For the particle-in-the-box, the stationary states we call φ_n. They have 2 important properties

1) Completeness: Any valid $\psi(x)$ can be written as a linear combination of φ_n. Guaranteed by Discrete Sine Series Fourier Theorem

2) Orthonormality: φ_n satisfy
$$\int \varphi_m^* \varphi_n \, dx = \delta_{mn} .$$

For the free particle we use continuous momentum eigenstates $\{e^{ikx}\}$. We have properties

1) Completeness: Any free particle wavefunction which is square integrable $\left(\int_{-\infty}^{\infty} |\psi|^2 dx = \text{finite} = 1\right)$ can be written as a continuous sum (integral) over the e^{ikx}: $\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \, \phi(k) \, e^{ikx}$ for some $\phi(k)$.

2) Do we have a orthonormality condition for the $\{e^{ikx}\}$? Answer: Yes. It is

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dk \left(e^{ikx}\right)\left(e^{-ikx'}\right) = \underbrace{\delta(x-x')}_{\text{Dirac Delta Function}}$$

(same k) (over k)

"Proof": Fourier Transform Theory:

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

Substitute $\phi(k)$ into integral for $F(x)$:

$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, e^{ikx} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx'\, e^{-ikx'} F(x') \right]$$

Use x' on RHS

interchange order of integration:

$$F(x) = \int_{-\infty}^{\infty} dx'\, F(x') \left[\frac{1}{2\pi} \int_{\infty}^{\infty} \left(e^{ikx}\right)\left(e^{-ikx'}\right) dk \right]$$

This looks like the definition of $\delta(x-x')$:

$$F(x) \equiv \int_{-\infty}^{\infty} dx'\, F(x')\, \delta(x-x') \leftarrow \text{Def. of } \delta(x-x')$$

if we identify

$$\boxed{\frac{1}{2\pi} \int_{-\infty}^{\infty} dk \left(e^{ikx}\right)\left(e^{-ikx'}\right) = \delta(x-x')}$$

~~Or the~~ Compare to:

$$\int_{-\infty}^{\infty} a_m^* a_n\, dx = \delta_{mn}$$

∴ The Dirac Delta can be thought of as the continuous version of the Kronecker Delta.

We usually write the orthonormality relation as

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-x')} = \delta(x-x')$$

By relabelling $x \leftrightarrow k$ we can also write it as

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{i(k-k')x} = \delta(k-k').$$

Physical Interpretation.

Suppose we have a quantum state which is a perfect plane wave:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} e^{ik^*x}$$, $k^* \Rightarrow$ some particular constant wavenumber

It extends forever to (+) & (−) ∞

The particle is equally likely to be found anywhere on the x-axis.

What is the momentum space wavefunction?

