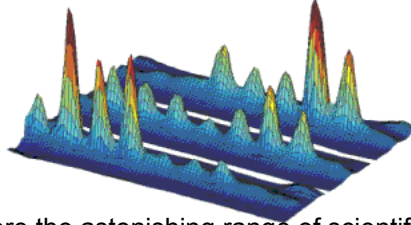


What happens when wires are so small that QM does determine their behavior? & can we take advantage of thi\$?



We virtually ignore the astonishing range of scientific and practical applications that quantum mechanics undergirds: today an estimated 30 percent of the U.S. gross national product is based on inventions made possible by quantum mechanics, from semiconductors in computer chips to lasers in compact-disc players, magnetic resonance imaging in hospitals, and much more.

Max Tegmark and John Archibald Wheeler Sci.American, Feb.2001

Phys 2130, Day 30:

Questions?

Review of Quantum Wells
& tunneling

Reminders:
Next up: Tunneling
HW Due Thurs

Updates

Shifting Instructors
(same team)



Same course Structure & Approach

Modest differences:

- slides (look at pre-lecture notes)
- different note-taking approach

Shifting to Applications

- **Week 12: Mar 14-16**
 - Mar 28: Prelecture Notes* and Full Notes from Class
 - * you are encouraged to download and bring these to class!

What happens when wires are so small that QM does determine their behavior? & can we take advantage of QM?



We virtually ignore the astonishing range of scientific and practical applications that quantum mechanics undergirds: today an estimated 30 percent of the U.S. gross national product is based on inventions made possible by quantum mechanics, from semiconductors in computer chips to lasers in compact-disk players, magnetic resonance imaging in hospitals, and much more.

Mike Tegmark and John Arthur III Wheeler Ed. American, Feb. 2001

Steve D'Angelo, Dept. 303, Question 2
 Member of Quantum Walls
 & Tunneling

Revisitors:
 Neilson, Tunneling
 SW/Dan Thum

Nanotechnology: how small does a wire have to be before movement of electrons starts to depend on size and shape due to quantum effects?

Look at energy level spacing compared to thermal energy.
 $kT = 540 \text{ eV}$ at room temp.

Calculate energy levels for electron in wire of length L .
 (Ignore spin, assume $m = m_0$, $E = 0$, $V = 0$, $\psi = 0$ at $x = 0, L$)

Use time independent Schrod. eq.

$$\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

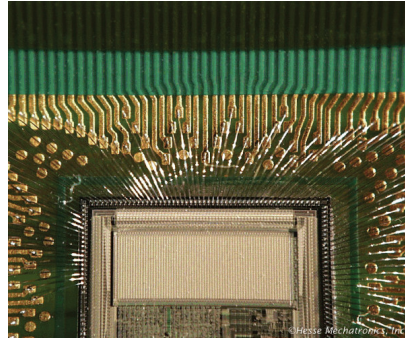
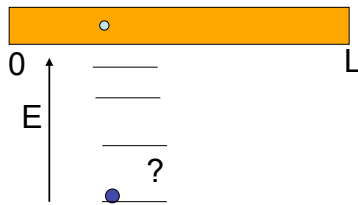
Figure out $V(x)$, then figure out how to solve, what solutions mean physically.

A whirlwind review!

Nanotechnology: how small does a wire have to be before movement of electrons starts to depend on size and shape due to quantum effects?

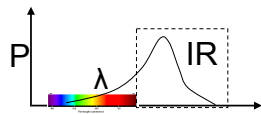
Look at energy level spacing compared to thermal energy, $kT = 1/40$ eV at room temp. [note: k is Boltzmann's const]

**Calculate energy levels for electron in wire of length L .
Know spacing big for 1 atom, what is L when E is $\sim 1/40$ eV?**



Wire (light bulb filament)

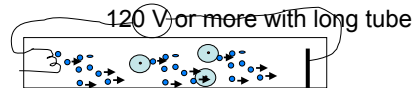
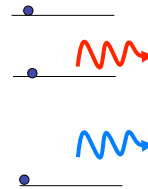
Hot electrons.
very large # close energy levels (metal)
Radiate spectrum of colors. Mostly IR.



Can think of classically)

Single atom (discharge lamps)

Electron jumps to lower levels.
Only specific wavelengths.

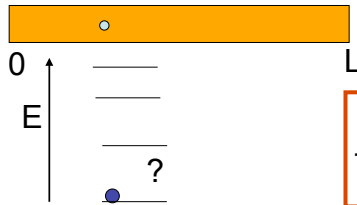


Need Quantum

Nanotechnology: how small does a wire have to be before movement of electrons starts to depend on size and shape due to quantum effects?

Look at energy level spacing compared to thermal energy, $kT = 1/40$ eV at room temp.

Calculate energy levels for electron in wire of length L. Know spacing big for 1 atom, what is L when E is ~1/40 eV?



Use time independ. Schrod. eq.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

Figure out $V(x)$, then figure out how to solve, what solutions mean physically.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

Most physical situations, like H atom, no time dependence in V !
 simplification #1 when $V(x)$ only. (works in 1D or 3D)
 (important, will use in all Shrod. Eq' n problems!!)

$\Psi(x,t)$ separates into position part $\psi(x)$ and time dependent part $\Phi(t) = \exp(-iEt/\hbar)$. $\Psi(x,t) = \psi(x)\Phi(t)$

plug in, get equation for $\psi(x)$
 You did this on your HW.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

what is in book
 With $V(x)$ for $U(x)$

“time independent Schrodinger equation”

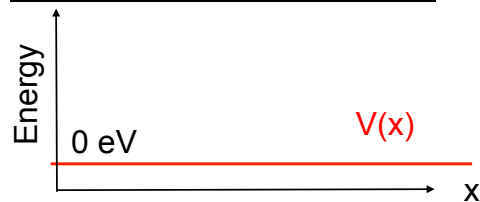
1. Figure out what $V(x,t)$ is, for situation given.

$V(x,t)$ = potential energy of the electron

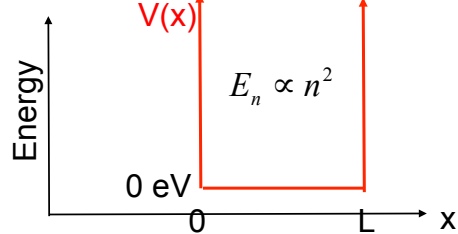
→ What is it as a function of position?

→ Is it changing with time? (Too complicated)

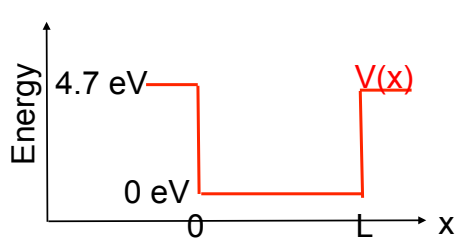
In free space, really long wire:



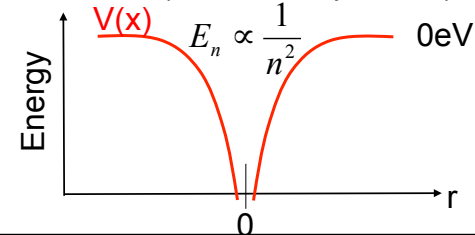
In an infinite square well:



In a wire:



In H-atom (3-D ... complicated):



Where does the electron want to be?

