7.4: The Schrödinger Equation

Learning Objectives

By the end of this section, you will be able to:

- Describe the role Schrödinger's equation plays in quantum mechanics
- Explain the difference between time-dependent and -independent Schrödinger's equations
- Interpret the solutions of Schrödinger's equation

In the preceding two sections, we described how to use a quantum mechanical wavefunction and discussed Heisenberg's uncertainty principle. In this section, we present a complete and formal theory of quantum mechanics that can be used to make predictions. In developing this theory, it is helpful to review the wave theory of light. For a light wave, the electric field $E(x,t)$ obeys the relation

$$\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2}, \tag{7.4.1}$$

where c is the speed of light and the symbol ∂ represents a *partial derivative*. (Recall from Oscillations that a partial derivative is closely related to an ordinary derivative, but involves functions of more than one variable. When taking the partial derivative of a function by a certain variable, all other variables are held constant.) A light wave consists of a very large number of photons, so the quantity $|E(x,t)|^2$ can interpreted as a probability density of finding a single photon at a particular point in space (for example, on a viewing screen).

There are many solutions to this equation. One solution of particular importance is

$$E(x,t) = A\,\sin(kx-\omega t), \tag{7.4.2}$$

where A is the amplitude of the electric field, k is the wave number, and ω is the angular frequency. Combing this equation with Equation 7.4.1 gives

$$k^2 = \frac{\omega^2}{c^2}, \tag{7.4.3}$$

According to de Broglie's equations, we have $p=\hbar k$ and $E=\hbar\omega$. Substituting these equations into Equation 7.4.3 gives

$$p = \frac{E}{c}, \tag{7.4.4}$$

or

$$E = pc. \tag{7.4.5}$$

Therefore, according to Einstein's general energy-momentum equation (Equation 5.10.26), Equation 7.4.5 describes a particle with a zero *rest mass*. This is consistent with our knowledge of a photon.

This process can be reversed. We can begin with the energy-momentum equation of a particle and then ask what wave equation corresponds to it. The energy-momentum equation of a nonrelativistic particle in one dimension is

$$E = \frac{p^2}{2m} + U(x,t), \tag{7.4.6}$$

where p is the momentum, m is the mass, and U is the potential energy of the particle. The wave equation that goes with it turns out to be a key equation in quantum mechanics, called **Schrödinger's time-dependent equation**.

THE TIME-DEPENDENT SCHRÖDINGER EQUATION

The equation describing the energy and momentum of a wavefunction is known as the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x,t)\,\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}. \tag{7.4.7}$$

As described in Potential Energy and Conservation of Energy, the force on the particle described by this equation is given by

$$F=-\frac{\partial U\left(x,t\right)}{\partial x}. \tag{7.4.8}$$

This equation plays a role in quantum mechanics similar to Newton's second law in classical mechanics. Once the potential energy of a particle is specified—or, equivalently, once the force on the particle is specified—we can solve this differential equation for the wavefunction. The solution to Newton's second law equation (also a differential equation) in one dimension is a function *x*(*t*) that specifies where an object is at any time *t*. The solution to Schrödinger's time-dependent equation provides a tool—the wavefunction—that can be used to determine where the particle is *likely* to be. This equation can be also written in two or three dimensions. Solving Schrödinger's time-dependent equation often requires the aid of a computer.

Consider the special case of a free particle. A free particle experiences no force ($F=0$).Based on Equation 7.4.8, this requires only that

$$U\left(x,t\right)=U_0=constant. \tag{7.4.9}$$

For simplicity, we set $U_0=0$. Schrödinger's equation then reduces to

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi\left(x,t\right)}{\partial x^2}=i\hbar\frac{\partial\Psi\left(x,t\right)}{\partial t}. \tag{7.4.10}$$

A valid solution to this equation is

$$\Psi\left(x,t\right)=Ae^{i(kx-\omega t)}. \tag{7.4.11}$$

Not surprisingly, this solution contains an **imaginary number** ($i=\sqrt{-1}$) because the differential equation itself contains an imaginary number. As stressed before, however, quantum-mechanical predictions depend only on $|\Psi\left(x,t\right)|^2$, which yields completely real values. Notice that the real plane-wave solutions, $\Psi\left(x,t\right)=A\,sin\left(kx-\omega t\right)$ and $\Psi\left(x,t\right)=A\,cos\left(kx-\omega t\right)$, do not obey Schrödinger's equation. The temptation to think that a wavefunction can be seen, touched, and felt in nature is eliminated by the appearance of an imaginary number. In Schrödinger's theory of quantum mechanics, the wavefunction is merely a tool for calculating things.

