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

Set parameters:

\[
\begin{align*}
n &= 300 \\
x_{\text{min}} &= -2 \\
x_{\text{max}} &= 12 \\
\Delta &= \frac{x_{\text{max}} - x_{\text{min}}}{n-1} \\
\mu &= 1 \\
D &= 2 \\
\beta &= 2 \\
x_e &= 0
\end{align*}
\]

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

\[
\begin{align*}
i &= 1 \ldots n & j &= 1 \ldots n \\
x_i &= x_{\text{min}} + (i - 1) \Delta \\
V_{i,j} &= \text{if} \left[ i = j, D \left[ 1 - \exp \left[ \beta (x_i - x_e) \right] \right]^2, 0 \right] \\
T_{i,j} &= \text{if} \left[ i = j, \frac{\pi^2}{6 \mu \Delta^2}, \frac{(-1)^{i-j}}{(i-j)^2 \mu \Delta^2} \right]
\end{align*}
\]

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

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

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

\[
\begin{array}{|r|}
\hline
E_m \\
0.8750 \\
1.8750 \\
2.0596 \\
\hline
\end{array}
\]
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:

\[ \langle T \rangle = 0.5n \langle V \rangle. \]

The calculations below show that virial theorem is not satisfied for the Morse oscillator. The reason is revealed in the following series expansion in \( \langle x \rangle \). The expansion contains cubic, quartic and higher order terms in \( \langle x \rangle \), so the virial theorem does not apply to the quartic oscillator.

\[ D (1 - \exp(-\beta x))^2 \] converts to the series \( D \beta^2 x^2 + (-D) \beta^3 x^3 + \frac{7}{12} D \beta^4 x^4 + O(x^5) \)

\[
\begin{pmatrix}
"Kinetic~Energy" & "Potential~Energy" & "Total~Energy"
\end{pmatrix} =
\begin{pmatrix}
0.3750 & 0.5000 & 0.8750 \\
0.3754 & 1.4996 & 1.8750 \\
0.3754 & 1.4996 & 1.8750 \\
\end{pmatrix}
\]