# Phys 486 Discussion 6 – Ehrenfest's Theorem

Below is a summary of the axioms of QM from this week's lectures. The axioms will be revised a bit when we introduce more mathematics, and a 6th axiom will be added when we learn about multiple identical particles.

• **STATE** axiom: A particle's state is described by a complex-valued **wavefunction** $\psi(x, t)$ that is **normalized** so that the probability of finding the particle *somewhere* is 1:

$$1 = \int_{-\infty}^{+\infty} |\psi(x,t)|^2 \, dx \,, \qquad \text{which requires that } \psi(x,t) \text{ goes to zero at } x = \pm\infty \text{ faster than } \frac{1}{\sqrt{x}} \,.$$

• **PROBABILITY** axiom: The magnitude squared of the wavefunction, $|\psi|^2 \equiv \psi^*\psi$, represents the **probability** $P(x, t)$ of finding the particle at location $x$ at a particular time $t$ :

$$P(x,t)\, dx \;=\; |\psi(x,t)|^2 \, dx \;\equiv\; \psi^*(x,t)\, \psi(x,t)\, dx$$

Further, when we measure a dynamical property $Q$ of the particle at a particular time $t$, the **expectation value** $\langle Q \rangle$ ≡ the **average value** that we will obtain is

$$\langle Q(t) \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t)\; \hat{Q} \;\; \psi(x,t)\, dx$$

• **OBSERVABLES** axiom: Each **dynamical[1] property** $Q$ of a particle is associated with an **operator** $\hat{Q}$ that acts on $\psi$. The position and momentum, from which all others can be built, are:

$$\hat{x} = x \,, \quad \hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

The **eigenstates**[2] of $\hat{Q}$ (notation: $\psi_q$) are the only states with **definite** $Q$, i.e. the only states where the observable $Q$ has a <u>specific, unique value</u>, which is the **eigenvalue** $q$. For all other states, *any* eigenvalue of $\hat{Q}$ can be measured, with a probability distribution $P(q)$ that can be calculated from the wavefunction (coming up).

• **MEASUREMENT** axiom: If we measure a dynamical property $Q$ of a system, the only values that we can obtain are the **eigenvalues** $q$ of the associated operator $\hat{Q}$. Once a particular value $q$ has been measured, the state of the system changes instantaneously into the **eigenstate** $\psi_q$.

• **TIME EVOLUTION** axiom: The wavefunction $\psi(x,t)$ of a non-relativistic particle of mass $m$ in a potential-energy field $V(x)$ evolves with time according to the **Schrödinger Equation** (**SE**) :

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \,, \qquad \text{or using operator symbols,} \quad \boxed{i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\, \psi} \; = \left( \frac{\hat{p}^2}{2m} + V \right) \psi$$

where $H = T + V$ is the particle's Hamiltonian.

**Problem 1 : Ehrenfest's Theorem**

**Ehrenfest's Theorem** is a hugely important result of the QM axioms :

| |
|---|
| Expectation Values Obey Classical Laws. |

Wow! We must explore this further! The theorem has multiple incarnations, all of which are important.

---

[1] A <u>dynamical property</u> is one that can change with time. These are the properties that have operators in QM. In contrast, an intrinsic property is one that can never change, like a particle's mass or charge; these are *not* associated with any operators in QM.

[2] In case you have forgotten, the <u>definition</u> of an eigenstate $\psi_q$ of an operator $\hat{Q}$ is: $\boxed{\hat{Q}\psi_q = q\psi_q}$, where $q$ is the eigenvalue.

(a) First, you need to do some calculus. Using Schrödinger's equation, show this important result :

$$i\hbar\frac{\partial}{\partial t}\left[\psi^*\psi\right] = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left[\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right] + (V - V^*)\,\psi^*\psi$$

It is really useful for several derivations but requires a non-trivial amount of work. Also, for the subsequent calculations, assume that **the potential energy *V* is real**. This removes the second term above. We will treat other cases soon enough, but for now, only consider real potential energies.

(b) Now consider the **expectation value of position** for a wavefunction $\psi$ :

$$\langle x(t)\rangle = \int_{-\infty}^{+\infty}\psi^*(x,t)\;x\;\psi(x,t)\,dx$$

This is the **average** position you would obtain if you prepared a huge ensemble of particles, each in state $\psi(x, t)$, and measured the position of each one at time $t$. <x> is the statistical average of all those position measurements. OK, so now let's try building an **expectation value for speed** : <v> = d<x>/dt. Using integration-by-parts show that

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\int_{-\infty}^{+\infty}\left[\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right]dx$$

(c) Using one more integration-by-parts, and the fact that all normalizable wavefunctions go to zero at infinity (see axiom 2) show that

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{m}\int_{-\infty}^{+\infty}\psi^*\frac{\partial\psi}{\partial x}\,dx = \frac{\langle p\rangle}{m} \quad\rightarrow\quad \text{Ehrenfest incarnation \#1 : } \boxed{\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}}$$

This is very nice indeed! The **expectation = average values** of momentum and position do indeed behave like their classical counterparts! ☺

(d) Now use the various tricks you have amassed to prove this :

$$\text{Ehrenfest incarnation \#2 : } \boxed{\frac{d\langle p\rangle}{dt} = \left\langle -\frac{dV}{dx}\right\rangle}$$

That is Newton's EOM "*F* = *dp* / *dt* " reincarnated using expectation values! Very nice. ☺

▶ **FYI #1**: A third incarnation can be found in Problem 4.20 of Griffith's book, namely the torque law:

$$\text{Ehrenfest incarnation \#3 : } \boxed{\frac{d\langle\vec{L}\rangle}{dt} = \langle\vec{r}\times-\vec{\nabla}V\rangle}.$$

▶ **FYI #2**: There is an exceedingly important **generalization** of Ehrenfest's theorem(s) that applies to *any* quantum observable *Q*. We will need it in a while to search for a system's <u>constants of motion</u> :

$$\text{Generalized Ehrenfest : } \boxed{\frac{d\langle Q\rangle}{dt} = \frac{1}{i\hbar}\langle[Q,H]\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle}$$

( Apparently this was proved by Heisenberg, but I've only ever heard it called "Ehrenfest's Theorem". )
This formula is our first encounter with the **commutator** of two operators : $\left[\hat{Q},\hat{H}\right] \equiv \hat{Q}\hat{H} - \hat{H}\hat{Q}$ .
Commutators play a crucial role in quantum mechanics, and one of those crucial roles is this formula!