9.10: Numerical Solutions for a Double-Minimum Potential Well

Schrödinger's equation is integrated numerically for a double minimum potential well: $V = bx^4 - cx^2$. The integration algorithm is taken from J. C. Hansen, ***J. Chem. Educ. Software,*** **8C2**, 1996.

Set parameters:

Increments: n = 100

Integration limits: xmin = -4

xmax = 4

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

Effective mass: μ = 1

Constants: b = 1 c = 6

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

$$V_{i,\,j} = if\left[i = j,\ b(x_i)^4 - c(x_i)^2,\ 0\right]$$

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

Hamiltonian matrix:

$$H = T + V$$

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

Display three eigenvalues: m = 1 .. 5

E_m =

-6.64272702
-6.64062824
-2.45118605
-2.3155705
0.41561275

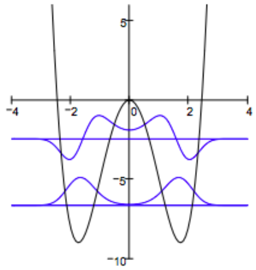
Calculate selected eigenvectors:

k = 1 .. 4

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

Display results:

First two even solutions:



First two odd solutions: