Chapter 6: The Classical Limit

Time evolution of the expectation value of an observable in state $|\psi\rangle$:

$$\frac{d}{dt}\langle\hat{\Omega}\rangle = \frac{d}{dt}\langle\psi|\hat{\Omega}|\psi\rangle = \langle\dot{\psi}|\hat{\Omega}|\psi\rangle + \langle\psi|\hat{\Omega}|\dot{\psi}\rangle + \langle\psi|\dot{\hat{\Omega}}|\psi\rangle$$

$$= \underbrace{\frac{i}{\hbar}\langle\psi|\hat{H}}_{\langle\dot{\psi}|}\hat{\Omega}|\psi\rangle - \frac{i}{\hbar}\langle\psi|\hat{\Omega}\,\hat{H}|\psi\rangle + \langle\psi|\dot{\hat{\Omega}}|\psi\rangle$$

$$= \left\langle -\frac{i}{\hbar}[\hat{\Omega},\hat{H}] + \frac{\partial\hat{\Omega}}{\partial t}\right\rangle$$

This equation is called Ehrenfest's theorem.

If $\hat{\Omega}$ has no explicit time dependence, the last term vanishes. Let us assume this to hold in the following.

<u>Example</u> $\hat{\Omega} = \hat{X}$, position of the particle:

$$\frac{d}{dt}\langle\hat{X}\rangle = -\frac{i}{\hbar}\left\langle[\hat{X},\hat{H}]\right\rangle = -\frac{i}{\hbar}\left\langle\left[\hat{X},\frac{\hat{P}^2}{2m} + \hat{V}(\hat{X})\right]\right\rangle$$

$$= -\frac{i}{2m\hbar}\left\langle\underbrace{[\hat{X},\hat{P}^2]}_{\hat{P}[\hat{X},\hat{P}] + [\hat{X},\hat{P}]\hat{P} = 2i\hbar\hat{P}}\right\rangle = \frac{1}{m}\langle\hat{P}\rangle$$

$$\Rightarrow \boxed{m\frac{d\langle\hat{X}\rangle}{dt} = \langle\hat{P}\rangle}$$ (c.f. $m\frac{dx}{dt} = p$ in class. mech.)

Writing $\frac{\hat{P}}{m} = \frac{\partial \hat{H}}{\partial \hat{P}} \implies \boxed{\frac{d\langle \hat{X}\rangle}{dt} = \left\langle \frac{\partial \hat{H}}{\partial \hat{P}} \right\rangle}$

Next

$$\frac{d\langle \hat{P}\rangle}{dt} = -\frac{i}{\hbar}\langle [\hat{P},\hat{H}]\rangle = -\frac{i}{\hbar}\langle [\hat{P},\hat{V}(\hat{X})]\rangle$$

In the x-basis, $\hat{P} \longrightarrow -i\hbar\frac{d}{dx}$, $V(\hat{X}) \longrightarrow V(x)$

and $[\hat{P},\hat{V}(\hat{X})] \longrightarrow \left[-i\hbar\frac{d}{dx}, V(x)\right] = -i\hbar\frac{dV}{dx}$

We conclude

$$[\hat{P},\hat{V}(\hat{X})] = -i\hbar\frac{d\hat{V}}{d\hat{X}} = -i\hbar\frac{\partial \hat{H}}{\partial \hat{X}}$$

$$\implies \boxed{\frac{d\langle \hat{P}\rangle}{dt} = \left\langle -\frac{\partial \hat{H}}{\partial \hat{X}} \right\rangle}$$

Again this reminds us of classical mechanics where

$$\dot{x} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial x}$$

Let us now study these "quantum equations of motion" for a macroscopic particle of mass, say, $m = 1g$.

Since we cannot fix its position and momentum exactly simultaneously, let us describe it instead by a narrow Gaussian wavepacket that is sufficiently well localized to satisfy classical laboratory precision:

$$|x_0 \, p_0 \, \Delta\rangle \longleftrightarrow \psi_{x_0 p_0 \Delta}(x) = \left(\frac{1}{\pi\Delta^2}\right)^{1/4} e^{ip_0 x/\hbar} \, e^{-(x-x_0)^2/2\Delta^2}$$

with, say, $\Delta \simeq 10^{-15}\,m = 1\,fm$ (the radius of a proton).

The corresponding momentum uncertainty $\Delta P = \frac{\hbar}{\sqrt{2}\Delta} = \frac{6.63\times 10^{-34}\,Js}{\sqrt{2}\cdot 10^{-15}\,m}$

$\approx 5\times 10^{-19}\,\frac{kg\,m}{s}$, or a velocity uncertainty $\Delta v = 5\times 10^{-16}\,\frac{m}{s}$.

This looks like pretty good precision – good enough for government work.

So this state has "well-defined" values x_0 and p_0 for $\hat{X}$ and $\vec{P}$, where "well-defined" is measured on the classical precision scale: the fluctuations around x_0 and p_0 are truly negligible.

The Ehrenfest equations of motion

$$\frac{dx_0}{dt} = \frac{d\langle\hat{X}\rangle}{dt} = \left\langle \frac{\partial \hat{H}(\hat{X},\hat{P})}{\partial \hat{P}} \right\rangle, \quad \frac{dp_0}{dt} = \frac{d\langle\hat{P}\rangle}{dt} = -\left\langle \frac{\partial \hat{H}}{\partial \hat{X}} \right\rangle$$

would look like classical equations of motion,

$$\dot{x}_0 = \frac{\partial \mathcal{H}(x_0,p_0)}{\partial p_0}, \quad \dot{p}_0 = -\frac{\partial \mathcal{H}(x_0,p_0)}{\partial x_0}$$

if we could replace

$$\left\langle \frac{\partial \hat{H}}{\partial \hat{P}} \right\rangle \approx \frac{\partial \hat{H}}{\partial \hat{P}}\bigg|_{\hat{X}=x_0,\,\hat{P}=p_0} = \frac{\partial \mathcal{H}(x_0,p_0)}{\partial p_0}, \quad \left\langle \frac{\partial \hat{H}}{\partial \hat{X}} \right\rangle \approx \frac{\partial \hat{H}}{\partial \hat{X}}\bigg|_{\hat{X}=x_0,\,\hat{P}=p_0} = \frac{\partial \mathcal{H}(x_0,p_0)}{\partial x_0}$$

So the question is: when is $\langle \hat{\Omega}(\hat{X},\hat{P})\rangle \approx \omega(x_0,p_0)$?

In other words, when is the mean of the functions $\frac{\partial \hat{H}}{\partial \hat{P}}$ etc. equal to the function $\frac{\partial \mathcal{H}}{\partial p_0}(x_0,p_0)$ of the mean values of $\hat{X},\hat{P}$?

Answer: when the fluctuations are small.

(The two are exactly the same *if* there are *no* fluctuations at all.)

Let's first consider $\dot{x}_0 = \frac{d\langle \hat{X} \rangle}{dt} = \left\langle \frac{\partial \hat{H}}{\partial \hat{P}} \right\rangle = \left\langle \frac{\hat{P}}{m} \right\rangle = \frac{p_0}{m}$

This takes the classical form <u>without approximation</u>.

In the second equation $\dot{p}_0 = \frac{d\langle \hat{P} \rangle}{dt} = -\left\langle \frac{\partial \hat{H}}{\partial \hat{X}} \right\rangle = -\left\langle \frac{d\hat{V}}{d\hat{X}} \right\rangle$

equivalence to the classical equation requires

$$\left\langle \frac{d\hat{V}}{d\hat{X}}(\hat{X}) \right\rangle \approx \frac{dV}{dx}(x = x_0).$$

To see when this is a good approximation, let's expand

$$V'(x) = V'(x_0) + (x - x_0) V''(x_0) + \frac{1}{2}(x - x_0)^2 V'''(x_0) + \dots$$

$$\Rightarrow \langle \hat{V}'(\hat{X}) \rangle = \underbrace{\langle V'(x_0) \hat{I} \rangle}_{V'(x_0)} + \langle \hat{X} - x_0 \hat{I} \rangle V''(x_0) + \frac{1}{2} \langle (\hat{X} - x_0 \hat{I})^2 \rangle V'''(x_0) + \dots$$

Since $\langle \hat{X} \rangle = x_0$, the linear term vanishes. The quadratic term is proportional to the uncertainty $(\Delta X)^2$ and can be neglected <u>iff</u> the width of the wavepacket is small and as long as it remains small. It tells us that the particle responds not only to the force at x_0, but (due to its position uncertainty) also to the force at neighboring points.

The classical approximation thus holds if, over the range of uncertainty ΔX for the particle position, the force is roughly constant. Of course, ΔX increases with time, so eventually this approximation breaks down, but for a single particle this uncertainty grows linearly in time (unless its motion is chaotic) and it takes (for a 1g particle) 300,000 years to grow to even 1mm.

There are, however, non-linear systems of interacting particles for which uncertainties in the initial position grow exponentially in time, due to classical or quantum chaotic dynamics. The growth rate can be millions of years (as for planetary orbits), days (as for weather patterns), or yoctoseconds (10^{-24}s) (as for certain types of classical gluon field configurations created in high energy collisions between protons or atomic nuclei). In such cases quantum uncertainties have a chance to become macroscopically relevant and important.

We summarize: for Ehrenfest's equations to really become equivalent to the classical equations of Newtonian dynamics, we must be able to ignore fluctuations, i.e. replace the mean of observable functions by the corresponding functions of the mean values $\langle\hat{X}\rangle = x_0$ and $\langle\hat{P}\rangle = p_0$.
i.e. $\boxed{\langle\Omega(\hat{X},\hat{P})\rangle = \Omega(\langle\hat{X}\rangle,\langle\hat{P}\rangle) = \omega(x_0,p_0)}$.
For Hamiltonians that are at most quadratic in $\hat{P}$ and $\hat{X}$, this replacement can be done without error.