

## 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:  $m = 1 \dots 3$

$E_m =$

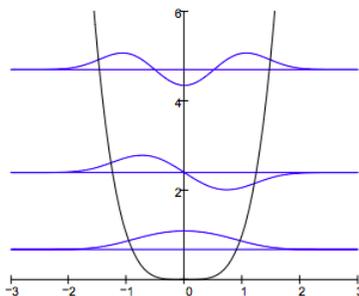
|        |
|--------|
| 0.6680 |
| 2.3936 |
| 4.6968 |

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  $n = 4$ .

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

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