Experiment 2.6: One-Dimensional Schroedinger Equation

Introduction

At the core of quantum mechanics lays the dualism between particles and waves, by which a particle – e.g. an electron – will display particle or wave behaviour according to the characteristics of the system (e.g. its typical lengths) and the quantities we want to measure. The Schroedinger Equation (SE) is the fundamental equation in quantum mechanics, and its solutions provide us with the wave description of particles, their time evolution when interacting among each other or with external potentials and their – quantised or not – corresponding energies.
In this experiment we will consider the time-independent Schroedinger Equation – a second order differential equation – for a single particle in one dimension, in an external confining potential given by a square box. The modulus square of the solution to this equation – the wave function – will give the probability that the particle is found at certain point x in space in an experimental measurement.
This SE equation is given by

$$\frac{d^2\psi(x)}{dx^2} + k^2(x)\psi(x) = 0, \tag{1}$$

with

$$k^2(x) = \frac{2m}{\hbar^2}[E - V(x)], \tag{2}$$

$\psi(x)$ the quantum mechanical wave function, m the mass of the particle and E its energy. The boundary conditions are given by $\psi(x \to \pm\infty) = 0$. The potential $V(x)$ is sketched in Fig.1. We will consider the dimensionless units $2m/\hbar^2 = 1$.
In this experiment we shall use the "shooting method" to calculate the correct particle energy E and the (2,2) Runge-Kutta method, as developed in experiment 2.2 to integrate the Schroedinger equation.

Objectives

- to solve computationally an eigenvalue problem, i.e. a differential equation of the form

  $$[-\frac{d^2}{dx^2} + V(x)]\psi(x) = E\psi(x), \tag{3}$$

  which presents multiple solutions and where both the solution(s) $\psi(x)$ and the number(s) E are unknown.

- to analyse computationally how the behaviour of the solutions $\psi(x)$ and the energies E changes as V(x) is varied

- to compare the numerical solution with an exact limiting case.

Experiment

The confining potential $V(x)$ presents a square-well structure characterised by its width $L = 4$ and its height V_0 (see Fig.1).

1. Find the lowest bound energy E_1 when $V_0 = 10$. Plot the corresponding wave function $\psi_1(x)$ (renormalise your plot so that its maximum or its integral – normalisation condition – is equal to 1) and the derivative of the logarithm of the solution (DLS) you have used to find the correct E_1.

2. Are there any other bound solutions $E_2,\ E_3 \ldots$ for this system? If so, estimate their values by plotting the corresponding DLS.

3. Study how E_1 and $\psi_1(x)$ change as V_0 is increased. Plot your results for E_1 versus V_0 and the wavefunctions $\psi_1(x)$ for some representative values of V_0. Renormalise your plot so that the wave functions are comparable, e.g. their integral is always equal to 1 (normalisation condition).

4. Compare your numerical solutions E_1 and $\psi_1(x)$ obtained for large V_0 with the exact solutions for an infinite square well ($V_0 = \infty$), which is given by:

$$E_n = \frac{n^2\pi^2}{L^2} \tag{4}$$

and

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L}). \tag{5}$$

Plot the comparison between the exact and the numerical $\psi_1(x)$. How large V_0 must be such that E_1 and $\psi_1(x)$ can be approximated by these limiting exact solutions?

5. How large V_0 must be such that also E_2 (E_3) and $\psi_2(x)$ ($\psi_3(x)$) can be approximated by the limiting exact solutions, with $|E_{n,num} - E_{n,exact}|/E_{n,exact}$ of the order of few percent? Plot the DLS used to support your answer and the comparison between the exact and the numerical wavefunctions.

(hint: to find the correct solutions you will have to integrate the SE over a box of width $l > L$, imposing the boundary conditions at its borders. The precision of your solution will depend on the size l of this box and on the interval dx you will use to integrate the SE with the Runge-Kutta method).

Shooting method

This method finds the solutions to a differential equation when the value of a parameter as well as the solution to the differential equation must be found at the same time.
In the case of Eq. (1) the parameter is the energy E and, for the particle in the box, solutions will be allowed only for specific, discrete values of E, i.e. $E_1,\ E_2, \ldots$.
Main idea: Eq. (1) will be solved many times by varying the value of E and only the values which will satisfy the boundary conditions and provide continuous solutions will be acceptable energies.

