Building a quantum system in Quantum Composer
Extension

1 The time-independent Schrödinger equation

Remember this equation, way back in Part I?

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi. \tag{1}$$

We call Equation 1 the *time-dependent* Schrödinger equation because Ψ can (and in the majority of cases does) change with time. In the main exercises, you have been solving Equation 1 *numerically*, in other words, using a computer algorithm that approximates the solution. Note that you never got out a function when solving for Ψ, but rather a set of numbers plotted on a graph. The aim of this extension exercise is to show you how to solve the equation *analytically*, in other words, using algebra.

In mathematics, a very common method of solving an equation is to make an educated guess at a solution, substitute it into the equation, and use the new equation you obtain to constrain the solution in some way. For example, consider the first order ordinary differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} + y = x. \tag{2}$$

One way we might solve this is to guess that the solution looks like $y = ax + b$. We substitute this in to obtain

$$a + ax + b = x. \tag{3}$$

For this to be true, $a = 1$ [1]. Furthermore, $a + b = 0$, so $b = -1$. Our solution is $y = x - 1$.

The Schrödinger equation is a bit more complicated, but the process of solving it is similar. We *assume* that Ψ is of the form "some function of x *only* multiplied by some function of t *only*".

$$\Psi(x,t) = \psi(x)\phi(t). \tag{4}$$

Substitute this into Equation 1. After a bit of algebra, we get

$$i\hbar\frac{1}{\phi(t)}\frac{\mathrm{d}\phi}{\mathrm{d}t} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x). \tag{5}$$

Now comes the most important part, so pay attention. The left hand side depends on t only, while the right hand side depends on x only (assuming that the potential is time-independent, which it always is in the *Quantum Composer* exercises you have been doing). So for the two sides to be equal, they must both equal an expression that is independent of both x and t, in other words, a constant.

Call this constant E. Then

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V = E. \tag{6}$$

Multiply by ψ and we obtain the time-*in*dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi. \tag{7}$$

Equation 7, it turns out, is much easier to solve than the time-dependent Schrödinger equation.

[1] There is one x on the right hand side, and there are a x's on the left hand side. Since this is an equation, $a = 1$.

2 The infinite potential well

In the infinite potential well, we define

$$V = \begin{cases} 0 & 0 < x < a, \\ \infty & \text{otherwise.} \end{cases} \tag{8}$$

The infinite potential well is contrived, and does not exist in real life. But it is a very useful example, because it is easy to solve analytically.

In the regions with infinite potential, the wave function does not exist because there is no way a particle can penetrate through an infinite barrier. Imagine throwing a ball over an infinitely high wall: no matter how much energy you give the ball, it will not go over.

And what about in the regions of zero potential? This is where Equation 7 comes in. Setting $V = 0$,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi. \tag{9}$$

Equation 9 belongs to a class of equations that have been studied extensively. Just as in the simple example in Equation 2, we guess a solution.

$$\psi(x) = A\sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) + B\cos\left(\frac{\sqrt{2mE}}{\hbar}x\right). \tag{10}$$

Rationalise the solution in Equation 10 this way: differentiating $\sin(kx)$ or $\cos(kx)$ twice gives $-k^2\sin(x)$ or $-k^2\cos(x)$. Dividing Equation 9 through by E,

$$-\frac{\hbar^2}{2mE}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \psi. \tag{11}$$

This means that $-k^2 = -(\frac{2mE}{\hbar^2})^2$, and $k = \frac{\sqrt{2mE}}{\hbar}$.

Try opening `Exercise1.flow` in *Quantum Composer* again, and type `infinity(0,a)` into the **Potential** box. Can you see that the wave functions look sinusoidal?

3 Deriving the energy expression

The use of E as the constant of separation was not a random choice. E stands for energy. Knowing this, we can derive the $E_n \propto n^2$ relationship you saw in Part II.

The key step here is that $\psi(x)$ must be zero at both $x = 0$ and $x = a$. We already know that $\psi(x)$ is zero *below* $x = 0$ and *above* $x = a$. This means that, if we are not to have a wave function that jumps abruptly at boundaries (in physics, things that jump like that rarely occur), $\psi(x)$ must also be zero *at* both $x = 0$ and $x = a$. We write

$$\psi(0) = 0, \psi(a) = 0. \tag{12}$$

We can immediately discard the cosine term in Equation 10 because the cosine function is not zero at $x = 0$, no matter what constant you slap in front of the x. We are left with

$$\psi(x) = A\sin\left(\frac{\sqrt{2mE}}{\hbar}x\right). \tag{13}$$

Now that we've dealt with the condition at $\psi(0) = 0$, we can turn our attention to the second condition, $\psi(a) = 0$. We know that the condition for $\sin(z)$ to be zero is

$$z = n\pi, \quad n = 0, \pm 1, \pm 2, ... \tag{14}$$

Hence, substituting $x = a$,

$$\frac{\sqrt{2mE_n}}{\hbar}a = n\pi, \tag{15}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}. \tag{16}$$

Since π, $\hbar$, m, and a are constants, $E_n \propto n^2$. Try checking the values given by Equation 16 with those provided by *Quantum Composer*.