

Notes on wavefunctions III: time dependence and the Schrödinger equation

We now understand that the wavefunctions for traveling particles with momentum p look like wavepackets with wavelength $\lambda = h/p$, but we haven't really said anything about the time-dependence. Our goal for this part of the notes is to learn how to predict what a wavefunction will look like in the future if we know the wavefunction now.

Time dependence of wavepackets

Suppose we have a wavepacket describing a particle with momentum p . Let's assume that it is a very broad wavepacket with a small uncertainty in momentum. How do we expect this to change with time?

One thing is fairly certain: since we know the particle is moving with momentum p , it should have a velocity $v = p/m$ (assuming $p \ll m$), so the wavepacket should move along at this velocity. If the wavepacket is centered at x_0 at time $t = 0$, then at a later time $t = T$, it should be centered somewhere near $x = x_0 + vT$.

In terms of wavelength, we can say that wavepackets with wavelength λ should travel at speed

$$v_{packet} = \frac{p}{m} = \frac{h}{m\lambda} . \quad (1)$$

It is interesting that the speed should depend on the wavelength. This does not happen for light in a vacuum or for waves on a string (assuming they obey the simplest wave equation) where waves with all possible wavelengths travel at one velocity. However, most realistic waves (e.g. water waves or light waves in air/water/glass) do have wavelength-dependent velocities.¹

Time dependence of pure waves

How does the wave velocity show up in a mathematical description of the waves? To understand this, it is simplest to start by thinking about the

¹For example, the index of refraction of a material is the speed of light in the vacuum divided by the speed of light in the material. A prism makes a rainbow because the index of refraction is different for the different colors; in other words, the light velocity in the glass is different for different wavelengths.

pure waves that describe momentum eigenstates. Our experience with other waves tells us that time dependent traveling sinusoidal waves are described mathematically as

$$\cos(kx - \omega t)$$

where k is related to the wavelength by $k = 2\pi/\lambda$ and $f = \omega/(2\pi)$ is the frequency of oscillations that we observe at a single point. For such a wave, the velocity of the “ripples” is

$$v_{ripples} = \frac{\omega}{k} \quad (2)$$

Similarly, for a traveling complex wave we would have

$$e^{i(kx - \omega t)} . \quad (3)$$

For any specific type of wave (water waves, light waves, sound waves, etc...), the frequency ω is always related somehow to the wavelength (or equivalently to $k = 2\pi/\lambda$). For light waves in the vacuum, we have $\frac{f=c}{\lambda}$ or $\omega = ck$. In this case, the equation (2) tells us that the ripple velocity is just c , independent of the wavelength. For other waves, the relationship $\omega(k)$ (known as the DISPERSION RELATION) between frequency and wavelength is more complicated, and then equation (2) will give us a ripple velocity that is different for different wavelengths.

Let’s now go back to thinking about momentum eigenstates. Since these are described by pure waves, the time-dependent wavefunctions should take the form (3). But how are k and ω related to the momentum p ? We know that the wavelength should be $\lambda = h/p$, so we have $k = 2\pi p/h$. What about the frequency? Based on (1) we might want to choose ω so that the velocity of the ripples in (2) matches the electron velocity p/m . But this isn’t quite right.

The reason is that if we form wavepackets out of these time-dependent pure waves, *the velocity of the packet is different from the velocity of the ripples*. In terms of wave jargon, the former is known as the GROUP VELOCITY and the latter is known as the PHASE VELOCITY. We already know that the phase velocity for waves of the form (3) is ω/k . But the group velocity can also be calculated in a simple way once we know how ω depends on k . The result is that if we form a wavepacket by adding a collection of pure waves with a narrow range of wavelengths near λ , the group velocity of this wavepacket will be

$$v_{group} = \frac{d\omega}{dk} , \quad (4)$$

evaluated at $k = 2\pi/\lambda$. For all the details, see the “notes on phase velocity and group velocity.”

For the wavepackets describing particles of mass m with momentum p , we decided earlier that the packet (i.e. group) velocity should be $p/m = h/(\lambda m) = hk/(2\pi m)$. According to (4), this will be true if

$$\frac{d\omega}{dk} = \frac{hk}{2\pi m} .$$

As we can easily check, this will be true if the relation between ω and k is:²

$$\omega = \frac{hk^2}{4\pi m}$$

Or, in terms of the momentum p , we want

$$\omega = \frac{2\pi}{h} \frac{p^2}{2m} . \tag{5}$$

There is a really simple interpretation of this result. Since $p^2/(2m)$ is just the energy of the electron (so far, we’re talking about “free” electrons traveling in regions without potential energy) and $\omega = 2\pi f$, what we have found is that

$$hf = E .$$

Thus, pure-wave wavefunctions with frequency f describe particles with energy $E = hf$, exactly the same relation between energy and frequency as we have for photons!

To summarize, our final result is the the time-dependent wavefunctions for particles with momentum p take the form (3) with $k = 2\pi p/h$ and ω given in (5). All together, we have:

$$\psi_p(x, t) = e^{i\frac{2\pi}{h}(px - \frac{p^2}{2m}t)} . \tag{6}$$

Time dependence of general wavefunctions

We have now solved the problem of time-dependence for the special case of momentum eigenstates. While this might seem like only a small step

²We could also add a constant to the right hand side here. We will understand the interpretation of such a constant term soon.

