Lecture 10: Ehrenfest Theorem

THEOREM: Quantum hermitic operators of coordinate and momentum fulfill the Newtonian laws of motion

$$\dot{x} = p_x / m_0 \text{ … kinetic equation of motion,}$$

$$\dot{p}_x = F_x = -\partial_x V(x) \text{ … dynamic equation of motion,}$$

in terms of their expectation values.

The proof is based on evaluation of the time-evolution for the expectation value for a given hermitic operator

$$\frac{d}{dt}\left\langle \hat{A} \right\rangle = \partial_t \int \psi^* \hat{A} \psi d\Gamma$$

$$= \int \left(\partial_t \psi^*\right) \hat{A} \psi d\Gamma + \int \psi^* \left(\partial_t \hat{A}\right) \psi d\Gamma + \int \psi^* \hat{A} \left(\partial_t \psi\right) d\Gamma$$

$$= \int \left(\frac{1}{i\hbar} \hat{H} \psi\right)^* \hat{A} \psi d\Gamma + \left\langle \partial_t \hat{A} \right\rangle + \int \psi^* \hat{\mathbf{A}} \left(\frac{1}{i\hbar} \hat{H} \psi\right) d\Gamma$$

$$= -\frac{1}{i\hbar} \int \psi^* \hat{H} \hat{A} \psi d\Gamma + \frac{1}{i\hbar} \int \psi^* \hat{A} \hat{H} \psi d\Gamma + \left\langle \partial_t \hat{A} \right\rangle$$

$$= \frac{1}{i\hbar} \int \psi^* \left[\hat{A}, \hat{H}\right] \psi d\Gamma + \left\langle \partial_t \hat{A} \right\rangle$$

$$= \frac{1}{i\hbar} \left\langle \left[\hat{A}, \hat{H}\right] \right\rangle + \left\langle \partial_t \hat{A} \right\rangle$$

from where there follows the time-dependent operator expectation equation:

$$i\hbar \frac{d}{dt}\left\langle \hat{A} \right\rangle = \left\langle \left[\hat{A}, \hat{H}\right] \right\rangle + i\hbar \left\langle \partial_t \hat{A} \right\rangle .$$

We are going now to apply this equation to space and momentum operators. However, since the commutator to evaluate involves Hamiltonian that contains the squared of momentum operator one needs to employ the distribution of multiplication commutator rule (easy to be checked out):

$$\left[\hat{A}, \hat{B}\hat{C}\right] = \left[\hat{A}, \hat{B}\right]\hat{C} + \hat{B}\left[\hat{A}, \hat{C}\right]$$

Therefore, for the space operator we have:

$$\left[\hat{x},\hat{H}\right]=\left[\hat{x},\frac{1}{2m_0}\hat{p}_x^2\right]+\underbrace{\left[\hat{x},V(\hat{x})\right]}_{0}=\frac{1}{2m_0}\underbrace{\left[\hat{x},\hat{p}_x\right]}_{i\hbar}\hat{p}_x+\frac{1}{2m_0}\hat{p}_x\underbrace{\left[\hat{x},\hat{p}_x\right]}_{i\hbar}=\frac{i\hbar}{m_0}\hat{p}_x$$

and assuming the Schrödinger picture of non-temporal operators (see also Section 2.2.5)

$$\left\langle\partial_t\hat{x}\right\rangle=0$$

the space operatorial time-dependent equation takes the form

$$\frac{d}{dt}\left\langle\hat{x}\right\rangle=\frac{1}{m_0}\left\langle\hat{p}_x\right\rangle$$

that consecrates the expectation value counterpart of the classical momentum definition.

