Chapter 6 Ehrenfest's Theorem

The telephone wouldn't shut up so he snapped the receiver from the wall. He could smell the booze through the telephone wires. No one said a word. After an eternity, the blond voice on the other end whispered "Ehrenfest...." He listened to the monotone humm that had lost the smell of cheap gin for a second eternity before he emptily laid the receiver in its cradle, and retreated staggering for his own bottle of whiskey.[1].

The Classical Limit

Classical mechanics is successful at predicting results in the classical realm. Since it is so successful, we expect quantum mechanics to give the same results as classical mechanics in the classical regime. The usual explanation of how this occurs is Bohr's correspondence principle, which states in the limit of large quantum numbers, the relations of quantum mechanics reduce to the relations of classical mechanics. Paul Ehrenfest originated a different answer. Erhenfest said replace the dynamical variables of classical mechanics with the expectation values of quantum mechanics and you get the same relations.

Derivation of Ehrenfest's Theorem

Start with the expectation value of a time independent operator,

$$<\mathcal{A}> = <\psi|\,\mathcal{A}\,|\psi>,$$

and take a time derivative. The wave function is assumed to be a function of time, so using the chain rule to take the derivative, we have

$$\frac{d}{dt}<\mathcal{A}> = <\dot{\psi}|\,\mathcal{A}\,|\psi> + <\psi|\,\dot{\mathcal{A}}\,|\psi> + <\psi|\,\mathcal{A}\,|\dot{\psi}>\,.$$

Since the operator is assumed to be time independent, the middle term is zero so the time derivative reduces to

$$\frac{d}{dt}<\mathcal{A}> = <\dot{\psi}|\,\mathcal{A}\,|\psi> + <\psi|\,\mathcal{A}\,|\dot{\psi}>\,. \qquad (6-1)$$

The Schrodinger equation is

$$\mathcal{H}\,|\psi> = i\hbar|\dot{\psi}> \;\;\Rightarrow\;\; |\dot{\psi}> = \frac{1}{i\hbar}\mathcal{H}\,|\psi> = -\frac{i}{\hbar}\mathcal{H}\,|\psi>\,.$$

Forming the adjoint of the last relation,

$$<\dot{\psi}| = <\psi|\,\mathcal{H}^{\dagger}\left(\frac{i}{\hbar}\right),$$

and since the Hamiltonian is Hermitian, this is

$$<\dot{\psi}| = \frac{i}{\hbar}<\psi|\,\mathcal{H}.$$

[1] Mickey Spillane, *Physics on the Streets* (Publisher, Location, Year), page.

Using these in equation (6–1),

$$\begin{aligned}\frac{d}{dt}<\mathcal{A}> &= \frac{i}{\hbar}<\psi|\,\mathcal{H}\,\mathcal{A}\,|\psi> - \frac{i}{\hbar}<\psi|\,\mathcal{A}\,\mathcal{H}\,|\psi> \\ &= \frac{i}{\hbar}\left(<\psi|\,\mathcal{H}\,\mathcal{A}\,|\psi> - <\psi|\,\mathcal{A}\,\mathcal{H}\,|\psi>\right) \\ &= \frac{i}{\hbar}<\psi|\left[\mathcal{H},\mathcal{A}\right]|\psi> \\ &= \frac{i}{\hbar}<\left[\mathcal{H},\mathcal{A}\right]> \qquad (6-2)\end{aligned}$$

which is Ehrenfest's theorem.

Canonical Commutation Relations

A commutator which is equivalent to multiplication by the factor $i\hbar$ *is called a* **canonical commutator**, *i.e.*, if

$$\left[\mathcal{A},\,\mathcal{B}\right] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A} = i\hbar,$$

then $\left[\mathcal{A}\,,\mathcal{B}\right]$ is a canonical commutation relation. Realize $i\hbar \to i\hbar\mathcal{I}$ in more than one dimension. The **fundamental canonical commutator**[2], which is included in postulate 2, is

$$\left[\mathcal{X},\,\mathcal{P}\right] = i\hbar. \qquad (6-3)$$

Note that if the order of the operators is reversed, we have the negative of equation (6–3), *i.e.*, $\left[\mathcal{P},\,\mathcal{X}\right] = -i\hbar$. Again, $-i\hbar\mathcal{I}$ is often implied.

