9.9: Numerical Solutions for the Harmonic Oscillator

Schrödinger's equation is integrated numerically for the first three energy states for the harmonic oscillator. The integration algorithm is taken from J. C. Hansen, ***J. Chem. Educ. Software,* 8C2**, 1996.

Set parameters:

Increments: n = 100

Integration limits: xmin = -5

xmax = 5

$$\Delta = \frac{xmax - xmin}{n-1}$$

Effective mass: μ = 1

Force constant: k = 1

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

$$i = 1 .. n \; j = 1 .. n \; x_i = xmin + (i - 1)\,\Delta$$

$$V_{i,\,j} = if\left[i = j,\ \frac{1}{2}k(x)^2,\ 0\right]$$

$$T_{i,\,j} = if\left[i = j,\ \frac{\pi^2}{6\mu\Delta^2},\ \frac{(-1)^{i-j}}{(i-j)^2\mu\Delta^2}\right]$$

Hamiltonian matrix: H = T + V

Find eigenvalues: E = sort(eigenvals(H))

Display three eigenvalues: m = 1 .. 3

E_m =

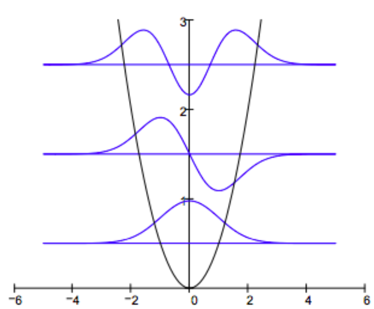
0.5000
1.5000
2.5000

Calculate associated eigenfunctions:

k = 1 .. 3

$$\psi(k) = eigenvec(H, E_k)$$

Plot the potential energy and selected eigenfunctions:



For V = ax^n the virial theorem requires the following relationship between the expectation values for kinetic and potential energy: <T> = 0.5n<V>. The calculations below show the virial theorem is satisfied for the harmonic oscillator for which n = 2.

$$\begin{pmatrix} \text{" Kinetic Energy "} & \text{" Potential Energy "} & \text{" Total Energy "} \\ \psi(1)^T T \Psi(1) & \psi(1)^T V \psi(1) & E_1 \\ \psi(2)^T T \Psi(2) & \psi(2)^T V \psi(2) & E_2 \\ \psi(3)^T T \Psi(3) & \psi(3)^T V \psi(3) & E_3 \end{pmatrix} = \begin{pmatrix} \text{" Kinetic Energy "} & \text{" Potential Energy "} & \text{" Total Energy "} \\ 0.2500 & 0.2500 & 0.5000 \\ 0.7500 & 0.7500 & 1.5000 \\ 1.2500 & 1.2500 & 2.5000 \end{pmatrix}$$