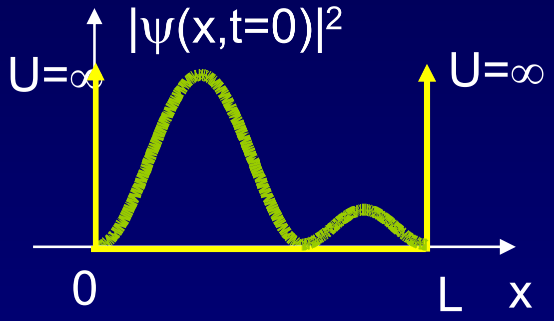
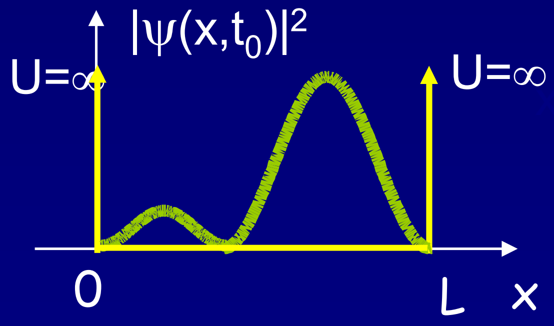
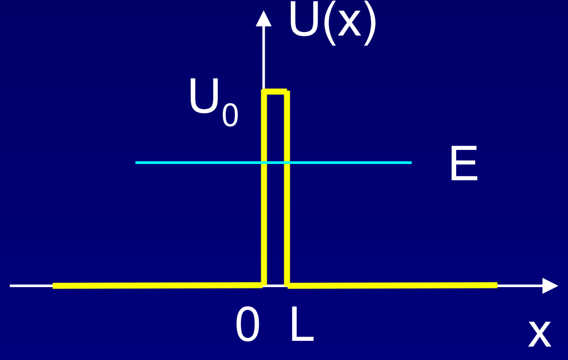
Lecture 15:
Time-Dependent QM & Tunneling
Review and Examples, Ammonia Maser







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

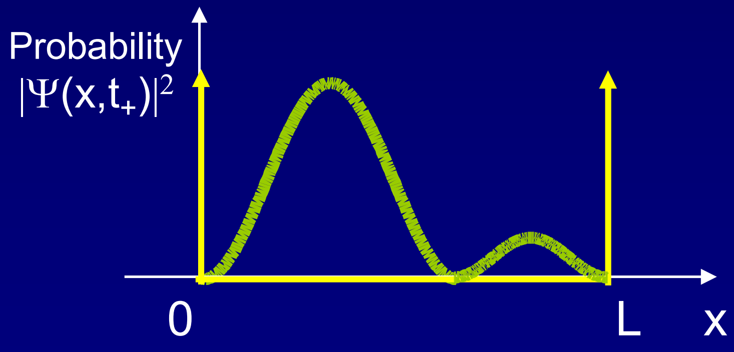
We used the identity:
$e^{i\theta} + e^{-i\theta} = 2\cos\theta$

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

In phase: (cos = +1)

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

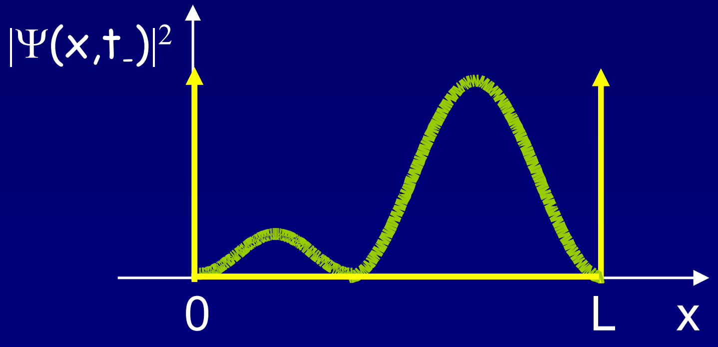
Particle localized on <u>left</u> side of well:



Out of phase: (cos = -1)

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

Particle localized on <u>right</u> side of well:



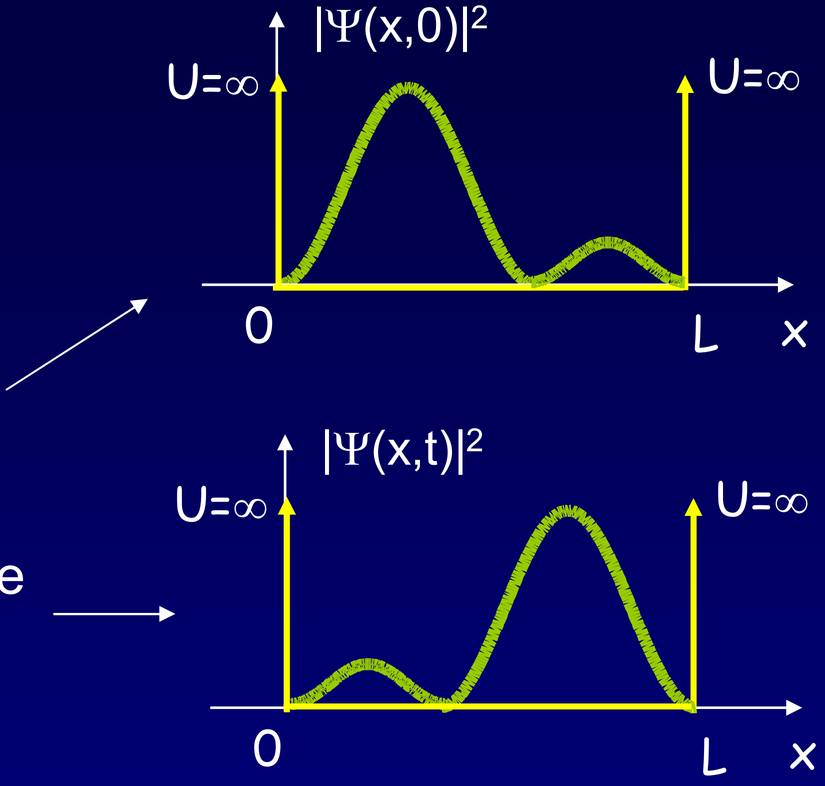
The frequency of oscillation is $\omega = \omega_2 - \omega_1 = (E_2 - E_1)/\hbar$, or $f = (E_2 - E_1)/h$.
This is precisely the frequency of a photon that would make a transition between the two states.

Example

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

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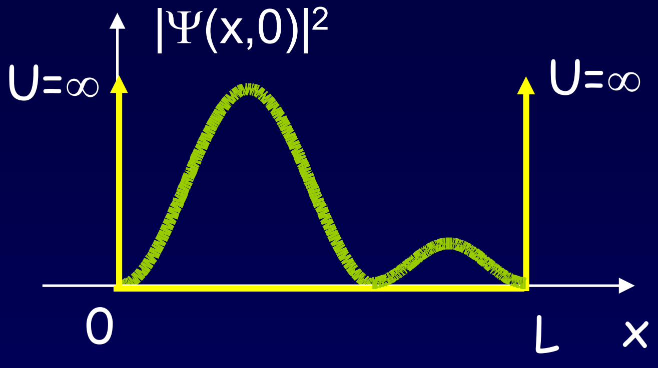

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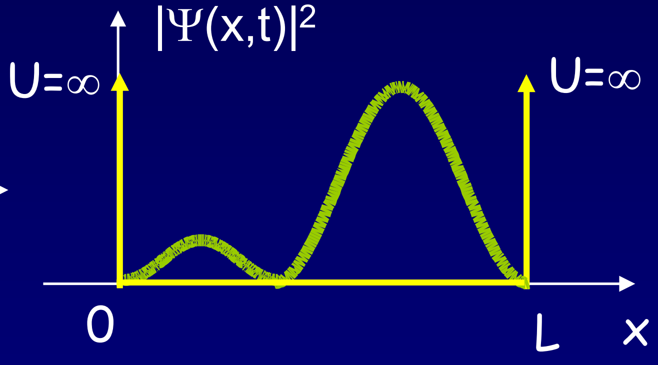


$$E_1 = \frac{1.505 \text{ eV}\cdot\text{nm}^2}{4L^2} = 1.505 \text{ eV}$$

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

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

Half a period.

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

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 !!

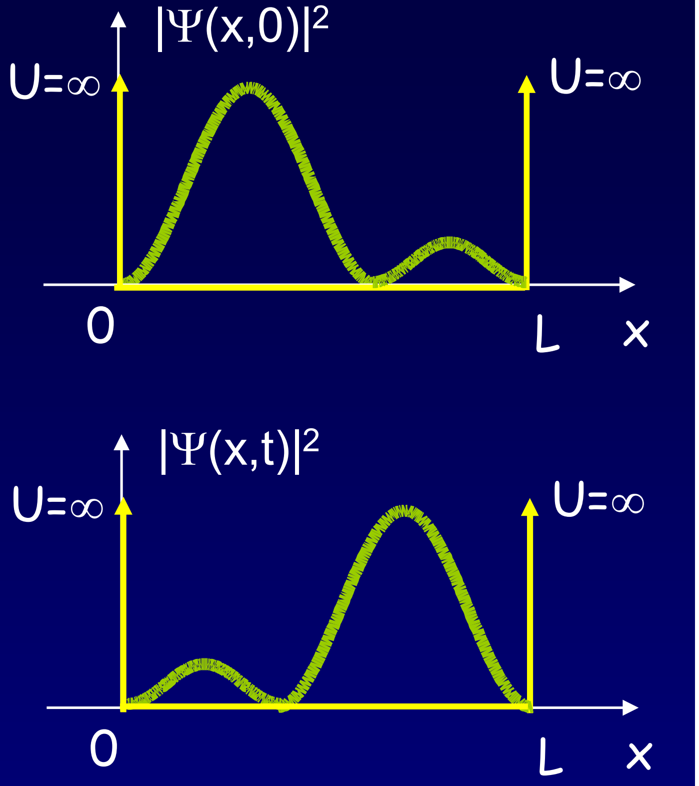
To be specific, we will never obtain $(E_1+E_2)/2$, or any other value.

