Reflection and Transmission at a Potential Step

Outline

- Review: Particle in a 1-D Box
- Reflection and Transmission - Potential Step
- Reflection from a Potential Barrier
- Introduction to Barrier Penetration (Tunneling)

Reading and Applets:

.Text on Quantum Mechanics by French and Taylor

.Tutorial 10 – Quantum Mechanics in 1-D Potentials

.applets at http://phet.colorado.edu/en/get-phet/one-at-a-time

Schrodinger: A Wave Equation for Electrons

$$E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi \qquad p_x\psi = \hbar k\psi = j\hbar\frac{\partial}{\partial x}\psi$$

$$E = \frac{p^2}{2m}$$ (free-particle)

$$-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$ (free-particle)

..The Free-Particle Schrodinger Wave Equation !

Erwin Schrödinger (1887–1961)
Image in the Public Domain

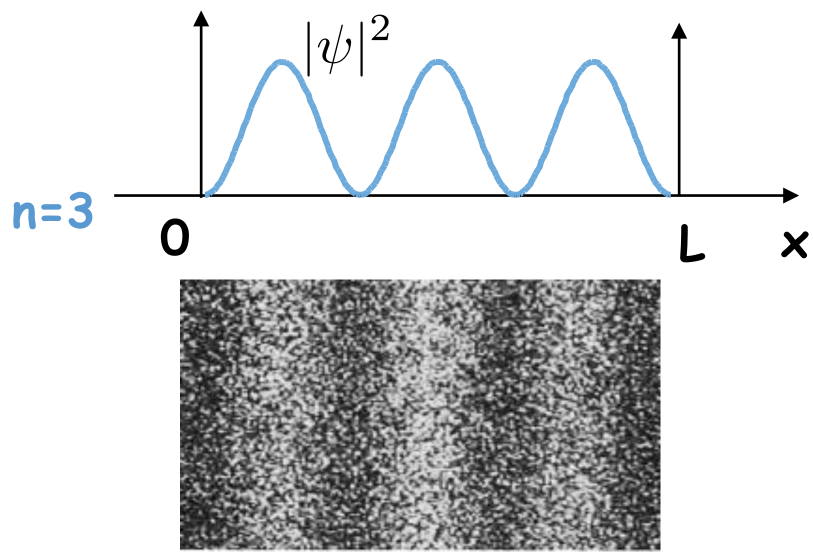
Schrodinger Equation and Energy Conservation

The Schrodinger Wave Equation

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

The quantity $|\psi|^2$ dx is interpreted as the probability that the particle can be found at a particular point *x* (within interval dx)

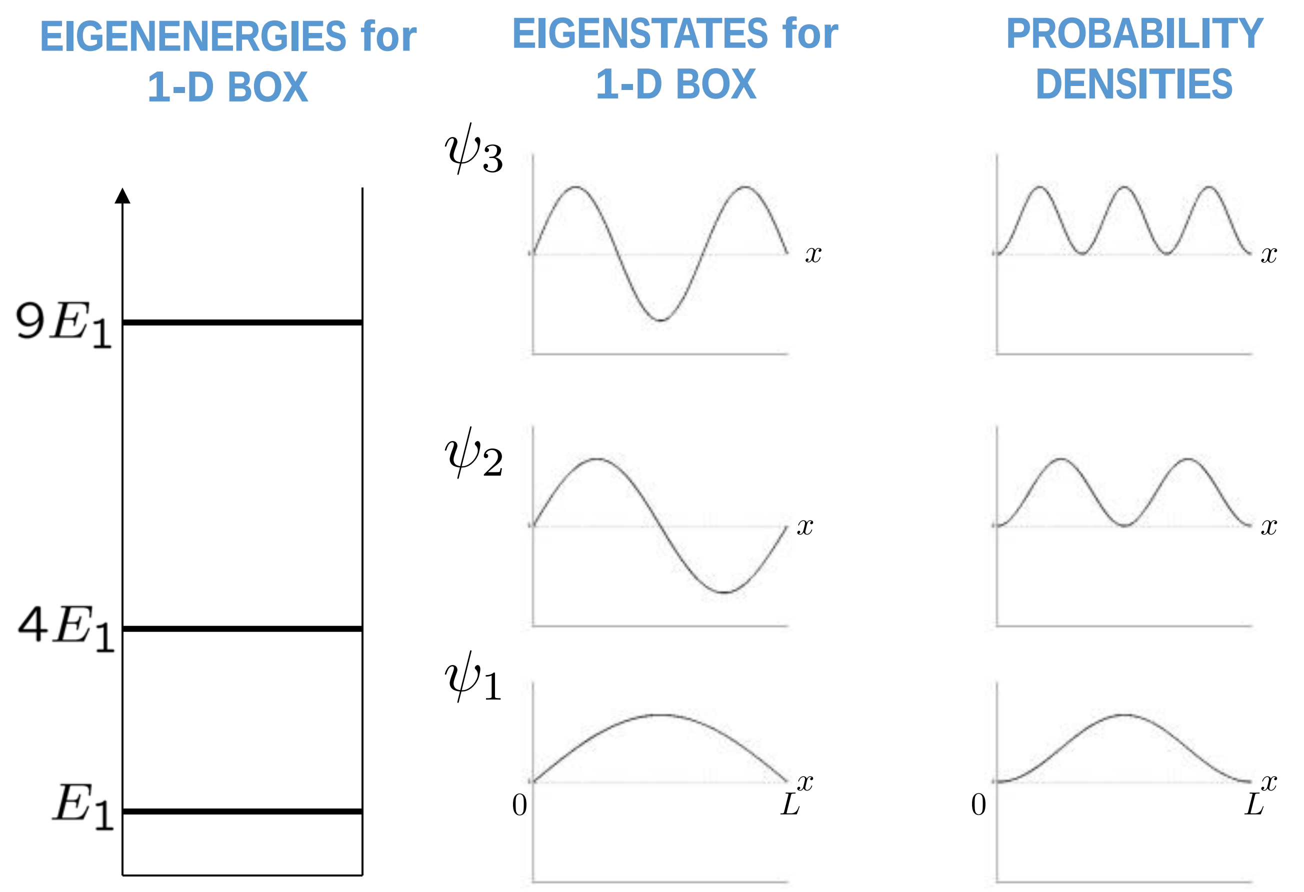
$$P(x) = |\psi|^2 dx$$



Schrodinger Equation and Particle in a Box

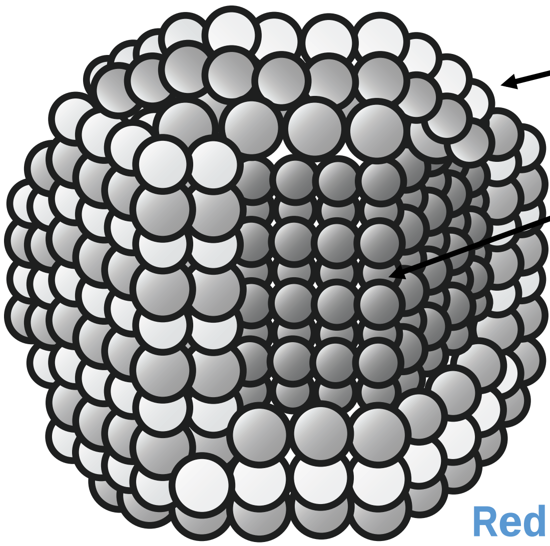
$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x)$$

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \qquad P(x) = |\psi(x)|^2\,dx$$



Semiconductor Nanoparticles

(aka: Quantum Dots)



Red: bigger dots!
Blue: smaller dots!

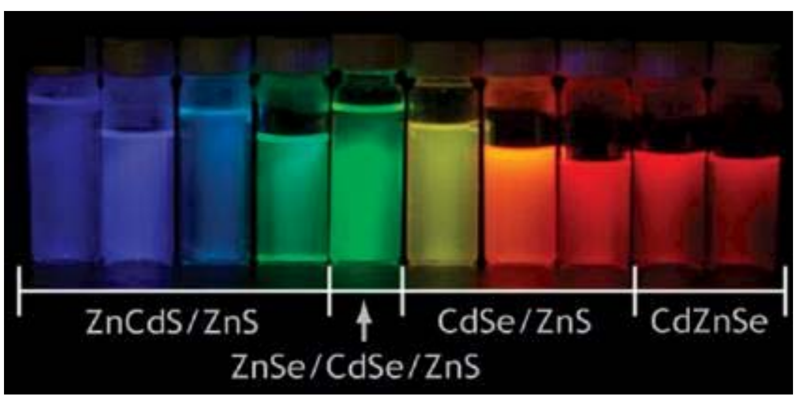
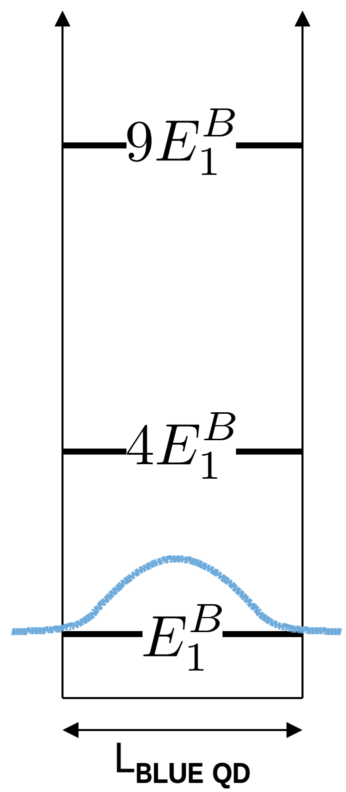
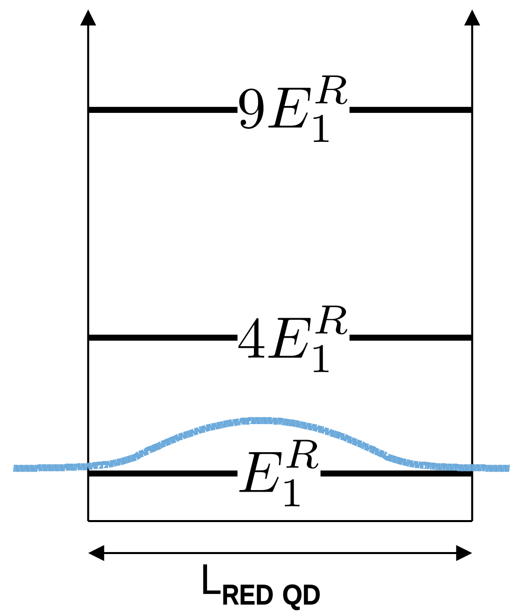


Photo by J. Halpert Courtesy of M. Bawendi Group, Chemistry, MIT

Determining QD energy using the Schrödinger Equation

$$E_1 = n^2 E_1 \qquad E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2}$$





Solutions to Schrodinger's Equation

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

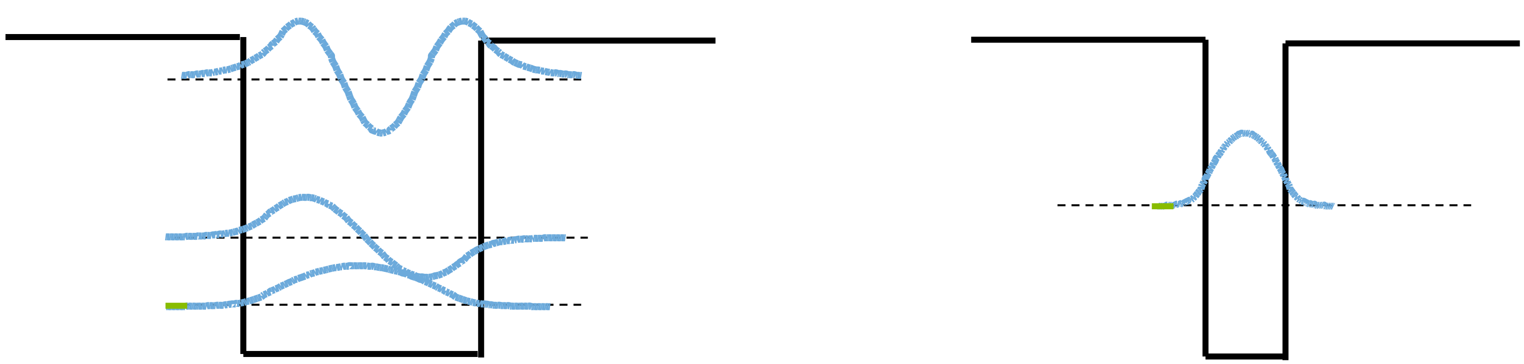
The kinetic energy of the electron is related to the curvature of the wavefunction

Tighter confinement → Higher energy

Even the lowest energy bound state requires some wavefunction curvature (kinetic energy) to satisfy boundary conditions

Nodes in wavefunction → Higher energy

The n-th wavefunction (eigenstate) has (n-1) zero-crossings



The Wavefunction

- $|\psi|^2\, dx$ corresponds to a physically meaningful quantity –
  - the probability of finding the particle near x
- $\left|\psi^* \frac{d\psi}{dx}\right| dx$ is related to the momentum probability density -
  - the probability of finding a particle with a particular momentum

PHYSICALLY MEANINGFUL STATES MUST HAVE THE FOLLOWING PROPERTIES:

ψ(x) must be single-valued, and finite

(finite to avoid infinite probability density)

ψ(x) must be continuous, with finite dψ/dx

(because dψ/dx is related to the momentum density)

In regions with finite potential, dψ/dx must be continuous

(with finite $d^2\psi/dx^2$, to avoid infinite energies)

There is usually no significance to the overall *sign* of ψ(x)

(it goes away when we take the absolute square)

(In fact, ψ(x,t) is usually complex !)

