Duane's Science Enrichment Series

Going From the Time-Dependent to the Time-Independent Schrödinger Equation

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Target: Graduate Physics, Physical Chemistry

This question has been asked repeatedly, and for good reason. Textbooks in physics and physical chemistry (as well as Wikipedia articles) may describe both versions of the Schrödinger equation. They start with the time-dependent version as the complete, general case:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=\left[\frac{-\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)\right]\Psi(\mathbf{r},t) \quad , \tag{I}$$

and progress right away to the time-independent version:

$$E\Psi(\mathbf{r},t)=\left[\frac{-\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)\right]\Psi(\mathbf{r},t) \quad , \tag{II}$$

which looks at the wave distribution at a fixed point in time.

The reason for this is simple. We can work with the time-independent version of the equation, at least to some extent, but the time-dependent version is a real headache. If we had a way to solve it in any practical manner, we wouldn't have to do chemistry in the lab; we could just calculate every reaction. But alas! Computers that can do that are probably 1000 years away and most scientists don't want to wait that long.

But those same textbooks never talk about how the two forms are related or how you get from the time-dependent case to the more specific time-independent case, and I've heard it asked more than once just how you do that. It's not a big secret; it's just that the answer is in another book: *Partial Differential Equations*.

The Schrödinger Equation is, of course, a partial differential equation, and partial differential equations have a reputation for being intractable. There is good reason for that reputation. If a textbook on the subject seems to rehearse chapter after chapter of special cases without discussing general methods, it's because there aren't many general methods. There are a small subset of partial differential equation cases that we know how to solve analytically, and, fortunately for quantum mechanics, the Schrödinger equation happens to fall into one of those: separable partial differential equations.

If you've studied ordinary differential equations, you've run into separable equations, where the variables can be split up on opposites sides of the equal sign. You might remember that doing so leads to a way to solve such equations using integration. In (I) you see the partial derivative with respect to time completely on the left and the partial derivative with respect to space completely on the right. What the textbooks don't normally mention at that point, but save for partial differential equations later, is that the only way that both sides, which are partial derivatives of two independent variables, can be equal under all conditions is that if they are equal to a constant. With this in mind, we can rewrite the time-dependent case as:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=C=\left[\frac{-\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)\right]\Psi(\mathbf{r},t) \tag{III}$$

At some point, we're going to want to know what that "C" is and there are two things to consider. First, that by "constant" we mean constant at each point in space and time, not necessarily constant over every point in space and time. If the second were true, there would be no meaning to a wavefunction at all. Second, since the C must be equal to the right side of the equation and the Hamiltonian is in terms of energy, the constant term must also be energy. Putting all this together, we discover that

$$C=E\Psi(\mathbf{r},t) \quad . \tag{IV}$$

Substituting this into (III) and taking the right-hand part gives us the familiar time-independent form (II). Viola!

But there is something else. This also means

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=E\Psi(\mathbf{r},t) \quad . \tag{V}$$

True, but you're only likely to see something like this in an advanced textbook or research paper dealing with quantum dynamics. But bear in mind that quantum dynamics is very, very hard. I know one researcher who gave it up because he got tired of doing it every day.