If the potential energy function (*U*) does not depend on time, it is possible to show that

$$\Psi\left(x,t\right)=\psi(x)\,e^{-i\omega t} \tag{7.4.12}$$

satisfies Schrödinger's time-dependent equation, where $\psi(x)$ is a *time*-independent function and e−iωte−iωt is a *space*-independent function. In other words, the wavefunction is *separable* into two parts: a space-only part and a time-only part. The factor $e^{-i\omega t}$ is sometimes referred to as a **time-modulation factor** since it modifies the space-only function. According to de Broglie, the energy of a matter wave is given by $E=\hbar\omega$, where E is its total energy. Thus, the above equation can also be written as

$$\Psi\left(x,t\right)=\psi(x)\,e^{-iEt/\hbar}. \tag{7.4.13}$$

Any linear combination of such states (mixed state of energy or momentum) is also valid solution to this equation. Such states can, for example, describe a localized particle (see Figure 7.3.1)

Exercise 7.4.1

A particle with mass *m* is moving along the *x*-axis in a potential given by the potential energy function $U(x)=0.5m\,\omega^2x^2$. Compute the product $\Psi\left(x,t\right)^*U(x)\,\Psi\left(x,t\right)$. Express your answer in terms of the time-independent wavefunction, $\psi(x)$.

Answer:

$0.5\,m\omega^2x^2\,\psi(x)^*\psi(x)$

Combining Equation 7.4.13 and Equation 7.4.7, Schrödinger’s time-dependent equation reduces to the **Schrӧdinger’s time-independent equation**.

THE TIME-inDEPENDENT SCHRÖDINGER EQUATION

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = E\,\psi(x), \tag{7.4.14}$$

where E is the total energy of the particle (a real number).

Notice that we use “big psi” (Ψ) for the time-dependent wavefunction and “little psi” (ψ) for the time-independent wavefunction. The wave-function solution to this equation must be multiplied by the time-modulation factor to obtain the time-dependent wavefunction.

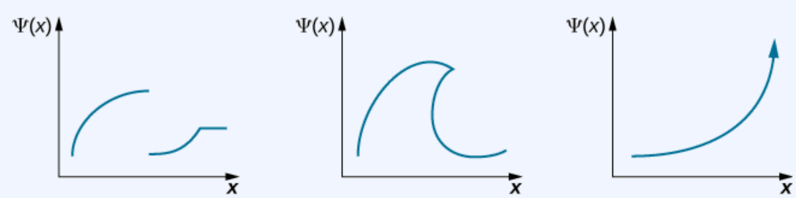
In the next sections, we solve Schrӧdinger’s time-independent equation for three cases: a quantum particle in a box, a simple harmonic oscillator, and a quantum barrier. These cases provide important lessons that can be used to solve more complicated systems. The time-independent wavefunction $\psi(x)$ solutions must satisfy three conditions:

- $\psi(x)$ must be a continuous function.
- The first derivative of $\psi(x)$ with respect to space, $d\psi(x)/dx$, must be continuous, unless $V(x) = \infty$.
- $\psi(x)$ must not diverge (“blow up”) at $x = \pm\infty$.

The first condition avoids sudden jumps or gaps in the wavefunction. The second condition requires the wavefunction to be smooth at all points, except in special cases. (In a more advanced course on quantum mechanics, for example, potential spikes of infinite depth and height are used to model solids). The third condition requires the wavefunction be normalizable. This third condition follows from Born’s interpretation of quantum mechanics. It ensures that $|\psi(x)|^2$ is a finite number so we can use it to calculate probabilities.

Exercise 7.4.2

Which of the following wavefunctions is a valid wave-function solution for Schrӧdinger’s equation?



Answer:

None. The first function has a discontinuity; the second curve is not even a function - it is double-valued; and the third function diverges so is not normalizable.

Contributors and Attributions

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