Physics 472 Lecture 5

Bra-ket notation revisited

Postulate 1 states that the dynamical state of a QM system can be represented by a wavefunction $\psi(x)$.

Postulate 2 states that any linear combination

$$\psi(x) = \sum_n c_n \psi_n(x)$$

of physically meaningful wavefunction is also a possible state of the system. For the case where $\psi_n(x)$, $n=1,2,\ldots$ form a complete set of orthonormal functions, we saw that $\psi(x)$ could also be represented by the column vector

$$\psi = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}.$$

Furthermore, we also made use of the Fourier transform

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

$$\tilde{\psi}(k) = \int_{-\infty}^{\infty} dx\, \psi(x)\, e^{-ikx}$$

All these different forms represent the same QM state, suggesting that a more general, representation-independent, description is possible.

Alternate form of Postulate 1

The dynamical state of a QM system can be represented by a state vector $|\psi\rangle$ in a complex vector/function (4

space known as Hilbert space.

This vector contains all the

information that can be known.

The specific representations

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

$$\tilde{\psi}(k) = \langle k | \Psi \rangle$$

$$c_n = \langle n | \Psi \rangle$$

are just the components of the vector $|\Psi\rangle$ in different bases.

Check

i) $\psi(x) = \sum_n c_n \psi_n(x)$

$\langle n'|\psi\rangle = \int dx\, \psi_{n'}^*(x)\, \psi(x) = \sum_n c_n \underbrace{\langle n'|n\rangle}_{\delta_{nn'}}$

$\langle n'|\psi\rangle = c_{n'}$ Q.E.D.

ii) $\tilde{\psi}(k) = \int_{-\infty}^{\infty} dx\, e^{-ikx}\, \psi(x)$

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

$\psi_k(x) = e^{ikx}$ plane wave = momentum eigenstate

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

$\Rightarrow \psi_x(x') = \delta(x'-x)$ position eigenstate

The set $\{\psi_n(x)\}$ could be the eigenfunctions of any Hermitian operator $\hat{Q}$:

$$\hat{Q}\,\psi_n = q_n\,\psi_n.$$

Properties of Hermitian operators

i) $q_n \in \mathbb{R}$

ii) $\langle n' | n \rangle = 0$ if $q_n \neq q_{n'}$

iii) The set $\{\psi_n(x)\}$ forms a complete basis in Hilbert space.

Properties (i) and (ii) were proven in Physics 371. Property (iii) can be proven for finite-dimensional vector spaces, but must be taken as an Axiom for infinite-dimensional vector spaces, the typical case in QM.

Since the states in Hilbert space are normalizable, property (ii) may be written

$$\langle n' | n \rangle = \delta_{nn'}.$$

However, this relation only holds if the spectrum $\{ \mathcal{E}_n \}$ is

<u>discrete.</u> For operators with a continuous spectrum, the eigenfunctions are not normalizable, and so lie outside Hilbert space, strictly speaking.

<u>Examples</u>

<u>Position</u> $\psi_x(x') = \delta(x'-x)$

$$\langle x|y\rangle = \int_{-\infty}^{\infty} dx' \, \delta^*(x'-x)\, \delta(x'-y)$$

$$= \delta(x-y) = \begin{cases} 0 & \text{if } x \neq y \\ \infty & \text{if } x = y \end{cases}$$

<u>Momentum</u> $\psi_k(x) = e^{ikx}$

$$\langle k|k'\rangle = \int_{-\infty}^{\infty} dx\ \psi_k^*(x)\,\psi_{k'}(x)$$

$$= \int_{-\infty}^{\infty} dx\ e^{-ikx}\, e^{ik'x}$$

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

Position and momentum eigenfunctions are orthogonal for different eigenvalues, but not normalizable. They possess "Dirac orthonormality", wherein $\delta_{nm} \longrightarrow \delta(n-m)$.

Physical states can only approximate position or momentum eigenstates $\longrightarrow$ wave packets.

Finite space

For the momentum operator, the eigenstates do lie in Hilbert space for a finite space with periodic boundary conditions:

$$\psi(x+L)=\psi(x)$$

position defined modulo L

$$\psi_k(x)=\frac{1}{\sqrt{L}}e^{ikx}$$

$$\psi_k(x+L)=\psi_k(x)\,e^{ikL}$$

$$\Rightarrow e^{ikL}=1\,,\quad k_n=\frac{2\pi n}{L}\,,\quad n\in\mathbb{Z}$$

$\Rightarrow$ discrete spectrum

$$\langle k|k'\rangle = \int_0^L dx \, \frac{e^{i(k'-k)x}}{L}$$

$$= \int_0^L \frac{dx}{L} \, e^{i\frac{2\pi}{L}(n'-n)x}$$

$$= \begin{cases} 1 \,, & n = n' \\ \dfrac{e^{i2\pi(n'-n)} - 1}{2\pi i} = 0 \,, & n \neq n' \end{cases}$$

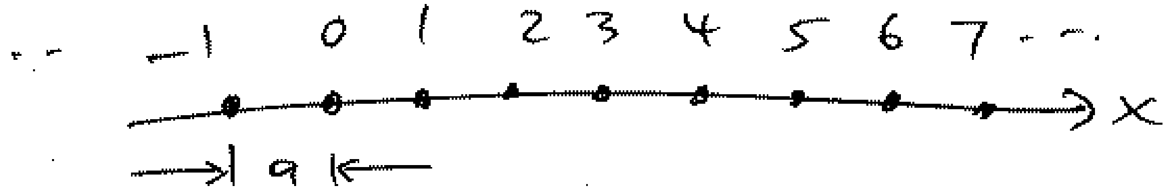
$$= \delta_{nn'} \quad \checkmark$$

Discrete space

In a similar way, position eigenstates become well-behaved

If we discretize space:

$x = na$, $n \in \mathbb{Z}$



$\psi(x) \to \{\psi_n\}$, where the amplitude ψ_n determines the probability $P_n = |\psi_n|^2$ to find the particle at $x = na$.

What happens to momentum in this case?

$$\psi_k(n) = e^{ikna} \quad \text{(plane wave)}$$

$$\psi_{k+\frac{2\pi}{a}}(n) = e^{ikna}\, e^{i2\pi n} = e^{ikna}$$

⇒ There is <u>no difference</u> between a plane wave with wave vector k and one with wave vector $k' = k + \frac{2\pi}{a}$

⇒ Momentum is defined only modulo $\frac{2\pi}{a}$, and may thus be chosen to lie in the interval

$$k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right),$$

known as the <u>first Brillouin zone</u>.

State vectors

An equation like

$$\Psi = \sum_n c_n \psi_n$$

holds in any basis, so we can write it in a basis-indep. vector notation

$$|\psi\rangle = \sum_n c_n |n\rangle .$$

But $c_n = \langle n|\psi\rangle$, so

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

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

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

$$\Rightarrow \boxed{\mathbb{1} = \sum_n |n\rangle\langle n|}$$

= unit operator.

similarly,

$$\boxed{\begin{aligned} \mathbb{1} &= \int dx\ |x\rangle\langle x| \\ \text{and}\quad \mathbb{1} &= \int \frac{dk}{2\pi}\ |k\rangle\langle k|. \end{aligned}}$$

These relations imply the <u>completeness</u> of the various bases.

<u>Proof</u>

$$\int dx\ \psi_n^*(x)\, \psi_{n'}(x) = \delta_{nn'}$$

$$\parallel$$

$$\int dx\ \langle x|n\rangle^* \langle x|n'\rangle$$

$$\parallel$$

$$\int dx\ \langle n|x\rangle\langle x|n'\rangle = \langle n|n'\rangle$$

$$\langle n | n' \rangle = \langle n | \left(\int dx\, |x\rangle\langle x| \right) | n' \rangle$$

$$\Rightarrow \int dx\, |x\rangle\langle x| = \mathbb{1} \,. \qquad \text{Q.E.D.}$$

We also have

$$\psi(x) = \int \frac{dk}{2\pi}\, \tilde{\psi}(k)\, e^{ikx} \,,$$

in other words

$$\langle x | \psi \rangle = \int \frac{dk}{2\pi}\, \langle k | \psi \rangle\, e^{ikx}$$

But $e^{ikx} = \psi_k(x) = \langle x | k \rangle$, so

$$\langle x | \psi \rangle = \int \frac{dk}{2\pi}\, \langle x | k \rangle \langle k | \psi \rangle$$

$$\Rightarrow \int \frac{dk}{2\pi}\, |k\rangle\langle k| = \mathbb{1} \,. \qquad \text{Q.E.D.}$$