

9.13: Numerical Solutions for the Lennard-Jones Potential

Merrill (Am. J. Phys. **1972**, 40, 138) showed that a Lennard-Jones 6-12 potential with these parameters had three bound states. This is verified by numerical integration of Schrödinger's equation. The integration algorithm is taken from J. C. Hansen, *J. Chem. Educ. Software*, **8C2**, 1996.

Set parameters:

- $n = 200$
- $x_{min} = 0.75$
- $x_{max} = 3.5$
- $\Delta = \frac{x_{max} - x_{min}}{n - 1}$
- $\mu = 1$
- $\sigma = 1$
- $\epsilon = 100$

Numerical integration algorithm:

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

$$V_{i,j} = if \left[i = j, 4\epsilon \left[\left(\frac{\sigma}{x_i} \right)^{12} - \left(\frac{\sigma}{x_i} \right)^6 \right], 0 \right]$$

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

Hamiltonian matrix: $H = T + V$

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

Display three eigenvalues: $m = 1 \dots 4$

$E_m =$

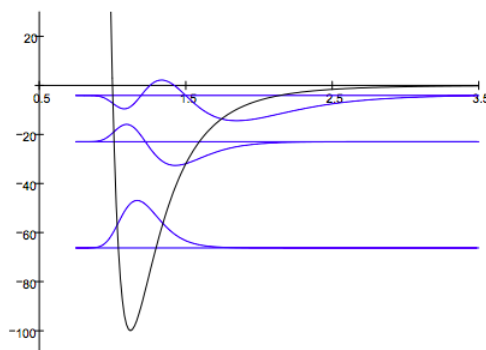
-66.269
-22.981
-4.132
1.096

Calculate eigenvectors:

$k = 1 \dots 3$

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

Display results:



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