Quantum Mechanics
Day 12

Today

I. Last Time

- We illustrated separation of variables on the Schrödinger PDE.
- We arrived at

  $$\hat{H}\psi = E\psi,$$

  which can also be written

  $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi,$$

  and at

  $$\varphi = e^{-iEt/\hbar}.$$

  The full wave function is

  $$\Psi(x,t) = \psi(x)\varphi(t).$$

- Julia derived

  $$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \qquad n = 1, 2, 3, \ldots,$$

  and

  $$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right).$$

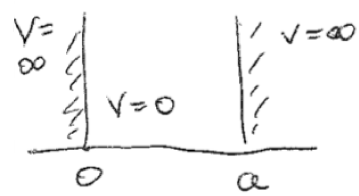

Figure 1: The potential $V(x)$ for the infinite square well.

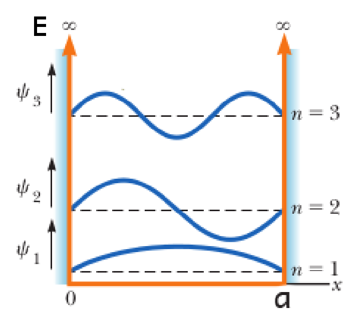

Figure 2: The first three energy eigenstates of the infinite square well.

II. Stationary States

These separable states are just special solutions of the Schrödinger equation. Who cares about them?! There are at least three reasons to care—we covered one last time, they are states of definite energy, and we'll cover two more now:

1. They are stationary states. The wave function

   $$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

   is time dependent, but the probability density

   $$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{+iEt/\hbar}\psi e^{-iEt/\hbar} = |\psi(x)|^2$$

   is time independent. You can check that this leads to all expectation values being time independent.

III. Building General States

Don't forget that the physical state is

$$Psi(x,t) = \psi(x)\varphi(t).$$

So, we put our findings together to find

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{n^2\pi^2\hbar}{2ma^2}t}$$

and a general state (that is, a general solution of the Schrödinger equation) is

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{n^2\pi^2\hbar}{2ma^2}t}.$$

Let's return to our question: why care about stationary states? Reason 3: Linear combinations of stationary states give a general solution of Schrödinger's PDE when $V = V(x)$, that is, when the potential is time independent.

Strategy: Tell me $V(x)$ and $\Psi(x,0)$, then using the completeness of the eigenfunctions we can expand

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

and then indeed

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n e^{-iE_n t/\hbar}$$

is a solution of Schrödinger's equation! Don't believe this claim, check it!! In words what it says is that once you know the initial wave function in a basis of eigenfunctions, you can time evolve each of the basis elements independently, add up the resulting time evolutions with the same weights as you did to get the initial wave function, and you will obtain the time evolution of the initial wave function.

This is an incredible strategy. Let's tackle an example.

IV. General Time Evolution from Energy Eigenstates

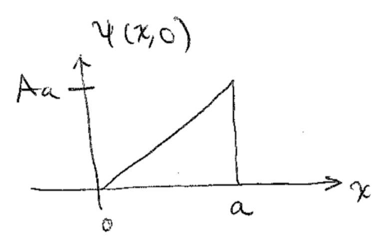

Figure 3: A particular initial wave funciton $\Psi(x,0) = Ax$.

Suppose $\Psi(x,0) = Ax$, for $0 \le x \le a$. This state is depicted at right.

We begin by normalizing this state:

$$\int_0^a A^2x^2\,dx = 1 \implies A^2\frac{a^3}{3} = 1 \implies A = \sqrt{\frac{3}{a^3}}.$$

Next, we use Fourier's trick to find the c_n:

$$c_n = \sqrt{\frac{3}{a^3}} \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) x\,dx,$$

which gives

$$c_n = \frac{\sqrt{6}}{a^2} \left. \frac{-a^2 \cos\left(\frac{n\pi}{a}x\right)}{n\pi} \right|_0^a = -\frac{\sqrt{6}\cos(n\pi)}{n\pi} = \frac{(-1)^{n+1}\sqrt{6}}{n\pi}.$$

So,

$$\boxed{\Psi(x,t) = \sqrt{\frac{2}{a}} \frac{\sqrt{6}}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin\left(\frac{n\pi}{a}x\right) e^{-i\frac{n^2\pi^2\hbar^2}{2ma^2}t}.}$$

We can use plotting an animation tools in Python to illustrate how rich this evolution is. In practice we have to truncate the sum over n. Experimenting with different values of n shows what the effects of this truncation are. I've implemented this in a jupyter notebook that you can download here.

With the default parameters that I have setup, it is great fun to look at what happens in the vicinity of $t = 63.5$ and $t = 127$. This unusual phenomenon is called wave packet revival.

From the formula

$$c_n = \langle \psi_n(x) | \Psi(x,0) \rangle$$

we see that we can think of the coefficients c_n as representing how much of the eigenstate ψ_n is present in $\Psi(x,0)$. But, is there a more physical understanding of the c_n? The answer is definitely yes.

We will prove this more carefully later in the course, but the c_n are the probability amplitudes for measuring energy E_n. That is,

$$|c_n|^2$$

represents the probability of measuring E_n. If this is right, it must be that

$$\sum_{n=1}^{\infty} |c_n|^2 = 1.$$

Let's check our case, we have

$$|c_n|^2 = \frac{6}{n^2\pi^2}$$

and indeed

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}! \ \checkmark.$$

Recall that we also have

$$\langle \heartsuit \rangle = \sum_n P_n \heartsuit_n.$$

Thus, we see that we can also write

$$\boxed{\langle \hat{H} \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n.}$$