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 $L = 0.5$ nm is (at $t=0$) described by the following wave function:

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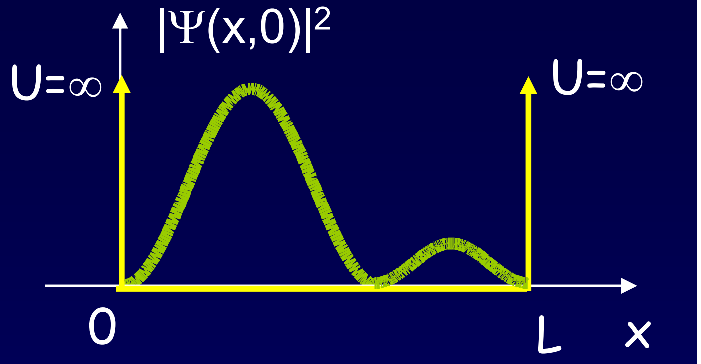

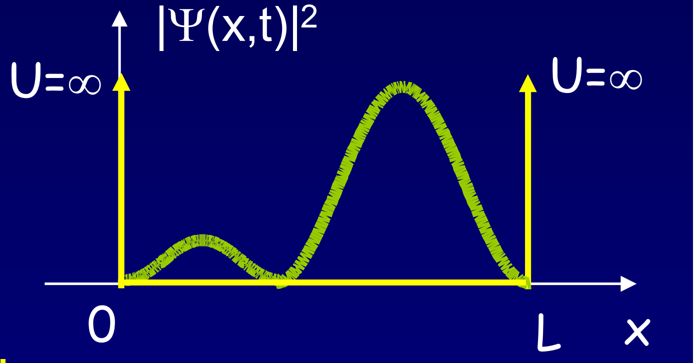

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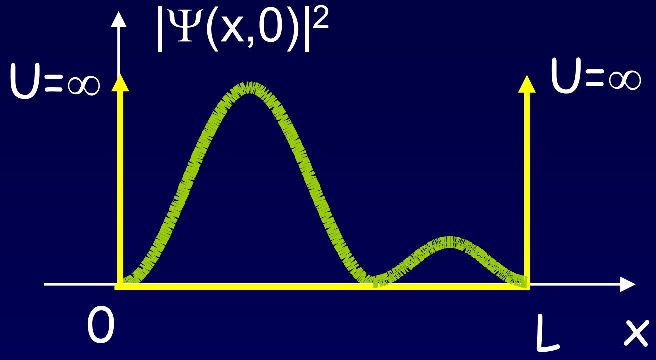

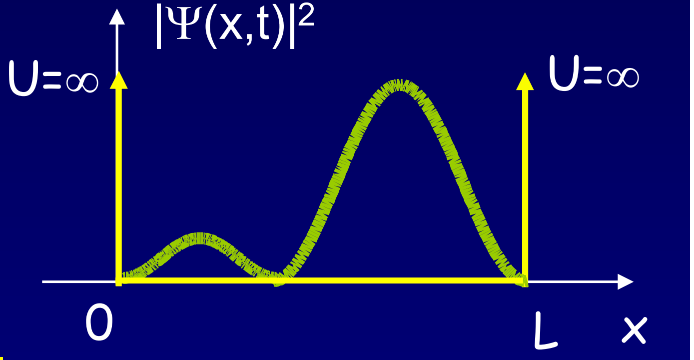

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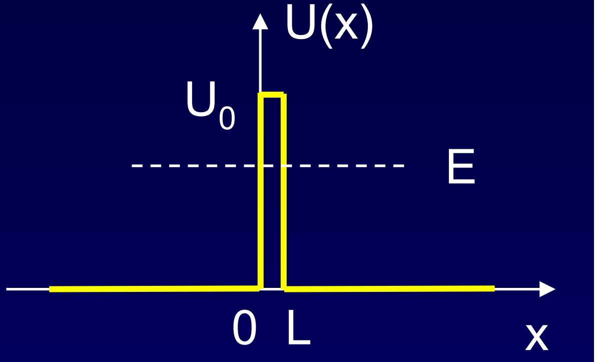
[✓ d) They don't vary with time.]

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

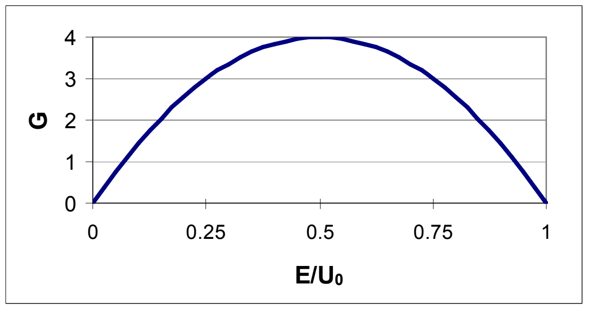


In many situations, the barrier width L is much larger than the 'decay length' 1/K of the penetrating wave (KL >> 1). In this case $B_1 \approx 0$ (why?), and the result resembles the infinite barrier. The tunneling coefficient simplifies:

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

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

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.)

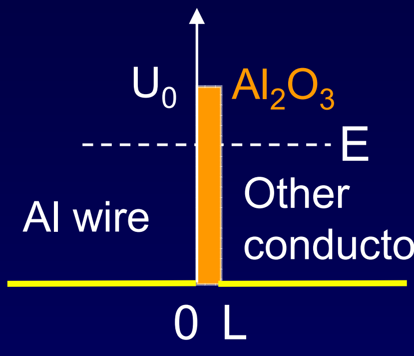
The important result is e^{-2KL}.

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 (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.)

Solution

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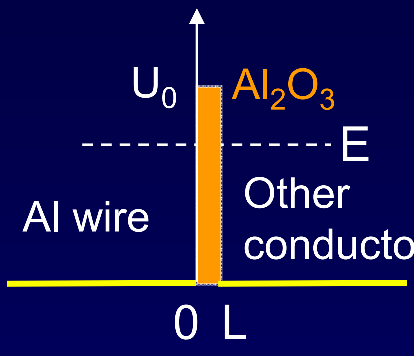

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Compute the maximum L:

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

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

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

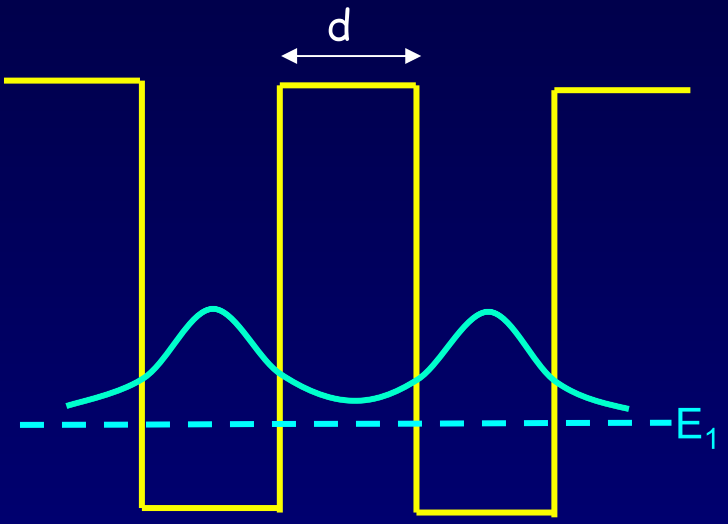
Oxide is thicker than this, so go with copper!
Al wiring in houses is illegal for this reason.

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.

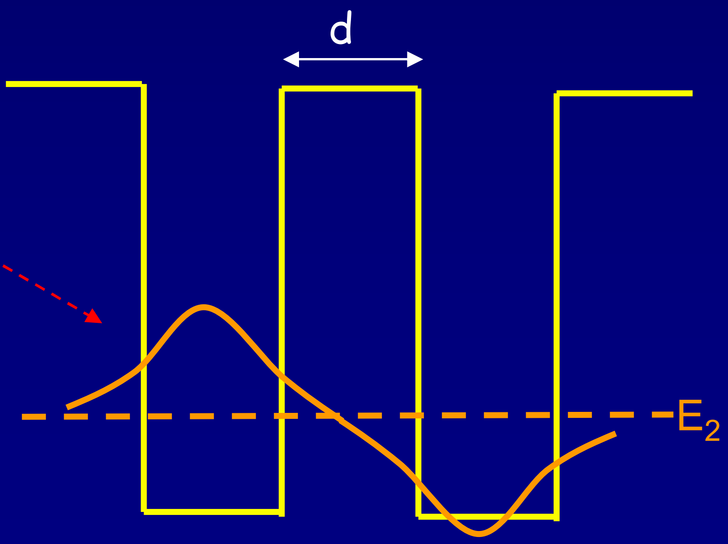
Is the particle on the left or right?

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



Lowest energy state:

ψ is small but non-zero inside the barrier.

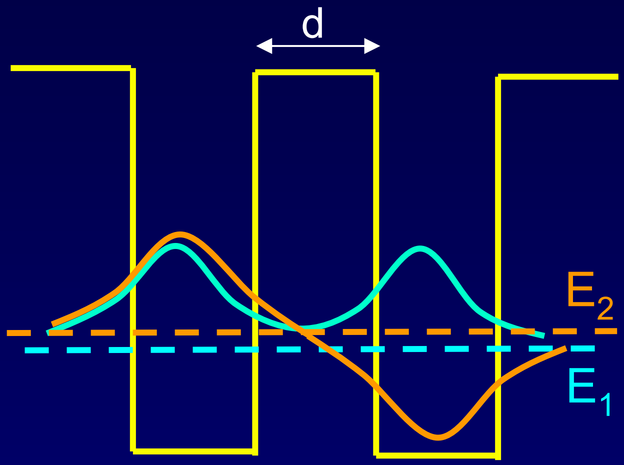


Here is the state with the next higher energy:

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 ψ, 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,
$T = h/(E_2 - E_1)$.

