Schrödinger's Equation in One Dimension

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1 Introduction

You may have been taught that an electron is a tiny ball, circling the nucleus of an atom like a planet around the Sun, with a position and speed that could be written down at any moment. It is a useful picture, and for many purposes a good enough one. However, on closer inspection, this simple model breaks down. We find that tiny particles such as electrons do not have a single, definite position; instead they are described by a *wavefunction*, $\psi(x)$, a function which doesn't tell us where a particle *is*, but where we are *likely* to find it. The equation that governs this wavefunction, proposed by Erwin Schrödinger in 1926, is not actually a single formula but a whole family of equations, with a different version for every physical situation we might wish to describe. In this article, we will cover the simplest form of Schrödinger's equation,

$$\hat{H}\psi = E\psi \tag{1}$$

This is called the **time-independent Schrödinger's equation**. We can use this remarkably simple equation to study a particle in a one-dimensional 'box'.

2 What is the wavefunction?

Before we start delving deeper into how to solve Schrödinger's equation, we first need to understand what it is we are actually solving for: the wavefunction, $\psi(x)$. $\psi(x)$ is a function that assigns a number to every position x along a line. On its own, the value ψ has no direct physical meaning: it can be positive, negative or even complex! Its usefulness comes from what happens when we *square* it. The quantity

$$|\psi(x)|^2$$

is called the **probability density**. If you have studied statistics this will be familiar: it is a curve where the height itself is not a probability, but the *area* underneath it is.

Basically, $|\psi(x)|^2$ tells us how probability is spread along the line, rather than the probability at any single point. Indeed, the chance of finding a particle at one exact position is zero. Instead we look at the probability of an *interval*. This is where integration comes in. The probability of finding the particle between $x = a$ and $x = b$ is given by

$$\int_a^b |\psi(x)|^2 \, \mathrm{d}x.$$

This is known as the **Born rule**, after the physicist Max Born.

Since the particle must be *somewhere*, the total probability must equal 1. Hence, wavefunctions must satisfy the **normalisation condition**

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x = 1. \tag{2}$$

Now that we have a better understanding of what $\psi(x)$ is, the remaining question is how to find it in the first place. That is exactly what Schrödinger's equation is for, but the equation needs a physical setting before it can give us an answer. So let us build one.

3 Building the box

Imagine a cricket ball rolling back and forth along a gutter that is sealed at both ends. Classically, this is the picture we are borrowing: a particle confined to a straight line between two impenetrable walls, placed at $x = 0$ and $x = L$. We define the potential energy of the system, $V(x)$, to be

$$V(x) = \begin{cases} 0, & 0 < x < L \quad \text{(inside the box)}, \\ \infty, & x \leq 0 \text{ or } x \geq L \quad \text{(outside the box)}. \end{cases} \tag{3}$$

Inside the box the particle feels no force at all; outside it would need infinite energy to enter, hence we have trapped the particle in the box. This is called the **infinite square well**.

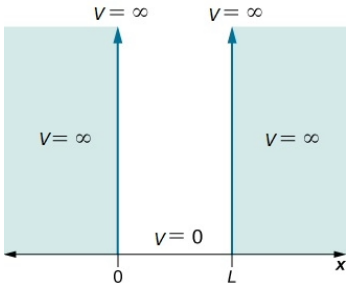

Figure 1: A particle in a one-dimensional box.

Because the particle can never be outside the box, its probability density must be zero there, so $\psi(x) = 0$ for $x \leq 0$ and $x \geq L$. A wavefunction cannot suddenly jump, so it must also be zero *at* the walls:

$$\psi(0) = 0, \qquad \psi(L) = 0.$$

These are the **boundary conditions**, and they follow directly from what we learnt about the wavefunction in the last section. Now we have everything we need to solve Schrödinger's equation.

4 Solving the equation

Step 1: Finding the general solution

To start with, let us define the terms in equation (1),

$$\hat{H}\psi = E\psi$$

E is the total energy of the particle and $\hat{H}$ is an operator called the **Hamiltonian**. An operator is simply an instruction that acts on a function (in this case $\psi(x)$) to produce a new function, just as $\frac{\mathrm{d}}{\mathrm{d}x}$ turns x^2 into $2x$. The Hamiltonian is defined as

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \tag{4}$$

Here m is the mass of the particle and $\hbar = \dfrac{h}{2\pi}$ is the reduced Planck constant, where $h \approx 6.63 \times 10^{-34}\,\mathrm{J\,s}$. The Hamiltonian has two parts, which mirror the two kinds of energy in classical mechanics:

- The first term, $-\dfrac{\hbar^2}{2m}\dfrac{\mathrm{d}^2}{\mathrm{d}x^2}$, represents the **kinetic energy**. It involves the second derivative of $\psi(x)$, which measures how sharply the wavefunction curves.
- The second term, $V(x)$, we have already defined as the **potential energy** at position x.

