

Numerical Solutions for the Infinite Potential Well with Internal Barrier

The purpose of this tutorial is to explore the impact of the presence of a large ($100 E_H$) thin ($0.10 a_0$) internal barrier on the solutions to the particle-in-a-box (PIB) problem. Schrodinger's equation is integrated numerically for the first five energy states. (Integration algorithm taken from J. C. Hansen, *J. Chem. Educ. Software*, **8C2**, 1996.)

For the one-bohr PIB the energy eigenvalues are:

$$m := 1..5 \quad E_m := \frac{m^2 \cdot \pi^2}{2} \quad E^T = (4.935 \quad 19.739 \quad 44.413 \quad 78.957 \quad 123.37)$$

Set parameters:

$$\begin{aligned} n &:= 400 & x_{\min} &:= 0 & x_{\max} &:= 1 & \Delta &:= \frac{x_{\max} - x_{\min}}{n - 1} \\ \mu &:= 1 & V_0 &:= 100 & l_b &:= .45 & r_b &:= .55 \end{aligned}$$

Calculate position vector, the potential energy matrix, and the kinetic energy matrix. Then combine them into a total energy matrix.

$$i := 1..n \quad j := 1..n \quad x_i := x_{\min} + (i - 1) \cdot \Delta \quad \text{Potential energy:} \quad V_{i,j} := \text{if}[(x_i \geq l_b) \cdot (x_i \leq r_b), V_0, 0]$$

$$\text{Kinetic energy:} \quad T_{i,j} := \text{if} \left[i = j, \frac{\pi^2}{6 \cdot \mu \cdot \Delta^2}, \frac{(-1)^{i-j}}{(i-j)^2 \cdot \mu \cdot \Delta^2} \right] \quad \text{Hamiltonian matrix:} \quad H := T + V$$

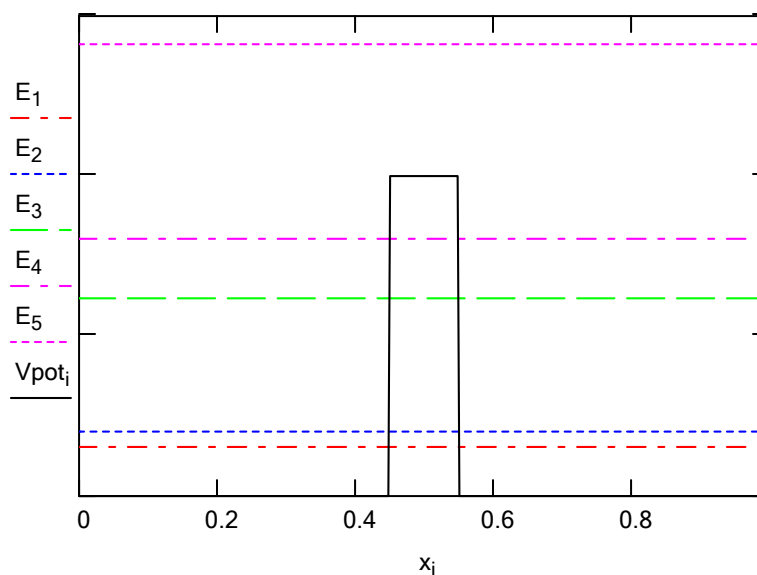
Find eigenvalues: $E := \text{sort}(\text{eigenvals}(H))$ Display selected eigenvalues: $m := 1..5$

$E_m =$
15.327
20.115
61.793
80.366
141.155

Calculate selected eigenvectors $k := 1..4$ $\Psi(k) := \text{eigenvec}(H, E_k)$

$$V_{\text{pot}_i} := V_{i,i}$$

Display energy level manifold in the presence of the internal potential barrier:



It is clear from the numeric and graphic display of the energy manifold that the presence of the internal barrier causes a bunching of the energy eigenstates for the four lowest levels. The explanation for this bunching is evident in the display of the four lowest wave functions. The presence of the barrier raises all energy levels relative to the simple PIB, but the $n = 2$ and $n = 4$ states have nodes in the barrier, thus reducing the barrier's effect on raising the energy. Thus the odd states are raised in energy more than the even states, causing the bunching.

Display selected eigenfunctions:

