

# Physics 342 Lecture 10

Okay, we've come a long way in the first three weeks from fundamental mathematical properties of linear operators to profound physical interpretation of it. We have developed the necessary background for finally deriving the fundamental equation of quantum mechanics, the Schrödinger equation.

Before our derivation, let's summarize our results thus far. Our summary will be important enough that we will refer to the following statements as the axioms of quantum mechanics:

Axiom 1: Observables (outcomes of physical experiment) correspond to Hermitian operators on a Hilbert space  $\mathcal{H}$ .

Axiom 2: The state of a system is represented by a wave function  $\psi$  on the Hilbert space  $\mathcal{H}$ , such that  $\langle \psi | \psi \rangle = 1$ .

Axiom 3: Expectation values of an observable corresponding to the Hermitian operator  $T$  on the state  $\psi$  is  $\langle \psi | T | \psi \rangle$ .

These axioms are called the Dirac-von Neumann axioms and, as we have discussed, their motivation lies firmly in linear algebra and analogy with probability axioms. Our goal in this lecture is to use these axioms, and our earlier results, to derive the fundamental equation of quantum mechanics.

Recall again what the fundamental goal of all of physics, nay, all of science is. The scientific method is to first make a hypothesis, motivated by all experimental data available thus far. Then, we test that hypothesis with new experimental data. Depending on the outcome of the experiment, we either modify our hypothesis, or gain confidence that ~~the~~ Nature works as our hypothesis suggests. As mentioned early in this class, there is a time ordering to the scientific method: we make a hypothesis in the present and test it in the future. Thus, our goal in physics is to predict how a system evolves forward in time, given data at the present.

Indeed, the fundamental equation of classical mechanics, Newton's second law, describes how the momentum of a system changes in time:

$$\vec{F} = \frac{d\vec{p}}{dt}$$

This is a differential equation in time can be solved for all future times  $t > 0$  given data of the momentum  $\vec{p}$  at  $t=0$ . If we know momentum (and position, etc.) at all times, we can definitively say we have "solved" the system. Our goal in quantum mechanics will be the same: we want the equation that governs time dependence of the wavefunction  $\psi(x,t)$ , as it is the wavefunction that ~~can~~ completely quantifies the physical state.

We have all of the pieces in place to do this. We want to figure out how the wavefunction  $\psi(x,t)$

transforms at a slightly later time:

$$\psi(x, t) \rightarrow \psi(x, t + \Delta t) = \psi(x, t) + \Delta t \frac{\partial}{\partial t} \psi(x, t) + \dots,$$

Where we have Taylor expanded on the right. We had earlier derived (well, really just motivated) that the energy/Hamiltonian operator  $\hat{H}$  translates forward in time. To translate an amount of time  $\Delta t$ , we act on  $\psi(x, t)$  with

$$U(\Delta t) = e^{-\frac{i\Delta t \hat{H}}{\hbar}}, \text{ so that}$$

$$\psi(x, t + \Delta t) = e^{-\frac{i\Delta t \hat{H}}{\hbar}} \psi(x, t) \approx \left(1 - \frac{i\Delta t \hat{H}}{\hbar}\right) \psi(x, t),$$

where again we Taylor expand to linear order in the time  $\Delta t$ . If these two expressions for  $\psi(x, t + \Delta t)$  are to equal one another, we must have that:

$$\frac{\partial}{\partial t} \psi(x, t) = -\frac{i\hat{H}}{\hbar} \psi(x, t), \text{ or, as it is usually written}$$

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi}$$

This is called the Schrödinger Equation, and describes the time evolution of the wavefunction  $\psi$  for a given Hamiltonian  $\hat{H}$  on a Hilbert space  $\mathcal{H}$ . It can be solved in generality in several ways; we'll consider one way here and another way later.

Throughout this course, we will, for simplicity, assume that the Hamiltonian is time-independent. Really, what this means in a basis independent way is that the eigenvalues of  $\hat{H}$  are independent of time.

Many interesting physical systems exhibit such a property, and this will allow us to express the Schrödinger equation in a more useful way. Assuming that the eigenvalues of the Hamiltonian  $\hat{H}$  are time independent, the eigenvalue equation for the Hamiltonian is:

$$\hat{H} \alpha_i(t) = E_i \alpha_i(t) = i\hbar \frac{\partial}{\partial t} \alpha_i(t), \text{ for an eigenfunction } \alpha_i(t),$$

and  $E_i$  is the energy eigenvalue of the Hamiltonian. With  $dE_i/dt = 0$ , the solution of this differential equation is:

$$\alpha_i(t) = \beta_i e^{-\frac{iE_i t}{\hbar}}, \text{ where } \beta_i \text{ is some constant complex number.}$$

As we mentioned a few lectures ago, we can always choose a time-independent basis in which to define the wavefunction  $|\psi\rangle$ , and with a time independent Hamiltonian, we have a natural basis in which to work. For a time-independent Hamiltonian  $\hat{H}$ , there exists a time-independent orthonormal, complete basis of functions  $\psi_i(x)$  such that

$$\hat{H} \psi_i(x) = E_i \psi_i(x), \text{ or } \hat{H} |\psi_i\rangle = E_i |\psi_i\rangle.$$

Then, a general wavefunction  $|\psi\rangle$  on Hilbert space can be written as:

$$|\psi\rangle = \sum_i \alpha_i(t) |\psi_i\rangle = \sum_i \beta_i e^{-\frac{iE_i t}{\hbar}} |\psi_i\rangle.$$

