The Schrödinger Equation

(Version: July 25, 2020)

A fairly general form of the equation

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

The main player in the equation is ψ, which is called by various names:

- The Quantum State
- The State Vector
- The Wave Function

These terms all mean the same thing. They all refer to ψ.

ψ represents the quantum state of some system (say a particle). Schrödinger's equation governs the evolution of ψ over time. Once we solve the equation we know what ψ is at a given time. Knowing ψ, we know *what we can know* about the state of the system we are modeling.

Notice that I've written ψ only as a function of t. ψ will of course have additional independent variables. But what they are will depend on the specific form of the equation.

A few words about the other symbols in the equation and then we'll talk more about ψ. I won't go into depth here, but just to get a basic understanding of what the equation "means."

i is, as usual, $\sqrt{-1}$.

$\hbar$ (pronounced "h bar") is something called *Planck's reduced constant*. If you haven't encountered $\hbar$ before, for the time being just think of it as an extremely small number.

$\dfrac{\partial}{\partial t}$ is the partial derivative with respect to t (remember that ψ actually has additional independent variables). $\dfrac{\partial}{\partial t}\psi$ is *how much ψ changes in a moment of time.*

$\hat{H}$ is an operator called the Hamiltonian. If you're familiar with the Hamiltonian from classical physics, this is the quantum operator version of that. If not, $\hat{H}$ is an operator which (at least in our initial simple problems) yields the total energy of the system.

So, if you step back and look at the whole equation (you can ignore the constants i and $\hbar$ for now) what it's basically telling you is that the change of the state of the system over time is proportional to how much energy the system has. This should sound plausible.

The wave function, or quantum state ψ

In "function talk" ψ is a complex function of real variables. Its *domain* is real and its *range* is complex. You plug in real numbers (like position and time) and you get out complex numbers (probability amplitudes).

In "vector space talk" ψ is a column vector. Like all quantum states, the elements in the vector are probability amplitudes. In this continuous space, ψ has an uncountable (continuous, nondenumerable) number of elements.

Take a specific example. Say that ψ represents the *position state* of a particle. (There's a reason that I say "position state" rather than just "position" as I hope will become clear.)

Here's a picture of the one dimensional position state of some particle which is somewhere along the x axis at a particular time:
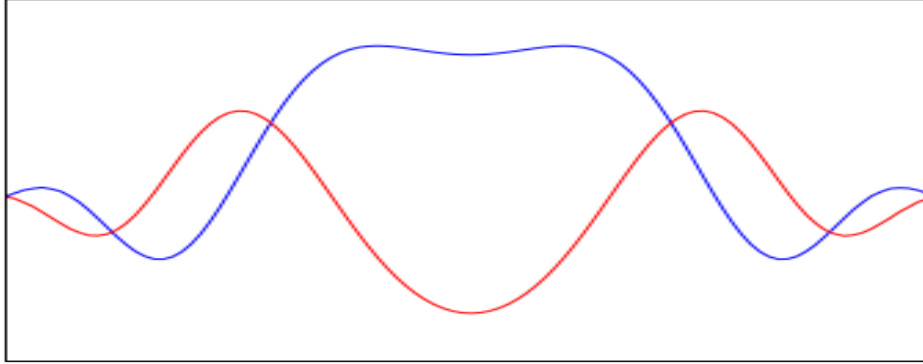
Since ψ is a complex function, we need to plot a complex value for every x position. We do this by plotting the real part in blue, and the imaginary part in red. So if you draw a vertical line through any x point, both the blue and red points constitute a single complex number: blue + red i.

So how does this complex function relate to the particle's actual position, as we might observe it in an experiment?

As you know from studying the discrete theory (quantum information), we find the probability of observing any particular outcome by taking the modulus squared of the complex probability amplitude given by the appropriate element of the state vector. The same thing is *almost* true here.

If you go back to the vertical line you drew above, the complex number you got is *almost* a probability amplitude for observing the particle at the given x position. But as you may recall from the "transition" lecture, all of these amplitudes are multiplied by an infinitesimal in order to normalize the (continuously infinite) state vector.

This means that, if we take one individual point on the function, we'll get an infinitesimally small probability. This makes sense, since in physical terms the probability that we could ever find something at one *exact* position would be vanishingly small (even if we were capable of measuring it with infinite precision).

