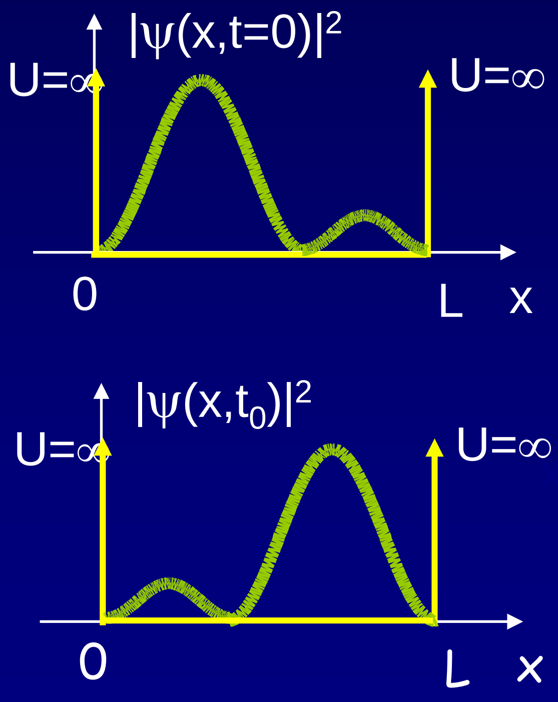
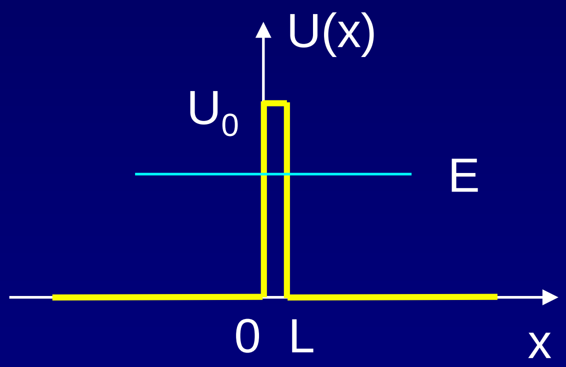
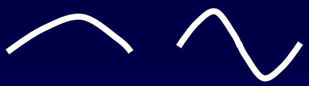
# Lecture 15:
# Time-Dependent QM & Tunneling
# Review and Examples, Ammonia Maser



# L14: Particle Motion in Infinite Well: in both n=1 and n=2 at the same time!

$$\Psi(x,t)=\frac{1}{\sqrt{2}}\left(\psi_1(x)e^{-i\omega_1 t}+\psi_2(x)e^{-i4\omega_1 t}\right)=\frac{1}{\sqrt{2}}e^{-i\omega_1 t}\left(\psi_1(x)+\psi_2(x)e^{-i3\omega_1 t}\right)$$



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

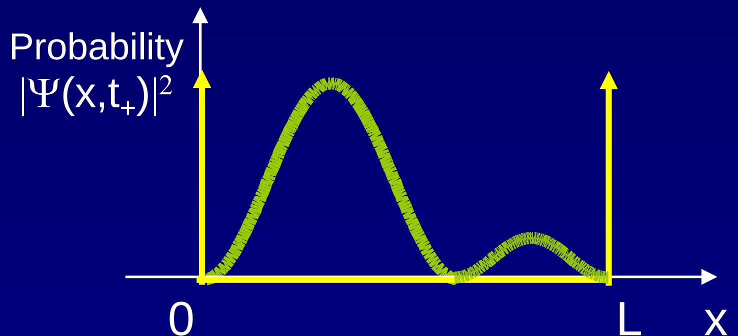
We used the identity:
$e^{i\theta}+e^{-i\theta}=2\cos\theta$

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

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

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

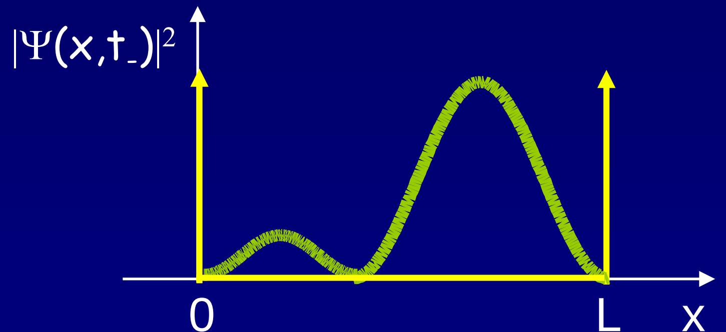
Particle localized on <u>left</u> side of well:




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

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

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



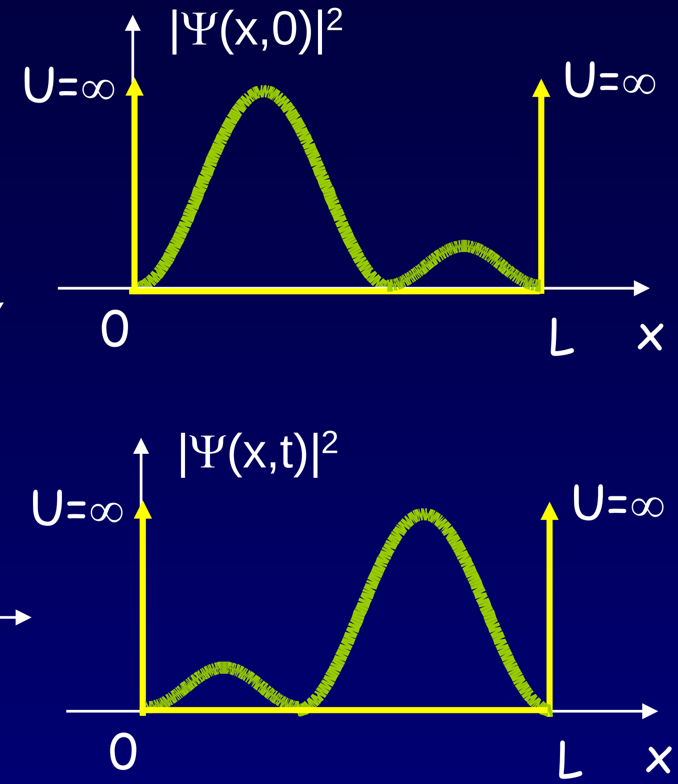

The frequency of oscillation is $\omega = \omega_2-\omega_1 = (E_2-E_1)/\hbar$, or $f = (E_2-E_1)/h$.
This is precisely the frequency of a photon that would make a transition between the two states.

# 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.



# L14: Measurements of Energy
# Fundamentals of Measurement Theory in Quantum Mechanics

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 $E_2$ !!

REALLY?? **YES!!!**

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

What about a and b? (In general these will be complex numbers.)

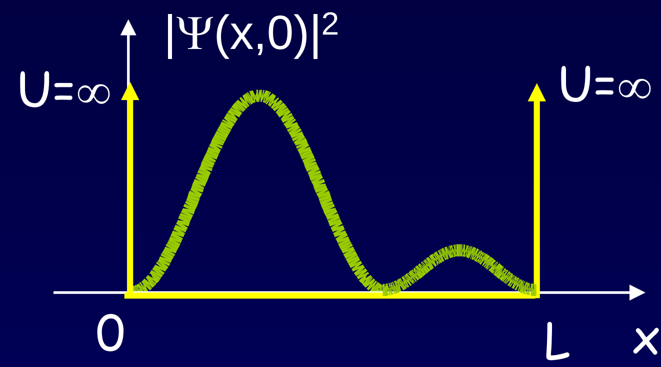
$|a|^2$ and $|b|^2$ are the probabilities of obtaining $E_1$ and $E_2$, respectively.

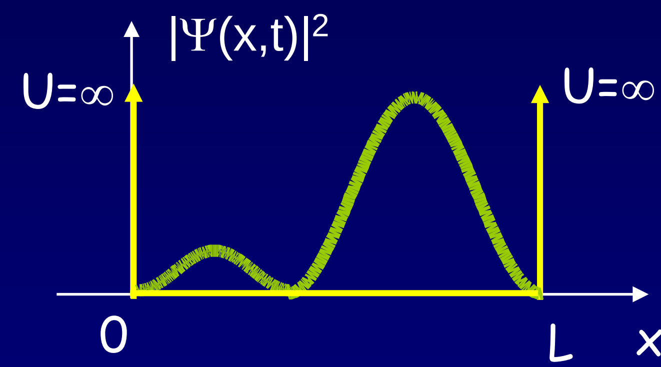
That's why we normalize the wave function to make $|a|^2 + |b|^2 = 1$.