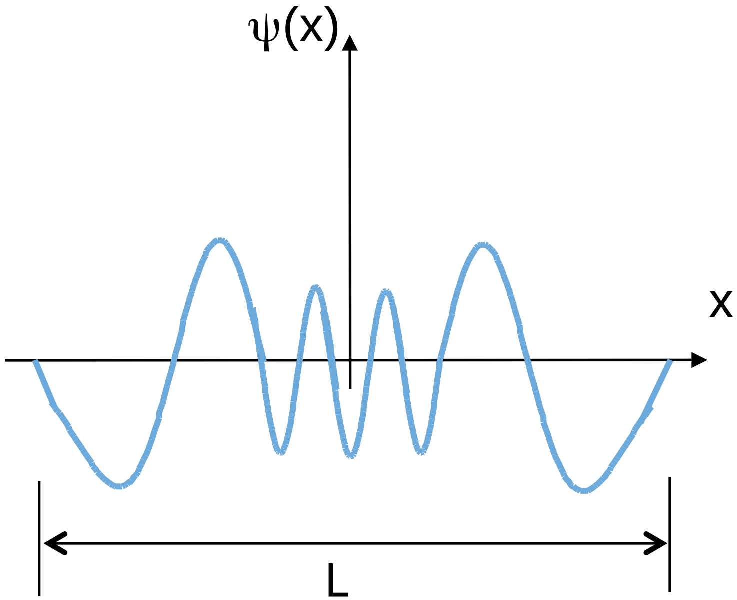
Solutions to Schrodinger's Equation

In what energy level is the particle? n = ...

(a) 7

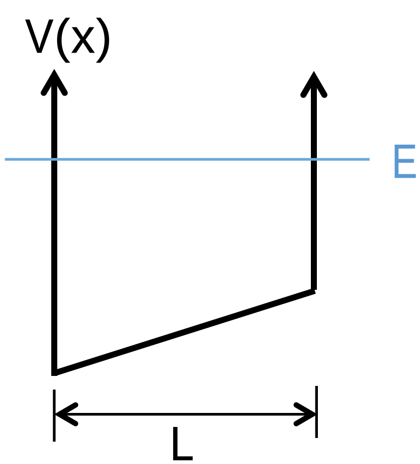
(b) 8

(c) 9

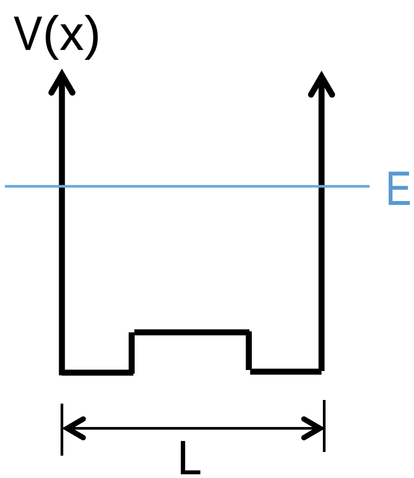


What is the approximate shape of the potential V(x) in which this particle is confined?

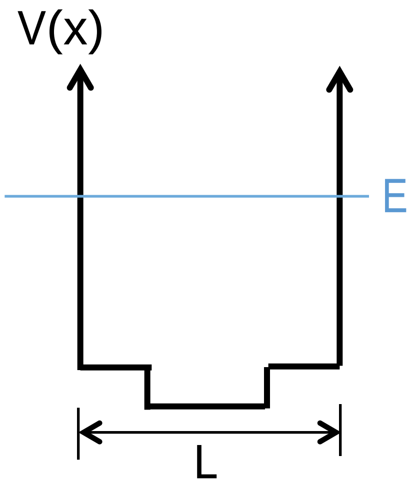
(a)



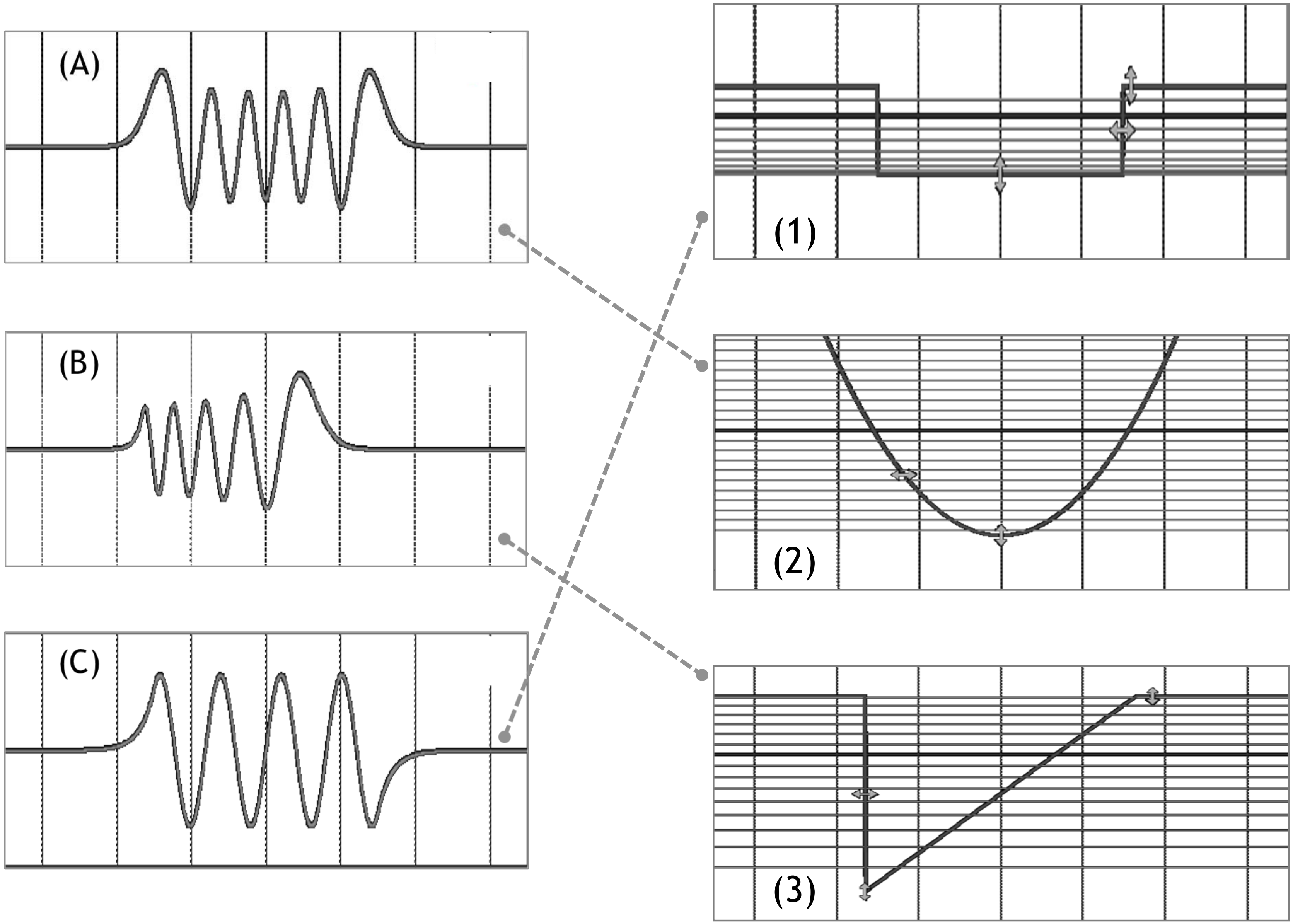
(b)



(c)



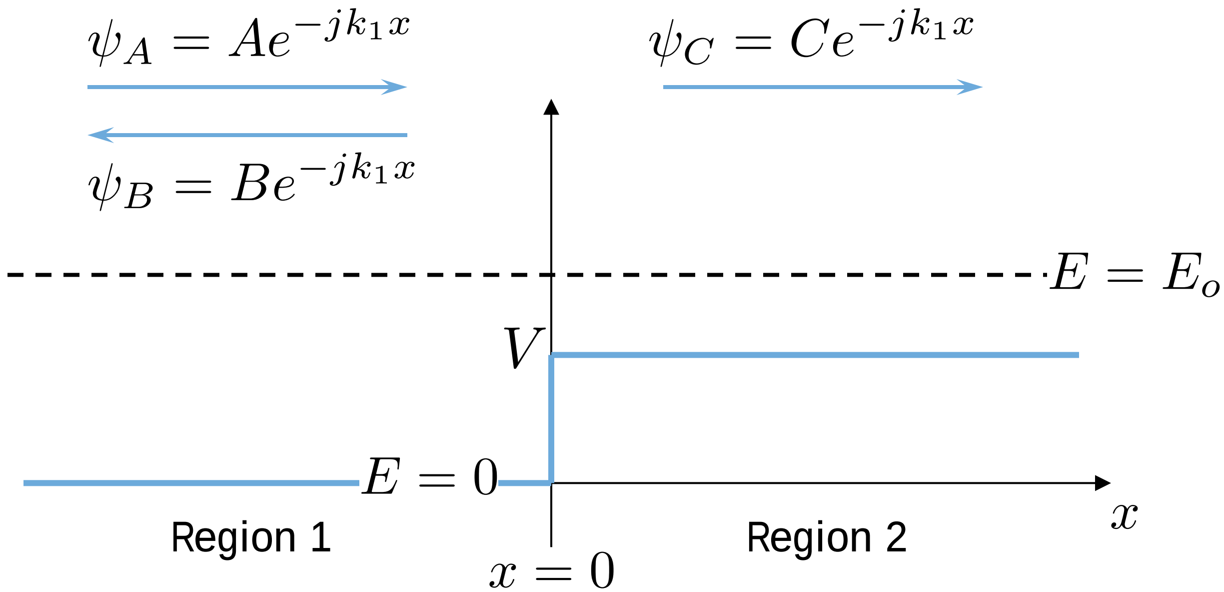
WHICH <u>WAVEFUNCTION</u> CORRESPONDS TO WHICH <u>POTENTIAL WELL</u> ?



NOTICE THAT FOR **<u>FINITE POTENTIAL WELLS</u>** WAVEFUNCTIONS ARE **<u>NOT ZERO</u>** AT THE WELL BOUNDARY

A Simple Potential Step

CASE I : $E_o > V$



In Region 1:

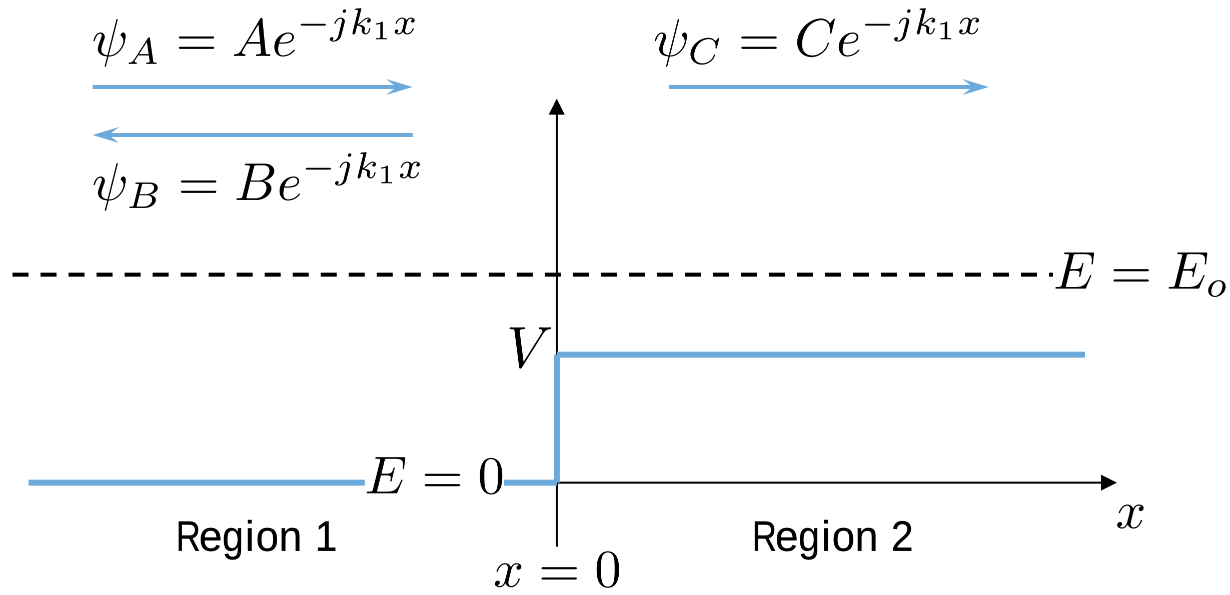
$$E_o\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \Rightarrow k_1^2 = \frac{2mE_o}{\hbar^2}$$

In Region 2:

$$(E_o - V)\,\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \Rightarrow k_2^2 = \frac{2m\,(E_o - V)}{\hbar^2}$$

A Simple Potential Step

CASE I : $E_o > V$



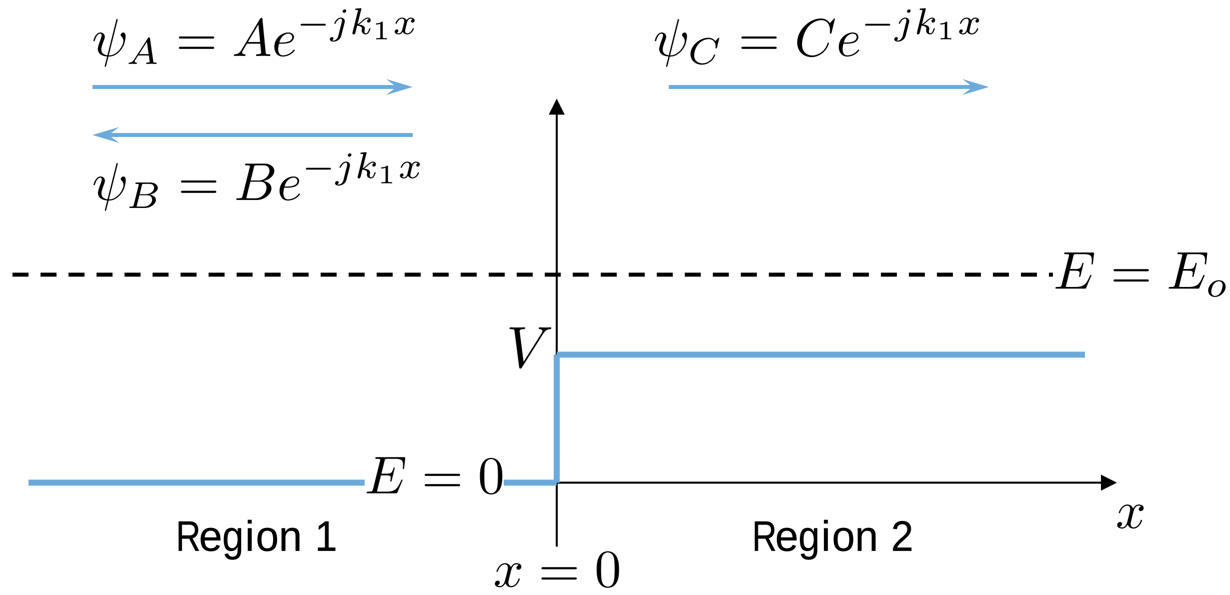
$$\psi_1 = Ae^{-jk_1x} + Be^{jk_1x} \qquad \psi_2 = Ce^{-jk_2x}$$

ψ is continuous: $\psi_1(0) = \psi_2(0)$ ⇒ $A + B = C$

$\frac{\partial \psi}{\partial x}$ is continuous: $\frac{\partial}{\partial x}\psi(0) = \frac{\partial}{\partial x}\psi_2(0)$ ⇒ $A - B = \frac{k_2}{k_1}C$

A Simple Potential Step

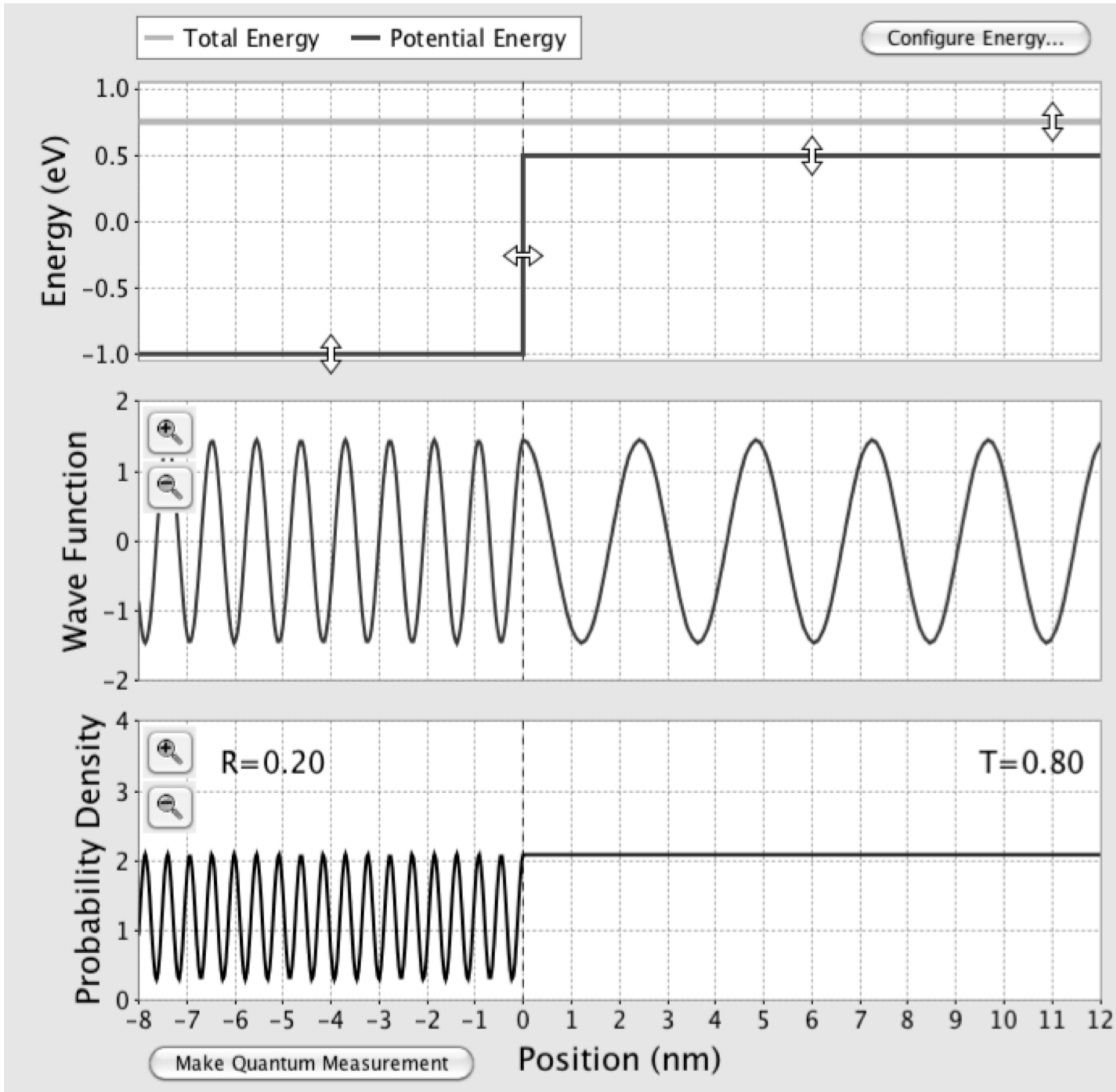
CASE I : $E_o > V$



$$\begin{cases} A + B = C \\ A - B = \dfrac{k_2}{k_1} C \end{cases}$$

$$\frac{B}{A} = \frac{1 - k_2/k_1}{1 + k_2/k_1} = \frac{k_1 - k_2}{k_1 + k_2}$$

$$\frac{C}{A} = \frac{2}{1 + k_2/k_1} = \frac{2k_1}{k_1 + k_2}$$



Example from: http://phet.colorado.edu/en/get-phet/one-at-a-time

Quantum Electron Currents

Given an electron of mass m

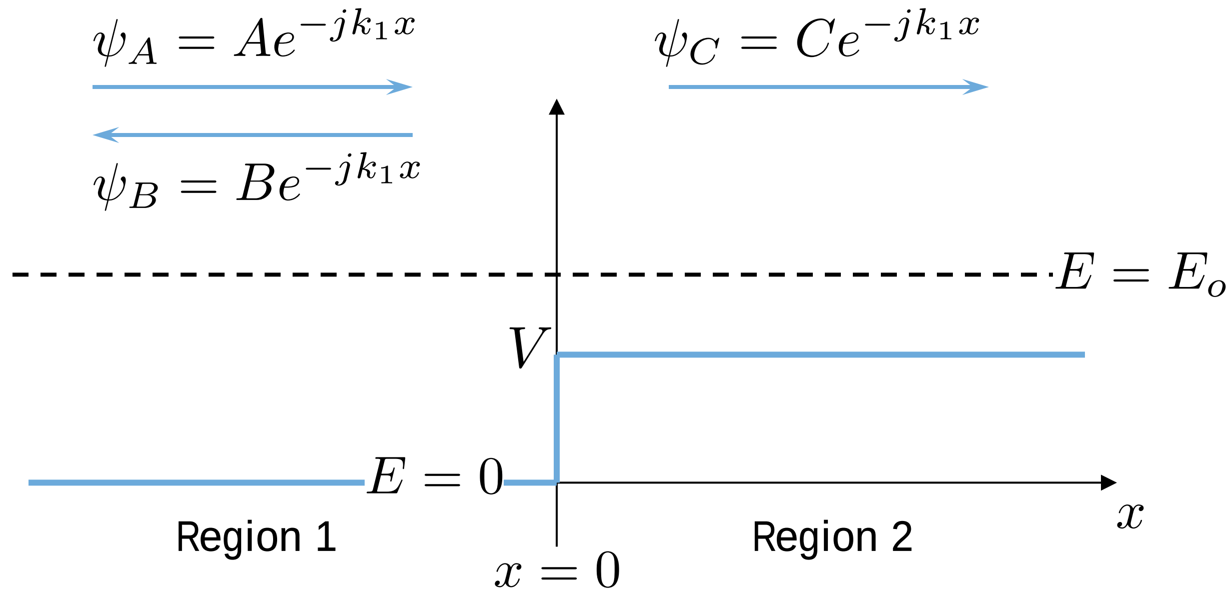
that is located in space with charge density $\rho = q \left|\psi(x)\right|^2$

and moving with momentum $< p >$ corresponding to $< v >= \hbar k/m$

... then the current density for a *single electron* is given by

$$J = \rho v = q \left|\psi\right|^2 (\hbar k/m)$$

A Simple Potential Step



CASE I : $E_o > V$

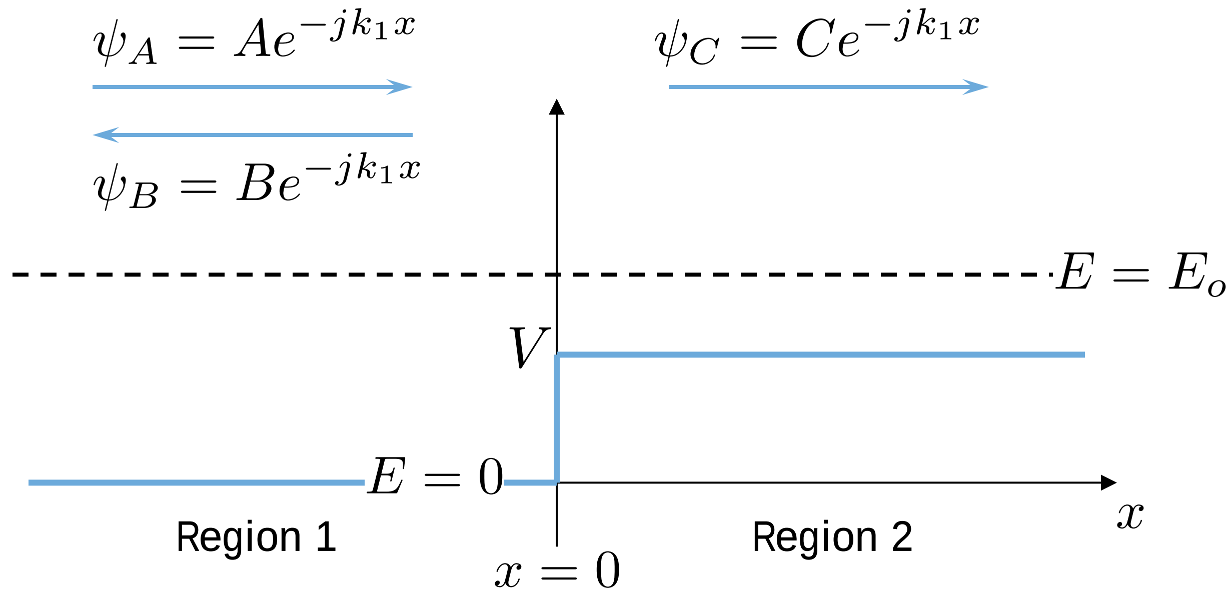
$$\text{Reflection} = R = \frac{J_{reflected}}{J_{incident}} = \frac{J_B}{J_A} = \frac{|\psi_B|^2(\hbar k_1/m)}{|\psi_A|^2(\hbar k_1/m)} = \left|\frac{B}{A}\right|^2$$

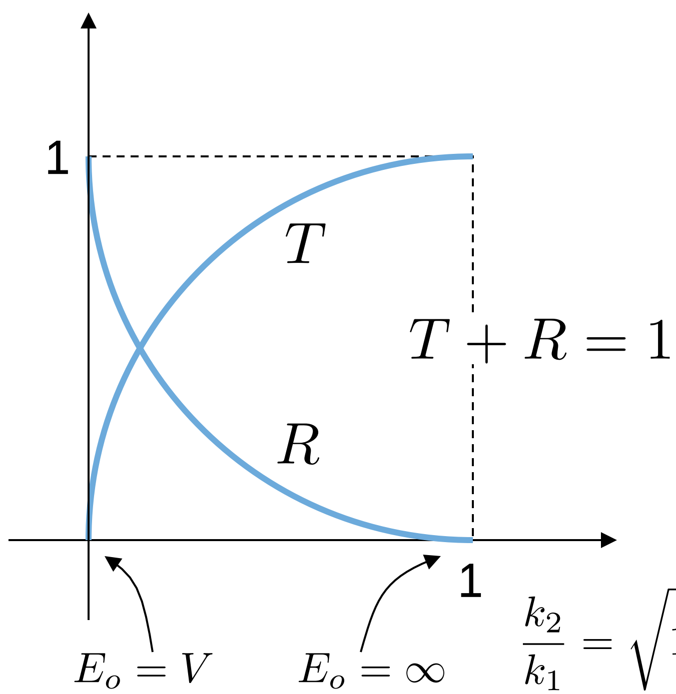
$$\text{Transmission} = T = \frac{J_{transmitted}}{J_{incident}} = \frac{J_C}{J_A} = \frac{|\psi_C|^2(\hbar k_2/m)}{|\psi_A|^2(\hbar k_1/m)} = \left|\frac{C}{A}\right|^2 \frac{k_2}{k_1}$$

$$\frac{B}{A} = \frac{1 - k_2/k_1}{1 + k_2/k_1} \qquad \frac{C}{A} = \frac{2}{1 + k_2/k_1}$$

A Simple Potential Step

CASE I : $E_o > V$



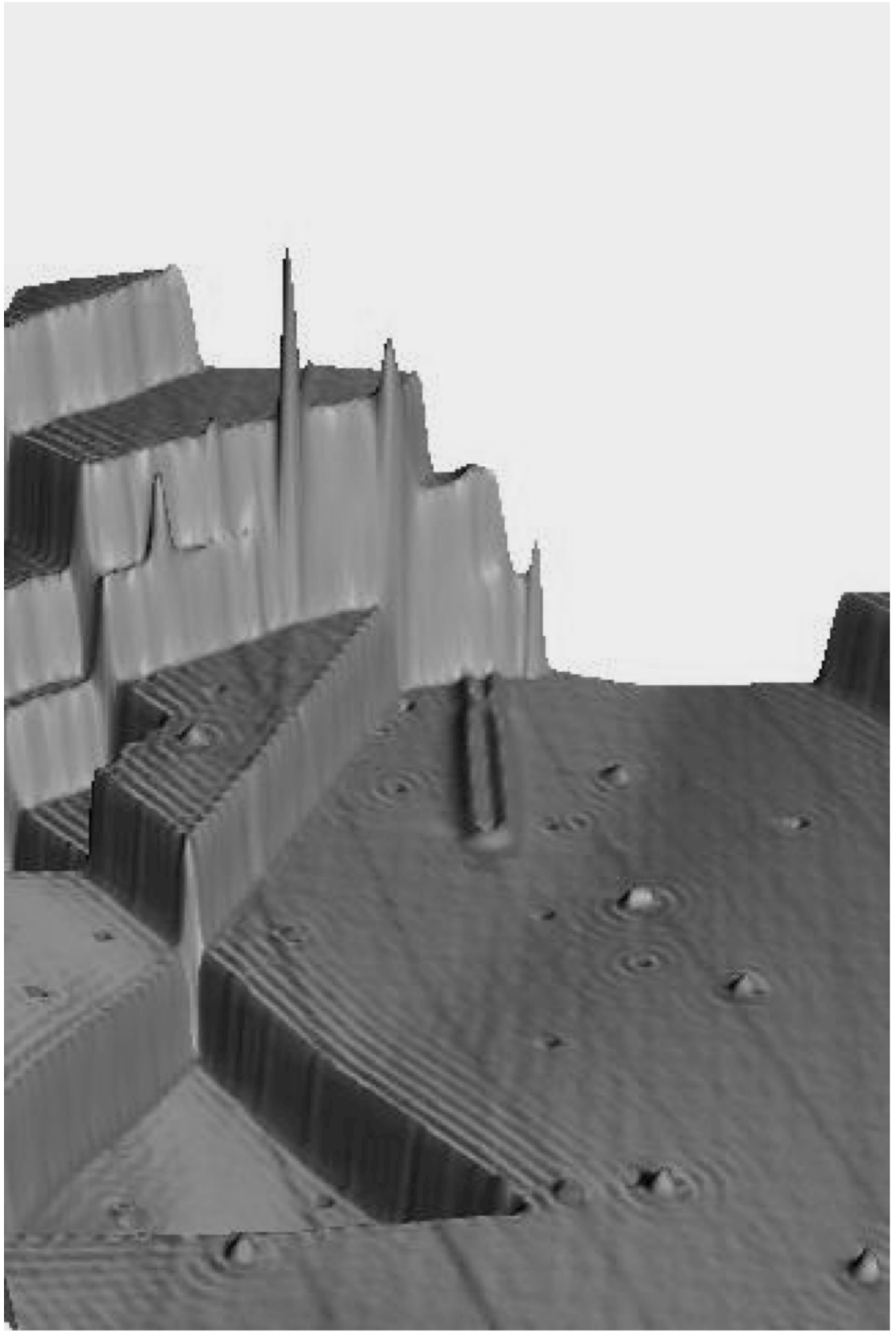


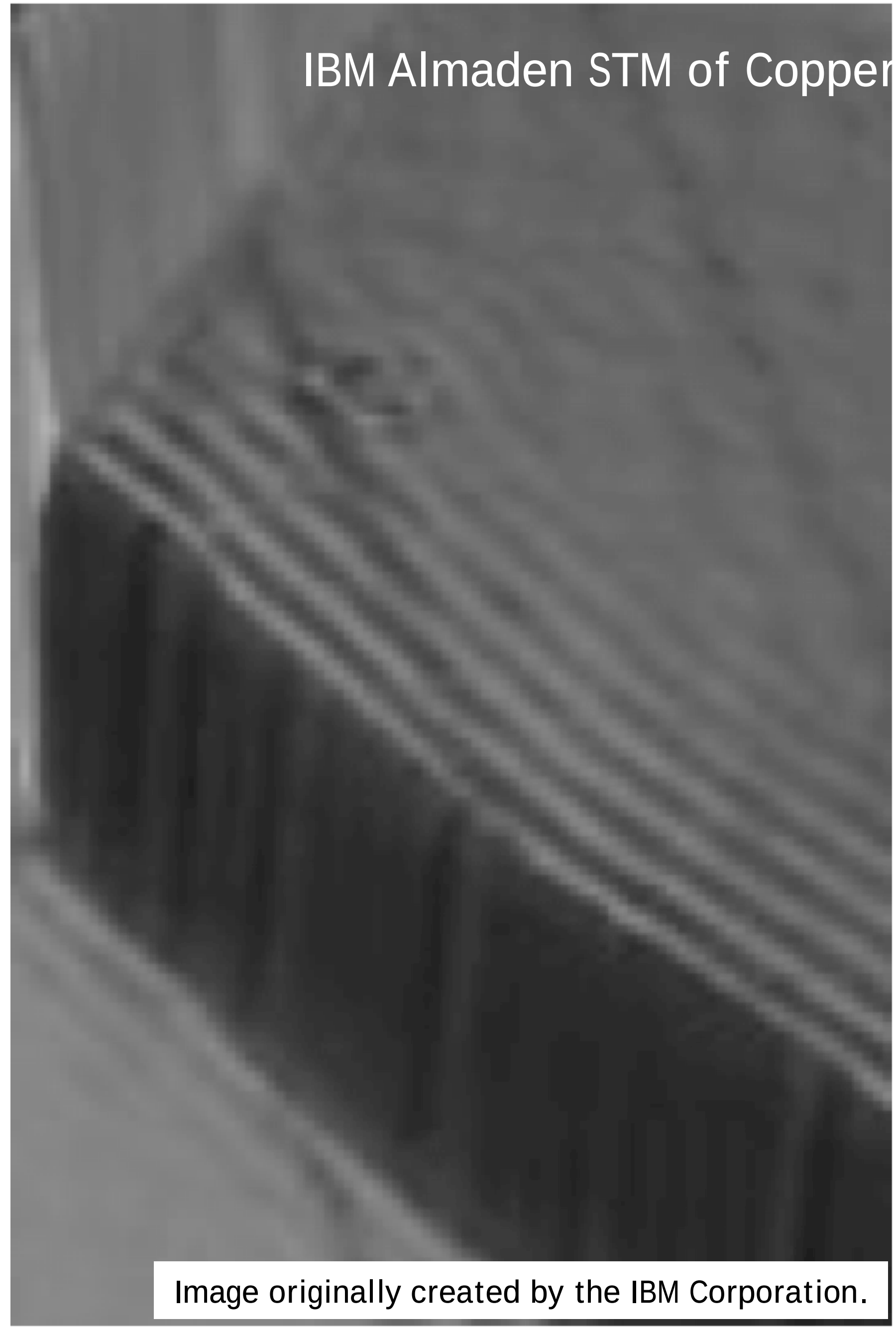
$$\frac{k_2}{k_1} = \sqrt{1 - \frac{V}{E_o}}$$

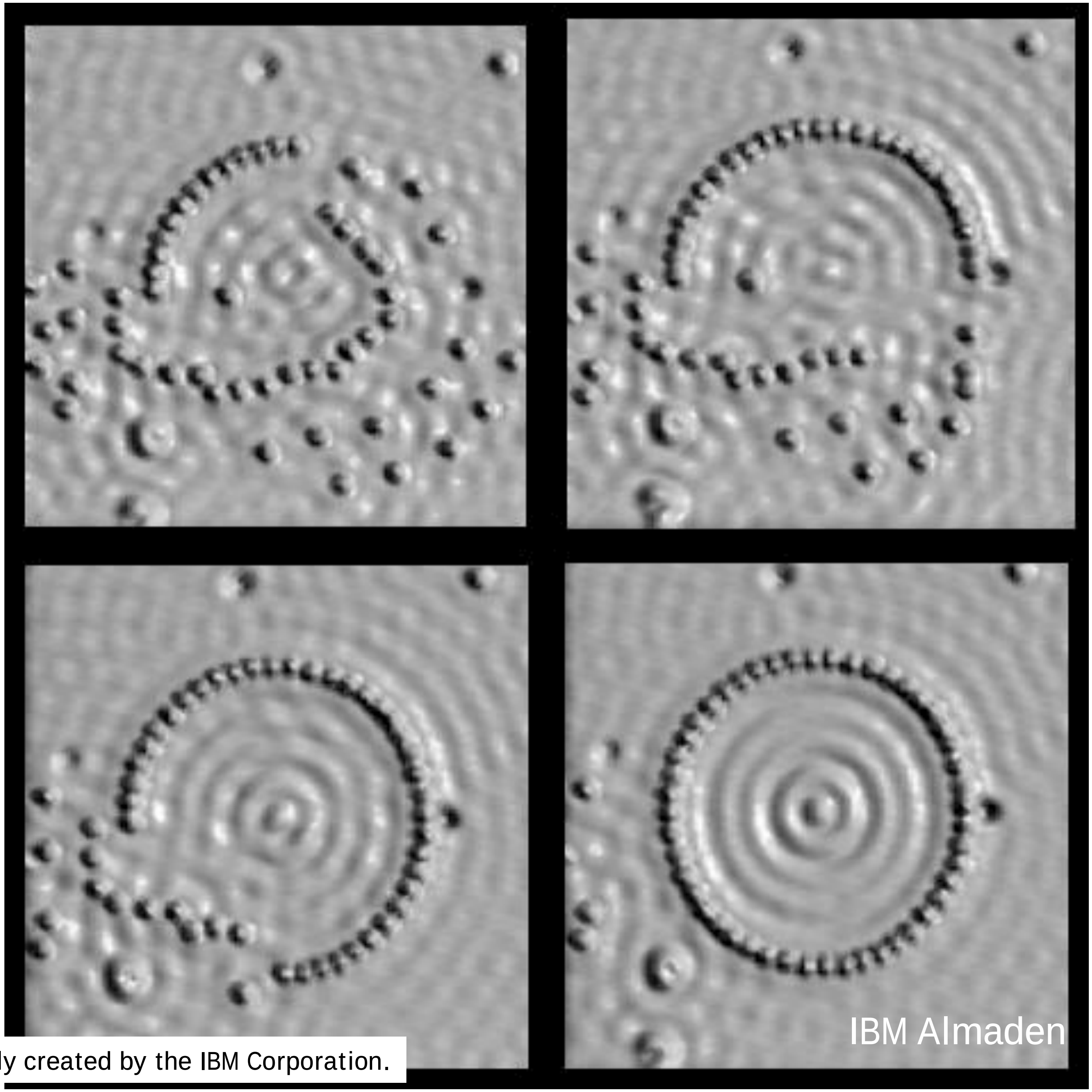
$$\text{Reflection} = R = \left|\frac{B}{A}\right|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2$$

$$\text{Transmission} = T = 1 - R$$

$$= \frac{4k_1k_2}{|k_1 + k_2|^2}$$




IBM Almaden STM of Copper
Image originally created by the IBM Corporation.



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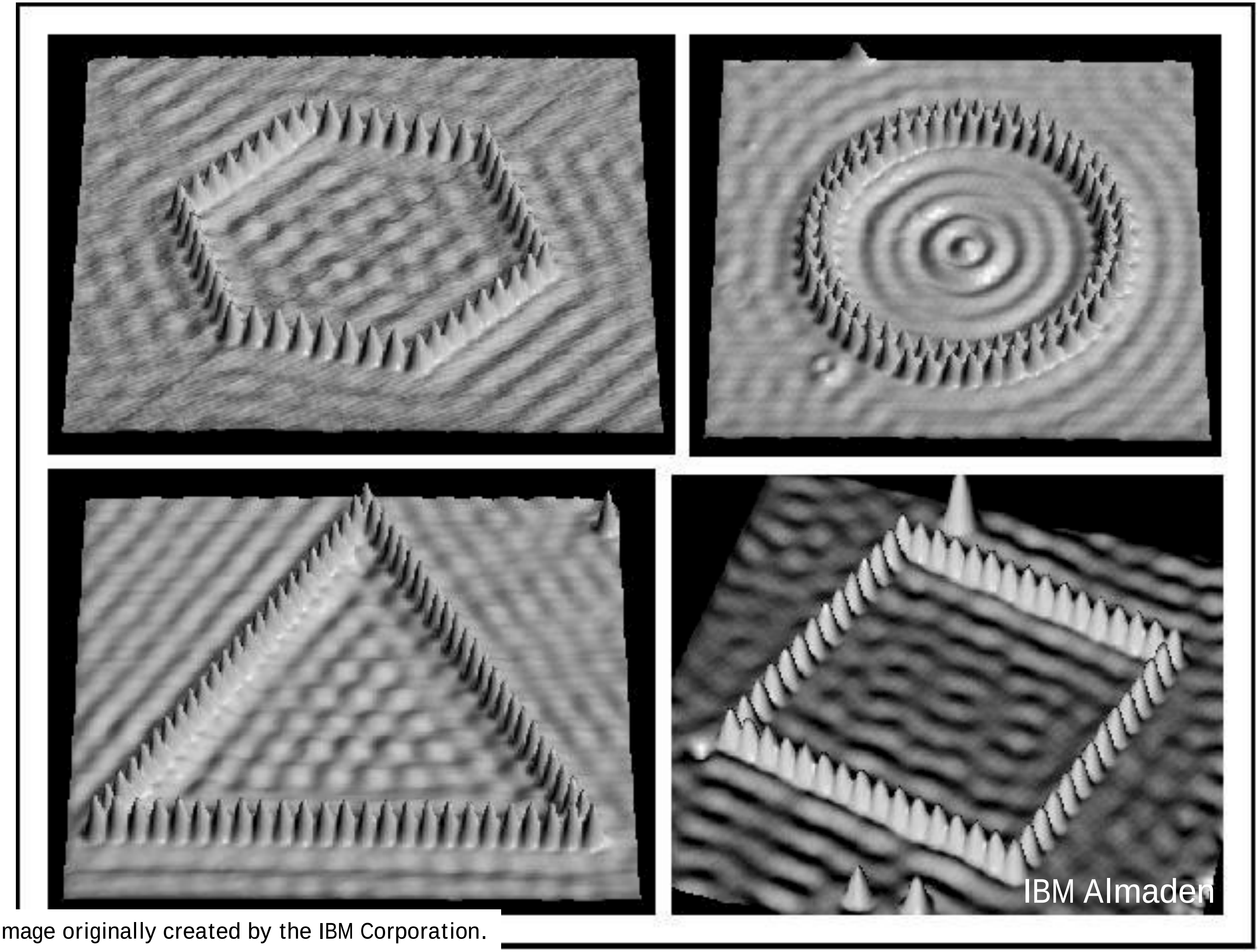

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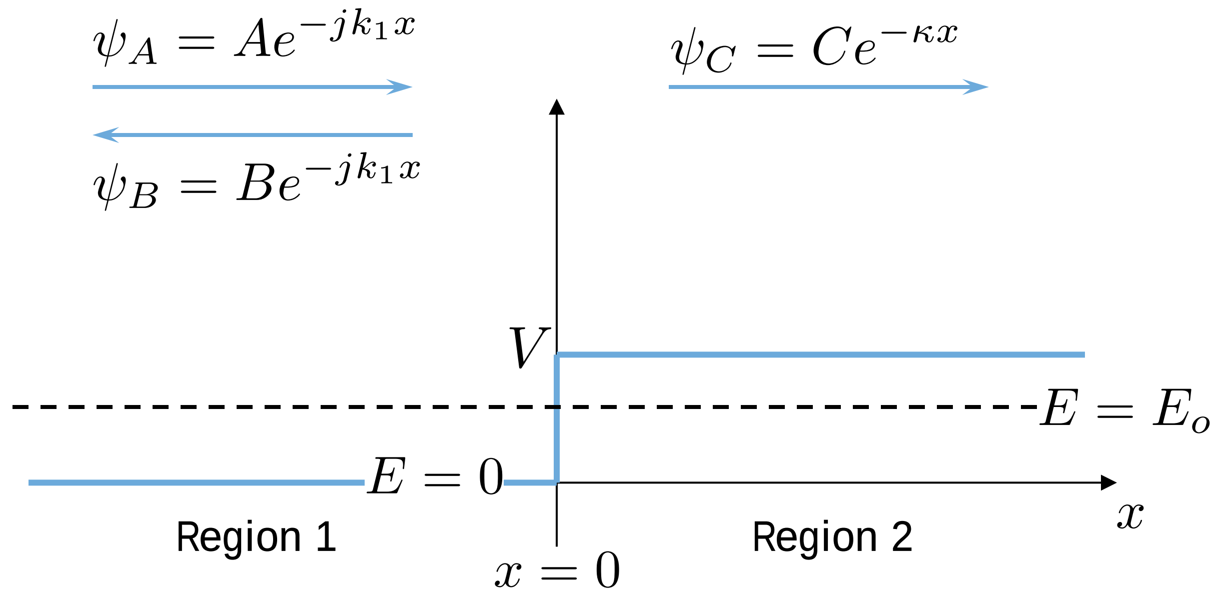
A Simple Potential Step

CASE II : $E_o < V$

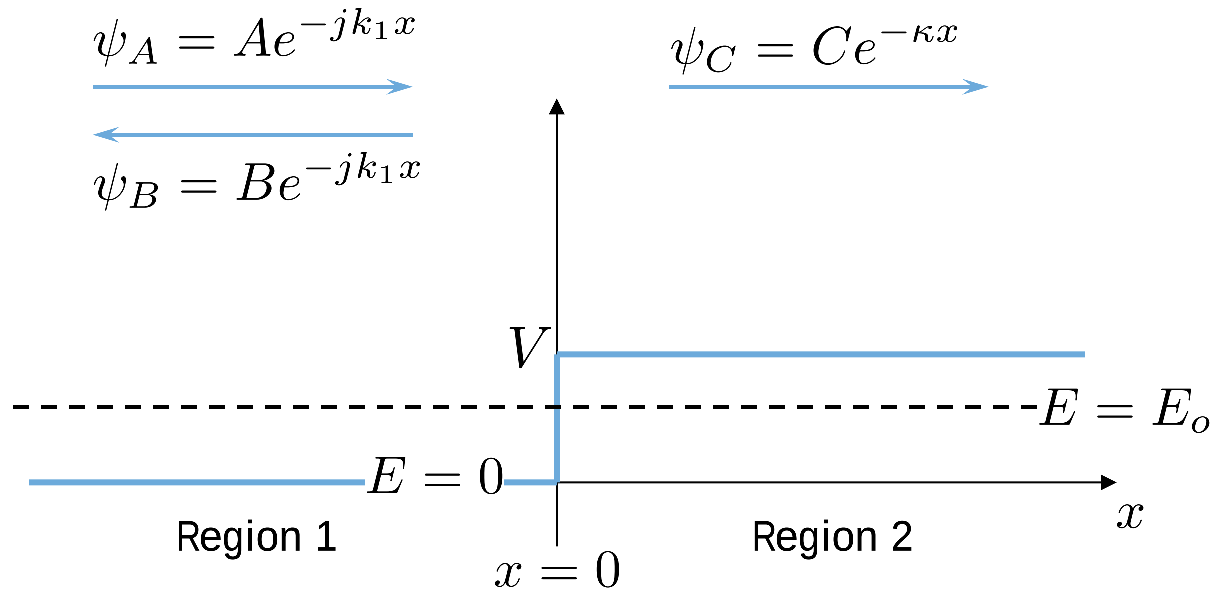


In Region 1:
$$E_o \psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \Rightarrow k_1^2 = \frac{2mE_o}{\hbar^2}$$

In Region 2:
$$\left(E_o - V\right)\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \Rightarrow \kappa^2 = \frac{2m\left(E_o - V\right)}{\hbar^2}$$

A Simple Potential Step

CASE II : $E_o < V$



$$\psi_1 = Ae^{-jk_1 x} + Be^{jk_1 x} \qquad \psi_2 = Ce^{-\kappa x}$$

ψ is continuous: $\psi_1(0) = \psi_2(0) \Rightarrow A + B = C$

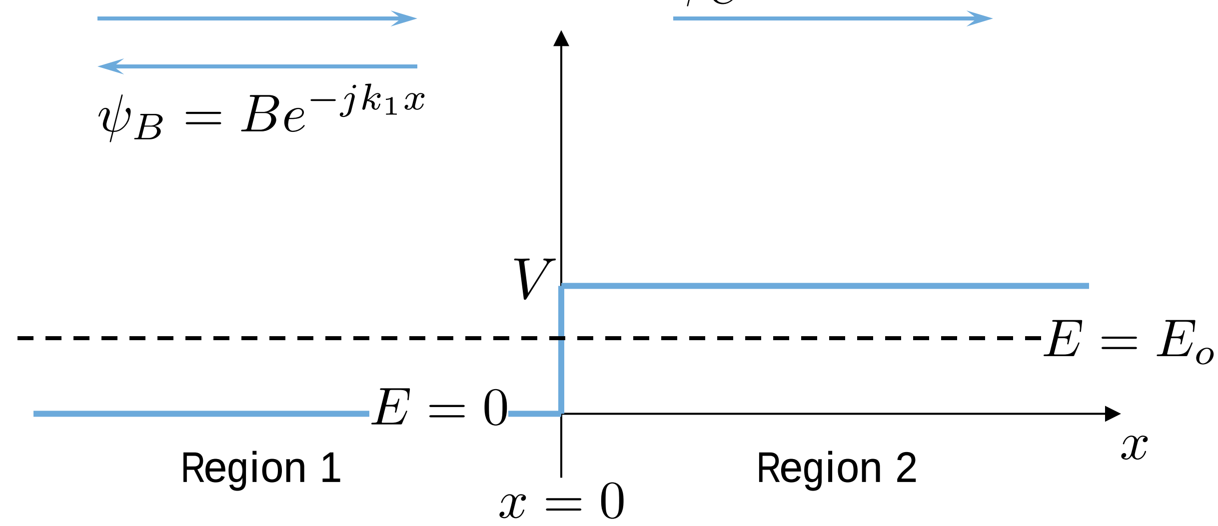
$\frac{\partial \psi}{\partial x}$ is continuous: $\frac{\partial}{\partial x}\psi(0) = \frac{\partial}{\partial x}\psi_2(0) \Rightarrow A - B = -j\frac{\kappa}{k_1}C$

A Simple Potential Step

$$\psi_A = Ae^{-jk_1 x}$$

$$\psi_C = Ce^{-\kappa x}$$

$$\psi_B = Be^{-jk_1 x}$$



CASE II : $E_o < V$

$$\begin{cases} A + B = C \\ A - B = -j\dfrac{\kappa}{k_1}C \end{cases}$$

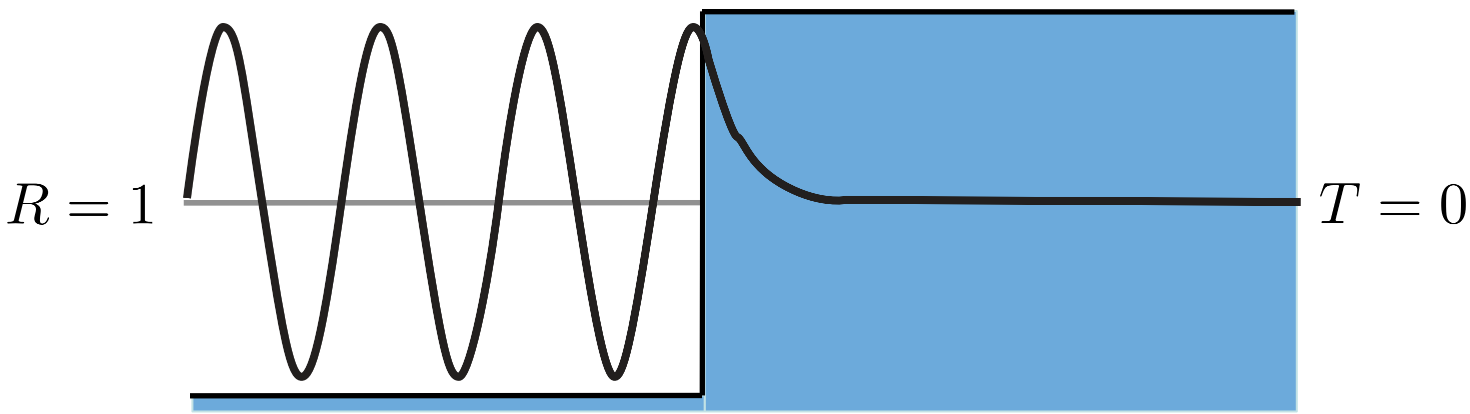
$$\frac{B}{A} = \frac{1 + j\kappa/k_1}{1 - j\kappa/k_1} \qquad \frac{C}{A} = \frac{2}{1 - j\kappa/k_1}$$

$$R = \left|\frac{B}{A}\right|^2 = 1 \qquad T = 0$$

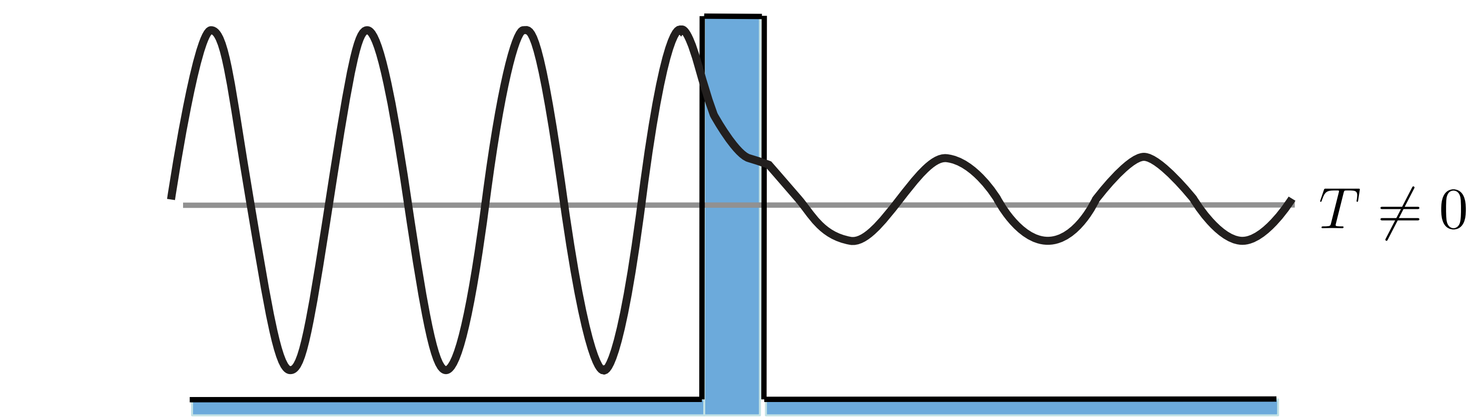
Total reflection → Transmission must be zero

Quantum Tunneling Through a Thin Potential Barrier

Total Reflection at Boundary



Frustrated Total Reflection (Tunneling)



KEY TAKEAWAYS

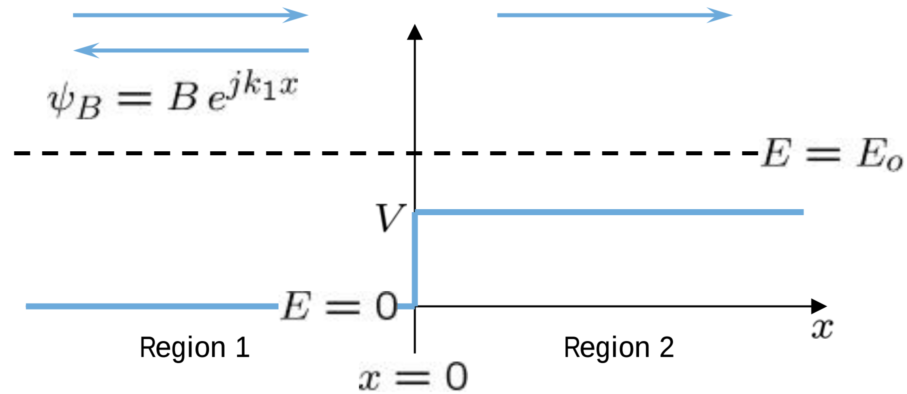
A Simple Potential Step

CASE I : $E_o > V$

$$\psi_A = A\, e^{-jk_1 x}$$

$$\psi_B = B\, e^{jk_1 x}$$

$$\psi_C = C\, e^{-jk_2 x}$$



$$Reflection = R = \left|\frac{B}{A}\right|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2$$

$$Transmission = T = 1 - R = \frac{4\, k_1 k_2}{|k_1 + k_2|^2}$$

PARTIAL REFLECTION

$$\psi_1 = A\, e^{-jk_1 x} + B\, e^{jk_1 x}$$

$$\psi_2 = C\, e^{-jk_2 x}$$

$$k_1^2 = \frac{2m\, E_o}{\hbar^2}$$

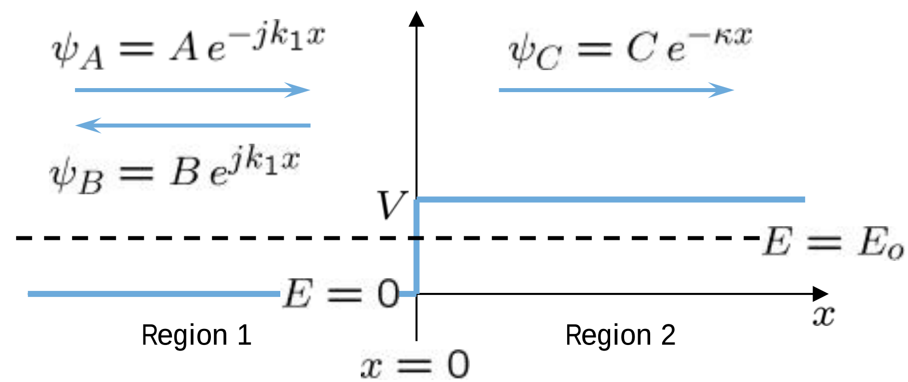
$$k_2^2 = \frac{2m\,(E_o - V)}{\hbar^2}$$

CASE II : $E_o < V$

$$\psi_A = A\, e^{-jk_1 x}$$

$$\psi_B = B\, e^{jk_1 x}$$

$$\psi_C = C\, e^{-\kappa x}$$



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

$$T = 0$$

TOTAL REFLECTION

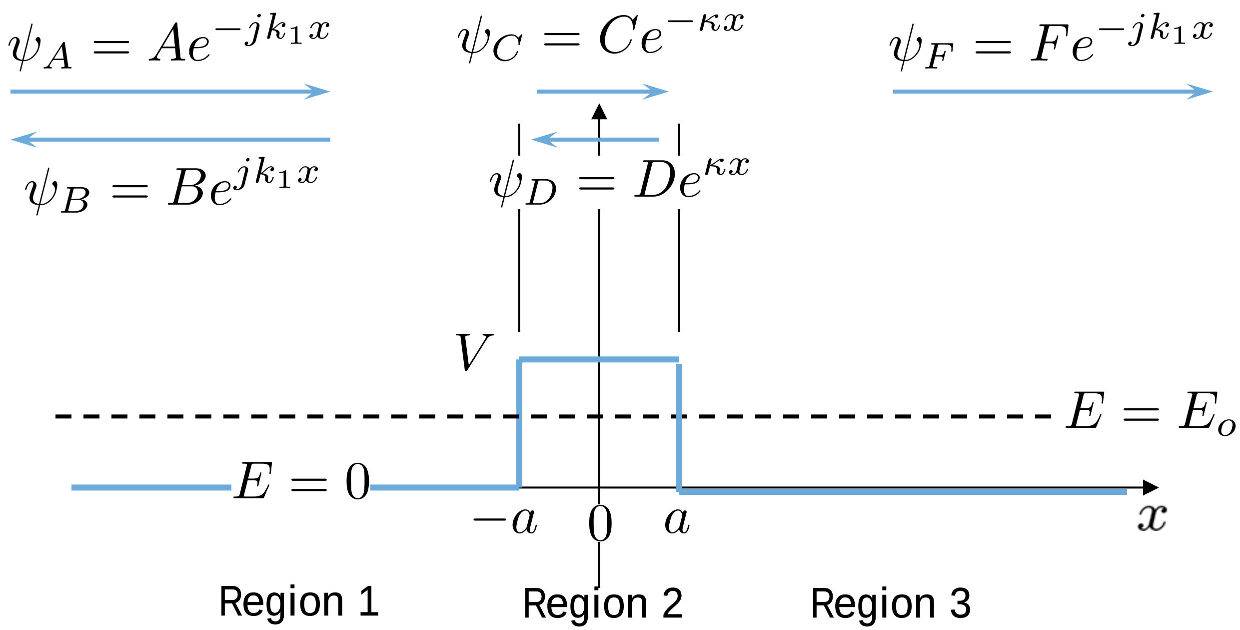
$$\psi_1 = A\, e^{-jk_1 x} + B\, e^{jk_1 x}$$

$$\psi_2 = C\, e^{-\kappa x}$$

$$k_1^2 = \frac{2m\, E_o}{\hbar^2}$$

$$\kappa^2 = \frac{2m\,(V - E_o)}{\hbar^2}$$

A Rectangular Potential Step



CASE II : $E_o < V$

In Regions 1 and 3:

$$E_o\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \quad \Rightarrow \quad k_1^2 = \frac{2mE_o}{\hbar^2}$$

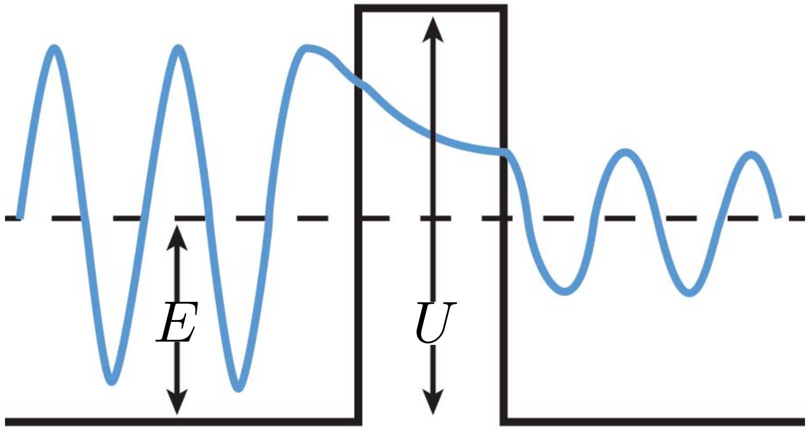
In Region 2:

$$(E_o - V)\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \quad \Rightarrow \quad \kappa^2 = \frac{2m(V - E_o)}{\hbar^2}$$

for $E_o < V$:

$$T = \left|\frac{F}{A}\right|^2 = \frac{1}{1 + \frac{1}{4}\frac{V^2}{E_o(V-E_o)}\sinh^2(2\kappa a)}$$

A Rectangular Potential Step



for $E_o < V$:

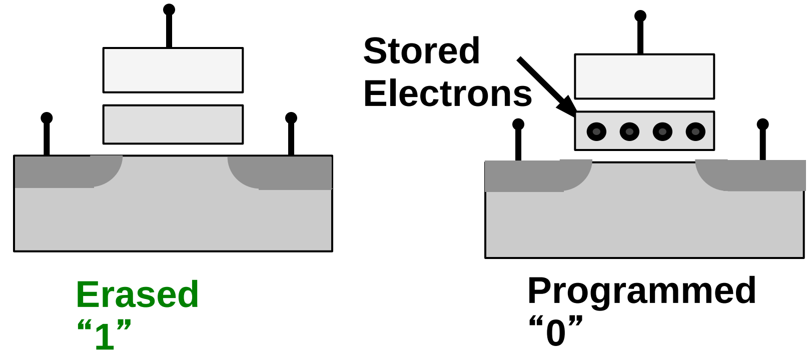
$$T = \left|\frac{F}{A}\right|^2 = \frac{1}{1 + \frac{1}{4}\frac{V^2}{E_o(V - E_o)}\sinh^2(2\kappa a)}$$

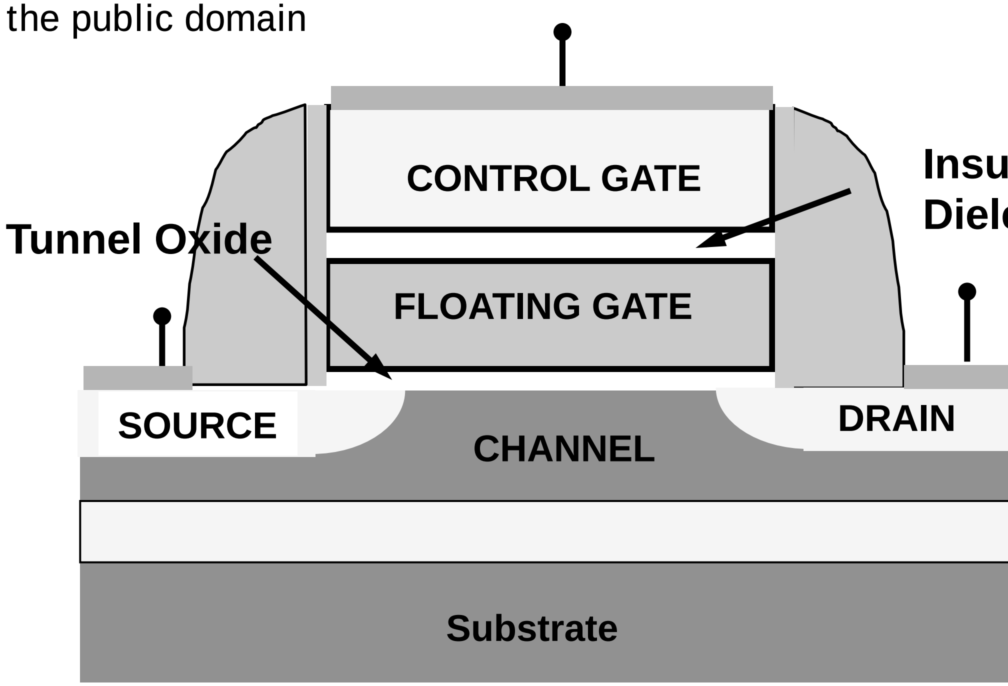
$$\sinh^2(2\kappa a) = \left[e^{2\kappa a} - e^{-2\kappa a}\right]^2 \approx e^{-4\kappa a}$$

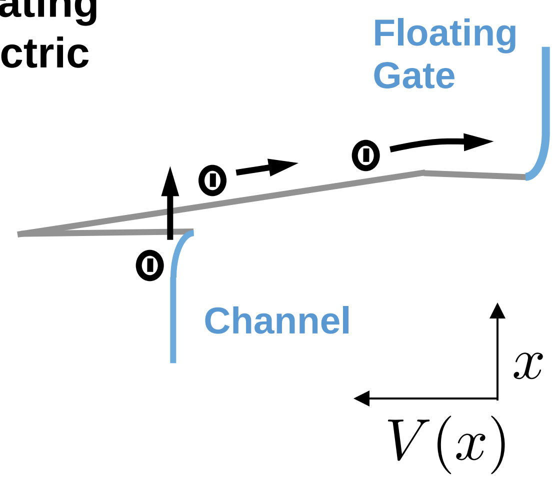
$$T = \left|\frac{F}{A}\right|^2 \approx \frac{1}{1 + \frac{1}{4}\frac{V^2}{E_o(V - E_o)}} e^{-4\kappa a}$$

