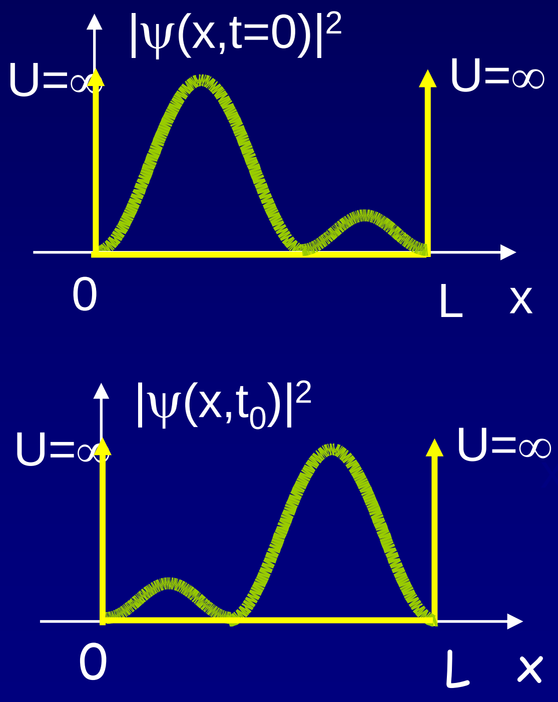
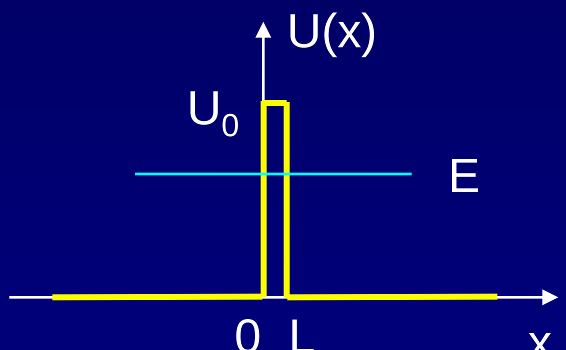
Lecture 15:
Time-Dependent QM & Tunneling
Review and Examples, Ammonia Maser





Measurements of Energy

What happens when we measure the energy of a particle whose wave function is a superposition of more than one energy state?

If the wave function is in an energy eigenstate (E_1, say), then we know with certainty that we will obtain E_1 (unless the apparatus is broken).

If the wave function is a superposition ($\psi = a\psi_1 + b\psi_2$) of energies E_1 and E_2, then we aren't certain what the result will be. However:

> We know with certainty that we will only obtain E_1 or E_2 !!

To be specific, we will never obtain $(E_1+E_2)/2$, or any other value.

What about a and b?

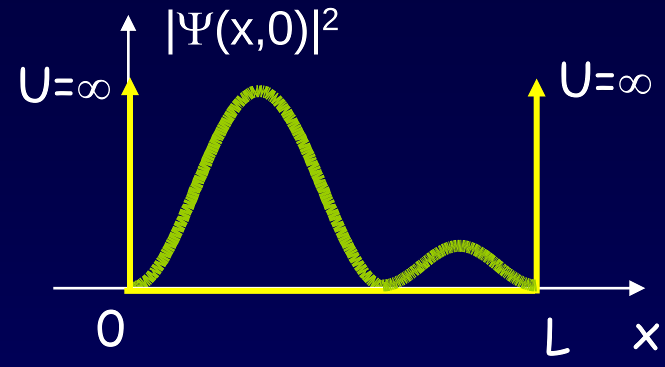
$|a|^2$ and $|b|^2$ are the probabilities of obtaining E_1 and E_2, respectively.

That's why we normalize the wave function to make $|a|^2 + |b|^2 = 1$.

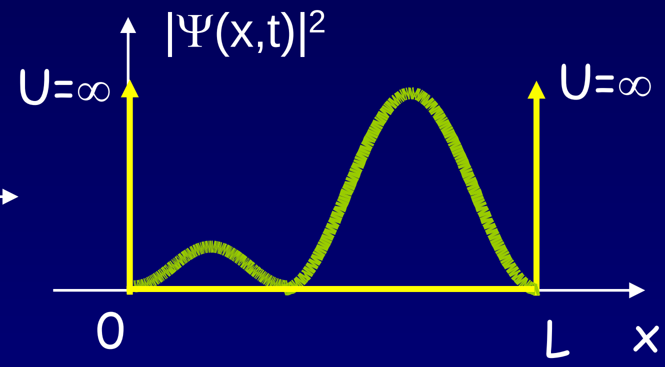
Example

An electron in an infinite square well of width L = 0.5 nm is (at t=0) described by the following wave function:

$$\Psi(x,t=0) = A\sqrt{\frac{2}{L}}\left(\sin\left(\frac{\pi}{L}x\right) + \sin\left(\frac{2\pi}{L}x\right)\right)$$



Determine the time it takes for the particle to move to the right side of the well.



