Quartic Oscillator

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

Set parameters:

Increments: $n := 100$ Integration limits: $xmin := -3$ $xmax := 3$ $\Delta := \frac{xmax - xmin}{n - 1}$

Effective mass: $\mu := 1$ Force constant: $k := 1$

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

$i := 1 .. n$ $j := 1 .. n$ $x_i := xmin + (i - 1)\cdot\Delta$

$$V_{i,j} := \text{if}\left[i = j, k\cdot(x_i)^4, 0\right] \qquad T_{i,j} := \text{if}\left[i = j, \frac{\pi^2}{6\cdot\mu\cdot\Delta^2}, \frac{(-1)^{i-j}}{(i-j)^2\cdot\mu\cdot\Delta^2}\right]$$

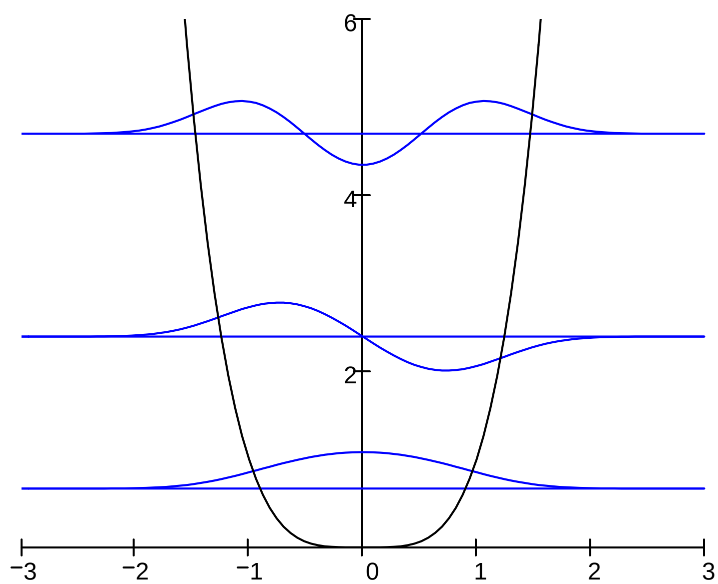
Form Hamiltonian energy matrix: $H := T + V$

Find eigenvalues: $E := \text{sort}(\text{eigenvals}(H))$ Display three eigenvalues: $m := 1 .. 3$ $E_m =$

0.6680
2.3936
4.6968

Calculate associated eigenfunctions: $k := 1 .. 3$ $\Psi(k) := \text{eigenvec}(H, E_k)$

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 quartic oscillator for which n = 4.

$$\begin{pmatrix} \text{"Kinetic Energy"} & \text{"Potential Energy"} & \text{"Total Energy"} \\ \Psi(1)^T \cdot T \cdot \Psi(1) & \Psi(1)^T \cdot V \cdot \Psi(1) & E_1 \\ \Psi(2)^T \cdot T \cdot \Psi(2) & \Psi(2)^T \cdot V \cdot \Psi(2) & E_2 \\ \Psi(3)^T \cdot T \cdot \Psi(3) & \Psi(3)^T \cdot V \cdot \Psi(3) & E_3 \end{pmatrix} = \begin{pmatrix} \text{"Kinetic Energy"} & \text{"Potential Energy"} & \text{"Total Energy"} \\ 0.4453 & 0.2227 & 0.6680 \\ 1.5958 & 0.7979 & 2.3936 \\ 3.1312 & 1.5656 & 4.6968 \end{pmatrix}$$