28/10/2025 Lec. 28. Ehrenfest and Virial Theorems

Ehrenfest Theorem

Consider a general QM system described the Hamiltonian $\hat{H}(t)$.

Suppose $|\Psi(t)\rangle$ is a general normalized state of the system and $\hat{A}(t)$ is an operator with possible explicit time-dependence. i.e.

$$\frac{\partial \hat{A}(t)}{\partial t} \neq 0 \quad \text{— (1)}$$

Then, the expectation value of $\hat{A}$, at any time, in the state $|\Psi(t)\rangle$ is

$$\langle \hat{A} \rangle_t = \langle \Psi(t) | \hat{A}(t) | \Psi(t) \rangle \quad \text{— (2)}$$
$$\equiv \langle \hat{A}(t) \rangle.$$

The rate at which it changes in time is given by

$$\frac{d\langle \hat{A} \rangle_t}{dt} = \left\langle \frac{\partial \Psi(t)}{\partial t} \right| \hat{A}(t) | \Psi(t) \rangle + \langle \Psi(t) | \hat{A}(t) \left| \frac{\partial \Psi(t)}{\partial t} \right\rangle + \langle \Psi(t) | \frac{\partial \hat{A}}{\partial t} | \Psi(t) \rangle \quad \text{— (3)}$$

The first 2 terms of (3) are simplified using the TDSE

$$i\hbar \frac{d|\Psi(t)\rangle}{dt} = \hat{H}(t)|\Psi(t)\rangle \quad -(4)$$

and its dual,

$$-i\hbar \frac{d\langle\Psi(t)|}{dt} = \langle\Psi(t)|\hat{H}(t) \quad -(5)$$

Thus,

$$\boxed{\frac{d\langle\hat{A}\rangle_t}{dt} = \frac{-i}{\hbar}\langle\Psi(t)|[\hat{A}(t),\hat{H}(t)]|\Psi(t)\rangle + \left\langle\frac{\partial\hat{A}(t)}{\partial t}\right\rangle.} \quad -(6)$$

This is general form of the Ehrenfest theorem.

Let's specialize some familiar cases.

First we consider time-independent Hamiltonians $\hat{H}$ such that

$$\hat{H}|E\rangle = E|E\rangle \quad \text{— (7)}$$

and lets consider an observable $\hat{A}$ s.t. $\frac{\partial \hat{A}}{\partial t} = 0$ (no explicit time-dependence)

For such an observable we have

$$\boxed{\frac{d\langle \hat{A}\rangle_t}{dt} = -\frac{i}{\hbar}\left\langle [\hat{A}, \hat{H}] \right\rangle} \quad \text{— (8)}$$

For any state $|\Psi(t)\rangle$.

If $[\hat{A}, \hat{H}] = 0$, (8) means that

$$\frac{d\langle \hat{A}\rangle_t}{dt} = 0 \quad \text{— (9)}$$

i.e. $\langle \hat{A} \rangle_t$ is "conserved" during state evolution. That is, it doesn't change in time.

But $[\hat{A}, \hat{H}] = 0$ also means that the 2 observables share a common set of eigenstates. More specifically

$$\hat{A} \, |E\rangle = a_E |E\rangle \quad \text{— (10)}$$

where a_E is an eigenvalue of $\hat{A}$ which may depend on E. Generically, we can then label the energy eigenstates as $\{ |a, E\rangle \}$ since we can determine both $\hat{A}$ & E simultaneously with arbitrary precision.

$\therefore$ a forms a "good" quantum number to label energy eigenstates.

We can combine (9) & (10) to state that

"Any observable that commutes with the Hamiltonian of a QM system will yield a good quantum number for the system and its expectation value is conserved during motion."

