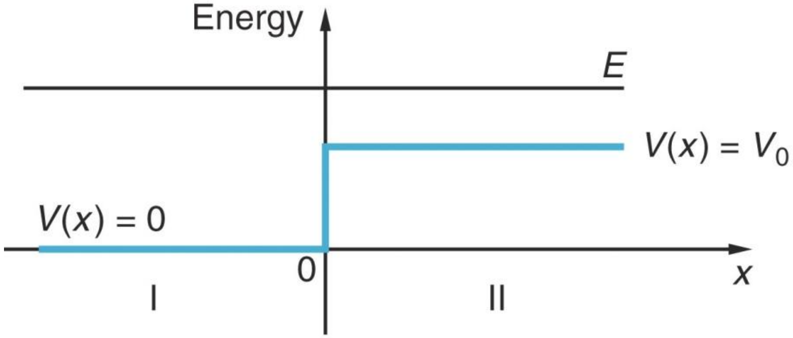
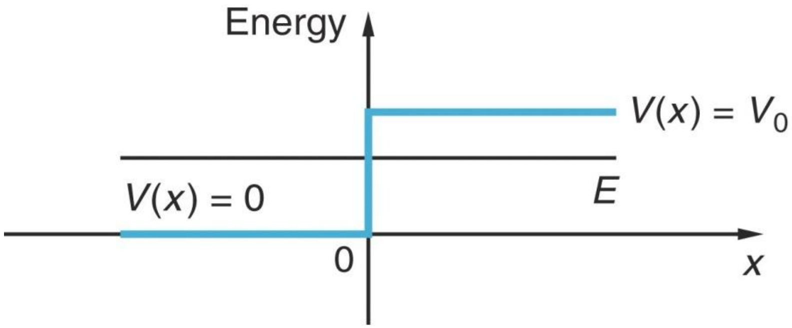
Questions:

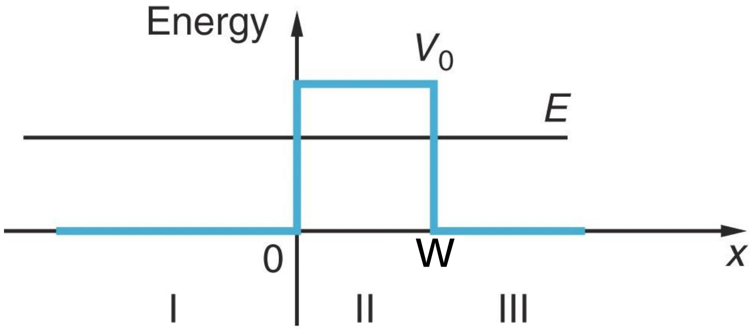
- What are the boundary conditions for tunneling problem?
- How do you figure out amplitude of wave function in different regions in tunneling problem?
- How do you determine probability of tunneling through a barrier?

Today: Answer these question for step potential:





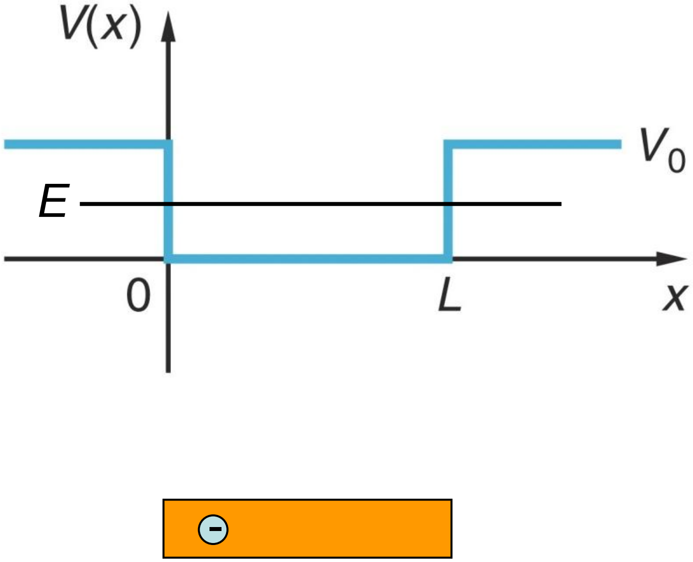
HW after spring break: You answer it for barrier potential (tunneling problem):



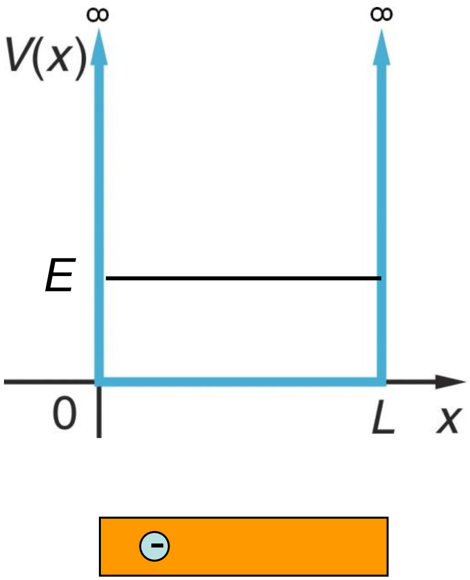
Big Picture:

- So far we’ve talked a lot about wave functions bound in potential wells:

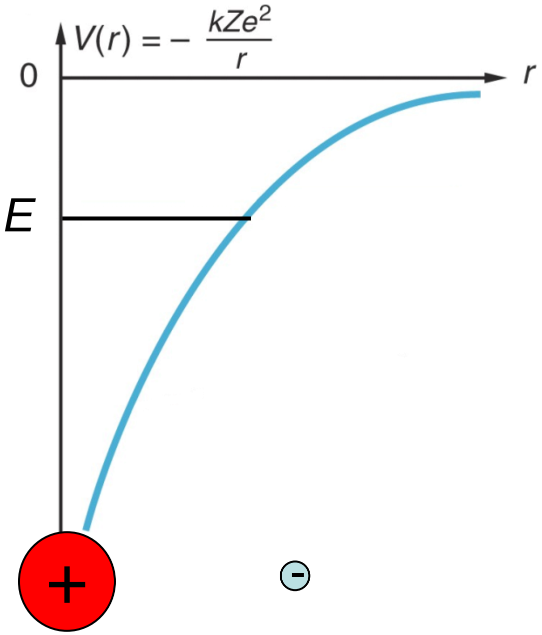
Finite Square Well/
Non-Rigid Box/
Electron in Wire



Infinite Square Well/
Rigid Box/
Electron in wire with work function ⑦ thermal energy



Coulomb Potential/
Hydrogen Atom/
Hydrogen-like Atom



- Here, generally looking at “energy eigenstates” – fixed energy levels.

Big Picture

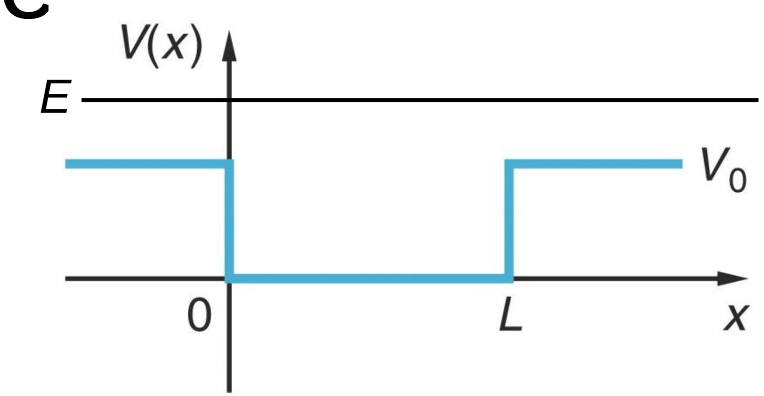
- Can also look at free electrons moving through space or interacting with potentials:
  - Plane wave spread through space:

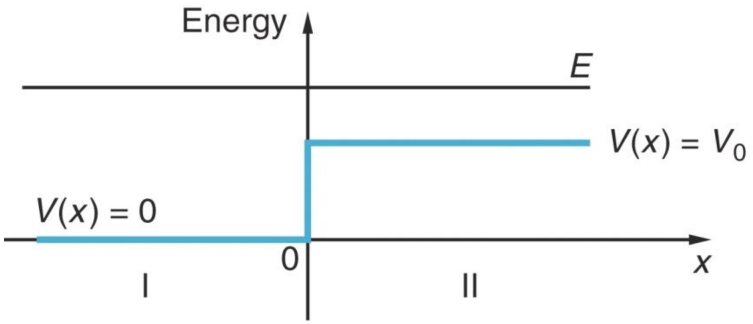
$$\Psi(x,t) = A\exp(ikx - iEt/\hbar)$$

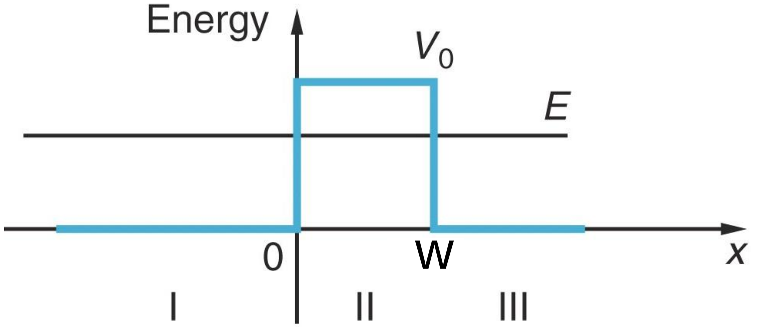
  - Wave packet localized in space:

$$\Psi(x,t) = \sum_n A_n \exp(ik_n x - iE_n t/\hbar)$$

- In these cases (tunneling, reflection/transmission from step, etc.) just pick some initial state, and see how it changes in time.







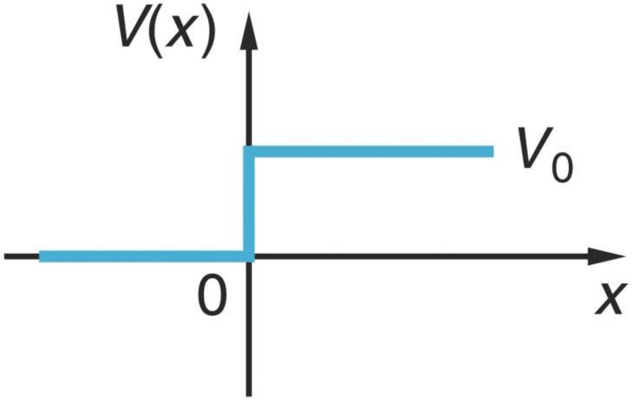
Tunneling

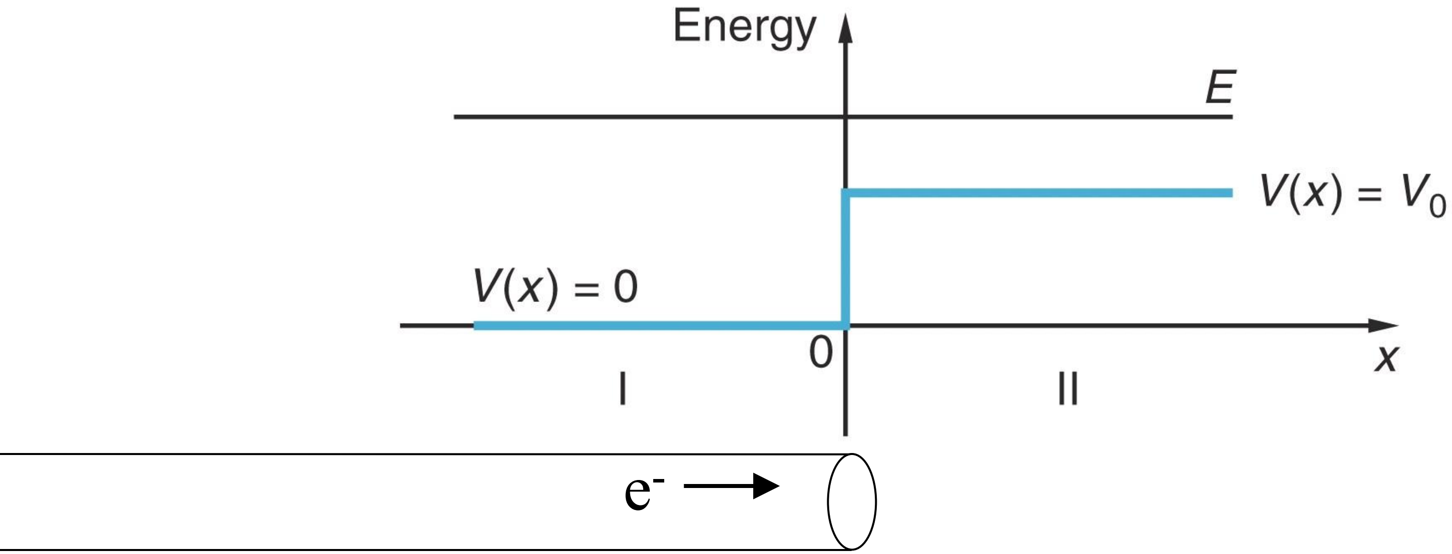
- Particle can “tunnel” through barrier even though it doesn’t have enough energy.
- Visualize with wave packets – show sim: http://phet.colorado.edu/new/simulations/sims.php?sim=QuantumTunneling
- Applications: alpha decay, molecular bonding, scanning tunneling microscopes, single electron tunneling transistors, electrons getting from one wire to another in your house wiring, corona discharge, etc.
- So far we’ve talked about how to determine general solutions in certain regions, wavelengths, decay constants, etc.
- Next step: How do you determine amplitudes of waves, probability of reflection and transmission?
  – Boundary conditions!
- Start with an easier problem…

- An electron is traveling through a very long wire, approaching the end of the wire:

- The potential energy of this electron as a function of position is given by:

$$V(x)=\begin{cases}0 & x<0\\ V_0 & x>0\end{cases}$$



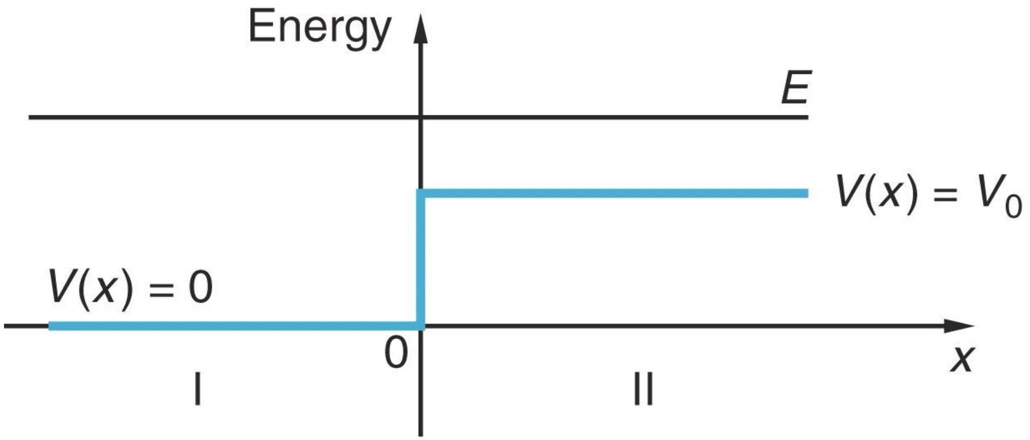


If the total energy E of the electron is GREATER than the work function of the metal, V_0, when the electron reaches the end of the wire, it will…

A. stop.
B. be reflected back.
C. exit the wire and keep moving to the right.
D. either be reflected or transmitted with some probability.
E. dance around and sing, “I love quantum mechanics!”

At this point you may be saying…

- “You said it would either be reflected or transmitted with some probability, but in the simulation it looks like part of it is reflected and part of it is transmitted. What’s up with that?”
- Can anyone answer this question?
- Wave function splits into two pieces – transmitted part and reflected part – but when you make a measurement, you always find a whole electron in one place or the other.
- Will talk about this more on Friday.



- Electron will either be reflected or transmitted with some probability.
- Why? How do we know?
- Solve Schro. equation

Solve time-independent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x) \text{ where } \Psi(x,t)=\psi(x)\exp(-iEt/\hbar)$$

Region I:

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

$$\frac{d^2\psi(x)}{dx^2}=-\underbrace{\frac{2mE}{\hbar^2}}_{k_1^2}\psi(x)$$

$$\psi_1(x)=A\exp(ik_1x)+B\exp(-ik_1x)$$

$$\Psi_1(x,t)=A\exp(i(k_1x-Et/\hbar))+B\exp(-i(k_1x+Et/\hbar))$$

Region II:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V_0\psi(x)=E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2}=-\underbrace{\frac{2m(E-V_0)}{\hbar^2}}_{k_2^2}\psi(x)$$

$$\psi_2(x)=C\exp(ik_2x)+D\exp(-ik_2x)$$

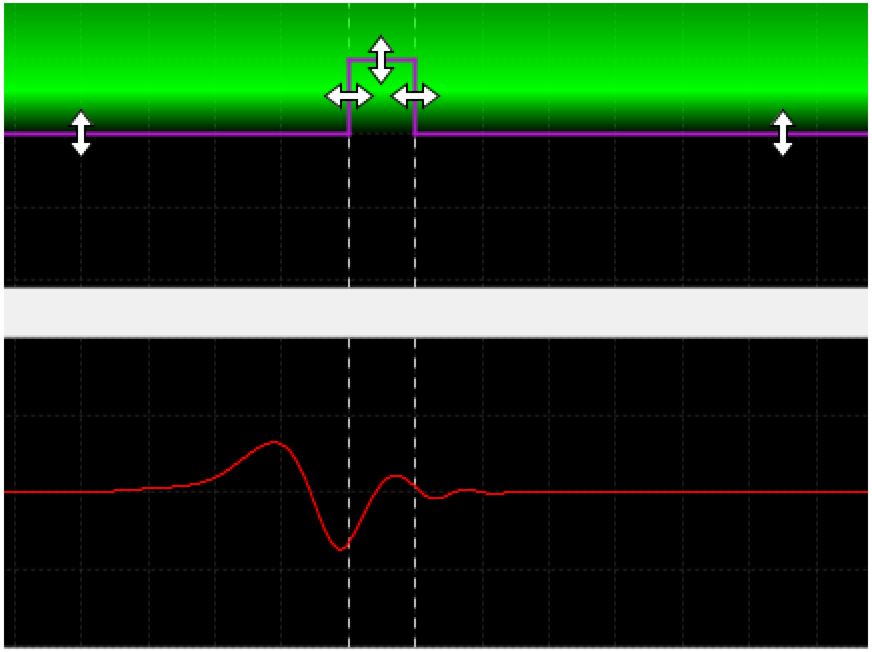
$$\Psi_2(x,t)=C\exp(i(k_2x-Et/\hbar))+D\exp(-i(k_2x+Et/\hbar))$$

Note that general solutions are plane waves:

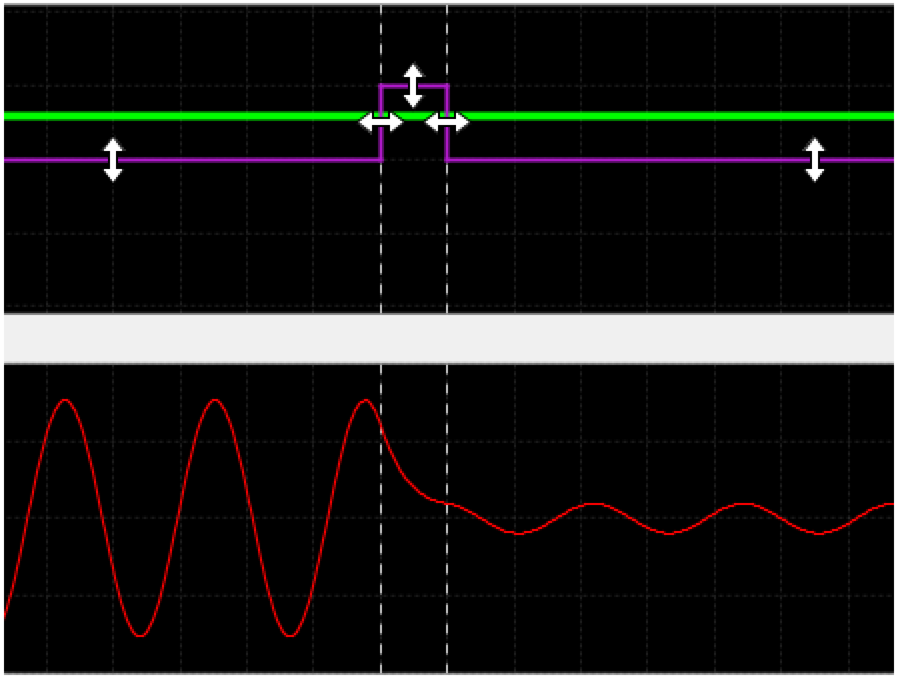
$$\Psi_1(x,t) = A\exp(i(k_1 x - Et/\hbar)) + B\exp(-i(k_1 x + Et/\hbar))$$

$$\Psi_2(x,t) = C\exp(i(k_2 x - Et/\hbar)) + D\exp(-i(k_2 x + Et/\hbar))$$

- Wave packets are more physical…



- But it’s easier to solve for plane waves!



- And you can always add up a bunch of plane waves to get a wave packet.

In region I, the general solution is:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x)$$

$$\Psi_1(x,t) = \psi(x)\exp(-iEt/\hbar) = A\exp(i(k_1x - Et/\hbar)) + B\exp(-i(k_1x + Et/\hbar))$$

What do the A and B terms represent physically?

A. A is the kinetic energy, B is the potential energy.

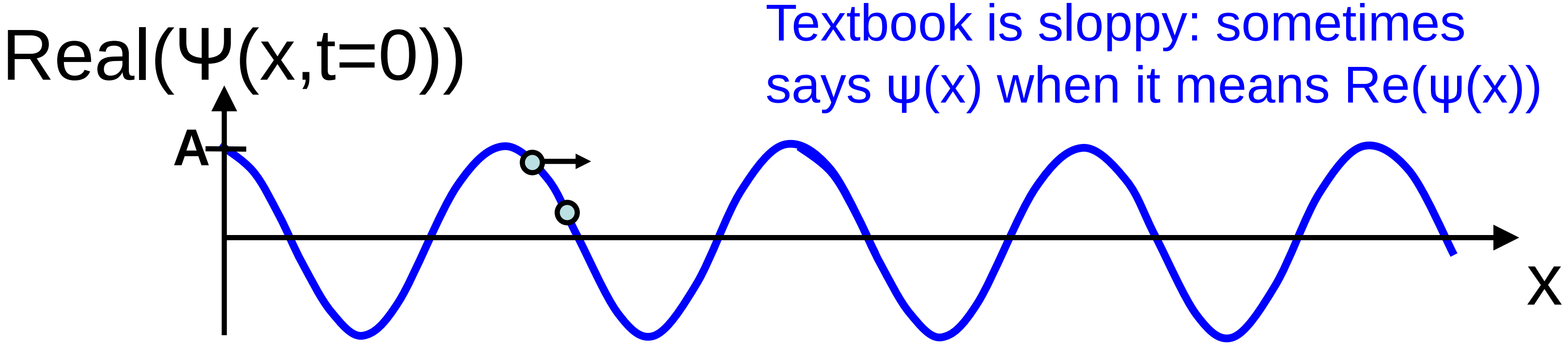
B. A is a wave traveling to the right, B is a wave traveling to the left.

C. A is a wave traveling to the left, B is a wave traveling to the right.

D. A and B are both standing waves.

E. These terms have no physical meaning.

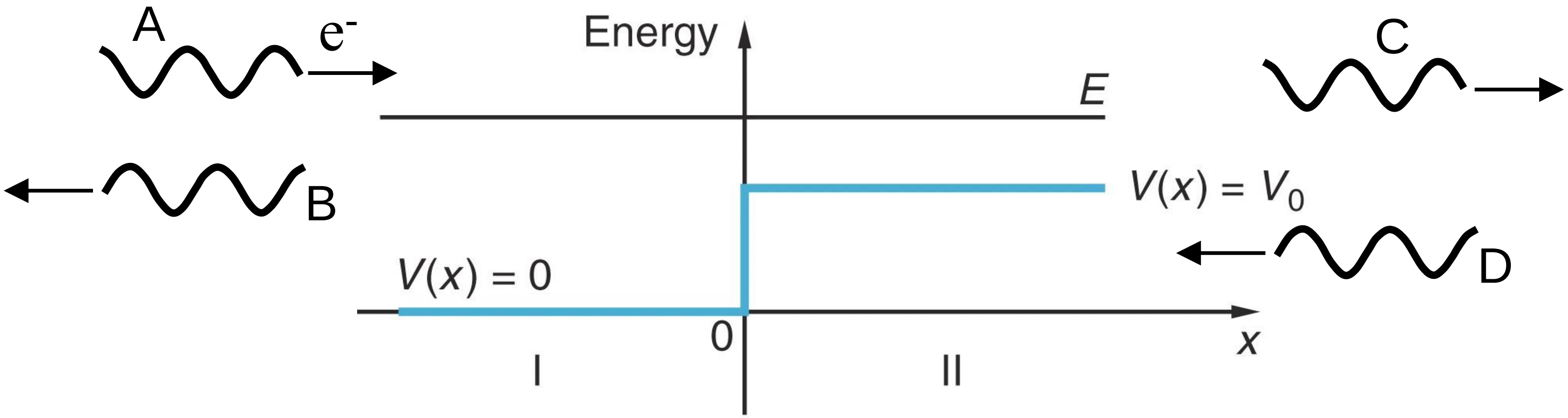
- If $\Psi(x,t) = A\exp(i(kx-\omega t))$, which way is this wave moving?
- Recall from HW: $\exp(i\theta)=\cos(\theta)+i\sin(\theta)$, so:
  - $\mathrm{Real}(\Psi) = A\cos(kx-\omega t)$
  - $\mathrm{Imaginary}(\Psi) = A\sin(kx-\omega t)$
- Real & imaginary parts of Ψ just differ by phase. Usually we just plot the real part:



Textbook is sloppy: sometimes says ψ(x) when it means Re(ψ(x))

- Increase t a little, Ψ same as a little bit to the left. $\Psi(x,t+\Delta t) = \Psi(x-\Delta x,t)$.

Wave moves to right.



Region I:

$$\frac{d^2\psi(x)}{dx^2} = -\underbrace{\frac{2mE}{\hbar^2}}_{k_1^2}\psi(x)$$

$$\psi_1(x) = \underbrace{A\exp(ik_1x)}_{\text{Wave traveling right}} + \underbrace{B\exp(-ik_1x)}_{\text{Wave traveling left}}$$

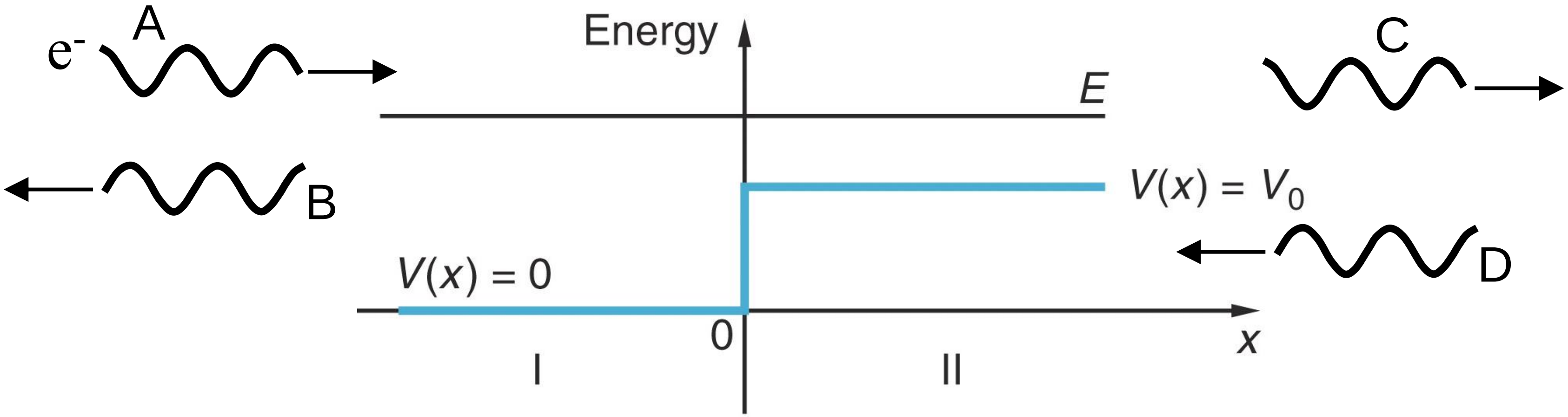
Region II:

$$\frac{d^2\psi(x)}{dx^2} = -\underbrace{\frac{2m(E-V_0)}{\hbar^2}}_{k_2^2}\psi(x)$$

$$\psi_2(x) = \underbrace{C\exp(ik_2x)}_{\text{Wave traveling right}} + \underbrace{D\exp(-ik_2x)}_{\text{Wave traveling left}}$$

What do each of these waves represent?

a) A = reflected, B = transmitted, C = incoming, D = incoming from right
b) A = transmitted, B = reflected, C = incoming, D = incoming from right
c) A = incoming, B = reflected, C = transmitted, D = incoming from right
d) A = incoming, B = transmitted, C = reflected, D = incoming from right
e) A = incoming from right, B = reflected, C = transmitted, D = incoming



Region I:

$$\psi_1(x)=\underbrace{A\exp(ik_1x)}_{\substack{\text{Wave traveling right}\\ \text{Incoming}}}+\underbrace{B\exp(-ik_1x)}_{\substack{\text{Wave traveling left}\\ \text{Reflected}}}$$

Region II:

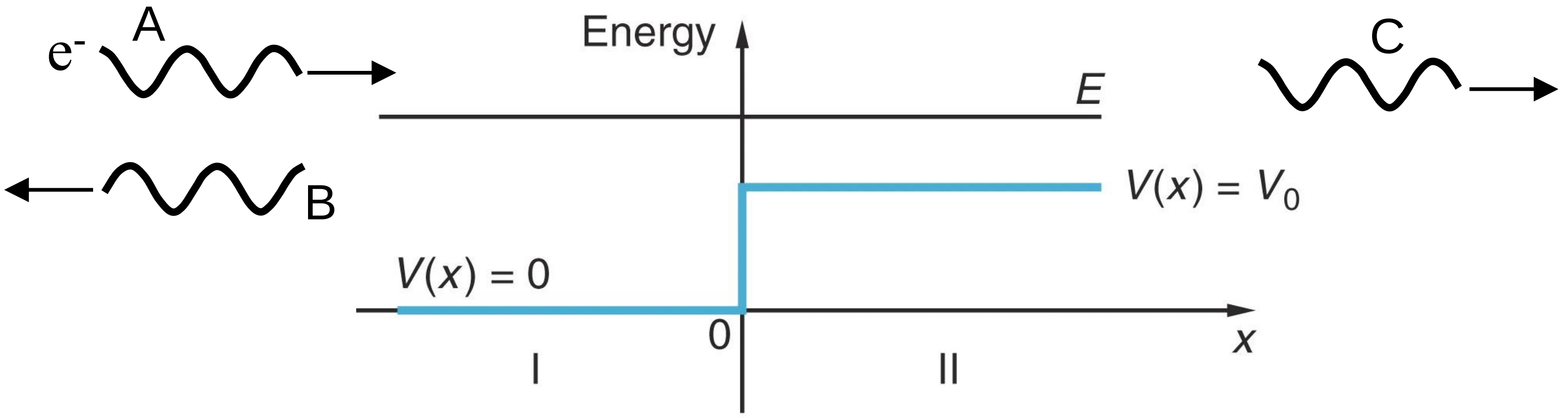
$$\psi_2(x)=\underbrace{C\exp(ik_2x)}_{\substack{\text{Wave traveling right}\\ \text{Transmitted}}}+\cancelto{0}{\underbrace{D\exp(-ik_2x)}_{\substack{\text{Wave traveling left}\\ \text{Incoming}\\ \text{from Right}}}}$$

Use initial/boundary conditions to determine constants:

Initial Conditions: Electron coming in from left $\Rightarrow$ D = 0

Boundary Conditions: $BC1.\quad \psi_1(0)=\psi_2(0)$ $\quad\Rightarrow$ A + B = C

$$BC2.\quad \frac{d\psi_1(0)}{dx}=\frac{d\psi_2(0)}{dx}\quad\Rightarrow ik_1(A-B)=ik_1C$$



Region I:

$$\psi_1(x) = \underbrace{A\exp(ik_1 x)}_{\text{Wave traveling right}} + \underbrace{B\exp(-ik_1 x)}_{\text{Wave traveling left}}$$

Incoming

Reflected

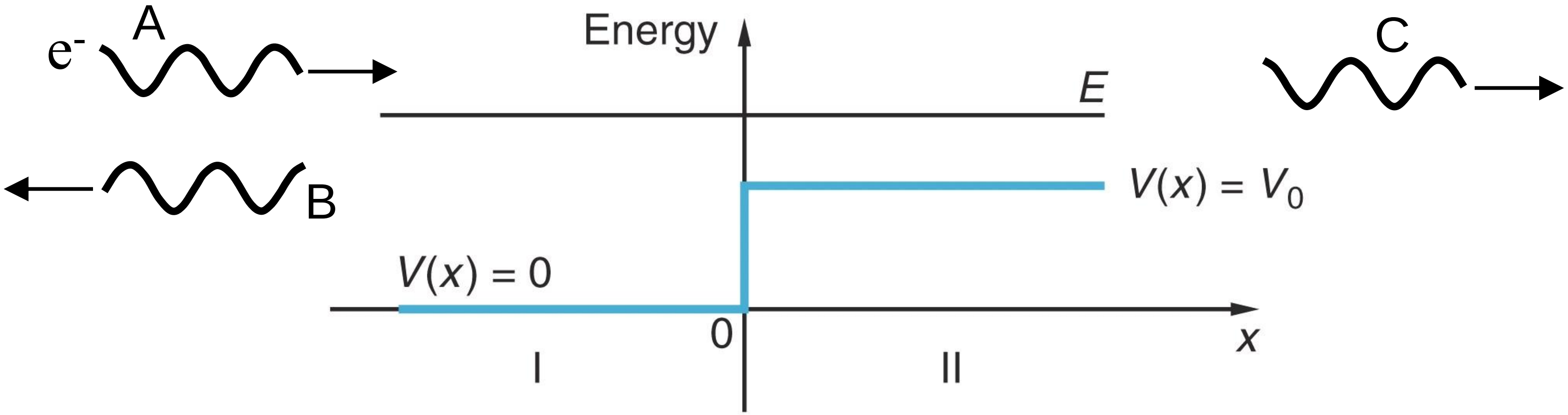
Region II:

$$\psi_2(x) = \underbrace{C\exp(ik_2 x)}_{\text{Wave traveling right}}$$

Transmitted

If an electron comes in with an amplitude A, what's the probability that it's reflected? What's the probability that it's transmitted?

a) P(reflection) = B, P(transmission) = 1 – B
b) P(reflection) = B/A, P(transmission) = 1 – B/A
c) P(reflection) = B^2, P(transmission) = 1 – B^2
d) P(reflection) = B^2/A^2, P(transmission) = 1 – B^2/A^2
e) P(reflection) = $|B|^2/|A|^2$, P(transmission) =1 – $|B|^2/|A|^2$



Region I:

$$\psi_1(x) = \underbrace{A\exp(ik_1x)}_{\text{Wave traveling right}} + \underbrace{B\exp(-ik_1x)}_{\text{Wave traveling left}}$$

Incoming Reflected

Region II:

$$\psi_2(x) = \underbrace{C\exp(ik_2x)}_{\text{Wave traveling right}}$$

Transmitted

If an electron comes in with an amplitude A, what’s the probability that it’s reflected? What’s the probability that it’s transmitted?

P(reflection) = “Reflection Coefficient”
= R = $|B|^2/|A|^2$,

P(transmission) = “Transmission Coefficient”
= T = 1 – $|B|^2/|A|^2$

To find R and T, use boundary conditions:

Wave Functions:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x)$$

$$\psi_2(x) = C\exp(ik_2x)$$

Boundary Conditions:

$$BC1. \quad \psi_1(0) = \psi_2(0)$$

$$BC2. \quad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$$

Write down the equations for Bound. Conds:

(1) $A+B=C$

(2) $ik_1(A–B) = ik_2C$

Solve for B and C in terms of A:

$B = A^*(k_1–k_2)/(k_1+k_2)$

$C = A^*2k_1/(k_1+k_2)$

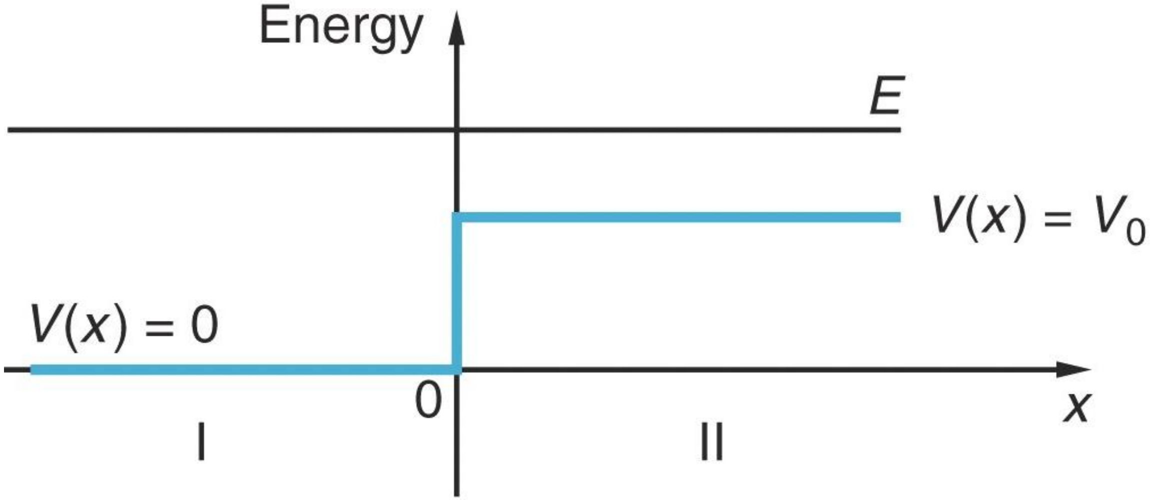
Find R and T:

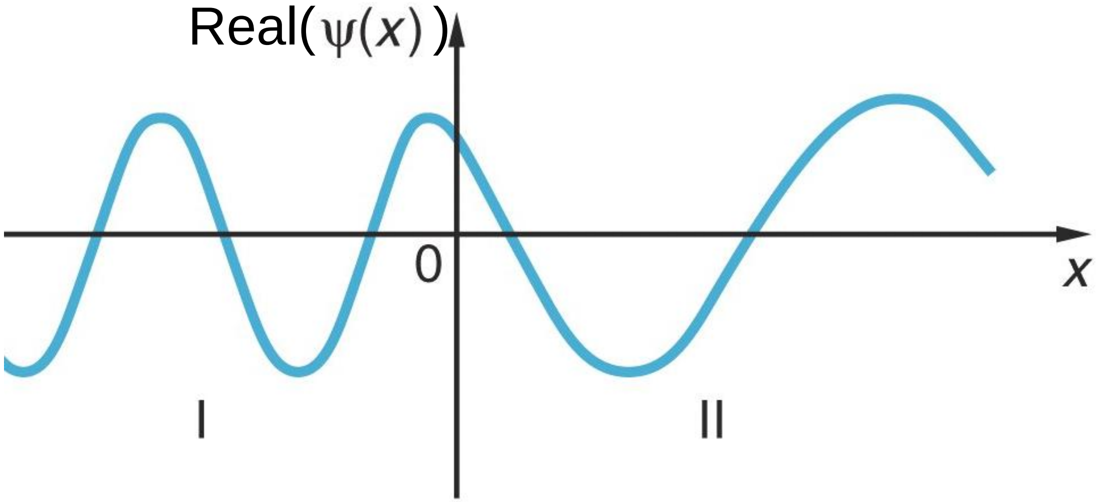
$R = |B|^2/|A|^2 = (k_1–k_2)^2/(k_1+k_2)^2$

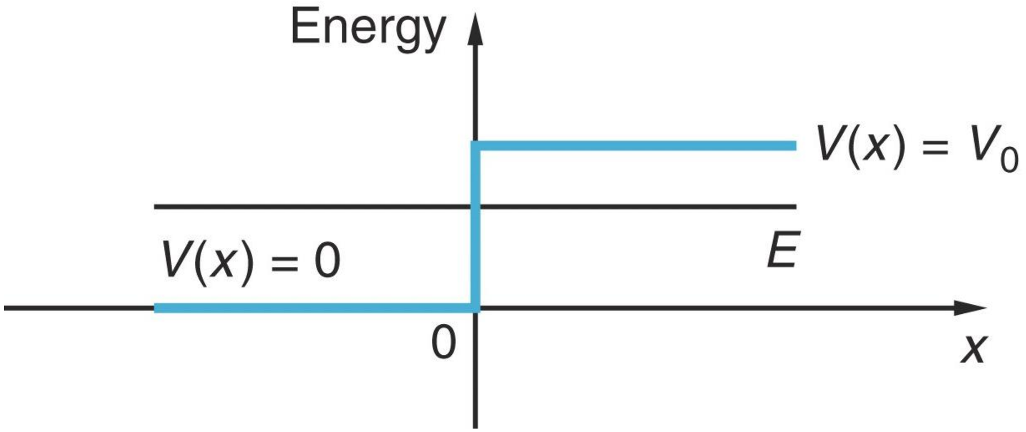
$T = 1 – |B|^2/|A|^2 = 4k_1k_2/(k_1+k_2)^2$

Note that you can't determine A from boundary conditions. It's the initial condition – must be given. But you don't need it to find R & T.

Once you have amplitudes, can draw wave function:

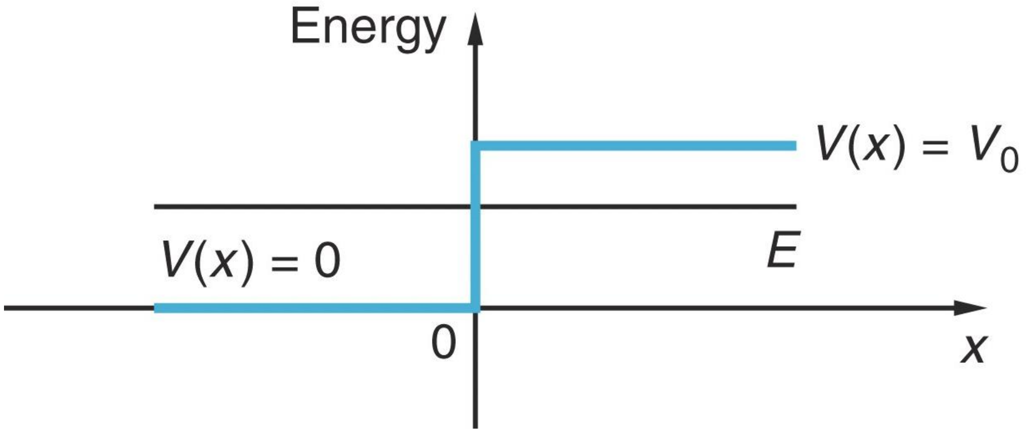






If the total energy *E* of the electron is LESS than the work function of the metal, V_0, when the electron reaches the end of the wire, it will…

A. stop.
B. be reflected back.
C. exit the wire and keep moving to the right.
D. either be reflected or transmitted with some probability.
E. dance around and sing, “I love quantum mechanics!”



Solve time-independent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x) \quad \text{where } \Psi(x,t)=\psi(x)\exp(-iEt/\hbar)$$

Region I (same as before):

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

$$\frac{d^2\psi(x)}{dx^2}=-\underbrace{\frac{2mE}{\hbar^2}}_{=\,k_1{}^2}\psi(x)$$

$$\psi_1(x)=A\exp(ik_1x)+B\exp(-ik_1x)$$

$$\Psi_1(x,t)=A\exp(i(k_1x-Et/\hbar)) \\ +B\exp(-i(k_1x+Et/\hbar))$$

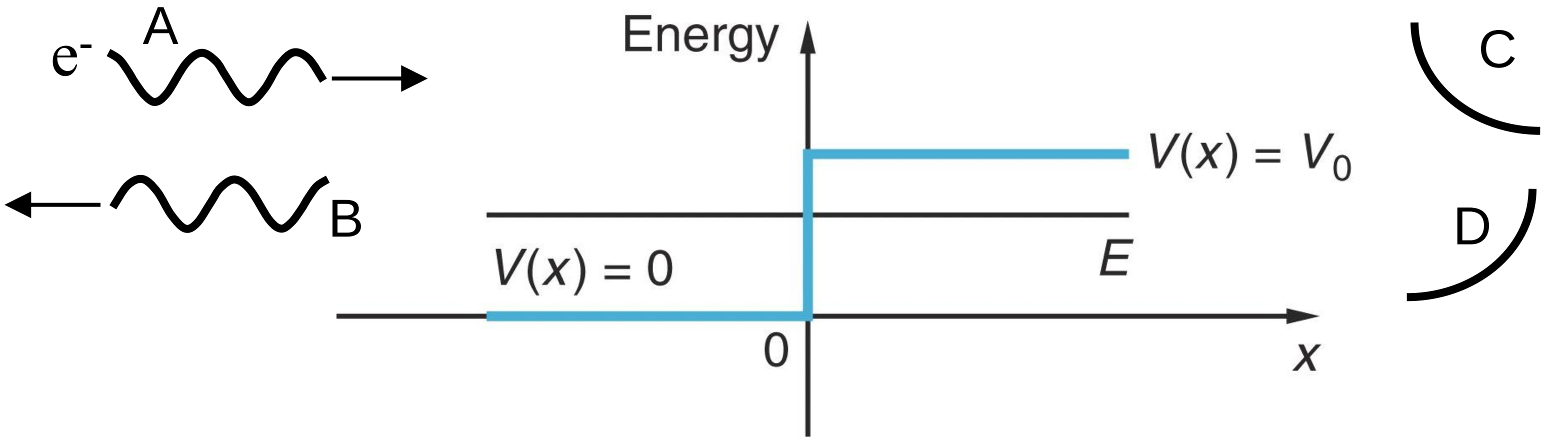
Region II:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V_0\psi(x)=E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2}=\underbrace{-\frac{2m(E-V_0)}{\hbar^2}}_{=\,\alpha^2}\psi(x)$$

$$\psi_2(x)=C\exp(-\alpha x)+D\exp(\alpha x)$$

$$\Psi_2(x,t)=C\exp(-\alpha x-iEt/\hbar) \\ +D\exp(\alpha x-Et/\hbar)$$



Region I:

$$\psi_1(x) = \underbrace{A\exp(ik_1x)}_{\text{Wave traveling right}} + \underbrace{B\exp(-ik_1x)}_{\text{Wave traveling left}}$$

Incoming Reflected

Region II:

$$\psi_2(x) = \underbrace{C\exp(-\alpha x)}_{\text{Exponential decay}} + \underbrace{\cancelto{0}{D\exp(\alpha x)}}_{\text{Exponential growth}}$$

Note: no transmitted wave appears in equations

Use boundary conditions to determine constants:

$$\boxed{R = \frac{|B|^2}{|A|^2} = 1}$$

Boundary Conditions:

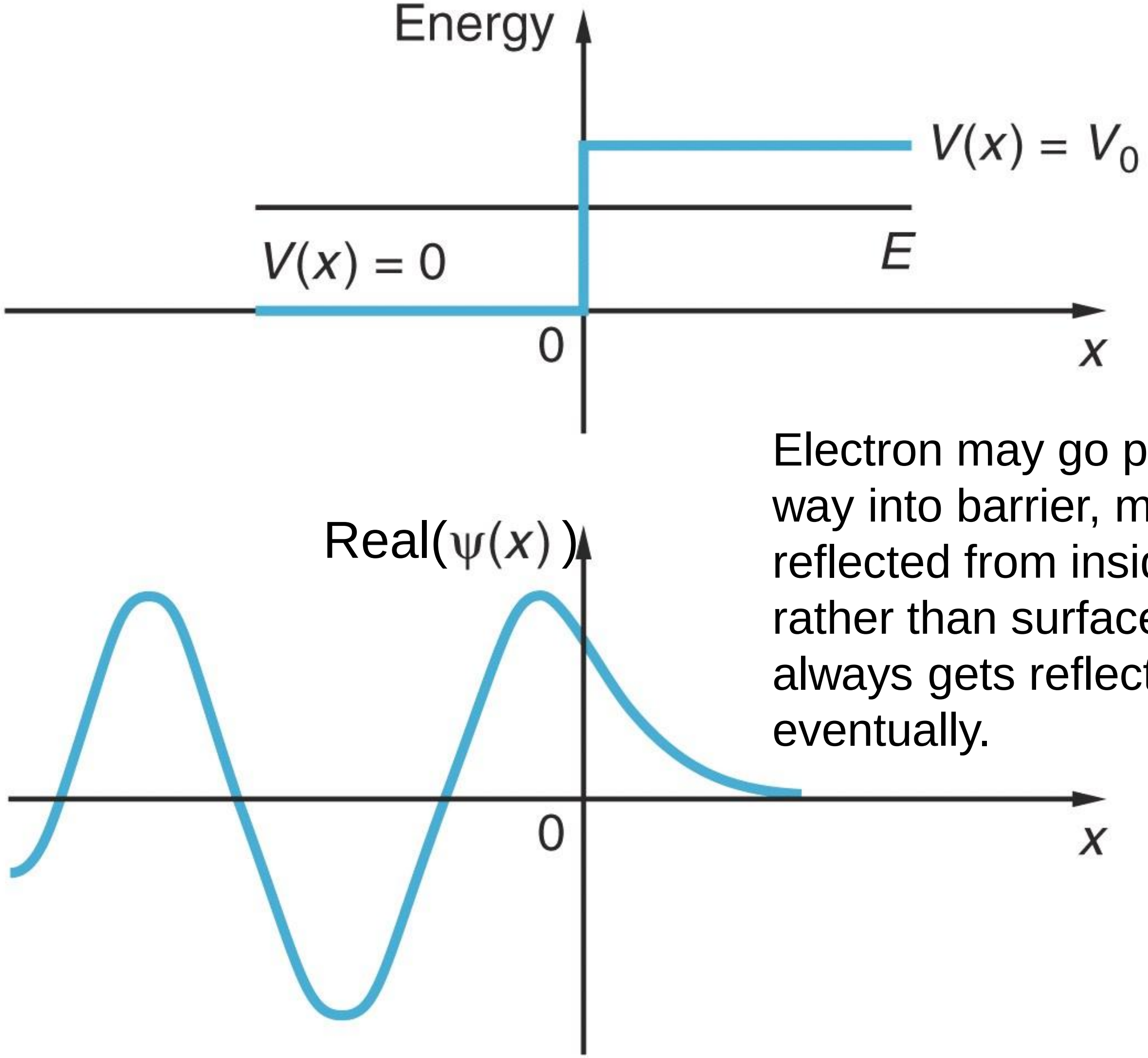
$$BC0. \quad \psi_2(x) \to 0 \quad \text{as} \quad x \to \infty$$

Solve for B in terms of A

$$BC1. \quad \psi_1(0) = \psi_2(0) \quad \Rightarrow \text{A + B = C}$$

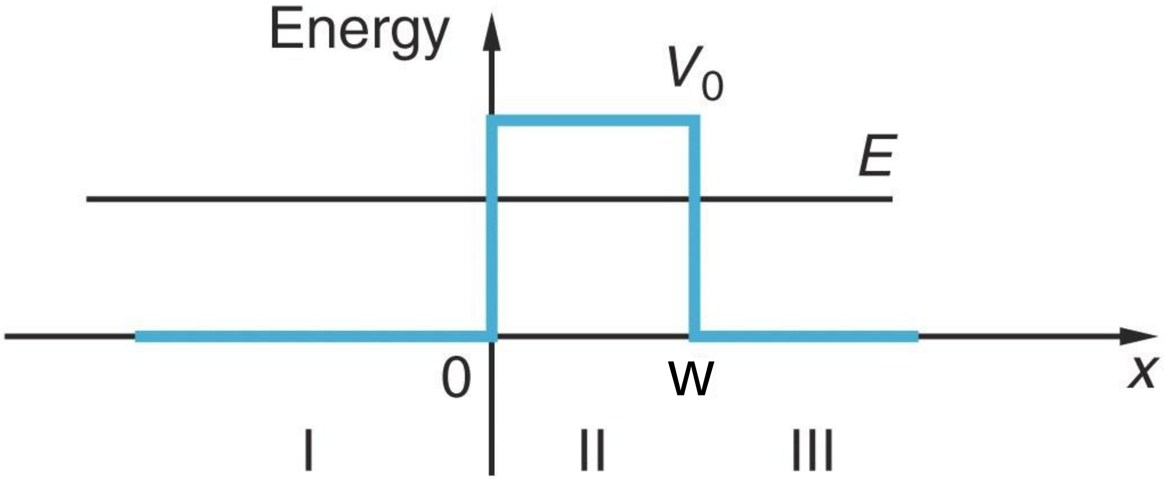
$$BC2. \quad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx} \quad \Rightarrow \text{ik(A – B) = –αC}$$

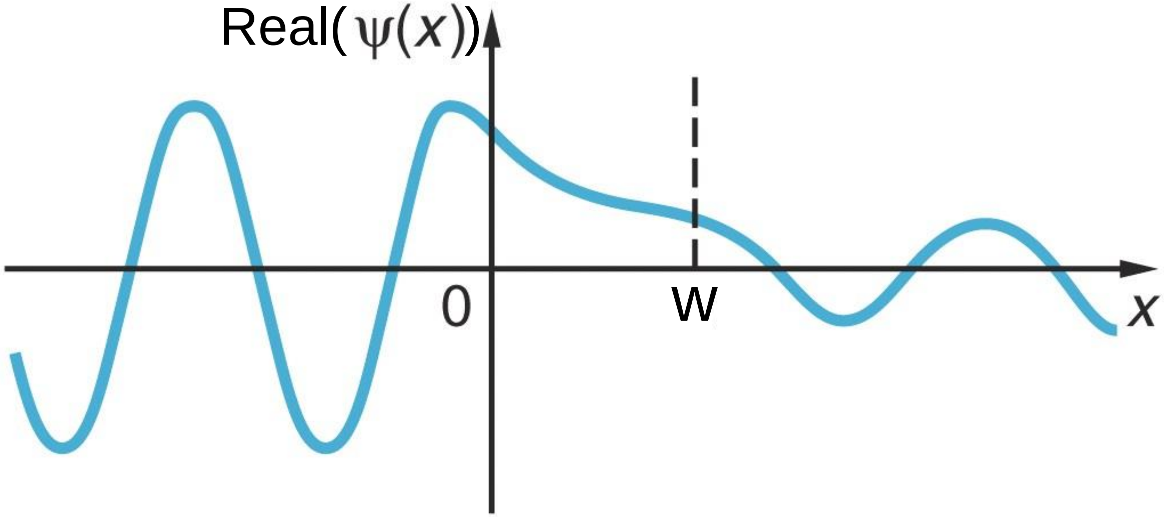
Once you have amplitudes, can draw wave function:



Electron may go part of the way into barrier, may be reflected from inside barrier rather than surface, but it always gets reflected eventually.

Tunneling Problem – in HW
Same as above but now 3 regions!





Tunneling Problem – in HW

- Find ψ in 3 regions: $$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x)$$ $$\psi_2(x) = C\exp(-\alpha x) + D\exp(\alpha x)$$ $$\psi_3(x) = F\exp(ik_1x) + G\exp(-ik_1x)$$
- Solve for B,C,D,F,G in terms of A
- Find probability of transmission/reflection:
- Final Result: $$T = \left[1+\frac{e^{\alpha w}-e^{-\alpha w}}{4\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1} \approx e^{-2\alpha w}$$

w = width of barrier

$\alpha = 1/\eta$ = decay constant = $\frac{\sqrt{2m(V_0 - E)}}{\hbar}$