Numerical Solutions for Schrodinger's Equation

Particle in a Box with an Internal Barrier

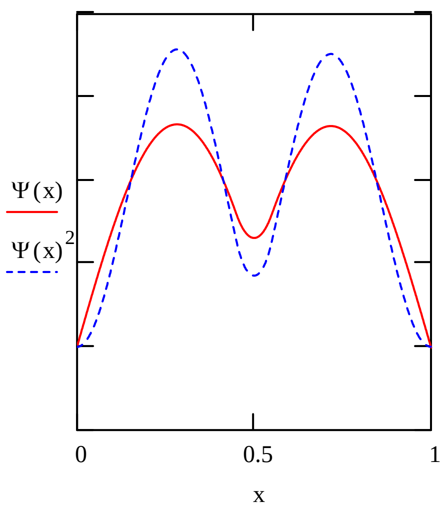
Numerical integration of Schrodinger's equation: Potential energy: $V(x) := \text{if}\left[(x \ge lb)\cdot(x \le rb), V_0, 0\right]$

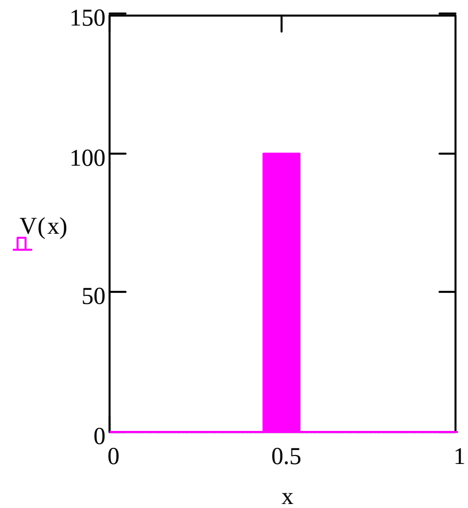
Given $\frac{-1}{2\cdot\mu}\cdot\frac{d^2}{dx^2}\Psi(x) + V(x)\cdot\Psi(x) = E\cdot\Psi(x)$ $\Psi(0) = 0$ $\Psi'(0) = 0.1$

$\Psi := \text{Odesolve}(x, x_{max})$ Normalize wave function: $\Psi(x) := \frac{\Psi(x)}{\sqrt{\int_0^{x_{max}} \Psi(x)^2\,dx}}$

Integration limit: $x_{max} \equiv 1$ Effective mass: $\mu \equiv 1$ Barrier height: $V_0 \equiv 100$

Barrier boundaries: $lb \equiv .45$ $rb \equiv .55$ Enter energy guess: $E \equiv 15.45$





Calculate potential energy: $PE := \int_{lb}^{rb} V_0\cdot\Psi(x)^2\,dx$ $PE = 4.932$

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

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

Calculate probability in barrier: $\frac{PE}{V_0} = 0.049$ $\int_{lb}^{rb} \Psi(x)^2\,dx = 0.049$

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 barrier are calculated above.

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

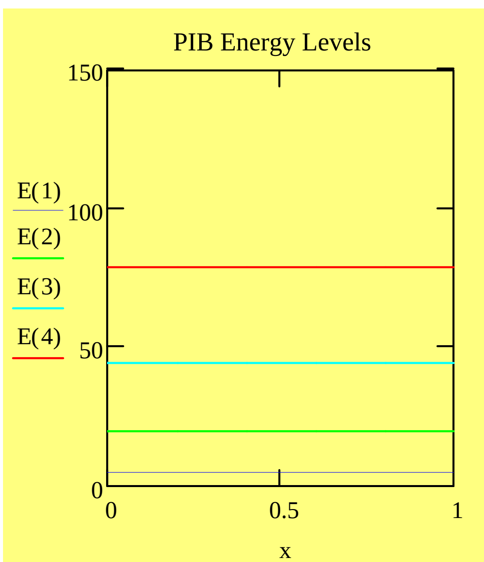
2. Interpret the results for energy in light of the fact that a 100 E_h (2720 eV) potential barrier of finite thickness exists in the center of the box.

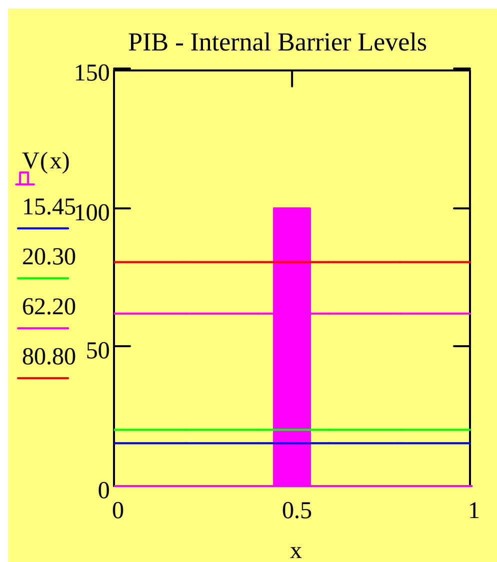
This is an excellent example of quantum mechanical tunneling. For the first four energy states the particle has probability of being found in the tunnel in spite of the fact that its energy is less than the barrier energy.

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: $E(n) := \frac{\pi^2}{2} \cdot n^2$

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.

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

The higher the mass the lower the energy because in quantum mechanics in E ~ 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 an m = 1 particle for barrier heights 50 and 150 Eh. Record your results in the table below and interpret them.

V_0	E	T	V	P
50	11.97	7.203	4.767	.095
100	15.45	10.518	4.932	0.049
150	17.32	13.024	4.296	0.029

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 barrier height and particle mass.

Tunneling is inversely proportional to mass and barrier height. It also is inversely proportional to barrier width, but we didn't look into this.

7. Calculate the energy of the particle using the PIB (no internal barrier) ground-state wave function.

$V_0 := 100$ $n := 1$

$$\frac{n^2 \cdot \pi^2}{2} + \int_{lb}^{rb} V_0 \cdot \left(\sqrt{2} \cdot \sin(n \cdot \pi \cdot x)\right)^2 dx = 24.771$$

8. Calculate the energy of the particle using the PIB (no internal barrier) first excited-state wave function.

$n := 2$

$$\frac{n^2 \cdot \pi^2}{2} + \int_{lb}^{rb} V_0 \cdot \left(\sqrt{2} \cdot \sin(n \cdot \pi \cdot x)\right)^2 dx = 20.384$$

9. Explain these results.

The n = 2 state has a lower energy than the n = 1 because its wave function has a node at the x = 0.5 where the potential barrier is centered.