Example 6–1: Show $\left[\mathcal{X},\,\mathcal{P}\right] = i\hbar$ in position space.

The commutator is an operator so we give it an arbitrary function in position space, $f(x)$, on which to operate, so

$$\begin{aligned}\left[\mathcal{X},\,\mathcal{P}\right]f(x) &= \left(\mathcal{X}\,\mathcal{P} - \mathcal{P}\,\mathcal{X}\right)f(x) \\ &= \mathcal{X}\,\mathcal{P}\,f(x) - \mathcal{P}\,\mathcal{X}\,f(x).\end{aligned}$$

In chapter 5, we used postulate 2 to derive the form of the position and momentum operators in position space. Using these results for a one dimensional case, specifically equations (5–36) and (5–39), the position/momentum commutator is

$$\left[\mathcal{X},\,\mathcal{P}\right]f(x) = (x)\left(-i\hbar\frac{d}{dx}\right)f(x) - \left(-i\hbar\frac{d}{dx}\right)x\,f(x)$$

where we need to use the chain rule to evaluate the last term. Differentiating,

$$\left[\mathcal{X},\,\mathcal{P}\right]f(x) = \cancel{-i\hbar\,x\frac{d\,f(x)}{dx}} + i\hbar\,f(x) + \cancel{i\hbar\,x\frac{d\,f(x)}{dx}} = i\hbar\,f(x).$$

Since $f(x)$ is an arbitrary function, the effect of the the commutator is

$$\left[\mathcal{X},\,\mathcal{P}\right] = i\hbar.$$

[2] Cohen-Tannoudji, *Quantum Mechanics* (John Wiley & Sons, New York, 1977), pp 149 – 151.

Note that since a commutator is an operator, the identity matrix is implied with the scalar on the right, *i.e.*

$$\left[\mathcal{X},\, \mathcal{P}\right] = i\hbar\mathcal{I}.$$

Were we to use the relations of equation (5–40) in momentum space, we would attain the same result for momentum space. Equation (6–3) is, in fact, basis independent.

Example 6–2: Calculate $<\dot{\mathcal{X}}>$.

We can calculate $<\dot{\mathcal{X}}>$ using Ehrenfest's theorem, which for the choice of $\mathcal{X}$ as the operator of interest, is

$$<\dot{\mathcal{X}}> = \frac{i}{\hbar} < \left[\mathcal{H},\, \mathcal{X}\right]>,$$

where we need an explicit form of a Hamiltonian. We use a Hamiltonian for a particle, which is

$$\mathcal{H} = \frac{\mathcal{P}^2}{2m} + \mathcal{V}\left(\mathcal{X}\right),$$

$$\begin{aligned} \Rightarrow\ <\dot{\mathcal{X}}> &= \frac{i}{\hbar} < \left[\frac{\mathcal{P}^2}{2m} + \mathcal{V}\left(\mathcal{X}\right), \mathcal{X}\right]> \\ &= \frac{i}{\hbar} < \left[\frac{\mathcal{P}^2}{2m}, \mathcal{X}\right] + \left[\mathcal{V}\left(\mathcal{X}\right), \mathcal{X}\right]>, \end{aligned}$$

We further assume $\mathcal{V}\left(\mathcal{X}\right)$ will be some function which is powers of $\mathcal{X}$, such as $\frac{1}{2}k\mathcal{X}^2$, or $e^{-\alpha\mathcal{X}}$. The significance of this assumption is that $\mathcal{V}\left(\mathcal{X}\right)$ will commute with $\mathcal{X}$. The second commutator in the expectation value is zero, so the time derivative is

$$\begin{aligned} <\dot{\mathcal{X}}> &= \frac{i}{\hbar} < \left[\frac{\mathcal{P}^2}{2m}, \mathcal{X}\right]> \\ &= \frac{i}{2m\hbar} < \left[\mathcal{P}^2, \mathcal{X}\right]> . \end{aligned} \qquad (6-4)$$

Evaluating the commutator in equation (6–4),

$$\begin{aligned} \left[\mathcal{P}^2, \mathcal{X}\right] &= \mathcal{P}^2\mathcal{X} - \mathcal{X}\mathcal{P}^2 \\ &= \mathcal{P}\mathcal{P}\mathcal{X} - \mathcal{X}\mathcal{P}\mathcal{P}. \end{aligned}$$

