Lecture 15 Physics 342

Welcome to Friday lecture! Please turn in homework and prepare yourself for physics.

In the previous couple of lectures, we have studied the infinite square well and its properties. Last lecture, we had studied the Heisenberg uncertainty principle for energy eigenstates and compared its features to classical probabilities of a particle stuck in a perfectly elastic box. This comparison motivated the understanding of the correspondence principle, which provided the concrete connection between quantum mechanics and its classical mechanics limit. This correspondence principle can be stated in many ways, but a particularly compact way is that:

In the limit of $\hbar \to 0$, the predictions of quantum mechanics reduce to those of classical mechanics.

Near the end of this course we will provide the sharpest statement of the correspondence principle.

In this lecture, we will introduce other features of quantum mechanics, using the infinite square well as our handrail. We assumed, through the axioms of quantum mechanics that probability is conserved which had the consequence that linear operators on the Hilbert space of states are unitary. Through identification of the Hamiltonian as the Hermitian operator that implements time evolution, we were lead to the Schrödinger equation, Ehrenfest's Theorem, and other results. The Schrödinger equation, for all of its virtues, has one glaring, awkward vice: it describes the time evolution of the wavefunction, which is only a probability amplitude, and not an actual, observable, probability. Can we use the formalism we have developed to determine how honest probabilities evolve in time? Then, with the infinite square well, can we understand the physical consequence of this time evolution?

Expressed ~~as~~ in ~~the~~ terms of the wavefunction $\psi(x)$, the probability density of a quantum system is

$$\rho(x) = \psi^*(x)\psi(x),$$ where I have suppressed

possible time dependence for now. This probability density is still a function of position x, and not just a single number. So, if we want to express this probability density in Dirac notation, we would not write it as

$$\rho(x) \neq \langle \psi | \psi \rangle = \int dx\, \psi^* \psi = 1,$$

which is not a function of position, because we ~~the~~ integrated over position. Okay, if the probability density is not the inner product of the state $|\psi\rangle$ with itself, what could it be? The only other operation we can perform with a bra $\langle\psi|$ and a ket $|\psi\rangle$ is the outer product. Therefore, the probability density must be the outer product:

$$\rho = |\psi\rangle\langle\psi| .$$

This argument is a good example of a "what else could it be?" proof in physics. If you have two options and one is eliminated, it must be the other option!

So, how does ρ evolve in time? That is, we would like to identify a differential equation in time for ρ. To do this, we do the usual Taylor expansion / time evolution trick. First if ρ is a function of time and we move forward in time by Δt, we have:

$$\rho(t+\Delta t) = \rho(t) + \Delta t \frac{\partial}{\partial t}\rho(t) + \mathcal{O}(\Delta t^2).$$

On the other hand, we can also just evolve the state $|\psi\rangle$ forward in time with the the Hamiltonian. That is:

$$|\psi\rangle\langle\psi| \to e^{\frac{-i\hat{H}\Delta t}{\hbar}} |\psi\rangle\langle\psi| e^{\frac{+i\hat{H}\Delta t}{\hbar}}$$

$$\cong \left(1 - \frac{i\hat{H}\Delta t}{\hbar} + \dots\right)|\psi\rangle\langle\psi|\left(1 + i\frac{\hat{H}\Delta t}{\hbar} + \dots\right)$$

$$= |\psi\rangle\langle\psi| - \frac{i\hat{H}\Delta t}{\hbar}|\psi\rangle\langle\psi| + |\psi\rangle\langle\psi|\frac{i\hat{H}\Delta t}{\hbar} + \dots$$

$$= |\psi\rangle\langle\psi| - \frac{i\Delta t}{\hbar}\left[\hat{H}, |\psi\rangle\langle\psi|\right] + \dots$$

Recall that the outer product of two vectors produced a matrix; i.e., a linear operator. Thus the commutator makes sense. Setting the two sides of the equation equal to one another, we find:

$$\rho + \Delta t \frac{\partial \rho}{\partial t} = |\psi\rangle\langle\psi| - \frac{i\Delta t}{\hbar}[\hat{H}, |\psi\rangle\langle\psi|], \text{ or}$$

identifying $\rho = |\psi\rangle\langle\psi|$, that

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}, |\psi\rangle\langle\psi|\right] = -\frac{i}{\hbar}[\hat{H}, \rho].$$

We'll come back to this equation at the end of this course, but it is called the Lindblad equation.

We can make further sense of this equation by expressing the Hamiltonian $\hat{H}$ on Hilbert space in terms of some explicit basis. Of course, the simplest basis is just the basis of energy eigenstates $|\psi_n\rangle$, for which

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle.$$

For the infinite square well, these energies are of course just:

$$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}$$

Then, we can express the Hamiltonian $\hat{H}$ as the outer product of energy eigenstates:

$$\hat{H} = \sum_n E_n |\psi_n\rangle\langle\psi_n|$$

Then, for this choice of basis, our time evolution of the probability density becomes:

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}\left(\hat{H}|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|\hat{H}\right)$$

$$= -\frac{i}{\hbar}\sum_n \left(E_n\langle\psi_n|\psi\rangle|\psi_n\rangle\langle\psi| - E_n\langle\psi|\psi_n\rangle|\psi\rangle\langle\psi_n|\right)$$

$$= -\frac{i}{\hbar}\sum_n E_n\left(\langle\psi_n|\psi\rangle|\psi_n\rangle\langle\psi| - \langle\psi|\psi_n\rangle|\psi\rangle\langle\psi_n|\right)$$

$$= \frac{2}{\hbar}\sum_n E_n \,\mathrm{Im}\left(\langle\psi_n|\psi\rangle|\psi_n\rangle\langle\psi|\right)$$

This can also be re~~ex~~expressed in terms of the position-dependent wave-function, if we note that

$\rho \to \psi^*\psi$, so that

$$\frac{\partial}{\partial t}(\psi^*\psi) = \frac{2}{\hbar}\sum_n E_n \,\mathrm{Im}\left[\left(\int dy\, \psi_n^*(y)\psi(y)\right)\psi_n(x)\psi^*(x)\right]$$

This formalism allows for some interesting analyses. First, the total probability of any state is of course 1 for all time, so the total probability must have vanishing time derivative. There is a nice way to calculate the inner product from the outer product. Given an outer product of some state $|\psi\rangle$: $|\psi\rangle\langle\psi|$, we can calculate its inner product through the trace, or sum of diagonal elements of the outer product matrix. That is, we can express $|\psi\rangle$ as a linear combination of energy eigenstates:

$|\psi\rangle = \sum_n \beta_n|\psi_n\rangle$, for some complex β_n, so that

$$|\psi\rangle\langle\psi| = \sum_{m,n}\beta_n^*\beta_m|\psi_m\rangle\langle\psi_n|$$

Then, note that the inner product calculated through the trace is:

$$\mathrm{tr}\left(|\psi\rangle\langle\psi|\right) = \sum_n \beta_n^* \beta_n |\psi_n\rangle\langle\psi_n| = \sum_n |\beta_n|^2 = 1,$$

as required if $\langle\psi|\psi\rangle = 1$.

With this insight, let's take the trace of the Lindblad equation:

$$\frac{d}{dt}\mathrm{tr}(\rho) = -\frac{i}{\hbar}\mathrm{tr}\left(\hat{H}|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|\hat{H}\right)$$

$$= -\frac{i}{\hbar}\left(\langle\psi|\hat{H}|\psi\rangle - \langle\psi|\hat{H}|\psi\rangle\right) = 0,$$

so, indeed, $\mathrm{tr}\,\rho = 1$ is time-independent, which is good!

