# 5.2: The Ehrenfest Theorem

In Sec. 4.7, we have derived all the basic relations of wave mechanics from the bra-ket formalism, which will also enable us to get some important additional results in that area. One of them is a pair of very interesting relations, together called the Ehrenfest theorem. To derive them, for the simplest case of 1D orbital motion, let us calculate the following commutator:

$$\left[\hat{x}, \hat{p}_x^2\right] \equiv \hat{x}\hat{p}_x\hat{p}_x - \hat{p}_x\hat{p}_x\hat{x}. \tag{5.2.1}$$

Let us apply the commutation relation (4.238) in the following form:

$$\hat{x}\hat{p}_x = \hat{p}_x\hat{x} + i\hbar\hat{I}, \tag{5.2.2}$$

to the first term of the right-hand side of Eq. (24) twice, with the goal to move the coordinate operator to the rightmost position:

$$\hat{x}\hat{p}_x\hat{p}_x = \left(\hat{p}_x\hat{x} + i\hbar\hat{I}\right)\hat{p}_x \equiv \hat{p}_x\hat{x}\hat{p}_x + i\hbar\hat{p}_x = \hat{p}_x\left(\hat{p}_x\hat{x} + i\hbar\hat{I}\right) + i\hbar\hat{p}_x \equiv \hat{p}_x\hat{p}_x\hat{x} + 2i\hbar\hat{p}_x. \tag{5.2.3}$$

The first term of this result cancels with the last term of Eq. (24), so that the commutator becomes quite simple:

$$\left[\hat{x}, \hat{p}_x^2\right] = 2i\hbar\hat{p}_x. \tag{5.2.4}$$

Let us use this equality to calculate the Heisenberg-picture equation of motion of the operator $\hat{x}$, by applying the general Heisenberg equation (4.199) to the $1\text{D}$ orbital motion described by the Hamiltonian (4.237), but possibly with a more general, time-dependent potential energy $U$ :

$$\frac{d\hat{x}}{dt} = \frac{1}{i\hbar}[\hat{x}, \hat{H}] = \frac{1}{i\hbar}\left[\hat{x}, \frac{\hat{p}_x^2}{2m} + U(\hat{x}, t)\right]. \tag{5.2.5}$$

The potential energy operator is a function of the coordinate operator and hence, as we know, commutes with it. Thus, the right-hand side of Eq. (28) is proportional to the commutator (27), and we get

$$\frac{d\hat{x}}{dt} = \frac{\hat{p}_x}{m}. \tag{5.2.6}$$

In this operator equality, we readily recognize the full analog of the classical relation between the particle's momentum and is velocity.

Now let us see what a similar procedure gives for the momentum's derivative:

$$\frac{d\hat{p}_x}{dt} = \frac{1}{i\hbar}\left[\hat{p}_x, \hat{H}\right] = \frac{1}{i\hbar}\left[\hat{p}_x, \frac{\hat{p}_x^2}{2m} + U(\hat{x}, t)\right]. \tag{5.2.7}$$

The kinetic energy operator commutes with the momentum operator and hence drops from the righthand side of this equation. To calculate the remaining commutator of the momentum and potential energy, let us use the fact that any smooth (infinitely differentiable) function may be represented by its Taylor expansion:

$$U(\hat{x}, t) = \sum_{k=0}^{\infty} \frac{1}{k!}\frac{\partial^k U}{\partial\hat{x}^k}\hat{x}^k, \tag{5.2.8}$$

where the derivatives of $U$ may be understood as $c$-numbers (evaluated at $x = 0$, and the given time $t$ ), so that we may write

$$[\hat{p}_x, U(\hat{x}, t)] = \sum_{k=0}^{\infty} \frac{1}{k!}\frac{\partial^k U}{\partial\hat{x}^k}\left[\hat{p}_x, \hat{x}^k\right] = \sum_{k=0}^{\infty} \frac{1}{k!}\frac{\partial^k U}{\partial\hat{x}^k}(\hat{p}_x\underbrace{\hat{x}\hat{x}\ldots\hat{x}}_{k\text{ times}} - \underbrace{\hat{x}\hat{x}\ldots\ldots\hat{x}}_{k\text{ times}}\hat{p}_x) \tag{5.2.9}$$

Applying Eq. (25) $k$ times to the last term in the parentheses, exactly as we did it in Eq. (26), we get

$$[\hat{p}_x, U(\hat{x}, t)] = -\sum_{k=1}^{\infty} \frac{1}{k!}\frac{\partial^k U}{\partial\hat{x}^k}ik\hbar\hat{x}^{k-1} \equiv -i\hbar\sum_{k=1}^{\infty} \frac{1}{(k-1)!}\frac{\partial^k U}{\partial\hat{x}^k}\hat{x}^{k-1}. \tag{5.2.10}$$

But the last sum is just the Taylor expansion of the derivative $\partial U/\partial x$. Indeed,

$$\frac{\partial U}{\partial \hat{x}}=\sum_{k'=0}^{\infty} \frac{1}{k'!} \frac{\partial^{k'}}{\partial \hat{x}^{k'}}\left(\frac{\partial U}{\partial \hat{x}}\right) \hat{x}^{k'}=\sum_{k'=0}^{\infty} \frac{1}{k'!} \frac{\partial^{k'+1} U}{\partial \hat{x}^{k'+1}} \hat{x}^{k'}=\sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{\partial^{k} U}{\partial \hat{x}^{k}} \hat{x}^{k-1} \tag{5.2.11}$$

where at the last step the summation index was changed from $k$ ' to $k-1$ . As a result, we may rewrite Eq. (5.32b) as

$$\left[\hat{p}_{x}, U(\hat{x}, t)\right]=-i \hbar \frac{\partial}{\partial \hat{x}} U(\hat{x}, t), \tag{5.2.12}$$

so that Eq. (30) yields:

$$\frac{d \hat{p}_{x}}{d t}=-\frac{\partial}{\partial \hat{x}} U(\hat{x}, t) \tag{5.2.13}$$

This equation also coincides with the classical equation of motion! Moreover, averaging Eqs. (29) and (35) over the initial state (as Eq. (4.191) prescribes), we get similar results for the expectation values: :[15]

$$\frac{d\langle x\rangle}{d t}=\frac{\left\langle p_{x}\right\rangle}{m}, \quad \frac{d\left\langle p_{x}\right\rangle}{d t}=-\left\langle\frac{\partial U}{\partial x}\right\rangle. \tag{5.2.14}$$

However, it is important to remember that the equivalence between these quantum-mechanical equations and similar equations of classical mechanics is superficial, and the degree of the similarity between the two mechanics very much depends on the problem. As one extreme, let us consider the case when a particle's state, at any moment between $t_{0}$ and $t$, may be accurately represented by one, relatively $p_{x}$-narrow wave packet. Then we may interpret Eqs. (36) as the equations of the essentially classical motion of the wave packet's center, in accordance with the correspondence principle. However, even in this case, it is important to remember the purely quantum mechanical effects of non-zero wave packet width and its spread in time, which were discussed in Sec. 2.2.

As an opposite extreme, let us revisit the "leaky" potential well discussed in Sec. $2.5-$ see Fig. 2.15. Since both the potential $U(x)$ and the initial wavefunction of that system are symmetric relative to point $x=0$ at all times, the right-hand sides of both Eqs. (36) identically equal zero. Of course, the result they predict (that the average values of the coordinate and the momentum stay equal to zero at all times) is correct, but this fact does not tell us much about the rich dynamics of the system: the finite lifetime of the metastable state, the formation of two wave packets, their waveform and propagation speed (see Fig. $2.17$), and about the insights the full solution gives for the quantum measurement theory and the system's irreversibility. Another similar example is the energy band theory (Sec. 2.7), with its purely quantum effect of the allowed energy bands and forbidden energy gaps, of which Eqs. (36) give no clue.

To summarize, the Ehrenfest theorem is important as an illustration of the correspondence principle, but its predictive power should not be exaggerated.

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[15] The equation set (36) constitutes the Ehrenfest theorem, named after its author, P. Ehrenfest.

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