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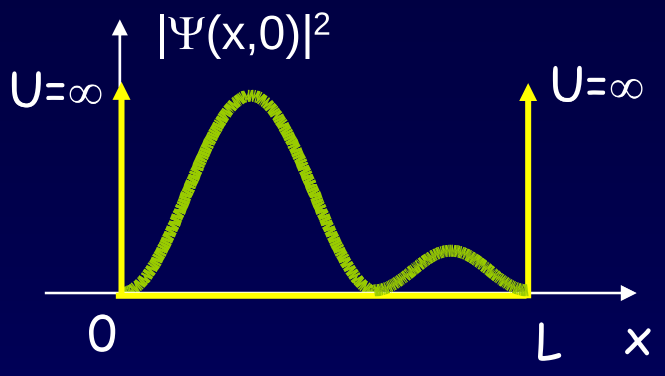

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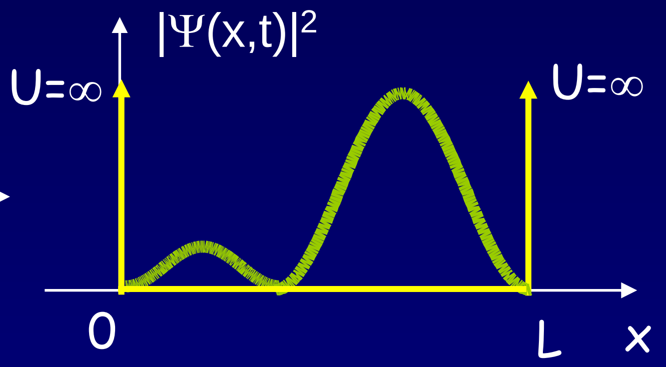

$$E_1 = \frac{1.505\ \text{eV}\cdot\text{nm}^2}{4L^2} = 1.505\ \text{eV}$$

$$\text{E}_2 = 4E_1 = 6.020\ \text{eV}$$

T = 1/f , where f = $(E_2 - E_1)/h$

Half a period.

$$t = \frac{T}{2} = \frac{h}{2(E_2 - E_1)} = \frac{4.136\times10^{-15}\ \text{eV}\cdot\text{sec}}{2(4.515\ eV)} = 4.6\times10^{-16}\ \text{sec}$$

ACT 1

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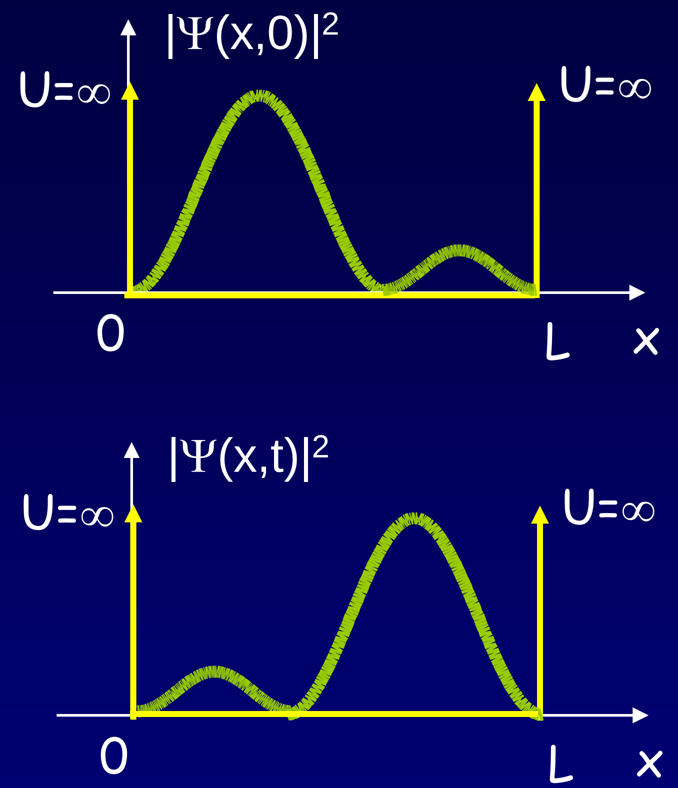

1) Suppose we measure the energy.
What results might we obtain?

a) E_1 b) E_2 c) E_3 d) Any result between E_1 and E_2

2) How do the probabilities of the various results depend on time?

a) They oscillate with $f = (E_2-E_1)/h$
b) They vary in an unpredictable manner.
c) They alternate between E_1 and E_2. (*i.e.*, it's always either E_1 or E_2).
d) They don't vary with time.

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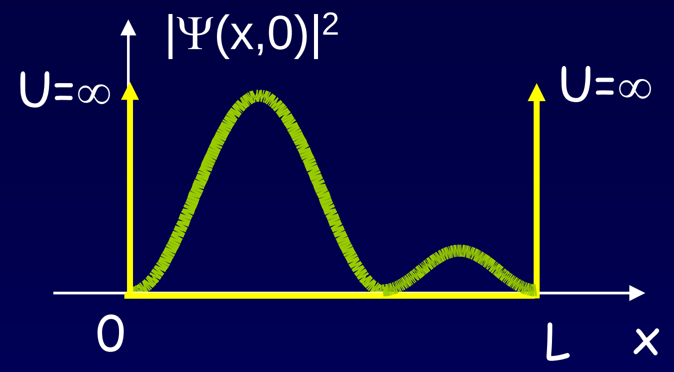

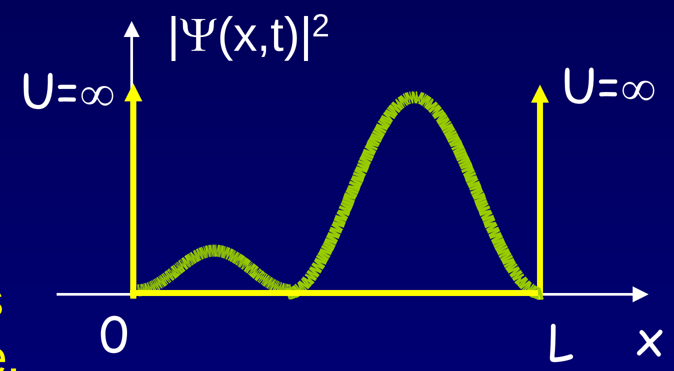

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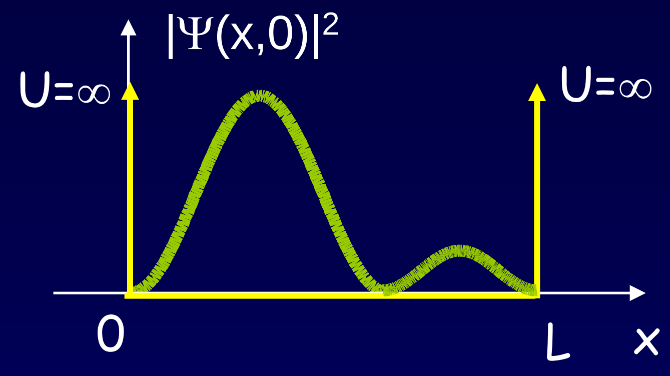

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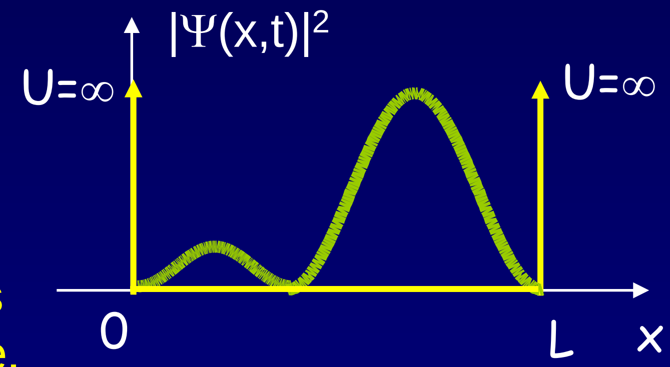

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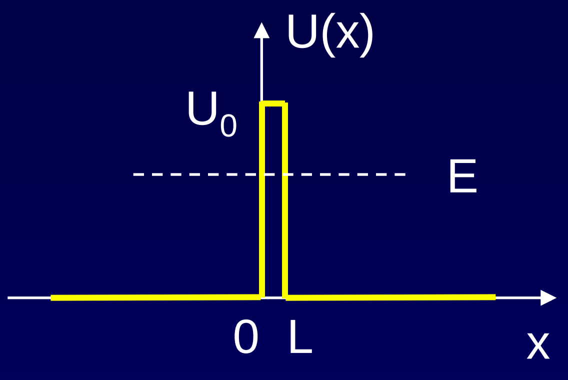
The probabilities depend on the coefficients, not on the various Ψ terms themselves. Because the coefficients are simply numbers ($A\sqrt{\frac{2}{L}}$), there is no time dependence.

Tunneling Through a Barrier

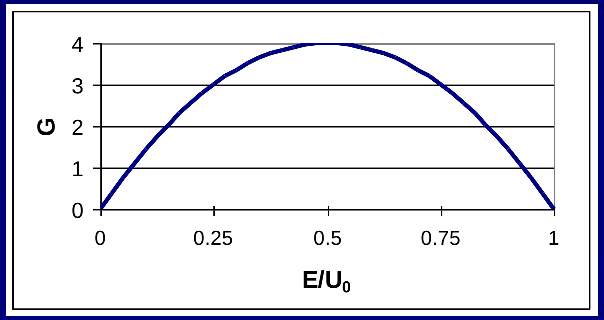
In many situations, the barrier width L is much larger than the 'decay length' 1/K of the penetrating wave (KL >> 1). In this case $B_1 \approx 0$ (why?), and the result resembles the infinite barrier. The tunneling coefficient simplifies:



$$T \approx Ge^{-2KL} \text{ where } G = 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right)$$

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

This is nearly the same result as in the "leaky particle" example! Except for G:



We will often ignore G.
(We'll tell you when to do this.)

The important result is e^{-2KL}.

ACT 2

What effect does a barrier have on probability?

Suppose T = 0.05. What happens to the other 95% of the probability?

a. It's absorbed by the barrier.
b. It's reflected by the barrier.
c. The particle "bounces around" for a while, then escapes.

Solution

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a. It's absorbed by the barrier.

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c. The particle "bounces around" for a while, then escapes.

Absorbing probability would mean that the particles disappear.
We are considering processes on which this can't happen.
The number of electrons remains constant.

