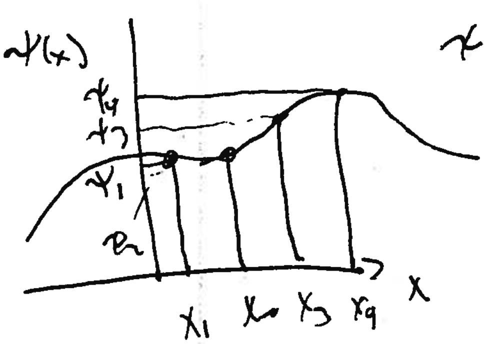
We've seen that the $\{a_n\}$ expansion coefficients for a particle-in-the-box can be written in Dirac Notation as

$$\underbrace{\langle n|}_{\text{one particular stationary state}}\underbrace{a\rangle}_{\text{any arbitrary particle-in-the box state}} = a_n = \text{amplitude to observe } E_n.$$

$$\Rightarrow |a_n|^2 = P(E_n).$$

But we have other types of amplitudes in QM, for example, $\psi(x)$ is an amplitude to observe a particular position: $|\psi|^2 dx = P(x)dx$.

The difference between $\psi(x)$ & $\{a_n\}$ is that x is a continuum of values, where (n) is discrete. But suppose we think of x as being discrete, with a very, very fine spacing. Then we could write $\psi(x)$ as a column vector:



$$\psi(x) \overset{\text{looks like}}{\sim} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \vdots \\ \vdots \end{pmatrix} \sim |\psi\rangle$$

where $\psi_1 = \psi(x_1)$
$\psi_2 = \psi(x_2)$
$\psi_3 = \psi(x_3)$

↓ infinitely many components

and $\psi^*(x) \overset{\text{looks like}}{\sim} (\psi_1^*, \psi_2^*, \psi_3^*, \ldots\ldots) \sim \langle\psi|$

With this bra-ket notation, the self multiplied bracket is

$$\langle\psi|\psi\rangle = (\psi_1^*, \psi_2^*, \psi_3^*, \ldots) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \vdots \end{pmatrix}$$

$$= \psi_1^*\psi_1 + \psi_2^*\psi_2 + \psi_3^*\psi_3 \ldots$$

Again, if ψ is a normalized state, this should sum up to 1:

$\langle\psi|\psi\rangle = 1 \leftarrow$ if ψ is correctly normalized.

Now let the discrete $\{x_i\}$s turn back into a continuum:

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

$$= \psi^*(x_1)\psi(x_1) + \psi^*(x_2)\psi(x_2) + \psi^*(x_3)\psi(x_3) + \ldots$$

In the true continuum limit, this sum is an integral:

$$= \int \psi^*(x)\,\psi(x)\,dx = 1 \text{ by normalization}$$

$\therefore$ To evaluate a bracket in a discrete representation, like the stationary states for the particle-in-the box, we do the dot-product by summing over the index.

In a continuum representation, we integrate over the variable.

Analogy:

Ordinary vectors: $\vec{a}\cdot\vec{b} = \sum_{i=1}^{3} a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3$

$\boxed{\text{Infinite length, discrete Dirac vectors:}}$ $\langle a|b\rangle = \sum_{n=1}^{\infty} a_n^* b_n = a_1^* b_1 + a_2^* b_2 + \ldots$

discrete (n)

$\boxed{\text{Infinite length, Continuous Dirac vectors:}}$ $\langle a|b\rangle = \int_{-\infty}^{\infty} a^*(x)\, b(x)\, dx$

sum over continuous x.

The tricky thing about these Dirac bra and ket vectors is that they take different forms depending on how you choose to represent them

$|arb\rangle$ ~~$|a\rangle$~~ is a ket vector ~~ass~~ symbolizing an arbitrary state

From the point-of-view of ~~the~~ energy ~~states~~

$|arb\rangle$ looks like $\{a_n\} = (a_1, a_2, a_3, \ldots\ldots)$

From the point of view of the position (x),

$|arb\rangle$ looks like $\psi_{arb}(x)$ or $a(x)$: $(\psi_1, \psi_2, \psi_3, \ldots)$

same thing.

but not ψ_1, ψ_2 are actually continuous

When we ~~fa~~ multiply an arbitrary state $|a\rangle$ by a particular ~~[illegible]~~ stationary state $\langle n|$, we get a_n:

$$\langle n|\underbrace{a}_{\text{an arbitrary state}}\rangle = a_n \text{ where } |a_n|^2 = P(E_n)$$

↑ an amplitude

$\psi(x)$ is also an amplitude. Can we multiply an arbitrary state $|\text{arb}\rangle$ by something to se $\psi(x)$?

$$\langle ?|\underbrace{\text{arb}}_{\text{an arbitrary state}}\rangle = \psi_{\text{arb}}(x^*) \text{ where } |\psi|^2 dx = P(x^*)\,dx$$

or $a(x)$

↑ an amplitude to observe the particle @ x^*

What should $\langle ?|$ be??

