Lecture 17: Wave Mechanics Recovered

Observables are eigenvalues of Hermitian operators, position $\hat{x}$, momentum $\hat{p}$. Eigenvalues are continuous. Label eigenstates by eigenvalue,

$$\hat{x}\,|x\rangle = x\,|x\rangle$$

$$\hat{p}\,|p\rangle = p\,|p\rangle$$

vector space of eigenstates is a Hilbert Space with inner product (see lec 4)

$$\langle x'|x\rangle = \delta(x'-x)$$

$$\langle p'|p\rangle = \delta(p'-p)$$

$\hat{x},\hat{p}$ operators do not have simultaneous eigenvalues: operators do not commute.
In general, commutation of Hermitian operators ($\hat{A},\hat{B},\hat{C}$ Hermitian)

$$[\hat{A},\hat{B}] = i\hat{C} \quad \text{implies} \quad \Delta A \Delta B \geq \frac{|\langle C\rangle|}{2}$$

Heisenberg uncertainty principle

$$\Delta x \Delta p \geq \frac{\hbar}{2} \quad \text{implies} \quad [\hat{x},\hat{p}] = i\hbar$$

$\hat{x},\hat{p}$ act on states representing position and momentum of particle: "space" part where

$$|\psi\rangle = |\text{space}\rangle\,|\text{spin}\rangle$$

<u>Wave function in position space</u>

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

(if not specified, all integrations are $-\infty$ to $+\infty$

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

$\psi(x)$ is amplitude to measure particle at x given state $|\psi\rangle$. Using δ-function we have the identity,

$$\langle x|\psi\rangle = \int dx'\, \underbrace{\langle x|x'\rangle}_{\delta(x-x')}\, \psi(x') = \psi(x)$$

Identical expansion in momentum-space (p-basis)

$$|\psi\rangle = \int dp\, |p\rangle\langle p|\psi\rangle = \int dp\, |p\rangle\, \tilde{\psi}(p)$$

$\tilde{\psi}(p)$ amplitude to measure momentum p.
Will show its the Fourier transform of $\psi(x)$

Inner product in Hilbert Space

$$\langle \phi | \psi \rangle = \langle \phi | \left(\int dx\, |x\rangle\langle x| \right) |\psi\rangle = \int dx\, \langle \phi | x \rangle \langle x | p \rangle$$

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

Postulating $[\hat{x}, \hat{p}] = i\hbar$, prove $\hat{p}$ is generator of translations. (here $\hat{p}$ is x-component of $\vec{p}$, $\hat{P}_x$)

$$\hat{T}(a) \equiv e^{-ia\hat{p}/\hbar}$$ a has dim. of length.

proof:

$$[\hat{x}, \hat{T}(a)] = \left[\hat{x},\ 1 + \frac{a}{i\hbar}\hat{p} + \frac{1}{2!}\left(\frac{a}{i\hbar}\hat{p}\right)^2 + \cdots\right]$$

$$= \frac{a}{i\hbar}[\hat{x}, \hat{p}] + \frac{1}{2!}\left(\frac{a}{i\hbar}\right)^2[\hat{x}, \hat{p}^2] + \cdots$$

easy to show $[\hat{x}, \hat{p}^2] = 2i\hbar \hat{P}_x$

in fact you will show $[\hat{x}, f(\hat{p})] = i\hbar \frac{\partial}{\partial \hat{p}} f(\hat{p})$

$$[\hat{x}, \hat{T}(a)] = i\hbar \frac{\partial}{\partial \hat{p}} e^{-ia\hat{p}/\hbar} = a\hat{T}(a)$$

Then $\hat{x}\left(\hat{T}(a)|x\rangle\right) = \left(\hat{T}\hat{x} + a\hat{T}\right)|x\rangle$

$$= (x+a)\left(\hat{T}(a)|x\rangle\right)$$

so $\underline{\hat{T}(a)|x\rangle = |x+a\rangle}$

Representation of $\hat{p}$ in position space

Infinitessimal translation ε

$$\hat{T}(\varepsilon) = 1 - \frac{i}{\hbar}\varepsilon\hat{p}$$

$$\hat{T}(\varepsilon)|\psi\rangle = \int dx\ \hat{T}(\varepsilon)\,|x\rangle\langle x|\psi\rangle$$

$$= \int dx\ |x+\varepsilon\rangle\langle x|\psi\rangle = \int dx'\ |x'\rangle\langle x'-\varepsilon|\psi\rangle$$

$x' = x+\varepsilon$

$$\langle x'-\varepsilon|\psi\rangle = \psi(x'-\varepsilon)$$
$$= \psi(x') - \varepsilon\frac{\partial\psi}{\partial x'}$$

Then

$$\left(1 - \frac{i}{\hbar}\varepsilon\hat{p}\right)|\psi\rangle = \int dx'\,|x'\rangle\left(\psi(x') - \varepsilon\frac{\partial\psi}{\partial x'}\right)$$

$$= |\psi\rangle - \varepsilon\int dx'\,|x'\rangle\frac{\partial\psi}{\partial x'}$$

$$\hat{p}|\psi\rangle = \int dx\ |x'\rangle\,\frac{\hbar}{i}\frac{\partial}{\partial x'}\psi(x')$$

or $\quad \langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x)$

"matrix" $\hat{p}$ in x-basis

$$\langle x|\hat{p}|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x')$$

$$= \frac{\hbar}{i}\delta(x-x')\frac{\partial}{\partial x'}$$

(See recitation #4)

So $\hat{p} \xrightarrow[x\text{-basis}]{} \frac{\hbar}{i}\frac{\partial}{\partial x}$

similarly

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

$$\langle x|\hat{x}|\psi\rangle = x\,\psi(x)$$
$$\langle x|\hat{x}|x'\rangle = x\,\delta(x-x')$$

$$\hat{x} \xrightarrow[x \to \text{basis}]{} x$$

<u>Plane wave state</u> definite p

$$\langle x|\hat{p}|p\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle$$

$$p\,\langle x|p\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle$$

$$\langle x|p\rangle \equiv \underbrace{\phi_p}_{p \text{ labeled by eigenvalue}}(x) = (\text{constant})\, e^{ipx/\hbar}$$

normalize so that $\langle p'|p\rangle = \delta(p'-p)$

$$\delta(p'-p) = \int dx\, \langle p'|x\rangle\langle x|p\rangle = c^2\int dx\, e^{ix(p'-p)/\hbar}$$
$$= c^2(2\pi\hbar)\,\delta(p'-p)$$

$$\phi_p(x) = \langle x|p\rangle = (2\pi\hbar)^{-1/2} e^{ipx/\hbar}$$

Wave function in momentum space

$$\psi(x) = \langle x|\psi\rangle = \int dp \, \langle x|p\rangle \langle p|\psi\rangle$$

$$= \int \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \langle p|\psi\rangle$$

so $\langle p|\psi\rangle = \tilde{\psi}(p) = \int \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \psi(x)$

Fourier transform of ψ

Schrödinger Equation:

classical $H(x,p) \xrightarrow{QM} \hat{H}(\hat{x},\hat{p})$

we have to worry about an 'xp' term in classical H.

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(\hat{x},\hat{p}) |\psi(t)\rangle$$

in position-space (x-basis)

$$i\hbar \frac{\partial}{\partial t} \langle x|\psi\rangle = \int dx' \underbrace{\langle x'|\hat{H}|x\rangle}_{\hat{H} \text{ matrix in } x\text{-basis}} \langle x'|\psi\rangle$$

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

Free particle $\hat{H} = \frac{\hat{p}^2}{2m}$

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = e^{-i\left(\frac{t}{2m\hbar}\right)\hat{p}^2}$$

$$\hat{H}|p\rangle = \frac{\hat{p}^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle$$

let $|\psi(0)\rangle = |p\rangle$

$$|\psi(t)\rangle = e^{-i\frac{t}{2m\hbar}\hat{p}^2}|p\rangle = e^{-it\left(\frac{p^2}{2m\hbar}\right)}|p\rangle$$

let $E(p) \equiv p^2/2m$

$$\langle x|\psi(t)\rangle = \psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{i}{\hbar}(px - E(p)t)}$$

plane wave moving in $+x$ direction

Momentum Space convenient for scattering

$\hat{x}$ generates translations in momentum space

$$\hat{W}(p_0) = e^{ip_0\hat{x}/\hbar}$$

$$[\hat{p}, \hat{x}] = -i\hbar \quad \text{so} \quad [\hat{p}, f(\hat{x})] = -i\hbar \frac{\partial}{\partial \hat{x}} f(\hat{x})$$

$$[p, \hat{W}(p_0)] = i\hbar \frac{\partial}{\partial \hat{x}} \left(e^{ip_0\hat{x}/\hbar} \right) = p_0 \hat{W}(p_0)$$

$$\hat{p} \left(\hat{W}(p_0)|p\rangle \right) = (p + p_0) \hat{W}(p_0)|p\rangle$$

so $\hat{W}(p_0)|p\rangle = |p + p_0\rangle$

infinitessimal $\hat{W}(\varepsilon) = 1 + i\varepsilon\hat{x}/\hbar$

$$\hat{W}(\varepsilon)|\psi\rangle = \int dp\, \hat{W}|p\rangle\langle p|\psi\rangle = \int dp' |p'\rangle\langle p' - \varepsilon|\psi\rangle$$

$p' = p + \varepsilon$

Taylor expand

$$\langle p' - \varepsilon|\psi\rangle = \langle p'|\psi\rangle - \varepsilon \frac{\partial}{\partial p'} \langle p'|\psi\rangle$$

$$\left(1 + \frac{i\varepsilon\hat{x}}{\hbar}\right)|\psi\rangle = \int dp' |p'\rangle \left(\langle p'|\psi\rangle - \varepsilon \frac{\partial}{\partial p'} \langle p'|\psi\rangle \right)$$

operate with $\langle p|$ to get

$$\frac{i\varepsilon}{\hbar} \langle p|\hat{x}|\psi\rangle = -\varepsilon \frac{\partial}{\partial p} \langle p|\psi\rangle$$

$$\langle p|\hat{x}|\psi\rangle = i\hbar \frac{\partial}{\partial p} \langle p|\psi\rangle$$

or

$$\langle p|\hat{x}|p'\rangle = i\hbar \frac{\partial}{\partial p}\delta(p-p') = i\hbar\delta(p-p')\frac{\partial}{\partial p'}$$

$\hat{x}$ in p-basis is $i\hbar\frac{\partial}{\partial p}$

check uncertainty

$$[\hat{x},\hat{p}]\,g(p) = i\hbar\frac{\partial}{\partial p}(pg) - i\hbar p\frac{\partial g}{\partial p} = i\hbar g(p)$$

or $[\hat{x},\hat{p}] = i\hbar$ an operator relation

just as in x-basis $\hat{p} \to \frac{\hbar}{i}\frac{\partial}{\partial x}$

$$[\hat{x},\hat{p}]\,f(x) = x\frac{\hbar}{i}\frac{\partial}{\partial x}f - \frac{\hbar}{i}\frac{\partial}{\partial x}(xf)$$

$$= -\frac{\hbar}{i}f(x) = i\hbar f(x)$$