Numerical Solutions for the Lennard-Jones Potential

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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 Schrodinger's equation. The integration algorithm is taken from J. C. Hansen, *J. Chem. Educ. Software*, **8C2**, 1996.

Set parameters:

$n := 200 \qquad xmin := .75 \qquad xmax := 3.5 \qquad \Delta := \frac{xmax - xmin}{n-1}$

$\mu := 1 \qquad \sigma := 1 \qquad \varepsilon := 100$

Numerical integration algorithm:

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

$$V_{i,j} := \mathrm{if}\left[i = j, 4\cdot\varepsilon\cdot\left[\left(\frac{\sigma}{x_i}\right)^{12} - \left(\frac{\sigma}{x_i}\right)^{6}\right], 0\right] \qquad T_{i,j} := \mathrm{if}\left[i = j, \frac{\pi^2}{6\cdot\mu\cdot\Delta^2}, \frac{(-1)^{i-j}}{(i-j)^2\cdot\mu\cdot\Delta^2}\right]$$

Total energy (Hamiltonian) matrix: $H := T + V$

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

Display eigenvalues: $m := 1..4$ $E_m =$

-66.269
-22.981
-4.132
1.096

Calculate eigenvectors $k := 1..3$ $\Psi(k) := \mathrm{eigenvec}(H, E_k)$

Display results: