Quantum Mechanics: Ehrenfest theorem

Heisenberg picture

Consider a particle of mass m, moving in one dimension, in a potential V. The Hamiltonian is then given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}). \tag{1}$$

The Heisenberg equation of motion for position can be written as

$$\frac{d}{dt}\hat{x}(t) = \frac{i}{\hbar}[\hat{H}, \hat{x}(t)], \tag{2}$$

where $\hat{x}(t) = \hat{U}_t\hat{x}(0)\hat{U}_t^\dagger$, $\hat{U}_t = \exp(i\hat{H}t/\hbar)$ being the unitary time evolution operator. Since $\hat{U}_t$ commutes with $\hat{H}$, and $\hat{x}$ commutes with $V(\hat{x})$, the above equation yields

$$m\frac{d}{dt}\hat{x}(t) = \hat{p}. \tag{3}$$

Similarly, the Heisenberg equation of motion for the momentum operator can be written as

$$\frac{d}{dt}\hat{p}(t) = \frac{i}{\hbar}[\hat{H}, \hat{p}(t)] = \frac{i}{\hbar}\hat{U}_t[V(\hat{x}), \hat{p}(0)]\hat{U}_t^\dagger. \tag{4}$$

Now let us assume that the potential V is an analytical function of x and it can be expanded in a Taylor series

$$V(x) = \sum_{n=0}^{\infty} \frac{V^{(n)}(0)}{n!}x^n, \tag{5}$$

where $V^{(n)}(0)$ denotes the nth derivative of $V(x)$ at $x = 0$. Using the series form of the potential, Heisenberg equation of motion for $\hat{p}$ can be written as

$$\begin{aligned} \frac{d}{dt}\hat{p}(t) &= \frac{i}{\hbar}\hat{U}_t\sum_{n=0}^{\infty}\frac{V^{(n)}(0)}{n!}[\hat{x}^n, \hat{p}]\hat{U}_t^\dagger \\ &= -\hat{U}_t\sum_{n=0}^{\infty}\frac{V^{(n)}(0)}{n!}n\hat{x}^{n-1}\hat{U}_t^\dagger \\ &= -\sum_{n=0}^{\infty}\frac{V^{(n)}(0)}{n!}n\hat{x}^{n-1}(t), \end{aligned} \tag{6}$$

where we have used the well known commutation relation $[\hat{x}^n, \hat{p}] = i\hbar n\hat{x}^{n-1}$. But $\sum_{n=0}^{\infty}\frac{V^{(n)}(0)}{n!}n\hat{x}^{n-1}$ is just the derivative of V, denoted by V'. Then the Heisenberg equation of motion for $\hat{p}$ assumes the form

$$\frac{d}{dt}\hat{p}(t) = -V'(\hat{x}(t)). \tag{7}$$

Using (3) and (7), one can write

$$m\frac{d^2}{dt^2}\hat{x}(t) = \frac{d}{dt}\hat{p}(t) = -V'(\hat{x}(t)). \tag{8}$$

This is a fully quantum mechanical equation involving operators, but has the exact form of the Newton's equation of motion. The only assumption that we made in arriving at this equation is that the potential is an analytical function which can be expanded in a Taylor series. For conciseness, the Taylor expansion was done around $x = 0$, but one can convince onself that the argument goes through for expansion around any other value. For example, for the potential $V(\hat{x}) = -1/\hat{x}$, the commutation relation $[\hat{p}, 1/\hat{x}] = i\hbar/\hat{x}^2$ leads to the equation of motion: $d\hat{p}(t)/dt = -1/\hat{x}^2(t)$.

Ehrenfest theorem

Now one can take the expectation value of both sides of equation (8) and get

$$m\frac{d^2}{dt^2}\langle\hat{x}\rangle = \frac{d}{dt}\langle\hat{p}\rangle = -\langle V'(\hat{x})\rangle, \tag{9}$$

where the angular brackets denote the expectation value. This is the familiar equation denoting Ehrefest theorem. It shows that the expection values of position and momentum *approximately* follow Newton's equations of motion. It is approximate because $\langle V'(\hat{x})\rangle \neq V'(\langle\hat{x}\rangle)$. For example, if $V'(\hat{x}) = \hat{x}^2$, then

$$\begin{aligned}\langle V'(\hat{x})\rangle =& \langle\hat{x}^2\rangle = \langle\hat{x}\rangle^2 + (\Delta x)^2 \\ =& V'(\langle\hat{x}\rangle) + (\Delta x)^2\end{aligned} \tag{10}$$

So, if the state is such that the uncertainty in position is small, then $\langle V'(\hat{x})\rangle \approx V'(\langle\hat{x}\rangle)$, and one can say that the expectation values follow classical dynamics.

Notice that for a Harmonic oscillator, the potential is $V(x) = \frac{1}{2}m\omega^2x^2$, and its derivative $V'(x) = m\omega^2 x$ is linear in x. Consequently $\langle V'(\hat{x})\rangle = V'(\langle\hat{x}\rangle)$, which means that the expectation value of the position always follows classical dynamics.