towards finding the time dependence of general wavefunctions, it actually gives us everything we need. The crucial point is that any state can be written as a superposition of momentum eigenstates (or equivalently, any wavefunction can be written as a superposition of pure waves). Suppose that our wavefunction at time $t = 0$ is $\psi(x)$. Then (from the previous notes) we know that we can write $\psi(x)$ as a superposition of pure waves:

$$\psi(x, t = 0) = \frac{1}{\sqrt{h}} \int A(p) e^{i \frac{2\pi p}{h} x} dp \quad (7)$$

where $A(p)$ can be determined using the Fourier transform formula. But we now know from equation (6) how all the individual pure waves evolve with time. Thus, to find out the wavefunction at a time t , we just take the same combination of pure waves, but evaluated at the later time:

$$\psi(x, t) = \frac{1}{\sqrt{h}} \int A(p) e^{i \frac{2\pi}{h} (px - \frac{p^2}{2m} t)} dp . \quad (8)$$

This gives a precise method to determine $\psi(x, t)$ for any wavefunction given $\psi(x, 0)$. While it may seem complicated to carry out in practice, this is a relatively easy calculation for a computer to do (or we can do it by hand for many possible forms of the initial wavefunction).

Time dependence from the Schrödinger equation

There is a very convenient way to summarize everything we've learned so far about how wavefunctions change with time, and that is by using a differential equation known as the SCHRÖDINGER EQUATION. Let's start by writing it down; it says that for a wavefunction $\psi(x, t)$

$$\frac{d\psi}{dt} = \frac{ih}{4\pi m} \frac{d^2\psi}{dx^2} \quad (9)$$

where the time derivative is taken with x fixed and the x derivatives are taken with t fixed. You may not have much experience with differential equations, let alone this more complicated variety with two different types of derivatives (known as a partial differential equation). But it's easy enough to figure out what this is telling us. First remember that the time derivative on the left hand side is defined to be

$$\frac{d\psi}{dt} \equiv \frac{\psi(x, t + \delta t) - \psi(x, t)}{\delta t}$$

in the limit where δt goes to zero. Rewriting our Schrödinger equation with this definition, we get:

$$\psi(x, t + \delta t) = \psi(x, t) + \delta t \frac{ih}{4\pi m} \frac{d^2\psi}{dx^2} . \quad (10)$$

In this way of writing things, we see that the left side is just the wavefunction evaluated at a time which is slightly later than t . The right hand side is just the wavefunction at time t plus a constant times some x derivatives of the wavefunction at time t . So the Schrödinger equation tells us what the wavefunction will be at a slightly later time based on what the wavefunction is now. So apparently it gives us a second way of finding the wavefunction $\psi(x, t)$ starting from the initial wavefunction $\psi(x, t = 0)$.³

We will now show that the Schrödinger equation predicts exactly the same time-dependence that we found in our general formula (8). First, it is easy to check that the momentum eigenstate wavefunction (6) satisfy the Schrödinger equation (9) for any value of p . We can just plug these functions into the equation and find that both sides give the same result. Next, we use a very special property of the Schrödinger equation: if ψ_1 is a solution and ψ_2 is a solution, then any linear combination $a\psi_1 + b\psi_2$ is a solution. For if

$$\frac{d\psi_1}{dt} = \frac{ih}{4\pi m} \frac{d^2\psi_1}{dx^2}$$

and

$$\frac{d\psi_2}{dt} = \frac{ih}{4\pi m} \frac{d^2\psi_2}{dx^2}$$

then adding a times the first equation plus b times the second equation gives

$$\frac{d(a\psi_1 + b\psi_2)}{dt} = \frac{ih}{4\pi m} \frac{d^2(a\psi_1 + b\psi_2)}{dx^2} ,$$

so $a\psi_1 + b\psi_2$ is also a solution. This works because the Schrödinger equation is LINEAR: each term has exactly one ψ in it (you can check that it would not work if there were any term with ψ^2 , etc...). In the same way, we could show that any linear combination of more than two solutions is also a solution.

³The equation (10) only works if δt is infinitesimal, so we have to break up the time t into many parts and then apply (10) a bunch of times. This is something that a computer can do easily. There are also analytical (i.e. calculating by hand) techniques for solving equations like this.

Now, suppose we have some initial wavefunction $\psi(x, t = 0)$. Then since the time-dependent wavefunction function (8) that we found earlier is just a linear combination of momentum eigenstates, and since we have checked that each momentum eigenstate wavefunction solves the Schrödinger equation, it must be that $\psi(x, t)$ is a solution to the Schrodinger equation. So if we just use the Schrödinger equation to determine $\psi(x, t)$ starting with the initial wavefunction $\psi(x, t = 0)$, the answer we get is exactly the one that we found before.

Newton's First Law v2.0

We've learned so far that in quantum mechanics, the description of the state of a particle is given by a wavefunction $\psi(x)$ instead of a position and velocity (x, v) . The Schrödinger equation (9) tells us how the wavefunction changes with time, but only in the special case where there are no forces on the particle. Thus, it is the quantum version of Newton's First Law ($m \frac{d^2x}{dt^2} = 0$ in the absence of forces). The solutions

$$\psi(x, t) = \frac{1}{\sqrt{h}} \int A(p) e^{i \frac{2\pi}{h} (px - \frac{p^2}{2m} t)} dp . \quad (11)$$

are the quantum version of constant velocity particles.

$$x = x_0 + vt .$$

An interesting difference between the classical picture and the quantum picture is that in classical physics, we need to know both the position and the time derivative of position (i.e. the velocity) at some time to determine what the position will be at later times. For the Schrödinger equation we only need to know the wavefunction, but not its time derivative to determine what the wavefunction will be at some later time. The reason for the difference is that the wavefunction contains all information about position *and* velocity (since we can figure out the momentum wavefunction directly from the position wavefunction).

Now that we know the quantum mechanical version of Newton's First Law, our next task is to understand what replaces Newton's Second Law; how do forces enter into the Schrödinger equation?