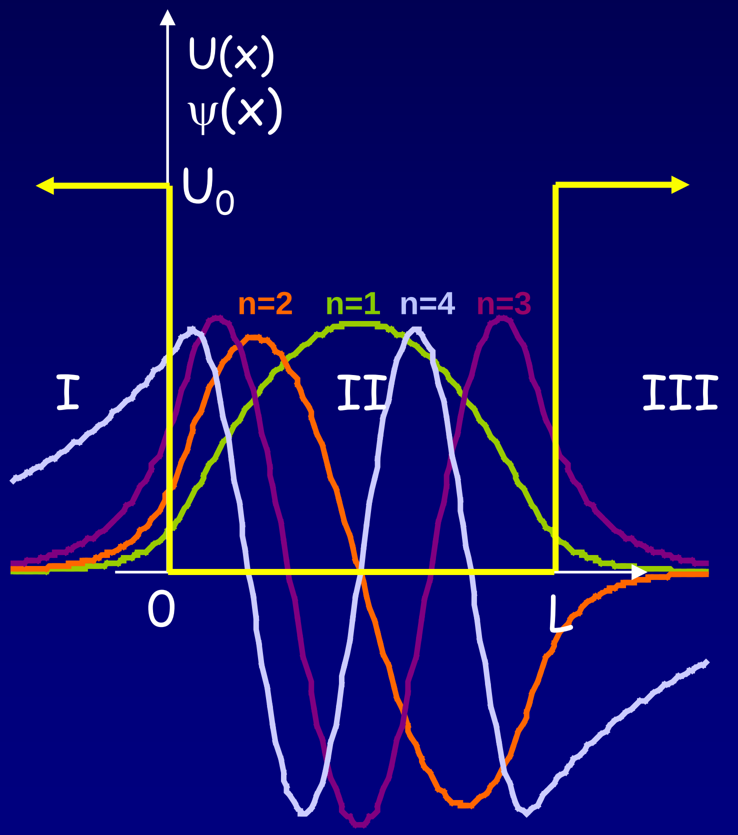
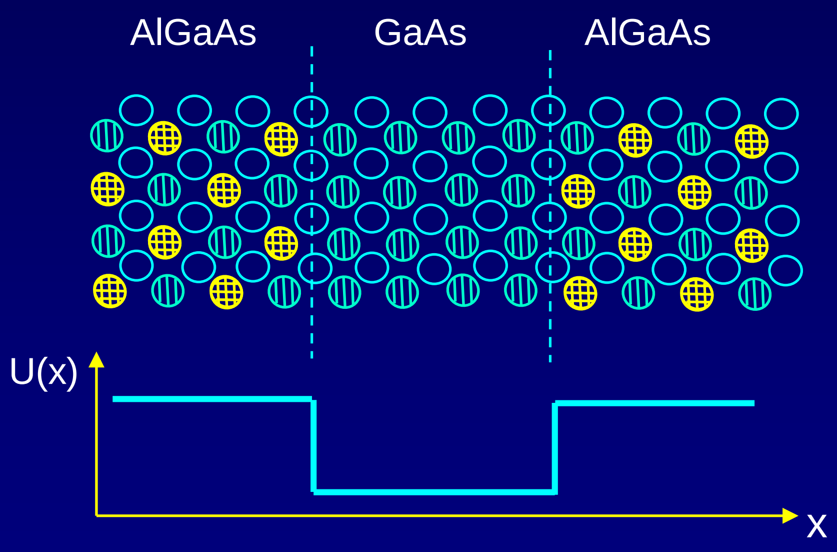
Lecture 11:
Particles in (In)finite Potential Wells

