Building a quantum system in Quantum Composer
Part I: Introduction

1 Introducing Schrödinger

1.1 Wave functions and potentials

Imagine a ball moving in a very deep well. Ignore gravity and friction for now and assume that the ball is constrained to move from one side of the well to the other, say on perfectly smooth rails. Given a set of initial conditions, you can use classical mechanics — Newton's laws, for example — to figure out precisely where the ball is at a given time. We say that such a system is *deterministic*.

Quantum mechanics, as you'll soon see, isn't deterministic. While some laws of physics still apply, we have to replace Newton's equations with something new. We call it the *Schrödinger equation*.

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

It looks complicated, but Equation 1 is just a statement that the total energy is constant. You don't really have to worry about solving the equation at the moment, as *Quantum Composer* will do it for you. But to understand the principles behind what you'll be learning, you should know what the symbols mean.

- x is a horizontal coordinate, t is time, m is the mass of the particle.

- Ψ is, in some sense, the whole point of the Schrödinger equation. We call it the *wave function*, and most problems in quantum mechanics involve solving the Schrödinger equation to find this function. But what *is* Ψ? Well, Ψ for a particle is a bit abstract. It's defined in such a way that its *magnitude* (think of this as its absolute value for now) is a probability density function of the particle's position. That is, if you have a well and you measure the position of the particle, $\int_a^b |\Psi(x)|^2 \, \mathrm{d}x$ is the probability of finding it between a and b. Figure 1 compares the classical ball in a well with various solutions to the Schrödinger equation describing an analogous situation in quantum mechanics.

- $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$ gives the kinetic energy. Think of it as the quantum mechanical equivalent of $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$.

- V is the *potential energy*. Just like when a ball rolls up the sides of a bowl, it loses kinetic energy and gains gravitational potential energy, so too the quantum particle has a different potential energy (and hence a different kinetic energy) at different displacements. In our classical analogy, if the sides of the bowl are so high that the ball cannot get out, the ball must be contained in the bowl. In quantum mechanics, particles may leak out of their potential wells. You will exploit this property in the tunnelling exercise later on.

- $\hbar$ and i are constants. Don't worry about what they mean for now.

1.2 Investigating the harmonic oscillator

Open the file `Exercise1.flow` in *Quantum Composer*. To do this, select **File** > **Open**, then choose the file you want to open. You should see something that looks like Figure 2. There are four boxes.

Quantum Composer is designed to have an intuitive interface. Each box is a single function which takes one or more inputs and produces one or more outputs. The inputs are represented by coloured circles on the left hand side of the box, while the outputs are represented by coloured circles on the right hand side. You can connect the inputs and outputs of different functions by clicking on a circle and dragging
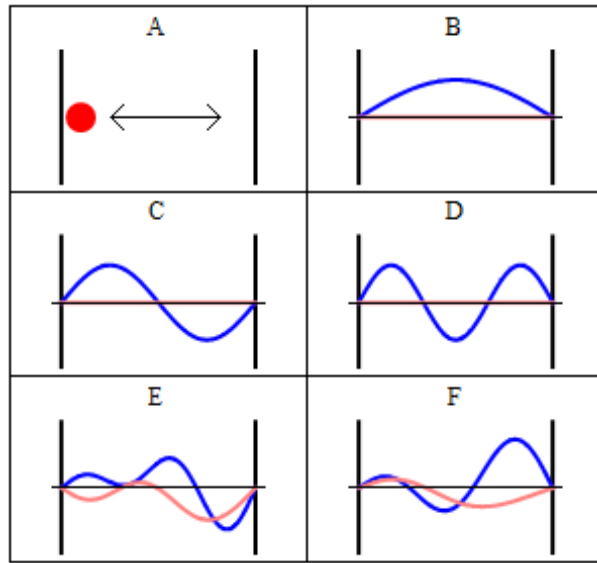
Figure 1: A ball moving in a potential well. (A) shows the classical picture, the other panels show various solutions of the Schrödinger equation for a quantum ball.
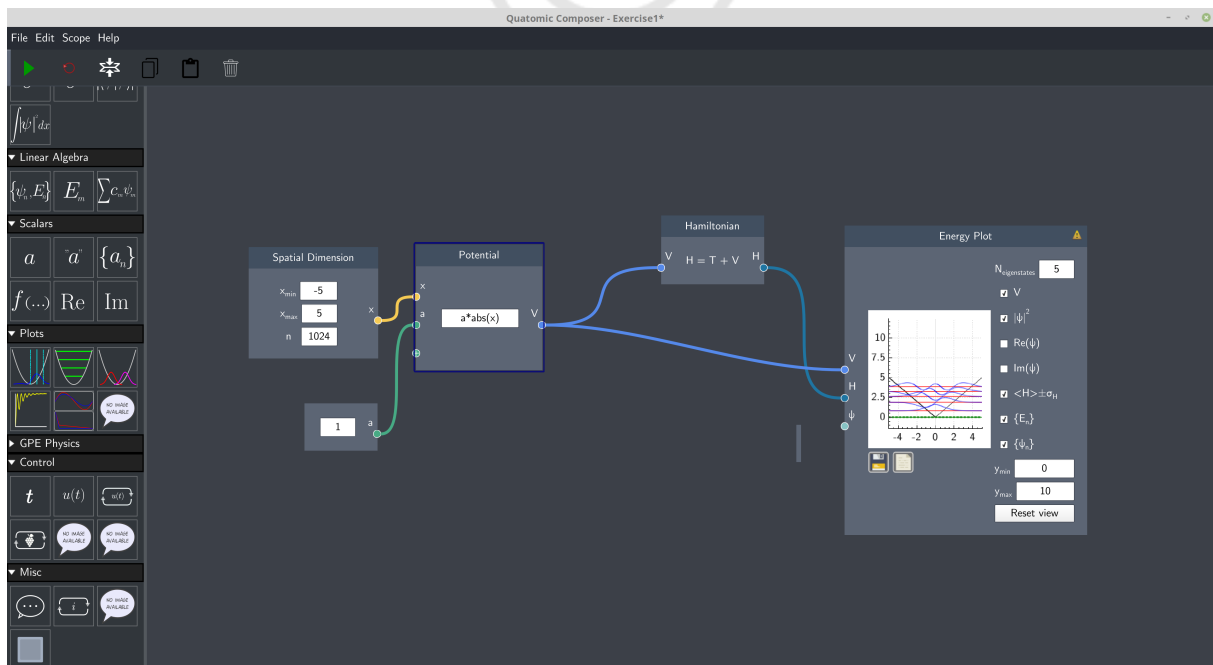