We are going to add zero, in a form convenient to us, with the intent of putting the last expression in some form related to the fundamental commutator. In other words, if we add and subtract $\mathcal{P}\mathcal{X}\mathcal{P}$, the last commutator becomes

$$\begin{aligned} \left[\mathcal{P}^2, \mathcal{X}\right] &= \mathcal{P}\mathcal{P}\mathcal{X} - \mathcal{X}\mathcal{P}\mathcal{P} + \mathcal{P}\mathcal{X}\mathcal{P} - \mathcal{P}\mathcal{X}\mathcal{P} \\ &= \mathcal{P}\mathcal{P}\mathcal{X} - \mathcal{P}\mathcal{X}\mathcal{P} + \mathcal{P}\mathcal{X}\mathcal{P} - \mathcal{X}\mathcal{P}\mathcal{P} \\ &= \mathcal{P}\Big(\mathcal{P}\mathcal{X} - \mathcal{X}\mathcal{P}\Big) + \Big(\mathcal{P}\mathcal{X} - \mathcal{X}\mathcal{P}\Big)\mathcal{P} \\ &= \mathcal{P}\Big[\mathcal{P},\, \mathcal{X}\Big] + \Big[\mathcal{P},\, \mathcal{X}\Big]\mathcal{P} \\ &= \mathcal{P}\big(-i\hbar\big) + \big(-i\hbar\big)\mathcal{P} = -2i\hbar\mathcal{P}. \end{aligned}$$

Using this in equation (6–4),

$$<\dot{\mathcal{X}}> = \frac{i}{2m\hbar} <\big(-2i\hbar\mathcal{P}\big)> = \frac{i}{2m\hbar}\big(-2i\hbar\big) <\mathcal{P}> = \frac{<\mathcal{P}>}{m}.$$

The result of example (6–2) says the expectation value of time rate of change of the position operator is equal to the expectation value of the momentum operator divided by mass. In position space, this is

$$\int_{-\infty}^{\infty} \psi^*(x)\left(\frac{dx}{dt}\right)\psi(x)\,dx = \int_{-\infty}^{\infty} \psi^*(x)\frac{1}{m}\left(-i\hbar\frac{d}{dx}\right)\psi(x)\,dx.$$

In momentum space, the result is

$$\int_{-\infty}^{\infty} \widehat{\psi}^*(p)\left(\frac{d}{dt}\right)\left(i\hbar\frac{d}{dp}\right)\widehat{\psi}(p)\,dp = \int_{-\infty}^{\infty} \widehat{\psi}^*(p)\frac{1}{m}(p)\widehat{\psi}(p)\,dp.$$

Example 6–3: Using a Gaussian wave packet, evaluate the expectation value of the time rate of change of the position operator in position space.

In chapter 6 we found the normalized Gaussian wave packet is

$$\psi(x) = \frac{e^{ip_0x/\hbar}e^{-x^2/2\triangle^2}}{(\pi\triangle^2)^{1/4}}.$$

Using the above expression for the expectation value of the time rate of change of the position operator in position space, we have

$$\begin{aligned} <\dot{\mathcal{X}}> &= \frac{-i\hbar}{m}\int_{-\infty}^{\infty} \frac{e^{-ip_0x/\hbar}e^{-x^2/2\triangle^2}}{(\pi\triangle^2)^{1/4}}\left(\frac{d}{dx}\right)\frac{e^{ip_0x/\hbar}e^{-x^2/2\triangle^2}}{(\pi\triangle^2)^{1/4}}\,dx \\ &= \frac{-i\hbar}{m\triangle\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-ip_0x/\hbar}e^{-x^2/2\triangle^2}\left(\frac{d}{dx}\right)e^{ip_0x/\hbar}e^{-x^2/2\triangle^2}\,dx. \end{aligned}$$

The derivative is

$$\frac{d}{dx}\left(e^{ip_0x/\hbar}e^{-x^2/2\triangle^2}\right) = \frac{ip_0}{\hbar}e^{ip_0x/\hbar}e^{-x^2/2\triangle^2} - \frac{x}{\triangle^2}e^{ip_0x/\hbar}e^{-x^2/2\triangle^2}.$$