Escaping after a delay would contribute to T.

Tunneling Exercise

Suppose an electron of KE = 0.1 eV approaches a barrier.

For what barrier height will it have a 50% chance of penetrating 1 nm into the forbidden region? What about 1 mm?

Here you can assume that the G term is not important.

Solution

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Solution:

In the forbidden region:

$K = \sqrt{(2m(U-E))} / \hbar$

$e^{-2KL} = ½$

U is the unknown barrier height and E = 0.1 eV.

The 2 in e^{-2KL} results from probability being $|\psi|^2$.

Note that all that really matters is U-E.

L = 1 nm:

$U = E + (\hbar\, ln(2)/2L)^2 / 2m$

$= 0.1\text{ eV} + 7.4\times10^{-22}\text{ J}$

$= 0.105\text{ eV}$

L = 1 mm:

$= 0.1\text{ eV} + 7.4\times10^{-28}\text{ J}$

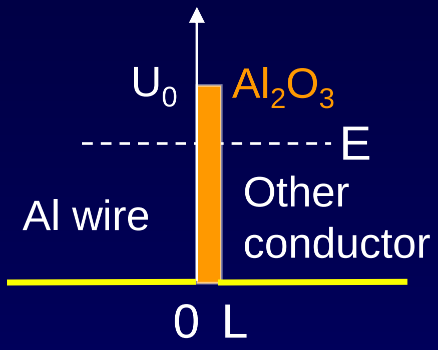
$= 0.100000005\text{ eV}$

Penetration a significant distance isn't possible unless E ~ U. The particle is at the top of the barrier.

Example: Aluminum wire

Why household electrical wire is not aluminum:

Aluminum is cheap and a good conductor. However, aluminum tends to form an oxide surface layer (Al_2O_3) which can be as much as several nanometers thick.



This layer could cause a problem in making electrical contacts, since it presents a barrier roughly 10 eV high to the flow of electrons in and out of the Al.

Your requirement is that your transmission coefficient across any contact must be $T > 10^{-10}$, or else the resistance will be too high for the high currents you're using, causing a fire risk. Should you use aluminum wiring or not? (You can neglect G here.)

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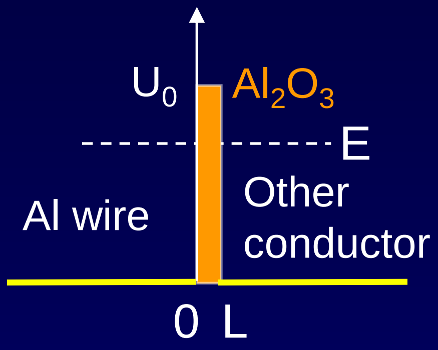

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Compute the maximum L:

$$K = 2\pi\sqrt{\frac{10\text{eV}}{1.505\text{eV-nm}^2}} \approx 16\text{nm}^{-1}$$

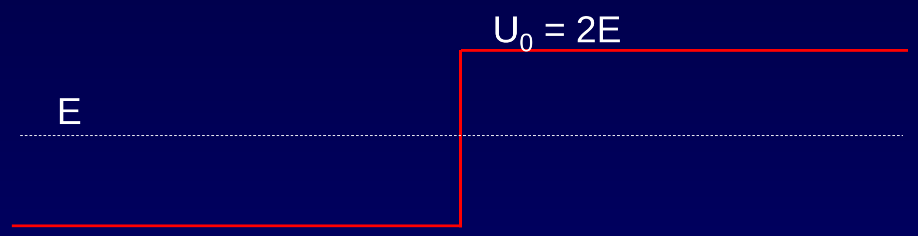
$$T \approx e^{-2KL} = 10^{-10}$$

$$L \approx -\frac{1}{2K}\ln\left(10^{-10}\right) \approx 0.72\text{ nm}$$

Oxide is thicker than this, so go with copper! Al wiring in houses is illegal for this reason.

Electron Approaching a Step

Suppose an electron with energy E approaches a step, effectively an infinitely wide barrier of height 2E. (I picked this ratio to simplify the math.)



What does the wave function look like, and what is happening?

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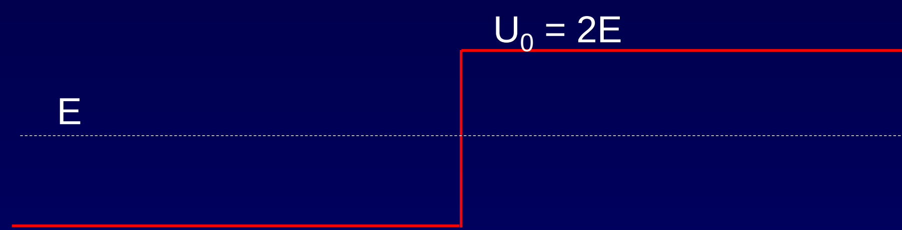


What does the wave function look like, and what is happening?

Here's the solution:

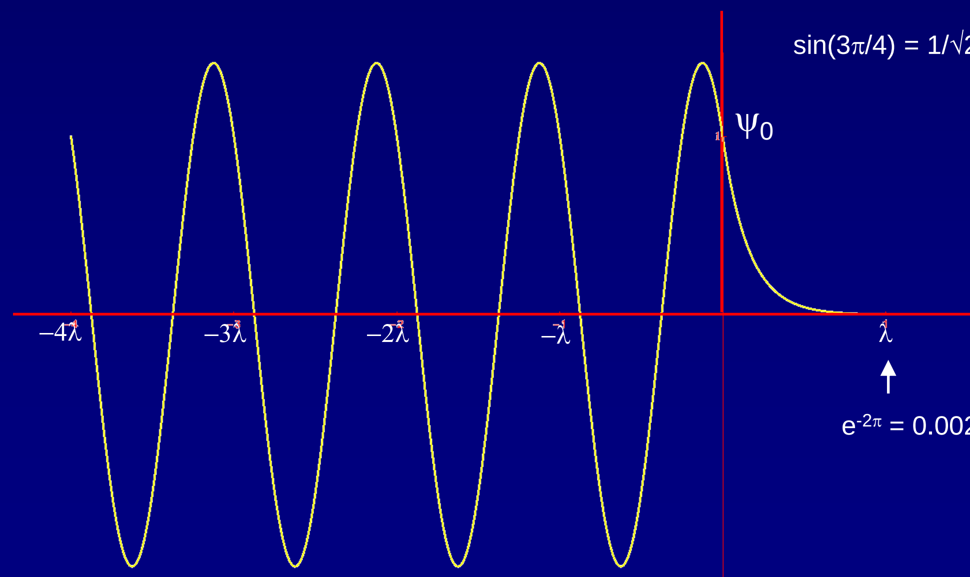
For x < 0: $\psi(x) = \psi_0 \sqrt{2} \sin\left(kx + \frac{3\pi}{4}\right)$

For x > 0: $= \psi_0 e^{-kx}$

K = k, because U_0-E = E.

The constants √2 and 3π/4 come from the boundary conditions.

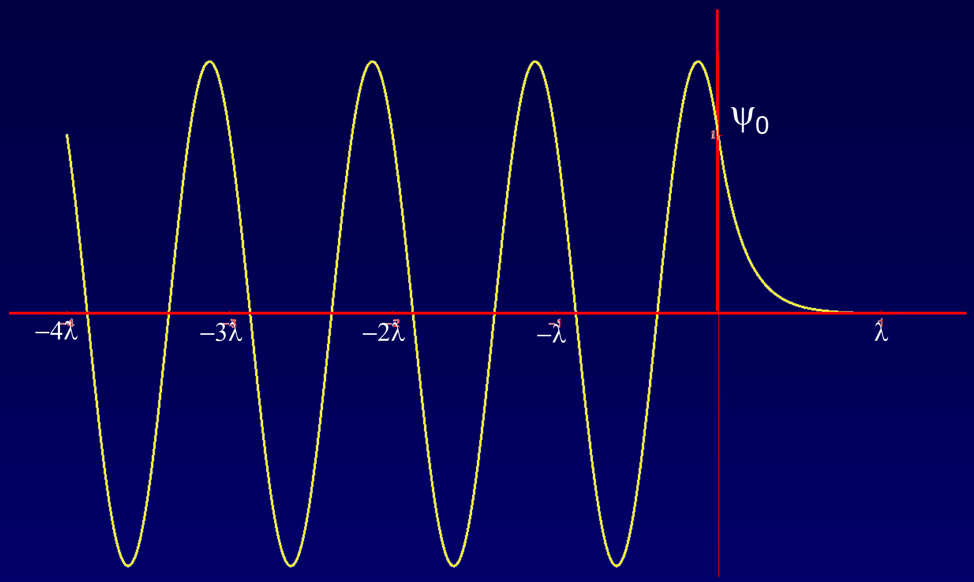
What is this graph telling us?



Solution

For legibility, I'm ignoring the $3\pi/4$ phase shift.

Sin(kx) is a standing wave.
It has nodes every $\lambda/2$.



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So, what do I mean when I say that the electron approaches the barrier?

Remember two things:

- The wave oscillates: $e^{-i\omega t}$.
- We can write: $\sin(kx) = (e^{ikx} - e^{-ikx}) / (2i)$

Thus, this standing wave is actually a superposition of two traveling waves:

$e^{i(kx-\omega t)}$ and $e^{i(-kx-\omega t)}$.

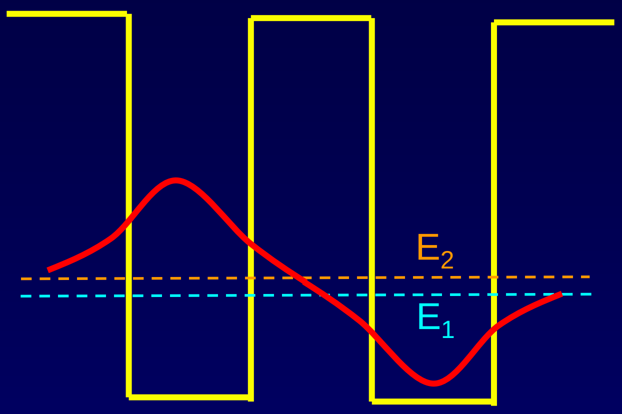
The incoming wave, traveling to the right.

