

"A vast time bubble has been projected into the future to the precise moment of the end of the universe.

This is, of course, impossible."

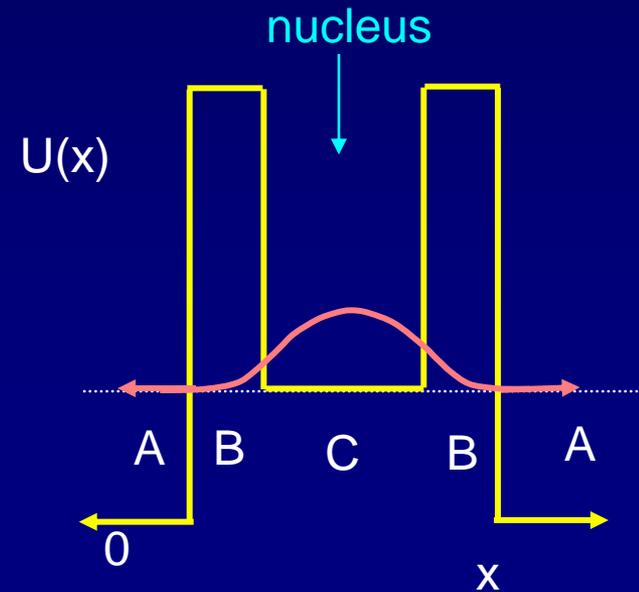
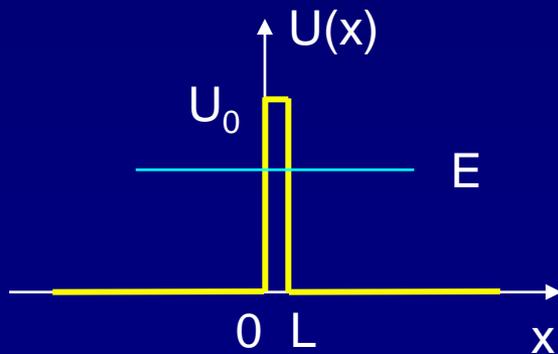
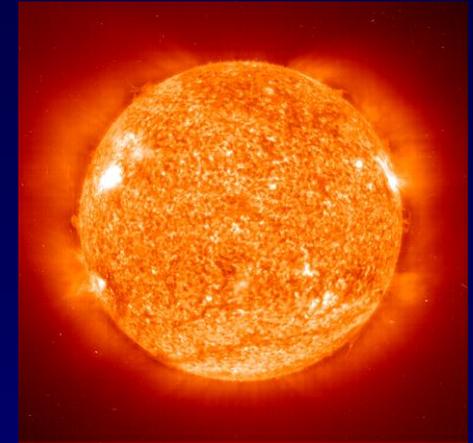
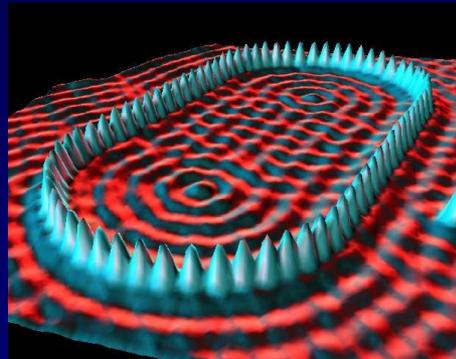
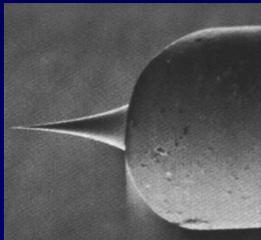
--D. Adams, *The Hitchhiker's Guide to the Galaxy*

"There is light at the end of the tunnel." -- proverb

"The light at the end of the tunnel is just the light of an oncoming train."

--R. Lowell

# Lecture 14: Barrier Penetration and Tunneling



# Act 0

The midterm exam was:

- a. Just right
- b. Too easy
- c. Too hard
- d. Too long
- e. Too long and too hard

# Today

## Tunneling of quantum particles

- Scanning Tunneling Microscope (STM)
- Nuclear Decay
- Solar Fusion
- The Ammonia Maser

## The rest of the course:

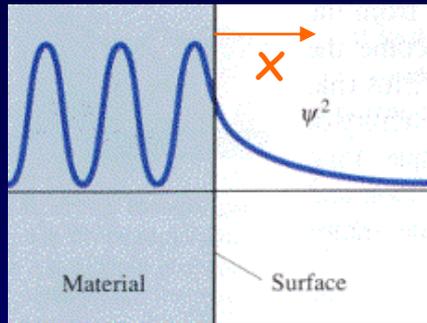
Next week: 3 dimensions - orbital and spin angular momentum  
H atom, exclusion principle, periodic table

Last week: Molecules and solids.  
Metals, insulators, semiconductors, superconductors,  
lasers, . .

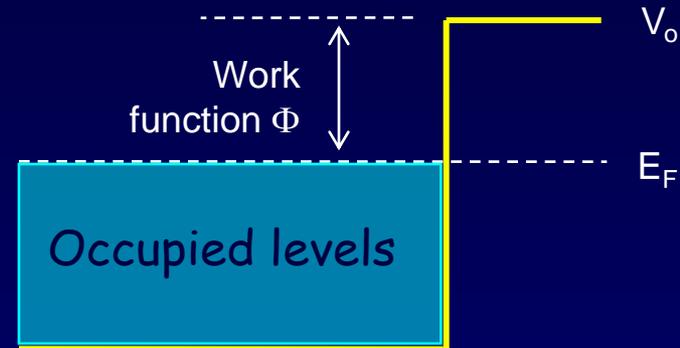
Good web site for animations <http://www.falstad.com/qm1d/>

# "Leaky" Particles: Revisited

Due to "barrier penetration", the electron density of a metal actually extends outside the surface of the metal!



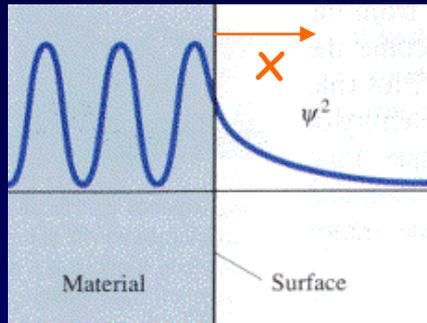
$x = 0$



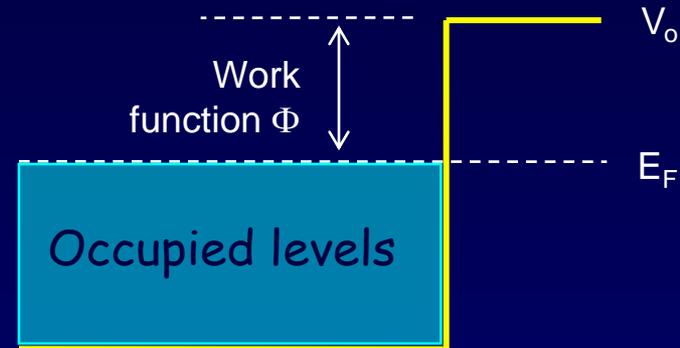
Assume that the work function (i.e., the energy difference between the most energetic conduction electrons and the potential barrier at the surface) of a certain metal is  $\Phi = 5 \text{ eV}$ . Estimate the distance  $x$  outside the surface of the metal at which the electron probability density drops to  $1/1000$  of that just inside the metal.

# "Leaky" Particles: Revisited

Due to "barrier penetration", the electron density of a metal actually extends outside the surface of the metal!



$$x = 0$$



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$$\frac{|\psi(x)|^2}{|\psi(0)|^2} = e^{-2Kx} \approx \frac{1}{1000} \quad \longrightarrow \quad x = -\frac{1}{2K} \ln\left(\frac{1}{1000}\right) \approx 0.3 \text{ nm}$$

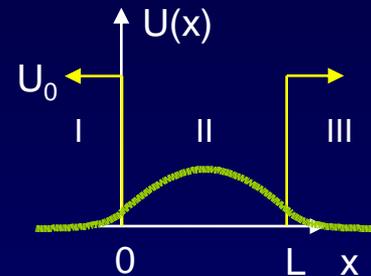
$$K = \sqrt{\frac{2m_e}{\hbar^2}(V_0 - E)} = 2\pi \sqrt{\frac{2m_e}{h^2} \Phi} = 2\pi \sqrt{\frac{5 \text{ eV}}{1.505 \text{ eV} \cdot \text{nm}^2}} = 11.5 \text{ nm}^{-1}$$

# Tunneling: Key Points

In quantum mechanics a particle can penetrate into a barrier where it would be classically forbidden.

The finite square well:

In region III,  $E < U_0$ , and  $\psi(x)$  has the exponential form  $D_1 e^{-Kx}$ . We did not solve the equations – too hard! You did it using the computer in Lab #3.



The probability of finding the particle in the barrier region decreases as  $e^{-2Kx}$ .

The finite-width barrier:

Today we consider a related problem – a particle approaching a finite-width barrier and “tunneling” through to the other side.

The result is very similar, and again the problem is too hard to solve exactly here:

The probability of the particle tunneling through a finite width barrier is approximately proportional to  $e^{-2KL}$  where  $L$  is the width of the barrier.

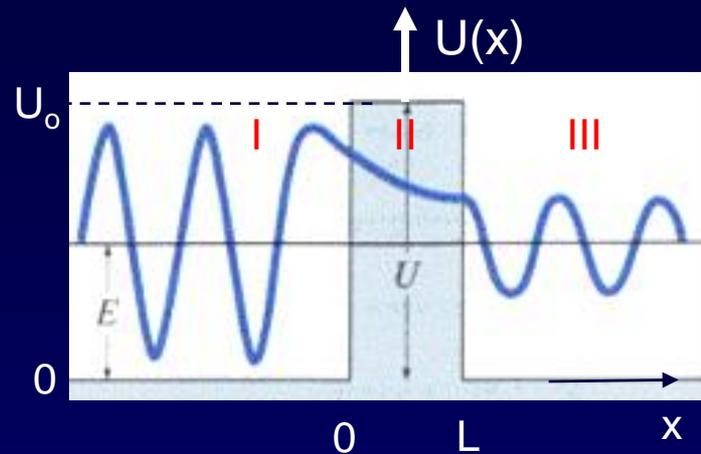
# Tunneling Through a Barrier (1)

What is the the probability that an incident particle tunnels through the barrier?

It's called the "Transmission Coefficient, T".

Consider a barrier (II) of height  $U_0$ .

$U = 0$  everywhere else.



Getting an exact result requires applying the boundary conditions at  $x = 0$  and  $x = L$ , then solving **six transcendental equations** for six unknowns:

$$\psi_I(x) = A_1 \sin kx + A_2 \cos kx$$

$$\psi_{II}(x) = B_1 e^{Kx} + B_2 e^{-Kx}$$

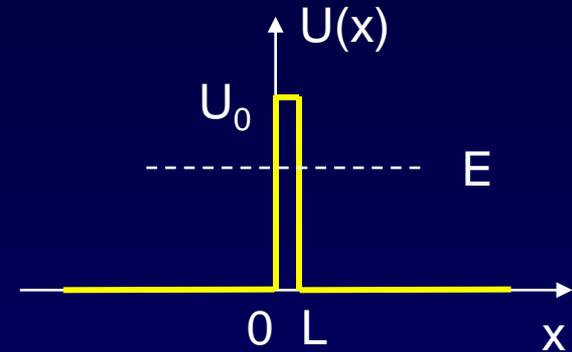
$$\psi_{III}(x) = C_1 \sin kx + C_2 \cos kx$$

$A_1, A_2, B_1, B_2, C_1,$  and  $C_2$  are unknown.  $K$  and  $k$  are known functions of  $E$ .

This is more complicated than the infinitely wide barrier, because we can't require that  $B_1 = 0$ . (Why not?)

# Tunneling Through a Barrier (2)

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:

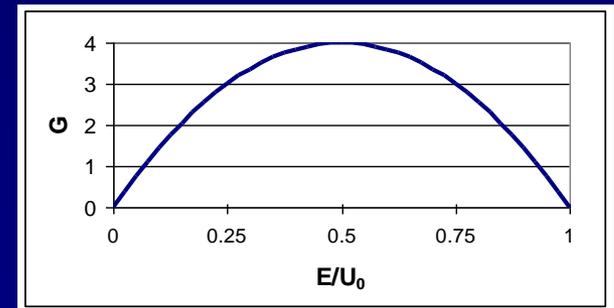


$$T \approx Ge^{-2KL} \text{ where } G = 16 \frac{E}{U_0} \left( 1 - \frac{E}{U_0} \right)$$

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

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.)



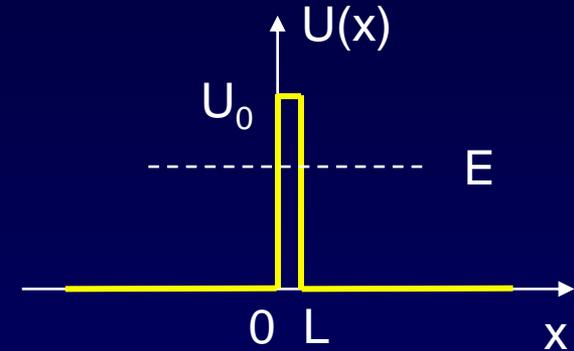
The important result is  $e^{-2KL}$ .

# Act 1

Consider a particle tunneling through a barrier.

1. Which of the following will increase the likelihood of tunneling?

- a. decrease the height of the barrier
- b. decrease the width of the barrier
- c. decrease the mass of the particle



2. What is the energy of the emerging particles?

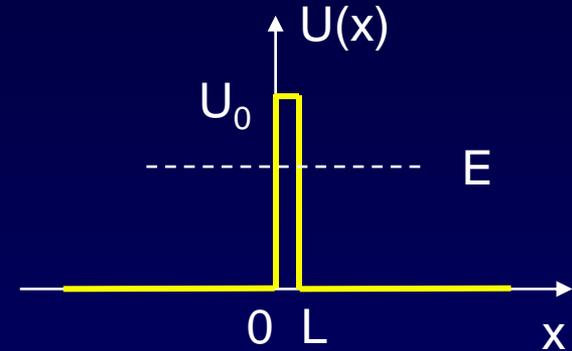
- a. < initial energy
- b. = initial energy
- c. > initial energy

# Solution

Consider a particle tunneling through a barrier.

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$$T \approx e^{-2KL} \quad \text{Decreasing } U_0 \text{ or } m_e \text{ will decrease } K.$$

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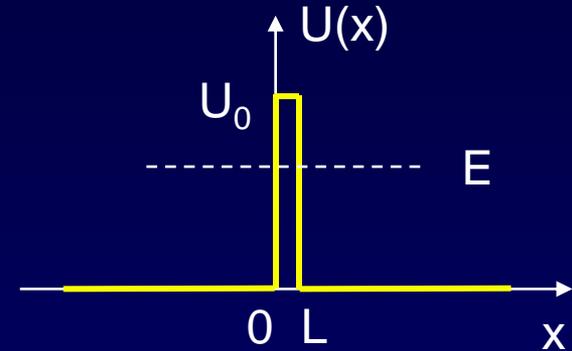
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# Solution

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2. What is the energy of the emerging particles?

- a. < initial energy
- b. = initial energy
- c. > initial energy

The barrier does not absorb energy from the particle. The amplitude of the outgoing wave is smaller, but the wavelength is the same.  $E$  is the same everywhere.

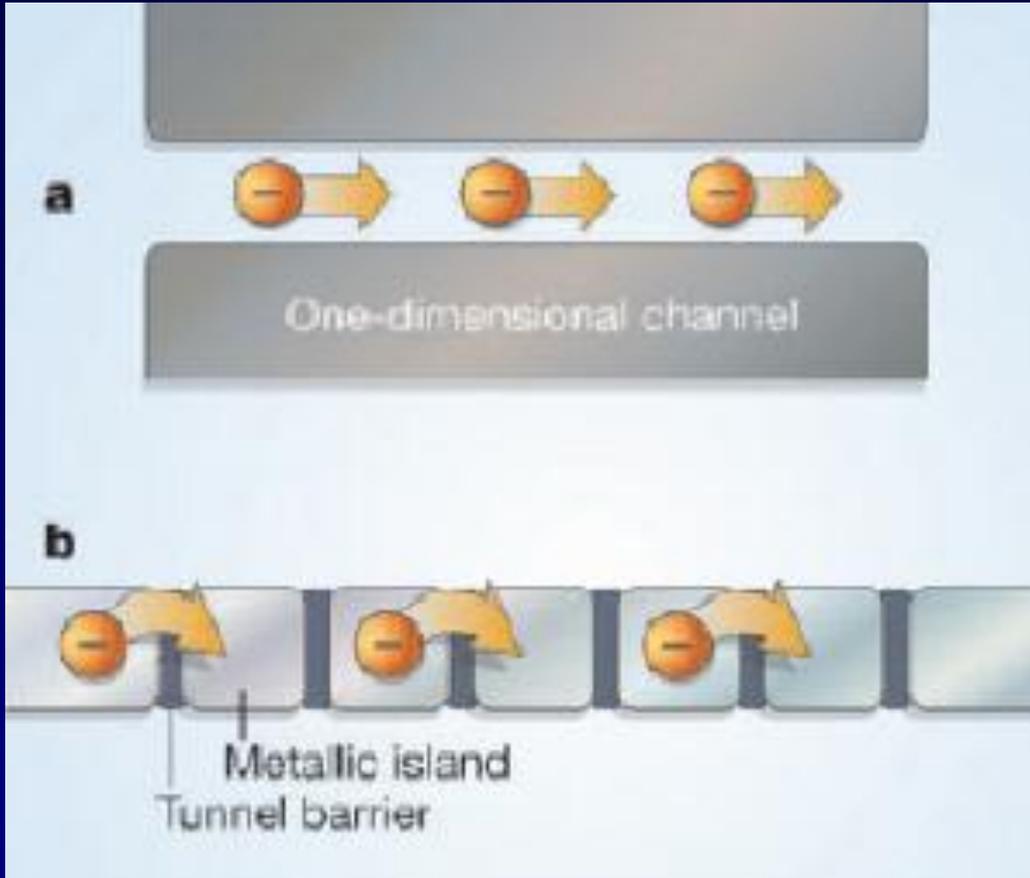
Probability  
 $\neq$  Energy

# Example: Electrons in Nanoscale devices

*Nature* 434, 361 - 364 (17 March 2005)

Current measurement by real-time counting of single electrons

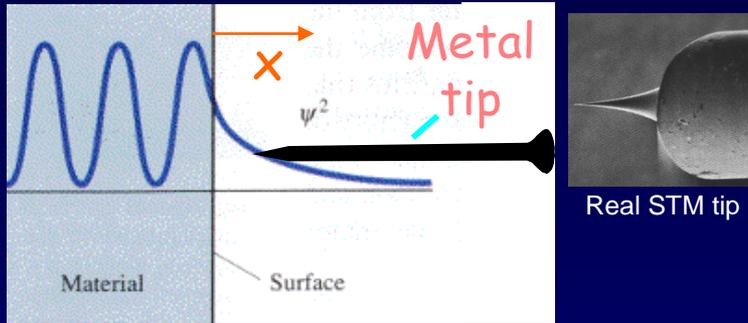
JONAS BYLANDER, TIM DUTY & PER DELSING



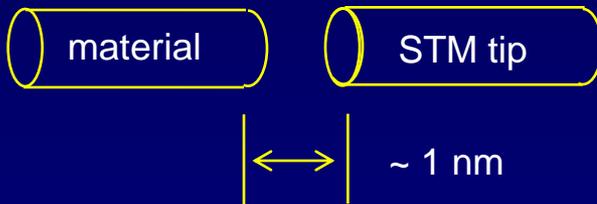
Electrons that successfully tunnel through the 50 junctions are detected using a fast single-electron transistor (SET).

# Application: Tunneling Microscopy

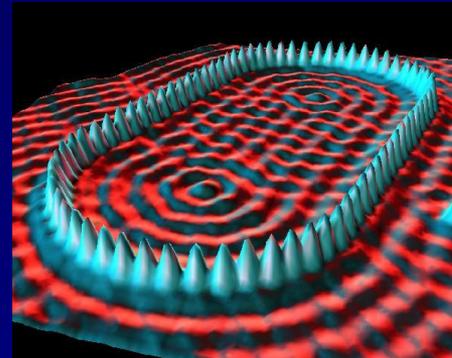
One can use barrier penetration to measure the electron density on a surface.



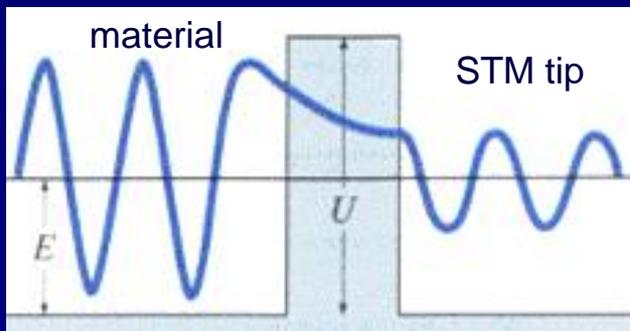
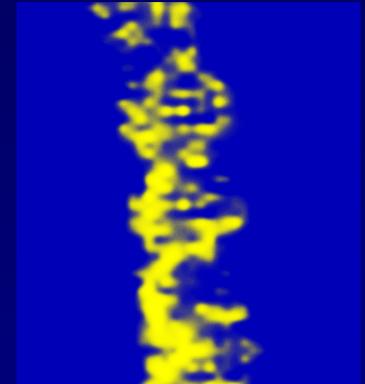
Scanning  
Tunneling  
Microscope  
images



Na atoms on metal:



DNA Double Helix:



STM demo:

<http://www.quantum-physics.polytechnique.fr/en/>

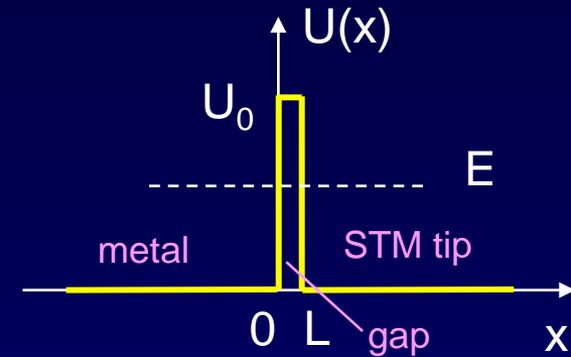
Barrier penetration is a wave phenomenon, not only QM. It is used in optical microscopes also. See:

[http://en.wikipedia.org/wiki/Total\\_internal\\_reflection\\_fluorescence\\_microscope](http://en.wikipedia.org/wiki/Total_internal_reflection_fluorescence_microscope)

# The STM

The STM (scanning tunneling microscope) tip is  $L = 0.18 \text{ nm}$  from a metal surface.

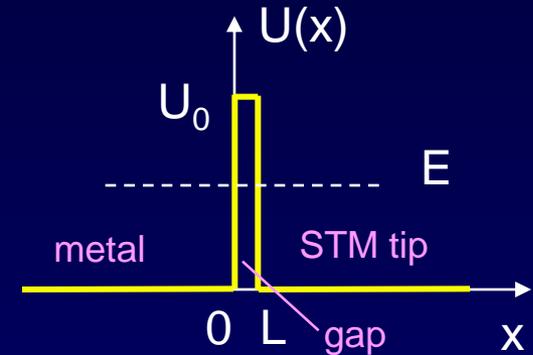
An electron with energy of  $E = 6 \text{ eV}$  in the metal approaches the surface. Assume the metal/tip gap is a potential barrier with a height of  $U_0 = 12 \text{ eV}$ . What is the probability that the electron will tunnel through the barrier?



# The STM

The STM (scanning tunneling microscope) tip is  $L = 0.18$  nm from a metal surface.

An electron with energy of  $E = 6$  eV in the metal approaches the surface. Assume the metal/tip gap is a potential barrier with a height of  $U_0 = 12$  eV. What is the probability that the electron will tunnel through the barrier?



$$T \approx Ge^{-2KL} = 4e^{-2(12.6)(0.18)} \\ = 4(0.011) = 4.3\%$$

$$G = 16 \frac{E}{U_0} \left(1 - \frac{E}{U_0}\right) = 16 \frac{1}{2} \left(1 - \frac{1}{2}\right) = 4$$

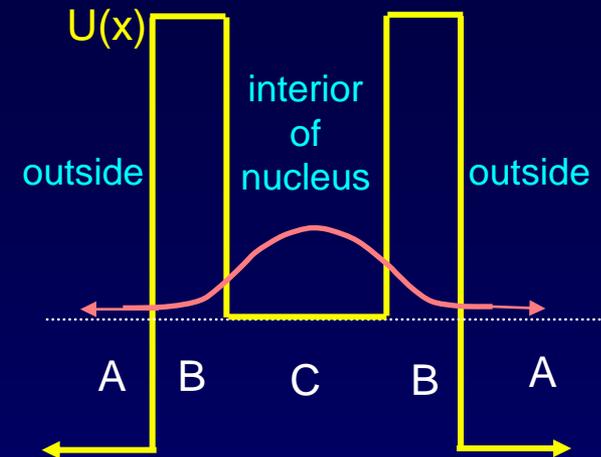
$$K = \sqrt{\frac{2m_e}{\hbar^2} (U_0 - E)} = 2\pi \sqrt{\frac{2m_e}{h^2} (U_0 - E)} \\ = 2\pi \sqrt{\frac{6 \text{ eV}}{1.505 \text{ eV}\cdot\text{nm}^2}} \approx 12.6 \text{ nm}^{-1}$$

$T \ll 1$ , so our use of the  $KL \gg 1$  approximation is justified.

Q: What will  $T$  be if we double the width of the gap?

# Tunneling and Radioactivity

In large atoms (e.g., Uranium), the nucleus can be unstable to the emission of an alpha particle (a He nucleus). This form of radioactivity is a tunneling process, involving transmission of the alpha particle from a low-energy valley through a barrier to a lower energy outside.



Why do we observe exponential decay?

- $\psi$  leaks out from C through B to A – the particle “tunnels” out.
- The leakage is slow ( $T \ll 1$ ), so  $\psi$  just outside the barrier stays negligible.
- The shape of  $\psi$  remaining in B-C shows almost no change: Its amplitude slowly decreases. That is,  $P_{\text{inside}}$  is no longer 1.
- The rate at which probability flows out is proportional to  $P_{\text{inside}}$  (by linearity)  $\Rightarrow$  exponential decay in time.

$$\frac{dx}{dt} = -Ax \quad \Rightarrow \quad x = e^{-At} = e^{-t/\tau}$$

$t_{1/2} = (\tau \ln 2)$  is the “half life” of the substance

# $\alpha$ -Radiation: Illustrations of the enormous range of decay rates in different nuclei

Consider a very simple model of  $\alpha$ -radiation:

Assume the alpha particle ( $m = 6.64 \times 10^{-27}$  kg) is trapped in a nucleus which presents a square barrier of width  $L$  and height  $U_0$ . To find the decay rate we consider:

(1) the “attempt rate” at which the alpha particle of energy  $E$  inside the nucleus hits the barrier

**Rough estimate with  $E \sim 5$  to  $10$  MeV:** the alpha particle makes about  $10^{21}$  “attempts” per second ( $\sim$ velocity/nuclear diameter)

(2) the tunneling probability for an alpha particle with energy  $E$  each time the particle hits the barrier. [For this order of magnitude calculation you may neglect  $G$ .] Here we use

$$T \approx e^{-2KL} \quad K = \sqrt{\frac{2m}{\hbar^2}(U_0 - E)}$$

Because of the exponential this factor can vary enormously!

## Act 2

Polonium has an effective barrier width of  $\sim 10$  fermi, leading to a tunneling probability of  $\sim 10^{-15}$ . Now consider Uranium, which has a similar barrier height, but an effective width of about  $\sim 20$  fermi.

Estimate the tunneling probability in Uranium:

- a.  $10^{-30}$
- b.  $10^{-14}$
- c.  $10^{-7}$

# Solution

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b.  $10^{-14}$

c.  $10^{-7}$

Think of it this way – there is a  $10^{-15}$  chance to get through the first half of the barrier, and a  $10^{-15}$  chance to then get through the second half.

Alternatively, when we double  $L$  in

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

this is equivalent to squaring the transmission  $T$ .

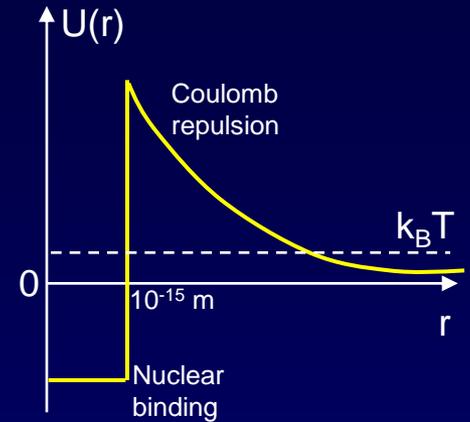
Polonium: Using  $10^{21}$  “attempts” at the barrier per second, the probability of escape is about  $10^6$  per second  $\rightarrow$  **decay time  $\sim 1$   $\mu$ s.**

Uranium: Actually has a somewhat higher barrier too, leading to  $P(\text{tunnel}) \sim 10^{-40} \rightarrow$  **decay time  $\sim 10^{10}$  years!**

# Tunneling Example: The Sun

The solar nuclear fusion process starts when two protons fuse together. In order for this reaction to proceed, the protons must “touch” (approach to within  $10^{-15}$  m of each other).

The potential energy,  $U(r)$ , looks something like this:



The temperature of the sun’s core is  $T \sim 1.3 \times 10^7$  K.

This corresponds to an average kinetic energy:

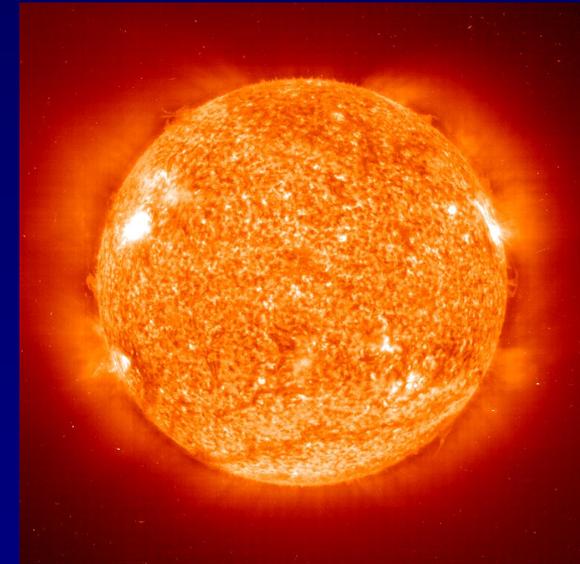
$$k_B T = 2 \times 10^{-16} \text{ J} \quad (k_B = \text{Boltzmann's constant})$$

At  $r = 10^{-15}$  m the height of the Coulomb barrier is:

$$\begin{aligned} U(r) &= (1/4\pi\epsilon_0)e^2/r = (9 \times 10^9) \times (1.6 \times 10^{-19} \text{ C})^2 / 10^{-15} \text{ m} \\ &= 2 \times 10^{-13} \text{ J} \end{aligned}$$

Thus, the protons in the sun very rarely have enough thermal energy to go over the Coulomb barrier.

How do they fuse then? **By tunneling through the barrier!**



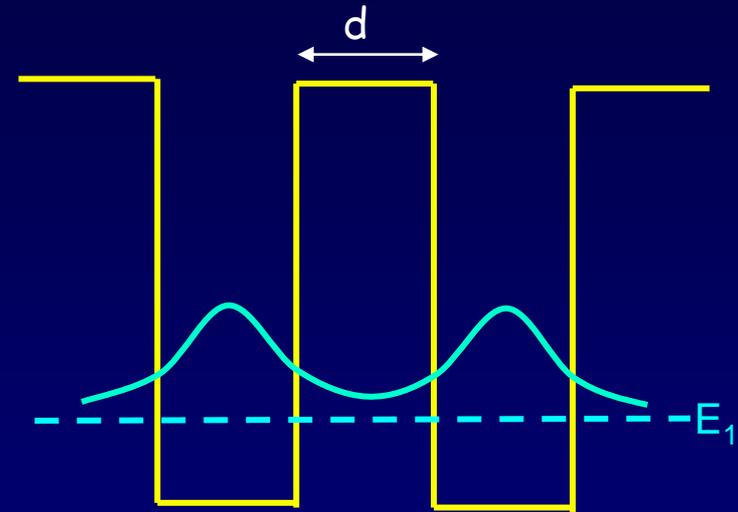
# Another Consequence of "Tunneling"

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?

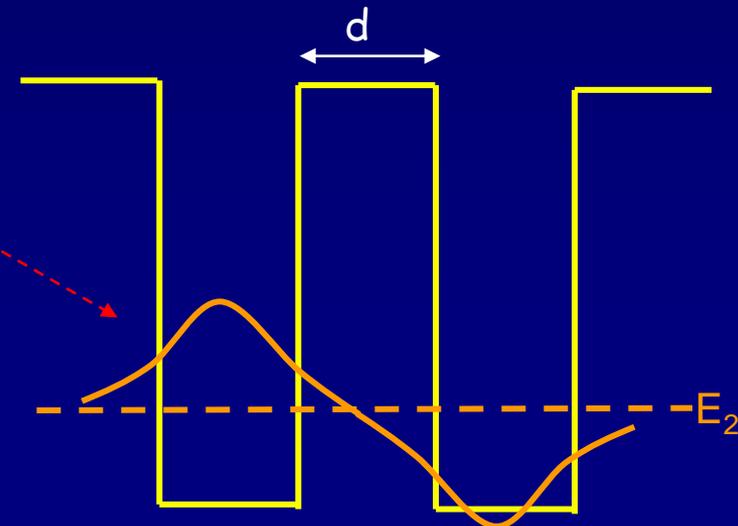
**Both!** If the barrier is finite, the wave function extends into both wells

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



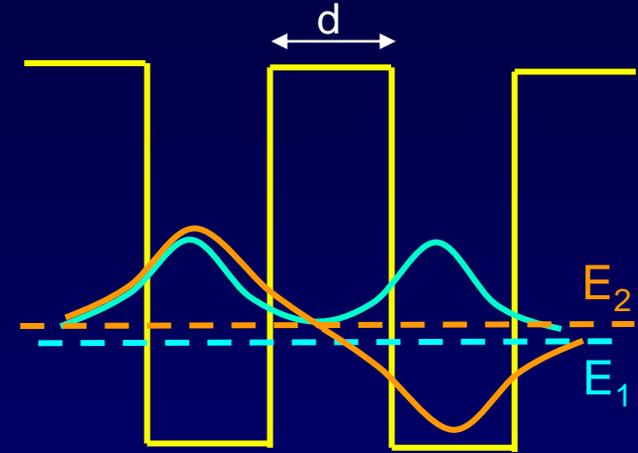
Here is the state with the next higher energy:  
Why does this state have higher energy?

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,  
 $T = h/(E_2 - E_1)$ .



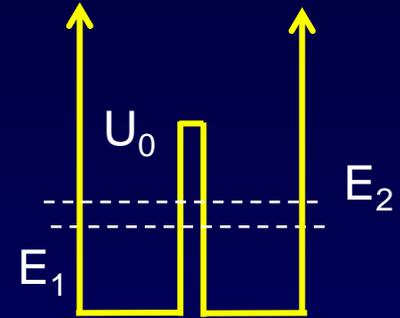
Therefore,  $\Delta E = E_2 - E_1$  depends on the tunneling rate.

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 3

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  $\lambda = 390 \text{ nm}$ .

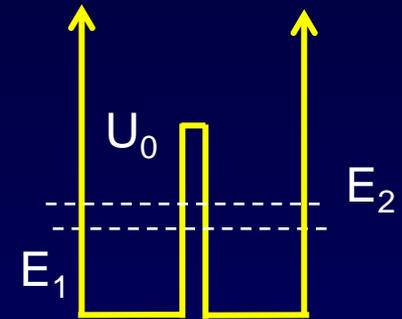


What could you modify to shift the wavelength to 400 nm?

- decrease the height of the barrier
- increase the height of the barrier
- decrease the width of the barrier

# Solution

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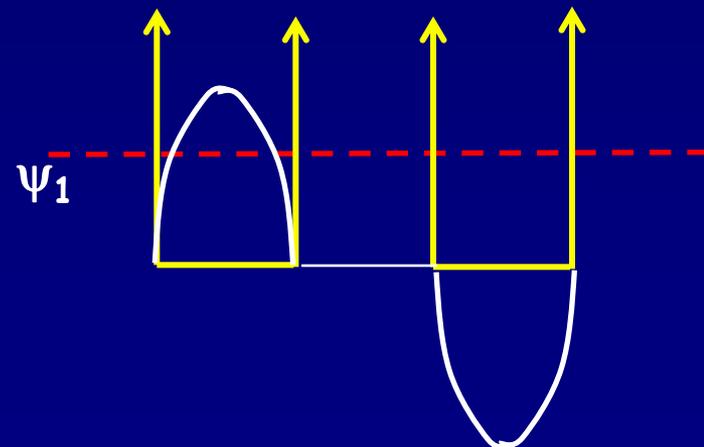
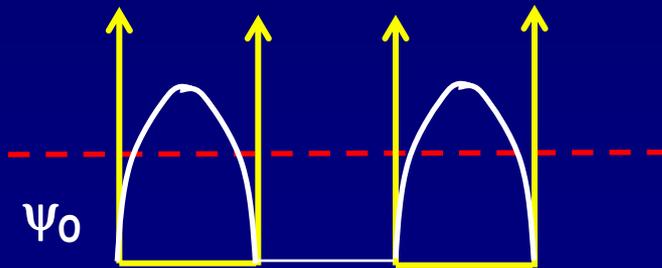
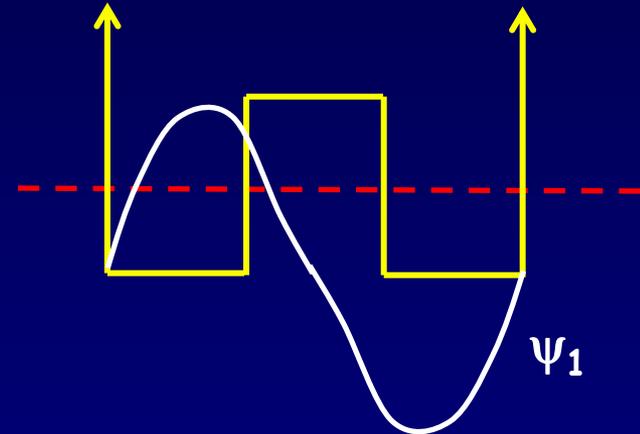
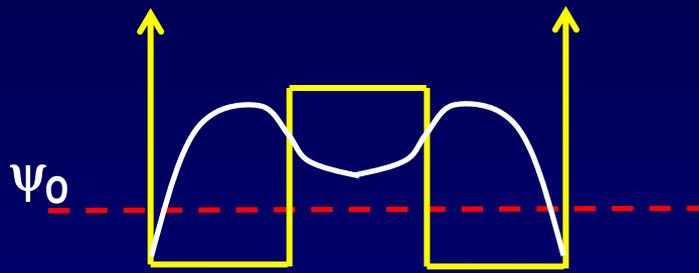
- a. decrease the height of the barrier
- b. increase the height of the barrier**
- c. decrease the width of the barrier

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.



# Next Week

3-Dimensional Potential Well

Schrödinger's Equation for the Hydrogen Atom