

4. We begin by considering the Schrödinger equation for the harmonic oscillator:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{m\omega^2 x^2}{2} \psi = E\psi \quad (1)$$

Firstly, to make some things easier, we will consider the values of  $\hbar$ ,  $\omega$ , and  $m$  to be 1. Now in order to approximate the second derivative in the equation above, we will use a finite difference scheme, namely a second order, centred difference. To do this, we first need to create a grid of  $x$  points, which we will consider on the interval  $[-5, 5]$  with 1000 grid points  $x_i$ . We will use the notation  $\psi(x_i) = \psi_i$ . Now we can discuss the approximation of the derivative:

$$\frac{d^2\psi}{dx^2} \approx \frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{\Delta x^2} \quad (2)$$

where  $\Delta x$  is  $10/1000$ , the distance between grid points.

Now we can rewrite our Schrödinger equation in its discretised form:

$$-\frac{1}{2} \frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{\Delta x^2} + \frac{x^2}{2} \psi_i = E\psi_i \quad (3)$$

We can simply inspect the equation to find the matrix that can act on  $\psi$  to give us  $E\psi$ , finding it to be

$$H = \begin{pmatrix} \frac{1}{\Delta x^2} + \frac{x^2}{2} & -\frac{1}{2\Delta x^2} & 0 & \dots & 0 \\ -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + \frac{x^2}{2} & -\frac{1}{2\Delta x^2} & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + \frac{x^2}{2} & -\frac{1}{2\Delta x^2} \\ 0 & \dots & 0 & -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + \frac{x^2}{2} \end{pmatrix} \quad (4)$$

We can use any method to solve this system for its eigenvalues and eigenvectors, and we chose to use the **Eigensystem** method from Mathematica. This method spits out all  $N$  eigenvalues and eigenvectors, for  $N$  being the size of the matrix, in our case 1000, so we simply chose the last 4, which were

$$E = 0.499997 \quad 1.49998 \quad 2.49996 \quad 3.49992$$

This is fairly close to the expected 0.5, 1.5, 2.5, 3.5, in units of  $\hbar\omega$  of course, and can be improved by increasing the number of grid points. The corresponding eigenvectors were