The reflected wave, traveling to the left.

The wave is entirely reflected. None is absorbed by the barrier.
It penetrates a short distance, but then bounces out.

Double Well Oscillation

Consider the double well shown. The two energy levels of interest are E_1 = 1.123 eV and E_2 = 1.124 eV. At t = 0, Ψ is in a superposition that maximizes its probability on the left side.



1) At what time will the probability be maximum on the right side?

2) If the barrier is made wider, will the time become larger or smaller? What about $E_2 - E_1$?

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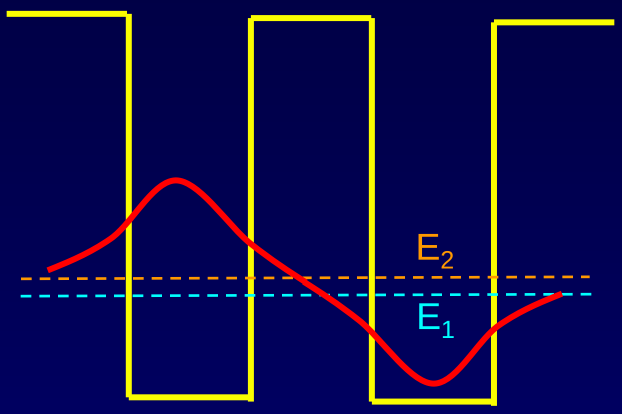

1) At what time will the probability be maximum on the right side?

The period of oscillation is:

$$T = h/(E_2-E_1) = 4.135\times10^{-15}\ \text{eV}\cdot\text{s} / 0.001\ \text{eV} = 4.1\times10^{-12}\ \text{s}.$$

We want a half period: $T/2 = 2.1\times10^{-12}$ s = 2.1 ps.

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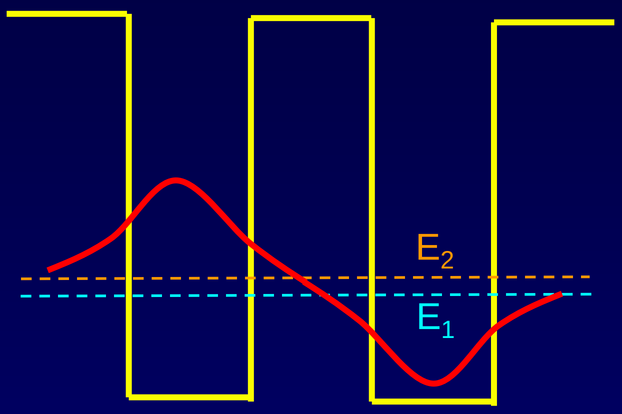

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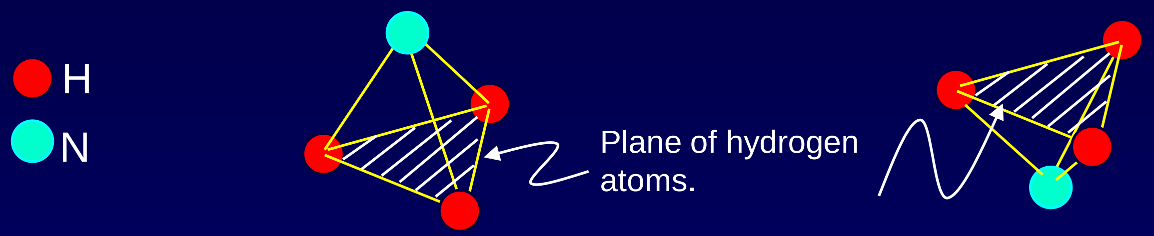
2) If the barrier is made wider, will the time become larger or smaller? What about E_2-E_1?

A wider barrier will have a smaller tunneling rate, so T/2 will increase. This implies that E_2-E_1 becomes smaller.

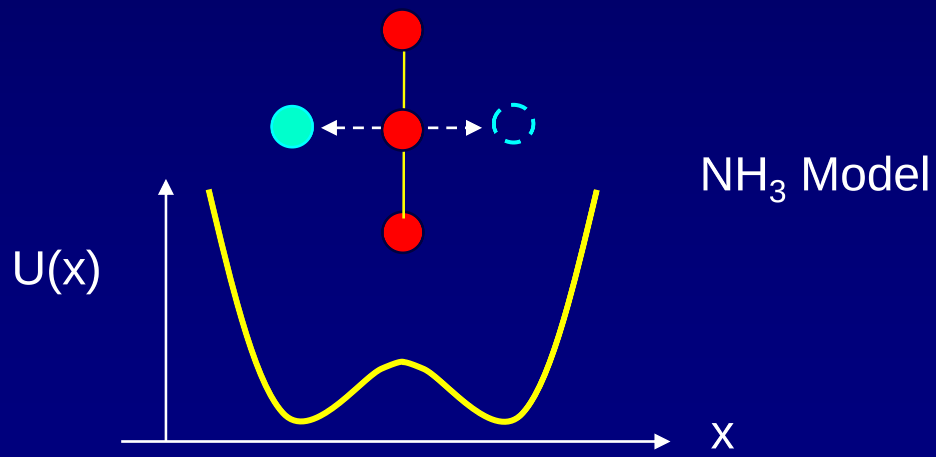
We'll see (week 7) that this effect is important in chemical bonding.

