OPTI 570 Th Sep 18

Known: $\hat{H}$, $|\psi(t_0)\rangle$

Main goal: $|\psi(t)\rangle$

Advanced goal: calculate quantities ex: prob., expect. values..

Challenges: many approaches

Problem 1:

Known: • free particle • mass m • moving in $\hat{x}$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \cancel{V(x)}^{\,0}$$

• $|\psi(t_0)\rangle$ corresponds to a Gaussian wavefunction in x

s.t. $\underline{\langle \hat{x} \rangle (t_0) = x_0}$, $\underline{\langle \hat{p} \rangle (t_0) = p_0}$

Calculate $\langle \hat{x} \rangle (t)$

Approach I use equations of motion for expectation values.

$$\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar}\langle [\hat{A},\hat{H}] \rangle + \langle \frac{\partial \hat{A}}{\partial t} \rangle \quad \text{FG p.44}$$

$\hat{x}, \hat{p}, \hat{H}$

$$\frac{d}{dt}\langle \hat{H} \rangle = \frac{1}{i\hbar}\underbrace{\langle [\hat{H},\hat{H}] \rangle}_{0} + \underbrace{\langle \frac{\partial \hat{H}}{\partial t} \rangle}_{0} =$$

$$\boxed{\frac{d}{dt}\langle \hat{H} \rangle = 0}$$

$$\frac{d}{dt}\langle \hat{x} \rangle = \frac{1}{i\hbar}\langle [\hat{x},\hat{H}] \rangle + \langle \frac{\partial \hat{x}}{\partial t} \rangle =$$

$$= \frac{1}{i\hbar}\left\{ \langle \underline{[\hat{x},\frac{\hat{p}^2}{2m}]} + \underbrace{[\hat{x},V(\hat{x})]}_{0} \rangle \right. + \underbrace{\langle \frac{\partial \hat{x}}{\partial t} \rangle}_{\text{no time dependence}} =$$

$$= \frac{1}{i\hbar}[\hat{x},\hat{p}]\frac{d}{d\hat{p}}\left(\frac{\hat{p}^2}{2m}\right) =$$

$$\boxed{\frac{d}{dt}\langle\hat{x}\rangle = i\hbar\ \frac{\hat{p}}{m}}$$

$$\frac{d}{dt}\langle\hat{p}\rangle = \frac{1}{i\hbar}\langle[\hat{p},\hat{H}]\rangle + \cancel{\left\langle\frac{d\hat{p}}{dt}\right\rangle}^{0} =$$

$$= \frac{1}{i\hbar}\Big\{\underbrace{\langle[\hat{p},\hat{p}^2/2m]\rangle}_{0} + \underbrace{\langle[\hat{p},V(\hat{x})]\rangle}\Big\} =$$

$$= \frac{1}{\cancel{i\hbar}}\left[-\cancel{i\hbar}\ \frac{\partial V(\hat{x})}{\partial\hat{x}}\right] =$$

$$\boxed{\begin{aligned}\frac{d}{dt}\langle\hat{p}\rangle &= -\left\langle\frac{dV(\hat{x})}{\partial\hat{x}}\right\rangle\\ \frac{d}{dt}\langle\hat{x}\rangle &= \frac{1}{m}\langle\hat{p}\rangle\end{aligned}}$$

Ehrenfest equations

in general $\left\langle\frac{dV(\hat{x})}{dx}\right\rangle \neq \frac{dV(\langle\hat{x}\rangle)}{dx}$

$$\frac{dp}{dt} = F = -\frac{dV}{dx}$$

$$\frac{dx}{dt} = \frac{p}{m} = v$$

Free particle:

$$\frac{d\langle\hat{p}\rangle}{dt} = 0$$

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}\rangle}{m} \Rightarrow \boxed{\begin{aligned}\langle\hat{p}\rangle(t) &= \langle\hat{p}\rangle(t_0) = p_0\\ \langle\hat{x}\rangle(t) &= \frac{p_0}{m}\cdot(t-t_0) + x_0\end{aligned}}$$