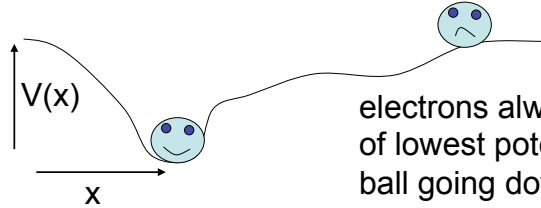
⇒ potential energy vs position, $V(x)$ & boundary conditions.

Electron wants to be at position where

- $V(x)$ is largest
- $V(x)$ is lowest
- Kin. Energy $> V(x)$
- Kin. E. $< V(x)$
- where elec. wants to be does not depend on $V(x)$

Electron wants to be at position where

- a. $V(x)$ is largest
- b. $V(x)$ is lowest**
- c. Kin. Energy $> V(x)$
- d. Kin. E. $< V(x)$
- e. where elec. wants to be does not depend on $V(x)$



electrons always want to go to position of lowest potential energy, just like ball going downhill.

c. and d. not right, because actual value of $V(x)$ is arbitrary, so can choose bigger or smaller than KE.
Only thing that matters is how changes.



Solving Schrod. equ.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

Before tackling wire, understand simplest case.

- **electron in free space**, no electric fields or gravity around.
 1. Where does it want to be? 1. no preference- all x the same
 2. What is $V(x)$? 2. constant.
 3. What are boundary conditions on $\psi(x)$? 3. none, could be anywhere.

smart choice
constant, $V(x) = 0!$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x)$$

what does this equation describe?

- a. nothing physical, just math exercise.
- b. only an electron in free space along the x axis with no electric fields around. →
- c. an electron flying along the x axis between two metal plates with a voltage between them as in photoelectric effect.
- d. an electron in an enormously long wire not hooked to any voltages.

e. more than one of the above

ans e. -- both b and d are correct. No electric field or voltage means potential energy constant in space and time, $V=0$.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x)$$

quick check on how well remember HW. No discussion

A solution to this diff. eq. is

- a. $A \cos(kx)$
- b. $A e^{-kx}$
- c. $B \sin(kx)$
- d. b. and c.
- e. a. and c.

ans. e. Both a. and c. are solutions. Check a., plug in.

$$\frac{\hbar^2}{2m} k^2 \cancel{A \cos kx} = E \cancel{A \cos kx} \quad \text{solution if } \frac{\hbar^2}{2m} k^2 = E$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x) \quad \psi(x) = A \cos kx$$

$$\frac{\hbar^2}{2m} k^2 = E$$

makes sense, because $p = \hbar k = \frac{h}{(2\pi)} \frac{(2\pi)}{\lambda}$

so condition on k is just saying that $(p^2)/2m = E$.

$V=0$, so $E = KE = \frac{1}{2} mv^2 = p^2/2m$

(graded) Total energy of electron is

a. quantized according to $E_n = (\text{constant}) \times n^2$, $n = 1, 2, 3, \dots$

b. quantized according to $E_n = \text{const} \times n$

c. quantized according to $E_n = \text{const.} \times 1/n^2$

d. quantized according to some other condition but don't know what it is.

e. not quantized, energy can take on any value.

e. no boundary, not quantized, energy can take on any value⁶⁵.

Electron in free space

$$\psi(x) = A \cos kx \quad \frac{\hbar^2}{2m} k^2 = E$$

No Boundary Conditions: k and therefore E can take on any value.

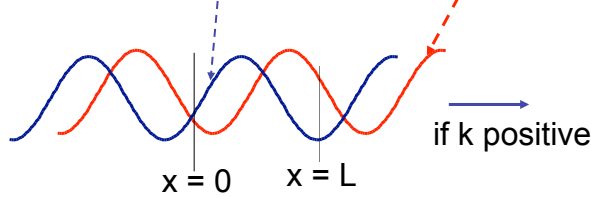
So almost have solution, but remember still have to include time dependence.

$$\Psi(x, t) = \psi(x)\phi(t) \quad \phi(t) = e^{-iEt/\hbar}$$

bit of algebra, including using identity that $e^{i\theta} = \cos\theta + i\sin\theta$

$$\Psi(x, t) = A \cos(kx - \omega t) + Ai \sin(kx - \omega t)$$

electron in free space or long wire with no voltage
 $\Psi(x,t) = A \cos(kx - \omega t) + Ai \sin(kx - \omega t)$



Using equation, probability of electron being in dx at $x = L$ is _____ than probability of being in dx at $x = 0$.

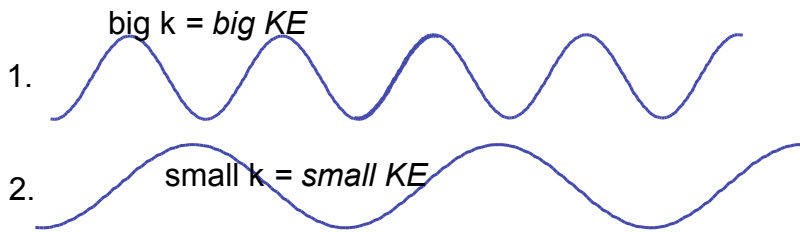
- a. always bigger, b. always same, c. always smaller
- d. oscillates up and down in time between bigger and smaller
- e. without being given k , can't figure out

ans. b. Prob $\sim \Psi^* \Psi = A^2 \cos^2(kx - \omega t) + A^2 \sin^2(kx - \omega t) = A^2$,
 so constant and equal, all x, t .

For 1 value of k , equal chance to find electron everywhere, like homework. Normal electron in wave packet, many k 's.

Which free electron has more kinetic energy?

- a. 1., b. 2., c. same



if $V=0$, then $E = \text{Kinetic energy}$.

So first term in Schrod. Eq. is always just kinetic energy!

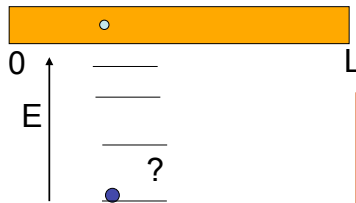
$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) = E\psi(x)$$

Curvature = KE. Bending ψ tighter = KE

Nanotechnology: how small (short) does a wire have to be before movement of electrons starts to depend on size and shape due to quantum effects?

Look at energy level spacing compared to thermal energy, $kT = 1/40$ eV at room temp.

Calculate energy levels for electron in wire of length L. Know spacing big for 1 atom, what L when $\sim 1/40$ eV?



Use time independ. Schrod. eq.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

Figure out $V(x)$, then figure out how to solve, what solutions mean physically.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$



Short copper wire, length L.

What is $V(x)$?

Consult with group.

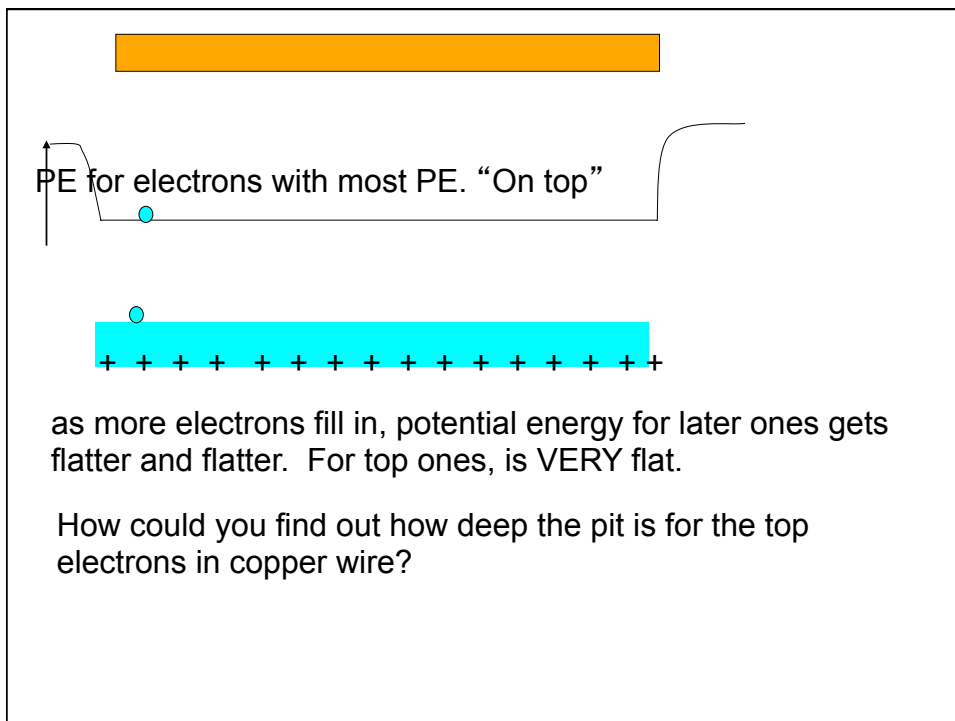
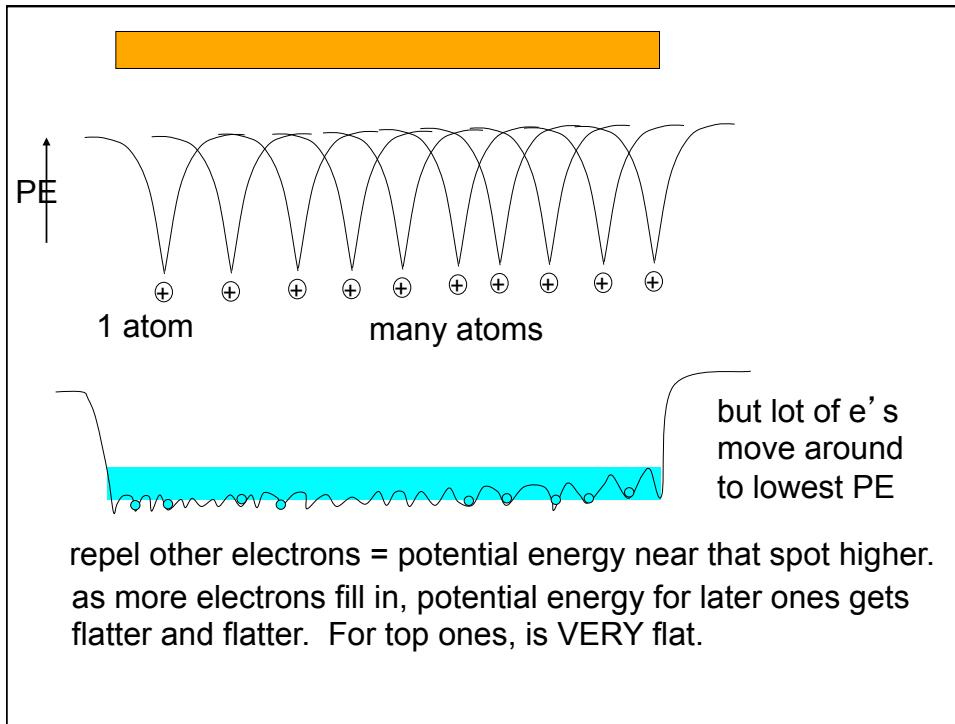
Will call on random groups for ideas.

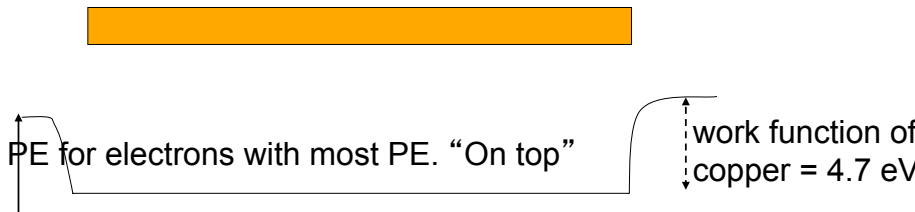
Remember photoelectric effect.

Took energy to kick electron out. So wants to be inside wire.

\Rightarrow inside is lower PE.

Everywhere inside the same?





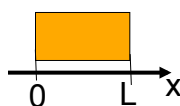
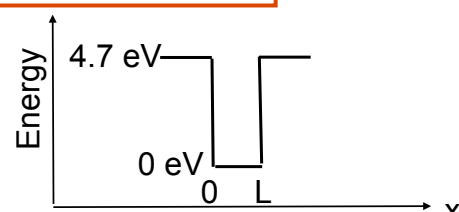
PE for electrons with most PE. "On top"

work function of copper = 4.7 eV

as more electrons fill in, potential energy for later ones gets flatter and flatter. For top ones, is VERY flat.

How could you find out how deep the pit is for the top electrons in copper wire?

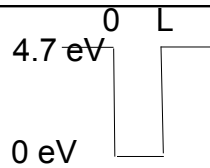
This is just the energy needed to remove them from the metal. That is the work function!!

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$



$x < 0, V(x) = 4.7 \text{ eV}$
 $x > L, V(x) = 4.7 \text{ eV}$
 $0 < x < L, V(x) = 0$

How to solve?

1. mindless mathematician approach:
 find Ψ in each region, make solutions match at boundaries, normalize.
 Works, but bunch of math.



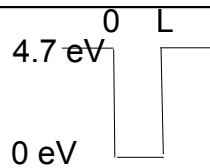
2. Clever physicist approach.

Reasoning to simplify how to solve.

Electron energy not much more than $\sim kT = 0.025$ eV.

Where is electron likely to be?

What is chance it will be outside of well?



mathematically

$$V(x) = 4.7 \text{ eV for } x < 0 \text{ and } x > L$$

$$V(x) = 0 \text{ eV for } 0 < x < L$$

2. Clever physicist approach.

Reasoning to simplify how to solve.

Electron energy not much more than $\sim kT = 0.025$ eV.

Where is electron likely to be?

What is chance it will be outside of well?

a. zero chance, b. very small chance, c. small, d. likely

b. $0.025 \text{ eV} \ll 4.7 \text{ eV}$. So very small chance ($e^{-4.7/0.025}$) an electron could have enough energy get out.

What does that say about boundary condition on $\psi(x)$?

a. $\psi(x)$ is the same for all regions: $x < 0$, $0 < x < L$, $x > L$,

b. $\psi(x < 0) \sim 0$, $\psi(x > 0) \neq 0$

c. $\psi(x) \sim 0$ except for $0 < x < L$

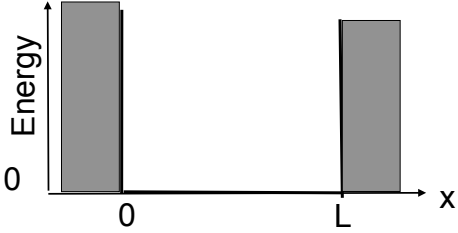
ans c.

$x < 0, V(x) \sim \text{infinite}$
 $x > L, V(x) \sim \text{infinite}$
 $0 < x < L, V(x) = 0$

so clever physicist just has to solve

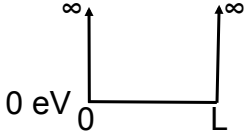
$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x)$$

with boundary conditions,
 $\psi(0) = \psi(L) = 0$



solution a lot like microwave & guitar string

NOTE:
 Book uses "rigid box" for "infinite square well"



$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x)$$

functional form of solution: $\psi(x) = A \cos(kx) + B \sin(kx)$

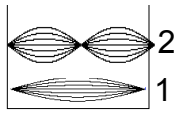
Apply boundary conditions

$x=0 \rightarrow ? \quad \psi(0) = A \rightarrow A=0$

$x=L \rightarrow \psi(L) = B \sin(kL) = 0 \Rightarrow ? \quad kL = n\pi \quad (n=1,2,3,4 \dots)$

$\rightarrow k = n\pi/L$

$k = \frac{2\pi}{\lambda} \quad \lambda = \frac{2L}{n}$



what is momentum p?
 $p = \hbar k = \hbar(n\pi / L)$

$$p = \hbar k = \hbar(n\pi / L) \quad \lambda = \frac{2L}{n}$$

E quantized by B. C.'s

$$E = \frac{p^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

What is E?

a. can be any value (not quantized).

$$\text{b.} = \frac{\pi^2 \hbar^2}{nmL^2} \quad \text{c.} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

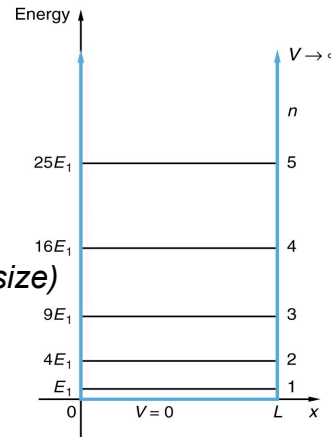
$$\text{d.} = \frac{n\pi^2 \hbar}{mL} + PE \quad \text{e.} = \frac{n^2 \pi^2 \hbar}{mL}$$

Does this L dependence make sense?

What value of L when $E_2 - E_1 = kT$?
(when motion of e's depends on wire size)

**you should check,
I estimate L ~100 atoms**

Answer = 6.6 nm ~30 Atoms.



Solving completely- everything there is to know about electron in small metallic object (flat $V(x)$ with high walls).

$$\Psi(x, t) = \psi(x)\phi(t) = B \sin\left(\frac{n\pi x}{L}\right) e^{-iEt/\hbar}$$

Normalize wavefunction ...

Probability of finding electron between $-\infty$ and ∞ must be 1.

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = \int_0^L \Psi^* \Psi dx = \int_0^L B^2 \sin^2(n\pi x / L) dx = 1$$

$$B = \sqrt{\frac{2}{L}} \quad (\text{in book and maybe was on hw})$$

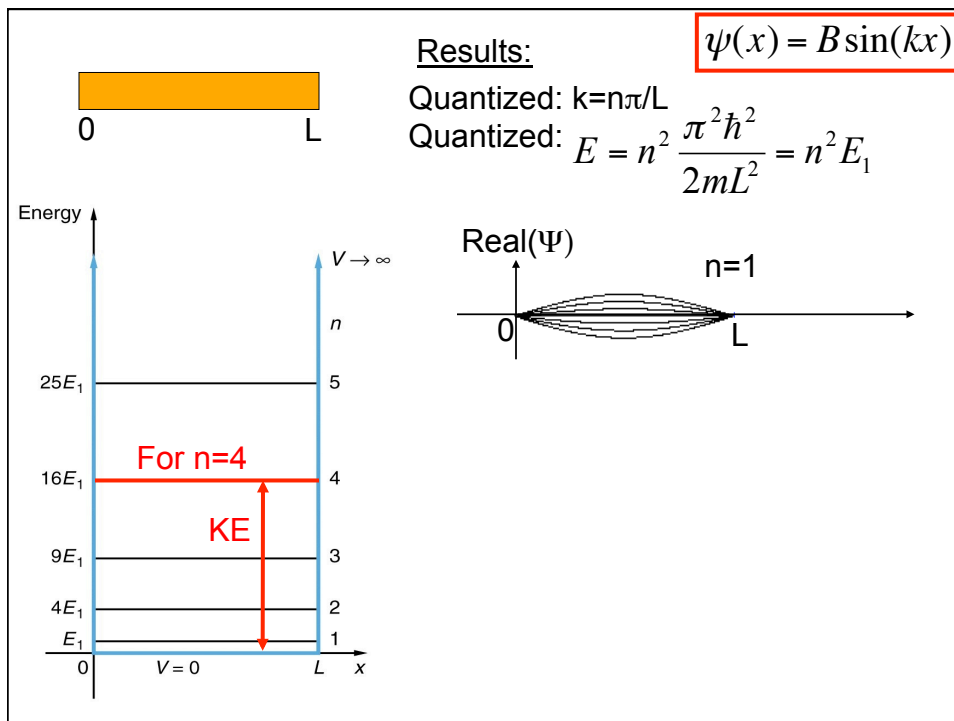
$$\Psi(x, t) = \psi(x)\phi(t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iEt/\hbar}$$

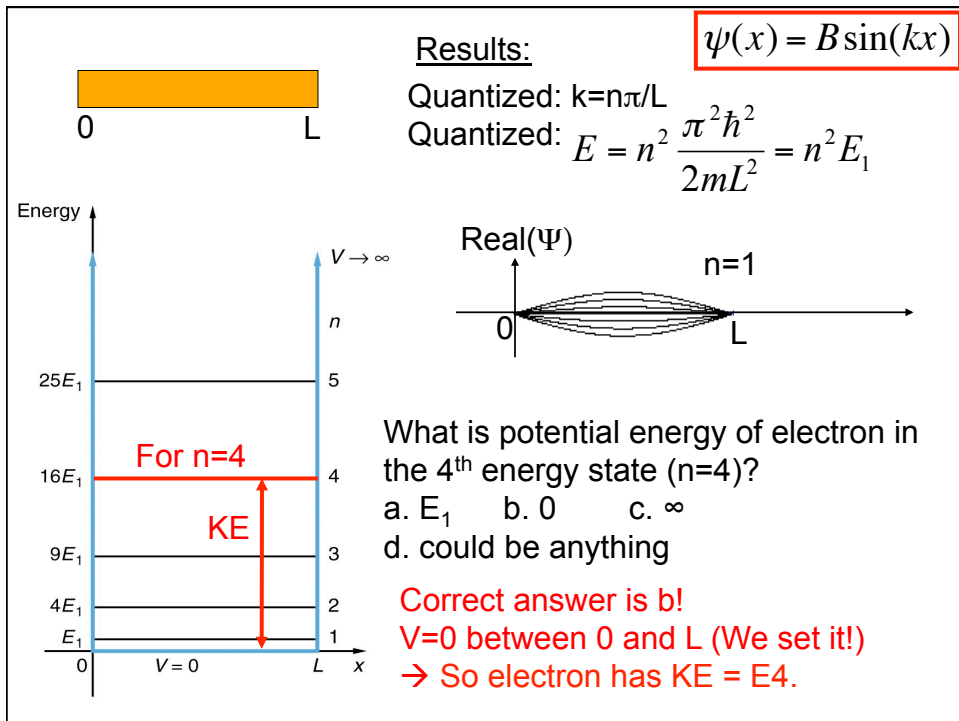
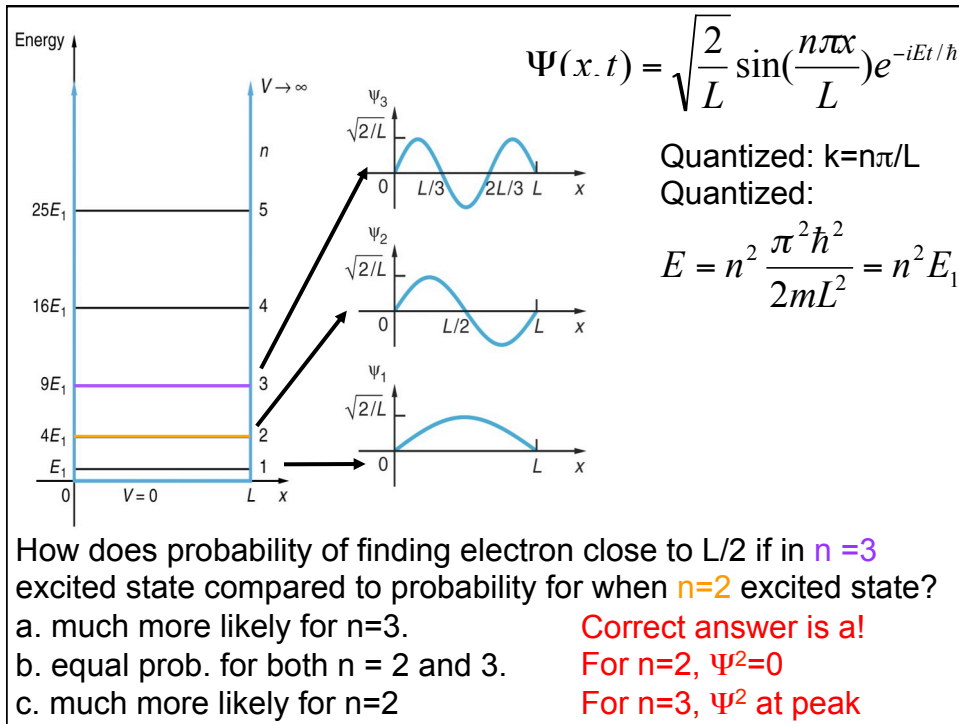
Solving completely- everything there is to know about electron in small metallic object (flat $V(x)$ with high walls).

$$\Psi(x, t) = \psi(x)\phi(t) = B \sin\left(\frac{n\pi x}{L}\right) e^{-iEt/\hbar}$$

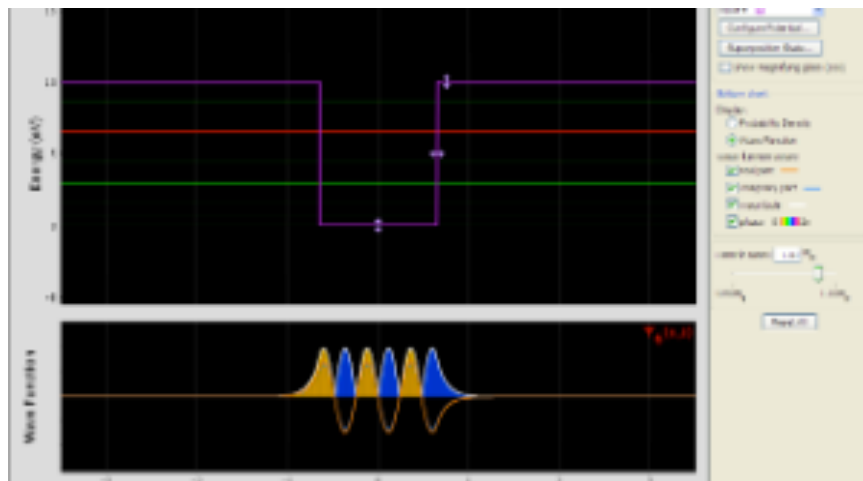
Normalizing:

$$\Psi(x, t) = \psi(x)\phi(t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iEt/\hbar}$$



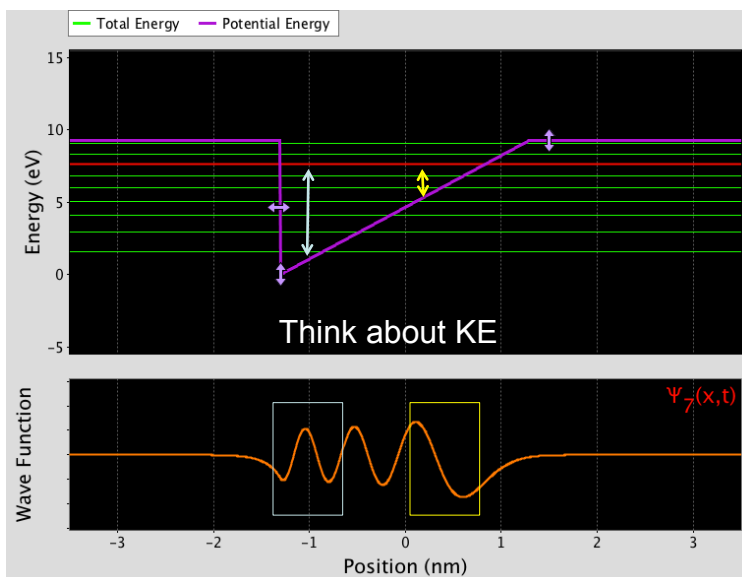


Quantum Bound States

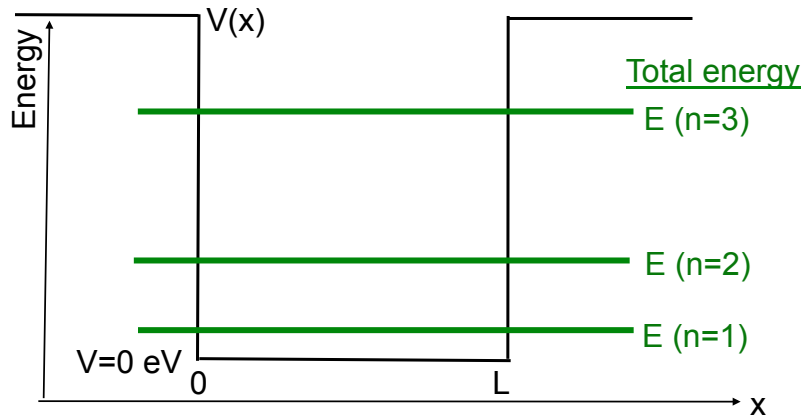


<http://phet.colorado.edu/en/simulation/bound-states>

A quick word about asymmetric wells

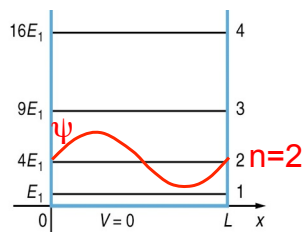


Careful about plotting representations....
Sometimes we're jerks



Careful... plotting 3 things on same graph: Potential Energy V(x)
Total Energy E
Wave Function $\psi(x)$

The small graph shows the wave function $\psi(x)$ for the n=2 state. It is a red curve that starts at zero at x=0, reaches a positive peak, crosses zero at x=L/2, reaches a negative peak, and returns to zero at x=L.



$$\Psi(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iEt/\hbar}$$

Quantized: $k = n\pi/L$

$$\text{Quantized: } E = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 E_1$$

What you expect classically:

What you get quantum mechanically:

Electron can have any energy

Electron can only have specific energies. (quantized)

Electron is localized

Electron is delocalized

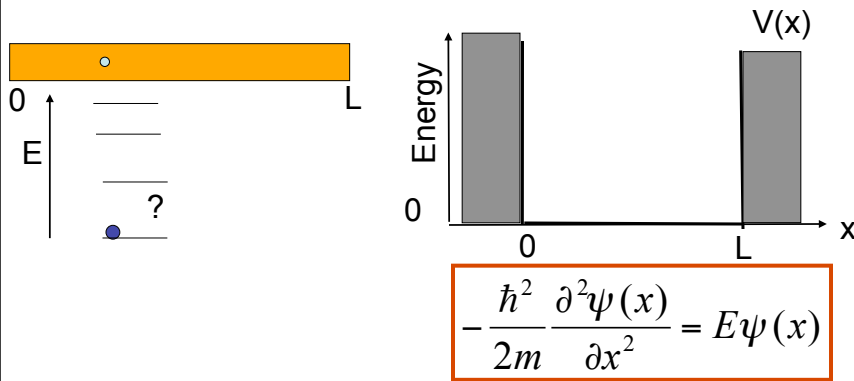
Electron equally likely anywhere in wire

Electron likely measured different places (depends on E!)

Nanotechnology:

How small does a wire have to be before movement of electrons starts to depend on size and shape due to quantum effects?

Look at energy level spacing compared to thermal energy, $kT = 1/40$ eV at room temp.



$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x)$$

The diagram shows two wires of length L on the x-axis. A vertical axis labeled E shows energy levels. A red horizontal line indicates an electron's energy level. The potential energy curve $V(x)$ shows two rectangular barriers at $x=0$ and $x=L$. A dashed red line represents the total energy E_{total} .

Good Approximation:
 Electrons never got out of wire
 $\psi(x < 0 \text{ or } x > L) = 0$.
 (OK when Energy \ll work function)

Exact Potential Energy curve (V):
 small chance electrons get out of wire
 $\psi(x < 0 \text{ or } x > L) \sim 0$, but not exactly 0!

What happens if electron Energy bigger?
 What if two wires very close to each other?

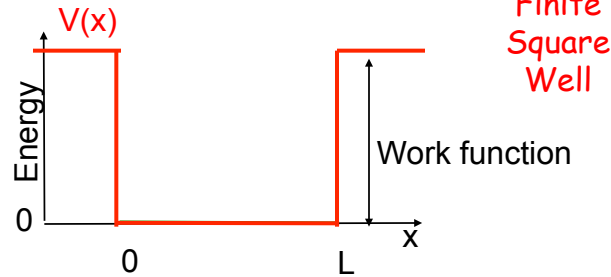
Then whether ψ leaks out a little or not, is very important.
 How much coupling to other wire?

Need to solve for exact Potential Energy curve:

$V(x)$: small chance electrons get out of wire

$\psi(x < 0 \text{ or } x > L) \sim 0$, but not exactly 0!

wire

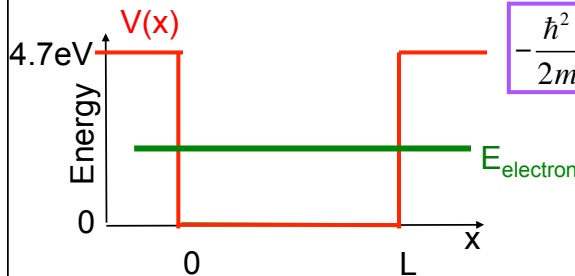


Important for thinking about “Quantum tunneling”:

Radioactive decay

Scanning tunneling microscope to study surfaces

wire



Need to solve Schrodinger Eqn:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x) \psi(x) = E\psi(x)$$

Region I | Region II | Region III

In Region II ... total energy $E >$ potential energy V

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2} (V - E)\psi(x) = -k^2\psi(x) \quad \boxed{k \text{ is real}}$$

Negative number

When $E > V$: Solutions = $\sin(kx)$, $\cos(kx)$, e^{ikx} .
Always expect sinusoidal functions



wire

4.7eV
Energy
0

0 L x

Region I Region II Region III

In Region III ... total energy $E <$ potential energy V

Need to solve Schrodinger Eqn:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2} (V - E)\psi(x) = \alpha^2\psi(x) \quad \boxed{\alpha \text{ is real}}$$

Positive

What functional forms of $\psi(x)$ work?

a. $e^{i\alpha x}$ b. $\sin(\alpha x)$ c. $e^{\alpha x}$ d. more than one of these

wire

4.7eV
Energy
0

0 L x

Region I Region II Region III

In Region III ... total energy $E <$ potential energy V

$$\psi_{III}(x) = Ae^{\alpha x} + Be^{-\alpha x}$$

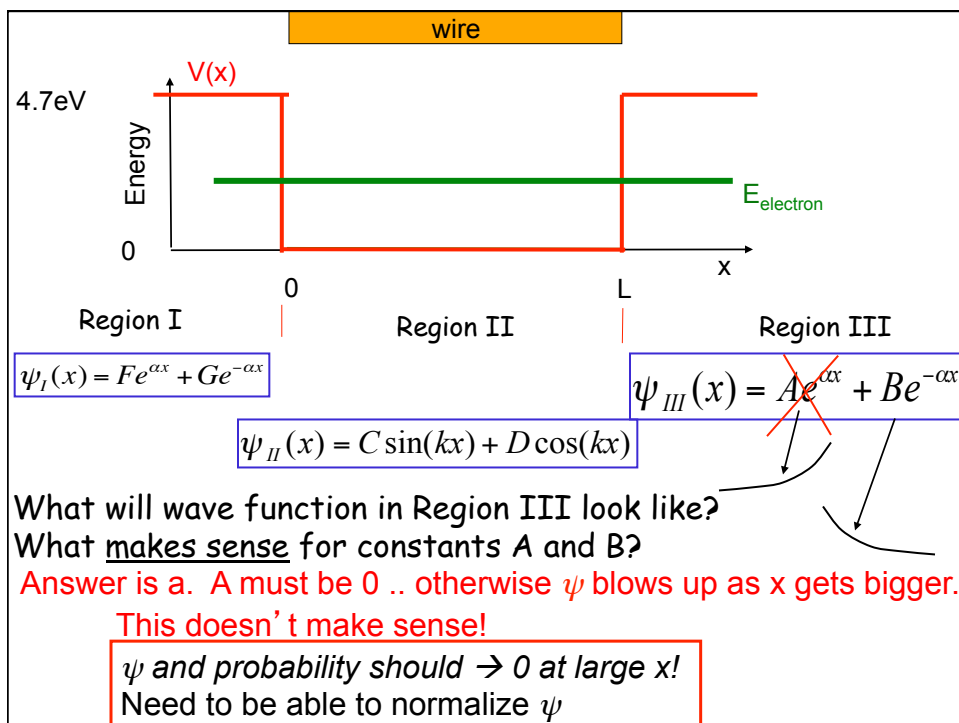
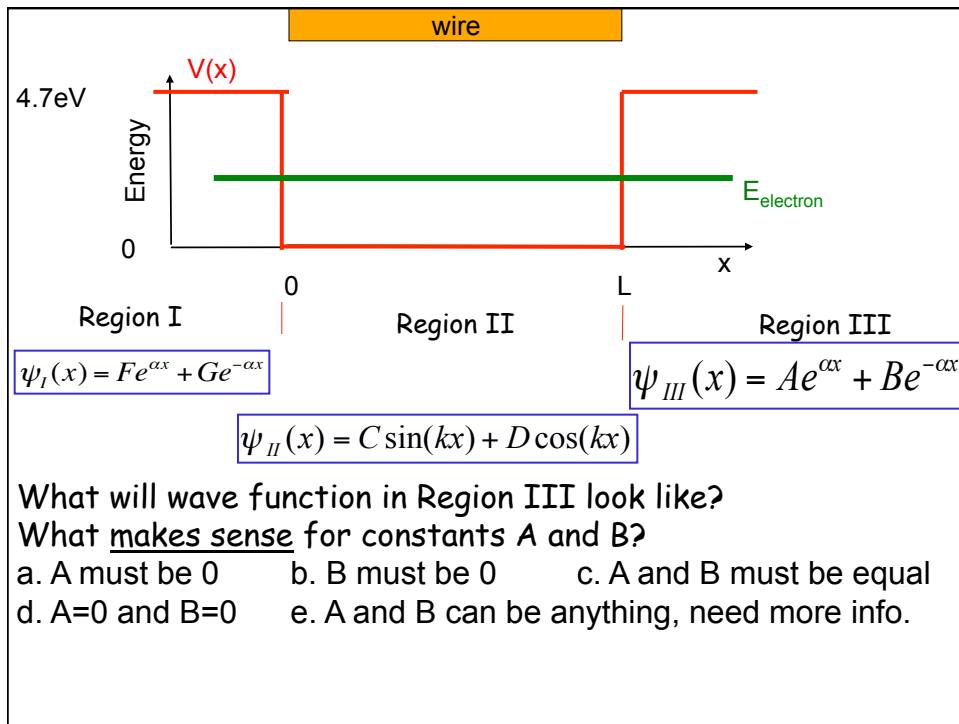
$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2} (V - E)\psi(x) = \alpha^2\psi(x) \quad \boxed{\alpha \text{ is real}}$$

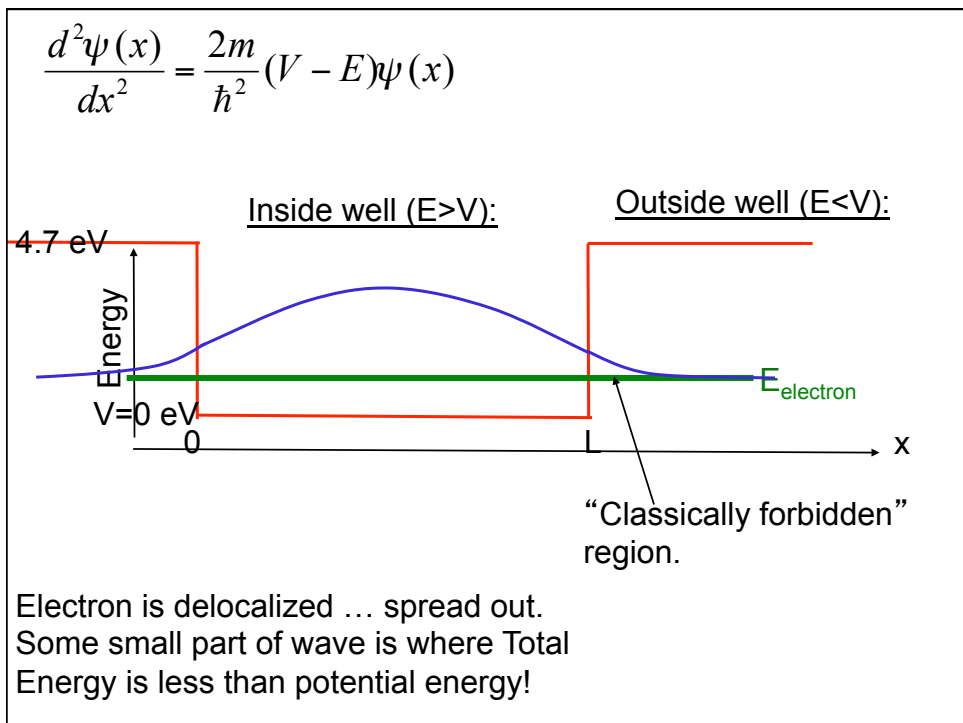
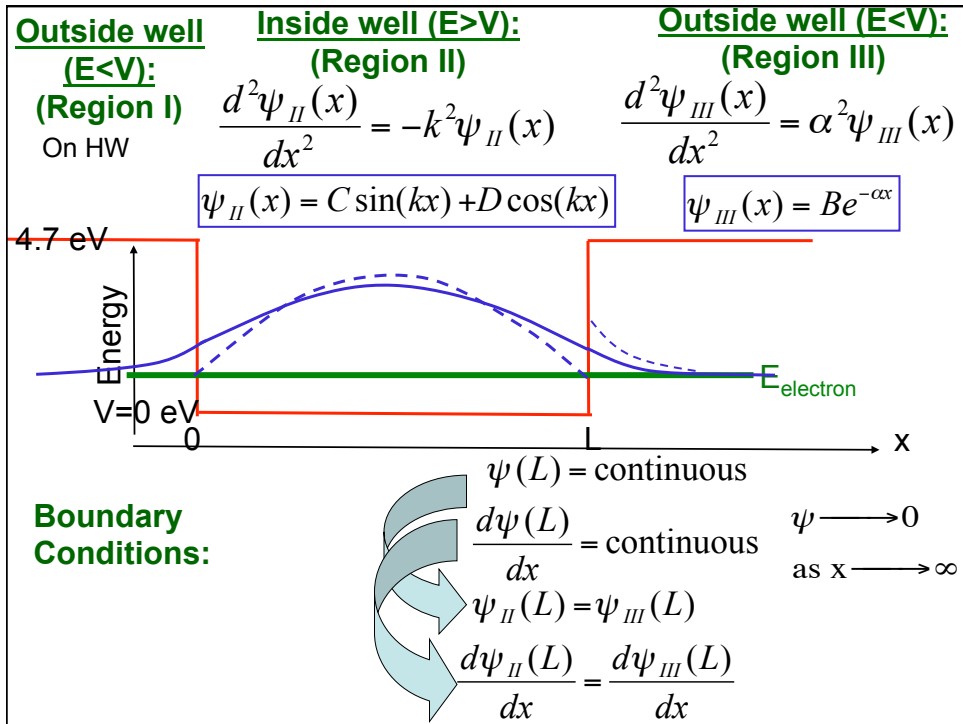
Positive