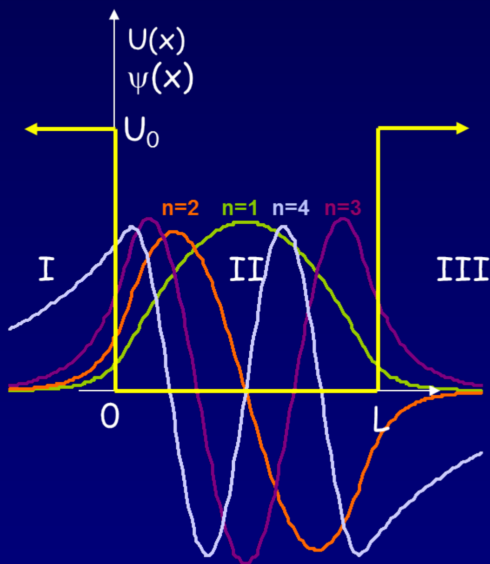




Last Time

Schrodinger's Equation (SEQ)

A wave equation that describes spatial and time dependence of $\Psi(x,t)$.
Expresses KE +PE = E_{tot}
Second derivative extracts $-k^2$ from wave function.



Constraints that $\psi(x)$ must satisfy

Existence of derivatives (implies continuity).
Boundary conditions at interfaces.

Infinitely deep 1D square well ("box")

Boundary conditions $\rightarrow$ Discrete energy spectrum:

$$E_n = n^2 E_1, \text{ where } E_1 = h^2/8mL^2.$$

Today

"Normalizing" the wave function

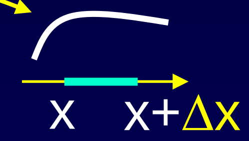
General properties of bound-state wave functions

Particle in a finite square well potential

- Solving boundary conditions
- Comparison with infinite-well potential

Constraints on the Form of $\psi(x)$

$|\psi(x)|^2$ corresponds to a physically meaningful quantity:
the probability density of finding the particle near x. → $|\psi(x)|^2\Delta x$



To avoid unphysical behavior, $\psi(x)$ must satisfy some conditions:

$|\psi(x)|^2$ is what you measure
$\psi(x)$ is what you calculate

$\psi(x)$ must be single-valued, and finite.

Finite to avoid infinite probability density.

$\psi(x)$ must be **continuous**, with finite $d\psi/dx$.

$d\psi/dx$ is related to the momentum.

In regions with finite potential, $d^2\psi/dx^2$ must be finite.

To avoid infinite energies.
This also means that $d\psi/dx$ must be continuous.

Note: The *sign* of ψ has nothing to do with charge!

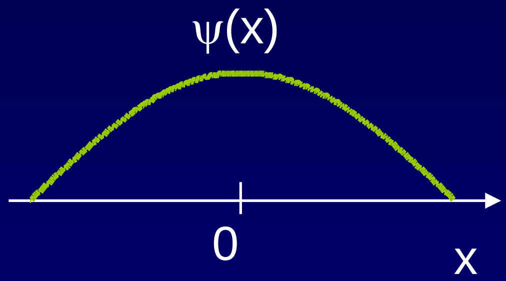
There is no significance to the overall *sign* of $\psi(x)$.
It goes away when we take the absolute square.

{In fact, we will see that $\Psi(x,t)$ is usually complex!}

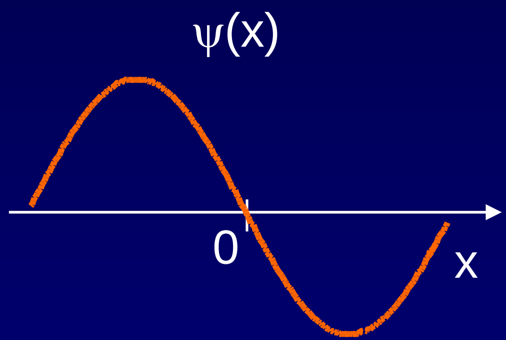
Act 1

1. Which of the following wave functions corresponds to a particle more likely to be found on the left side?

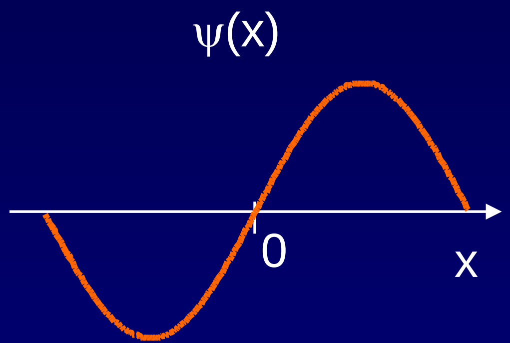
(a)



(b)



(c)



Probabilities

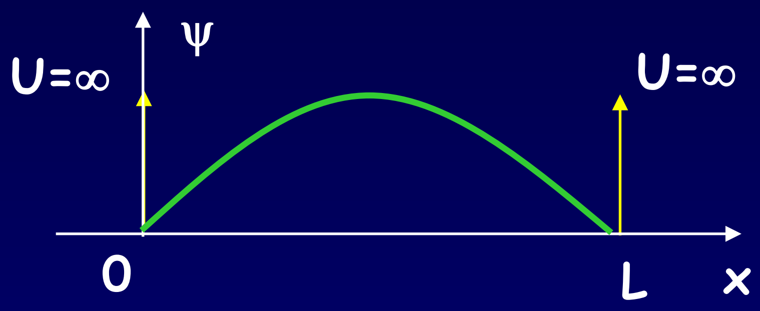
Often what we measure in an experiment is the probability density, $|\psi(x)|^2$.

$$\psi_n(x) = B_1 \sin\left(\frac{n\pi}{L}x\right)$$

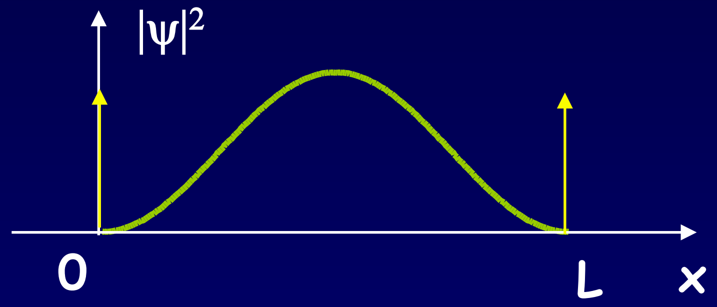
Wavefunction = Probability amplitude

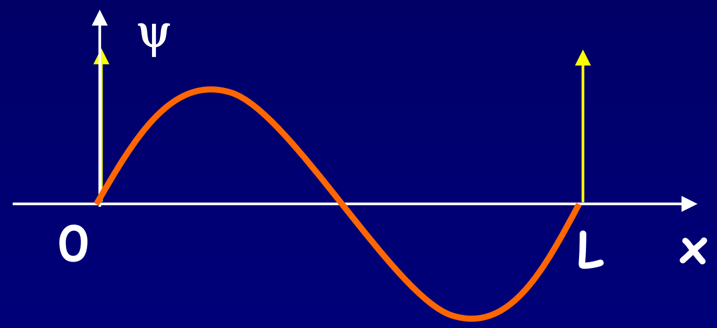
$$|\psi_n(x)|^2 = B_1^2 \sin^2\left(\frac{n\pi}{L}x\right)$$

Probability per unit length (in 1-dimension)