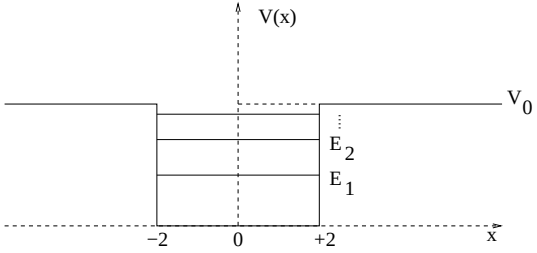

Figure 1: Confining potential $V(x)$

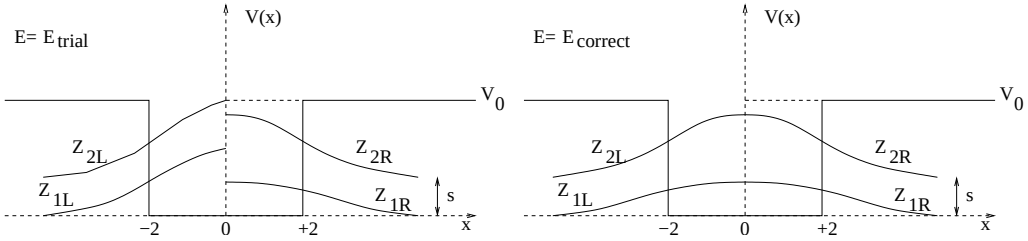

Figure 2: shooting method

In our case, since the boundary conditions are set at the border of the box, we will solve Eq. (1) from left ($\psi_L(x;E)$) and right ($\psi_R(x;E)$) using the Runge-Kutta method. The correct energies E will be the values for which the solutions and their derivatives match at the centre $x = 0$. This is described in Fig.2, with the notation $z_1(x) = \psi(x)$ and $z_2(x) = d\psi/dx$.
Boundary conditions: $\psi_{L,R}(x \to \infty) = 0$; $d\psi_L(x \to \infty)/dx = s$, $d\psi_R(x \to \infty)/dx = -s$. (hint: you can choose $s = 1$; if your box is very large, you may want to reduce the value of s)
Since both $\psi(x)$ and $\alpha\psi(x)$ are solutions of the SE, the matching conditions $z_{1L}(0) = z_{1R}(0)$ and $z_{2L}(0) = z_{2R}(0)$ reduce to a single condition

$$\frac{z_{2L}(0)}{z_{1L}(0)} = \frac{z_{2R}(0)}{z_{1R}(0)}, \tag{6}$$

i.e. the derivative of the logarithm of the solution (DLS) must match at the centre. By plotting DLS for the R and L solutions versus the parameter E it is then possible to find the solutions to Eq.6 and to our problem.

(2,2) Runge-Kutta method

Eq. (1) can be rewritten as a system of two coupled differential equations

$$\frac{dy_1}{dt} = f_1(t, y_1, y_2) \tag{7}$$

$$\frac{dy_2}{dt} = f_2(t, y_1, y_2). \tag{8}$$

The time interval of interest is then discretised in n steps of width h. This parameter will determine the accuracy of the solution, the error being of order $o(h^3)$.

The solutions to Eq. (7) and (8) at the $(i+1)$-th step are given by

$$y_{1,i+1} = y_{1,i} + \frac{K_{11} + K_2}{2} \tag{9}$$

$$y_{2,i+1} = y_{2,i} + \frac{K_{22} + K_1}{2} \tag{10}$$

with

$$K_{11} = hf_1(t_i, y_{1,i}, y_{2,i}) = K_{21} \tag{11}$$

$$K_{22} = hf_2(t_i, y_{1,i}, y_{2,i}) = K_{12} \tag{12}$$

$$K_1 = hf_2(t_i + h, y_{1,i} + K_{21}, y_{2,i} + K_{22}) \tag{13}$$

$$K_2 = hf_1(t_i + h, y_{1,i} + K_{11}, y_{2,i} + K_{12}). \tag{14}$$

To initialise the calculation it is sufficient to provide the values of y_1 and y_2 at the chosen initial time t_0.
To test the method it is convenient to consider, as a first step, a system of differential equations whose solution is known. In any case it is important to check if the value chosen for h is appropriate for the precision required by the problem.