Define: $\underbrace{\hat{S}(x_0)}_{\text{unitary}} = e^{-ix_0\hat{p}/\hbar}$ scalar, units of length; Hermitian

Q: What does $\hat{S}(x_0)$ do to state $|\psi\rangle$?

$$|\varphi\rangle = \hat{S}(x_0)|\psi\rangle$$

1. $\langle x|\varphi\rangle = \langle x|\hat{S}(x_0)|\psi\rangle = \langle x|e^{-ix_0\hat{p}/\hbar}|\psi\rangle =$

$$= \langle x|\int_p e^{-ix_0\hat{p}/\hbar}\ |p\rangle\langle p|\psi\rangle\, dp =$$

$$= \int_p e^{-ix_0\hat{p}/\hbar} \underbrace{\langle x|p\rangle} \underbrace{\langle p|\psi\rangle} dp =$$

$$= \int_p e^{-ix_0 p/\hbar} \cdot \left(\frac{1}{\sqrt{2\pi\hbar}} e^{ixp/\hbar}\right) \tilde{\psi}(p)\, dp =$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \underbrace{\int_p e^{i(x-x_0)p/\hbar} \tilde{\psi}(p)\, dp}$$

$$= FT^{-1}\{\tilde{\psi}(p)\big|_{x-x_0} =$$

$$= \psi(x)\big|_{x-x_0} =$$

$$\boxed{\langle x|\hat{S}(x_0)|\psi\rangle = \psi(x - x_0)}$$ – translates ψ by x_0 in position

2. $\langle \underline{x}| \underline{\hat{S}(x_0)|\psi\rangle} = e^{-x_0 \frac{\partial}{\partial x}} \psi(x) =$

$$= \ldots = \underline{\psi(x-x_0)}$$

3. General, no representation (CT II E)

$$[\hat{x}, \hat{S}(x_0)] = [\hat{x}, e^{-ix_0\hat{p}/\hbar}] = [\hat{x}, \hat{p}] \frac{d\hat{S}}{d\hat{p}} =$$

$$= x_0 \hat{S}(x_0)$$

$\underline{\text{so}}$: $[\hat{x}, \hat{S}(x_0)] = \hat{x}\hat{S}(x_0) - \hat{S}(x_0)\hat{x} = x_0\hat{S}(x_0)$

$$\Rightarrow \hat{x}\hat{S}(x_0) = \hat{S}(x_0)\cdot(\hat{x} + x_0)$$

$$\hat{x}\hat{S}(x_0)|x\rangle = \hat{S}(x_0)(\hat{x} + x_0)|x\rangle =$$

$$= \hat{S}(x_0)(x + x_0)|x\rangle =$$

$$\hat{x}\underbrace{\left(\hat{S}(x_0)|x\rangle\right)} = (x + x_0)\underbrace{\left(\hat{S}(x_0)|x\rangle\right)}$$

eigenket of $\hat{x}$ associated eigenvalue is $(x+x_0)$

$$\hat{S}(x_0)|x\rangle = |x+x_0\rangle$$

$$\hat{S}(-x_0)|x\rangle = |x-x_0\rangle$$

In position representation : $\langle x|\hat{S}(x_0)|\psi\rangle = \langle x-x_0|\psi\rangle = \boxed{= \psi(x-x_0)}$

Similarly : $\hat{T}(p_0) = e^{ip_0\hat{x}/\hbar}$

$$\Rightarrow \langle p|\hat{T}(p_0)|\psi\rangle = \bar{\psi}(p-p_0)$$

$$\langle x|\hat{T}(p_0)|\psi\rangle = \langle x|e^{ip_0\hat{x}/\hbar}|\psi\rangle = $$

$$= e^{ip_0x/\hbar}\langle x|\psi\rangle$$

$$\Rightarrow \langle x|\hat{T}(p_0)\hat{S}(x_0)|\psi\rangle = e^{ip_0x/\hbar}\psi(x-x_0)$$

$$\langle x|\hat{S}(x_0)\hat{T}(p_0)|\psi\rangle = e^{ip_0(x-x_0)/\hbar}\psi(x)\Big|_{x\to x-x_0} =$$

