# Phys 570 A    Lecture 14

## Equations of Motion for Operators

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Two ways to define $f(\hat{A})$:

$$f(\hat{A}) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \hat{A}^n \qquad \text{(Taylor series)}$$

$$f(\hat{A}) = \sum_{\alpha} f(\alpha) |\alpha\rangle\langle\alpha| \qquad \text{(specrtal rep.)}$$

Here $\hat{A}|\alpha\rangle = \alpha|\alpha\rangle$. The later definition also works for functions lacking a Taylor expansion, e.g.,

$$\delta(x - \hat{A}) = \sum_{\alpha} \delta(x-\alpha) |\alpha\rangle\langle\alpha| .$$

For time evolution, we are particularly interested in the exp. function:

$$e^{\lambda \hat{A}} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \hat{A}^n$$

Care must be taken with functions of operators that don't commute:

$$e^{\hat{A}+\hat{B}} \neq e^{\hat{A}} e^{\hat{B}} \quad \text{if} \quad [\hat{A},\hat{B}] \neq 0.$$

For the special case where $[\hat{A},\hat{B}]$ is a c-number, we have

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-[\hat{A},\hat{B}]/2}$$ Weyl's formula.

## Time-evolution

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle$$

Let $|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle$. $\hat{U}(t)$ obeys

$$i\hbar \frac{d}{dt} \hat{U}(t) = \hat{H}(t) \hat{U}(t)$$

i) Consider the case where $\hat{H}$ is independent of $t$.

$$\hat{U}(t) = \exp\left(-i\frac{\hat{H}t}{\hbar}\right)$$

$$\langle \psi(t)| = \langle \psi(0)| e^{\frac{i\hat{H}t}{\hbar}}$$

## Expectation values

$$\langle \hat{A} \rangle|_t = \langle \psi(t)| \hat{A} |\psi(t)\rangle$$

$$= \langle \psi(0)| e^{\frac{i\hat{H}t}{\hbar}} \hat{A} e^{-\frac{i\hat{H}t}{\hbar}} |\psi(0)\rangle$$

## Heisenberg picture

So far, we have been working in the Schrödinger picture, where quantum states evolve in time according to the Sch. eq., and operators are typically time-independent. In the Heisenberg picture, it is the other way around:

$$\boxed{\text{Define } \hat{A}_H(t) \equiv e^{\frac{i\hat{H}t}{\hbar}} \hat{A} e^{-\frac{i\hat{H}t}{\hbar}} \quad \text{Then } \langle \hat{A} \rangle|_t = \langle \psi(0)| \hat{A}_H(t) |\psi(0)\rangle}$$

## Heisenberg equation of motion

$$i\hbar \frac{d\hat{A}_H(t)}{dt} = e^{\frac{i\hat{H}t}{\hbar}} \left[ -\hat{H}\hat{A} + \hat{A}\hat{H} + i\hbar \frac{\partial \hat{A}}{\partial t} \right] e^{-\frac{i\hat{H}t}{\hbar}}$$

$$= \left[ \hat{A}_H(t), \hat{H} \right] + \underbrace{i\hbar \frac{\partial \hat{A}_H}{\partial t}}_{\text{let's drop this for now}}$$

What about $\hat{H}$ itself?

If $\hat{H}$ is indep. of $t$ in the Sch. picture, then

$$\hat{H}_H(t) = e^{+\frac{i\hat{H}t}{\hbar}} \hat{H} e^{-\frac{i\hat{H}t}{\hbar}} = \hat{H}.$$

$\hat{H}$ is a constant of the motion.

## Particle in 3D

$$\hat{H} = \frac{\vec{P}^2}{2m} + V(\vec{r}) = \frac{\vec{P}_H^2(t)}{2m} + \hat{V}_H(\vec{r}, t)$$

$$\frac{d\vec{r}_H(t)}{dt} = \frac{1}{i\hbar} \left[ \vec{r}_H(t), \hat{H} \right]$$

$$\left[\hat{r}_i(t), \hat{p}_j(t)\right] = e^{i\hat{H}t/\hbar}\left(\hat{r}_i\hat{p}_j - \hat{p}_j\hat{r}_i\right)e^{-i\hat{H}t/\hbar}$$

$$= i\hbar\,\delta_{ij}$$ same as in Sch. picture.

(not true if not at equal times)

$$\frac{d\vec{r}_H(t)}{dt} = \frac{1}{i\hbar}\left[\vec{r}_H(t), \frac{\vec{p}_H^{\,2}(t)}{2m}\right]$$

$$= \frac{1}{2i\hbar m}\left(\vec{p}_H\left[\vec{r}_H, \vec{p}_H\right] + \left[\vec{r}_H, \vec{p}_H\right]\vec{p}_H\right)$$

$$\boxed{\frac{d\vec{r}_H(t)}{dt} = \frac{\vec{p}_H(t)}{m}}$$

$$\frac{d\vec{p}_H(t)}{dt} = \frac{1}{i\hbar}\left[\vec{p}_H(t), \hat{H}\right] = \frac{1}{i\hbar}\left[\vec{p}_H(t), V(\vec{r}, t)\right]$$

$$= \frac{1}{i\hbar}e^{i\hat{H}t/\hbar}\underbrace{\left[\vec{p}, V(\vec{r})\right]}_{\frac{\hbar}{i}\nabla V(\vec{r})}e^{-i\hat{H}t/\hbar}$$

$$\boxed{\frac{d\vec{p}_H(t)}{dt} = -\nabla V_H(\vec{r}(t))}$$

The operators obey the classical equations of motion in the Heisenberg picture. The Ehrenfest theorem then follows trivially.

