9.8: Numerical Solutions for a Particle in a V-Shaped Potential Well

Schrödinger's equation is integrated numerically for a particle in a V-shaped potential well. The integration algorithm is taken from J. C. Hansen, ***J. Chem. Educ. Software,*** **8C2**, 1996.

Set parameters:

$$n = 100 \quad xmin = -4 \quad xmax = 4 \quad \Delta = \frac{xmax - xmin}{n-1} \quad \mu = 1 \quad Vo = 2$$

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

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

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

Hamiltonian matrix: $H = T + V$

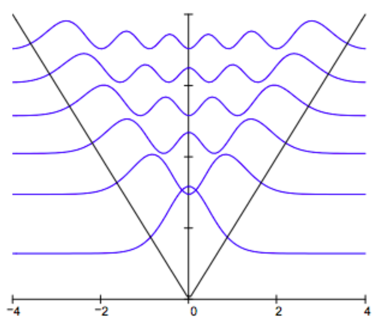
Calculate eigenvalues: $E = \text{sort}(\text{eigenvals}(H))$

Selected eigenvalues: $m = 1 .. 6$

$E_m =$

1.284
2.946
4.093
5.153
6.089
7.030

Display solution:



For $V = ax^n$ the virial theorem requires the following relationship between the expectation values for kinetic and potential energy: $\langle T \rangle = 0.5n\langle V \rangle$. The calculations below show the virial theorem is satisfied for this potential for which n = 1.

$$\begin{pmatrix} \text{" Kinetic Energy "} & \text{" Potential Energy "} & \text{" Total Energy "} \\ \psi(1)^T T \psi(1) & \psi(1)^T V \psi(1) & E_1 \\ \psi(2)^T T \psi(2) & \psi(2)^T V \psi(2) & E_2 \\ \psi(3)^T T \psi(3) & \psi(3)^T V \psi(3) & E_3 \end{pmatrix} = \begin{pmatrix} \text{" Kinetic Energy "} & \text{" Potential Energy "} & \text{" Total Energy "} \\ 0.428 & 0.857 & 1.284 \\ 0.982 & 1.964 & 2.946 \\ 1.365 & 2.728 & 4.093 \end{pmatrix}$$