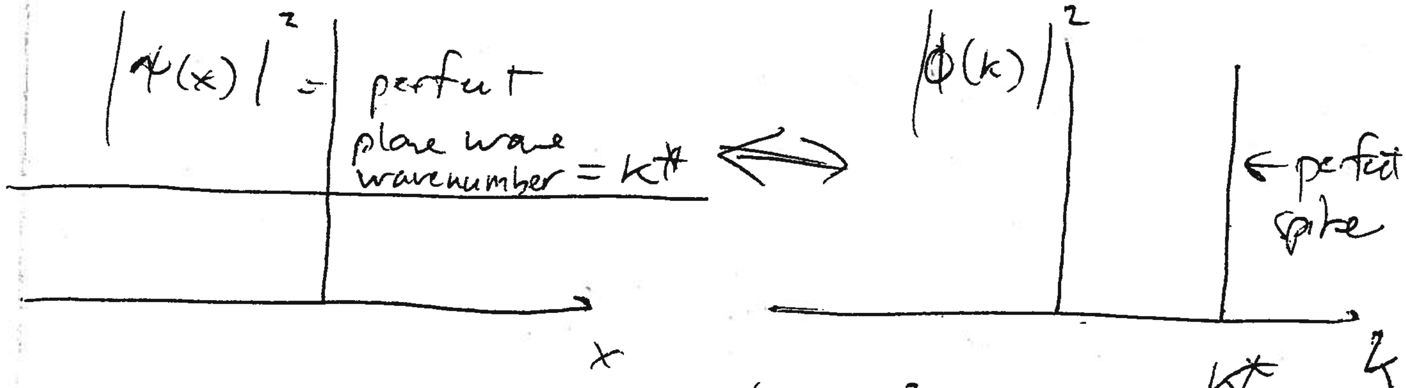
Answer

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, \psi(x) e^{-ikx} = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx \left(e^{ik^*x}\right)\left(e^{-ikx}\right)$$

$$= \delta(k-k^*)$$

$\therefore$ $\phi(k) = \delta(k - k^*)$: The p-space wavefunction is a perfect spike at $k = k^*$.

$\Rightarrow$ If our particle is a perfect plane wave with one and only one wavenumber, k^*, its $\phi(k)$ is a perfect spike at $k = k^*$.



What is the width of $|\psi(x)|^2$? Answer: $\Delta x \to \infty$.
What is the width of $\phi(k)$? Answer: $\Delta k \to 0$.

Again, we have an inverse relationship.

$$(\Delta x) \sim \frac{1}{(\Delta k)} \Rightarrow (\Delta x)(\Delta k) \sim 1.$$

This is an extreme illustration of the uncertainty principle

Dirac Notation

For the Free Particle, we have seen that there are two equivalent ways of thinking about the QM state:

$|amp|^2 =$ Probability

$\psi(x)$: tells us the amplitude to find the particle at x: $|\psi|^2 dx = P(x)\,dx$

$\phi(k)$: tells us the amplitude to find the particle with momentum at $\hbar k$: $|\phi|^2 dk = P(k)\,dk$.

$\psi(x)$ & $\phi(k)$ are equivalent representations of the QM state. We say "$\psi(x)$ represents the state in the position basis, and $\phi(k)$ represents the state in the momentum basis".

For the particle in a box, we also have $\psi(x)$

$\psi(x)$: amplitude of the QM particle in x-space

We also have the $\{a_n\}$, which represents the state ~~ene~~ in the energy basis. $\Rightarrow a_n = \int_0^L \varphi_n^*(x)\,\psi(x)\,dx$

$\{a_n\}$: tells us the amplitude to measure energy $E_n \Rightarrow |a_n|^2 = P(E_n)$.

$\{a_n\}$ is the analog of $\phi(k)$ for a system with discrete stationary states.

If we know the $\{a_n\}$ for a particular system, then we know everything about the system.

For example, if $a_1 = 1$, $a_2, a_3 \ldots a_\infty = \emptyset$,

then $\psi(x) = \phi_1(x) = \sqrt{\frac{2}{L}} \sin(\pi x/L)$

If $a_1 = \emptyset$, $a_2 = \frac{1}{\sqrt{2}}$, $a_3 = \frac{i}{\sqrt{2}}$, $a_4 = a_5 = \emptyset$.

then $\psi(x) = \frac{1}{\sqrt{2}} \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) + \frac{i}{\sqrt{2}} \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right)$

We can think of the $\{a_n\}$ for a system as being a vector. We call it a state vector:

$$\{a_n\} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}$$

Column vector

$\downarrow$ infinite # of components

The complex conjugates are also a state vector:

$$\{a_n^*\} = (a_1^*, a_2^*, a_3^*, \ldots) \quad \text{Row vector.}$$

$\longrightarrow$ infinite # of components

These column & Row vectors are sometimes useful, but we usually write them more compactly as bra's and ket vectors:

$|\text{a column vector}\rangle \leftarrow$ ket vector

$\langle \text{a row vector}| \leftarrow$ bra vector

This notation is due to Dirac.

Inside a bra vector or ket vector, we put a label to remind us what type of QM state the vector stands for:

$$|\text{the } n=3 \text{ e.f. of the particle-in-the-box}\rangle$$

As a column vector this looks like: $\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$

As a wavefunction it looks like $\sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right)$.

