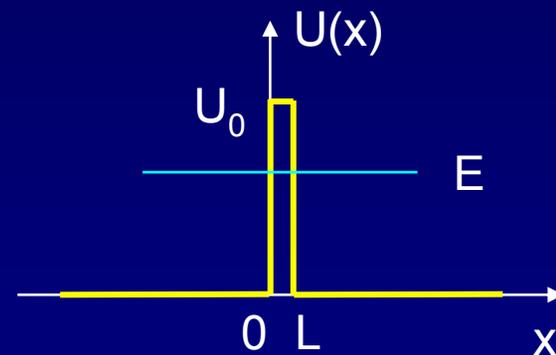
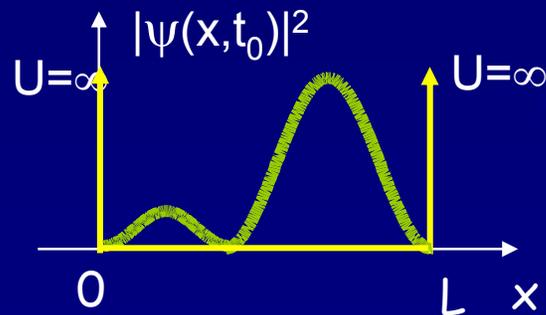
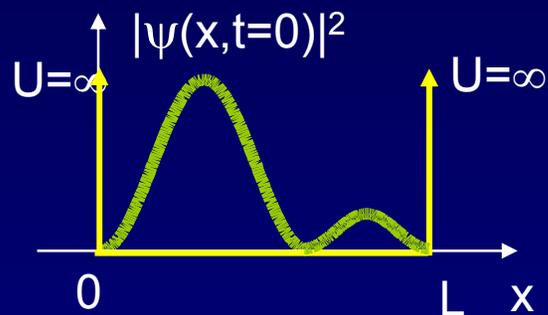


# Lecture 15:

## Time-Dependent QM & Tunneling

### Review and Examples, Ammonia Maser



# Special (Optional) Lecture

## “Quantum Information”

- One of the most modern applications of QM
  - quantum computing
  - quantum communication – cryptography, teleportation
  - quantum metrology
  - nonlocality
- Prof. Kwiat will give a special 214-level lecture on this topic
  - Sunday, Sept. 29
  - 3 pm, 141 Loomis
- Attendance is optional, but encouraged.

# L14: Particle Motion in a Well

The probability density is given by:  $|\Psi(x,t)|^2$  :

$$|\Psi(x,t)|^2 = \psi_1^2 + \psi_2^2 + 2\psi_1\psi_2 \cos((\omega_2 - \omega_1)t)$$

Interference term

We used the identity:

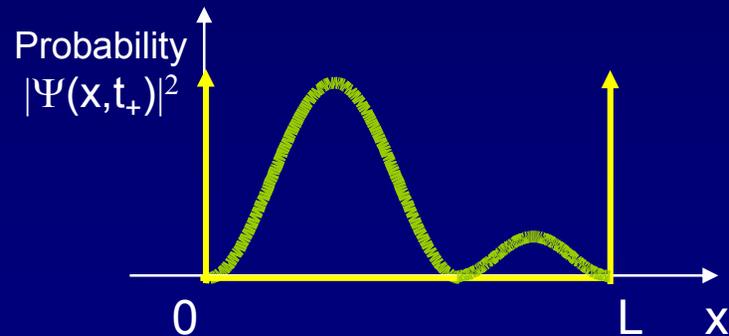
$$e^{i\theta} + e^{-i\theta} = 2\cos\theta$$

So,  $|\Psi(x,t)|^2$  oscillates between:

In phase: ( $\cos = +1$ )

$$|\Psi(x,t)|^2 = (\psi_1 + \psi_2)^2$$

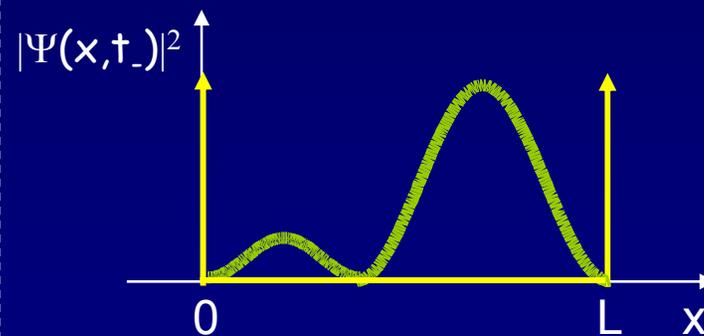
Particle localized on left side of well:



Out of phase: ( $\cos = -1$ )

$$|\Psi(x,t)|^2 = (\psi_1 - \psi_2)^2$$

Particle localized on right side of well:



The frequency of oscillation is  $\omega = \omega_2 - \omega_1 = (E_2 - E_1)/\hbar$ , or  $f = (E_2 - E_1)/h$ .

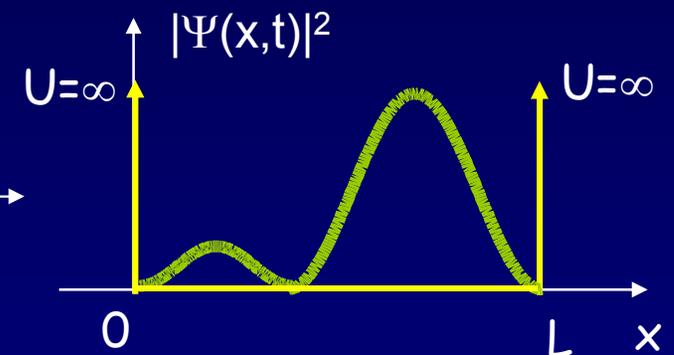
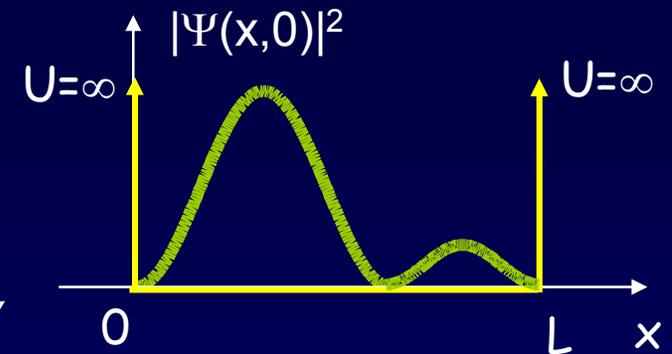
This is precisely the frequency of a photon that would make a transition between the two states.

# Example

An electron in an infinite square well of width  $L = 0.5 \text{ nm}$  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.



# Solution

An electron in an infinite square well of width  $L = 0.5 \text{ nm}$  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.

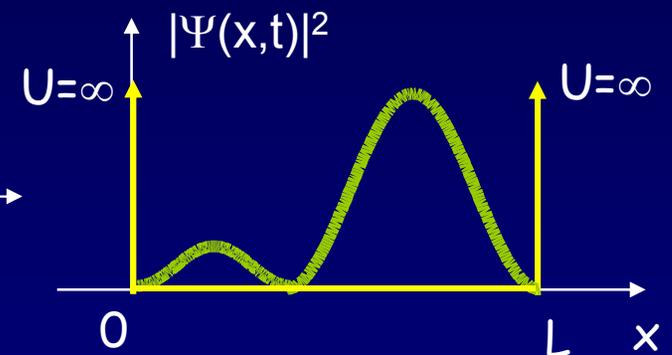
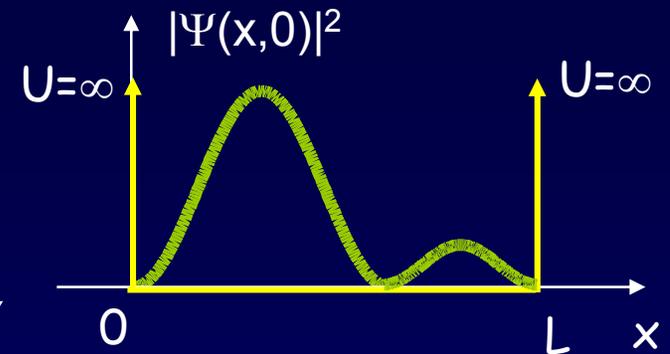
$$E_1 = \frac{1.505 \text{ eV} \cdot \text{nm}^2}{4L^2} = 1.505 \text{ eV}$$

$$E_2 = 4E_1 = 6.020 \text{ eV}$$

$$T = 1/f, \text{ where } f = (E_2 - E_1)/h$$

Half a period.

$$t = \frac{T}{2} = \frac{h}{2(E_2 - E_1)} = \frac{4.136 \times 10^{-15} \text{ eV} \cdot \text{sec}}{2(4.515 \text{ eV})} = 4.6 \times 10^{-16} \text{ sec}$$



# L14: 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  $|a|^2 + |b|^2 = 1$ .

# ACT 1

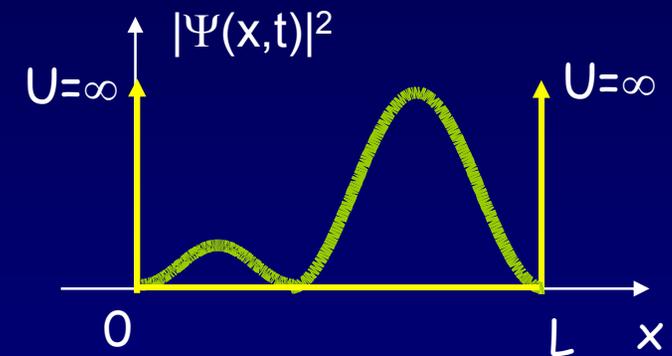
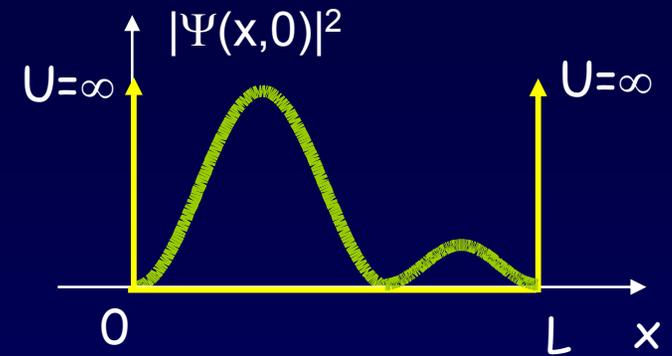
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1) Suppose we measure the energy.

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.

# Solution

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

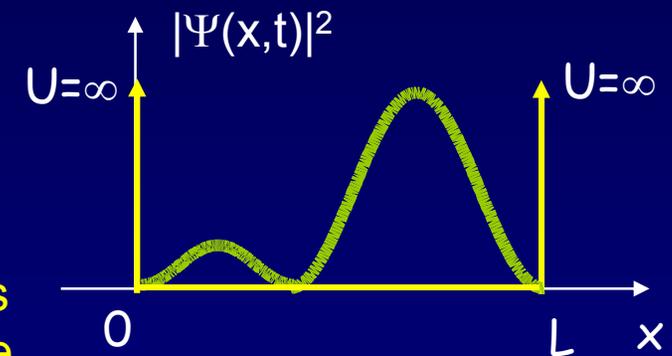
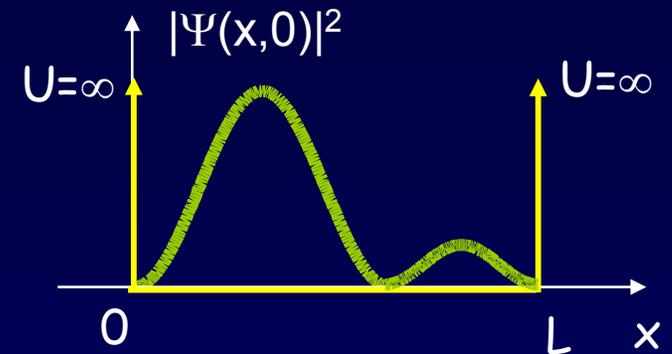
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- a)  $E_1$    b)  $E_2$    c)  $E_3$    d) Any result between  $E_1$  and  $E_2$

We will only obtain results that correspond to the terms appearing in  $\Psi$ . Therefore, only  $E_1$  and  $E_2$  are possible.



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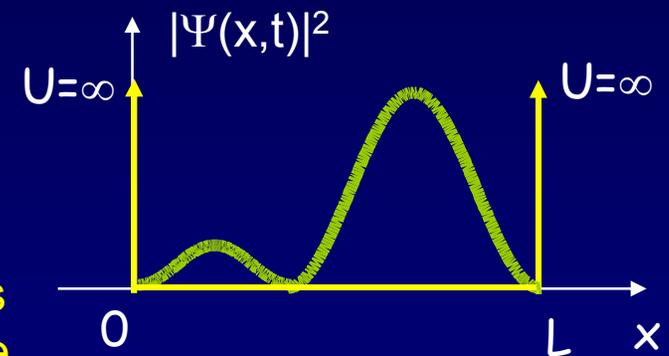
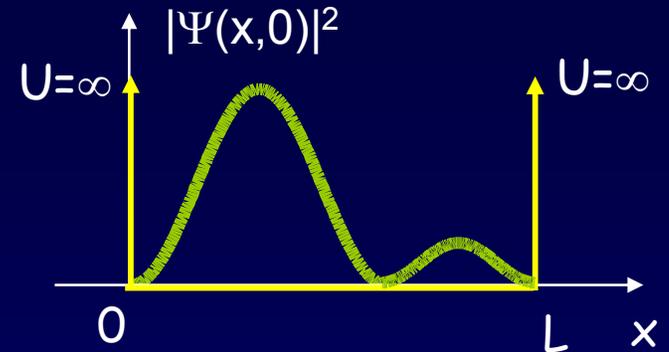
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1) Suppose we measure the energy.

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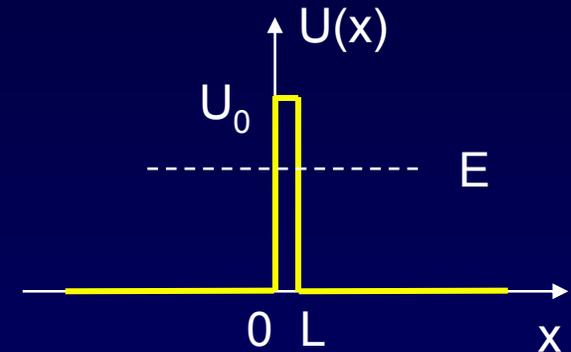
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(i.e., it's always either  $E_1$  or  $E_2$ ).  
d) They don't vary with time.

The probabilities depend on the coefficients, not on the various  $\Psi$  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 ( $KL \gg 1$ ). In this case  $B_1 \approx 0$  (why?), and the result resembles the infinite barrier. The tunneling coefficient simplifies:



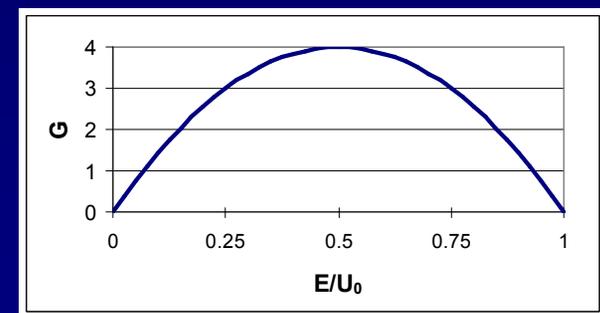
$$T \approx Ge^{-2KL} \text{ where } G = 16 \frac{E}{U_0} \left( 1 - \frac{E}{U_0} \right)$$

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

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  $e^{-2KL}$ .



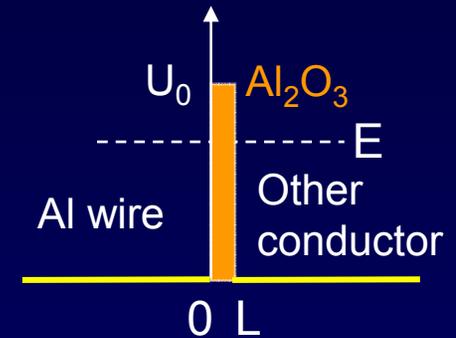
# Example: Aluminum wire

Why household electrical wire is not aluminum:

Aluminum is cheap and a good conductor. However, aluminum tends to form an oxide surface layer ( $\text{Al}_2\text{O}_3$ ) 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.)