Generally speaking, the Heisenberg eq.s of motion are harder to solve than the classical eq.s of motion due to the non-commutativity of the operators. However, they do permit explicit solutions for some simple cases.

a) free particle $\qquad \hat{V}_H = 0$

$$\frac{d \vec{p}_H}{dt} = 0 \qquad \vec{p}_H(t) = \text{const.}$$

$$\vec{r}_H(t) = \vec{r}_H(0) + \frac{\vec{p}_H}{m} t$$

b) Harmonic oscillator

$$\frac{d x_H}{dt} = \frac{p_H(t)}{m}$$

$$\frac{d p_H(t)}{dt} = -m\omega^2 x_H(t)$$

solution:

$$x_H(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t$$

$$p_H(t) = p(0)\cos\omega t - m\omega x(0)\sin\omega t,$$

exactly as for the classical oscillator.

ii) $\hat{H}_s = \hat{H}_s(t)$

e.g. $\hat{H}_s = \frac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{r}}) - \vec{F}(t)\cdot\hat{\vec{r}}$

$\vec{F}(t) =$ t-dep. external driving force

$$i\hbar \frac{d}{dt}\hat{U}(t) = \hat{H}_s(t)\,\hat{U}(t)$$

same as before

and

$$\hat{U}(0) = \mathbb{1}.$$

Let us construct the Heisenberg rep. in this case.

$$\langle \hat{A} \rangle|_t = \langle \psi(t) | \hat{A} | \psi(t) \rangle = \langle \psi(0) | \hat{U}^\dagger(t) \hat{A} \hat{U}(t) | \psi(0) \rangle$$

$$\boxed{\hat{A}_H(t) \equiv \hat{U}^\dagger(t) \hat{A} \hat{U}(t).}$$

To find the eq. of motion, differentiate:

$$i\hbar \frac{d}{dt} \hat{A}_H(t) = i\hbar \frac{d\hat{U}^\dagger(t)}{dt} \hat{A} \hat{U}(t) + \hat{U}^\dagger(t) \hat{A} \left( i\hbar \frac{d\hat{U}(t)}{dt} \right)$$

$$\left(\text{assuming } \frac{\partial \hat{A}}{\partial t} = 0\right).$$

$$-i\hbar \frac{d\hat{U}^\dagger(t)}{dt} = \hat{U}^\dagger(t) \hat{H}_s(t)$$

$$i\hbar \frac{d\hat{A}_H}{dt} = \hat{U}^\dagger(t) \left[ -\hat{H}_s(t) \hat{A} + \hat{A} \hat{H}_s(t) \right] \hat{U}(t)$$

$$= \left[ \hat{A}_H(t), \hat{H}_H(t) \right],$$

where $\hat{H}_H(t) \equiv \hat{U}^\dagger(t) H_S(t) \hat{U}(t) \neq \hat{H}_S(t)$ in general.

$\hat{H}_H(t)$ is no longer a constant of the motion, but obeys

$$\frac{d\hat{H}_H(t)}{dt} = \frac{1}{i\hbar}\underbrace{\left[\hat{H}_H(t), \hat{H}_H(t)\right]}_{0} + \hat{U}^\dagger(t)\frac{\partial \hat{H}_S(t)}{\partial t}\hat{U}(t)$$

$$= \hat{U}^\dagger(t)\frac{\partial \hat{H}_S(t)}{\partial t}\hat{U}(t) \equiv \frac{\partial \hat{H}_H(t)}{\partial t}$$

as in classical mechanics.

For the example Hamiltonian,

$$\frac{d\vec{r}_H(t)}{dt} = \frac{\vec{p}_H(t)}{m}$$

$$\frac{d\vec{p}_H(t)}{dt} = -\nabla V_H(\vec{r}_H(t)) + \vec{F}(t)$$

Formal solution for $\hat{U}(t)$ in the case of a t-dep. $\hat{H}$.

$$i\hbar \frac{d\hat{U}(t)}{dt} = \hat{H}_s(t)\,\hat{U}(t), \qquad \hat{U}(0) = \mathbb{1}$$

$$\hat{U}(\Delta t) \simeq \mathbb{1} - \frac{i}{\hbar}\hat{H}_s(0)\,\Delta t$$

$$\hat{U}(2\Delta t) \simeq \left(\mathbb{1} - \frac{i}{\hbar}\hat{H}_s(\Delta t)\,\Delta t\right)\hat{U}(\Delta t)$$

$$\vdots$$

$$\hat{U}(N\Delta t) \simeq \prod_{n=1}^{N-1}\left(\mathbb{1} - \frac{i\Delta t}{\hbar}\hat{H}_s(n\Delta t)\right),$$

where later terms are ordered to the left in the product. Taking the limit where $\Delta t = t/N$ and $N \to \infty$,

$$\hat{U}(t) = T\left(\exp\left[-\frac{i}{\hbar}\int_0^t dt\;\hat{H}_s(t)\,dt\right]\right),$$

where
$$T\left(\hat{A}(t)\,\hat{B}(t')\right) = \begin{cases} \hat{A}(t)\,\hat{B}(t'), & t \geq t' \\ \hat{B}(t')\,\hat{A}(t), & t' > t \end{cases}$$

denotes the time-ordered product.