Usually we just use (n) as the label:

$|n\rangle \leftarrow$ a ~~bra~~ ket vector for e.f. n.

note that n is not really a variable or index or integer here, it's really just a name to remind ourselves that this stands for the n^{th} energy e.f.

We can multiply a bra-vector with a ket-vector

$$\langle \text{my QM state} | | \text{my QM state}\rangle$$

same state

$$= (a_1^*, a_2^*, a_3^*, \ldots) \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = a_1^* a_1 + a_2^* a_2 + a_3^* a_3 + \ldots$$

$$= |a_1|^2 + |a_2|^2 + |a_3|^2$$

$$= \sum_{n=1}^{\infty} |a_n|^2 .$$

We already know the physical interpretation of $|a_n|^2$. It is a probability, so $\sum_{n=1}^{\infty} |a_n|^2$ must be 1.

$$\langle \text{my QM state} | \, | \text{my QM state} \rangle = \sum_{n=1}^{\infty} |a_n|^2 = 1$$

~~Whether When we multiply two states together this way~~

When we multiply a bra vector & a ket vector, we call the combination a bracket. We also drop the double-line in the middle:

$$\langle \text{my QM state} | \text{my QM state} \rangle = \text{a bracket} = 1.$$

~~The bracket represents a dot-product between a bra vector & a ket vector. The bracket will always be a number, often a complex number.~~

For $\langle \text{my QM state} | \text{my QM state} \rangle = 1$, the result was 1 because we implicitly assumed that the $\{a_n\}$ had been calculated for a properly normalized state. In fact, any normalized state should always ~~[illegible]~~ result in 1 when its bra vector is multiplied with its ket vector.

More generally, the bracket represents a dot-product of two Dirac vectors. Compare

$$\langle a | b \rangle = a_1^* b_1 + a_2^* b_2 + \ldots = \sum_{n=1}^{\infty} a_i^* b_i$$

a label, a label, a c-number, a c-number

In ordinary vectors, the dot-product is

$$\vec{a} \cdot \vec{b} = a_x b_x + a_y b_y + a_z b_z = \sum_{n=1}^{3} a_n b_n$$

where $1 \rightarrow x$
$2 \rightarrow y$
$3 \rightarrow z$.

The Dirac bracket generalizes this to the complex state vecters we have in QM.

In Dirac notation, the particle-in-a-box stationary states are written as vectors:

$|n\rangle$ ← a ket vector for energy e.f. (n).
↑ a label

† $\langle n|$ ← a bra vector for the same state

We can multiply:

$$\underbrace{\langle n|n\rangle}_{\text{a bracket}} = 1$$ if $|n\rangle$ is properly normalized.

Explicitly, $$\langle n|n\rangle = (a_1^*, a_2^*, a_3^*, \ldots) \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}$$

$$= \sum_{n=1}^{\infty} a_n^* a_n = \sum_{n=1}^{\infty} |a_n|^2 = 1$$

Here we have multiplied a state by itself and got 1 because we assume it is normalized correctly.

We can also multiply an arbitrary state with a ~~another~~ ~~states~~ different arbitrary state:

$$\langle \underbrace{a}_{\substack{\text{any state}\\ \text{at all}}}|\underbrace{b}_{\substack{\text{any other}\\ \text{state at all}}}\rangle = \sum_{n=1}^{\infty} a_n^* b_n = \text{could be any complex number.}$$

A bracket like this ~~idea~~ has a deep significance which we illustrate

Suppose we take the bracket of an arbitrary state with an energy e.f.:

2

$\langle n | a \rangle$ ← any arbitrary state

$|a\rangle$ = an arbitrary QM state in ket form

$$= \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} \quad \text{in column vector form}$$

$\langle n|$ = a bra vector for an energy e.f.