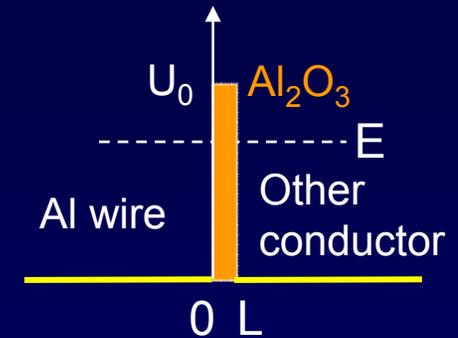
# Solution

Why household electrical wire is not aluminum:

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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.)



Compute the maximum  $L$ :

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

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

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

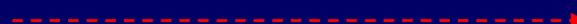
Oxide is thicker than this, so go with copper!  
Al wiring in houses is illegal for this reason.

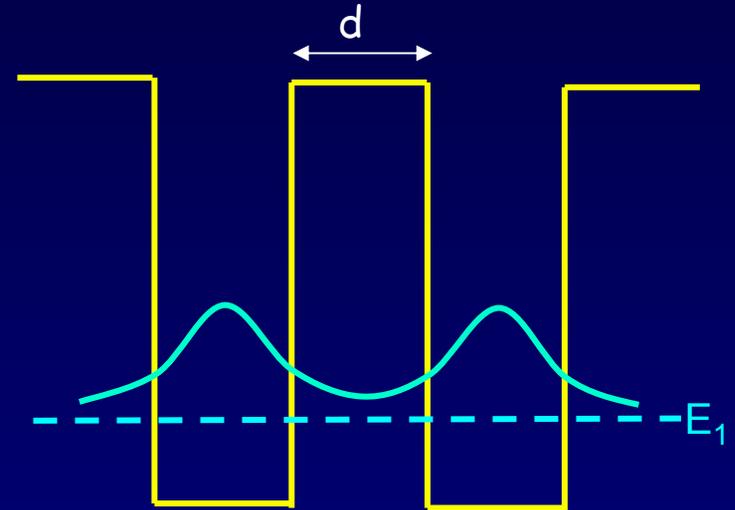
# Another Consequence of "Tunneling"

Consider a situation in which a particle (e.g., an electron or an atom) can be in either of two wells separated by a potential barrier.

Is the particle on the left or right?

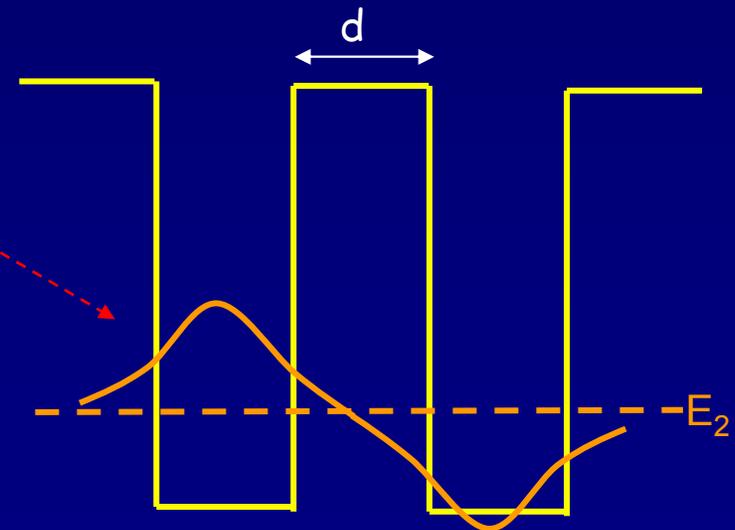
**Both!** If the barrier is finite, the wave function extends into both wells

Lowest energy state:   $\psi$  is small but non-zero inside the barrier.



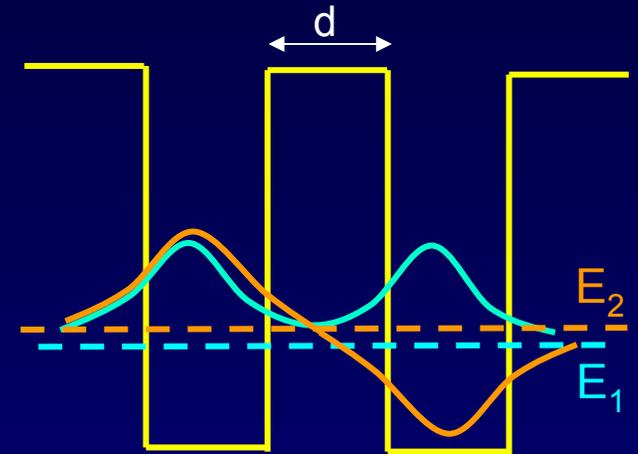
Here is the state with the next higher energy:  
Why does this state have higher energy?

Note that the potential is symmetric about the middle of the barrier. Therefore, the energy states must be either symmetric or antisymmetric. Also, remember that there are  $n-1$  nodes.



# Energy Splitting in a Double Well

Suppose the particle starts out in the left well.  
What is the time dependence of the probability?  
From the graphs of  $\psi$ , we can see that, initially,  
 $\psi = \psi_1 + \psi_2$  (to get cancellation on the right).  
As discussed last lecture, the particle oscillates  
between the wells with an oscillation period,  
 $T = h/(E_2 - E_1)$ .



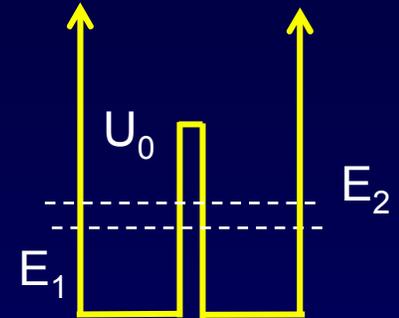
Therefore,  $\Delta E = E_2 - E_1$  depends on the tunneling rate.

A double well with a high or wide barrier will have a smaller  $\Delta E$  than one with a low or narrow barrier.

Also,  $\Delta E$  will become larger as the energy increases (*i.e.*, as  $U_0 - E$  decreases).

# Act 2

You are trying to make a laser that emits violet light ( $\lambda = 400 \text{ nm}$ ), based on the transition an electron makes between the ground and first-excited state of a double quantum well as shown. Your first sample emitted at  $\lambda = 390 \text{ nm}$ .

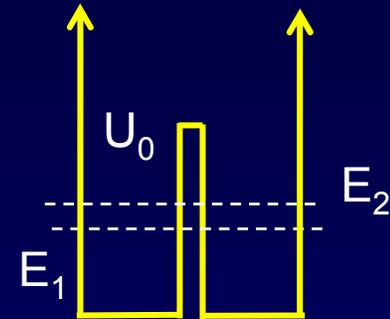


What could you modify to shift the wavelength to 400 nm?

- a. decrease the height of the barrier
- b. increase the height of the barrier
- c. decrease the width of the barrier

# Solution

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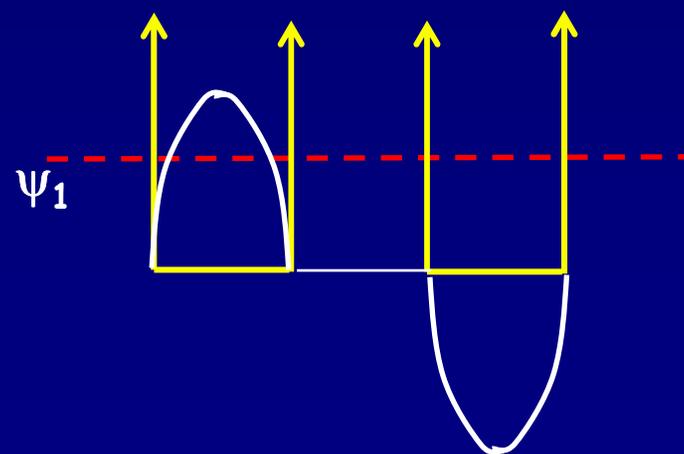
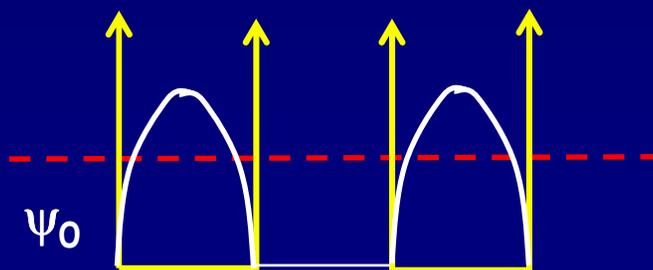
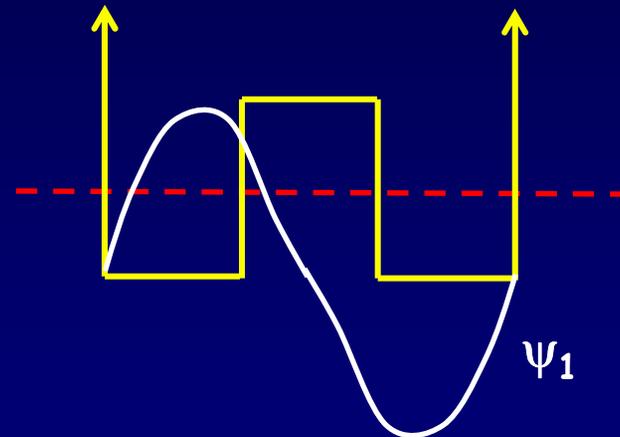
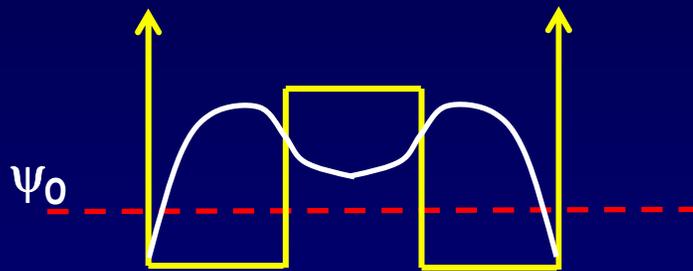
- a. decrease the height of the barrier
- b. increase the height of the barrier**
- c. decrease the width of the barrier

The frequency of the electron oscillating between the left and right well was too high  $\rightarrow$  the probability to “tunnel” was too high! You can reduce this by increasing the barrier height.