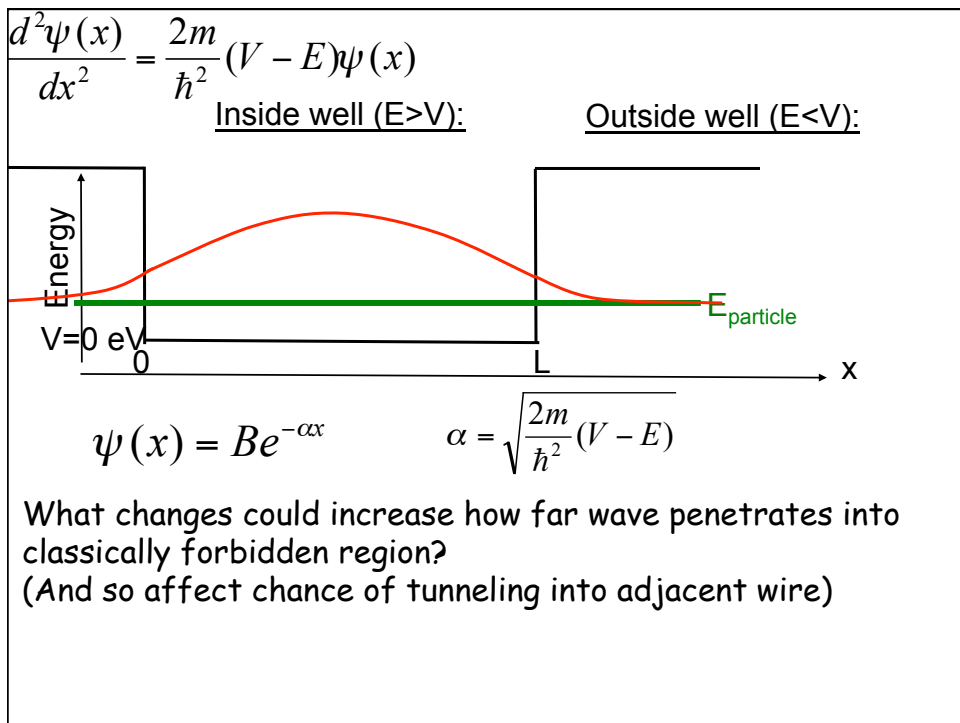
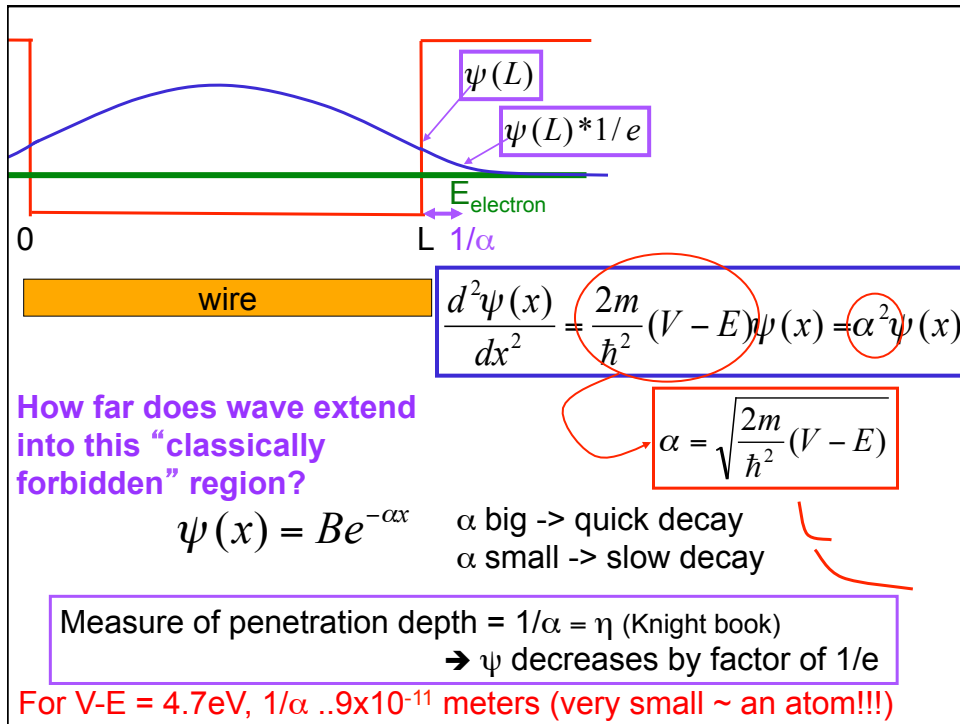
Answer is C: $e^{\alpha x}$... could also be $e^{-\alpha x}$.
Exponential decay or growth

Why not $e^{i\alpha x}$?

LHS	RHS
$-\alpha^2\psi(x)$	$\neq \alpha^2\psi(x)$







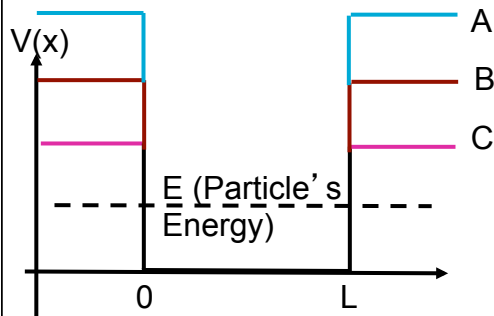
Thinking about α and penetration distance

Under what circumstances would you have a largest penetration?

Order each of the following case from smallest to largest.

$$\psi(x) = Be^{-\alpha x} \quad \alpha = \sqrt{\frac{2m}{\hbar^2}(V - E)}$$

To get largest penetration (tunneling), which Potential curve for a given energy level?



Thinking about α and penetration distance

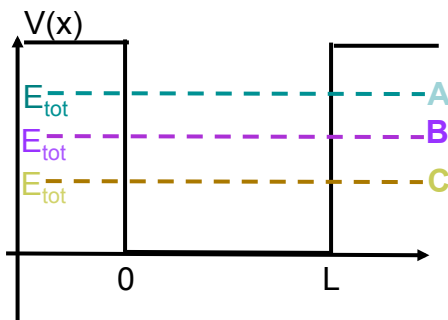
Under what circumstances would you have a largest penetration?

Order each of the following case from smallest to largest.

To get largest penetration (tunneling), which total energy level for a fixed potential curve?

$$\psi(x) = Be^{-\alpha x}$$

$$\alpha = \sqrt{\frac{2m}{\hbar^2}(V - E)}$$



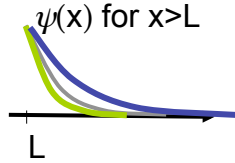
Thinking more about what α means

Putting these together!

$$\alpha = \sqrt{\frac{2m}{\hbar^2}(V - E)}$$

$$\psi(x) = Be^{-\alpha x}$$

Smaller difference
between V & E ,
smaller α
Slower decay
Larger penetration



And bigger diff
btwn V and E ,
Larger α
Faster decay
Smaller penetration