So, our problem of finding the wave function for all times  $t$  is reduced to solving for the time-independent eigensystem  $|\psi_i\rangle, E_i$ , where

$$\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle.$$

As an eigenvalue equation, we will typically drop the subscripts  $i$ . We will often also just consider the time-independent wavefunction (or  $t=0$  wavefunction) as:

$$|\psi(t=0)\rangle = \sum_i \beta_i |\psi_i\rangle, \text{ and the coefficients}$$

$\beta_i$  can be found through orthonormality of the  $|\psi_i\rangle$ :

$$\langle \psi_i | \psi(t=0) \rangle = \sum_j \beta_j \langle \psi_i | \psi_j \rangle = \sum_j \beta_j \delta_{ij} = \beta_i.$$

So, we can claim victory in completely solving a quantum system if we know all eigenvalues of  $\hat{H}$ . We sometimes colloquially say that our goal is to "diagonalize the Hamiltonian", as when the Hamiltonian only has non-zero elements on the diagonal, the elements on the diagonal are just the eigenvalues.

So, let's figure out what:  $\hat{H}|\psi\rangle = E|\psi\rangle$  means. In classical mechanics, the energy of a particle consists of two components: kinetic energy and potential energy. For a particle of mass  $m$ , its kinetic energy  $K$  is

$$K = \frac{1}{2}mv^2 = \frac{p^2}{2m}, \text{ where } p \text{ is the momentum of the particle.}$$

The potential energy  $U$  of a particle can depend on the particle's position  $x$ . We denote this as

$U = V(x)$ , and will often just refer to  $V(x)$  as the "potential" (dropping "energy" word).

Thus, the total energy classically is:

$$E = K + U = \frac{p^2}{2m} + V(x).$$

Quantum mechanically, energy is something that is measured as the outcome of experiment, so we need to interpret this "Kinetic + potential" as some Hermitian operator with appropriate energy eigenvalues. All we have to do in this case is to reinterpret the classical  $p$ , a coordinate or function on phase space, as a quantum operator,  $\hat{p}$ :

$$\begin{aligned} \hat{K} + \hat{U} &= \frac{\hat{p}^2}{2m} + V(x) = \frac{1}{2m} \left( -i\hbar \frac{\partial}{\partial x} \right)^2 + V(x) \\ &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x). \end{aligned}$$

All we have done here is replace  $p \rightarrow \hat{p} = -i\hbar \frac{\partial}{\partial x}$ . Thus, the time-independent, eigenvalue equation for the Hamiltonian  $\hat{H}$  can be expressed as a second-order differential equation:

$$\hat{H}|\psi\rangle = E|\psi\rangle \Rightarrow \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x) = E\psi(x).$$

In this class, we'll go back and forth from the differential formulation of the Hamiltonian to the more abstract operator form. Either way, the physical system of interest is completely specified by the form

of the potential,  $V(x)$ . In this course, we will study the free particle,  $V(x)=0$ , the harmonic oscillator,  $V(x)=\frac{1}{2}kx^2$ , the hydrogen atom,  $V(x)=-\frac{k}{x}$ , and these different potentials will produce different eigenstates and energy values. (We'll consider some other potentials, as well, and the hydrogen atom is a three-dimensional problem, which adds its own interesting complications.)

One thing to re-emphasize is that because the Hamiltonian is Hermitian, the Schrödinger equation preserves the normalization of the wave function  $\Psi(x,t)$  for all time. This was an assumption/axiom we used to derive the Schrödinger equation, and simply follows because general time evolution is implemented by the unitary operator

$$U(t) = e^{-\frac{i\hat{H}t}{\hbar}}$$

The Schrödinger equation is nothing more than the infinitesimal form of the action of  $U(t)$  on the wave function  $\Psi(x,t)$ . Indeed, consider the wave function at time  $t$ :

$$\Psi(x,t) = U(t) \Psi(x,t=0) = e^{-\frac{i\hat{H}t}{\hbar}} \Psi(x,t=0),$$

which assures that the Hamiltonian is time independent. We can just explicitly check that this solves the Schrödinger equation:

~~$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = i\hbar \frac{\partial}{\partial t} \left( e^{-\frac{i\hat{H}t}{\hbar}} \Psi(x,t=0) \right) = i\hbar \left( -\frac{i\hat{H}}{\hbar} \right) e^{-\frac{i\hat{H}t}{\hbar}} \Psi(x,t=0) = \hat{H} e^{-\frac{i\hat{H}t}{\hbar}} \Psi(x,t=0) = \hat{H} \Psi(x,t)$$~~

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = i\hbar \frac{\partial}{\partial t} e^{\frac{-it\hat{H}}{\hbar}} \psi(x, t=0) = i\hbar \left( -\frac{i\hat{H}}{\hbar} \right) e^{\frac{-it\hat{H}}{\hbar}} \psi(x, t=0)$$

$= \hat{H} \psi(x, t)$ , which is indeed the Schrödinger equation.

Thus, given an initial wave function  $\psi(x, t=0)$ , we can find the wave function at any later time by acting on it by  $U(t)$ :

$$\psi(x, t) = e^{\frac{-it\hat{H}}{\hbar}} \psi(x, t=0).$$

For now, this exact solution of the Schrödinger equation will be a novelty, but we'll come back to it later in the course.