Flash Memory

Image is in the public domain

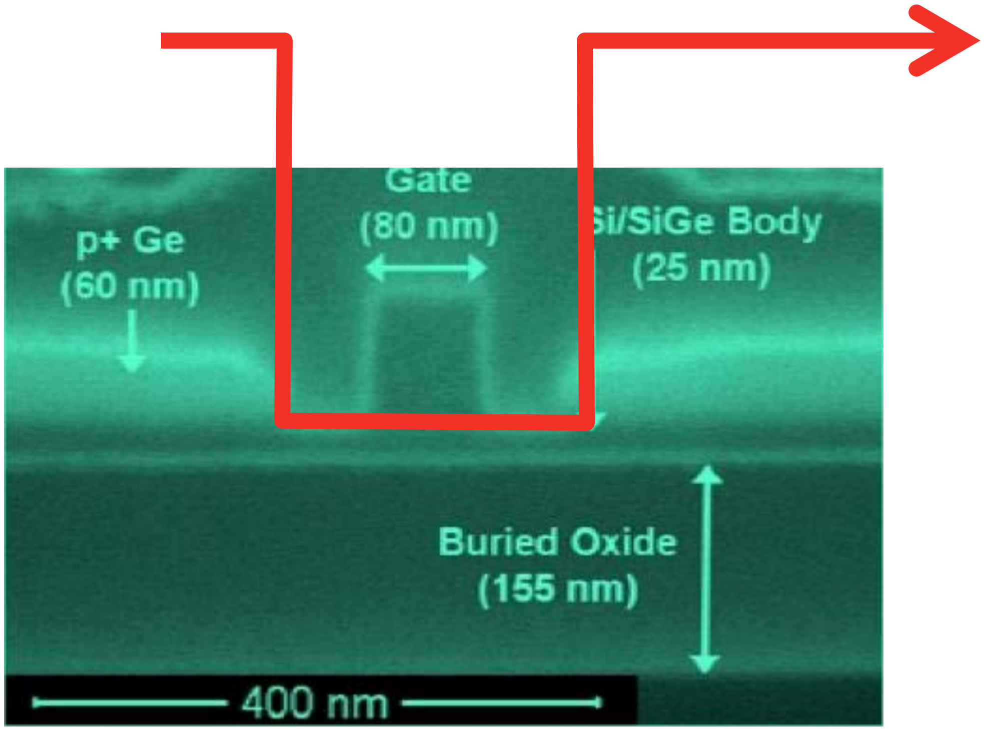






Electrons tunnel preferentially when a voltage is applied

MOSFET: Transistor in a Nutshell



Conduction electron flow

Image courtesy of J. Hoyt Group, EECS, MIT. Photo by L. Gomez

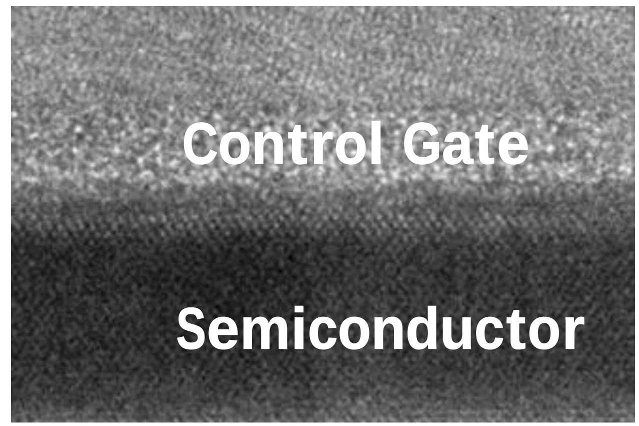


Image courtesy of J. Hoyt Group, EECS, MIT
Photo by L. Gomez

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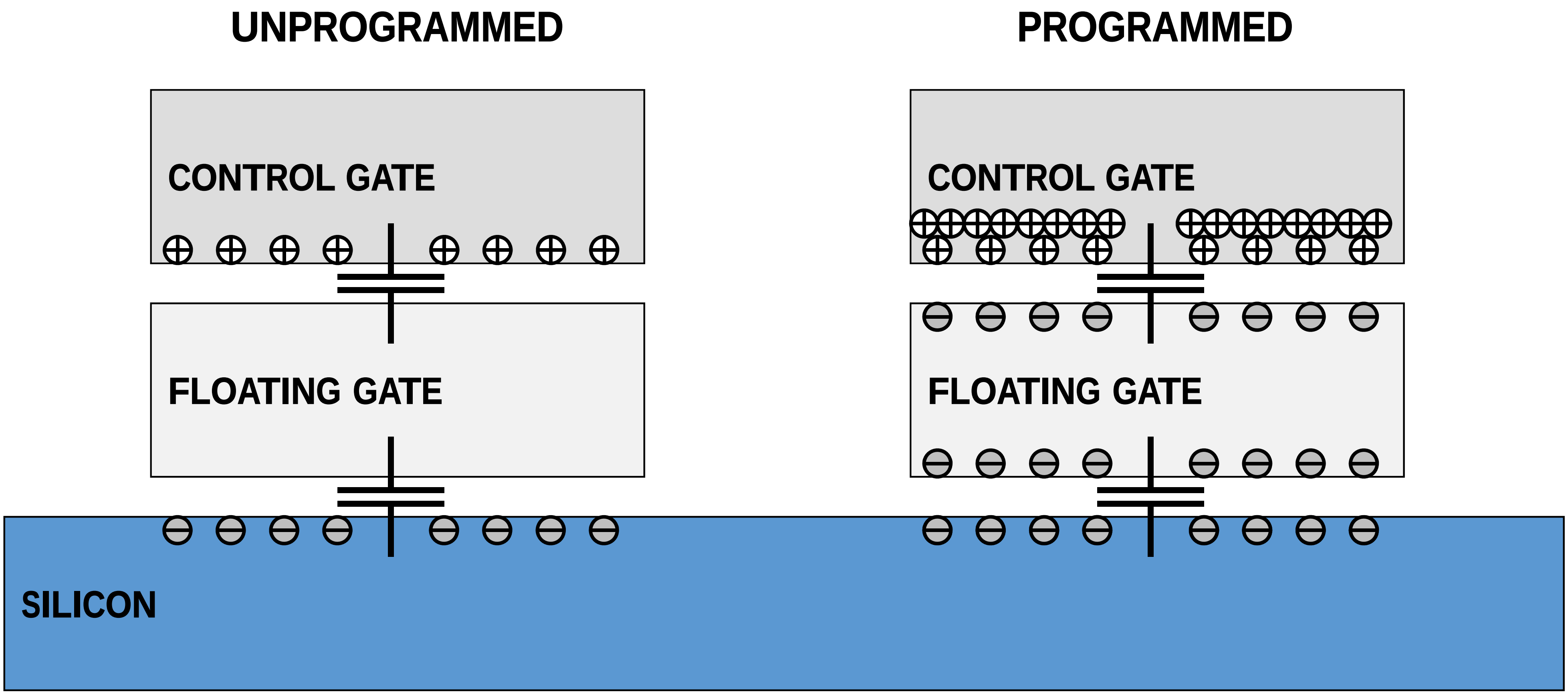
Tunneling causes thin insulating layers
to become leaky !

Reading Flash Memory



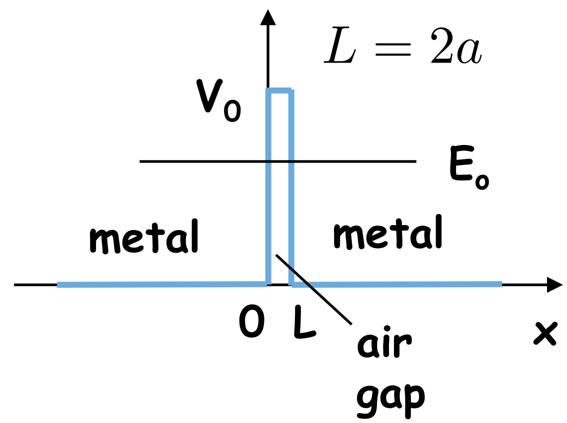
To obtain the same channel charge, the programmed gate needs a higher control-gate voltage than the unprogrammed gate

How do we WRITE Flash Memory ?

Example: Barrier Tunneling

- Let's consider a tunneling problem:

An electron with a total energy of E_o= 6 eV approaches a potential barrier with a height of V_0 = 12 eV. If the width of the barrier is L = 0.18 nm, what is the probability that the electron will tunnel through the barrier?



$$T = \left|\frac{F}{A}\right|^2 \approx \frac{16E_o(V - E_o)}{V^2} e^{-2\kappa L}$$

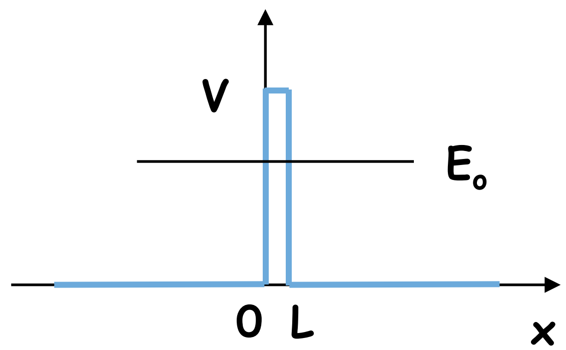
$$\kappa = \sqrt{\frac{2m_e}{\hbar^2}(V - E_o)} = 2\pi\sqrt{\frac{2m_e}{h^2}(V - E_o)} = 2\pi\sqrt{\frac{6\text{eV}}{1.505\text{eV-nm}^2}} \approx 12.6\ \text{nm}^{-1}$$

$$T = 4e^{-2(12.6\ \text{nm}^{-1})(0.18\ \text{nm})} = 4(0.011) = \boxed{4.4\%}$$

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

Multiple Choice Questions

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 particles that have successfully "escaped"?

   a. < initial energy

   b. = initial energy (boxed)

   c. > initial energy

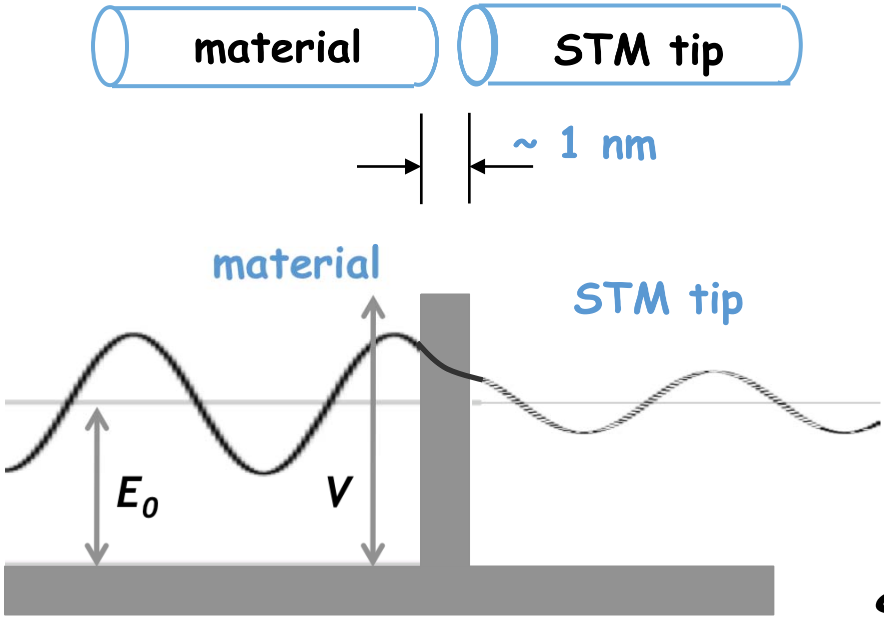
Although the *amplitude* of the wave is smaller after the barrier, no energy is lost in the tunneling process

Application of Tunneling:

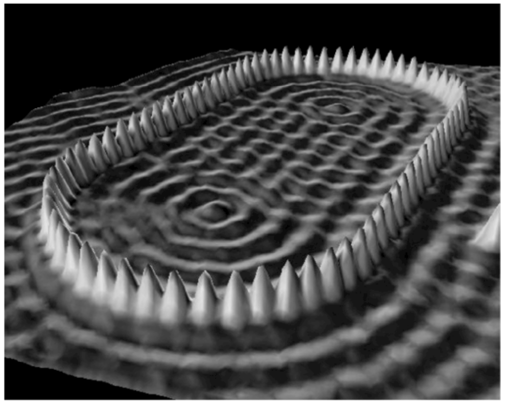
Scanning Tunneling Microscopy (STM)

Due to the quantum effect of "barrier penetration," the electron density of a material extends beyond its surface:

One can exploit this to measure the electron density on a material's surface:



Sodium atoms on metal:



STM images

Image originally created by IBM Corporation

Single walled carbon nanotube:

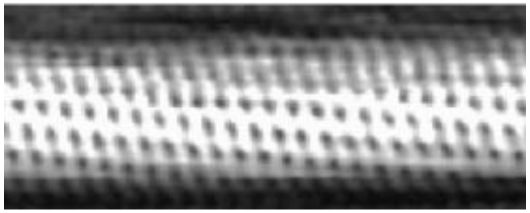


Image is in the public domain

6.007 Electromagnetic Energy: From Motors to Lasers
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