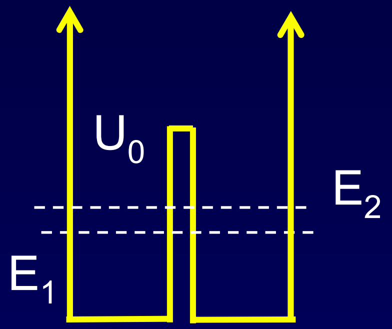
Therefore, $\Delta E = E_2 – E_1$ depends on the tunneling rate.

A double well with a high or wide barrier will have a smaller ΔE
than one with a low or narrow barrier.

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

Act 3

You are trying to make a laser that emits violet light (λ = 400 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 λ = 390 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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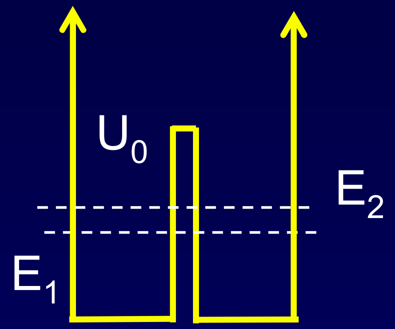

What could you modify to shift the wavelength to 400 nm?

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b. increase the height of the barrier

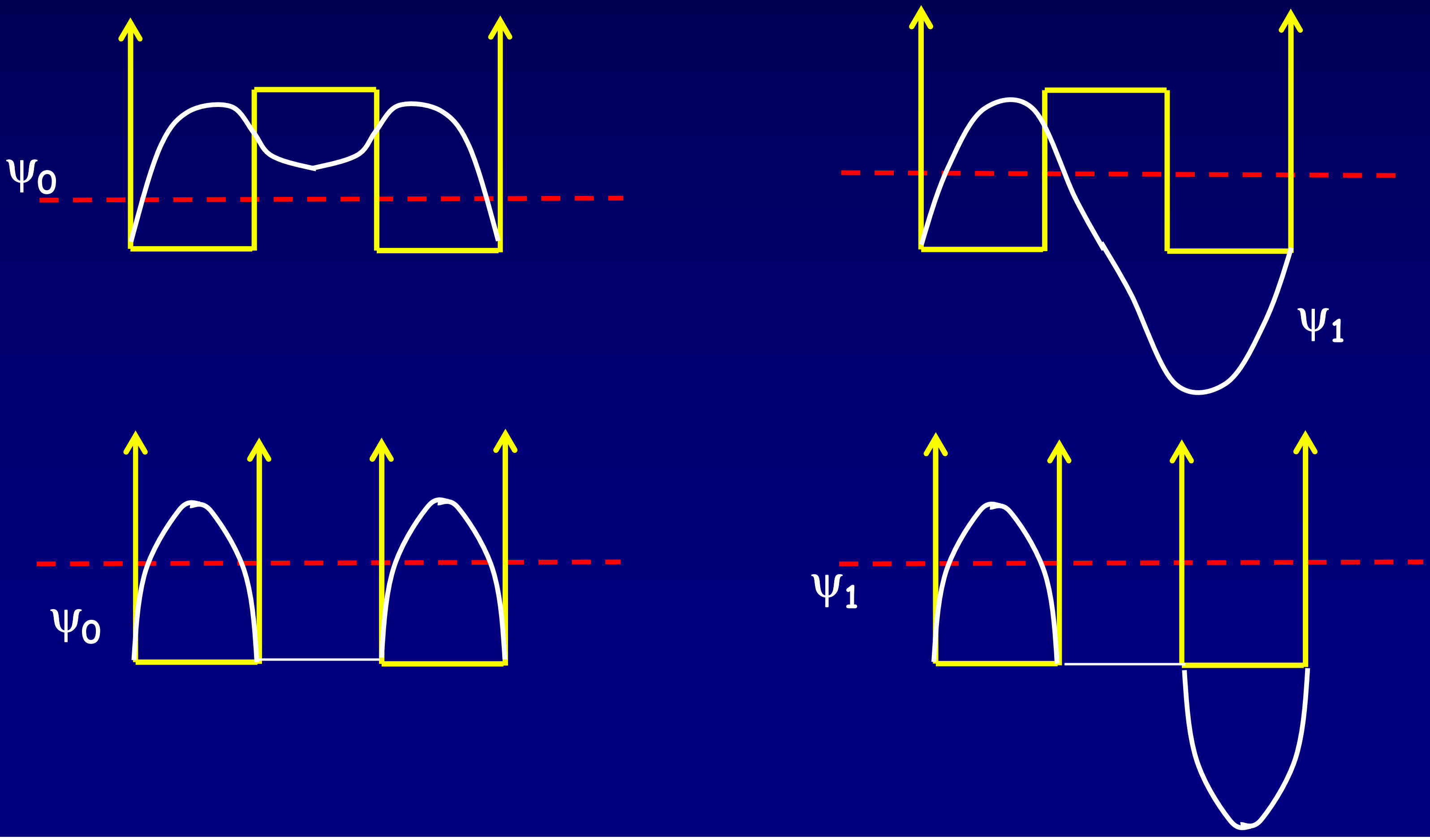
c. decrease the width of the barrier

The frequency of the electron oscillating between the left and right well was too high → 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 → the frequency of the photon was too high → 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?

