The Double Morse Oscillator

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

Set parameters:

$n := 200$ $\quad xmin := -10$ $\quad xmax := 10$ $\quad \Delta := \frac{xmax - xmin}{n - 1}$

$\mu := 1$ $\quad D := 2$ $\quad \beta := 1$ $\quad x_0 := 1$

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

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

$$V_{i,j} := \text{if}\left[i = j, D\cdot\left[1 - \exp\left[-\beta\cdot\left(|x_i| - x_0\right)\right]\right]^2, 0\right] \qquad T_{i,j} := \text{if}\left[i = j, \frac{\pi^2}{6\cdot\mu\cdot\Delta^2}, \frac{(-1)^{i-j}}{(i-j)^2\cdot\mu\cdot\Delta^2}\right]$$

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

Find eigenvalues: $E := \text{sort}(\text{eigenvals}(H))$ Display four eigenvalues: $m := 1 .. 4$ $E_m =$

0.8092
0.9127
1.8284
1.8975

Calculate associated eigenfunctions: $k := 1 .. 4$ $\quad \Psi(k) := \text{eigenvec}\left(H, E_k\right)$

Plot the potential energy and bound state eigenfunctions: $Vpot_i := V_{i,i}$