So here's how you get probabilities. Take the modulus squared of the entire wave function: $|\psi|^2 = \psi\psi^*$. This is the same thing as taking the modulus squared of each individual (blue and red) point, by the way.

What you get is a real, positive function:
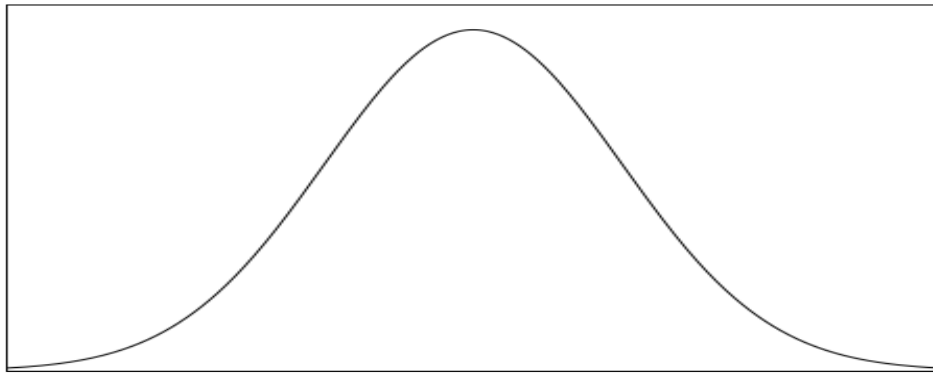
This is a *probability density function* as we discussed in the last couple of lectures. In order to get the probability of finding the particle between two points a and b, you integrate $|\psi|^2$ between those two points.
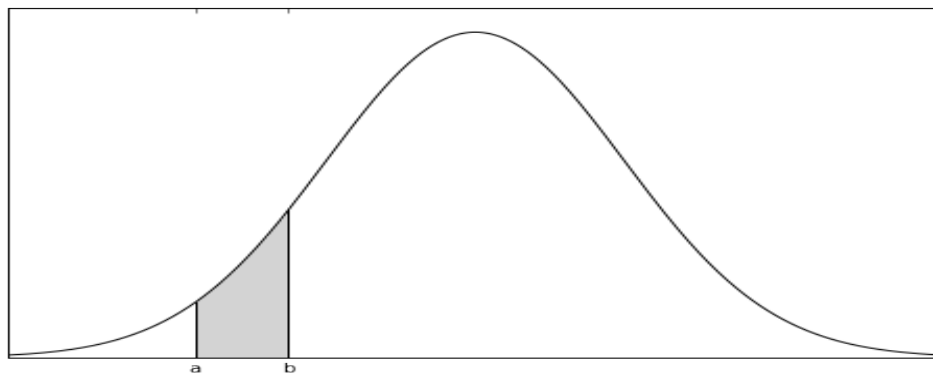
Integrate between a and b to find the probability of seeing the particle between those two points.

That's basically it. To summarize: The wave function gives the (infinitesimal) probability amplitudes of seeing particular outcomes in an experiment. In order to find out the probability of seeing any specific range of outcomes we take the modulus squared of the wave function and integrate over the desired range.

There's a very important point to bear in mind for when we talk about the underlying "interpretational" questions related to quantum theory. Unlike the temperature function in the heat equation, the wave function has no obvious *direct* relationship to physical reality. The only relationship is the indirect one, where we can find out probabilities of things happening.

In particular, the position wave function is definitely *not* a picture of the position of the particle. The particle is *not* "spread out in space" until we measure it, or something like that. It is not a wave that "becomes a particle" when you measure it.

We don't know what the wave function is (and we don't know what a "particle" is, for that matter). But we do know how to connect the mathematical object called the wave function with probabilities for the results of experiments.

One dimensional position examples

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

All of the examples that we're going to work on for the next few meetings involve the position of a small "particle" (an electron, for example) along one dimensional axes. Situations like this use the Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$\hbar$ is still Plank's reduced constant, m is the mass of the particle, and the main part of the operator is the second spatial derivative. $V(x)$ is the potential that the particle is being subjected to at position x. (I'll explain where all these values came from later.)

We can simplify things further by taking a particle which is not subjected to any potential. Then the equation becomes:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

This is the form of Schrödinger's equation that we'll use for the *free particle* and *infinite well* examples. Note that, if you ignore all the constants, this is exactly the same as the heat equation which we previously discussed. The mathematical methods for solving it are exactly the same. And the behaviour of the system has *some* similar attributes (for example the "spreading" of ψ which is reminiscent of the heat/diffusion equation).

