

TIME-INDEPENDENT SCHRÖDINGER EQUATION

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Once we have the Schrödinger equation, most of non-relativistic quantum mechanics is devoted to finding solutions to this equation for various potential functions. Since it is a second-order partial differential equation, the number of cases for which an exact solution may be found is depressingly small. As a result there are a lot of approximation techniques that allow solutions in various cases, and of course there is always the option of a numerical solution using a computer.

An important feature of the Schrödinger equation is that it is *linear*, meaning that the function Ψ and its derivatives occur to the first power only, and there are no products or other non-linear functions of Ψ to be found. This has the important consequence that if we find two different solutions of the Schrödinger equation, then any linear combination of these two solutions is also a solution. A *linear combination* of two solutions Ψ_1 and Ψ_2 has the form

$$\Psi = a\Psi_1 + b\Psi_2 \quad (1)$$

where a and b are complex constants.

There are, however, several important potentials for which exact solutions may be found, and many of these potentials are *time-independent*, meaning that they depend only on position. In such a case, the Schrödinger equation may be simplified by the trick of *separation of variables*. To see how this works, let's start with the general Schrödinger equation:

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

The only place in this equation where an explicit time dependence can occur is in the potential function $V(x, t)$ (of course the wave function itself will have an explicit time dependence, but that's what we're trying to solve for!). In the situation where the potential depends only on space, the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (3)$$

Not much of an improvement, you might think. But suppose we propose a solution for the wave function that is the product of one function $\psi(x)$ that depends on space (x) only and another function $\Xi(t)$ (the Greek capital 'xi') that depends only on time (t). That is

$$\Psi(x,t) = \psi(x)\Xi(t) \quad (4)$$

The partial derivatives become a little simpler:

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial^2 \psi}{\partial x^2} \Xi(t) \quad (5)$$

$$\frac{\partial \Psi}{\partial t} = \psi(x) \frac{\partial \Xi}{\partial t} \quad (6)$$

Substituting this back into the Schrödinger equation we get

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \Xi(t) + V(x)\psi(x)\Xi(t) = i\hbar \frac{\partial \Xi}{\partial t} \psi(x) \quad (7)$$

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = i\hbar \frac{1}{\Xi(t)} \frac{\partial \Xi}{\partial t} \quad (8)$$

where in the last line we have divided the first line through by $\psi(x)\Xi(t)$.

Notice that a magical thing has happened here: the left side of the equation depends only on x and the right side depends only on t . We have therefore *separated* the two independent variables in the equation. How does that help us? Well, since x and t are *independent* variables, we can vary either of them without changing the other. If we varied x for example, then in principle the left side of the equation would change while the right side, which does not depend on x wouldn't. So it looks like we've ended up with an impossible situation.

Not quite. The equation can still be satisfied if both sides of the equation are equal to the same constant, which we'll call E . That is, we must have

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = E \quad (9)$$

$$i\hbar \frac{1}{\Xi(t)} \frac{\partial \Xi}{\partial t} = E \quad (10)$$

which we can rewrite as two separate *ordinary* (not partial) differential equations, since each equation now has only one independent variable:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (11)$$

$$i\hbar \frac{d\Xi(t)}{dt} = E\Xi(t) \quad (12)$$

The clever thing about this separation of variables is that the potential function has disappeared from the second equation, so we can solve for the time part of the equation in general, and get

$$\int \frac{d\Xi}{\Xi} = -\frac{i}{\hbar} E \int dt \quad (13)$$

$$\ln \Xi = -\frac{i}{\hbar} Et + \ln C \quad (14)$$

$$\Xi(t) = Ce^{-iEt/\hbar} \quad (15)$$

where C is a constant of integration, and will be determined by the normalization of the wave function.

But what is this constant E ? To get an idea of what E represents, we can rewrite the ψ equation like this:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x) \quad (16)$$

$$\left[\frac{1}{2m} \left(\frac{\hbar}{i} \frac{d}{dx} \right)^2 + V(x) \right] \psi(x) = E\psi(x) \quad (17)$$

Now if we remember the expression of the momentum as an operator:

$$p = \frac{\hbar}{i} \frac{d}{dx} \quad (18)$$

(whether we use a total or partial derivative doesn't matter when the function being operated on depends on x only), we can see that the ψ equation can be written as:

$$\left[\frac{p^2}{2m} + V(x) \right] \psi(x) = E\psi(x) \quad (19)$$

The terms in square brackets are the kinetic plus the potential energy, so we can view this as an operator equation, where the operator in square brackets operates on the spatial part of the wave function with the result of giving the same wave function back again, but multiplied by the constant E which can therefore be interpreted as the total energy in the state.

In more advanced language, the function $\psi(x)$ is an *eigenfunction* of the operator $\frac{p^2}{2m} + V(x)$ with *eigenvalue* E . (If you're just starting out in quantum mechanics and these terms are unfamiliar, don't worry about them right now.)

We can look at this the other way round as well, as is done by, for example, Landau & Lifshitz and Messiah. That is, we can start by looking for states with fixed energies E_n . Since the quantum operator that corresponds to energy is $i\hbar \frac{\partial}{\partial t}$, we are therefore looking for solutions of

$$i\hbar \frac{\partial \Xi}{\partial t} = E_n \Xi \quad (20)$$

which gives us the result 15 above.

All this may look a bit arbitrary, since from the appearance of the ψ equation, it looks like we can just pick any old value (including complex numbers) for E . However, the magic of this equation is that when we solve it for particular potential functions, we discover that only certain values of E (and they are all real, too) are allowed. This equation, therefore, puts the 'quantum' in 'quantum mechanics', since it shows that energies can be only certain discrete values. More on this when we discuss some of the individual potentials.

For now, it is worthwhile summarizing the chain of logic that got us this far. Starting with the Schrödinger equation (which can be accepted as a postulate, or you can review the argument we presented to justify it), we considered the special case of a time-independent potential. This led to a solution using the mathematical technique of separation of variables, which in turn led to the interpretation of the spatial part of the solution as an equation that gives the allowed energy levels in the system. Note that the prediction of the energy levels is an entirely mathematical consequence of the assumption that the Schrödinger equation is the correct equation for describing nature.

In general, the solutions $\psi(x)$ of the spatial equation 16 depend, of course, on the specific form of the potential $V(x)$. Suppose we have found such a set, and found that only a discrete set of energies E_n are permitted. The spatial function $\psi_n(x)$ that corresponds to energy E_n can then be combined with the solution 15 of the time part of the equation to give the total solution for this energy. That is, the full solution becomes

$$\Psi_n(x) = \psi_n(x) e^{-iE_n t/\hbar} \quad (21)$$

where we've absorbed the normalization constant C into the spatial function $\psi_n(x)$.

Because the Schrödinger equation is linear, we can build up other solutions that are linear combinations of the $\Psi_n(x)$ functions in 21. The general solution thus becomes

$$\Psi(x) = \sum_n c_n \Psi_n(x) \quad (22)$$

$$= \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar} \quad (23)$$

Here, the c_n are (in general, complex) constants. This is the most general solution of the time-independent Schrödinger equation for a given potential.

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