~~Well, write the dot product in vector form~~

Well, $\langle ?|$ must ~~localize the particle~~ be an eigenstate of position, by analogy with $\langle n|a\rangle = a_n$.

We call it $\langle x|$, a bra vector which represents an eigenstate of position.

In vector form, $\langle x|$ looks like

$$\langle x| \sim (\ldots 0, 0, 0, 1, 0, 0, \ldots) \leftarrow$$

↑ the x position

From the point of view of discrete x

has to be ∞ for continuity

$$\sim (\ldots 0, 0, 0, \infty, 0, 0, 0 \ldots)$$

↑ the x position

$\langle x|$ "picks out" the amplitude to be seen at position x: $\langle x|\text{arb}\rangle = \psi_{\text{arb}}(x)$ ~~or $a(x)$~~

just like $\langle n|\text{arb}\rangle = a_n$

We use $\{|n\rangle\}$ to mean a set of states which are the discrete stationary state of the particle in the box. These are eigenfunctions of $\hat{H}$.

In the position basis, they look like

$$|n\rangle \overset{\text{looks like}}{\sim} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad \text{in } x\text{-space}$$

In the energy basis they look like

$$|n\rangle \overset{\text{looks like}}{\sim} \begin{pmatrix} \vdots \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \quad \text{in energy basis.}$$

← nth position

We use $\{|x\rangle\}$ to mean a set of states which are the continuous eigenstates of position.

$|x^*\rangle$ means a state with particle 100% localized at $x = x^*$.

In the position basis, they look like

$$|x^*\rangle \overset{\text{looks like}}{\sim} \delta(x - x^*) \quad \text{in position basis.}$$

We use these states to get $\psi(x)$ from an arbitrary state:

$$\underbrace{\langle x|}_{\text{position eigenstates}}\underbrace{\text{arb}\rangle}_{\text{arbitrary state}} = \psi_{arb}(x) \text{ or } \left(a(x)\right)$$

Since the label "a" ~~is arbitrary~~ could be anything, people usually use ψ:

$$\langle x|\psi\rangle = \psi(x)$$

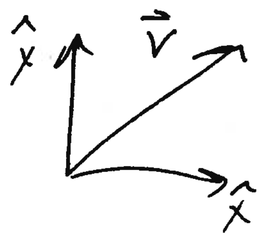
$$\& \quad \langle n|\psi\rangle = a_n \text{ where } \psi(x) = \sum_n a_n \phi_n(x)$$

These bases, $\{|x\rangle\}$ & $\{|n\rangle\}$ are different because $\{|x\rangle\}$ is continuous, & $\{|n\rangle\}$ is discrete. But we can "project" an arbitrary state onto either one:

$$\langle n|\psi\rangle = a_n \leftarrow \text{discrete series}$$

$$\langle x|\psi\rangle = \psi(x). \leftarrow \text{continuous function.}$$

The ket vector $|\psi\rangle$ represents an abstract state which has not yet been projected onto any basis. With ordinary vectors, we have

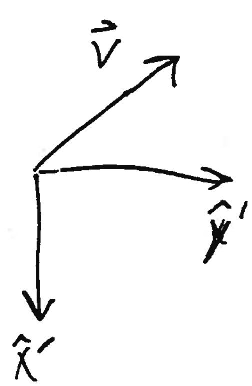


an abstract vector $\vec{V}$ looks like

$$\vec{V} = V_x\hat{x} + V_y\hat{y} \quad \text{projected on } \hat{x} \,\&\, \hat{y}$$

$$= (\vec{V}\cdot\hat{x})\,\hat{x} + (\vec{V}\cdot\hat{y})\,\hat{y}$$

But we could choose a different coordinate system.



