

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:

$n = 100$	$x_{\min} = -3$	$x_{\max} = 3$	$\Delta = \frac{x_{\max} - x_{\min}}{n-1}$
$\mu = 1$	$lb = -1$	$rb = 1$	$V_0 = 4$

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

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

Form Hamiltonian energy matrix: $H = TV$

Find eigenvalues: $E = \text{sort}(\text{eigenvals}(H))$

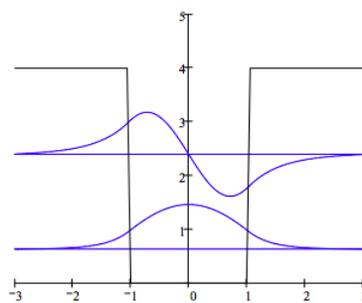
Display three eigenvalues: $m = 1 \dots 3$

$E_m =$

0.63423174
2.39691438
4.4105828

Calculate associated eigenfunctions: $k = 1 \dots 2 \quad \psi(k) = \text{eigenvec}(H, E_k)$

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



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