Numerical Solutions for a V-Shaped Potential Well

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Schrodinger'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:

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

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

$i := 1..n \qquad j := 1..n \qquad x_i := xmin + (i-1)\cdot\Delta \qquad V_{i,i} := Vo\cdot|x_i| \qquad T_{i,j} := \text{if}\left[i = j, \frac{\pi^2}{6\cdot\mu\cdot\Delta^2}, \frac{(-1)^{i-j}}{(i-j)^2\cdot\mu\cdot\Delta^2}\right]$

Hamiltonian matrix: $H := T + V$

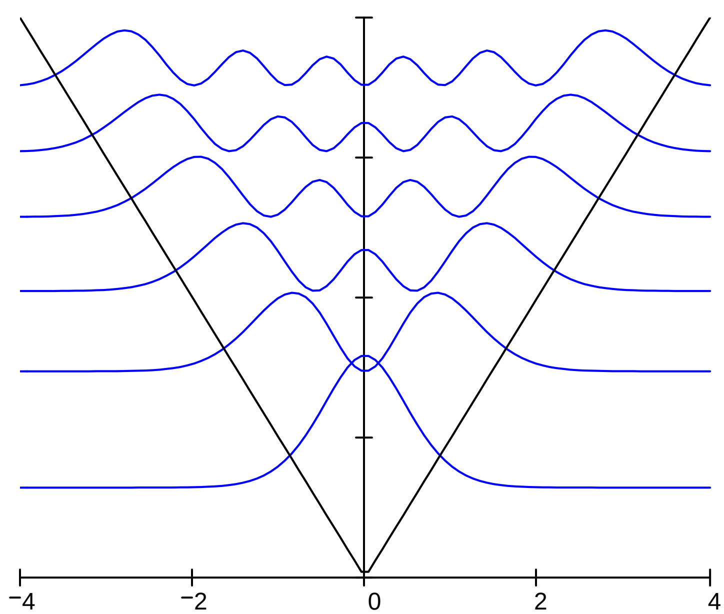
Calculate eigenvalues: $E := \text{sort}(\text{eigenvals}(H))$

Selected eigenvalues: $m := 1..6$ $E_m =$

1.284
2.946
4.093
5.153
6.089
7.030

Calculate eigenfunctions: $k := 1..6 \qquad \Psi(k) := \text{eigenvec}(H, E_k)$

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.

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