Lecture # 17

The Schrödinger versus the Heisenberg picture

First recall properties of unitary transformations.

$|\alpha\rangle \Rightarrow \hat{U}|\alpha\rangle = |\alpha'\rangle$

$|\beta\rangle \Rightarrow \hat{U}|\beta\rangle = |\beta'\rangle$ $\Rightarrow$ $\langle\beta|\alpha\rangle \Rightarrow \langle\beta|\hat{U}^{+}\hat{U}|\alpha\rangle = \langle\beta|\alpha\rangle = \langle\beta'|\alpha'\rangle$

$$\langle\beta|\hat{A}|\alpha\rangle \Rightarrow \langle\beta|\hat{U}^{+}\hat{A}\hat{U}|\alpha\rangle = $$

arbitrary observable

$$= \langle\beta'|\hat{A}|\alpha'\rangle =$$

$$= \langle\beta|\underbrace{\hat{A}'}_{=\hat{U}^{+}\hat{A}\hat{U}}|\alpha\rangle$$

This says that if we change the states of the system, i.e. go from $\overbrace{|\alpha\rangle \Rightarrow |\alpha'\rangle, \ |\beta\rangle \Rightarrow |\beta'\rangle}^{\text{Case 1}}$

and leave the operator $\hat{A}$ unchanged $\Rightarrow$ this would be <u>equivalent</u> to leaving the same states $|\alpha\rangle$, $|\beta\rangle$ and changing the operator to $\underbrace{\hat{U}^{+}\hat{A}\hat{U} = \hat{A}'}_{\text{Case 2}}$

Example: translation in space $\Rightarrow \hat{U}_{d\vec{x}} = I - \frac{i}{\hbar}\vec{P}\cdot d\vec{x}$ (2)

Let's find out how the expectation value of the position operator changes upon translation:

1) Case 1

$$|\alpha\rangle \Rightarrow |\alpha'\rangle = \hat{U}_{d\vec{x}}|\alpha\rangle = \left(\hat{I} - \frac{i}{\hbar}\vec{P}\cdot d\vec{x}\right)|\alpha\rangle$$

$X \Rightarrow X$ (does not change)

$$\langle X\rangle = \langle\alpha'|X|\alpha'\rangle = \langle\alpha|\left(\hat{I} + \frac{i}{\hbar}\vec{P}\cdot d\vec{x}\right)X\left(\hat{I} - \frac{i}{\hbar}\vec{P}\cdot d\vec{x}\right)|\alpha\rangle = \langle X\rangle + \langle dx\rangle$$

2) Case 2

$|\alpha\rangle \Rightarrow |\alpha\rangle$ (does not change)

$$X \Rightarrow X' = \hat{U}^{\dagger}_{d\vec{x}}\hat{X}\hat{U}_{d\vec{x}} = \left(\hat{I} + \frac{i}{\hbar}\vec{P}\cdot d\vec{x}\right)\hat{X}\cdot\left(\hat{I} - \frac{i}{\hbar}\vec{P}\cdot d\vec{x}\right) = \hat{X} + \frac{i}{\hbar}[\underbrace{\vec{P}\cdot d\vec{x}}_{= P_x dx + P_y dy + P_z dz}, \hat{X}] =$$

$$= \hat{X} + \frac{i}{\hbar}d\hat{x}\,[\underbrace{P_x, X}_{= -i\hbar}] = \hat{X} + d\hat{x}$$

So, the expectation value $\langle\hat{X}\rangle \Rightarrow \langle\hat{X}\rangle + \langle d\hat{x}\rangle$ is the same in both cases!

Now back to time translations $\Rightarrow$

$$\left.\begin{aligned} |\alpha\rangle &\Rightarrow |\alpha'\rangle = \hat{U}(t, t_0)|\alpha\rangle \\ A &\Rightarrow A \quad (\text{does } \underline{\underline{\text{not}}} \text{ change}) \end{aligned}\right\} \text{the Schrödinger picture}$$

$$\left.\begin{aligned} |\alpha\rangle &\Rightarrow |\alpha\rangle \quad (\text{does } \underline{\underline{\text{not}}} \text{ change}) \\ A &\Rightarrow A' = \hat{U}^{+} A \hat{U} \end{aligned}\right\} \text{the Heisenberg picture}$$

$$\Downarrow$$

$$|\alpha, t_0; t\rangle_S = \underbrace{\hat{U}(t, t_0)}_{= e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}} |\alpha, t_0\rangle$$

Schrödinger picture

$$|\alpha, t_0; t\rangle_H = |\alpha, t_0\rangle$$

Heisenberg picture

$$A_S(t) = A_S(0) = A_H(0)$$

$$A_H(t) = \hat{U}^{+}(t, t_0) \underbrace{A_H(0)}_{= A_S} \hat{U}(t, t_0)$$

Expectation values at time t:

$$\langle A \rangle_S = \langle \alpha, t_0; t | A_S | \alpha, t_0; t \rangle =$$

$$= \langle \alpha, t_0 | \hat{U}^+ A_S \hat{U} | \alpha, t_0 \rangle = \langle \alpha, t_0 | A_H(t) | \alpha, t_0 \rangle =$$

$$= \langle A \rangle_H$$

So, in the Schrödinger's picture $\Rightarrow$ solve Schrödinger's equation to find time evolution of $|\alpha, t_0; t\rangle$

In the Heisenberg's picture $\Rightarrow$ solve the Heisenberg equation of motion to find how the operator A_H changes with time. What is this equation of motion? $\Rightarrow$ $A_H(t) = \hat{U}^+(t, t_0) A_S \hat{U}(t, t_0)$

$$\frac{dA_H}{dt} = \frac{\partial \hat{U}^+}{\partial t} A_S \hat{U} + \hat{U}^+ \underbrace{\frac{\partial A_S}{\partial t}}_{=0} \hat{U} + \hat{U}^+ A_S \frac{\partial \hat{U}}{\partial t} =$$

since A_S does not depend on time!

$$= -\frac{1}{i\hbar} \hat{U}^+ \hat{H} A_S \hat{U} + \hat{U}^+ A_S \hat{H} \hat{U} \cdot \frac{1}{i\hbar} =$$

Recall Eq.(15.1) from Lecture #15 (Schrodinger equation for the propagator $i\hbar \frac{\partial \hat{U}}{\partial t} = \hat{H}\hat{U}$)

$$= \frac{1}{i\hbar} \hat{U}^+ [A_s, \hat{H}] \hat{U} = \frac{1}{i\hbar} \Big(-\hat{H} \underbrace{\hat{U}^+ A_s \hat{U}}_{= A_H} +$$

for time-independent $H \Rightarrow$

$$\hat{U}(t, t_0) = e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} \Rightarrow$$

$$[\hat{U}, \hat{H}] = 0$$

$$+ \underbrace{\hat{U}^+ A_s \hat{U}}_{= A_H} \hat{H} \Big) = \frac{1}{i\hbar} [A_H, H] = \frac{dA_H}{dt}$$

equation of motion in the Heisenberg picture

$\Downarrow$

very similar form to what we had last time for the expectation values!

Example

Derive the equations of motion of a free particle of mass m for the position and momentum.

$\Downarrow$

Free-particle Hamiltonian $\Rightarrow$ $H = \frac{P_x^2 + P_y^2 + P_z^2}{2m}$

$$\frac{dP_i}{dt} = \frac{1}{i\hbar} [P_i, H] = \frac{1}{i\hbar} \left[P_i, \frac{P_x^2 + P_y^2 + P_z^2}{2m} \right] = 0 \Rightarrow$$

$(i = x, y, z)$

for a free particle P_i is a constant of motion ⑥

What about $\vec{R}$? $\Rightarrow$ $\vec{R} = (X, Y, Z) \equiv \equiv \{R_i\}$, $i = x, y, z$

position operator in 3D

$$\frac{dR_i}{dt} = \frac{1}{i\hbar}[R_i, H] =$$

$$= \frac{1}{i\hbar}\left[R_i, \frac{P_x^2 + P_y^2 + P_z^2}{2m}\right] = \frac{1}{2mi\hbar}\left([X, P_x^2] \text{ or } [Y, P_y^2] \text{ or } [Z, P_z^2]\right) =$$

depending on i

$$[X, P_x^2] = [X, P_x]P_x + P_x[X, P_x] = 2i\hbar P_x$$

$$= \frac{1}{m} P_i$$

Since we just obtained that P_i is a constant of motion, i.e. $P_i \neq f(t)$ $\Rightarrow$ integrate $\frac{dR_i}{dt} = \frac{P_i}{m}$ out

$$R_i(t) = R_i(0) + \frac{P_i}{m} t$$

(Note: very similar to classical-mechanical trajectory equation!)

What's not classical-mechanics-like though is that $[R_i(t), R_i(0)] \neq 0$!

Although we know that $[R_i(0), R_j(0)] = 0$ for any i, j (e.g. $[X, Y] = [Y, Z] = 0$, $[X(0), X(0)] = 0$)

$$[R_i(t), R_i(0)] = \left[\frac{P_i}{m}t, R_i(0)\right] = -\frac{i\hbar t}{m}$$

So that the uncertainty relation in its general form $\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}\cdot |\langle[A,B]\rangle|^2$

in the case of $A = R_i(t)$ is
$B = R_i(0)$

$$\langle(\Delta R_i(t))^2\rangle \cdot \langle(\Delta R_i(0))^2\rangle \geq \frac{1}{4} \cdot |\langle -\frac{i\hbar t}{m}\rangle|^2 = \frac{\hbar^2 t^2}{4m^2}$$

This means that if the particle is well-localized at $t=0$, i.e. $\Delta R_i(0)$ is small $\Rightarrow$ $\Delta R_i(t)$ is large, i.e. with time the position of the particle becomes more and more uncertain!

Homework: spreading of the wave-packet with time.

Now place the particle in a potential $V(\vec{R})$

$$\Downarrow$$

$$H = \frac{\vec{P}^2}{2m} + V(\vec{R}) \Rightarrow$$

Equations of motion $\Rightarrow$ $$\frac{dP_i}{dt} = \frac{1}{i\hbar}[P_i, H] = -\frac{\partial V(\vec{R})}{\partial R_i} \neq 0$$

$\uparrow$ see Lecture # 16

$$\frac{dR_i}{dt} = \frac{1}{i\hbar}[R_i, H] = \frac{P_i}{m}$$ $\leftarrow$ still the same, but now P_i is not a constant of motion.

$$\Downarrow$$

$$\frac{d^2R_i}{dt^2} = \frac{1}{m}\frac{dP_i}{dt} = -\frac{1}{m}\underbrace{\nabla_i}_{= \frac{\partial}{\partial R_i}} V(\vec{R}) \Rightarrow$$ back to vectorial form

$$m\frac{d^2\vec{R}}{dt^2} = -\vec{\nabla} V(\vec{R})$$ $\leftarrow$ QM analog of the Newton's law!! (has meaning only in the Heisenberg picture)

$$\Downarrow$$

$$m\frac{d^2}{dt^2}\langle \vec{R} \rangle = -\langle \vec{\nabla} V(\vec{R}) \rangle$$ $\leftarrow$ expectation values law

$\Downarrow$

valid for both $\Leftarrow$ Ehrenfest theorem

Schrödinger & Heisenberg pictures since expectation values are picture-independent