Another thing we can do is a partial trace: only sum over a subset of the diagonal elements of $|\psi\rangle\langle\psi|$. This is much more interesting than a complete trace. Recall that, given a complete set of orthonormal basis ~~the~~ states $\{|\psi_n\rangle\}$ can be completely summed to produce the identity matrix:

$$\mathbb{I} = \sum_{\text{all } m} |\psi_m\rangle\langle\psi_m|$$

For a matrix $\mathbb{M}$, of course its trace is identical if multiplied by $\mathbb{I}$ or not:

$$\mathrm{tr}\,\mathbb{M} = \mathrm{tr}\,\mathbb{M}\mathbb{I}.$$

For an incomplete or partial trace, we simply subtract the basis states we don't want to sum over. For example, let's <u>not</u> include $|\psi_1\rangle$, the ground state in the trace. This is accomplished by subtracting $|\psi_1\rangle\langle\psi_1|$ from the identity:

$$\mathrm{tr}_{\mathbb{I}-|\psi_1\rangle\langle\psi_1|}\, \mathbb{M} = \mathrm{tr}\left(\mathbb{M}\left(\mathbb{I}-|\psi_1\rangle\langle\psi_1|\right)\right)$$

Let's see what doing this partial trace means for our Lindblad equation. First, we have

$$\mathrm{tr}\left(\rho\left(\mathbb{I}-|\psi_1\rangle\langle\psi_1|\right)\right) = \langle\psi|\psi\rangle - \langle\psi|\psi_1\rangle\langle\psi_1|\psi\rangle$$
$$= 1 - |\langle\psi|\psi_1\rangle|^2.$$

The right side of Lindblad is:

$$-\frac{i}{\hbar}\,\mathrm{tr}\left[\left(\hat{H}|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|\hat{H}\right)\left(\mathbb{I}-|\psi_1\rangle\langle\psi_1|\right)\right]$$
$$= +\frac{i}{\hbar}\left[\langle\psi_1|\hat{H}|\psi\rangle\langle\psi|\psi_1\rangle - \langle\psi_1|\psi\rangle\langle\psi|\hat{H}|\psi_1\rangle\right]$$

$= 0$, because $|\psi_1\rangle$ is an eigenstate of $\hat{H}$. Actually,

if you subtract any energy eigenstate you just find 0; that is, the time evolution of $|\langle\psi_n|\psi\rangle|^2$ is 0; it remains unchanged from $t=0$.

This partial trace is much more interesting when we subtract a state that is not an energy eigenstate. Let's consider just a simple state that is a constant complex linear combination of the first two eigenstates:

$$|\chi\rangle = \alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle, \text{ such that } |\alpha_1|^2 + |\alpha_2|^2 = 1.$$

Now, the partial trace of ρ with this state is:

$$\mathrm{tr}\left(\rho\left(\mathbb{I}-|\chi\rangle\langle\chi|\right)\right)=\langle\psi|\psi\rangle-\langle\psi|\chi\rangle\langle\chi|\psi\rangle$$

$$=1-|\langle\psi|\chi\rangle|^2.$$

The right side is:

$$-\frac{i}{\hbar}\,\mathrm{tr}\left[\left(\hat{H}|\psi\rangle\langle\psi|-|\psi\rangle\langle\psi|\hat{H}\right)\left(\mathbb{I}-|\chi\rangle\langle\chi|\right)\right]$$

$$=+\frac{i}{\hbar}\left(\langle\chi|\hat{H}|\psi\rangle\langle\psi|\chi\rangle-\langle\chi|\psi\rangle\langle\psi|\hat{H}|\chi\rangle\right)$$

For arbitrary, complex α_1, α_2 (normalized appropriately) this is non-zero. You'll study this more in Homework, but this partial trace produces the time dependence equation:

$$\frac{\partial}{\partial t}|\langle\psi|\chi\rangle|^2=-\frac{i}{\hbar}\left(\langle\chi|\hat{H}|\psi\rangle\langle\psi|\chi\rangle-\langle\chi|\psi\rangle\langle\psi|\hat{H}|\chi\rangle\right)$$

$$=+\frac{2}{\hbar}\,\mathrm{Im}\left(\langle\chi|\hat{H}|\psi\rangle\langle\psi|\chi\rangle\right).$$

Next week, we'll move on to the harmonic oscillator...