Using this, the integral becomes

$$\begin{aligned} <\dot{\mathcal{X}}> &= \frac{-i\hbar}{m\triangle\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-ip_0x/\hbar}e^{-x^2/2\triangle^2}\left(\frac{ip_0}{\hbar}e^{ip_0x/\hbar}e^{-x^2/2\triangle^2} - \frac{x}{\triangle^2}e^{ip_0x/\hbar}e^{-x^2/2\triangle^2}\right)dx \\ &= \frac{-i\hbar}{m\triangle\sqrt{\pi}}\frac{ip_0}{\hbar}\int_{-\infty}^{\infty} e^{-x^2/\triangle^2}\,dx + \frac{i\hbar}{m\triangle\sqrt{\pi}}\frac{1}{\triangle^2}\int_{-\infty}^{\infty} x\,e^{-x^2/\triangle^2}\,dx \\ &= \frac{p_0}{m\triangle\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-x^2/\triangle^2}\,dx + \frac{i\hbar}{m\triangle^3\sqrt{\pi}}\int_{-\infty}^{\infty} x\,e^{-x^2/\triangle^2}\,dx. \end{aligned}$$

The second integrand is the product of an odd and even function, so is an odd function. The integral of an odd function evaluated between symmetric limits is zero, so the second integral is zero. The first integral is Gaussian, so can be evaluated using the result of example 6–3, for $a = 1/\triangle^2$. The first integral is $\sqrt{\pi\triangle^2} = \triangle\sqrt{\pi}$. The expectation value then, is

$$< \dot{\mathcal{X}} > = \frac{p_0}{m\triangle\sqrt{\pi}}\triangle\sqrt{\pi} = \frac{p_0}{m} = \frac{mv_0}{m} = v_0,$$

which you should recognize from introductory physics.

Example 6–3 amplifies the fact the objects $\mathcal{X}$ and $\mathcal{P}$ in the equation

$$< \dot{\mathcal{X}} > = \frac{< \dot{\mathcal{P}} >}{m}$$

are operators. You need to establish a representation in a basis where the operators may be evaluated. Example 6–3 further illustrates the usefulness of having a reasonable form, a Gaussian form, for a wave packet. Remember, if the wave packet is Gaussian in position space, it is also Gaussian in momentum space. We expect the arguments and normalization constants to change when we did the Fourier transform to attain the Gaussian wave packet in momentum space. Nevertheless, were we to do the calculation in momentum space, it would look much the same as example 6–3, because we would have a Gaussian wave function in momentum space also.

Contrast with Hamilton's Equations

Hamilton's equations of classical mechanics are[3]

$$\dot{x} = \frac{\partial H}{\partial p} \qquad \text{and} \qquad \dot{p} = -\frac{\partial H}{\partial x}.$$

In calculation similar to example (6–2), we can find the quantum mechanical equivalents,

$$< \dot{\mathcal{X}} > = < \frac{\partial \mathcal{H}}{\partial \mathcal{P}} > \qquad \text{and} \qquad < \dot{\mathcal{P}} > = < -\frac{\partial \mathcal{H}}{\partial \mathcal{X}} >$$

The similarity is striking. The quantum mechanical equivalents say the center of mass of the wave packet follows the classical equations of motion. Another way of saying the same thing is the motion looks classical when we can replace the expectation value with the mean value of x and p, or

$$< \frac{\partial \mathcal{H}}{\partial \mathcal{A}} > \approx \frac{\partial H}{\partial A}\bigg|_{x_0,\ p_0},$$

where x_0 is the location of the center of the wave packet, and p_0 is the central momentum of the wave packet. For a particle modelled by a wave packet, these statements are *usually* applicable.

Applicability of Ehrenfest's Theorem

Ehrenfest's theorem is applicable when a classical force is uniform over the width of the particle wave packet. Classically,

$$F = -\frac{d}{dx}V(x).$$

[3] Goldstein, *Classical Mechanics* (Addison–Wesley Publishing Company, Reading, Massachusetts, 1980), pp 339 – 343.

Also in classical terms, if the packet is large and the potential varies over that width, the derivatives at various locations also varies, as illustrated in figure 6–1.

Figure 6 – 1. A Large Wave Packet over a Varying Potential.

If the wave packet is small compared to the variation in the potential, as illustrated in figure 6–2, the particle feels a uniform force and Ehrenfest's theorem applies.

Figure 6 – 2. A Small Wave Packet over a Varying Potential.