9.15: Particle in a Box with an Internal Barrier

Numerical integration of Schrödinger's equation:

Potential energy:

$$V(x) = \Big|^{V_0 \; if \; (x \geq lb)(x \leq rb)}_{0 \; otherwise}$$

Given:

$$\frac{-1}{2\mu}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

$$\psi(0) = 0$$

$$\psi'(0) = 0.1$$

$$\psi = \text{Odesolve}(x, x_{max})$$

Normalize wave function:

$$\psi(x) = \frac{\psi(x)}{\sqrt{\int_0^x \psi(x)^2 dx}}$$

Integration limit: $x_{max} = 1$

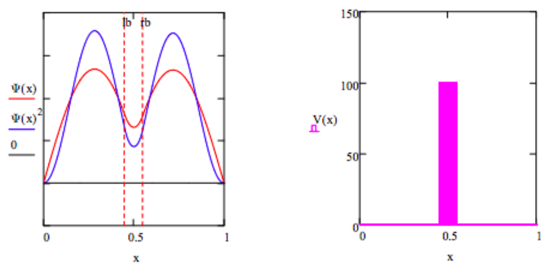
Effective mass: $\mu = 1$

Barrier height: $V_0 = 100$

Barrier boundaries: lb = 0.45

rb = 0.55

Enter energy guess: E = 15.45



Calculate potential energy: $PE = \int_0^1 V(x)\psi(x)^2 dx$ PE = 4.932 $\int_0^1 \psi(x)^2 dx = 1.00$

Calculate kinetic energy: $KE = E - PE$ E = 10.518

Ratio of potential energy to total energy: $\frac{PE}{E} = 0.319$

Calculate probability in barrier: $\frac{PE}{V_0} = 0.049$

$$P = \int_{lb}^{rb} \psi(x)^2 dx = 0.049$$

1. Find the first four energy levels, sketch ψ^2 for each state, and fill in the table below. KE, PE and the probability in the electron is in the barrier are calculated above.

$$\begin{pmatrix} E & KE & PE & P \\ 15.45 & 10.518 & 4.932 & 0.049 \\ 20.30 & 19.827 & 0.473 & 0.0047 \\ 62.20 & 47.745 & 14.455 & 0.145 \\ 80.80 & 78.968 & 1.832 & 0.018 \end{pmatrix}$$

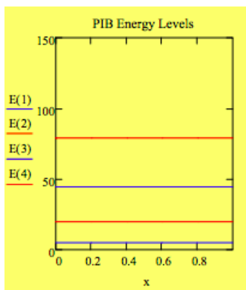
2. Interpret the results for energy in light of the fact that a 100 E_h (2720 eV) potential barrier of finite thickness exists in the center of the box.

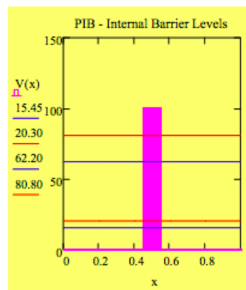
This is an excellent example of quantum mechanical tunneling. For the first four energy states the particle has probability of being found in the tunnel in spite of the fact that its energy is less than the barrier energy.

3. Explain the obvious bunching of energy states in pair in terms of the impact of the internal barrier. In other words why is the probability of being in the potential barrier larger for the n = 1 and 3 states than it is for the n = 2 and 4 states.

The PIB energy levels without an internal barrier are: $E(n) = \frac{\pi^2}{2} n^2$

The bunching can be seen by comparing the two energy manifolds. The n = 2 and 4 states have nodes at the middle of the box where the internal barrier is situated. Thus their potential energy does not increase as much as the n = 1 and 3 states which do not have nodes in the barrier.





4. Find the ground state energy for particle masses of 0.5 and 1.5. Record your results in the table below and interpret them.

$$\begin{pmatrix} Mass & E & T & V & P \\ 0.5 & 23.95 & 14.411 & 9.539 & 0.095 \\ 1.0 & 15.45 & 10.518 & 4.932 & 0.049 \\ 1.5 & 11.55 & 8.684 & 2.866 & 0.029 \end{pmatrix}$$

The higher the mass the lower the energy because in quantum mechanics in $E \sim \frac{1}{mass}$. The greater the mass the lower the probability that tunneling will occur. This is due to the fact that the deBroglie wavelength is inversely proportional to mass.

5. Find the ground state energy for a m = 1 particle for barrier heights 50 and 150 Eh. Record your results in the table below and interpret them.

$$\begin{pmatrix} V_0 & E & T & V & P \\ 50 & 11.97 & 7.203 & 4.767 & 0.095 \\ 100 & 15.45 & 10.518 & 4.932 & 0.049 \\ 150 & 17.32 & 13.024 & 4.296 & 0.029 \end{pmatrix}$$

The higher the barrier energy the higher the ground-state energy and the lower the tunneling probability.

6. On the basis of your calculations in this exercise describe quantum mechanical tunneling. In your answer you should consider the importance of particle mass, barrier height and barrier width. Perform calculations for widths of 0.05 and 0.15 in atomic units.

Tunneling is inversely proportional to mass, barrier height and barrier width.

$$\begin{pmatrix} Width & E & T & V & P & \frac{P}{Width} \\ 0.05 & 11.65 & 7.326 & 4.324 & 0.043 & 0.860 \\ 0.10 & 15.45 & 10.518 & 4.932 & 0.049 & 0.490 \\ 0.15 & 18.35 & 13.317 & 5.033 & 0.050 & 0.333 \end{pmatrix}$$