Physics 472 Lecture 6

1) The inner product $\langle \phi | \psi \rangle$

Let $\hat{Q}$ be a Hermitian operator, with $\hat{Q}\psi_n = q_n \psi_n$. From the completeness of $\{\psi_n\}$, we may write

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

$$\phi(x) = \sum_n d_n \psi_n(x).$$

kets: $|\psi\rangle \longleftrightarrow \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \qquad |\phi\rangle \longleftrightarrow \begin{pmatrix} d_1 \\ d_2 \\ \vdots \end{pmatrix}$

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

$$= \sum_n d_n^* c_n = (d_1^* \; d_2^* \cdots) \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$

Thus the inner product of two quantum states is the scalar product of the corresponding vectors of coefficients, but where the left vector is complex conjugated:

$$\langle \psi | \longleftrightarrow (c_1^* \; c_2^* \ldots)$$

<u>bras:</u>

$$\langle \phi | \longleftrightarrow (d_1^* \; d_2^* \ldots)$$

$$\boxed{\text{Kets are equivalent to column vectors, while bras are equivalent to complex conjugated row vectors.}}$$

The standard definition

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

is just the expression in the position basis.

2) Operators in bra-ket notation

When an operator $\hat{Q}$ acts on a state vector $|\psi\rangle$, it creates another (not necessarilly normalized) state vector $|\phi\rangle$:

$$|\phi\rangle = \hat{Q}|\psi\rangle.$$

Taking the components of this equation in an orthonormal basis $|n\rangle$, $n=1,2,\ldots$, gives

$$\langle n|\phi\rangle = \langle n|\hat{Q}|\psi\rangle = \sum_{n'} \langle n|\hat{Q}|n'\rangle\langle n'|\psi\rangle$$

Using $d_n = \langle n|\phi\rangle$, $c_n = \langle n|\psi\rangle$, and $Q_{nn'} = \langle n|\hat{Q}|n'\rangle$, this becomes

$$d_n = \sum_{n'} Q_{nn'}\, c_{n'}. \quad \text{or}$$

$$\begin{pmatrix} d_1 \\ d_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & \cdots \\ Q_{21} & Q_{22} & \\ \vdots & & \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}.$$

The action of an operator on a state vector is completely analogous to the action of a matrix on a column vector.

If $\hat{Q}$ is Hermitian, then

$$\hat{Q}^{+} = \hat{Q} \quad \text{or} \quad Q_{ij}^{*} = Q_{ji}.$$

$\Rightarrow$ diagonal elements are real.

The corresponding bra equation is

$$\langle \phi | = \langle \psi | \hat{Q}^{+}$$

$$\langle \phi | n \rangle = \langle \psi | \hat{Q}^{+} | n \rangle = \sum_{n'} \langle \psi | n' \rangle \langle n' | \hat{Q}^{+} | n \rangle$$

$$d_n^{*} = \sum_{n'} a_{n'}^{*} \left(\hat{Q}^{+}\right)_{n'n} \qquad \text{or}$$

$$(d_1^* \; d_2^* \; \cdots) = (c_1^* \; c_2^* \; \cdots) \begin{pmatrix} Q_{11}^\dagger & Q_{12}^\dagger & \cdots \\ Q_{21}^\dagger & Q_{22}^\dagger & \\ \vdots & & \end{pmatrix}$$

If $\hat{Q}$ is Hermitian, then $\hat{Q}^\dagger = \hat{Q}$, i.e., the matrix which acts to the left on row vectors is the <u>same matrix</u> which acts to the right on column vectors.

3) <u>Operators in the $|x\rangle$ basis</u>

$$|\phi\rangle = \hat{Q}\,|\psi\rangle$$

$$\langle x|\phi\rangle = \langle x|\hat{Q}|\psi\rangle = \int dx' \, \langle x|\hat{Q}|x'\rangle\langle x'|\psi\rangle$$

$$\phi(x) = \int dx' \, Q(x,x') \, \psi(x')$$

i) <u>Position operator</u> $\langle x|\hat{x}|x'\rangle = x'\langle x|x'\rangle$

$$= x' \, \delta(x-x')$$

$$= x \, \delta(x-x')$$

Formally, we can write

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

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

$$= \int_{-\infty}^{\infty} dx' \, |x'\rangle \, x' \psi(x')$$

$$\langle x|\hat{x}|\psi\rangle = \int_{-\infty}^{\infty} dx' \underbrace{\langle x|x'\rangle}_{\delta(x-x')} x' \psi(x')$$

$$= x \, \psi(x)$$

ii) <u>momentum operator</u>

$$\langle \phi|\hat{p}_x|\psi\rangle = \int_{-\infty}^{\infty} dx \, \phi^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x)$$

$$= \int_{-\infty}^{\infty} dx \, \langle \phi | x \rangle \frac{\hbar}{i} \frac{\partial}{\partial x} \langle x | \psi \rangle$$

$$= \langle \phi | \left(\int_{-\infty}^{\infty} dx \, |x\rangle \frac{\hbar}{i} \frac{\partial}{\partial x} \langle x | \right) | \psi \rangle$$

$$\Rightarrow \quad \hat{P}_x = \int_{-\infty}^{\infty} dx \, |x\rangle \frac{\hbar}{i} \frac{\partial}{\partial x} \langle x |$$

Similarly,

$$\hat{H} = \int_{-\infty}^{\infty} dx \, |x\rangle \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \langle x |$$

4) <u>Operators in the $|k\rangle$ basis</u>

$$\langle k | \phi \rangle = \langle k | \hat{Q} | \psi \rangle$$

$$\langle k | \phi \rangle = \int \frac{dk'}{2\pi} \langle k | \hat{Q} | k' \rangle \langle k' | \psi \rangle$$

$$\tilde{\phi}(k) = \int \frac{dk'}{2\pi} \, Q(k, k') \, \tilde{\psi}(k')$$

$$\hat{Q} = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \, |k\rangle \, Q(k,k') \, \langle k'|$$

i) <u>momentum operator</u>

$$\langle k | \hat{P}_x | k' \rangle = \hbar k' \langle k | k' \rangle = \hbar k' \, 2\pi \delta(k-k')$$

$$\hat{P}_x = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \, |k\rangle \, \hbar k \, 2\pi \delta(k-k') \langle k'|$$

$$= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \, \hbar k \, |k\rangle\langle k|$$

In three dimensions, one would have

$$\vec{P} = \int \frac{d^3k}{(2\pi)^3} \, \hbar \vec{k} \, |\vec{k}\rangle\langle\vec{k}|$$

ii) <u>Potential energy</u>

$$\langle k | V | k' \rangle = \int_{-\infty}^{\infty} dx \, e^{-ikx} \, V(x) \, e^{ik'x}$$

$$V(k,k') = \int_{-\infty}^{\infty} dx\; V(x)\, e^{i(k'-k)x}$$

$$\equiv \tilde{V}(k-k')$$ Fourier transform

$$\hat{V} = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi}\, |k\rangle\, V(k,k') \langle k'|$$

$$= \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi}\, \tilde{V}(k-k')\, |k\rangle\langle k'|$$

$$= \int \frac{dq}{2\pi} \int \frac{dk}{2\pi}\, \tilde{V}(q)\, |k+q\rangle\langle k|$$

Feynman diagram: