Lecture 28: **04/01/09**

- Expectation values in momentum space
- Free particle I (at $t=0$)

IV$_1$ Position and Momentum Space: Recap

	position space	momentum space
$\vert\psi\rangle$ in terms of basis states:	$\vert\Psi\rangle = \int \vert x\rangle\langle x\vert\Psi\rangle\, dx$	$\vert\Psi\rangle = \int \vert p\rangle\langle p\vert\Psi\rangle\, dp$
projection ampl.:	$\langle x\vert\Psi\rangle = \Psi(x,t)$: position space wavefunction $\vert\langle x\vert\Psi\rangle\vert^2 dx = \vert\Psi(x,t)\vert^2 dx$ = prob. of finding particle between x and $x+dx$	$\langle p\vert\Psi\rangle = C_p \equiv \Phi(p,t)$: momentum space wave function $\vert\langle p\vert\Psi\rangle\vert^2 dp = \vert\Phi(p,t)\vert^2 dp$ = prob. that measurement of momentum will give result within p to $p+dp$

→ Position space and momentum space wavefunction:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Phi(p,t)\, e^{i\frac{px}{\hbar}}\, dp$$

Fourier transform $\Updownarrow$

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Psi(x,t)\, e^{-i\frac{px}{\hbar}}\, dx$$

IV$_2$ Expectation Values in Position and Momentum Space:

→ in position space:

position operator: $\hat{x} = x$

momentum operator: $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$

write as function of position and momentum

⇒ expectation value of a quantity $Q(x,p)$

$$\underbrace{\langle Q(x,p)\rangle}_{\text{average value of results measured on a large number of identical quantum systems}} = \langle \Psi | \hat{Q} | \Psi \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\, \hat{Q}\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi(x,t)\, dx$$

"replace" x by x

replace every p in $Q(x,p)$ by operator $\hat{p}$ to get $\hat{Q}$

→ in momentum space: How to calculate $\langle Q(x,p)\rangle$ from $\Phi(p,t)$?

• start with $\langle p\rangle$:

$$\langle p\rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\,\frac{\hbar}{i}\frac{\partial}{\partial x}\,\Psi(x,t)\,dx$$

$$= \int_{-\infty}^{+\infty} dx \left\{\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} \Phi^*(p',t)\,e^{-i\frac{p'x}{\hbar}}\,dp'\right\}\frac{\hbar}{i}\frac{\partial}{\partial x}\left\{\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\Phi(p,t)\,e^{+i\frac{px}{\hbar}}\,dp\right\}$$

$$= \int_{-\infty}^{+\infty} dx\,\frac{1}{2\pi\hbar}\left\{\int_{-\infty}^{+\infty}\Phi^*(p',t)\,e^{-\frac{ip'x}{\hbar}}\,dp'\right\}\frac{\hbar}{i}\frac{i}{\hbar}\left\{\int_{-\infty}^{+\infty}\Phi(p,t)\,p\,e^{ipx/\hbar}\,dp\right\}$$

$$= \int_{-\infty}^{+\infty} dp'\,dp\,\Phi^*(p',t)\,\Phi(p,t)\,p\,\underbrace{\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx\,e^{i\frac{x}{\hbar}(p-p')}}_{=\langle f_{p'}|f_p\rangle = \delta(p-p')}$$

$$= \int_{-\infty}^{+\infty} \Phi^*(p,t)\,p\,\Phi(p,t)\,dp = \underbrace{\int_{-\infty}^{+\infty} |\Phi(p,t)|^2\,p\,dp}_{\text{weighted average over momentum}}$$

prob. density function of momentum

$$\boxed{\Rightarrow\ \hat{p} = p \text{ in momentum space}}$$

• for $\langle x \rangle$ in momentum space:

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) \, x \, \Psi(x,t) \, dx$$

$$= \int_{-\infty}^{+\infty} dx \left\{ \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Phi^*(p',t) \, e^{-i\frac{p'x}{\hbar}} dp' \right\} x \left\{ \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Phi(p,t) \, e^{+i\frac{px}{\hbar}} dp \right\}$$

$$= \int_{-\infty}^{+\infty} dx \, \frac{1}{2\pi\hbar} \left\{ \int_{-\infty}^{+\infty} \Phi^*(p',t) \, e^{-i\frac{p'x}{\hbar}} dp' \right\} \left(\frac{\hbar}{i} \right) \left\{ \underbrace{\int_{-\infty}^{+\infty} \Phi(p,t) \frac{\partial}{\partial p} e^{i\frac{px}{\hbar}} dp}_{} \right\}$$

next: integration by parts:

$$\int f g' = - \int f' g + \underbrace{f g \Big|_{-\infty}^{+\infty}}_{}$$

$= 0$ here, since $\Phi(\pm\infty, t) = 0$ to be normalizable

$$\Rightarrow \langle x \rangle = \int_{-\infty}^{+\infty} dx \, \frac{1}{2\pi\hbar} \left\{ \int_{-\infty}^{+\infty} \Phi^*(p',t) \, e^{-i\frac{p'x}{\hbar}} dp' \right\} \frac{\hbar}{i} \left\{ - \int_{-\infty}^{+\infty} \frac{\partial \Phi(p,t)}{\partial p} e^{i\frac{px}{\hbar}} dp \right\}$$

$$\Rightarrow \langle x \rangle = \int_{-\infty}^{+\infty} dp'\, dp\, \Phi^*(p',t)\left(-\frac{\hbar}{i}\right)\frac{\partial \Phi(p,t)}{\partial p}\, \underbrace{\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx\, e^{i\frac{x}{\hbar}(p-p')}}_{=\langle f_{p'} | f_p \rangle = \delta(p-p')}$$

$$\Rightarrow \langle x \rangle = \int_{-\infty}^{+\infty} \Phi^*(p,t) \underbrace{\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}\right)}\Phi(p,t)\, dp$$

$$\left(\begin{array}{l}\text{position operator} \\ \text{in momentum space}\end{array}\right) = \hat{x} = -\frac{\hbar}{i}\frac{\partial}{\partial p}$$

<u>Note</u>: this makes sense in momentum space:

$$\underbrace{\hat{x}\,\Phi_y(p)}_{\substack{\text{state of definite} \\ \text{position } x=y \text{ in} \\ \text{momentum space}}} \stackrel{?}{=} y\,\Phi_y(p) = \left(-\frac{\hbar}{i}\frac{\partial}{\partial p}\right)\left(\frac{1}{\sqrt{2\pi\hbar}}e^{ipy/\hbar}\right) \stackrel{!}{=} y\,\Phi_y(p)$$

$g_y(x) = \delta(x-y)$ in position space

$\updownarrow$ fourier transformation

$$\Phi_y(p) = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipy/\hbar}$$

→ Result:

operator	position space	momentum space
position $\hat{x}$	x	$-\frac{\hbar}{i}\,\partial/\partial p$
momentum $\hat{p}$	$\frac{\hbar}{i}\frac{\partial}{\partial x}$	p

$$\langle Q(x,p)\rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\,\hat{Q}\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi(x,t)\,\underline{\underline{dx}}$$

$$= \int_{-\infty}^{+\infty} \Phi^*(p,t)\,\hat{Q}\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}, p\right)\Phi(p,t)\,\underline{\underline{dp}}$$

replace every x by $-\frac{\hbar}{i}\frac{\partial}{\partial p}$ in $Q(x,p)$

"replace" p by p

IV_3 The Free Particle I (at $t = 0$):

→ free particle → no forces → choose $V(x) = 0$ for all x

→ $\langle p \rangle = \text{const}$

⇒ time indep. Schrödinger Equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} = E\Psi \quad \text{, since } V = 0$$

⇒ stationary state solutions: $\Psi(x) = A e^{ipx/\hbar} + B e^{-ipx/\hbar}$

with $E = p^2/2m$

⇒ with time dependence:

$$\Psi(x,t) = A \underbrace{e^{i(px/\hbar - E/\hbar \cdot t)}}_{\substack{\text{traveling wave representing a} \\ \text{"particle" with definite energy} \\ \text{and momentum } +p}} + B \underbrace{e^{-i(px/\hbar + E/\hbar \cdot t)}}_{\substack{\text{traveling wave representing} \\ \text{a "particle" with definite energy } E \\ \text{and definite momentum } -p}}$$

simple de Broglie particle wave

$p = \hbar k$, $E = \hbar\omega$

⇒ Problem: not normalizable ⇒ not physical ?

<u>Solution</u>: Superposition of states of definite momentum (complete, orthonormal set of basis functions!)

$$\Psi(x,t) = \int_{-\infty}^{+\infty} \underbrace{\Phi(p,t)}_{\text{projection amplitude}} \underbrace{\frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}}_{\text{state of definite momentum}} dp$$

projection amplitude $= \langle p | \Psi \rangle = C_p(p,t)$

$=$ momentum space wave function $\Phi(p,t)$

$\Rightarrow$ can built up <u>localized</u> <u>wave packets</u>!

<u>Note</u>: these are solutions of the time-<u>dep.</u> S.E. and <u>not</u> of the time-indep. S.E!