A more direct way to see this:

$$\langle A\rangle_t = \langle \Psi(t)|\hat{A}|\Psi(t)\rangle$$

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

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

$$= \langle \Psi(0)|\hat{A}|\Psi(0)\rangle = \langle \hat{A}\rangle_0$$

$$(\because [\hat{H},\hat{A}]=0) \qquad \text{— (11)}$$

Now consider $\hat{A} = \hat{x}$ for a 1-particle 1-d problem.

$$\Rightarrow \hat{H} = \frac{\hat{p}_x^2}{2m} + V(\hat{x}) \quad \text{—} (12)$$

$\because \frac{\partial \hat{x}}{\partial t} = 0$, (8) implies

$$\frac{d\langle \hat{x} \rangle_t}{dt} = \frac{-i}{\hbar} \langle [\hat{x}, \hat{H}] \rangle \quad \text{—} (13)$$

Now,
$$[\hat{x}, \hat{H}] = \frac{1}{2m} [\hat{x}, \hat{p}_x^2]$$
$$= i\hbar \frac{\hat{p}_x}{m} \quad \text{—} (14)$$

$$\therefore \frac{d\langle \hat{x} \rangle_t}{dt} = \frac{\langle \hat{p}_x \rangle}{m} \quad \text{—} (15)$$

If we pretend that $\langle \hat{x} \rangle_t$ represents classical position of particle & $\langle \hat{p}_x \rangle_t$ its classical momentum, then

(15) is analogous to the equ.

$$\dot{x}(t) = \frac{p(t)}{m} = v(t) \quad \text{—(16)}$$

Now, $$\frac{d\langle \hat{p}_x \rangle}{dt} = \frac{-i}{\hbar} \langle [\hat{p}_x, \hat{H}] \rangle$$

$$= -\left\langle \frac{d\hat{V}}{dx} \right\rangle \quad \text{—(17)}$$

$$\therefore \frac{d^2\langle x \rangle_t}{dt^2} = \frac{1}{m} \frac{d\langle \hat{p}_x \rangle}{dt}$$

or

$$m \frac{d^2\langle x \rangle_t}{dt^2} = -\underbrace{\left\langle \frac{d\hat{V}}{dx} \right\rangle}_{\text{Force}} \quad \text{—(18)}$$

(18) is the analog of the Newton's equ. of motion

$$F = ma = m\ddot{x}(t) \quad \text{—(19)}$$

The 2 eqns.

$$\boxed{\begin{aligned} \frac{d\langle \hat{x}\rangle_t}{dt} &= \frac{\langle \hat{p}_x\rangle}{m} \\ m\frac{d^2\langle \hat{x}\rangle_t}{dt^2} &= -\left\langle \frac{d\hat{V}}{dx}\right\rangle \end{aligned}}$$

are together called the Ehrenfest theorem. They help illustrate the correspondence between quantum and classical notions.

If $|\Psi(t)\rangle$ is a stationary state then the corresponding wavefunction is separable in space & time.

i.e. $\Psi(x,t) = \psi(x)\phi(t)$ — (20)

where $\phi = \exp\left(-i\frac{Et}{\hbar}\right)$

& ψ is eigenfunction for E.

$$\Rightarrow \langle \hat{x} \rangle_t = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, x\, \psi(x) \quad -(21)$$

The RHS can be evaluated (converges) if $\psi(x)$ is a bound state.

$$\Rightarrow \frac{d\langle \hat{x} \rangle_t}{dt} = 0 \quad \text{for such a state!} \quad -(22)$$

$$\therefore \langle \hat{p}_x \rangle = 0 \quad \text{from } (15) \rightarrow (23)$$

$\therefore$ For a stationary bound state the expectation value of momentum is 0 at all times.

Hypervirial Theorem :

Now consider a QM system of N (1-d) particles or 1 particle and N-d.

We define the generalized coordinates and momenta $\{\hat{q}_i, \hat{p}_i\}_{i=1,N}$ to describe the dynamic variables, such that

$$\left.\begin{aligned} [\hat{q}_i, \hat{p}_j] &= i\hbar\,\delta_{ij} \\ [\hat{q}_i, \hat{q}_j] &= [\hat{p}_i, \hat{p}_j] = 0 \end{aligned}\right\} \quad (24)$$

i.e. they still obey the same commutation relations part of our postulates.

The Hamiltonian would then be

$$\hat{H} = \sum_{i=1}^{N} C_i\, \hat{p}_i^2 + V(q_1, q_2, q_3 \cdots q_N) \quad (25)$$

where C_i are some constants that depend on the choice of coordinates.