Example: The Ammonia Molecule

This example will bring together several things you've learned so far.
Consider the ammonia (NH_3) molecule:



The N atom in the ammonia molecule (NH_3) can has two equilibrium positions: above or below the plane of the H atoms, as shown. If we graph the potential as the N atom moves along the line joining these positions, we get:

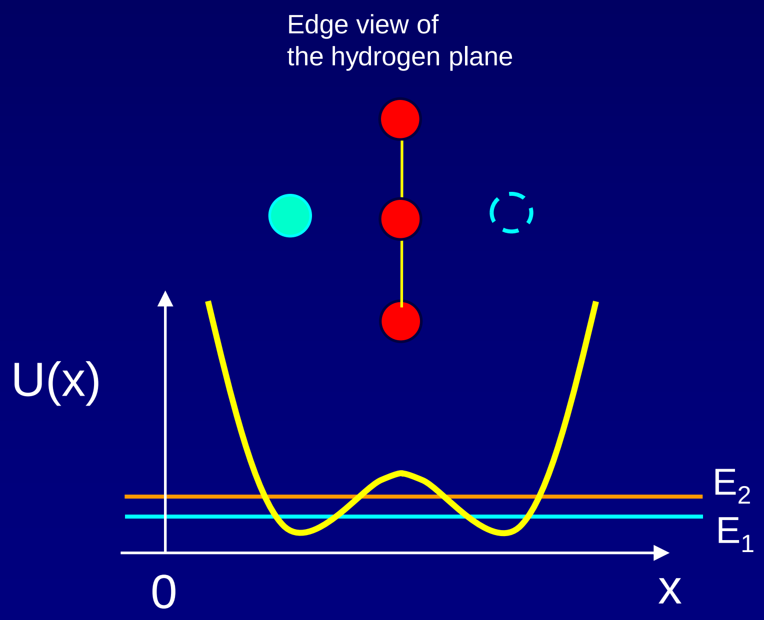


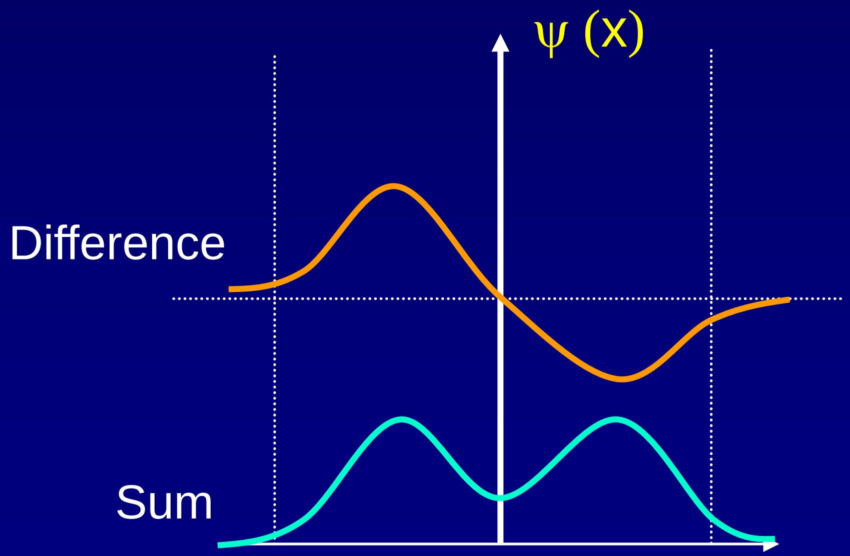
The nitrogen atom can tunnel between these two equivalent positions.

Example: The Ammonia Molecule (2)

These are not square wells, but the idea is the same. The lowest energy state is the symmetric superposition of the two single-well wave functions.

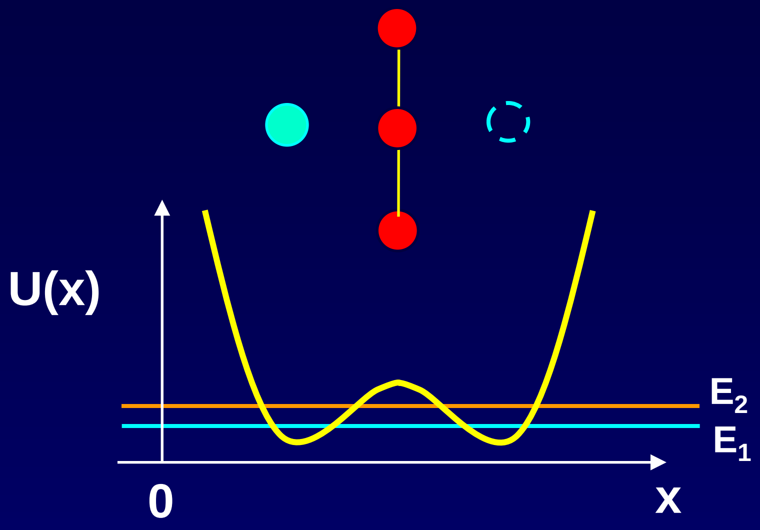
The antisymmetric state has slightly higher energy: $\Delta E = 1.8 \times 10^{-4}$ eV.





