9.14: Numerical Solutions for the Double Morse Potential

Schrödinger'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

xmin = -10

xmax = 10

$$\Delta = \frac{xmax - xmin}{n - 1}$$

μ = 1

D = 2

β = 1

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 j = 1 .. n x_i = xmin + (i - 1) Δ

$$V_{i,\,j} = if\left[i = j,\ D\left[1 - exp\left[-\beta\left(\left|x_i\right| - x_0\right)\right]\right]^2,\ 0\right]$$

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

Hamiltonian matrix: H = T + V

Find eigenvalues: E = sort(eigenvals(H))

Display four eigenvalues: m = 1 .. 4

E_m =

0.8092
0.9127
1.8284
1.8975

Calculate associated eigenfunctions:

k = 1 .. 4

$$\psi(k) = eigenvec(H, E_k)$$

Plot the potential energy and bound state eigenfunctions:

$$Vpot_i = V_{i,\,i}$$