CLASSICAL LIMIT OF QUANTUM MECHANICS - EHRENFEST'S THEOREM

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We've met Ehrenfest's theorem earlier, where the theorem had the form

$$\frac{\partial\langle p\rangle}{\partial t}=-\left\langle \frac{\partial V}{\partial x}\right\rangle \tag{1}$$

This says that, in one dimension, the rate of change of the mean momentum equals the negative of the mean of the derivative of the potential V, which is assumed to depend on x only. In this case, the behaviour of the means of the quantum variables reduces to the corresponding classical relation, in this case, Newton's law $F=\frac{dp}{dt}$, where the force is defined in terms of the gradient of the potential: $F=-\frac{dV}{dx}$.

Shankar treats Ehrenfest's theorem a bit more generally. For an operator Ω we can use the product rule to state that

$$\frac{d}{dt}\langle\Omega\rangle = \frac{d}{dt}\langle\psi\left|\Omega\right|\psi\rangle \tag{2}$$

$$= \left\langle\dot{\psi}\left|\Omega\right|\psi\right\rangle+\left\langle\psi\left|\Omega\right|\dot{\psi}\right\rangle+\left\langle\psi\left|\dot{\Omega}\right|\psi\right\rangle \tag{3}$$

where a dot indicates a time derivative. If Ω does not depend explicitly on time, we have

$$\frac{d}{dt}\langle\Omega\rangle=\left\langle\dot{\psi}\left|\Omega\right|\psi\right\rangle+\left\langle\psi\left|\Omega\right|\dot{\psi}\right\rangle \tag{4}$$

The time derivative of ψ can be found from the Schrödinger equation:

$$\left|\dot{\psi}\right\rangle=-\frac{i}{\hbar}H\left|\psi\right\rangle \tag{5}$$

$$\left\langle\dot{\psi}\right|=\frac{i}{\hbar}\left\langle\psi\right|H \tag{6}$$

The second equation follows since H is hermitian, so $H^{\dagger}=H$. Plugging these into 4 we have

$$\frac{d}{dt}\langle\Omega\rangle = \frac{i}{\hbar}\left[\langle\psi|H\Omega|\psi\rangle - \langle\psi|\Omega H|\psi\rangle\right] \tag{7}$$

$$= -\frac{i}{\hbar}\langle\psi|[\Omega, H]|\psi\rangle \tag{8}$$

$$= -\frac{i}{\hbar}\langle[\Omega, H]\rangle \tag{9}$$

That is, the rate of change of the mean of an operator can be found from its commutator with the Hamiltonian. It is this result that Shankar refers to as Ehrenfest's theorem. This relation is similar to that from classical mechanics, where the rate of change of a dynamical variable ω is equal to its Poisson bracket with the classical Hamiltonian. In the Hamiltonian formulation of classical mechanics, dynamical variables depend on generalized coordinates q_i and their corresponding momenta p_i, so we have:

$$\frac{d\omega}{dt} = \sum_i \left(\frac{\partial\omega}{\partial q_i}\dot{q}_i + \frac{\partial\omega}{\partial p_i}\dot{p}_i\right) \tag{10}$$

$$= \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial H}{\partial q_i}\right) \tag{11}$$

$$\equiv \{\omega, H\} \tag{12}$$

We can work out 9 for the particular cases where $\Omega = X$, the position operator and $\Omega = P$, the momentum operator. For a Hamiltonian of the form

$$H = \frac{P^2}{2m} + V(x) \tag{13}$$

and using the commutation relation

$$[X, P] = i\hbar \tag{14}$$

we have

$$\frac{d\langle X\rangle}{dt} = -\frac{i}{\hbar}\langle[X, H]\rangle \tag{15}$$

$$= -\frac{i}{2m\hbar}\left\langle\left[X, P^2\right]\right\rangle \tag{16}$$

We can evaluate this commutator using the theorem

$$[AB, C] = A[B, C] + [A, C]B \tag{17}$$

In this case, $A = B = P$ and $C = X$, so we have

$$\left[P^2,X\right]=P\left[P,X\right]+\left[P,X\right]P \tag{18}$$

$$=-2i\hbar P \tag{19}$$

$$\left[X,P^2\right]=2i\hbar P \tag{20}$$

$$\frac{d\left\langle X\right\rangle}{dt}=\frac{\left\langle P\right\rangle}{m} \tag{21}$$

This is equivalent to the classical relation $p=mv$ for velocity v. We can write this result in terms of the Hamiltonian, provided that it's legal to take the derivative of the Hamiltonian with respect to an operator (which works if we can expand the Hamiltonian as a power series):

$$\frac{d\left\langle X\right\rangle}{dt}=\frac{\left\langle P\right\rangle}{m}=\left\langle\frac{\partial H}{\partial P}\right\rangle \tag{22}$$

This looks a lot like one of Hamilton's canonical equations in classical mechanics:

$$\dot{q}_i=\frac{\partial H}{\partial p_i} \tag{23}$$

The main difference between the quantum and classical forms is that the quantum version is a relation between mean values, while the classical version is exact. We can make the correspondence exact provided that it's legal to take the averaging operation inside the derivative and apply it to each occurrence of X and P. That is, is it legal to say that

$$\left\langle\frac{\partial H}{\partial P}\right\rangle=\left\langle\frac{\partial H\left(P,X\right)}{\partial P}\right\rangle=\frac{\partial H\left(\left\langle P\right\rangle,\left\langle X\right\rangle\right)}{\partial\left\langle P\right\rangle} \tag{24}$$

This depends on the precise functional form of H. In the case 13 we're considering here, we have

$$\left\langle\frac{\partial H}{\partial P}\right\rangle=\left\langle\frac{P}{m}\right\rangle=\frac{\left\langle P\right\rangle}{m}=\frac{\partial}{\partial\left\langle P\right\rangle}\left(\frac{\left\langle P\right\rangle^2}{2m}+V\left(\left\langle X\right\rangle\right)\right) \tag{25}$$

So in this case it works. In general, if H depends on P either linearly or quadratically, then its derivative with respect to P will be either constant or linear, and we can take the averaging operation inside the function without changing anything. However, if, say, $H=P^3$ (unlikely, but just for the sake of argument), then

$$\left\langle\frac{\partial H}{\partial P}\right\rangle=\left\langle 3P^2\right\rangle\neq 3\left\langle P\right\rangle^2=\frac{\partial H\left(\left\langle P\right\rangle,\left\langle X\right\rangle\right)}{\partial\left\langle P\right\rangle} \tag{26}$$

since, in general, the mean of the square of a value is not the same as the square of the mean.

Shankar goes through a similar argument for $\dot{P}$. We have

$$\left\langle \dot{P}\right\rangle = -\frac{i}{\hbar}\left\langle [P,H]\right\rangle \tag{27}$$

In this case, we can use the position basis form of P which is

$$P = -i\hbar\frac{d}{dx} \tag{28}$$

and the position space version of the potential $V(x)$ to get

$$[P,H]\psi = -i\hbar\left(\frac{d(V\psi)}{dx} - V\frac{d\psi}{dx}\right) \tag{29}$$

$$= -i\hbar\psi\frac{dV}{dx} \tag{30}$$

Using this in 27 we have

$$\left\langle \dot{P}\right\rangle = -\left\langle \frac{dV}{dx}\right\rangle \tag{31}$$

Writing this in terms of the Hamiltonian, we have

$$\left\langle \dot{P}\right\rangle = -\left\langle \frac{\partial H}{\partial x}\right\rangle \tag{32}$$

Again, this looks similar to the second of Hamilton's canonical equations from classical mechanics:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{33}$$

and again, we're allowed to make the correspondence exact provided we can take the averaging operation inside the derivative on the RHS of 32. This works provided that V is either linear or quadratic in x (such as in the harmonic oscillator). Other potentials such as the $\frac{1}{r}$ potential in the hydrogen atom do not allow an exact correspondence between the quantum average and the classical Hamilton equation, but this shouldn't worry us too much since the hydrogen atom is quintessentially quantum anyway, and any attempt to describe it classically will not work.

Shankar provides a lengthly discussion on when the reduction to classical mechanics is valid, and shows that in any practical experiment that we could do with a classical particle, the difference between the average quantum behaviour and the classical measurements should be so small as to be undetectable. It is only when we deal with systems that are small enough that quantum effects dominate that we need to abandon classical mechanics.