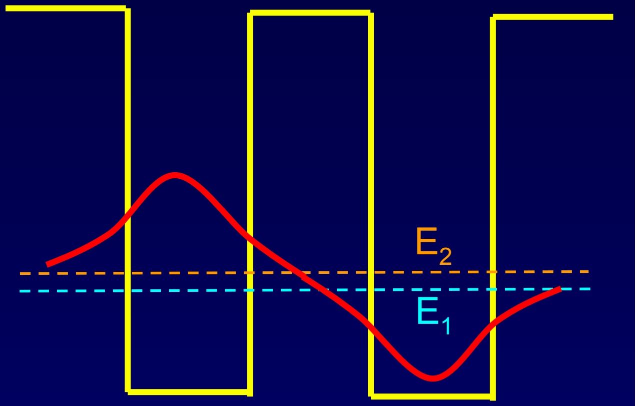
Solution - More

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 → same wavefunction curvature for both the symmetric (ground state) and anti-symmetric (1st excited state) wavefunctions → same kinetic energy, i.e., degenerate solutions.



Double Well Oscillation

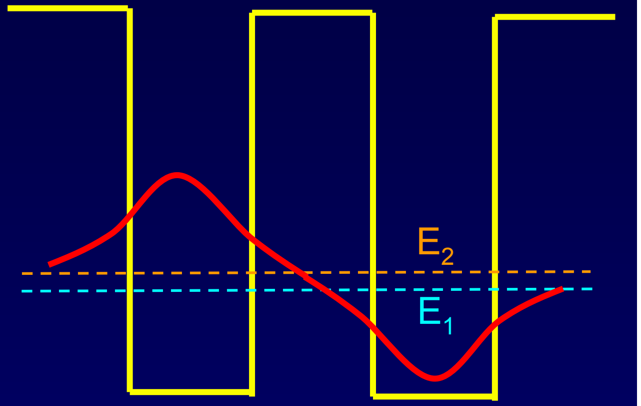
Consider the double well shown. The two energy levels of interest are E_1 = 1.123 eV and E_2 = 1.124 eV. At t = 0, Ψ is in a superposition that maximizes its probability on the left side.



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 $E_2 - E_1$?

Solution



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

The period of oscillation is:

$T = h/(E_2 - E_1) = 4.135\times10^{-15}$ eV·s / 0.001 eV = 4.1×10^{-12} s.

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

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

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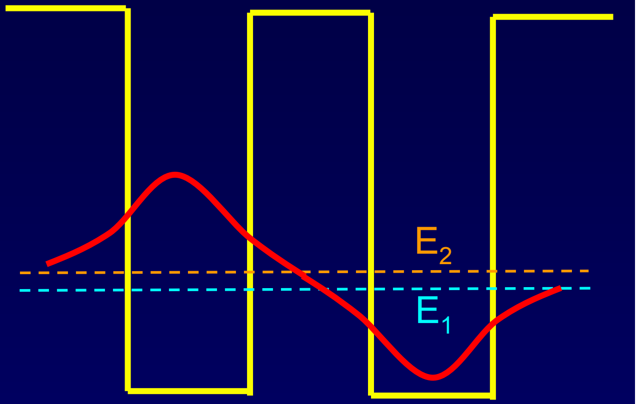

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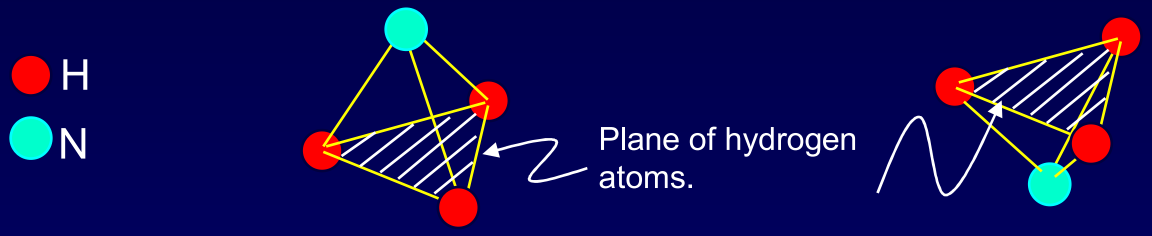
2) If the barrier is made wider, will the time become larger or smaller? What about E_2-E_1?

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

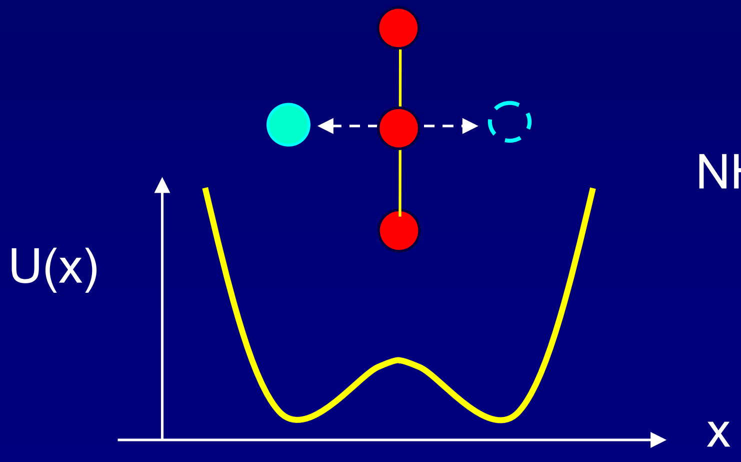
We'll see (week 7) that this effect is important in chemical bonding.

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:



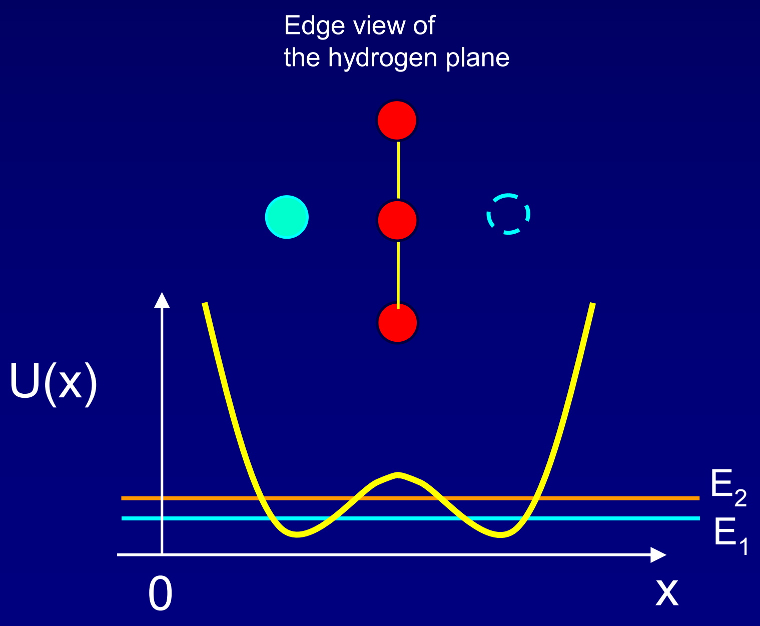
NH_3 Model

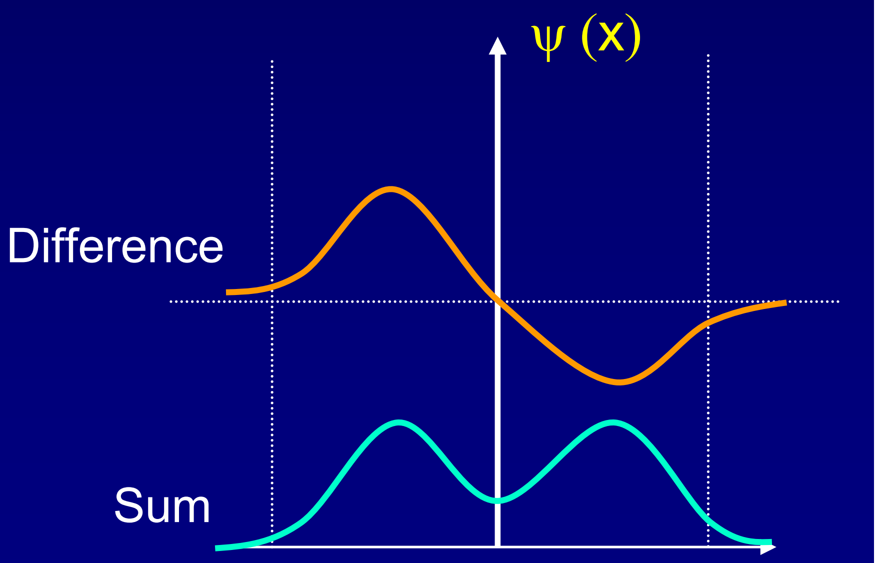
The nitrogen atom can tunnel between these two equivalent positions.

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.

