
Set parameters:

Increments: \( n = 100 \)

Integration limits: \( xmin = -5 \)

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

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.

\[
i = 1 \ldots n \quad j = 1 \ldots n \quad x_{i} = x_{min} + (i - 1) \Delta
\]

\[
V_{i,j} = \begin{cases} \frac{1}{2} k (x)^2, & i = j \\ 0, & j \neq i \end{cases}
\]

\[
T_{i,j} = \begin{cases} \frac{\pi^2}{6 \mu \Delta^2}, & i = j \\ \frac{(-1)^{i-j}}{(i-j)^2 \mu \Delta^2}, & j \neq i \end{cases}
\]

Hamiltonian matrix: \( H = T + V \)

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

Display three eigenvalues: \( m = 1 \ldots 3 \)

\[
E_m =
\begin{array}{l}
0.5000 \\
1.5000 \\
2.5000
\end{array}
\]

Calculate associated eigenfunctions:
$k = 1 \ldots 3$

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

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 harmonic oscillator for which $n = 2$.

\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} \\
0.2500 & 0.2500 & 0.5000 \\
0.7500 & 0.7500 & 1.5000 \\
1.2500 & 1.2500 & 2.5000
\end{pmatrix}