The Finite Potential and Tunneling

CHEM 361B: Introduction to Physical Chemistry

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Lecture 8

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Learning Objective: Develop an understanding on how boundary conditions link wavefunctions in regions with different potentials to describe quantum effects.

References:

- McQuarrie Problems 4-51 and 4-54

Particle in a Box - Finite Potential Well

Consider the finite square well potential

$$U(x) = \begin{cases} 0 & \text{for } -a < x < a \\ U_0 & \text{for } |x| > a \end{cases}$$

For this case, assume that $E < U_0$. This is called a bound state.

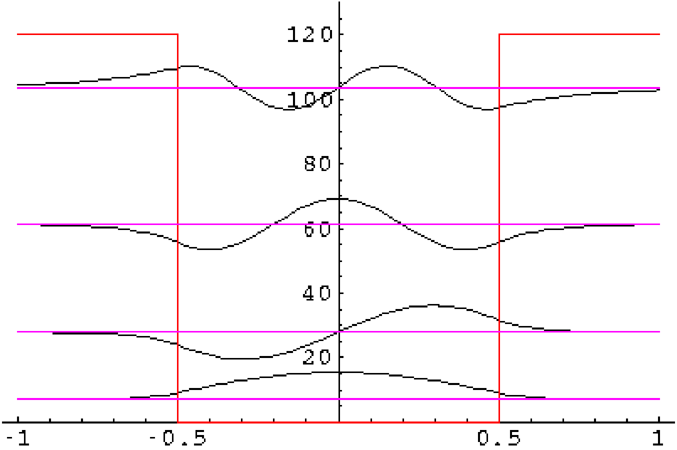
1. Find $\psi(x)$ for $x < -a$

   Answer: $\psi(x) = Ae^{\frac{\sqrt{2m(U_0-E)}x}{\hbar}}$
2. Find $\psi(x)$ for $-a < x < a$

   Answer: $\psi(x) = C\cos(\frac{\sqrt{2mE}x}{\hbar}) + D\sin(\frac{\sqrt{2mE}x}{\hbar})$
3. Find $\psi(x)$ for $x > a$

   Answer: $\psi(x) = Fe^{-\frac{\sqrt{2m(U_0-E)}x}{\hbar}}$

Graphical Solutions to the Finite Square Well



Particle in a Box - Finite Potential Well (cont.)

We will assume that

- $\psi(x)$ and $d\psi/dx$ are continuous at $-a$ and a

We will evaluate these boundary conditions where:

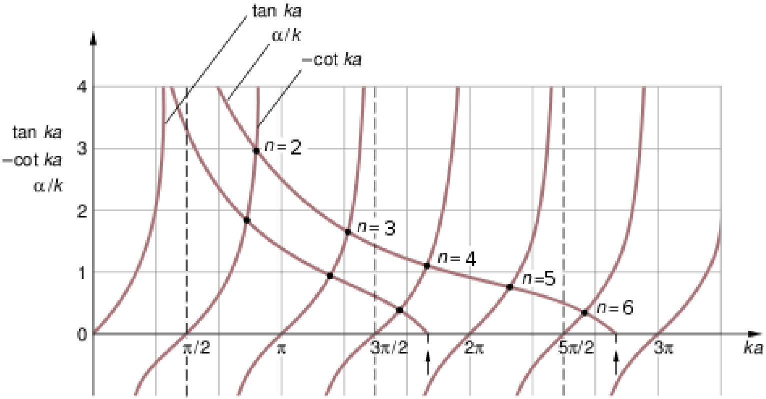
$$\psi(x) = \begin{cases} Fe^{-\alpha x} & x > a \\ C\cos(kx) + D\sin(kx) & -a < x < a \\ Ae^{\alpha x} & x < -a \end{cases}$$

where $k = \frac{\sqrt{2mE}}{\hbar}$ and $\alpha = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$

We will find that the energy of the bound states are quantized and are defined by

$$\tan(ka) = \frac{\alpha}{k} = -\cot(ka)$$

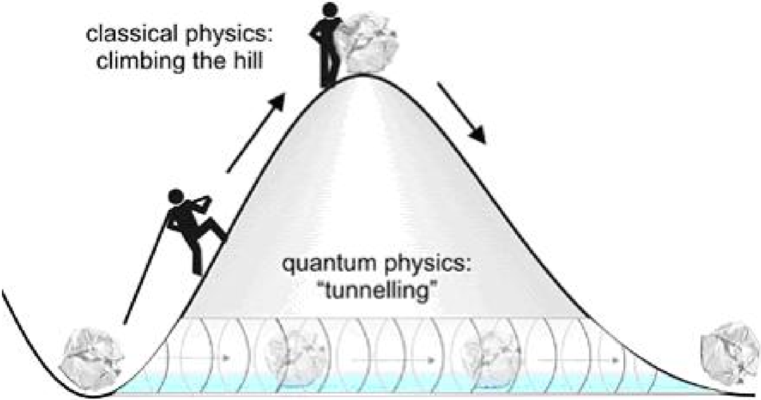
Particle in a Box - Finite Potential Well (cont.)



Particle in a Box - Finite Potential Well (cont.)

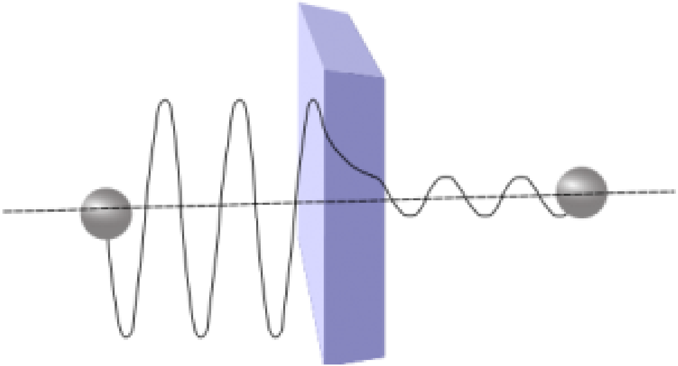
- Energy levels are calculated as when the line α/k crosses either $tan(ka)$ (even) or $-cot(ka)$ (odd) solutions. As a result there are only a finite number of energy levels trapped in the well.
- As U_0 gets bigger then the spot α/k crosses the x-axis moves to the right. This means
  - for every $\pi/2$ increase, a new energy state is trapped in the well.
  - that when $U_0 \to \infty$, all the energy levels present in the infinite square well appear here.
- As U_0 goes to zero (but is never equal to zero), the spot α/k crosses the x-axis moves to the left. This means
  - energy levels become free from the potential well.
  - regardless of the depth of the well, there will always be at least one bound state.

Lifting Boulders Classically vs Quantum Mechanically



Quantum Tunneling

Since ψ can exist in a finite potential barrier then there is a chance that the particle can penetrate the barrier even if $E < U_0$.



A Note on Traveling Waves

Given the typical solution to the Schrödinger equation

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

where k is some constant that is a function of energy, if we apply the momentum operator to each solution individually then

$$\begin{aligned}\hat{P}Ae^{ikx} &= -i\hbar\frac{d}{dx}Ae^{ikx} \\ &= -i\hbar A(ik)e^{ikx} \\ &= k\hbar Ae^{ikx}\end{aligned}$$

$$\begin{aligned}\hat{P}Be^{-ikx} &= -i\hbar\frac{d}{dx}Be^{-ikx} \\ &= -i\hbar B(-ik)e^{-ikx} \\ &= -k\hbar Be^{ikx}\end{aligned}$$

The solution is a combination of a wave moving to the right, and a wave moving to the left with the same momentum $k\hbar$ (hence why $\langle p \rangle = 0$ in the particle in a box problem)

Quantum Tunneling Setup

Consider the potential barrier

$$U(x) = \begin{cases} 0 & \text{for } x < 0 \\ U_0 & \text{for } 0 \leq x \leq a \\ 0 & \text{for } x > a \end{cases}$$

For this case, assume that $E < U_0$ so that classically a particle traveling from the left can not overcome the barrier.

1. Find $\psi(x)$ for $x < 0$

   Answer: $\psi(x) = Ae^{i\frac{\sqrt{2mE}}{\hbar}x} + Be^{-i\frac{\sqrt{2mE}}{\hbar}x}$
2. Find $\psi(x)$ for $0 \leq x \leq a$

   Answer: $\psi(x) = Ce^{\frac{\sqrt{2m(U_0-E)}}{\hbar}x} + De^{-\frac{\sqrt{2m(U_0-E)}}{\hbar}x}$
3. Find $\psi(x)$ for $x > a$

   Answer: $\psi(x) = Ee^{i\frac{\sqrt{2mE}}{\hbar}x}$

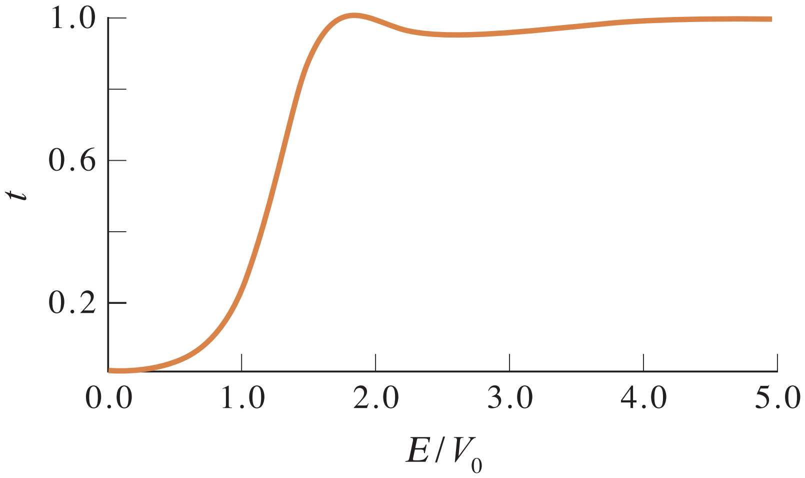
Finding Tunneling Probabilities

It can be assumed that B can be used to determine the probability of a particle reflecting off the barrier ($|B|^2/|A|^2$), and E can be used to determine the probability of a particle tunneling through the barrier ($|E|^2/|A|^2$).

Rearranging the three wavefunctions and using the fact that $\psi(x)$ and $\frac{d\psi}{dx}$ must be continuous at the boundaries of the potential then

$$|E|^2/|A|^2 = \frac{1}{1 + \frac{(e^{\kappa a} - e^{-\kappa a})^2}{4(E/U_0)(1-E/U_0)}} \quad \text{where } \kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

Plot of Transmission Probability



Tunneling Examples

1. What is the tunneling probability of a 2000 kg truck moving through a square speed bump 0.1 m high and 0.1 m long traveling at 1.39 m/s?
2. What is the tunneling probability of an electron moving through a 8.0109×10^{-18} J barrier that is 1 angstrom wide traveling at 1% the speed of light?

Summary

- Finite potentials more closely resemble real systems
- The finite potential well gives a proper example on how to match up wavefunctions at the boundaries. The solution shows that the particle exists in the barrier.
- Since the wavefunction is non-zero in finite potential barriers, there are instances where quantum particles can tunnel through the barrier even if it does not have the energy to go over it.