# ACT 1

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

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




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

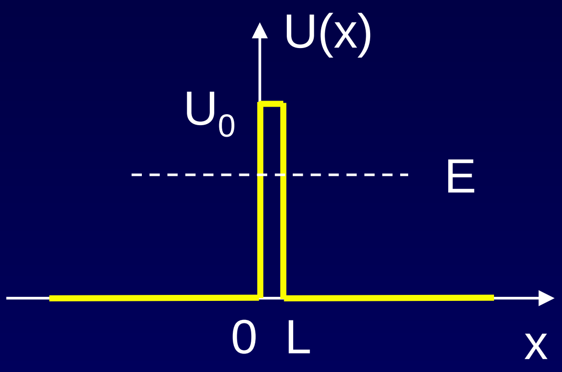
a) $E_1$ b) $E_2$ c) $E_3$ d) Any result between $E_1$ and $E_2$

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.

# Tunneling Through a Barrier

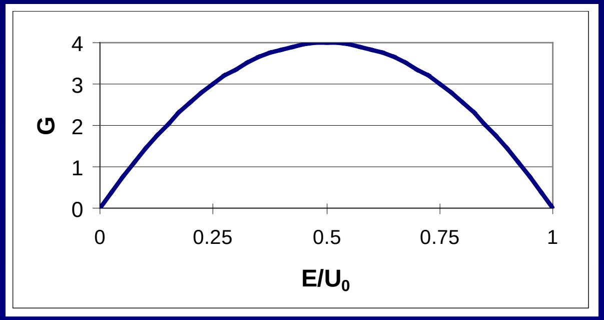
In many situations, the barrier width L is much larger than the 'decay length' 1/K of the penetrating wave (KL >> 1). In this case $B_1 \approx 0$ (why?), and the result resembles the infinite barrier. The tunneling coefficient simplifies:




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

$$K = \sqrt{\frac{2m}{\hbar^2}\underbrace{(U_0 - E)}_{\text{Energy deficit in the barrier}}}$$

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.)

$\boxed{\text{The important result is } e^{-2KL}.}$

# 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.

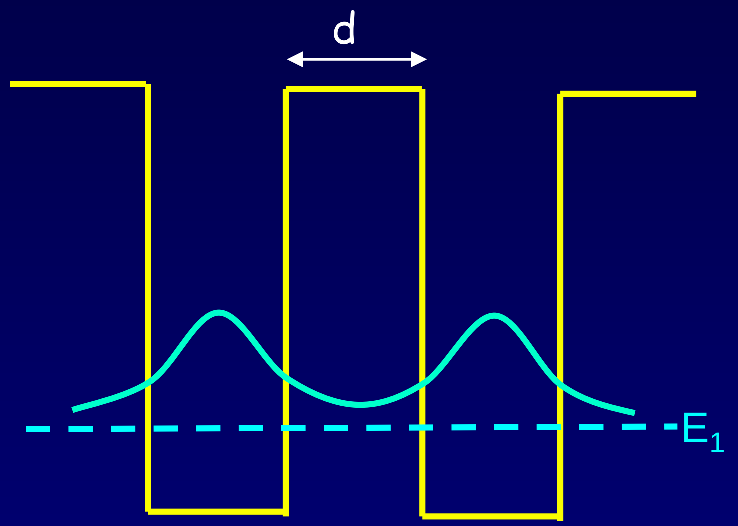
b. It's reflected by the barrier.

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

# 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. Here we find an entirely new ground state:

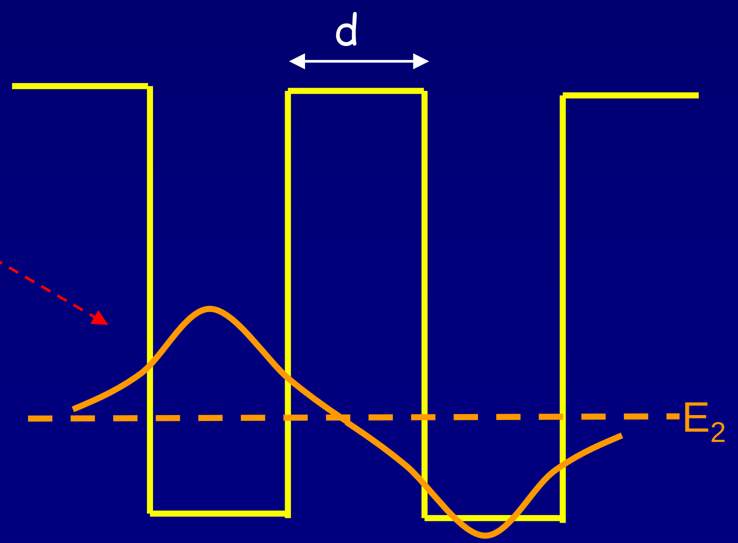
Is the particle on the left or right?




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.

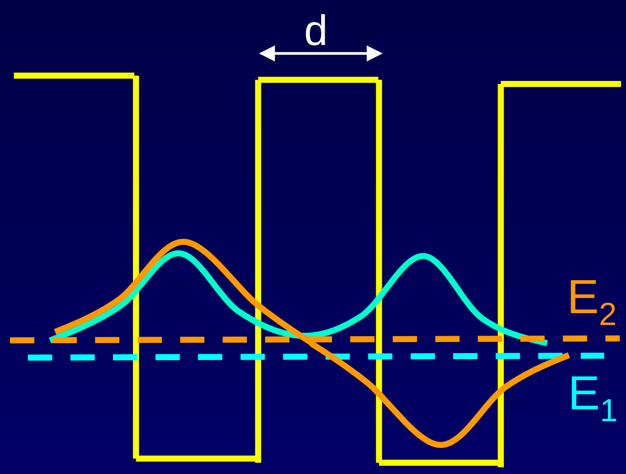
Here is the state with the next higher energy:
Why does this state have higher energy?




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.
(NOT AN ENERGY EIGENSTATE…)
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,
$T = h/(E_2 - E_1) = 1/f$.

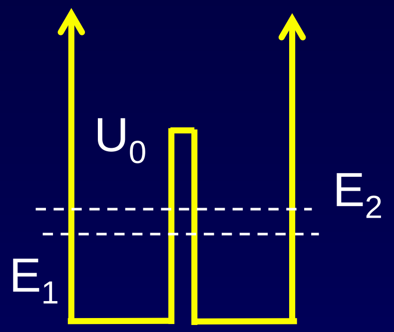
Therefore, $\Delta E = E_2 – E_1$ determines the tunneling rate.

A double well with a high or wide barrier will have a smaller $\Delta E$ than one with a low or narrow barrier. (Less coupling.) It will have a smaller tunneling rate and a slower sloshing back and forth of probability density.

Also, $\Delta E$ 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 ($\lambda$ = 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 $\lambda$ = 390 nm.




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

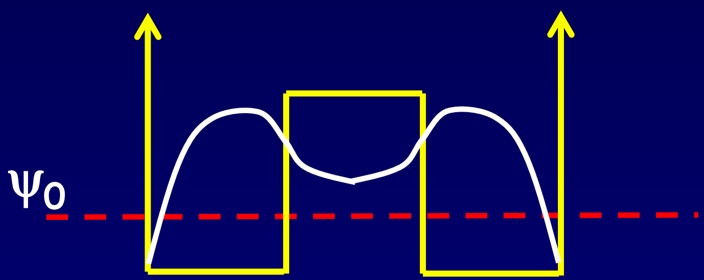
a. decrease the height of the barrier

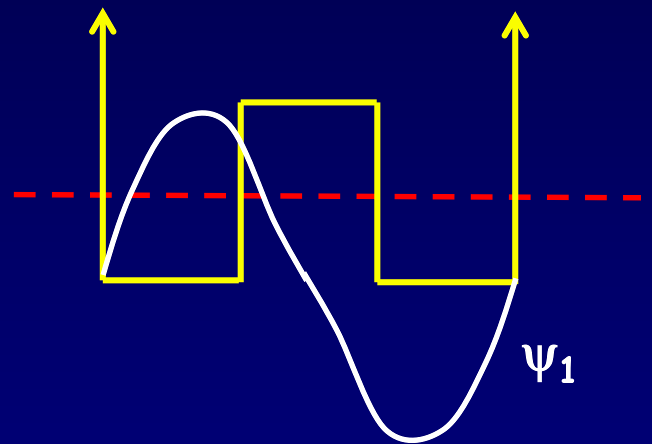
b. increase the height of the barrier

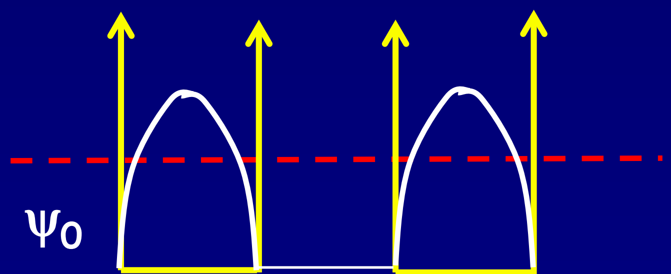
c. decrease the width of the barrier

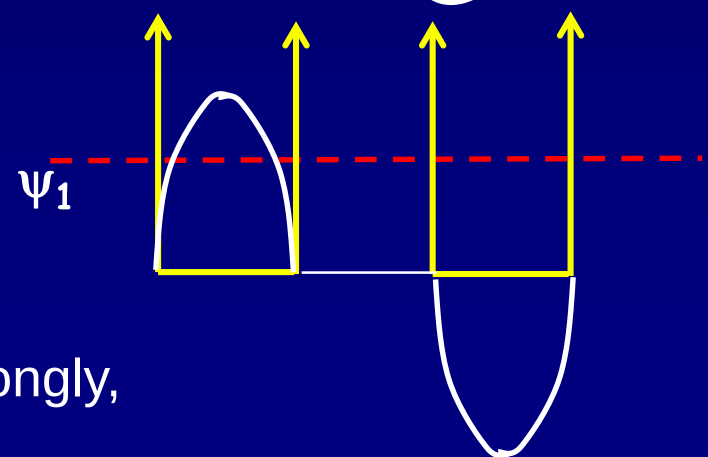
# Solution - More

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.



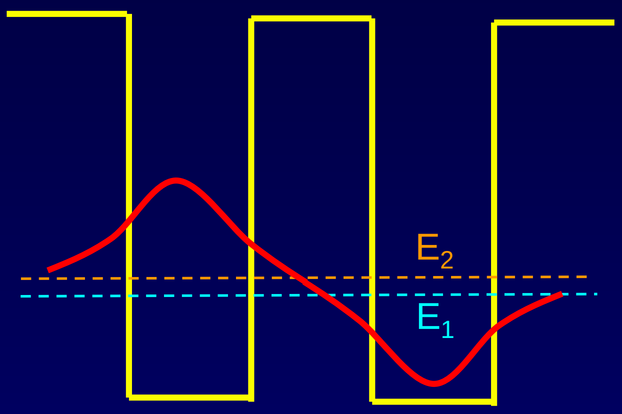




Conversely, if they are coupled more strongly, they will split more in energy.

# Double Well Oscillation



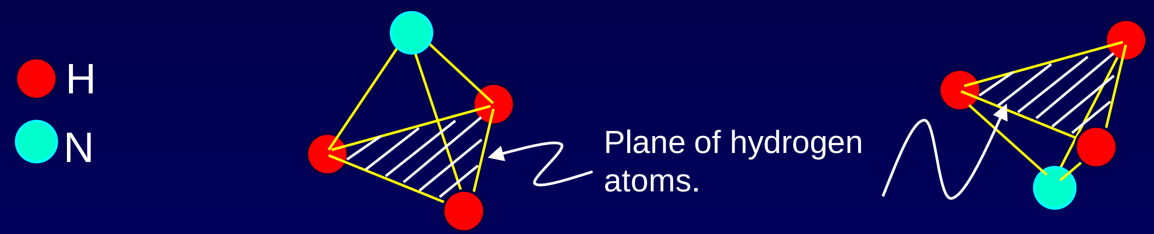

Consider the double well shown. The two energy levels of interest are $E_1$ = 1.123 eV and $E_2$ = 1.124 eV. At t = 0, $\Psi$ is in a superposition that maximizes its probability on the left side. What does this mean??

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

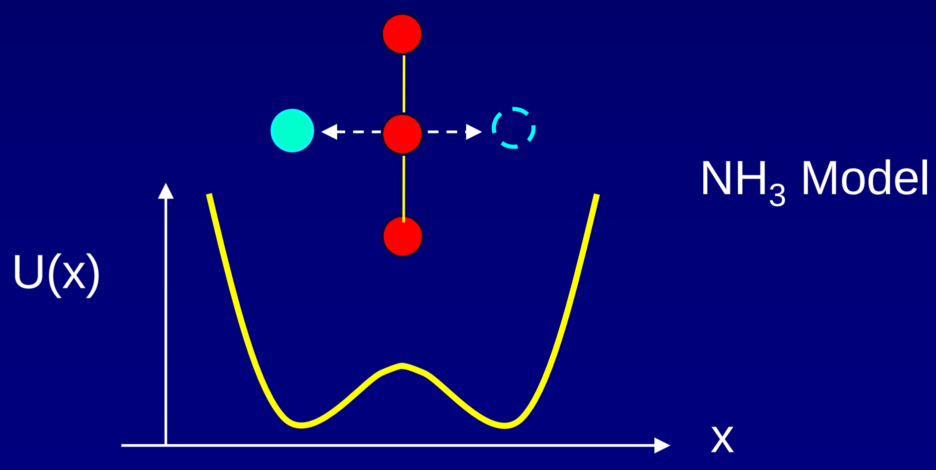
2) If the barrier is made wider, will the time become larger or smaller? What about $E_2 - E_1$?

# Example: The Ammonia Molecule
## double well in disguise

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:

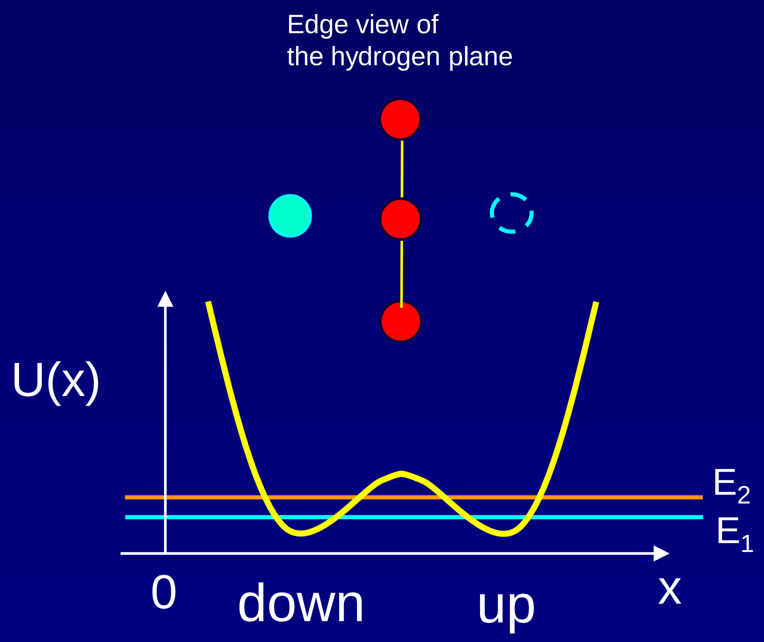


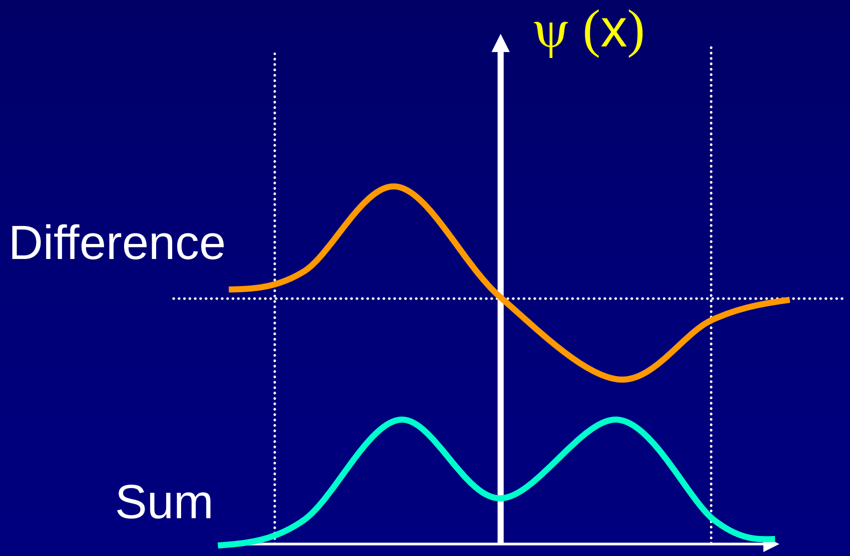

The nitrogen atom can tunnel between these two equivalent positions.

# 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.

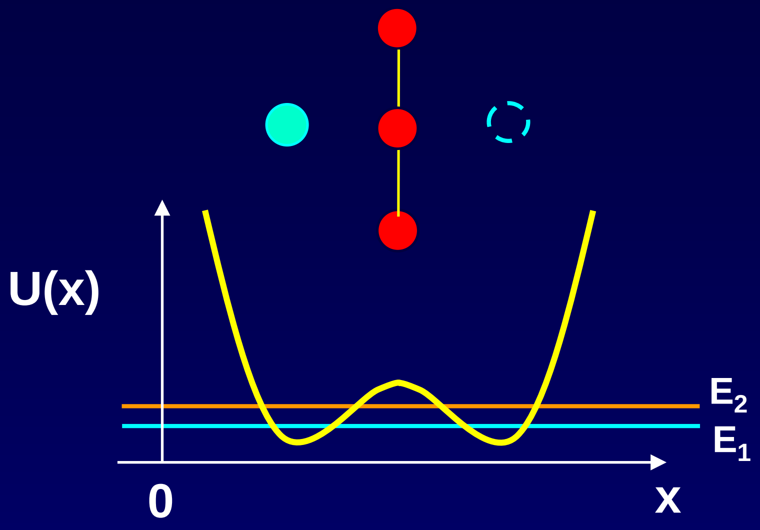
The anti-symmetric state has slightly higher energy: $\Delta E = 1.8\times10^{-4}$ eV.



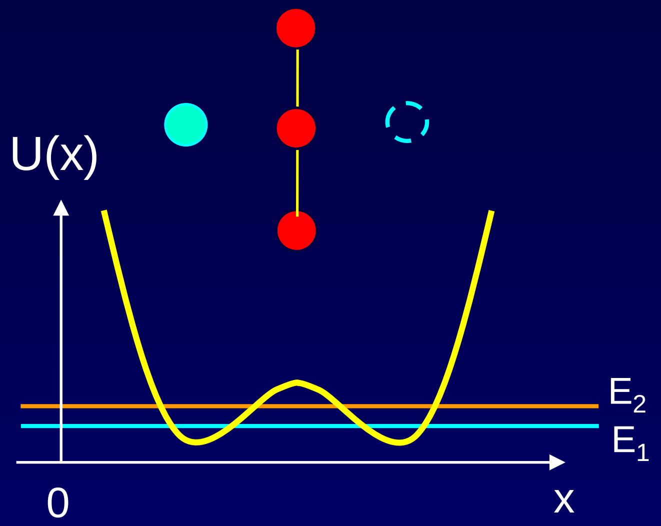
# Example: The Ammonia Molecule (3)

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



# 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?




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