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## Lecture 6

### *Time Evolution and the Schrödinger Equation*

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#### Assigned Reading:

E&R	3 <sub>all</sub> , 5 <sub>1,3,4,6</sub>
Li.	2 <sub>5-8</sub> , 3 <sub>1-3</sub>
Ga.	2 <sub>all≠4</sub>
Sh.	3, 4

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The Schrödinger equation is a partial differential equation. For instance, if

$$\hat{E} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2},$$

then the Schrödinger equation becomes

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{m\omega^2 x^2}{2} \psi.$$

Of course,  $\hat{E}$  depends on the system, and the Schrödinger equation changes accordingly.

To fully solve this for a given  $\hat{E}$ , there are a few different methods available, and those are through brute force, extreme cleverness, and numerical calculation. An elegant way that helps in all cases though makes use of superposition.

Suppose that at  $t = 0$ , our system is in a state of definite energy. This means that

$$\psi(x, 0; E) = \phi(x; E),$$

where

$$\hat{E}\phi(x; E) = E \cdot \phi(x; E).$$

Evolving it in time means that

$$i\hbar \frac{\partial \psi_E}{\partial t} = E \cdot \psi_E.$$

Given the initial condition, this is easily solved to be

$$\psi(x, t; E) = e^{-i\omega t} \phi(x; E)$$

through the de Broglie relation

$$E = \hbar\omega.$$

Note that

$$\mathbf{p}(x, t) = |\psi(x, t; E)|^2 = |\phi(x; E)|^2,$$

so the time evolution disappears from the probability density! That is why wavefunctions corresponding to states of definite energy are also called *stationary states*.

So are all systems in stationary states? Well, probabilities generally evolve in time, so that cannot be. Then are any systems in stationary states? Well, nothing is eternal, and like the plane wave, the stationary state is only an approximation. So why do we even bother with this?

The answer lies in superposition! If

$$\psi_n(x, t) = e^{-i\omega_n t} \phi_n(x)$$

solves the Schrödinger equation, then so does

$$\psi(x, t) = \sum_n c_n \psi_n(x, t) = \sum_n c_n e^{-i\omega_n t} \phi_n(x) \quad (0.1)$$

thanks to the linearity of that equation. This means that *any*  $\psi(x)$  at any time satisfying appropriate boundary conditions can be expressed as a superposition of energy eigenfunctions. But what do these energy eigenstates look like anyway? The answer depends on the particular form of  $\hat{E}$ , which depends on the system in question.

For example, let us consider a free particle. This means that

$$V(x) = 0,$$

so

$$\hat{E} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}.$$

We need to solve for the eigenfunctions given by

$$\hat{E}\phi_E = E \cdot \phi_E,$$

so

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi_E}{\partial x^2} = E \cdot \phi_E.$$

Making the substitution

$$k^2 \equiv \frac{2mE}{\hbar^2}$$

yields the general solution

$$\phi(x; E) = \alpha e^{ikx} + \beta e^{-ikx}$$

where  $\alpha$  and  $\beta$  are complex constant coefficients satisfying normalization.

Another way to get this would be through the knowledge that the eigenfunctions of  $\hat{p}$  are  $e^{ikx}$  and  $e^{-ikx}$ . Note that

$$E = \frac{\hbar^2 k^2}{2m}$$

is the energy of both the states  $e^{ikx}$  and  $e^{-ikx}$ . This is an example of a degeneracy: sometimes, different states happen to share the same eigenvalue for a particular observable operator.

Take note of the normalization: multiplying an eigenfunction by a constant leaves it still as an eigenfunction. We want to fix the normalization such that

$$\langle \phi_E | \phi_{E'} \rangle = \delta(E - E').$$

In the previous case, it makes sense to choose the normalization

$$\langle \phi_k | \phi_{k'} \rangle = \delta(k - k')$$

as  $k$  is continuous, so

$$\phi(x; k) = \frac{1}{\sqrt{2\pi}} e^{ikx}.$$

Continuing with that example,

$$E = \frac{\hbar^2 k^2}{2m}$$

implies that

$$\omega = \frac{\hbar k^2}{2m},$$

so the solution for all time is a traveling wave

$$\psi(x, t; E) = e^{i(kx - \omega t)}$$

disregarding normalization. Note that the phase velocity

$$v_p = \frac{\omega}{k} = \frac{\hbar k}{2m}$$

is half of the classical velocity of a free particle, while the group velocity

$$v_g = \frac{\partial \omega}{\partial k} = \frac{\hbar k}{m}$$

is exactly the classical velocity. In general, the group velocity is more representative of the classical velocity than is the phase velocity, as the group velocity is observable while the phase velocity is not.

Let us move on to an example of a nontrivial potential. The infinite square well, also known as the particle in a box, is an idealization of a large, deep potential. It is given by

$$V(x) = \{0 \text{ for } 0 \leq x \leq \ell, \infty \text{ otherwise}\}.$$

The implication of this is that

$$\mathbb{P}(x > \ell) = \mathbb{P}(x < 0) = 0,$$

implying that  $\psi(x) = 0$  outside of the box. Inside, we can use the energy eigenvalue equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi_E}{\partial x^2} = E \cdot \phi_E$$

and define

$$\hbar^2 k^2 \equiv 2mE$$

so that the solutions are

$$\phi(x; E) = A \sin(kx) + B \cos(kx).$$

The boundary conditions

$$\psi(0) = \psi(\ell) = 0$$

imply  $B = 0$  and

$$k\ell = \pi(n + 1),$$

so

$$k_n = \frac{\pi}{\ell}(n + 1).$$

This means that the allowed energies are

$$E_n = \frac{\pi^2 \hbar^2 (n + 1)^2}{2m\ell^2}.$$

Note that the energies are discrete, and that  $E_0 > 0$ , which is also thanks to the uncertainty principle. This is very different from a classical particle in a box! Also, the eigenfunctions are

$$\phi_n(x) = A_n \sin(k_n x),$$

and the time-evolved eigenfunctions are

$$\psi_n(x, t) = A_n e^{-\frac{iE_n t}{\hbar}} \sin(k_n x).$$

Note again that for energy eigenstates, the probability density

$$\mathbf{p}_n(x, t) = |\psi_n(x, t)|^2 = |A_n|^2 \sin^2(k_n x)$$

is independent of time. Also note the normalization requirement

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1$$

means that the coefficients are

$$A_n = \sqrt{\frac{2}{\ell}} e^{i\varphi}.$$

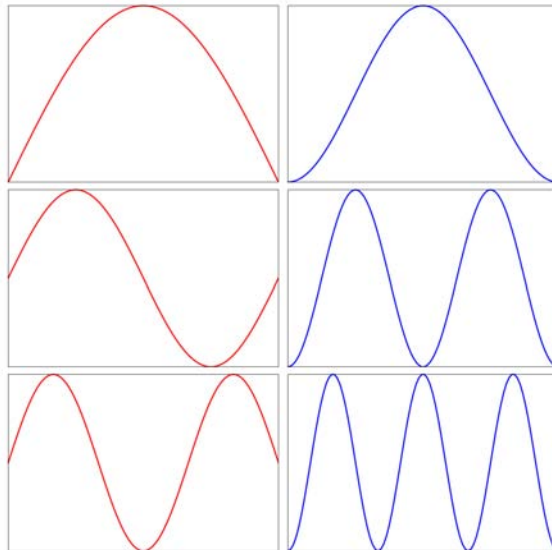


Figure 1: First, second, and third lowest-energy eigenfunctions (red) and associated probability densities (blue) for the infinite square well potential

Once again, the overall phase is not physical, so for convenience,  $\varphi = 0$ , so that

$$A_n = \sqrt{\frac{2}{\ell}}.$$

**Any good wavefunction  $\psi(x)$  at a given time  $t$  can be expanded in terms of the energy eigenfunctions  $\phi_n$  as**

$$\boxed{\psi(x) = \sum_n c_n \phi(x; n)} \quad (0.2)$$

for some  $c_n$ , where we normalize

$$\langle \phi_i | \phi_j \rangle = \int_{-\infty}^{\infty} \phi^*(x; i) \phi(x; j) dx = \delta_{ij} \quad (0.3)$$

so that the normalization

$$\langle \psi | \psi \rangle = \sum_{i,j} c_i^* c_j \delta_{ij} = \sum_j |c_j|^2 = 1 \quad (0.4)$$

holds for the wavefunction.

