Numerieke methoden in de natuurwetenschappen

Ex. 1: Bound states in a finite square well

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

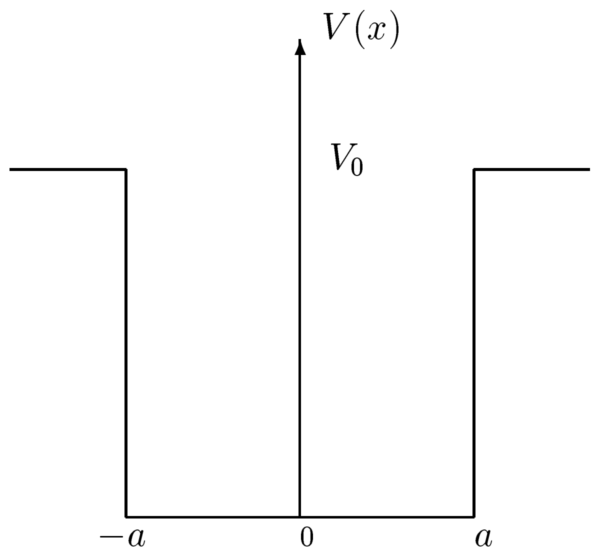

Figure 1: Finite potential well

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:

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

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

$$\begin{aligned}
\Psi_I(x) &= A \ \exp^{\beta x} + B \ \exp^{-\beta x} \qquad x < -a \\
\Psi_{II}(x) &= C \ \sin \alpha x + D \ \cos \alpha x \qquad -a < x < a \\
\Psi_{III}(x) &= E \ \exp^{\beta x} + F \ \exp^{-\beta x} \qquad x > a \\
\alpha &= \sqrt{\frac{2mE}{\hbar^2}} \\
\beta &= \sqrt{2m(V_0 - E)/\hbar^2}
\end{aligned}$$

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:

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

A more convenient form is:

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

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:

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

   Do not forget to label the axis 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. If you use gnuplot, you could plot the eigenvalues with linespoints so that you can trace back for which values of V_0 the calculations has been performed.

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

[1]

[1] More details on this problem and on computational strategy can be found in: P.L. De Vries *A first course in computational Physics*, J. Wiley & sons, N.Y. 1994