For instance if $\{q_i\}$ were just Cartesian coordinates $c_i = 1/2m_i$

$\lambda \hat{p}_i \leftrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x_i}$

Now consider the operator

$$\hat{A} = \sum_{i=1}^{N} \hat{q}_i \hat{p}_i \quad — (26)$$

and a stationary bound state $|\Psi(t)\rangle$.

Then,

$$\frac{d\langle \hat{A}\rangle}{dt} = 0 \quad — (27)$$

as we saw in (22).

But $\frac{d\langle \hat{A}\rangle}{dt} = \frac{i}{\hbar}\langle [\hat{A}, \hat{H}]\rangle$ by (8)

$$\Rightarrow \langle [\hat{A}, \hat{H}]\rangle = 0 \quad — (9)$$

for A given by (28)

$$[\hat{A}, \hat{H}] = \sum_{i=1}^{N} [\hat{q}_i \hat{p}_i, \hat{H}]$$

$$= \sum_{i=1}^{N} C_i \, [\hat{q}_i \hat{p}_i, \hat{p}_i^2]$$

$$+ \; [\hat{q}_i \hat{p}_i, V(q)] \qquad (27)$$

where we have used the fact that $[q_i p_i, \hat{p}_j^2] = 0$ if $i \neq j$.

$$\therefore [\hat{A}, \hat{H}] = \sum_{i=1}^{N} \Big\{ C_i \, [\hat{q}_i, \hat{p}_i^2] \, \hat{p}_i + q_i [\hat{p}_i, V(q)] \Big\}$$

(using $[\hat{A}B, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$)

$$= \sum_{i=1}^{N} \Big\{ C_i \cdot 2i\hbar \, \hat{p}_i^2 + \frac{\hbar}{i} \hat{q}_i \frac{\partial \hat{V}}{\partial q_i} \Big\}$$

$$= i\hbar \Big\{ 2\hat{T} - \sum_{i=1}^{N} \hat{q}_i \frac{\partial \hat{V}}{\partial q_i} \Big\} \qquad (28)$$

$\therefore \langle [\hat{A}, \hat{H}] \rangle = 0$

$$\Rightarrow \boxed{2\langle \hat{T} \rangle = \left\langle \sum_{i=1}^{N} \hat{q}_i \frac{\partial \hat{V}}{\partial q_i} \right\rangle} \quad (29)$$

This is called the Hypervirial theorem. Since $|\Psi(t)\rangle$ is a stationary bound state, (29) is especially true for eigenfunction.

The RHS is like a virial

$\vec{r} \cdot \vec{F}$ ↳ force.

Virial Theorem: Now consider a special class of potential energy functions called homogeneous fns.

$V(q_1, q_2 .. q_N)$ is said to be homogeneous of degree n if

$$V(\lambda q_1, \lambda q_2 .. \lambda q_N) = \lambda^n V(q_1, q_2, q_3 .. q_N) \quad — (30)$$

for some $\lambda \in \mathbb{C}$

Then, differentiation of (30) with respect to λ yields

$$\text{LHS} = \sum_{i=1}^{N} \frac{\partial V(\lambda q_i)}{\partial(\lambda q_i)} \cdot \frac{\partial(\lambda q_i)}{\partial \lambda}$$

$$= \sum_{i=1}^{N} \frac{\partial V(\lambda q_1, \lambda q_2 \cdots)}{\partial(\lambda q_i)} q_i \quad \text{— (31)}$$

$$\text{RHS} = n \lambda^{n-1} V(q_1, q_2 \cdots q_N) \quad \text{— (32)}$$

Since (30), (31) & (32) are true for any λ, we can set $\lambda = 1$ which yields

$$\boxed{\sum_{i=1}^{N} \frac{\partial V}{\partial q_i} \cdot q_i = n V(q_1, q_2 \cdots q_N)}$$

— (33)

For such a potential the hypervirial theorem, for a stationary bound state, yields

$$\boxed{2\langle \hat{T} \rangle = n \langle \hat{V} \rangle} \quad — (34)$$

This is called the Virial Theorem (due to V. Fock). It relates the averge K.E & P.E of any eigen state of a QM system.