

## 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:  $x_{min} = -4$

$x_{max} = 4$

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

Effective mass:  $\mu = 1$

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.

$$i = 1 \dots n \quad j = 1 \dots n \quad x_i = x_{min} + (i - 1) \Delta$$

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

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

Hamiltonian matrix:

$$H = T + V$$

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

Display three eigenvalues:  $m = 1 \dots 5$

$E_m =$

-6.64272702
-6.64062824
-2.45118605
-2.3155705
0.41561275

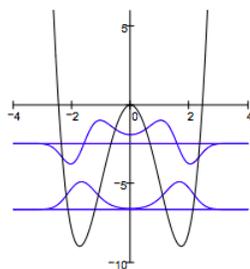
Calculate selected eigenvectors:

$k = 1 \dots 4$

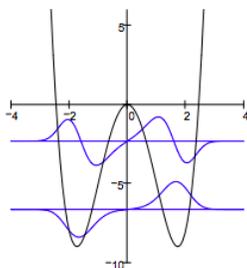
$$\psi(k) = \text{eigenvec}(H, E_k)$$

Display results:

First two even solutions:



First two odd solutions:




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