L12-Ehrenfest Theorem: Momentum Operator

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* In classical mechanics, we can convert Newton's law $F(x) = ma = m\ddot{x}$, which is 2nd order in position x, into two first order equations by singling out a second independent variable, momentum p:

a) $p = mv = m\dot{x}$ b) $F = -\nabla V = m\ddot{x} = \dot{p}$

We have already seen the two variables are complementary in Q.M., through the Heisenberg Uncertainty Principle: $\Delta p \cdot \Delta x \geq \hbar/2$

The "symplectic" symmetry of these two coupled equations becomes more aparent by introducing the Hamiltonian:

$\mathcal{H} = \frac{p^2}{2m} + V(x)$, which is the total energy in terms of (p, x).

Then we get Hamilton's equations: [note: $\frac{\partial}{\partial p}\frac{p^2}{2m} = \frac{p}{m}$, $\frac{\partial V}{\partial x} = -F$]

a) $\frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m} = \dot{x}$ b) $-\frac{\partial \mathcal{H}}{\partial x} = F = \dot{p}$ [symplectic refers to the lone (-)]

* Later on we will discover other parallels between Hamilton's eq's and Q.M., but for now we can at least explore the classical correspondence "Ehrenfest theorems" which relate the Q.M. expectation values to their classical equations.

* Ehrenfest theorems for x, p (Griffiths 1.5, Gasiorowicz 2-7)

a) $\boxed{\frac{d}{dt}\langle x \rangle = \frac{\langle p \rangle}{m}}$ [This is similar to the proof that $\frac{d}{dt}\int_{-\infty}^{\infty} |\psi|^2 dx = 0$.]

$$\frac{d}{dt}\langle x \rangle = \frac{d}{dt}\int_{-\infty}^{\infty} x|\psi|^2 dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} x\, \psi^* \psi\, dx = \int dx\, \frac{\partial}{\partial t} \underbrace{\psi^* x \psi}$$

[it is customary to put x between ψ^* and ψ]

$$= \int_{-\infty}^{\infty} dx\; \partial_t \psi^* \cdot x\psi + \psi^* x\, \partial_t \psi \qquad [\partial_t x = 0]$$

$$= \int dx \underbrace{\left[\frac{-i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{V}{-i\hbar}\cancel{\psi^*}\right]}_{\text{using the T.D.S.E.}} x\psi + \psi^* x \underbrace{\left[\frac{i\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi + \frac{V}{i\hbar}\cancel{\psi}\right]}_{\text{using the T.D.S.E.}}$$

TDSE and complex conjugate:

$$i\hbar\partial_t \psi = \frac{-\hbar^2}{2m}\partial_x^2 \psi + V(x)\psi$$

$$-i\hbar\partial_t \psi^* = \frac{-\hbar^2}{2m}\partial_x^2 \psi^* + V(x)\psi^*$$

$$= \frac{-i\hbar}{2m}\int_{-\infty}^{\infty} dx \left[\underbrace{\frac{\partial^2 \psi^*}{\partial x^2} x \psi}_{A} - \underbrace{\psi^* x \frac{\partial^2 \psi}{\partial x^2}}_{B}\right]$$

$$= \frac{-i\hbar}{2m}\int_{-\infty} dx \left[\underbrace{\frac{\partial^2\psi^*}{\partial x^2} x \psi}_{A} - \underbrace{\psi^* x \frac{\partial^2\psi}{\partial x^2}}_{B} \right]$$

Integrate by parts 3 times to simplify A and B:

i) $0 = \int_{-\infty}^{\infty} dx \frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x} x \psi\right) = \int_{-\infty}^{\infty} dx \left[\underbrace{\frac{\partial^2\psi^*}{\partial x^2} x \psi}_{A} + \underbrace{\frac{\partial\psi^*}{\partial x}\cdot 1\cdot \psi}_{C} + \underbrace{\frac{\partial\psi^*}{\partial x} x \frac{\partial\psi}{\partial x}}_{D} \right]$

ii) $0 = \int_{-\infty}^{\infty} dx \frac{\partial}{\partial x}\left(\psi^* x \frac{\partial\psi}{\partial x}\right) = \int_{-\infty}^{\infty} dx \left[\underbrace{\frac{\partial\psi^*}{\partial x} x \frac{\partial\psi}{\partial x}}_{D} + \underbrace{\psi^*\cdot 1\cdot\frac{\partial\psi}{\partial x}}_{E} + \underbrace{\psi^* x \frac{\partial^2\psi}{\partial x^2}}_{B} \right]$

iii) $0 = \int_{-\infty}^{\infty} dx \frac{\partial}{\partial x}(\psi^*\psi) = \int_{-\infty}^{\infty} dx \left[\underbrace{\frac{\partial\psi^*}{\partial x}\cdot\psi}_{C} + \underbrace{\psi^*\cdot\frac{\partial\psi}{\partial x}}_{E} \right]$

Thus $A - B = (-C - \cancel{D}) - (-\cancel{D} - E) = 2E$ and therefore:

$$\frac{d}{dt}\int_{-\infty}^{\infty} dx\, \psi^* \underbrace{x}_{\hat{x}} \psi = \frac{1}{m}\int_{-\infty}^{\infty} \psi^* \underbrace{[-i\hbar\partial_x]}_{\hat{p}} \psi \quad \text{or} \quad \frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle$$

* Note we have written expectation values using operators using the pattern: $\langle G\rangle = \int_{-\infty}^{\infty} dx\, \psi^* \hat{G} \psi \equiv \langle\psi|\hat{G}|\psi\rangle$, [new notation!] which works for both regular values like $\hat{x} = x$ [regular weighted average] as well as more complicated operators like $\hat{p} = -i\hbar\frac{\partial}{\partial x}$, which should operate on ψ, not multiply by $|\psi|^2$ as above.

* We will come back and formalize this idea in Chapter 3.

b) $\boxed{\frac{d}{dt}\langle p\rangle = \langle F\rangle = \langle -\frac{\partial V}{\partial x}\rangle}$ [Also similar to the proof that $\frac{d}{dt}\int_{-\infty}^{\infty}|\psi|^2 dx = 0$]

$$\frac{d}{dt}\langle p\rangle = \frac{d}{dt}\int_{-\infty}^{\infty} dx\, \psi^*(-i\hbar\partial_x)\psi = \int_{-\infty}^{\infty} dx\,(-i\hbar)\left[\partial_t\psi^*\cdot\partial_x\psi + \psi^*\partial_x\partial_t\psi\right]$$

$$= \int_{-\infty}^{\infty} dx \left[\underbrace{\frac{-\hbar^2}{2m}\partial_x^2}_{\hat{T}}\psi^* + V\psi^*\right]\partial_x\psi + \psi^*\partial_x\left[\underbrace{\frac{\hbar^2}{2m}\partial_x^2}_{-\hat{T}}\psi - V\psi\right] \qquad \hat{T} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$= \int_{-\infty}^{\infty} dx\,(\cancel{\psi\hat{T}\psi^* - \psi^*\hat{T}\psi}) + \cancel{V\psi^*\partial_x\psi} - \psi^*[\partial_x V\cdot\psi + \cancel{V\partial_x\psi}]$$

see below

$$= \int_{-\infty}^{\infty} dx\, \psi^* \frac{-\partial V}{\partial x}\psi = \langle -\frac{\partial V}{\partial x}\rangle$$

* Ex: show that the expectation values of $\hat{p}$, $\hat{p}^2$, $\hat{T} = \hat{p}^2/2m$ are real-valued. We call operators that have this property "Hermitian"

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$$\langle p \rangle = \int_{-\infty}^{\infty} dx\, \Psi^* \hat{p}\, \Psi = \int_{-\infty}^{\infty} dx\, \Psi^* (-i\hbar\partial_x) \Psi = -i\hbar \int_{-\infty}^{\infty} \Psi^* d\Psi$$

$$= -i\hbar\, \overbrace{\Psi^*\Psi\Big|_{-\infty}^{\infty}}^{0} + i\hbar \int_{-\infty}^{\infty} \Psi\, d\Psi^*$$ [integration by parts]

$$= \int_{-\infty}^{\infty} dx\, \Psi (-i\hbar\partial_x \Psi)^* = \int dx\, (\hat{p}\Psi)^* \Psi = \langle p \rangle^*$$

$$\langle p^2 \rangle = \int dx\, \Psi^* p^2 \Psi = \int dx\, (\hat{p}\Psi)^* p \Psi = \int dx\, (\hat{p}^2\Psi)^* \Psi = \langle p^2 \rangle^*$$

$$\langle T \rangle = \int dx\, \Psi^* \frac{p^2}{2m} \Psi = \int dx\, \Psi^* \frac{-\hbar^2}{2m} \partial_x^2 \Psi = \langle T \rangle^*$$

We will also formalize the concept of Hermitian operators as "observables" in the sense that they correspond to real-valued measurements. We will also show that these operators have real eigenvalues, which turn out to be the possible values we can observe in an experiment.