Numerical Solutions for the Finite Potential Well

Schrodinger's equation is integrated numerically for the first three energy states for a finite potential well. The integration algorithm is taken from J. C. Hansen, *J. Chem. Educ. Software*, **8C2**, 1996.

Set parameters:

$n := 100$ $\quad xmin := -3$ $\quad xmax := 3$ $\quad \Delta := \frac{xmax - xmin}{n - 1}$

$\mu := 1$ $\quad lb := -1$ $\quad rb := 1$ $\quad V_0 := 4$

Calculate position vector, the potential energy matrix, and the kinetic energy matrix. Then combine them into a total energy matrix.

$i := 1 .. n$ $\quad j := 1 .. n$ $\quad x_i := xmin + (i - 1)\cdot\Delta$

$$V_{i,i} := if\left[\left(x_i \geq lb\right)\cdot\left(x_i \leq rb\right), 0, V_0\right] \qquad T_{i,j} := if\left[i = j, \frac{\pi^2}{6\cdot\mu\cdot\Delta^2}, \frac{(-1)^{i-j}}{(i-j)^2\cdot\mu\cdot\Delta^2}\right]$$

Form Hamiltonian energy matrix: $H := T + V$

Find eigenvalues: $E := sort(eigenvals(H))$ Display three eigenvalues: $m := 1 .. 3$ $E_m =$

0.63423174
2.39691438
4.4105828

Calculate associated eigenfunctions: $k := 1 .. 2$ $\quad \Psi(k) := eigenvec\left(H, E_k\right)$

Plot the potential energy and bound state eigenfunctions: $Vpot_i := V_{i,i}$