$\vec{V}$ looks like $\vec{V} = (\vec{V}\cdot\hat{x}')\,\hat{x}' + (\vec{V}\cdot\hat{y}')\,\hat{y}'$

In this coordinate system.

The particular components $(\vec{V}\cdot\hat{x},\ \vec{V}\cdot\hat{y})$ & $(\vec{V}\cdot\hat{x}',\ \vec{V}\cdot\hat{y}')$ depend on the choice of coordinate system. But $\vec{V}$ exists no matter how you choose to project it.

We say that a basis is complete when all relevant states can be represented by linear combinations of them.

For the particle-in-the-box, the energy eigenfunctions are complete:

$$\psi(x) = \sum_n a_n \psi_n(x) \quad \text{for appropriate } \{a_n\}.$$

In Dirac notation we write

$$|\psi\rangle = \sum_n a_n |n\rangle = \sum_n |n\rangle a_n \qquad \langle n|\psi\rangle = a_n$$

$$= \sum_n \underset{\text{basis vector}}{|n\rangle} \underset{\text{projection}}{\langle n|\psi\rangle}$$

This is analogous to

$$\vec{v} = (\vec{v}\cdot\hat{x})\,\hat{x} + (\vec{v}\cdot\hat{y})\,\hat{y} = \sum_{i=1}^{2} \hat{x}_i\,(\vec{v}\cdot\hat{x}_i)$$

$$\therefore\ |\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle \quad \text{if } \{|n\rangle\} \text{ is complete}$$

Often we write this as

$$|\psi\rangle = \left(\sum_n |n\rangle\langle n|\right)|\psi\rangle$$

take the dot product with each $|n\rangle$.

Since $|\psi\rangle$ appears on both sides,

$$\left(\sum_n |n\rangle\langle n|\right) \text{ must be the Identity Operator}$$

$$\boxed{\hat{I} = \text{multiply by one} = \sum_n |n\rangle\langle n|}$$

$$|\psi\rangle = \hat{I}\,|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$$

This is how we say that the $\{|n\rangle\}$ are complete

∴ For our complete, orthonormal basis, we have

a number $\rightarrow$ $\langle m|n\rangle = \delta_{mn}$ $\leftarrow$ orthonormality condition

$\sum_n |n\rangle\langle n| = \hat{I}$ $\leftarrow$ completeness condition

an operator $\rightarrow$

We can insert $\hat{I}$ into the middle of a bracket:

$$\langle a|b\rangle = \langle a|\,|b\rangle = \langle a|\hat{I}|b\rangle$$
$$= \langle a|\sum_n |n\rangle\langle n|\,|b\rangle$$
$$= \sum_n \langle a|n\rangle\langle n|b\rangle$$
$$\langle a|b\rangle = \sum_n a_n^* b_n$$

This is the correct rule for the dot product; analogous to $\vec{a}\cdot\vec{b} = \sum_{i=1}^{3} a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3$.

For a continuous basis, the sum in the Identity operator is an integral: For example $\{|x\rangle\}$ is complete, so

$$\hat{I} = \int dx\ |x\rangle\langle x|$$

and we can do

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

same dot product evaluated in the position basis $\rightarrow$ $= \int dx\ a^*(x)\, b(x)$

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

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

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

(This is ~~the~~ analogous to

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

We can make this statement more concrete, and easier to understand by <u>projecting</u> 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

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

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

Common set of Base ~~set~~ States in QM.

1. $\{|n\rangle\}$: Bound state energy eigenstates. Discrete
2. $\{|x\rangle\}$: Position eigenstates, Continuous
3. $\{|k\rangle\}$: momentum eigenstates, Continuous for a free particle.

We can project these states into the position basis. This gives us their spatial wavefunctions:

$$\langle x|n\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad \langle x|x^*\rangle = \delta(x-x^*)$$

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

For each of these bases, we have completeness and orthonormality:

$$\underbrace{\langle m|n\rangle = \delta_{mn}}_{\text{orthonormality}} \leftarrow \text{Kronecker Delta}, \quad \underbrace{\hat{I} = \sum_n |n\rangle\langle n|}_{\text{completeness}}$$

$$\langle x|x^*\rangle = \delta(x-x^*) \leftarrow \text{Dirac Delta}, \quad \hat{I} = \int |x\rangle\langle x|$$

$$\langle k|k^*\rangle = \delta(k-k^*) \leftarrow \text{Dirac Delta}, \quad \hat{I} = \int |k\rangle\langle k|$$

