha|\underbrace{\hat{A}|\beta\rangle}_{\text{to the right}}$$

For all $|\alpha\rangle$ & $|\beta\rangle$

Example 1 Let $\hat{D}$ be $\frac{d}{dx}$ in position space. What is $\hat{D}^\dagger$?

Evaluate $\langle\alpha|\left(\hat{D}|\beta\rangle\right)$ in position space:

$$\langle\alpha|\left(\hat{D}|\beta\rangle\right) = \int_{-\infty}^{\infty}\psi_\alpha^*(x)\frac{d}{dx}\psi_\beta(x)\,dx = \underbrace{\left(\psi_\alpha^*(x)\psi_\beta(x)\right)_{-\infty}^{\infty}}_{0-0,\text{ if }\psi_\alpha\,\&\,\psi_\beta\text{ are normalizable.}} - \int_{-\infty}^{\infty}\left(\frac{d}{dx}\psi_\alpha^*(x)\right)\psi_\beta(x)\,dx$$

$$= \int_{-\infty}^{\infty}\left(-\frac{d}{dx}\psi_\alpha^*(x)\right)\psi_\beta(x)\,dx$$

$$\equiv \left(\langle\alpha|\hat{D}^\dagger\right)|\beta\rangle \text{ by definition of } \hat{D}^\dagger$$

The def. is confusing because it is legal to apply a Hermitian Conjugate to a ket state: $A^\dagger|\beta\rangle$ is legal. But the def. of $A^\dagger$, it sets applied to the bra $\langle\alpha|A^\dagger$

To keep track of which way the operator is applied, we sometimes move the operator inside the bra or ket symbol:

$A^\dagger|\beta\rangle \equiv |A^\dagger\beta\rangle$ $\quad\langle\alpha|A^\dagger = \langle A^\dagger\alpha|$

partners

$$\therefore \quad \boxed{\hat{D}^+ = -\frac{d}{dx} \iff \hat{D} = \frac{d}{dx}}$$

Since $\hat{D}^+ \neq \hat{D}$, $\hat{D}$ is not Hermitian, and it cannot represent an observable.

~~[illegible]~~

The momentum operator $\hat{p}$ includes a factor of (i) so it will be Hermitian. $\hat{p} = -i\hbar\frac{d}{dx} = \hat{p}^+$.

<u>Example 2</u> IF $\hat{A}$ = multiplication by a number c,
Then $\hat{A}^+$ = multiplication by c^*.

Proof: $\langle\alpha|\left(\hat{A}|\beta\rangle\right) = \langle\alpha|\left(c|\beta\rangle\right) = c\langle\alpha|\beta\rangle$

$$= c\int_{-\infty}^{\infty}\psi_\alpha^*(x)\psi_\beta(x)\,dx$$

$$= \int_{-\infty}^{\infty}\left(c^*\psi_\alpha(x)\right)^*\psi_\beta(x)\,dx$$

$$\overset{\text{by def. of } \hat{A}^+}{=} \left(\langle\alpha|\hat{A}^+\right)|\beta\rangle = \int_{-\infty}^{\infty}\left(\psi_\alpha(x)\hat{A}^+\right)^*\psi_\beta(x)\,dx$$

$\therefore$ $\hat{A}^+$ = multiplication by c^*.

Now we prove <u>the two</u> important consequences of an operator being Hermitian:

Important Property ① IF $\hat{A} = \hat{A}^+$, then the eigenvalues of $\hat{A}$ are real: $\hat{A}|n\rangle = a_n|n\rangle$, where $a_n = a_n^*$, and $|n\rangle$ = eigenvector of $\hat{A}$

<u>Proof</u>

Evaluate $\langle n|\left(\hat{A}|n\rangle\right) = \langle n|a_n|n\rangle = a_n\langle n|n\rangle$

$|||$ by def of A^+ $\qquad = \int(\hat{A}\psi_n(x))^*\psi_n(x)\,dx \qquad$ b/c $\hat{A}=\hat{A}^+$ $\quad a_n^*\langle n|n\rangle$

$$\left(\langle n|\hat{A}^+\right)|n\rangle = \int\left(\psi_n^*(x)\hat{A}^+\right)^*\psi_n\,dx = \int a_n^*\psi_n^*(x)\psi_n(x)\,dx$$

$\therefore \quad a_n = a_n^*$, and a_n = real number.

~~Pr~~

Important Property 2

If $|n\rangle$ & $|m\rangle$ are eigenvectors of $\hat{A}$, and $\hat{A} = \hat{A}^\dagger$ then

$\langle m|n\rangle = \delta_{mn}$ ← the eigenvectors are orthogonal.

Proof : $\hat{A}|n\rangle = a_n|n\rangle$ and $\langle n|\hat{A} = a_n\langle n|$ by I.P. 1.

$\hat{A}|m\rangle = a_m|m\rangle$ and $\langle m|\hat{A} = a_m\langle m|$

Therefor $\langle m|\hat{A}|n\rangle = \langle m|(\hat{A}|n\rangle) = a_n\langle m|n\rangle$

$$\begin{aligned} &\parallel \\ (\langle m|\hat{A})\,|n\rangle &= a_m\langle m|n\rangle \end{aligned}$$

$\therefore \quad a_m\langle m|n\rangle = a_n\langle m|n\rangle$

$(a_m - a_n)\langle m|n\rangle = \emptyset.$

Three ~~two~~ cases ~~1 $a_m \neq a_n$. Then $\langle m|n\rangle = \emptyset$.~~
~~2 $a_m = a_n$:~~

1. $m = n$. Thus we have $\overbrace{(a_m - a_m)}^{\emptyset}\langle m|m\rangle = \emptyset$

   If $|m\rangle$ is normalized, $\langle m|m\rangle = 1$.

2. $m \neq n$, $a_m \neq a_n$. Thus

$$\underbrace{(a_m - a_n)}_{\neq 0}\underbrace{\langle m|n\rangle}_{\emptyset} = \emptyset$$

$$\langle m|n\rangle = \emptyset$$

3. $m \neq n$, but $a_m = a_n$.

In this case two different states $|m\rangle$ & $|n\rangle$ have the same eigenvalue. We call this situation "degenerate eigenstates"

In the case of degenerate eigenstates, it turns out that we can make linear combinations of the states which are orthogonal. We'll ignore this detail and jump straight to the conclusion.

$$\boxed{\langle m|n\rangle = \delta_{mn}}$$ For ~~orthog~~ the eigenstates of a Hermitian operator