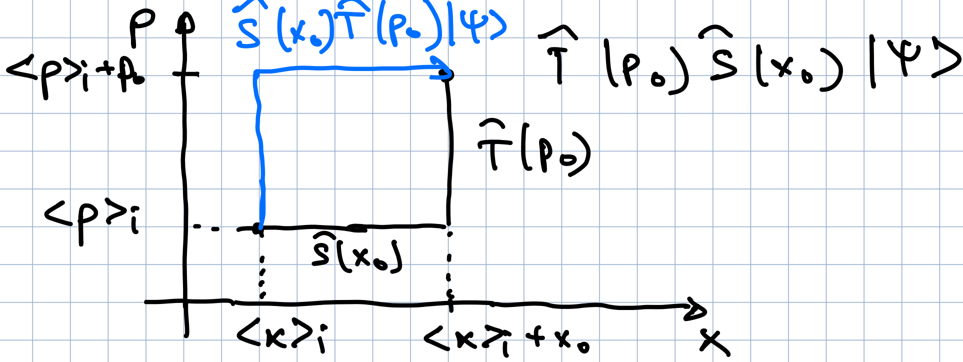
$$= e^{ip_0(x-x_0)/\hbar}\psi(x-x_0) =$$

$$= \underbrace{e^{-ip_0x_0/\hbar}}_{\text{global phase factor}}\underline{e^{ip_0x/\hbar}\psi(x-x_0)}$$

- similarly in momentum representation :

$$\langle p|\hat{S}(x_0)|\psi\rangle = e^{-ix_0p/\hbar}\tilde{\psi}(p)$$

. . . .



$$\left(\hat{S}(x_0) + \hat{T}(p_0)\right)|\psi\rangle$$

<u>Special cases</u>: $|\psi\rangle$ – even and odd functions

<u>Ex:</u> $\psi(x) = c e^{-\frac{x^2}{2w^2}}$ – Gaussian

$$\langle x\rangle = 0$$

$$\langle\hat{p}\rangle = 0 = \int dx \underbrace{\psi^*(x)}_{\text{even}} \Big[\underbrace{-i\hbar \frac{d}{dx} \underbrace{\psi(x)}_{\text{even}}}_{\text{odd}} \Big] = 0 \checkmark$$

if: $e^{ip_0 x/\hbar}\psi(x) = \langle x|\hat{T}(p_0)|\psi\rangle$

$\Rightarrow \langle\hat{p}\rangle = p_0$

<u>In general</u>:

$\psi(x)$ is even or odd about x_0 $\Rightarrow$ $\langle\hat{x}\rangle = x_0$, $\langle\hat{p}\rangle = 0$

$\psi(p)$ —— // —————— p_0 $\Rightarrow$ $\langle\hat{p}\rangle = p_0$, $\langle\hat{x}\rangle = 0$

	$\langle x\rangle$	$\langle p\rangle$
• $\psi(x) = c\, e^{-\lvert x\rvert/w}$	0	0
• $\psi(x) = c\, \underbrace{e^{-ip_0 x/w}}_{\hat{T}(-p_0)} e^{-\lvert x\rvert/w}$	0	$-p_0$
• $\tilde{\psi}(p) = c\, e^{\underbrace{-ip/p_1}} e^{-\left(p - \underline{\hbar/(lm)}\right)^2/2a}$	$\frac{\hbar}{p_1}$	$\frac{\hbar}{lm}$

$x_0/\hbar = 1/p_1 \Rightarrow x_0 = \frac{\hbar}{p_1}$

Approach II

Gaussian wave packet s.t. $|\tilde{\psi}(p)|^2$ has 1/e half-width of a

$\langle \hat{p} \rangle = p_0$, $\langle \hat{x} \rangle = x_0$

$$\boxed{\langle p | \psi \rangle = \left(\frac{1}{\pi a^2}\right)^{1/4} e^{-i x_0 p/\hbar} \, e^{-(p-p_0)^2/2a^2}}$$