Computational Methods and Data Analysis 2002

Ex. 1: Bound states in a finite square well

This exercise covers the topics of the first two lectures, numerical differentiation, root finding and numerical integration.

Consider a square potential well of finite height V_0 and width $2a$, as in figure 1.

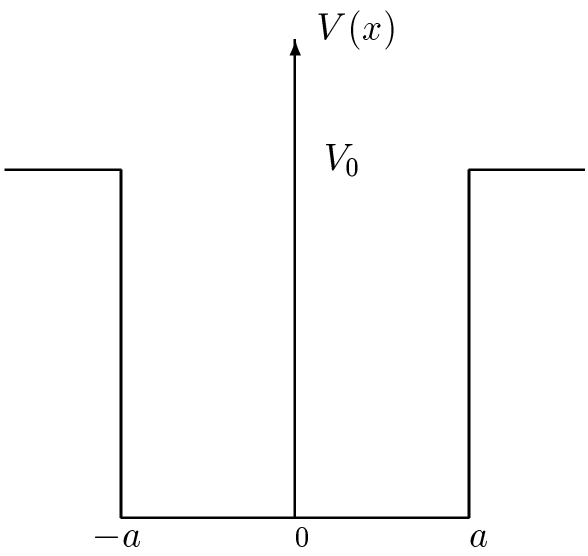

Figure 1: Finite potential well

The Schrödinger equation:

$$\frac{d^2\Psi}{dx^2} - \frac{2m}{\hbar^2}\left[V(x) - E\right]\Psi = 0$$

with $V(x)$ given by:

$$\begin{aligned} V(x) &= V_0 \qquad x < -a \qquad && \text{region } I \\ V(x) &= 0 \qquad -a < x < a \qquad && \text{region } II \\ V(x) &= V_0 \qquad x > a \qquad && \text{region } III \end{aligned}$$

has general solutions for the bound states at energy less than V_0 in the three regions given by:

$$\begin{aligned} \Psi_I(x) &= A\ \exp^{\beta x} + B\ \exp^{-\beta x} \qquad && x < -a \\ \Psi_{II}(x) &= C\ \sin\alpha x + D\ \cos\alpha x \qquad && -a < x < a \\ \Psi_{III}(x) &= E\ \exp^{\beta x} + F\ \exp^{-\beta x} \qquad && x > a \end{aligned}$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}}$$
$$\beta = \sqrt{2m(V_0 - E)/\hbar^2}$$

The boundary conditions require continuity of the wavefunction and of its derivative at the boundary, whence

Even states: $B = E = 0, C = 0, D \neq 0, A = F \qquad \alpha \tan \alpha a = \beta$
Odd states: $B = E = 0, C \neq 0, D = 0, A = -F \qquad \alpha \cot \alpha a = -\beta$

Therefore eigenvalues of the Schrödinger equation are found by solving numerically:

$$\alpha tg(\alpha a) - \beta = 0 \quad \text{for even states}$$
$$\alpha ctg(\alpha a) + \beta = 0 \quad \text{for odd states}$$

A more convenient form is:

$$\alpha sin(\alpha a) - \beta cos(\alpha a) = 0 \quad \text{for even states}$$
$$\alpha cos(\alpha a) + \beta sin(\alpha a) = 0 \quad \text{for odd states}$$

Use $2a$=10 Å, $m = 1\ m_e$. It is useful to use $\hbar^2 = 7.6199682 m_e$ eV Å^2

1. The repetitive nature of the tangent suggests that there might be several solutions, one per each cycle of the function. Establish the intervals in which roots exist. Remember that, in one dimension, a square well has always at least one bound state at $E \neq 0$.

2. Find all bound states with precision 10^{-4} eV by use of the bisection, Newton and secant methods for several values of V_0 between V_0=0.2 eV and V_0=5 eV.

3. Make a plot of the eigenvalues as a function of V_0, comparing also to the limiting case of an infinite well:

$$E_n = \frac{\hbar^2}{2m_e}\left(\frac{n\pi}{2a}\right)^2. \tag{1}$$

   Give some of the data also in a Table in order to check that the results are correct within the desired precision. Do not forget to label the axis of the figures and to make clear table and figure captions, giving the used units and for which values of the parameters (e.g which value of a) the calculation is done.

   The idea is that, even without the text of the exercise, by reading the report one can understand and reproduce the calculation. Comment briefly the results.

4. Facultative: Make a plot of the eigenvalues as a function of a for V_0=3 eV.

5. Calculate (and plot) the normalized wavefunction corresponding to the first two bound states for two values of V_0 and comment the results. To perform the integral needed to normalize the wavefunction you need to specify the range of integration. This obviously requires an approximation, the desired range is in principle from minus to plus infinity. However, once you know the energy of a given state you can estimate the decay length of the wavefunctions in the forbidden barrier regions in order to define a sensible range for integration. Describe your reasoning in doing this. Test convergence of your results as a function of the number of points on which the integral is evaluated. In defining the grid of points on which the wavefunction is calculated to perform the integration choose a spacing which fits into the well.

6. Check numerically that, as expected from quantum mechanics, the eigenfunctions corresponding to different eigenvalues are orthogonal.