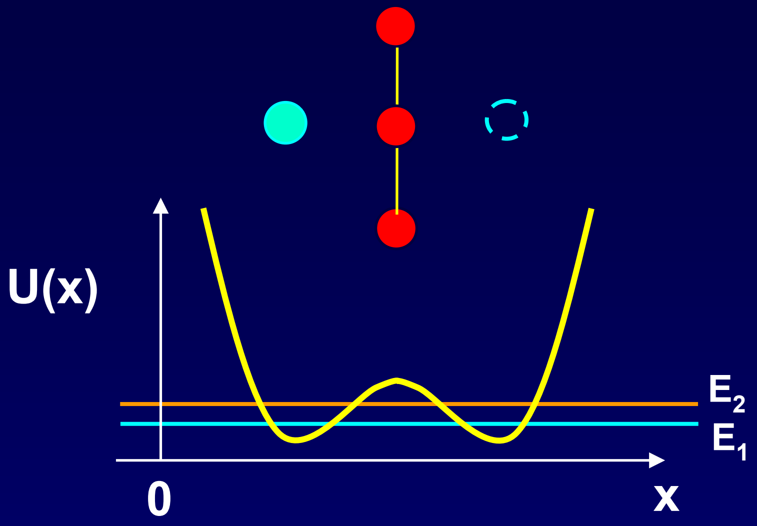
The antisymmetric state has slightly higher energy: $\Delta E = 1.8\times10^{-4}$ eV.





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 NH_3 molecule to the other?



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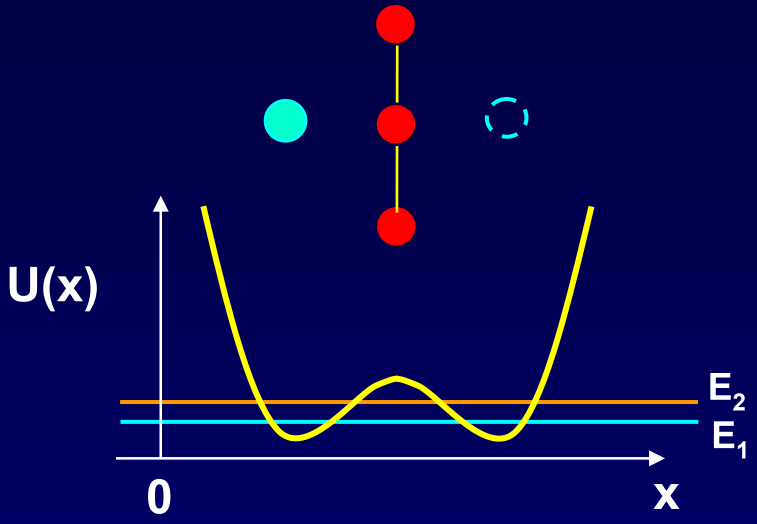
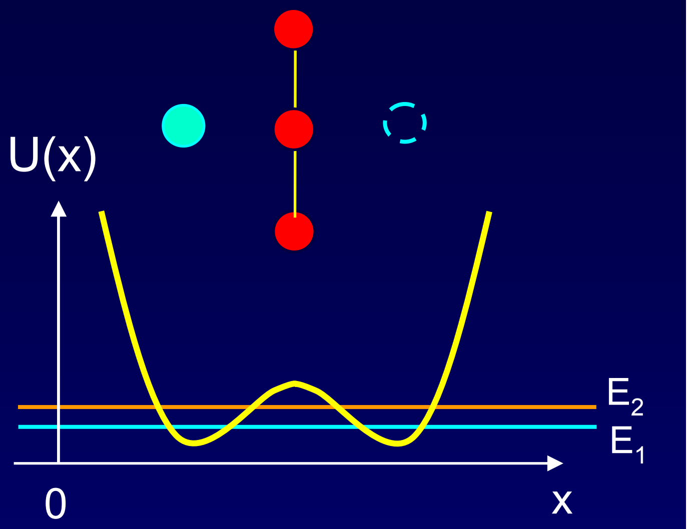


This takes a half the oscillation period, $T = h/(E_2-E_1)$:

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

The Ammonia Maser

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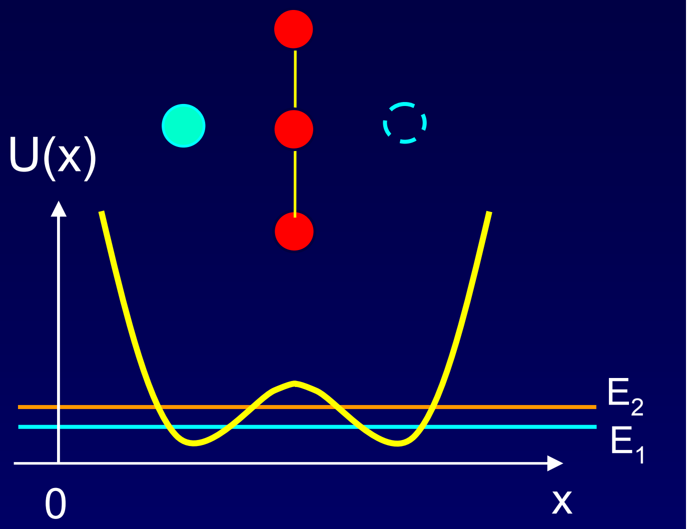

Solution:

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

$\lambda = hc/(E_2-E_1) = 1240\text{ eV}\cdot\text{nm}/1.8\text{x}10^{-4}\text{ eV}$ $\boxed{= 6.88\times10^{6}\text{ nm} \\ = 6.88\text{ mm}}$

microwaves

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