Example: The Ammonia Molecule (3)

Given the energy difference between the ground and first excited states, E_2 - E_1 = 1.8×10^{-4} eV, estimate how long it takes for the N atom to "tunnel" from one side of the NH_3 molecule to the other?



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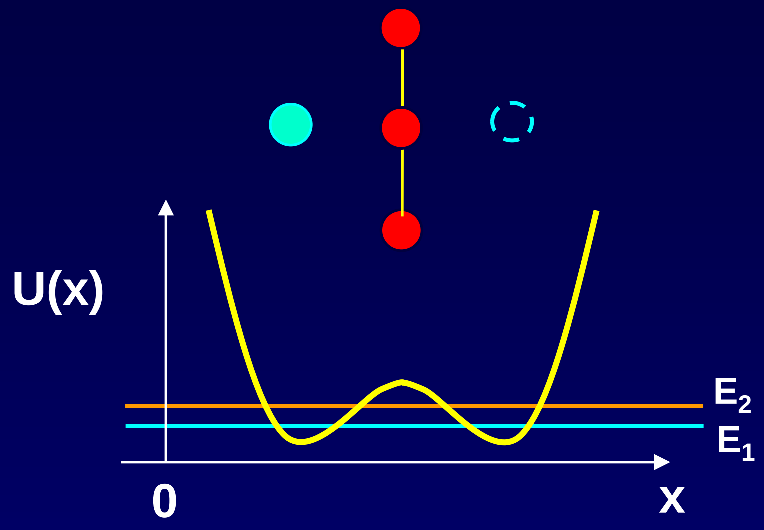


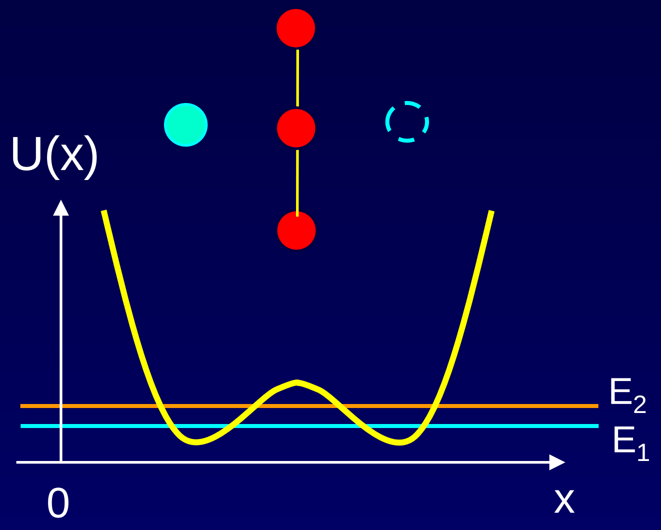
This takes a half the oscillation period, T = h/(E_2-E_1):

$$t_o = \frac{T}{2} = \frac{h}{2\left(E_2 - E_1\right)} = \frac{4.136\times10^{-15} eV \cdot \text{sec}}{2\left(1.8\times10^{-4} eV\right)} = 1.1\times10^{-11}\,\text{sec}$$

The Ammonia Maser

Stimulated emission of radiation between these two lowest energy states of ammonia ($\Delta E = 1.8 \times 10^{-4}$ eV) was used to create the ammonia maser, by C. Townes in 1954 (for which he won the Nobel prize in 1964).

What wavelength of radiation does the maser emit?



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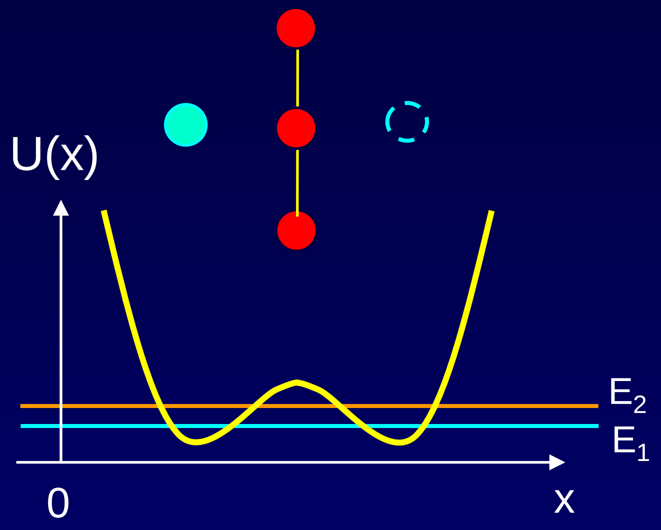

Solution:
By energy conservation, $E_2 - E_1 = E_{photon} = hc/\lambda$
$\lambda = hc/(E_2-E_1) = 1240\ \text{eV}\cdot\text{nm}/1.8\times10^{-4}\ \text{eV}$ $= 6.88\times10^{6}$ nm
$= 6.88$ mm

microwaves

The maser was the precursor to the laser. The physics is the same (more later).