In fact, the only constant that does anything other than scale the result is i. And i does make all the difference. The complex nature of solutions to Schrödinger's equation have an oscillatory nature, which we don't see in solutions to the heat equation.

Now remember that from the "vector space perspective" what we have here is: $i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$, where the operator $\hat{H}$ happens to equal $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$. And what we want are particular vectors ψ_n which are eigenvectors (or eigenfunctions) of that operator, giving: $\hat{H}\psi_n = E_n\psi_n$, where E_n is the eigenvalue of ψ_n and represents one particular energy value. The ψ_n provide a *basis* in which we can construct a solution to our problem. The point of the following "separation of variables" is to find those specific ψ_n.

Separation of variables

We have the PDE:

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t)$$

and we want to:

(1) Assume $\psi(x,t)$ equals the product of two functions: $\psi(t)$ and $\psi(x)$.

(2) Get all the ts on one side and all the xs on the other.

(3) Set both sides to the same constant.

In this case, which is common for Schrödinger's equation, the separation constant represents energy.

First I'll replace $\psi(x,t)$ with $\psi(t)\psi(x)$:

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

Then do the derivatives:

$$i\hbar\, \psi(x) \frac{\partial}{\partial t} \psi(t) = -\frac{\hbar^2}{2m} \psi(t) \frac{\partial^2}{\partial x^2} \psi(x)$$

Then I'm going to divide through by: $\psi(t)$, $\psi(x)$, and $\hbar$, leaving i on the left hand side:

$$i \frac{1}{\psi(t)} \frac{\partial}{\partial t} \psi(t) = -\frac{\hbar}{2m} \frac{1}{\psi(x)} \frac{\partial^2}{\partial x^2} \psi(x)$$

Now the left hand side is a function only of t and the right hand side only of x. I'll set both sides equal to the separation constant E_n, and rearrange things a bit, giving the two ODEs:

(1) $\quad \dfrac{\partial}{\partial t} \psi(t) = -iE_n \psi(t)$

(2) $\quad \dfrac{\partial^2}{\partial x^2} \psi(x) = -\dfrac{2m}{h} E_n \psi(x)$

(1) Is the time evolution equation, which is easily solved as: $\psi(t) = e^{-iE_n t}$. The time evolution always has the same form, as long as the Hamiltonian itself is time-independent.

(2) is the *eigenvalue problem* (also called the time-independent Schrödinger equation). It's called the eigenvalue problem because this is the equation we need to solve in order to get the ψ_n eigenfunctions mentioned above, which form our solution basis. The solution to *this* equation will depend on the boundary conditions for the specific situation.

Once we find our basis functions, whatever they may be, we can write a single solution to the equation for our wave function as:

$$\psi_n(x,t) = \psi_n(x)\, e^{-iE_n t}$$

We then project the initial state of the wave function, $\psi(x,0)$ onto the solution basis, in order to get the weights of the individual basis functions:

$$c_n = \int_a^b \psi_n^*(x)\, \psi(x,0)\, dx$$

Finally, we can add up all the individual solutions, with their corresponding weights, to obtain the final solution:

$$\psi(x,t) = \sum_n c_n \psi_n(x)\, e^{-iE_n t}$$

Note that, in vector space terms, this is simply a linear combination of basis vectors being summed (with the appropriate weights) to yield the (time evolving) state vector or wave function.

Of course, we will only do the summation above if we have a countably infinite number of basis functions. If we have a continuously infinite number, the summation will become an integral.

Infinite Well (or "particle in a box")

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

$$0 \le x \le \pi$$

$$\psi(0) = \psi(\pi) = 0$$

We know the time evolution will be: $e^{-iE_n t}$.

The eigenvalue problem is: $\dfrac{\partial^2}{\partial x^2}\psi(x) = -\dfrac{2m}{\hbar}E_n\psi(x)$

From the physical nature of the problem we know that we want sine waves as the eigenfunctions. The sines that solve the eigenvalue problem are: (1) $\sin\left(\sqrt{2mE_n/\hbar}\, x\right)$.

When we solve the boundary conditions for the sine functions we get (2) $\sin(nx)$.

Comparing (1) and (2) we can see that nth energy level must be: $E_n = \dfrac{n^2\hbar}{2m}$

Finally, we need to normalize the eigenfunctions: $\sqrt{\dfrac{2}{\pi}}\sin(nx)$.