The wavelength of the emitted photon was too low  $\rightarrow$  the frequency of the photon was too high  $\rightarrow$  the energy splitting between the ground and first-excited state was too large. Raising the barrier makes the difference in energy  $E_2 - E_1$  smaller. Why?

## Solution - More

As we raise the height of the central barrier, the coupling between the two wells decreases. In the limit of an infinite barrier, it looks like two independent wells  $\rightarrow$  same wavefunction curvature for both the symmetric (ground state) and anti-symmetric ( $1^{\text{st}}$  excited state) wavefunctions  $\rightarrow$  same kinetic energy, i.e., degenerate solutions.

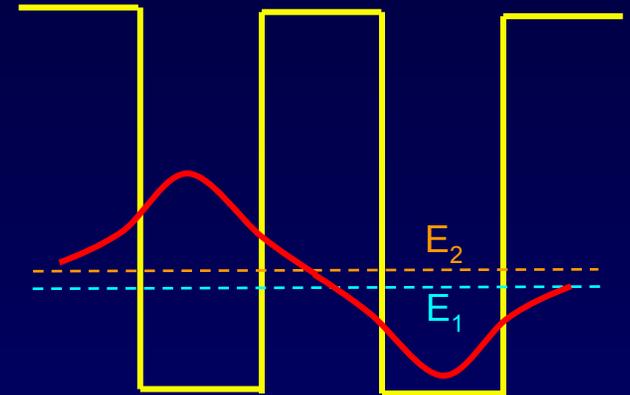


# Double Well Oscillation

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

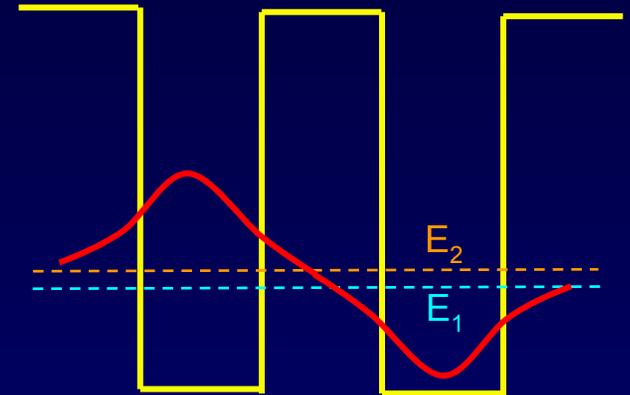
1) At what time will the probability be maximum on the right side?

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



# Solution

Consider the double well shown. The two energy levels of interest are  $E_1 = 1.123$  eV and  $E_2 = 1.124$  eV. At  $t = 0$ ,  $\Psi$  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?

The period of oscillation is:

$$T = h/(E_2 - E_1) = 4.135 \times 10^{-15} \text{ eV}\cdot\text{s} / 0.001 \text{ eV} = 4.1 \times 10^{-12} \text{ s}.$$

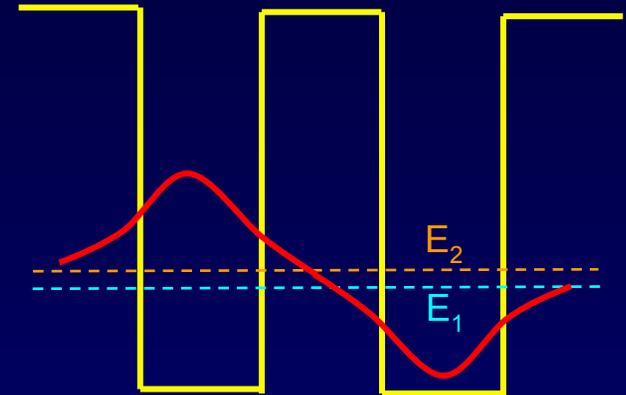
We want a half period:  $T/2 = 2.1 \times 10^{-12} \text{ s} = 2.1 \text{ ps}.$

2) If the barrier is made wider, will the time become larger or smaller?

What about  $E_2 - E_1$ ?

# Solution

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



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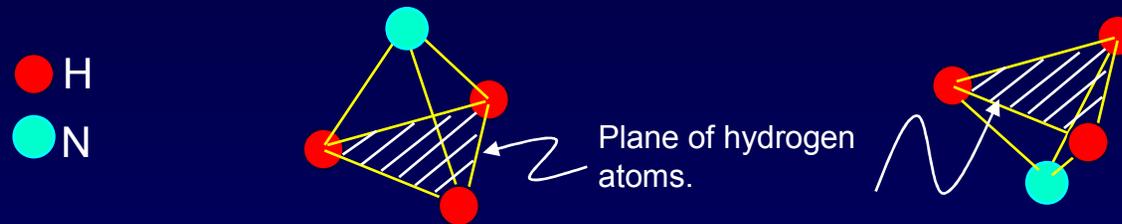
A wider barrier will have a smaller tunneling rate, so  $T/2$  will increase.

This implies that  $E_2 - E_1$  becomes smaller.

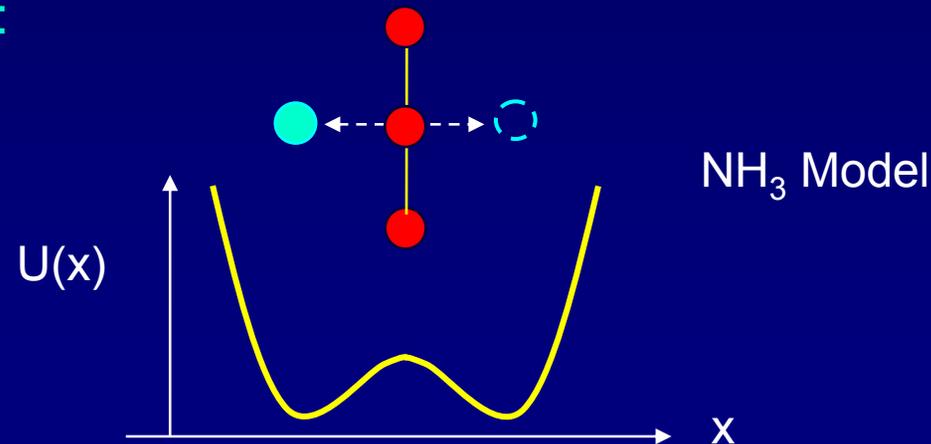
We'll see (week 7) that this effect is important in chemical bonding.

# Example: The Ammonia Molecule

This example will bring together several things you've learned so far. Consider the ammonia ( $\text{NH}_3$ ) molecule:



The N atom in the ammonia molecule ( $\text{NH}_3$ ) can have 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:

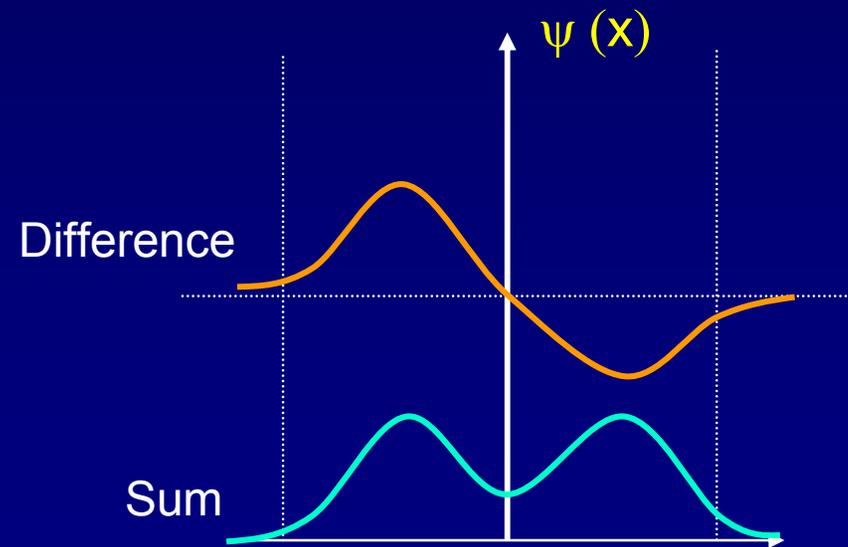
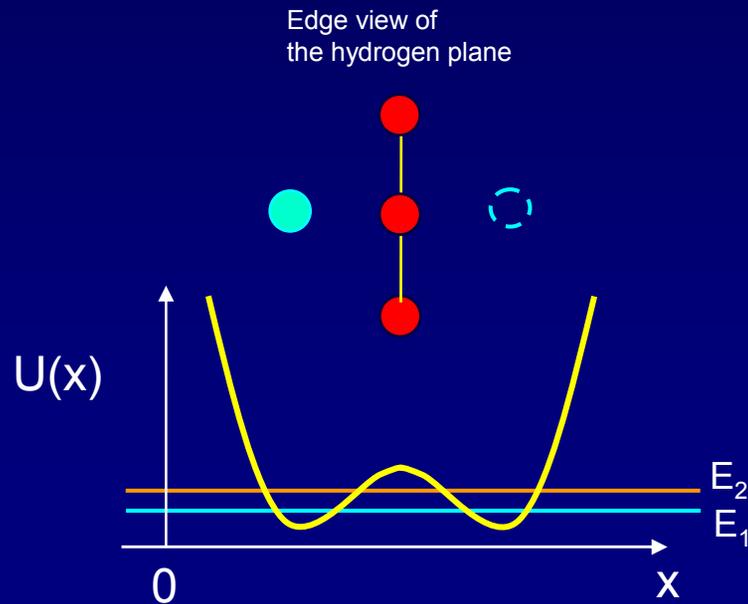


The nitrogen atom can tunnel between these two equivalent positions.

# Example: The Ammonia Molecule (2)

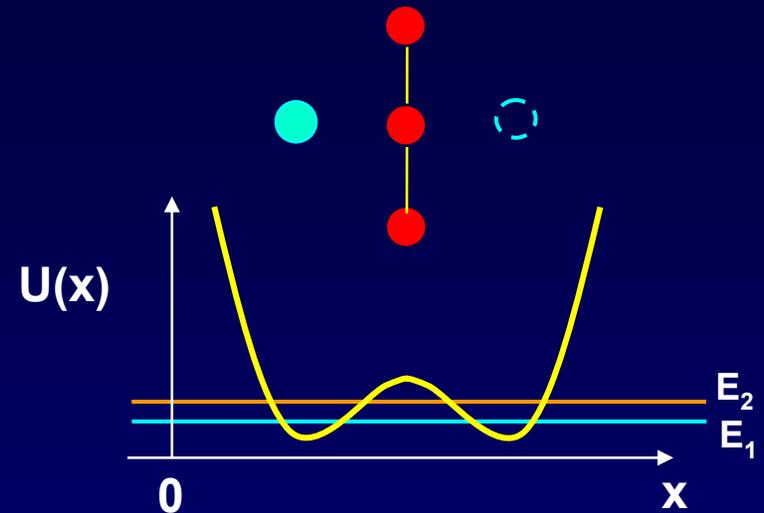
These are not square wells, but the idea is the same. The lowest energy state is the symmetric superposition of the two single-well wave functions.

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



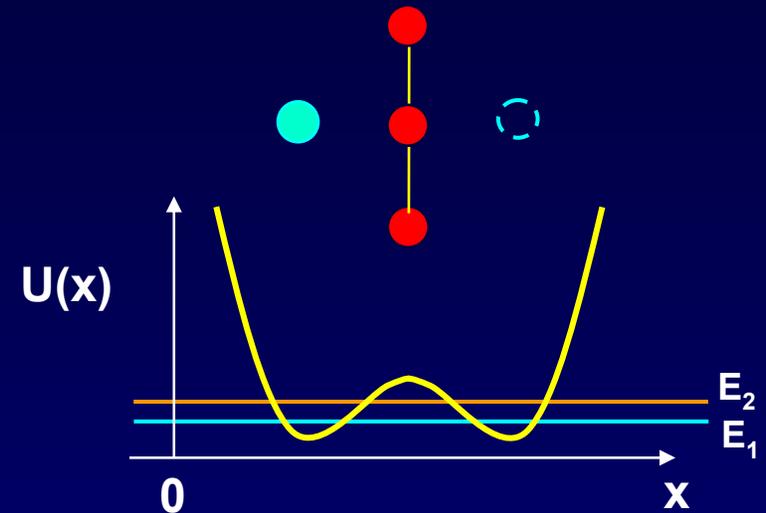
# Example: The Ammonia Molecule (3)

Given the energy difference between the ground and first excited states,  $E_2 - E_1 = 1.8 \times 10^{-4}$  eV, estimate how long it takes for the N atom to “tunnel” from one side of the  $\text{NH}_3$  molecule to the other?



# Example: The Ammonia Molecule (3)

Given the energy difference between the ground and first excited states,  $E_2 - E_1 = 1.8 \times 10^{-4}$  eV, estimate how long it takes for the N atom to “tunnel” from one side of the  $\text{NH}_3$  molecule to the other?

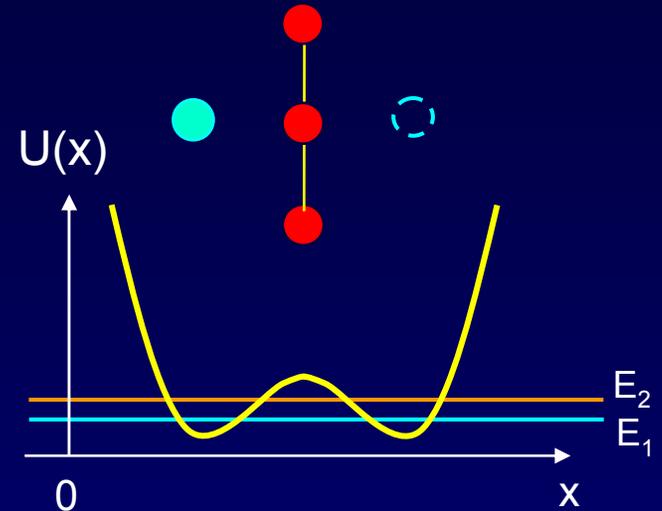


This takes a half the oscillation period,  $T = h/(E_2 - E_1)$ :

$$t_o = \frac{T}{2} = \frac{h}{2(E_2 - E_1)} = \frac{4.136 \times 10^{-15} \text{ eV} \cdot \text{sec}}{2(1.8 \times 10^{-4} \text{ eV})} = 1.1 \times 10^{-11} \text{ sec}$$

# The Ammonia Maser

Stimulated emission of radiation between these two lowest energy states of ammonia ( $\Delta E = 1.8 \times 10^{-4} \text{ eV}$ ) 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?

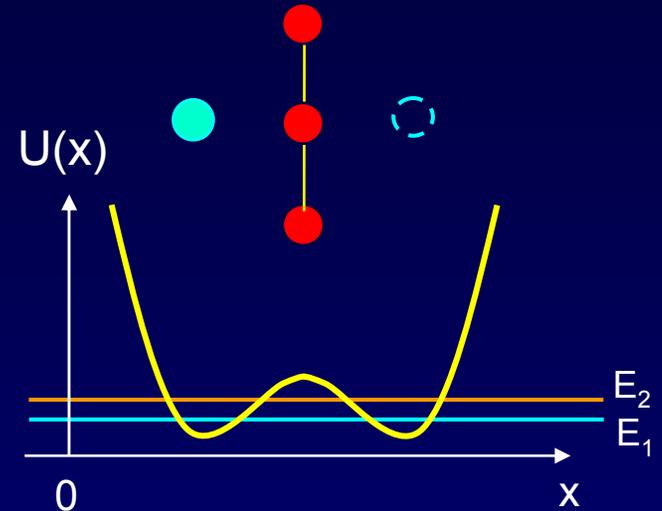


The maser was the precursor to the laser. The physics is the same (more later).

# The Ammonia Maser

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What wavelength of radiation does the maser emit?



**Solution:**

By energy conservation,  $E_2 - E_1 = E_{\text{photon}} = hc/\lambda$

$$\lambda = hc/(E_2 - E_1) = 1240 \text{ eV}\cdot\text{nm}/1.8 \times 10^{-4} \text{ eV} = 6.88 \times 10^6 \text{ nm} = 6.88 \text{ mm}$$

microwaves

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