Putting equation (4) into $\hat{H}\psi = E\psi$ gives the full equation in the form we will actually solve:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\,\psi = E\,\psi. \tag{5}$$

Recall from Section 3 that inside the box, $V(x) = 0$. This simplifies our equation to

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\,\psi \qquad \Longrightarrow \qquad \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2mE}{\hbar^2}\psi. \tag{6}$$

Now, we can group the constant terms together and express them as k^2 such that

$$k = \frac{\sqrt{2mE}}{\hbar}, \qquad \text{and} \qquad \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -k^2\psi. \tag{7}$$

This equation asks for a function that, when differentiated twice, returns a multiple of itself: $-k^2\psi$. Sine and cosine both have this exact property, and the equation is known as the equation of **simple harmonic motion**. Its general solution is

$$\psi(x) = A\sin(kx) + B\cos(kx), \tag{8}$$

where A and B are constants.

Step 2: Applying the boundary conditions

At the left wall, $\psi(0) = 0$ gives

$$A\sin 0 + B\cos 0 = 0$$

since $\sin 0 = 0$ and $\cos 0 = 1$,

$$\begin{aligned} A(0) + B(1) &= 0 \\ B &= 0 \end{aligned}$$

so the cosine term disappears and we are left with

$$\psi(x) = A\sin(kx). \tag{9}$$

At the right wall, $\psi(L) = 0$ gives

$$A\sin(kL) = 0.$$

Either $A = 0$, which would mean the wavefunction is always zero (so there is no particle), or $\sin(kL) = 0$. The sine function is zero only at integer multiples of π, so

$$kL = n\pi \quad \Longrightarrow \quad k_n = \frac{n\pi}{L}, \qquad n \in \mathbb{Z}^+ \tag{10}$$

Step 3: Finding an expression for E

Now that we have two equations for k (equation (7) and equation (10)), we can equate them and solve for the total energy, E:

$$\begin{aligned} \frac{\sqrt{2mE_n}}{\hbar} &= \frac{n\pi}{L} \\ 2mE_n &= \left(\frac{n\pi\hbar}{L}\right)^2 \\ E_n &= \frac{n^2\pi^2\hbar^2}{2mL^2} \end{aligned}$$

Remembering that $\hbar = \frac{h}{2\pi}$, we obtain the final expression for energy,

$$E_n = \frac{n^2h^2}{8mL^2}, \qquad n \in \mathbb{Z}^+ \tag{11}$$

An interesting observation here is that the energy is **quantised**, meaning it can only take certain discrete values corresponding to different values of n. Crucially, it can never be zero. Even in its lowest energy state, a confined particle always retains some kinetic energy. This minimum energy is known as the **zero-point energy**, E_1. The zero-point energy for an electron in a 1nm box is 6×10^{-20}J (about 0.4eV), while a 0.16kg cricket ball in a 1 m gutter has E_1 of order 10^{-67}J. While this means the cricket ball is technically moving, the scale is unfathomably small; in 13.8 *billion* years (the age of the universe), the ball will have covered a distance of 10^{-15}m, about the size of a single proton.

Step 4: Normalising the wavefunction

One thing is still missing: the constant A. To find it, we can use the normalisation condition outlined in equation (2):

$$\int_0^L |\psi_n(x)|^2 \, \mathrm{d}x = 1$$

Substituting k_n into equation (9) gives $\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$.

$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) \mathrm{d}x = 1$$

Using the identity $\sin^2\theta = \frac{1}{2}(1 - \cos 2\theta)$,

$$\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) \mathrm{d}x = \frac{1}{2}\int_0^L \left(1 - \cos\frac{2n\pi x}{L}\right) \mathrm{d}x = \frac{1}{2}\left[x - \frac{L}{2n\pi}\sin\frac{2n\pi x}{L}\right]_0^L = \frac{L}{2},$$

so we now have

$$A^2\frac{L}{2} = 1 \qquad \Longrightarrow \qquad A = \sqrt{\frac{2}{L}}.$$

Our complete solution is therefore

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad 0 \le x \le L} \tag{12}$$

5 Conclusion

We have seen that a particle is not a tiny ball with a definite position, but is described by a wavefunction, $\psi(x)$, whose square gives the probability of finding it. By solving $\hat{H}\psi = E\psi$ for a particle in a one-dimensional box, we found that the energy is **quantised**, with $E_n = \frac{n^2h^2}{8mL^2}$, and that the lowest energy is never zero. From a single differential equation and two boundary conditions, we have uncovered one of the strangest and most important ideas in modern science: that for a confined particle, energy comes in discrete steps and is never zero.