In the same manner for the momentum operator we have:

$$\left[\hat{p}_x,\hat{H}\right]=\left[\hat{p}_x,\frac{1}{2m_0}\hat{p}_x^2\right]+\left[\hat{p}_x,V(\hat{x})\right]$$

$$=\frac{1}{2m_0}\underbrace{\left[\hat{p}_x,\hat{p}_x\right]}_{0}\hat{p}_x+\frac{1}{2m_0}\hat{p}_x\underbrace{\left[\hat{p}_x,\hat{p}_x\right]}_{0}+\left[\hat{p}_x,V(\hat{x})\right]$$

$$=\left[\hat{p}_x,V(\hat{x})\right];$$

The evaluation of the last commutator we unfold as successively acting on a trial wave-function to get:

$$\underbrace{\left[\hat{p}_x,f(\hat{x})\right]}_{\mapsto}\varphi=\left[-i\hbar\partial_x,f(x)\right]\varphi=-i\hbar\partial_x\left[f(x)\varphi\right]+i\hbar f(x)\partial_x\varphi=\underbrace{-i\hbar\left[\partial_x f(x)\right]}_{\uparrow}\varphi\,;$$

With this the momentum-Hamiltonian commutator becomes:

$$\left[\hat{p}_x,\hat{H}\right]=-i\hbar\partial_x V(x)\,,$$

that together with the expectation of the time change in momentum,

$$\left\langle\partial_t\hat{p}_x\right\rangle=-i\hbar\left\langle\partial_t\left(\partial_x\right)\right\rangle=0\,,$$

the associate time evolution of the momentum expectation yields

$$\partial_t\left\langle\hat{p}_x\right\rangle=-\left\langle\partial_x V(x)\right\rangle$$

proofing the second part or the Ehrenfest theorem.

Overall, the Ehrenfest theorem shows that quantum description is compatible with classical mechanics, under the expectation values of its main operators, i.e. the space, momentum and energy (Hamiltonian). Moreover, it says us that what we can know from quantum mechanical description of Nature is not the detailed evolution but its average; nevertheless, it seems that *quantum mechanically we can not know everything in causes but the remaining knowledge is not absolutely necessary to be revealed for explaining the observed world*! With this answer we opened the direction in which the first Kantian universal interrogative may be approached with the quantum theory.

However, worth remarking that the time-dependent operator expectation equation simply becomes:

$$\frac{d}{dt}\left\langle \hat{A}\right\rangle = \left\langle \partial_t \hat{A}\right\rangle ,$$

i.e. the expectation value of the given observable is computed over stationary eigen-functions, if the concerned observable commutes with Hamiltonian:

$$\left[\hat{A},\hat{H}\right] = 0 \; .$$

The fundamental consequence of this assertion is that *the stationary eigen-functions of a quantum system may be found from the eigen-problems of the operators that commute with the Hamiltonian of the system*. Moreover, if two operators give eigen-values on the same eigen-function of a quantum system,

$$\hat{A}\psi = a\psi \;;\; \hat{B}\psi = b\psi \;;\; a,b \in \Re e \, ,$$

they necessary commute:

$$\left[\hat{A},\hat{B}\right]\psi = \left(\hat{A}\hat{B}\text{-}\hat{B}\hat{A}\right)\psi = \left(ba - ab\right)\psi = 0 \; .$$

Combining the last two ideas, one may conclude that all operators that commute among them and commute with Hamiltonian build up the so called *complete set of commutative operators:*

$$\text{CoSCOpe: } \left\{\hat{A},\hat{B},\ldots,\hat{H}\right\} \;\Big|\; \left[\hat{A},\hat{B}\right] = 0,\ldots,\left[\hat{A},\hat{H}\right] = 0,\left[\hat{B},\hat{H}\right] = 0$$

with the help of which all stationary eigen-values and eigen-functions of a system may be determined throughout the associate eigen-problems:

$$\begin{aligned} &\hat{A}\psi = a\psi \\ &\hat{B}\psi = b\psi \\ &\ldots \\ &\hat{H}\psi = E\psi \end{aligned}$$

This is a fundamental property of operators and will be of the first importance in furnishing the complete solution of the Hydrogen atomic problem.