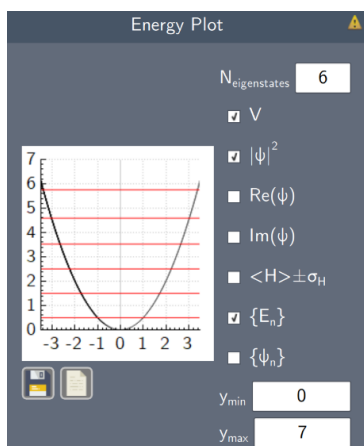Figure 2: The *Quantum Composer* interface.

Figure 3: The form of the harmonic oscillator potential.

to another circle. This produces a line between two boxes. However, since the flow charts have already been constructed for you, you should not have to do this. Drag the boxes around by left-clicking on them to arrange the workspace, and move around the page by using right-click. Zoom using the scroll wheel. The boxes are defined as follows:

- **Spatial Dimension** lets you adjust the range of x values plotted on the graphs. The parameter n affects the accuracy of the solution — the larger n, the better the solution, but the slower the simulation runs.

- **Potential** lets you define the potential energy as a function of x. You can use parameters in your definitions, but these have to be specified in a **Scalar** box and connected to the potential. One such box is labelled `a` in the flow chart you have opened. Changing the value in the box allows you to adjust the potential.

- **Hamiltonian** solves the Schrödinger equation for the given potential. The term *Hamiltonian* is simply a technical name for the sum of the kinetic and potential energies in Equation 1.

- **Energy Plot** plots the form of the potential. It also plots a set of very special energies and their corresponding wave functions. You'll see lots more of these in the next exercise.

You'll be investigating a special parabolic potential, which we call the *harmonic potential*. Harmonic potentials occur all over the place. The potential experienced by a mass oscillating on a spring or a simple pendulum is harmonic, while the potential experienced by the atoms in a diatomic molecule is harmonic for small oscillations. Perhaps you know that the equation for the potential energy in a stretched spring is

$$V(x) = \frac{1}{2}kx^2, \tag{2}$$

where k is the spring constant. We define the angular frequency ω to be

$$\omega := \sqrt{\frac{k}{m}}. \tag{3}$$

Thus we can eliminate k to give $V(x) = \frac{1}{2}m\omega^2 x^2$. We will use a instead of ω because this is easier to type, and set $m = 1$.

Type `0.5*a^2*x^2` in the **Potential** box. You should see something that looks like Figure 3. The black line represents the form of the potential, a parabola. The red lines are the energy levels that *Quantum Composer* has calculated. The blue lines are the wave functions corresponding to each of the energy levels. The check boxes on the right of the plot control which lines are displayed. Try checking and unchecking them now to see their effects. Now display the energy levels. What do you notice about their spacing?