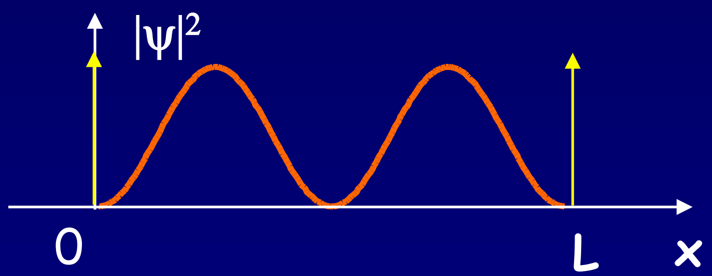


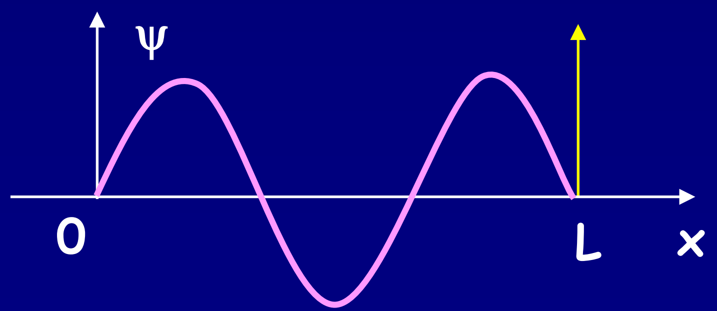
n=1



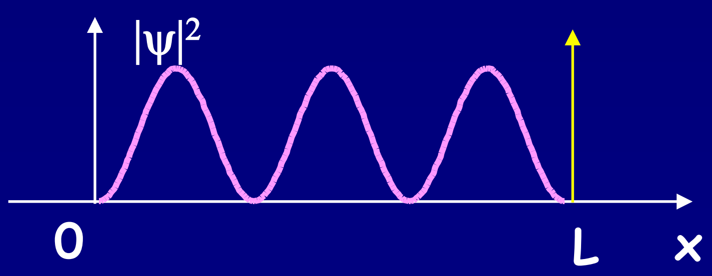


n=2





n=3

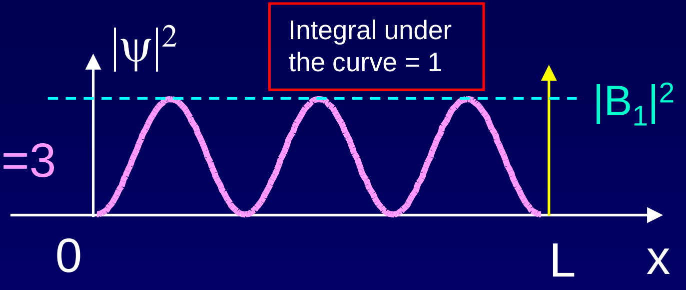


Probability and Normalization

We now know that $\psi_n(x) = B_1 \sin\left(\frac{n\pi}{L}x\right)$. How can we determine B_1?

We need another constraint. It is the requirement that total probability equals 1.

The probability density at x is $|\psi(x)|^2$:



Therefore, the total probability is the integral:

$$P_{tot} = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx$$

In our square well problem, the integral is simpler, because ψ = 0 for x < 0 and x > L:

$$P_{tot} = |B_1|^2 \int_0^L \left| \sin\left(\frac{n\pi}{L}x\right) \right|^2 dx$$

$$= |B_1|^2 \frac{L}{2}$$

Requiring that P_{tot} = 1 gives us: $\boxed{B_1 = \sqrt{\frac{2}{L}}}$

Probability Density

In the infinite well: $P(x) = N^2 \sin^2\left(\frac{n\pi}{L}x\right)$. (Units are m^{-1}, in 1D)

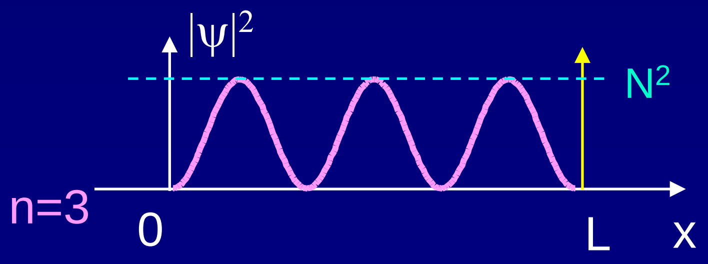
Notation: The constant is typically written as "N", and is called the "normalization constant". For the square well:

$$\boxed{N = \sqrt{\frac{2}{L}}}$$

One important difference with the classical result:

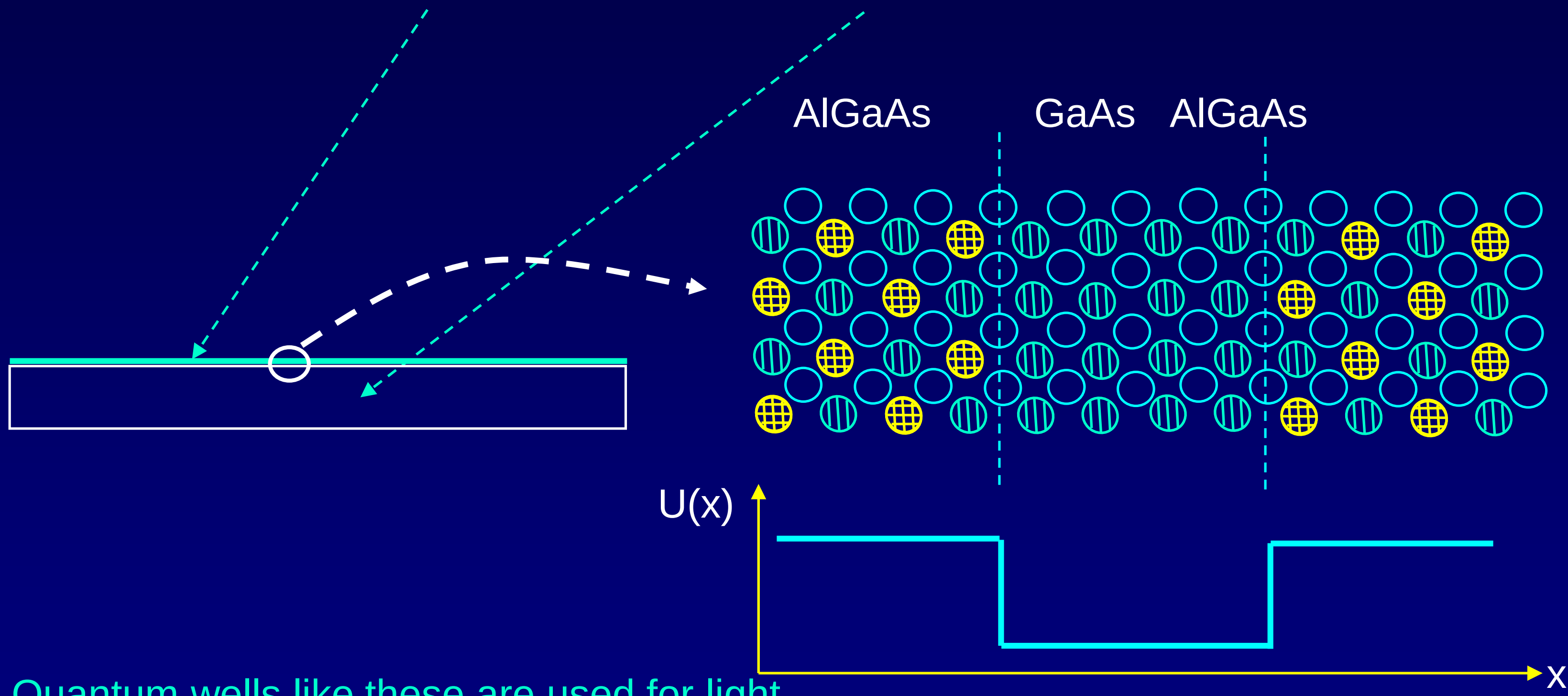
For a classical particle bouncing back and forth in a well, the probability of finding the particle is equally likely throughout the well.

For a quantum particle in a stationary state, the probability distribution is not uniform. There are "nodes" where the probability is zero!



Example of a microscopic potential well -- a semiconductor "quantum well"

Deposit different layers of atoms on a substrate crystal:



Quantum wells like these are used for light emitting diodes and laser diodes, such as the ones in your CD player.

The quantum-well laser was invented by Charles Henry, PhD UIUC '65.

This and the visible LED were developed at UIUC by Nick Holonyak.

An electron has lower energy in GaAs than in AlGaAs. It may be trapped in the well – but it "leaks" into the surrounding region to some extent

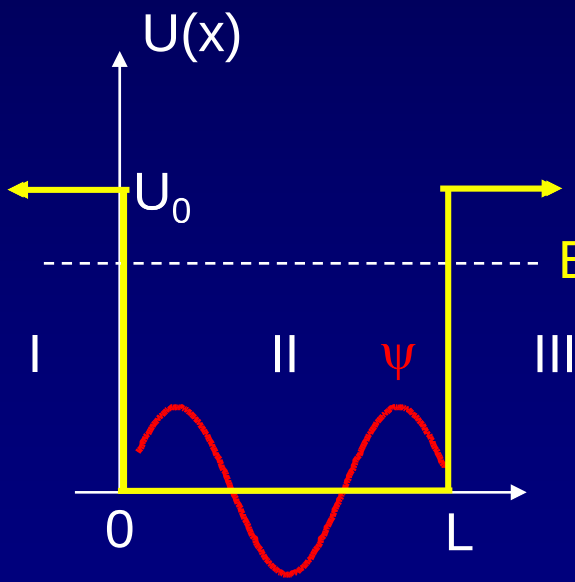
Particle in a Finite Well (1)

What if the walls of our "box" aren't infinitely high?

We will consider finite U_0, with $E < U_0$, so the particle is still trapped.

This situation introduces the very important concept of "barrier penetration".

As before, solve the SEQ in the three regions.



Region II:
U = 0, so the solution is the same as before:

$$\psi_{II}(x) = B_1 \sin kx + B_2 \cos kx$$

We do not impose the infinite well boundary conditions, because they are not the same here.
We will find that B_2 is no longer zero.

Before we consider boundary conditions,
we must first determine the solutions in regions I and III.

Particle in a Finite Well (2)

Regions I and III:
$U(x) = U_o$, and $E < U_0$

Because $E < U_0$, these regions are "forbidden" in classical particles.

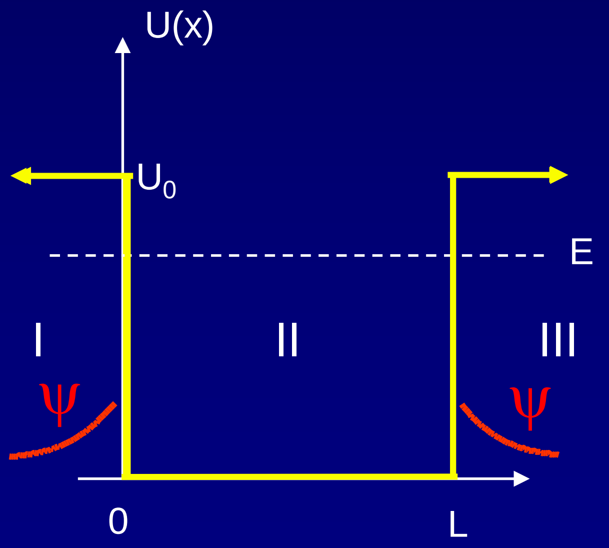
The SEQ $\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E-U)\psi(x) = 0$ can be written:

$$\frac{d^2\psi(x)}{dx^2} - K^2\psi(x) = 0$$

In region II this was a + sign.

where: $K = \sqrt{\frac{2m}{\hbar^2}(U_0 - E)}$

$U_0 > E$:
K is real.



The general solution to this equation is:

Region I: $\psi_I(x) = C_1 e^{Kx} + C_2 e^{-Kx}$

Region III: $\psi_{III}(x) = D_1 e^{Kx} + D_2 e^{-Kx}$

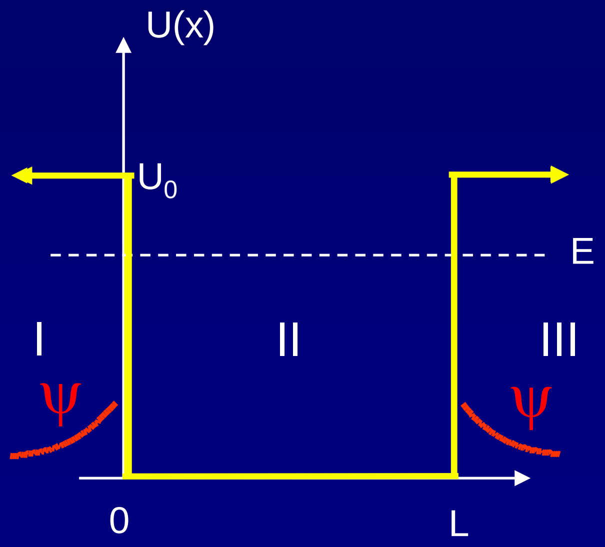
C_1, C_2, D_1, and D_2, will be determined by the boundary conditions.

Particle in a Finite Well (3)

Important new result! (worth putting on its own slide)

For quantum entities, there is a finite probability amplitude, ψ, to find the particle inside a "classically-forbidden" region, *i.e.*, inside a barrier.

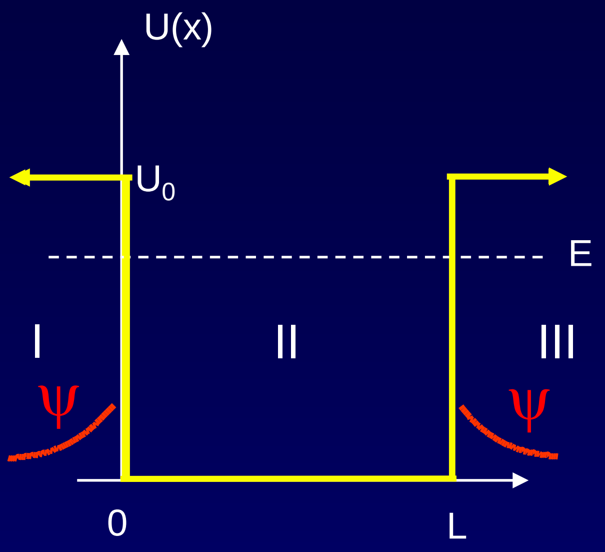
$$\psi_I(x) = C_1 e^{Kx} + C_2 e^{-Kx}$$



Act 2

In region III, the wave function has the form

$$\psi_{III}(x) = D_1 e^{Kx} + D_2 e^{-Kx}$$



1. As x → ∞, the wave function must vanish. (why?) What does this imply for D_1 and D_2?

a. $D_1 = 0$ b. $D_2 = 0$ c. D_1 and D_2 are both nonzero.

2. What can we say about the coefficients C_1 and C_2 for the wave function in region I?

$$\psi_{I}(x) = C_1 e^{Kx} + C_2 e^{-Kx}$$

a. $C_1 = 0$ b. $C_2 = 0$ c. C_1 and C_2 are both nonzero.

Particle in a Finite Well (4)

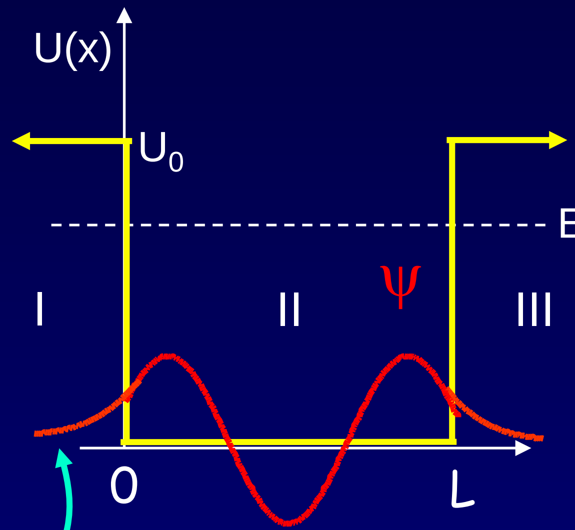
Summarizing the solutions in the 3 regions:

Region I: $\psi_I(x) = C_1 e^{Kx}$

Region II: $\psi_{II}(x) = B_1 \sin(kx) + B_2 \cos(kx)$

Region III: $\psi_{III}(x) = D_2 e^{-Kx}$

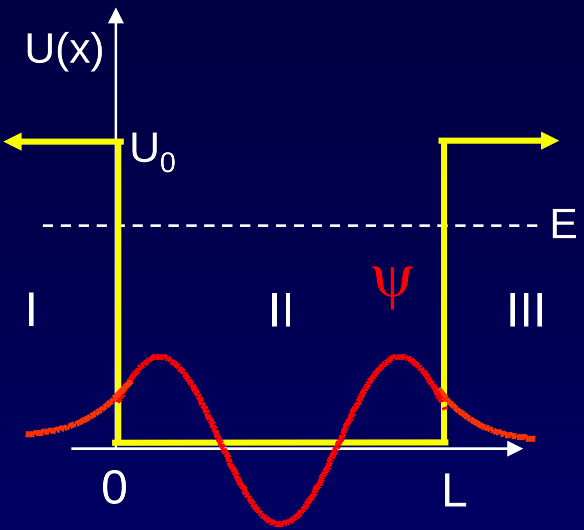
As with the infinite square well, to determine parameters (K, k, B_1, B_2, C_1, and D_2) we must apply boundary conditions.



Useful to know:
In an allowed region, ψ curves toward 0.
In a forbidden region, ψ curves away from 0.

Particle in a Finite Well (5)

The boundary conditions are not the same as for the finite well. We no longer require that $\psi = 0$ at $x = 0$ and $x = L$.



Instead, we require that $\psi(x)$ and $d\psi/dx$ be continuous across the boundaries:

	ψ is continuous	$d\psi/dx$ is continuous
At x = 0:	$\psi_I = \psi_{II}$	$\dfrac{d\psi_I}{dx} = \dfrac{d\psi_{II}}{dx}$
At x = L:	$\psi_{II} = \psi_{III}$	$\dfrac{d\psi_{II}}{dx} = \dfrac{d\psi_{III}}{dx}$

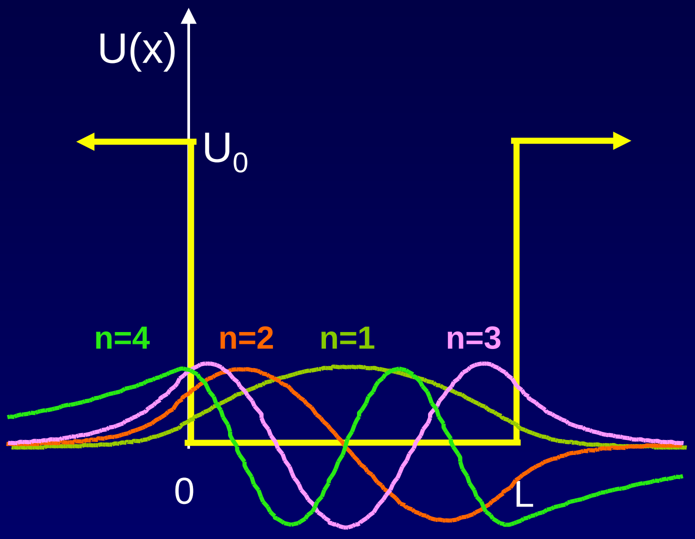
Unfortunately, this gives us a set of four transcendental equations. They can only be solved numerically (on a computer). We will discuss the qualitative features of the solutions.

Particle in a Finite Well (6)

What do the wave functions for a particle in the finite square well potential look like?

They look very similar to those for the infinite well, except …

The particle has a finite probability to "leak out" of the well !!



Some general features of finite wells:

- Due to leakage, the wavelength of ψ_n is longer for the finite well. Therefore E_n is lower than for the infinite well.
- K depends on U_0 - E. For higher E states, e^{-Kx} decreases more slowly. Therefore, their ψ penetrates farther into the forbidden region.
- A finite well has only a finite number of bound states. If E > U_0, the particle is no longer bound.

Very nice Java applet: http://www.falstad.com/qm1d/

Act 3

1. Which has more bound states?

   a. particle in a finite well
   b. particle in an infinite well
   c. both have the same number of bound states.

2. For a particle in a ***finite*** square well, which of the following will ***decrease*** the number of bound states?

   a. decrease well depth U_0
   b. decrease well width L
   c. decrease m, mass of particle

3. Compare the energy $E_{1,finite}$ of the lowest state of a finite well with the energy $E_{1,infinite}$ of the lowest state of an infinite well of the same width L.

a. $E_{1,finite} < E_{1,infinite}$ b. $E_{1,finite} > E_{1,infinite}$ c. $E_{1,finite} = E_{1,infinite}$

Summary

Particle in a finite square well potential

- Solving boundary conditions:
  You'll do it with a computer in lab. We described it qualitatively here.

- Particle can "leak" into forbidden region.
  We'll discuss this more later (tunneling).

- Comparison with infinite-well potential:
  The energy of state n is lower in the finite square well potential
  of the same width.
  We can understand this from the uncertainty principle.