

9.11: Numerical Solutions for the Quartic Oscillator

Schrödinger'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: $x_{\min} = -3$

$x_{\max} = 3$

$$\Delta = \frac{x_{\max} - x_{\min}}{n - 1}$$

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.

$$i = 1 \dots n \quad j = 1 \dots n \quad x_i = x_{\min} + (i - 1) \Delta$$

$$V_{i,j} = if \left[i = j, k(x_i)^4, 0 \right]$$

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

Hamiltonian matrix: $H = T + V$

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

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

$E_m =$

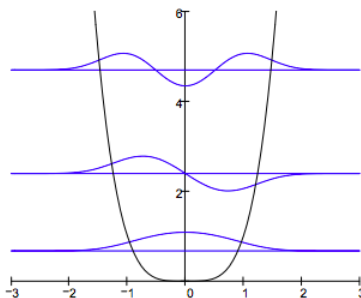
0.6680
2.3936
4.6968

Calculate associated eigenfunctions:

$k = 1 \dots 3$

$$\psi(k) = \text{eigenvec}(H, E_k)$$

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: $\langle T \rangle = 0.5n\langle V \rangle$. The calculations below show the virial theorem is satisfied for the harmonic oscillator for which $n = 4$.

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

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