$= \cancel{(\ldots, 0, 0, \ldots 1, 0, 0, \ldots)}$

$= (\ldots, 0, 0, 1, 0, 0, \ldots\ldots)$

↑ the n^{th} position

The bracket is

$$\underbrace{\langle n | a \rangle}_{\text{a bracket}} = a_n \leftarrow \text{the } n^{th} \text{ coefficient in the } \{a_n\} \text{ series.}$$

↑ a complex number

The dot-product of our arbitrary state with the energy e.f. for state (n) "picks out" the n^{th} coeff. of the $\{a_n\}$ expansion.

This is exactly the same as the way that ordinary dot product works: $\vec{V} = (V_x, V_y, V_z)$, $\vec{V} \cdot \hat{x} = V_x$ i.e. → This dot product picks out

We already know that $|a_n|^2 = P(E_n) \leftarrow$ prob. to observe E_n

$\therefore |\langle n | a \rangle|^2 = P(E_n)$. ⟹ Dirac brackets are QM amplitudes → specifically complex numbers.

Suppose that our arbitrary state is another energy e.f. with index (m):

What is $\langle n | m \rangle$?

↑ an eigenstate of energy — ↑ another eigenstate of energy

(any bra vector / any ket vector)

= complex #

= QM amplitude

Well, $\langle n| = (\ldots 0, 0, 0, 1, 0, 0, \ldots)$ ← nth position

$$|m\rangle = \begin{pmatrix} \vdots \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \leftarrow m\text{th position}$$

So $\langle n|m\rangle$ either is 1 or 0; 1 if $m=n$
ϕ if $m \neq n$

$\boxed{\langle n|m\rangle = \delta_{mn}}$ This is how we write orthonormality in Dirac notation.

Previously we wrote this in position space as $\int_0^L \psi_n^*(x)\, \psi_m(x)\, dx = \delta_{mn}$.

This is one reason we love Dirac Notation $\Longrightarrow$ It is very compact and elegant.

<u>Compare Dirac vectors</u> to ordinary vectors:

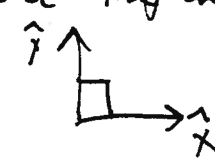
Call $\hat{x} = \hat{x}_1$, $\hat{y} = \hat{x}_2$, $\hat{z} = \hat{x}_3$.

Then we have

$$\hat{x}_1 \cdot \hat{x}_2 = \phi$$
$$\hat{x}_1 \cdot \hat{x}_3 = \phi$$
$$\hat{x}_1 \cdot \hat{x}_1 = 1$$

etc

because they are $\perp$



or $\underbrace{\hat{x}_i \cdot \hat{x}_j}_{\text{ordinary dot product}} = \delta_{ij}$

$\overbrace{\langle n|m\rangle}^{\text{Dirac dot product}} = \delta_{mn}$ is the analagous statement for bra and ket vectors.

$\hat{x}$ & $\hat{y}$ "have no overlap" because they point in orthogonal directions:

$$\hat{x} \cdot \hat{y} = 0$$

~~A rot can never turn an $\hat{x}$ vector into a $\hat{y}$ vector~~

~~Says~~ Similary, we say that different energy eigenfunctio "have no overlap" because their dot-product $\langle m | n \rangle$ is zero unless $m = n$.

Going back to $\underbrace{\langle n |}_{\text{a stationary state}} \underbrace{a \rangle}_{\text{an arbitrary state}} = a_n$ = amplitude to observe E_n in state $|a\rangle$.

We see the physical interpretation of this bracket: it ~~tells us~~ represents the amplitude to observe E_n in state $|a\rangle$. But we have other types of amplitudes in QM. For example $\psi(x)$ is an amplitude to observe ~~position~~ the particle at position x:

$$\psi^*(x)\psi(x)\,dx = P(x)\,dx$$

$\psi(x)$ is a <u>continuum of amplitudes</u> for the continuous <u>varible x</u>.

$\{a_n\}$ is a <u>discrete</u> set of amplitudes for the discrete energies $\{E_n\}$.

If $a_n = \underbrace{\langle n|}_{\text{one particular stationary state}}\underbrace{a\rangle}_{\text{any arbitrary state}}$,

Can we write the $\psi(x)$ amplitude as a bracket??

The answer is <u>yes</u>.