

## SCHRÖDINGER EQUATION: THE MOTIVATION

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Chapter 1.

Although it is perfectly acceptable to begin a study of quantum mechanics by simply stating the Schrödinger equation, it is interesting to have a look at some of the motivation for it. Before we do, however, it is important to realize that the Schrödinger equation cannot be *derived* from any other underlying physical principles. It is a statement of how physics works and can be viewed as a postulate that must be accepted without proof. In that sense, it plays the same role as the equation  $F = ma$  in Newton's view of physics, and the same role as Maxwell's four equations in the classical theory of electromagnetism. All of these physical theories were written down in an attempt to explain experimental results; none of them was derived from any deeper physical theory (although it is possible, of course, that it *may* be possible to derive them from some deeper theory that we have not yet discovered, but so far that hasn't happened).

Although there are a fair number of experiments whose explanation requires some modification to classical physics, the ideas that gave rise to Schrödinger's equation came from the observation that the behaviour of light (or more precisely, electromagnetic radiation, which includes light and other radiation such as X-rays and radio waves) in some cases requires that we assume it to be composed of particles (photons). Max Planck's original proposal was that the energy of a photon was directly proportional to its frequency, which he wrote as

$$E = h\nu \tag{1}$$

where  $\nu$  (the Greek letter 'nu') is the frequency of the photon in cycles per second, and  $h$  is the constant of proportionality, now known as Planck's constant for obvious reasons.

A wave of any sort is characterized by three quantities: its frequency  $\nu$ , or number of times per second a peak of the wave passes a fixed point, its wavelength  $\lambda$ , or distance between two adjacent peaks, and its velocity  $v$ , or the speed at which one particular peak moves (try not to get  $\nu$  and  $v$  confused). Note that these three quantities are related:

$$\lambda\nu = v \quad (2)$$

That is, the speed of a wave is its frequency multiplied by its wavelength. A wave with a particular wavelength can move faster, so that more peaks pass a fixed point in a given time; thus its frequency is larger.

One of the consequences of the theory of special relativity, devised by Einstein and first published in 1905, is the famous equation  $E = mc^2$ , but what is not often realized is that the  $m$  in the equation is the particle's *apparent* mass, which depends on its speed relative to the observer. If a particle is at rest relative to the observer, then  $m = m_0$  where  $m_0$  is the rest mass of the particle. If the particle is moving relative to the observer, then it will appear to have a momentum  $p$  and one of the predictions of relativity is the energy of a moving particle is given by the equation:

$$E = mc^2 = \sqrt{(pc)^2 + m_0^2c^4} \quad (3)$$

Note that if the particle is at rest relative to the observer, then it has zero momentum ( $p = 0$ ), and the equation reduces to  $E = m_0c^2$  as it should.

Now notice that if the particle has *zero* rest mass ( $m_0 = 0$ ), then the energy becomes

$$E = pc \quad (4)$$

According to relativity, a massless particle is the only type of particle that can travel at the speed of light  $c$  and in fact a massless particle *must* travel at the speed of light at all times. (By the way, it is sometimes said that light travels more slowly when passing through a dense transparent substance such as glass. Although it may take a beam of light more time to pass through the glass, the individual photons still travel at speed  $c$  inside the glass. They have to bounce between the atoms of the glass in order to pass through it, so it is this process which appears to slow the light beam down.)

So we now have two very simple equations from which we can calculate the energy of a photon. One gives the energy in terms of the frequency; the other gives the energy in terms of the velocity. However, since the velocity is related to the frequency as we saw above, we can rewrite the first equation as

$$E = \frac{hc}{\lambda} \quad (5)$$

Comparing this with the second equation, we get

$$pc = \frac{hc}{\lambda} \quad (6)$$

$$p = \frac{h}{\lambda} \quad (7)$$

So far, all these calculations have been done for photons (which is why the velocities involved have all been equal to  $c$ ). In 1924, Louis de Broglie proposed (in his PhD thesis no less) that *all* particles can be represented by waves and that the formula for the momentum of a photon also applies to all particles, whether or not they have rest mass. That is, he proposed that  $p = h/\lambda$  for all particles.

At this point we should pause for a moment and modify these equations slightly to bring them into line with what is usually seen in textbooks. Rather than use the frequency  $\nu$  (which is expressed in cycles per second) it is more usual to use the frequency measure  $\omega = 2\pi\nu$  (which is expressed in radians per second). With this alteration, the energy-frequency equation becomes

$$E = h\nu \quad (8)$$

$$= \frac{h}{2\pi}\omega \quad (9)$$

$$= \hbar\omega \quad (10)$$

where  $\hbar \equiv h/2\pi$  is pronounced “h-bar”.

The momentum relation is usually written using a quantity  $k \equiv 2\pi/\lambda$  called the *wave number*, so the momentum-wavelength equation becomes

$$p = \hbar k \quad (11)$$

Now, in non-relativistic physics, the energy of a free particle (that is, a particle not being acted on by any force) is entirely kinetic, and can be written as

$$E = \frac{1}{2}mv^2 \quad (12)$$

$$= \frac{p^2}{2m} \quad (13)$$

$$= \frac{\hbar^2 k^2}{2m} \quad (14)$$

since the momentum of a particle is  $p = mv$ . Equating this to the other expression for the energy, we get

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \quad (15)$$

$$\omega = \frac{\hbar k^2}{2m} \quad (16)$$

This is a relation between the frequency  $\omega$  and the wave number  $k$  (and thus with the wavelength  $\lambda$ ) and in classical wave theory is known as a *dispersion relation*, since it describes how rapidly a localized packet of waves with various wavelengths (or wave numbers) will disperse over time. Remember that the velocity is  $v = \omega/k$  and for particles that have rest mass, the velocity can be anything less than the speed of light, so the relation between the frequency and wave number need not be constant. Thus waves with different frequencies can travel at different velocities and with a dispersion relation like we have here, they will travel at different velocities.

You could be forgiven for thinking that we haven't got much closer to writing down the Schrödinger equation, but in fact there isn't much more to do. Since we want to represent particles as waves, we need to think up an equation whose solution is a wave of some sort. (Remember, we're jumping from postulate to postulate at this stage; there is no rigorous mathematical derivation.) The simplest form of wave is that represented by a sine or cosine wave, so if we want a wave with a particular frequency and wave number, we can postulate a function (in one dimension) of form

$$\Psi(x, t) = A \cos(kx - \omega t) \quad (17)$$

where  $A$  is the amplitude (height) of the wave.

If you're not convinced this represents a wave, you can do a few tests on it. The cosine repeats after every change of  $2\pi$  in its argument, so if we fix the time at, say,  $t = 0$  and then measure the distance  $\Delta x$  between successive peaks, we get  $k\Delta x = 2\pi$ . Now remember that the wave number is related to the wavelength by  $k = 2\pi/\lambda$ , so the distance between two peaks is found from

$$k\Delta x = 2\pi \quad (18)$$

$$\frac{2\pi}{\lambda}\Delta x = 2\pi \quad (19)$$

$$\Delta x = \lambda \quad (20)$$

so the distance between two peaks is indeed one wavelength.

For the frequency, we can fix our sights on one position, say  $x = 0$ , and then measure how long ( $\Delta t$ ) it takes for one complete wave to pass that point. The first complete wave will have passed when  $\omega\Delta t = 2\pi$ . Since  $\omega = 2\pi\nu$ , we get  $\Delta t = 1/\nu$  so the number of complete wavelengths to pass the point in one second is  $1/\Delta t = \nu$  which again is correct.

Finally, we can measure the velocity of the wave by looking at one fixed point on the wave. That is, we can examine a point on the wave where  $kx - \omega t = C$  for some constant  $C$ . If we take the derivative with respect to  $t$  of this equation, we get

$$k \frac{dx}{dt} - \omega = 0 \quad (21)$$

$$\frac{dx}{dt} = \frac{\omega}{k} \quad (22)$$

so the velocity of the wave is  $\omega/k$ .

Now in classical physics, it is common to use complex numbers to represent a wave by using the relation

$$e^{i\theta} = \cos\theta + i\sin\theta \quad (23)$$

with the understanding that the part that represents the wave is always the real part of the equation. If we try the same trick here, we can represent a wave by the quantity

$$\Psi(x, t) = Ae^{i(kx - \omega t)} \quad (24)$$

$$= A(\cos(kx - \omega t) + i\sin(kx - \omega t)) \quad (25)$$

Now, finally, we are ready to get to the Schrödinger equation. What we want, then is a differential equation with a wave-like solution given by  $\Psi(x, t)$  above that also has the dispersion relation  $\omega = \frac{\hbar k^2}{2m}$ . There are various equations that could satisfy these requirements, but the simplest one appears to be the Schrödinger equation for a free particle:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = i\hbar \frac{\partial \Psi}{\partial t} \quad (26)$$

We can check that  $\Psi(x, t)$  above satisfies this equation by taking its derivatives:

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A e^{i(kx - \omega t)} \quad (27)$$

$$= -k^2 \Psi \quad (28)$$

$$\frac{\partial \Psi}{\partial t} = -i\omega A e^{i(kx - \omega t)} \quad (29)$$

$$= -i\omega \Psi \quad (30)$$

Plugging these back into the Schrödinger equation we get

$$\frac{\hbar^2 k^2}{2m} = \hbar\omega \quad (31)$$

$$\omega = \frac{\hbar k^2}{2m} \quad (32)$$

so the dispersion relation is satisfied.

That's really all there is to it. If it looks like a series of kludges, that's because it is; the physicists who contributed the various stages in the argument really were groping in the dark and postulating various equations and conditions and hoping for the best. In fact, there was one more kludge which Schrödinger made to get the final form of the equation that is satisfied by a particle moving under the influence of a potential, and that was just to add the potential term  $V(x, t)$  onto the left hand side, so the final form is

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x, t) \Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (33)$$

One final note about this equation. While the use of complex numbers in classical physics was just a computational convenience with the understanding that the function that described the physical wave was just the real part, in quantum mechanics, the wave function  $\Psi$  *must* be a complex function because of the  $i$  that multiplies the right hand side of the Schrödinger equation. This leads to the consequence that  $\Psi$  itself cannot represent a physically measurable quantity, a consequence that was resolved by Max Born's assumption that the square modulus of the function (which *is* real) represented the probability density for finding the particle at a particular location and time.

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