9.5: Particle in a Finite Potential Well

Numerical Solutions for the Finite Potential Well

Schrödinger'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	xmin = -3	xmax = 3	$\Delta = \frac{xmax - xmin}{n-1}$
μ = 1	lb = -1	rb = 1	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	j = 1 .. n	x_i = xmin + (i - 1) Δ

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

Form Hamiltonian energy matrix: H = TV

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 ψ(k) = eigenvec(H, E_k)

Plot the potential energy and bound state eigenfunctions: $V_{pot1} := V_{i,i}$