We can use the completeness statement to calculate the Dirac Bracket of arbitrary states, if we know how those states are represented in one of these bases:

$$\langle a|b\rangle = \langle a|\underset{\uparrow \text{ Identity}}{\hat{I}}|b\rangle = \langle a|\left(\sum_n |n\rangle\langle n|\right)|b\rangle$$

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

we can use this if we know the $\{a_n\}$ & $\{b_n\}$. $\longrightarrow$ $= \sum_n a_n^* b_n$

Similarly,

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

$$= \int \langle a|x\rangle\langle x|b\rangle\,dx$$

We can use this if we know the spatial wavefunctions for ~~~~ $|a\rangle$ & $|b\rangle$.

$$= \int \psi_a^*(x)\,\psi_b(x)\,dx$$

And

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

$$= \int \underbrace{\langle a|k\rangle}_{\phi_a^*(k)}\,\underbrace{\langle k|b\rangle}_{\phi_b(k)}\,dk$$

We can use this if we know the momentum space wavefunction for $|a\rangle$ & $|b\rangle$.

$$= \int \phi_a^*(k)\,\phi_b(k)\,dk$$

In all three cases we are <u>projecting</u> these abstract bra & ket vectors onto a particular basis. This makes them more down-to-earth, and ~~~~ allows us to use their <u>explicit</u> forms, in these bases.

Note: most people & textbooks use the symbol "$|\psi\rangle$" to represent an arbitrary QM state. Remember, "ψ" is a label. Strictly speaking

$$\langle x|\psi\rangle = \psi(x)$$

a label — a label — a real variable — a complex #

Dictionary for translating Wave Mechanics Into Dirac Notation

~~Eigenfunction Eqn~~

	Wave Mech.	Dirac Notation
Eigenvalue Eq:	$\hat{A}\,\alpha = a\,\alpha$	$\hat{A}\,\lvert\alpha\rangle = a\,\lvert\alpha\rangle$
Momentum Eigenstates:	$\alpha(k) = \frac{1}{\sqrt{2\pi}} e^{ikx}$	$\langle x \mid k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$
TISE:	$\hat{H}\,\alpha_n = E_n\,\alpha_n$	$\hat{H}\,\lvert n\rangle = E_n\,\lvert n\rangle$
General Solution e t=0:	$\psi(x) = \sum_n a_n \alpha_n(x)$	$\lvert\psi\rangle = \sum_n a_n \lvert n\rangle$
For all t:	$\Psi(x,t) = \sum_n a_n \alpha_n(x) e^{-i\omega_n t}$	$\lvert\Psi\rangle = \sum_n a_n \lvert n\rangle e^{-i\omega_n t}$
Fourier's Trick	$a_n = \int \alpha_n^* \psi(x)\,dx$	$a_n = \langle n \mid \psi\rangle$
orthonormality for bound state	$\int \alpha_m^*(x)\,\alpha_n(x)\,dx = \delta_{mn}$	$\langle m \mid n\rangle = \delta_{mn}$
Orthonormality for momentum eigenstates	$\frac{1}{2\pi}\int_{-\infty}^{\infty} \left(e^{ikx}\right)^* \left(e^{ik'x}\right) dx = \delta(k-k')$	$\langle k \mid k'\rangle = \delta(k-k')$
Orthonormality for position eigenstates	$\frac{1}{2\pi}\int_{-\infty}^{\infty} \left(e^{ikx}\right)^* \left(e^{ikx'}\right) dk = \delta(x-x')$	$\langle x \mid x'\rangle = \delta(x-x')$
Free Particle	$\psi(x) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{ikx}\,dk$	$\lvert\psi\rangle = \int \lvert k\rangle\,\phi(k)\,dk$
Expectation Value	$\langle C\rangle = \int \psi^*(x)\,\hat{C}\,\psi(x)\,dx$	$\langle\psi \mid \hat{C} \mid \psi\rangle$

$\cancel{\lvert\psi\rangle = \int \lvert k\rangle\langle k \mid \psi\rangle\,dk}$ ($\phi(k)$)

$\cancel{\psi(x) = \langle x \mid \psi\rangle = \int \langle x \mid k\rangle\,\phi(k)\,dk}$

$\cancel{\frac{1}{\sqrt{2\pi}}\int e^{ikx}\,\phi(k)\,dk}$