Going back to the example of the infinite square well, the eigenfunctions are

$$\phi(x; n) = \sqrt{\frac{2}{\ell}} \sin(k_n x)$$

with

$$k_n = \frac{\pi}{\ell}(n + 1),$$

so the expansion

$$\psi(x) = \sum_n \sqrt{\frac{2}{\ell}} c_n \sin(k_n x)$$

is just a usual Fourier series! Similarly, for a free particle, the eigenfunctions are

$$\phi(x; k) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

with the normalization

$$\langle \phi_k | \phi_{k'} \rangle = \delta(k - k'),$$

so the expansion

$$\psi(x) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \tilde{\psi}(k) e^{ikx} dk$$

is just a normal inverse Fourier transform!

Note that

$$c_n = \langle \phi_n | \psi \rangle$$

is consistent with any general expansion

$$\psi(x) = \sum_n c_n \phi(x; n),$$

and the continuous analogue is likewise true. We can check this in the discrete case as

$$\begin{aligned} c_n &= \langle \phi_n | \psi \rangle = \int_{-\infty}^{\infty} \phi^*(x; n) \psi(x) dx \\ &= \sum_s c_s \int_{-\infty}^{\infty} \phi^*(x; n) \phi(x; s) dx \\ &= \sum_s c_s \delta_{ns} = c_n \end{aligned}$$

as expected by orthonormality. We can also check an example of the continuous case through the free particle:

$$\begin{aligned} \tilde{\psi}(k) &= \langle \phi_k | \psi \rangle = \int_{-\infty}^{\infty} \phi^*(x; k) \psi(x) dx \\ &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-ikx} \psi(x) dx = \int \frac{1}{\sqrt{2\pi}} e^{-ikx} \int \frac{1}{\sqrt{2\pi}} \tilde{\psi}(k') e^{ik'x} dk' dx \\ &= \int \tilde{\psi}(k') \delta(k - k') dk' = \tilde{\psi}(k) \end{aligned}$$

again by orthonormality.

All operators corresponding to measurable observables have real eigenvalues which are the values of those observables that can be measured, and the eigenfunctions are orthonormal. Any wavefunction representing a quantum state can then be expanded in terms of those eigenfunctions:

$$\psi(x) = \sum_A c_A \phi(x; A)$$

in the discrete case, or

$$\psi(x) = \int c(A) \phi(x; A) dA$$

in the continuous case for an observable  $A$  with a corresponding operator  $\hat{A}$ . The expansion coefficients do have meaning. If the measurable values of a certain observable are discrete, then

$$\mathbb{P}(A) = |c_A|^2$$

is the probability of measuring the value  $A$  for that observable, while in the continuous case,

$$\mathbf{p}(A) = |c(A)|^2$$

is likewise the probability density of measuring that value.

In the case of energy,

$$\psi(x) = \sum_n c_n \phi(x; n),$$

where the eigenstates are given by

$$\hat{E} \phi(x; n) = E_n \cdot \phi(x; n).$$

The probability of measuring the energy to be  $E_n$  is therefore

$$\mathbb{P}(E_n) = |c_n|^2.$$

In the case of momentum, the expansion coefficient is the Fourier transform of the wavefunction, so the probability density of measuring a momentum  $p = \hbar k$  in that state is

$$\mathbf{p}(k) = |\tilde{\psi}(k)|^2.$$

In the case of position, the expansion coefficient is exactly the same wavefunction at a differently-labeled position because the position eigenfunctions are Dirac delta functions, so the probability density of measuring a position  $x_0$  in that state is

$$\mathbf{p}(x_0) = |\psi(x_0)|^2.$$

But there is an even better reason to expand wavefunctions in terms of energy eigenfunctions. If

$$\psi(x, 0) = \sum_n c_n \phi(x; n),$$

then

$$\psi(x, t) = \sum_n c_n e^{-i\omega_n t} \phi(x; n) \tag{0.5}$$

describes how the state evolves in time. The reason this works is because the energy operator  $\hat{E}$  and the Schrödinger equation respect superposition!

Note that if  $\phi(x; n)$  is postulated to not evolve in time, then the expansion coefficients must evolve in time:

$$c_n(t) = c_n e^{-i\omega_n t}.$$

However,

$$\mathbb{P}(E_n, t) = |c_n(t)|^2 = |c_n|^2$$

is independent of time as the time evolution is simply a complex phase. Similarly,

$$\langle E \rangle = \sum_n E_n \mathbb{P}(E_n, t) = \sum_n E_n |c_n|^2$$

is independent of time. However, it can be shown that quantities such as  $\langle x \rangle$  in general do depend on time. This is because physical state wavefunctions are not pure energy eigenfunctions but are superpositions thereof!



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