# 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
- $x_{min} = 0.75$
- $x_{max} = 3.5$
- $\Delta = \frac{xmax - xmin}{n-1}$
- $\mu$ = 1
- $\sigma$ = 1
- $\varepsilon$ = 100

Numerical integration algorithm:

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

$$V_{i,\,j} = if\left[i = j,\ 4\varepsilon\left[\left(\frac{\sigma}{x_i}\right)^1 2 - \left(\frac{\sigma}{x_i}\right)^6\right], 0\right]$$

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

Hamiltonian matrix: H = T + V

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

Display three eigenvalues: m = 1 .. 4

$E_m$ =

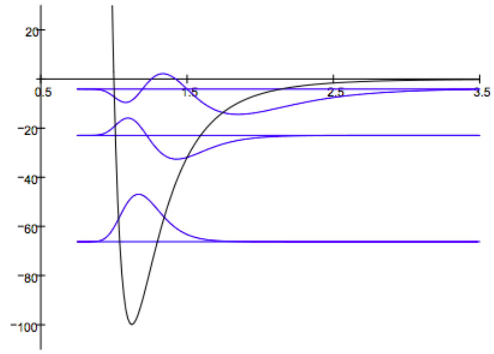
| |
|---|
| $-66.269$ |
| $-22.981$ |
| $-4.132$ |
| $1.096$ |

Calculate eigenvectors:

k = 1 .. 3

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

Display results:



20
-20
-40
-60
-80
-100
0.5
1.5
2.5
3.5