Lecture 12: Schrödinger Equation

Outline

- Wave Equations from ω-k Relations
- Schrodinger Equation
- The Wavefunction
- Particle in a box
- Reflection and transmission at a potential step
- Barrier Penetration (tunneling)

TRUE / FALSE

1. The momentum p of a photon is proportional to its wavevector k. ____
2. The energy E of a photon is proportional to its phase velocity v_p. ____
3. We do not experience the wave nature of matter in everyday life because the wavelengths are too small. ____

Photon Momentum

IN FREE SPACE:

$$E = cp \Rightarrow p = \frac{E}{c} = \frac{\hbar\omega}{c} = \hbar k$$

IN OPTICAL MATERIALS:

$$E = v_p p \Rightarrow p = \frac{E}{v_p} = \frac{\hbar\omega}{v_p} = \hbar k_{vac} n$$

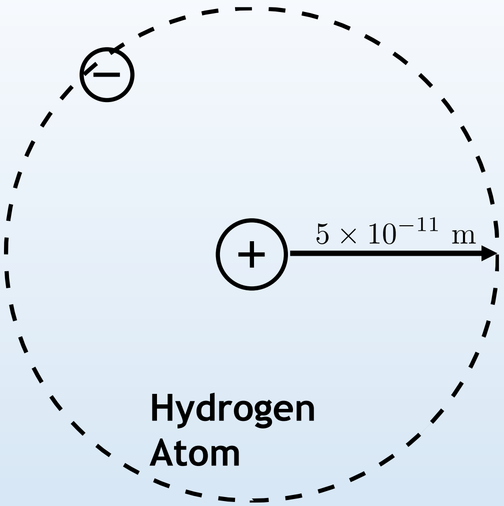
Heisenberg's Uncertainty Principle

uncertainty
in momentum

$$\Delta x \Delta p \geq \frac{h}{4\pi} = \frac{\hbar}{2}$$

uncertainty
in position

The more accurately you know the position (i.e., the smaller Δx is), the less accurately you know the momentum (i.e., the larger Δp is); and vice versa



Consider a single hydrogen atom:

an electron of *charge* = -*e* free to move around in the electric field of a fixed proton of *charge* = +*e* (proton is ~2000 times heavier than electron, so we consider it fixed).

The electron has a potential energy due to the attraction to proton of:

$$V(r) = -\frac{e^2}{4\pi\epsilon_o r}$$

where *r* is the electron-proton separation

The electron has a kinetic energy of $K.E. = \frac{1}{2}mv^2 = \frac{p^2}{2m}$

The total energy is then

$$E(r) = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_o r}$$

Classically, the minimum energy of the hydrogen atom is $-\infty$

the state in which the electron is on top of the proton → p = 0, r = 0.

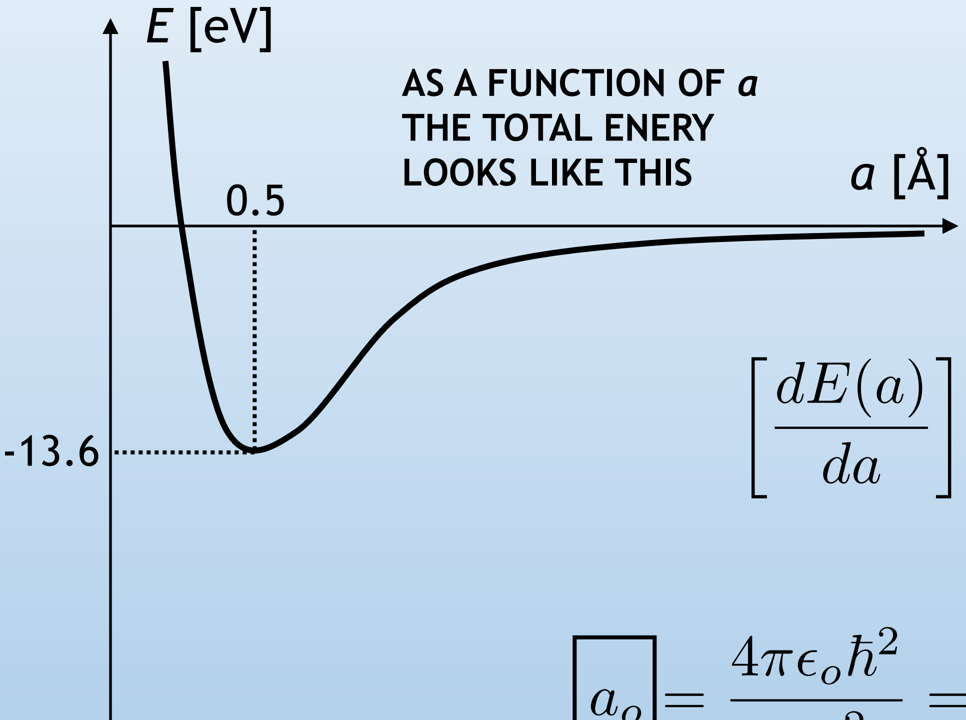
Quantum mechanically, the uncertainty principle forces the electron to have non-zero momentum and non-zero expectation value of position.

If ***a*** is an average distance electron-proton distance,
the uncertainty principle informs us that the minimum electron momentum is on the order of ***ħ/a***.

The energy as a function of ***a*** is then:

$$E(a) = \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\epsilon_o a}$$

The minimum energy state, quantum mechanically, can be estimated by calculating the value of $a=a_o$ for which $E(a)$ is minimized:



$$E(a) = \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\epsilon_o a}$$

$$\left[\frac{dE(a)}{da}\right]_{a_o} = -\frac{\hbar^2}{ma_o^3} + \frac{e^2}{4\pi\epsilon_o a_o^2} = 0$$

$$\boxed{a_o} = \frac{4\pi\epsilon_o\hbar^2}{me^2} = \frac{10^{-10}\cdot 10^{-68}}{10^{-30}\cdot 2\cdot 10^{-38}} m \approx \boxed{0.5\ \mathring{A}}$$

By preventing localization of the electron near the proton, the Uncertainty Principle

RETARDS THE CLASSICAL COLLAPSE OF THE ATOM,

PROVIDES THE CORRECT DENSITY OF MATTER,

and YIELDS THE PROPER BINDING ENERGY OF ATOMS

One might ask:
"If light can behave like a particle, might particles act like waves"?

YES !
Particles, like photons, also have a wavelength given by:

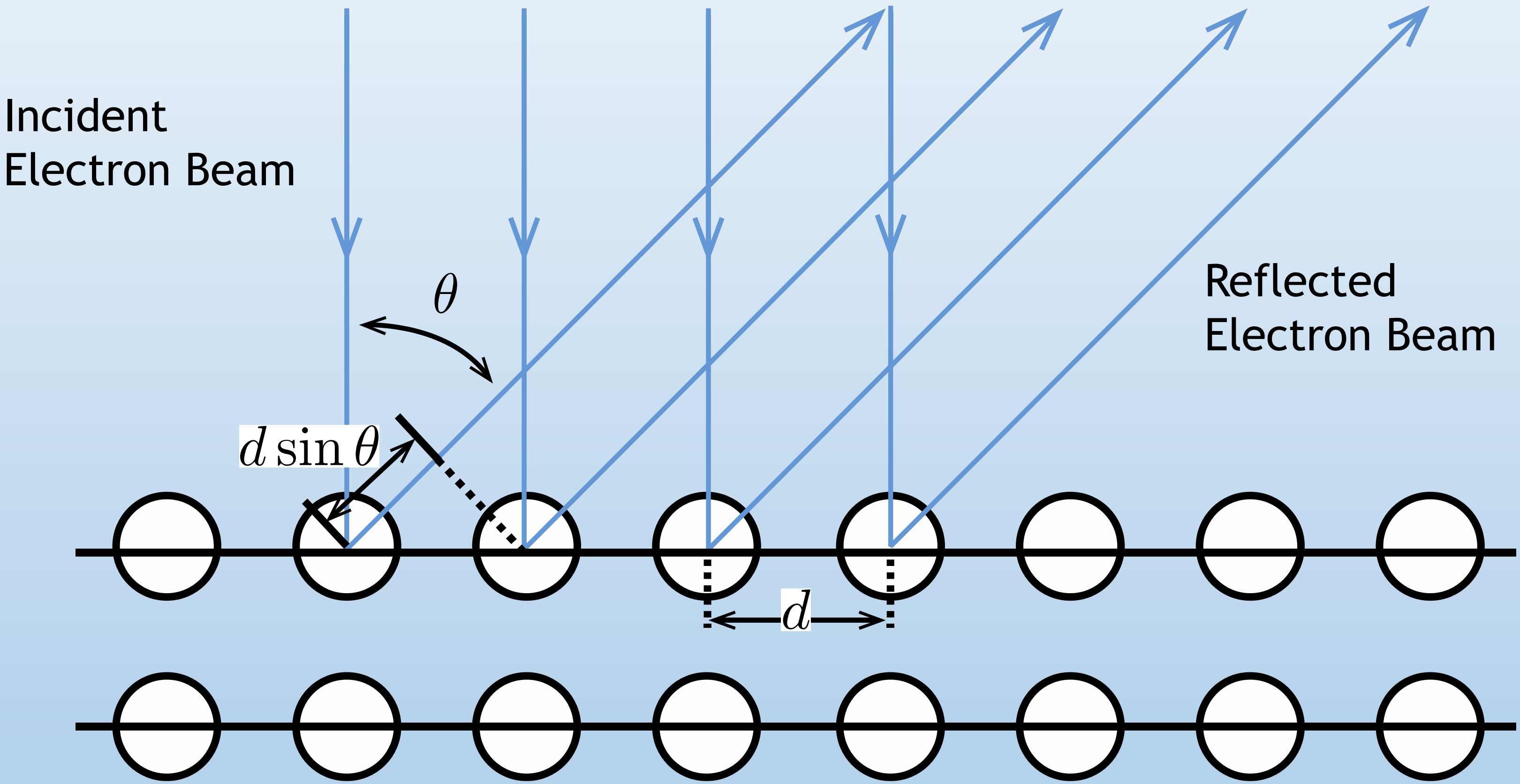
$$\boxed{\lambda = h/p = h/mv}$$

de Broglie wavelength

The wavelength of a particle depends on its momentum, just like a photon!

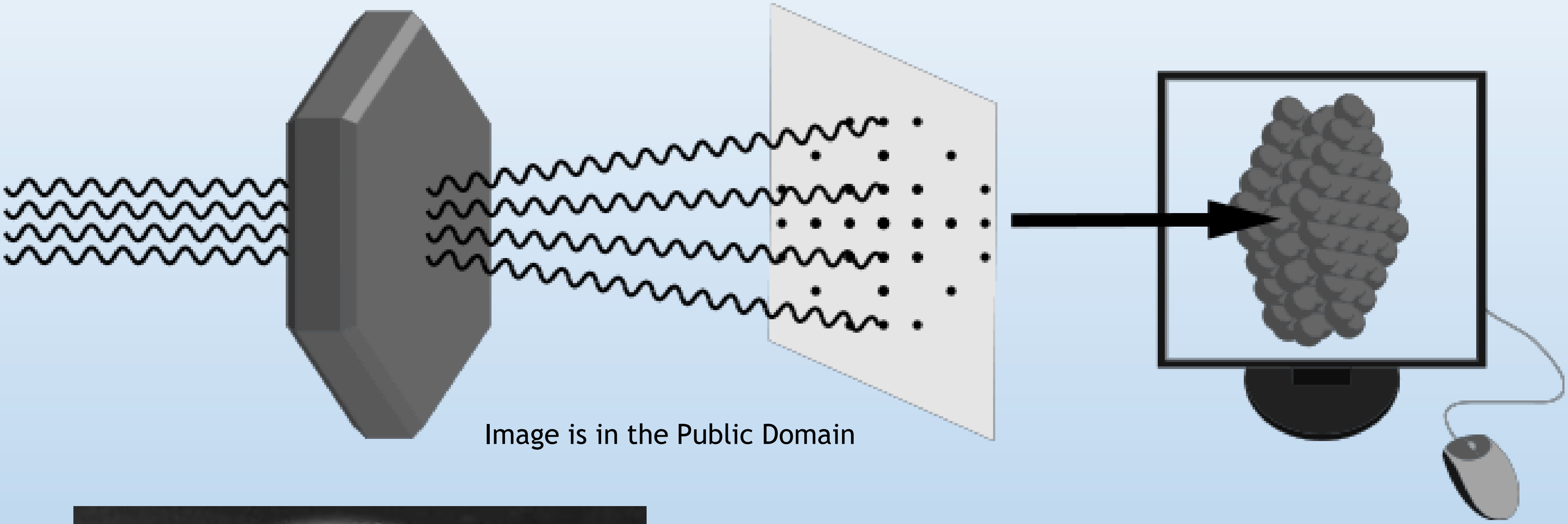
The main difference is that matter particles have mass, and photons don't !

Electron Diffraction



Positive Interference: $d\sin\theta = n\lambda$

Electron diffraction for characterizing crystal structure



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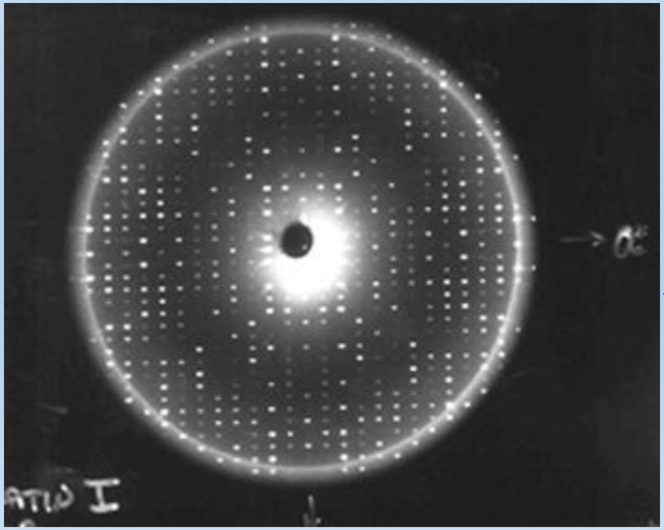

Image from the NASA gallery
http://mix.msfc.nasa.gov/abstracts.php?p=2057

From Davisson-Germer Experiment

Theory:

$$E = 54 \text{ eV}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.109 \times 10^{-31} \times 54 \times 1.602 \times 10^{-19}}}$$

$$= 0.167 \text{ nm}$$

Experiment:

$$d = 0.215 \text{ nm}$$

$$\theta = 50^\circ$$

$$\lambda = d \sin\theta = 0.165 \text{ nm}$$

Schrodinger: A prologue
Inferring the Wave-equation for Light

$$\psi \approx e^{j(\omega t - k_x x)}$$

$$\frac{\partial}{\partial t}\vec{E} = j\omega\vec{E} \qquad\qquad \frac{\partial}{\partial x}\vec{E} = -jk_x\vec{E}$$

$$\omega = ck$$

$$\Downarrow$$

$$\omega^2 = c^2 k^2$$

$$\Downarrow$$

$$-\frac{\partial^2}{\partial t^2}\vec{E} = -c^2\frac{\partial^2}{\partial x^2}\vec{E}$$

… so relating ω to k allows us to infer the wave-equation

Schrodinger: A Wave Equation for Electrons

$$E = \hbar\omega \qquad\qquad p = \hbar k$$

Schrodinger ***guessed*** that there was some wave-like quantity that could be related to energy and momentum …

$$\psi \approx e^{j(\omega t - k_x x)}$$ wavefunction

$$\frac{\partial}{\partial t}\psi = j\omega\psi \quad \Rightarrow \quad E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi$$

$$\frac{\partial}{\partial x}\psi = -jk_x\psi \quad \Rightarrow \quad p_x\psi = \hbar k_x\psi = j\hbar\frac{\partial}{\partial x}\psi$$

Schrodinger: A Wave Equation for Electrons

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

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

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

..The Free-Particle Schrodinger Wave Equation !

Erwin Schrödinger (1887–1961)
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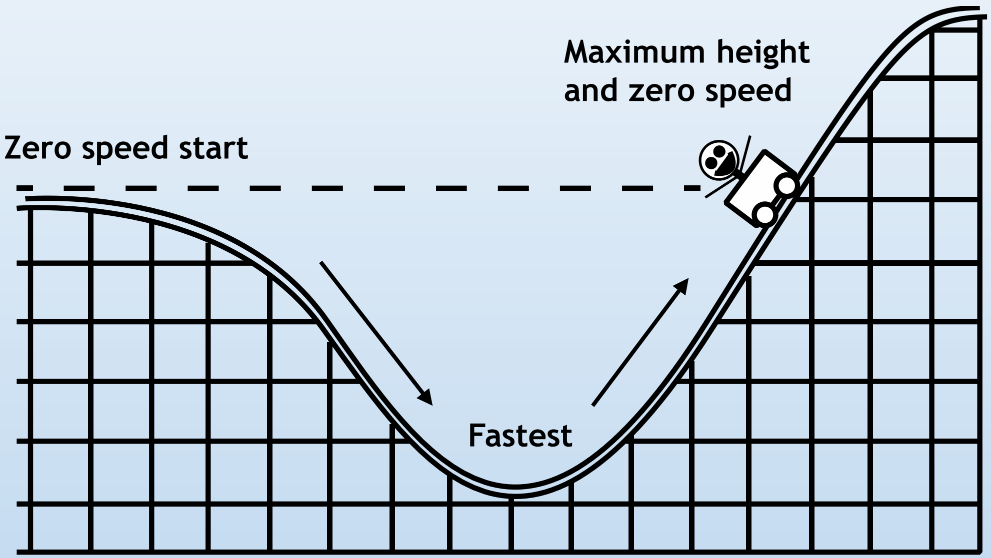
Classical Energy Conservation



- total energy = kinetic energy + potential energy
- In classical mechanics, $E = K + V$
- *V* depends on the system
  - e.g., gravitational potential energy, electric potential energy

Schrodinger Equation and Energy Conservation

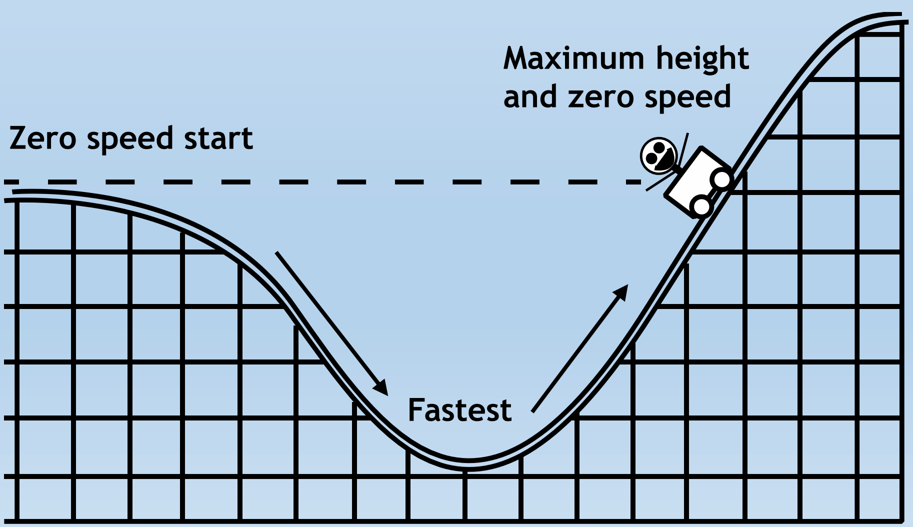
... The Schrodinger Wave Equation !

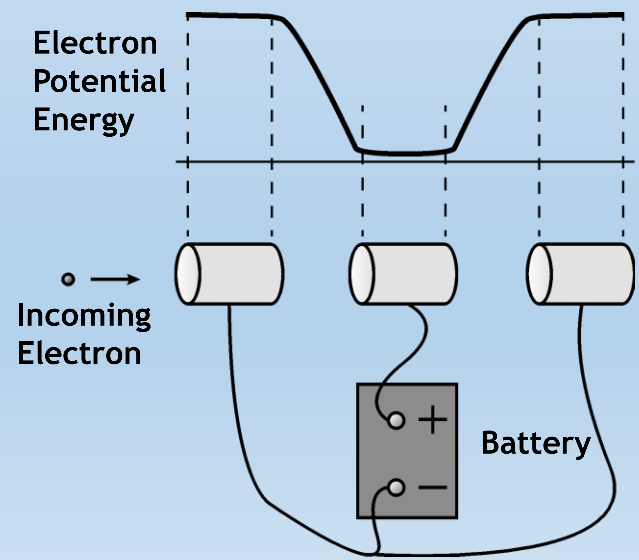
$$E = K + V \quad \Rightarrow \quad \boxed{-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi}$$

Total E term **K.E. term** **P.E. term**

... In physics notation and in 3-D this is how it looks:

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





Time-Dependent Schrodinger Wave Equation

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

PHYSICS NOTATION

Total E term

K.E. term

P.E. term

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

Time-Independent Schrodinger Wave Equation

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

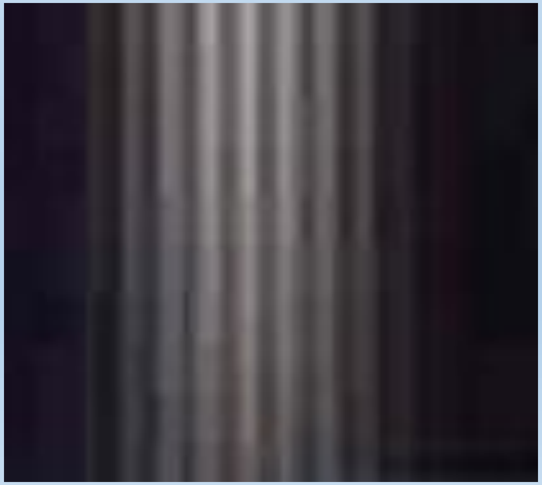
Electronic Wavefunctions

$$\psi(x) \approx e^{j(\omega t - k_x x)}$$ free-particle wavefunction

- Completely describes all the properties of a given particle
- Called $\psi = \psi\,(x,t)$ - is a complex function of position x and time t
- What is the meaning of this wave function?

  - The quantity $|\psi|^2$ is interpreted as the probability that the particle can be found at a particular point x and a particular time t

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



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Werner Heisenberg (1901–1976)
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Copenhagen Interpretation of Quantum Mechanics

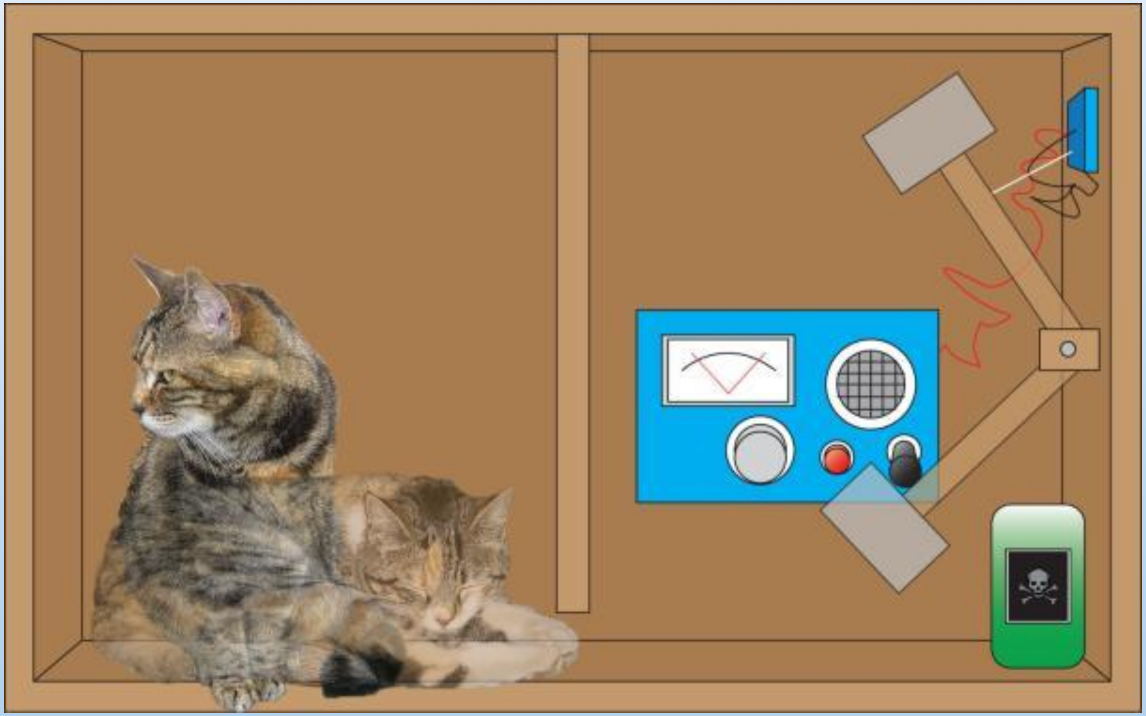
- A system is completely described by a wave function ψ, representing an observer's subjective knowledge of the system.
- The description of nature is essentially probabilistic, with the probability of an event related to the square of the amplitude of the wave function related to it.
- It is not possible to know the value of all the properties of the system at the same time; those properties that are not known with precision must be described by probabilities. (Heisenberg's uncertainty principle)
- Matter exhibits a wave–particle duality. An experiment can show the particle-like properties of matter, or the wave-like properties; in some experiments both of these complementary viewpoints must be invoked to explain the results.
- Measuring devices are essentially classical devices, and measure only classical properties such as position and momentum.
- The quantum mechanical description of large systems will closely approximate the classical description.

Today’s Culture Moment

Schrödinger's cat

“It is typical of these cases that an indeterminacy originally restricted to the atomic domain becomes transformed into macroscopic indeterminacy, which can then be resolved by direct observation. That prevents us from so naively accepting as valid a "blurred model" for representing reality. In itself, it would not embody anything unclear or contradictory. There is a difference between a shaky or out-of-focus photograph and a snapshot of clouds and fog banks.”

-Erwin Schrodinger, 1935



SCHRÖDINGER'S CAT IS DEAD

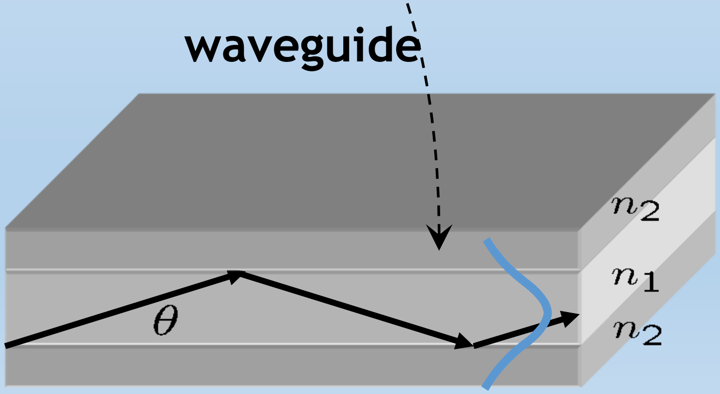
Comparing EM Waves and Wavefunctions

EM WAVES

$$\omega^2 = c^2 k^2$$

$$-\frac{\partial^2}{\partial t^2}\vec{E} = -c\frac{\partial^2}{\partial x^2}\vec{E}$$

$$I = \frac{|E|^2}{\eta}$$

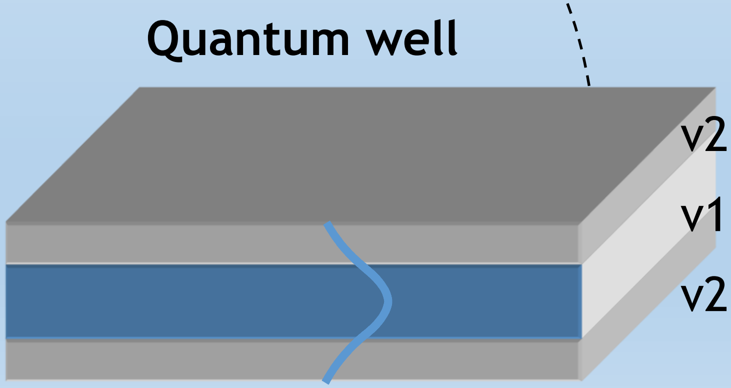


QM WAVEFUNCTIONS

$$E = \frac{p^2}{2m} + V(x)$$

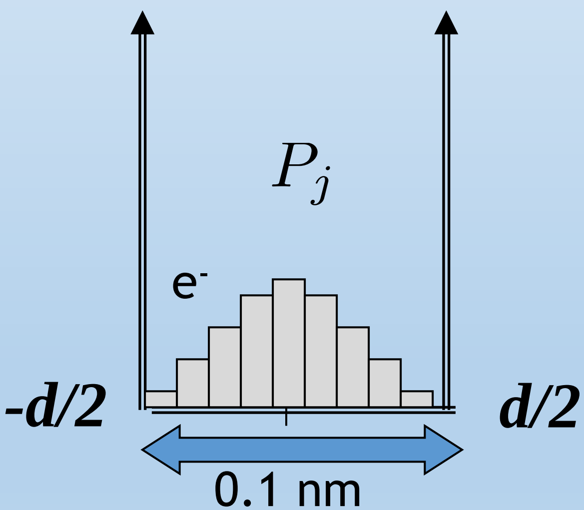
$$-j\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

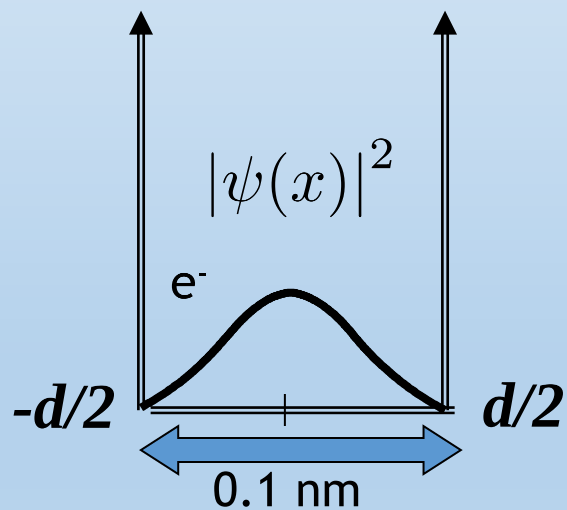
$$P(x)dx = |\psi|^2$$



Expected Position

$$\langle x \rangle = \sum_{j=-\infty}^{\infty} x\, P_j \qquad \langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx$$





$$< x >= 0 \qquad < x >= 0$$

Expected Momentum

$$< p >= \int_{-\infty}^{\infty} p \left|\psi(x)\right|^2 dx$$

$$= \int_{-\infty}^{\infty} j\hbar \frac{\partial}{\partial x} \left|\psi(x)\right|^2 dx$$

imaginary

real

Doesn't work !
Need to guarantee <p> is real

… so let's fix it by rewriting the expectation value of p as:

$$< p >= \int_{-\infty}^{\infty} \psi^*(x) \left(j\hbar \frac{\partial}{\partial x} \right) \psi(x) dx$$

free-particle wavefunction

$$\psi \approx e^{j(\omega t - k_x x)}$$

$$< p >= \hbar k$$

Maxwell and Schrodinger

Maxwell's Equations

$$\oint_C \vec{E} \cdot d\vec{l} = -\frac{d}{dt}\left(\int_S \vec{B} \cdot d\vec{l}\right)$$

$$\oint_C \vec{H} \cdot d\vec{l} = \int \vec{J} \cdot d\vec{A} + \frac{d}{dt}\int_S \epsilon \vec{E} \cdot d\vec{A}$$

The Wave Equation

$$\frac{\partial^2 E_y}{\partial z^2} = \epsilon\mu \frac{\partial^2 E_y}{\partial t^2}$$

Dispersion Relation

$$\omega^2 = c^2 k^2$$

$$\omega = ck$$

Energy-Momentum

$$E = \hbar\omega = \hbar ck = cp$$

Quantum Field Theory

The Schrodinger Equation

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

(free-particle)

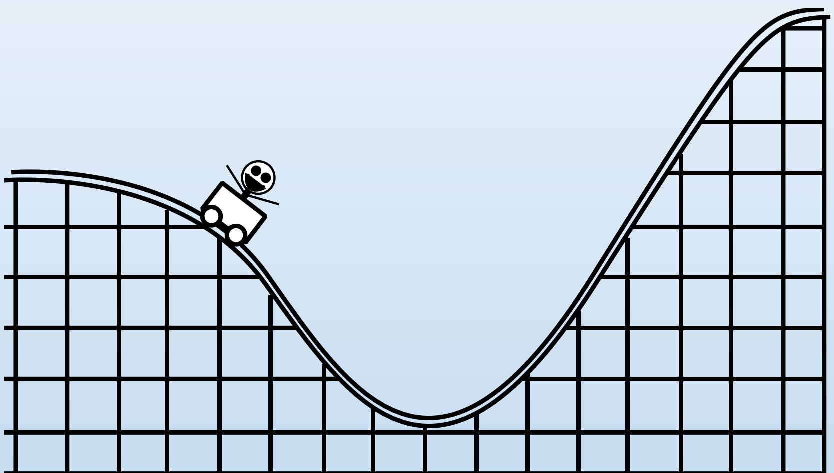
Dispersion Relation

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

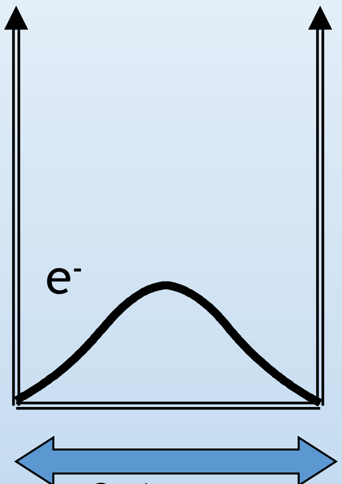
Energy-Momentum

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

Particle in a Box



$$\hbar = 1.054 \times 10^{-34}\,[\mathrm{J \cdot s}]$$



The particle the box is bound within certain regions of space.
If bound, can the particle still be described as a wave ?
→ YES … as a standing wave
(wave that does not change its $P(x) = |\Psi(x,t)|^2\, dx$ with time)

$$\Psi(x,t) \approx e^{j(\omega t - k_x x)} = \psi(x) e^{j\omega t} \Rightarrow \boxed{P(x) = |\psi|^2\, dx}$$

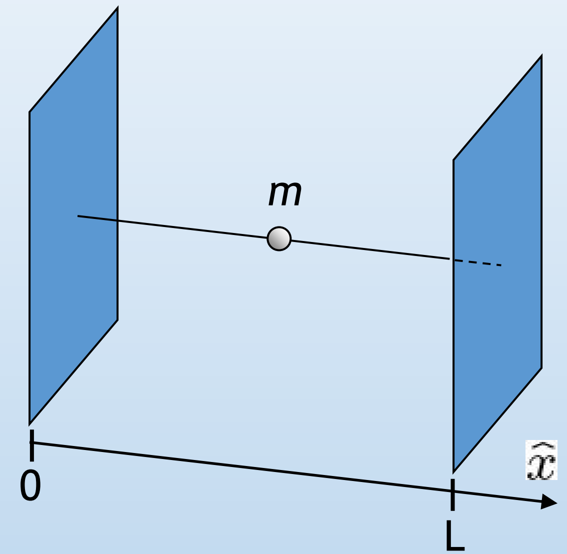
A point mass *m* constrained to move on an infinitely-thin, frictionless wire which is strung tightly between two impenetrable walls a distance *L* apart

for $(x \leq 0, x \geq L)$

$$V(x) = \infty$$

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

$$\Rightarrow \psi = 0$$



for $(0 < x < L)$

$$V(x) = 0$$

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

WE WILL HAVE MULTIPLE SOLUTIONS FOR ψ, SO WE INTRODUCE LABEL n

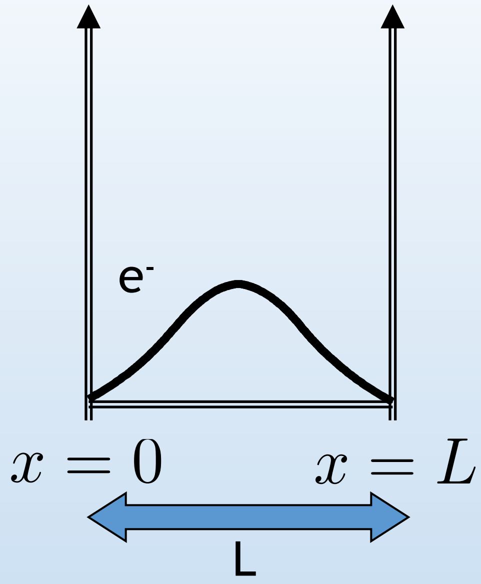
$$\Rightarrow \psi(0) = \psi(L) = 0$$

ψ IS CONTINUOUS

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

$$E_n \psi_n = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi_n}{\partial x^2}$$

WE WILL HAVE MULTIPLE SOLUTIONS FOR ψ, SO WE INTRODUCE LABEL *n*



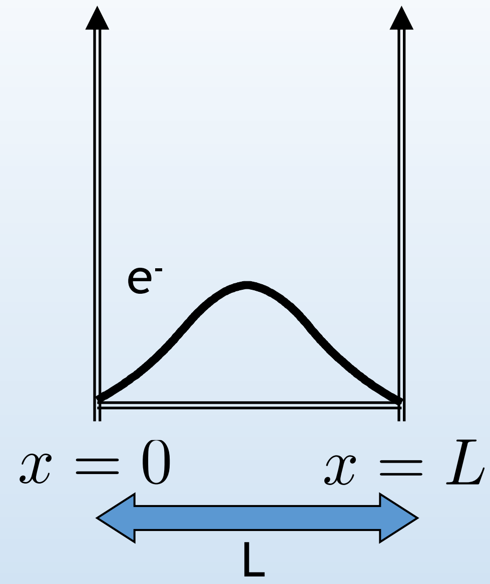
REWRITE AS:

$$\frac{\partial^2 \psi_n}{\partial x^2} + k_n^2 \psi_n = 0 \qquad \text{WHERE} \qquad k_n^2 = \frac{2mE_n}{\hbar^2}$$

GENERAL SOLUTION:

$$\psi_n(x) = A \sin k_n x + B \cos k_n x \qquad \text{OR} \qquad \psi_n = C_1 e^{jk_n x} + C_2 e^{-jk_n x}$$

USE BOUNDARY CONDITIONS TO DETERMINE COEFFICIENTS A and B



$$\Rightarrow \quad k_n L = n\pi$$

$$\Rightarrow \quad B = 0 \text{ since } \quad \psi(0) = 0$$

NORMALIZE THE INTEGRAL OF PROBABILITY TO 1

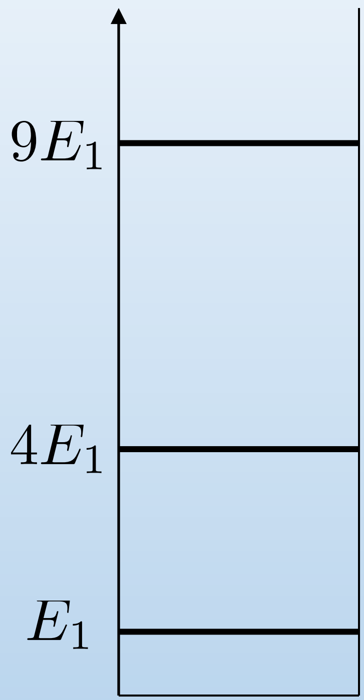
$$\Downarrow$$

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

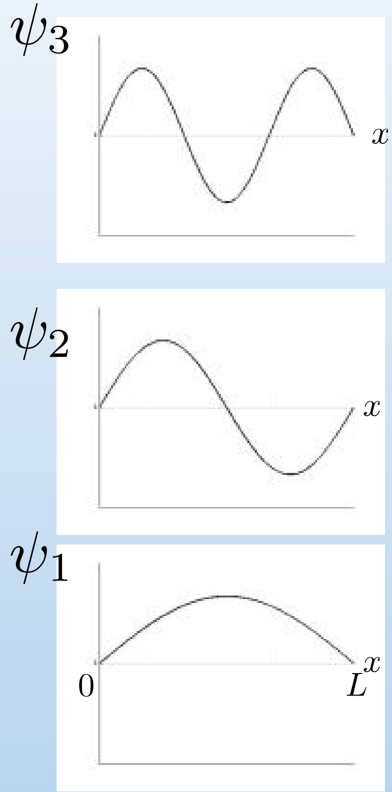
$$k_n^2 = \frac{2mE_n}{\hbar^2}$$

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

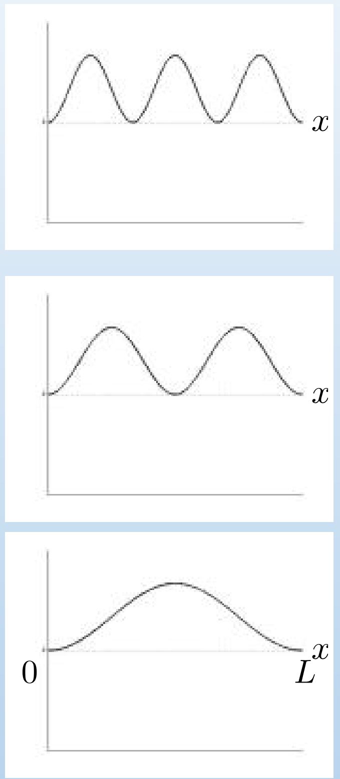
EIGENENERGIES for 1-D BOX



EIGENSTATES for 1-D BOX



PROBABILITY DENSITIES



$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

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

Today’s Culture Moment

Max Planck

- Planck was a gifted musician. He played piano, organ and cello, and composed songs and operas.
- The Munich physics professor Jolly advised Planck against going into physics, saying, “in this field, almost everything is already discovered, and all that remains is to fill a few holes.”
- In 1877 he went to Berlin for a year of study with physicists Helmholtz and Kirchhoff. He wrote that Kirchhoff spoke in carefully prepared lectures which were dry and monotonous. He eventually became Kirchhoff’s successor in Berlin.
- The concept of the photon was initially rejected by Planck. He wrote "The theory of light would be thrown back not by decades, but by centuries, into the age when Christian Huygens dared to fight against the mighty emission theory of Isaac Newton.“
- In his *Scientific Autobiography and Other Papers,* he stated Planck's Principle, which holds that "A new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die and a new generation grows up that is familiar with it."

1858 - 1947

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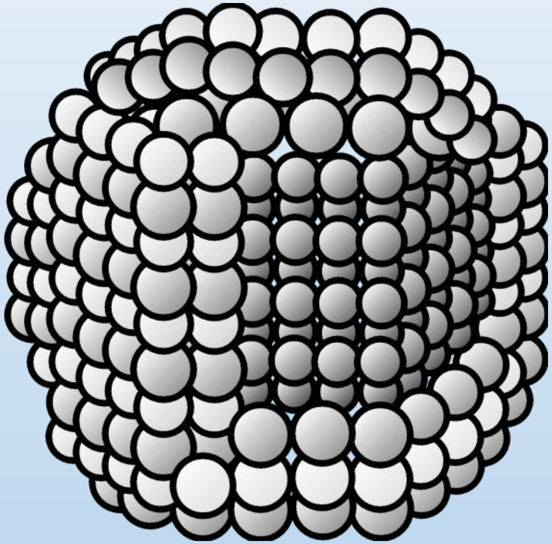
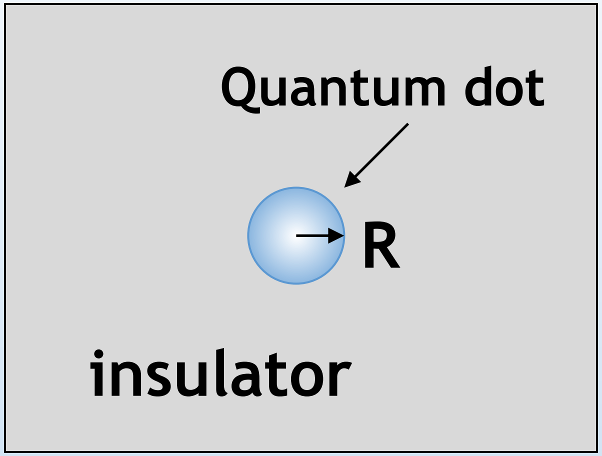
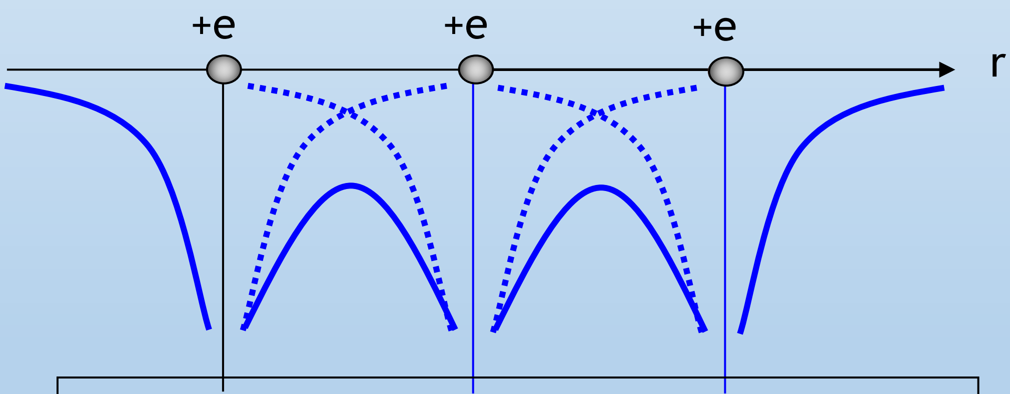
Quantum Confinement

another way to know Δx





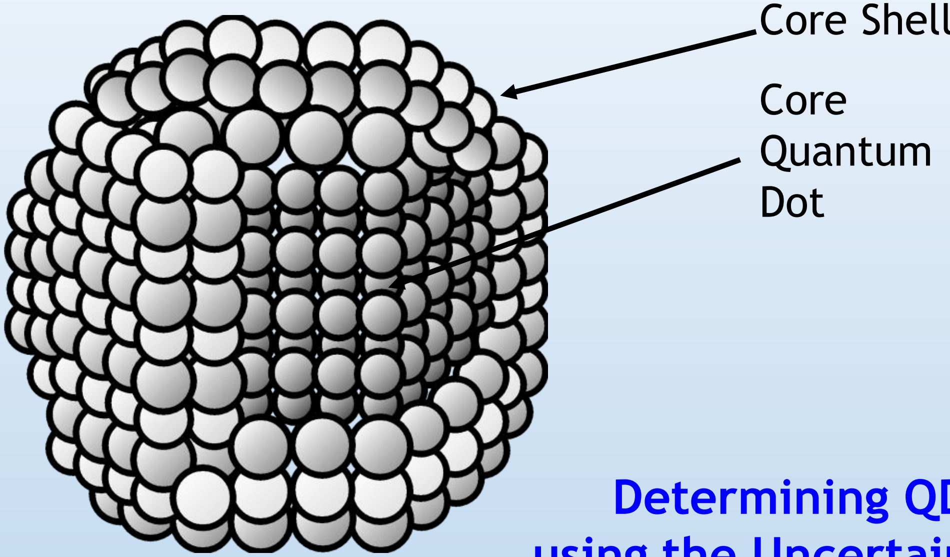


electron can be anywhere in the dot

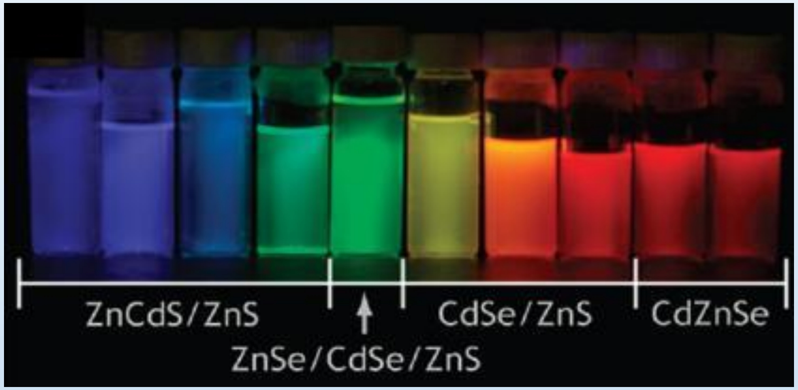
$$< \Delta x^2 > \sim R^2$$

Semiconductor Nanoparticles

(aka: Quantum Dots)



Red: bigger dots!
Blue: smaller dots!



Determining QD energy using the Uncertainty Principle

$$< \Delta x^2 > \sim R^2$$

$$< \Delta x^2 > = < x^2 > - < x >^2$$

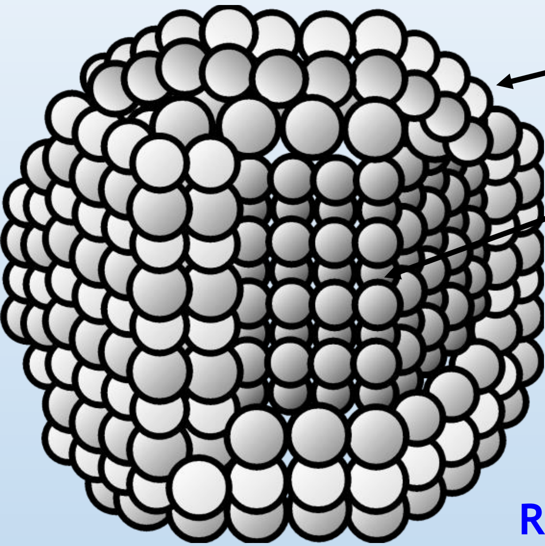
$$\Delta x \Delta p \geq \frac{h}{4\pi} = \frac{\hbar}{2}$$

$$< \Delta p^2 > \sim \left(\frac{\hbar^2}{2R} \right)^2$$

$$< E > = \frac{< p^2 >}{2m} = \frac{< \Delta p^2 >}{2m} \approx \frac{1}{R^2}$$

Semiconductor Nanoparticles

(aka: Quantum Dots)



Determining QD energy using the Schrödinger Equation

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

Red: bigger dots!
Blue: smaller dots!

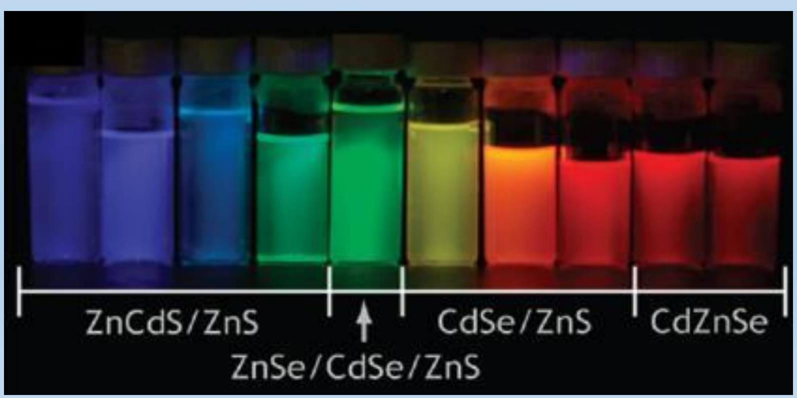
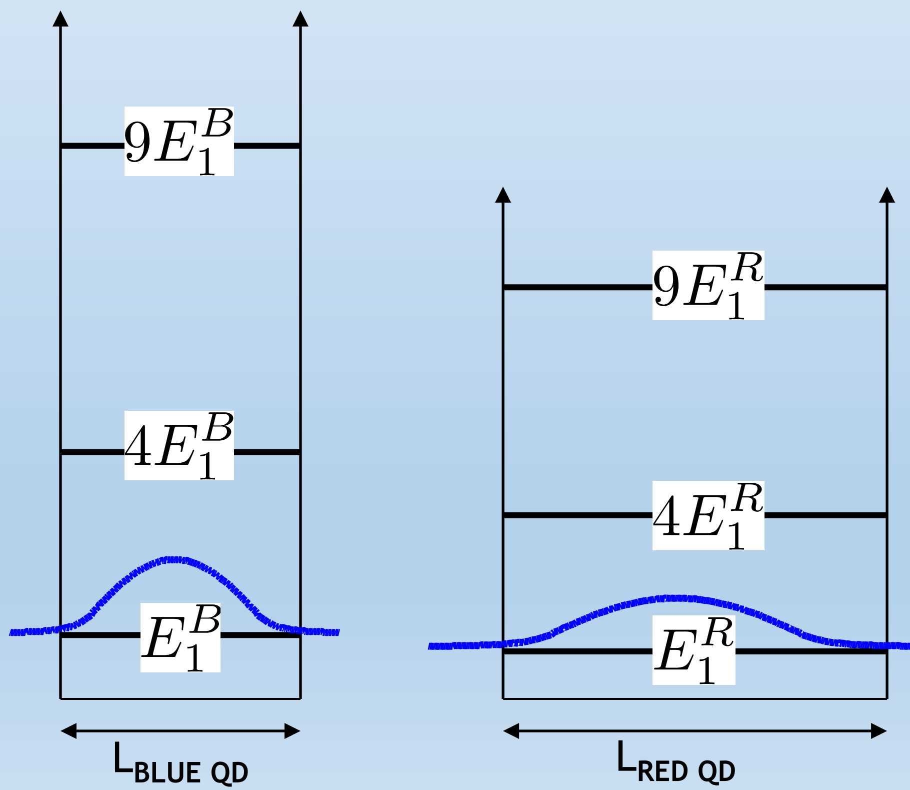


Photo by J. Halpert
Courtesy of M. Bawendi Group, Chemistry, MIT



The Wavefunction

- $|\psi|^2 \, dx$ corresponds to a physically meaningful quantity –
  - the probability of finding the particle near x
- $\left|\psi^* \dfrac{d\psi}{dx}\right| dx$ 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)

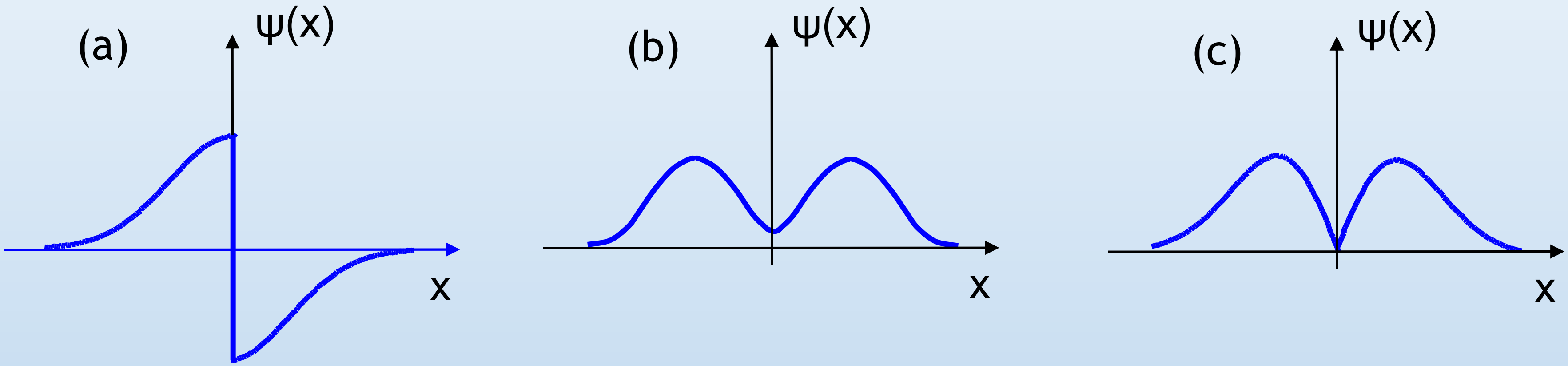
ψ(x) must be continuous, with finite dψ/dx
(because dψ/dx is related to the momentum density)

In regions with finite potential, dψ/dx must be continuous
(with finite $d^2\psi/dx^2$, to avoid infinite energies)

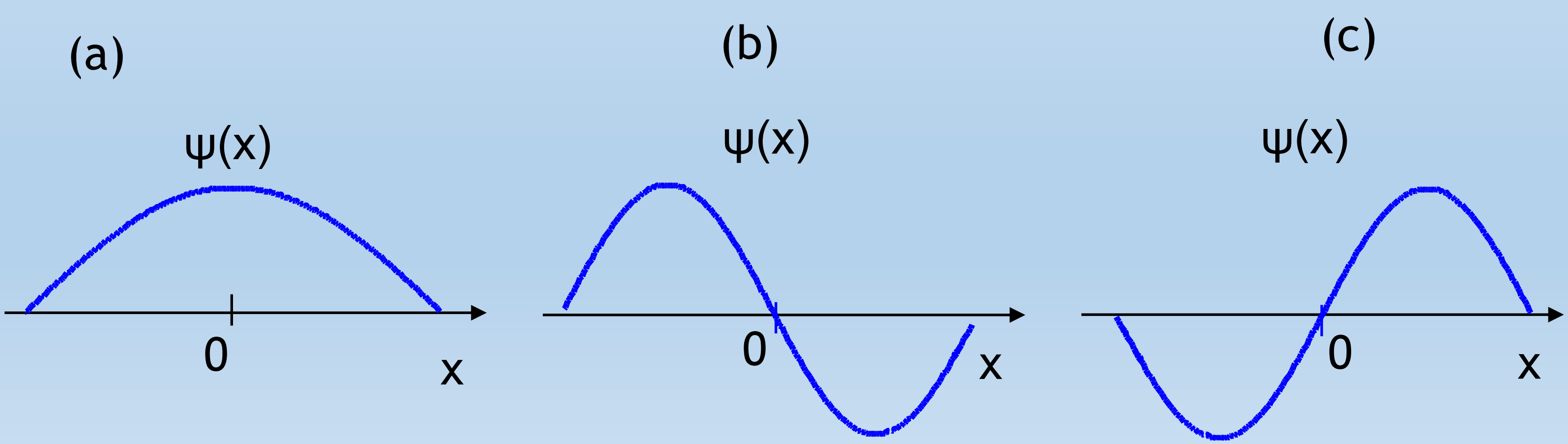
There is usually no significance to the overall *sign* of ψ(x)
(it goes away when we take the absolute square)
(In fact, ψ(x,t) is usually complex !)

Physically Meaningful Wavefunctions

1. Which of the following hypothetical wavefunctions is acceptable for a particle in some realistic potential V(x)?



2. Which of the following wavefunctions corresponds to a particle more likely to be found on the left side?



Schrodinger Equation and Energy Conservation

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

- Notice that if V(x) = constant, this equation has the simple form:

$$\frac{\partial^2\psi}{\partial x^2} = C\psi$$

where $C = \frac{2m}{\hbar^2}(V-E)$ is a constant that might be positive or negative.

For positive C, what is the form of the solution?

a) sin kx b) cos kx c) e^{ax} d) e^{-ax}

For negative C, what is the form of the solution?

a) sin kx b) cos kx c) e^{ax} d) e^{-ax}

Solutions to Schrodinger's Equation

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

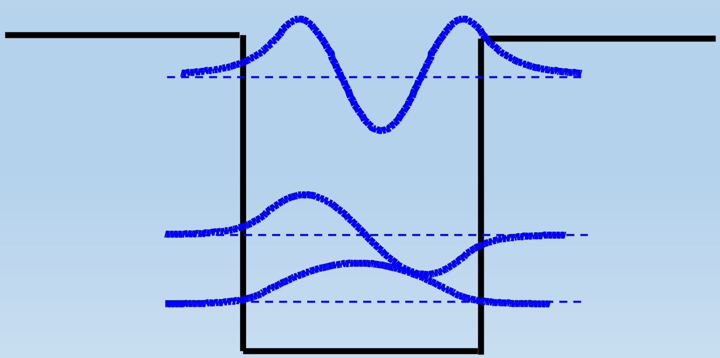
The kinetic energy of the electron is related to the curvature of the wavefunction

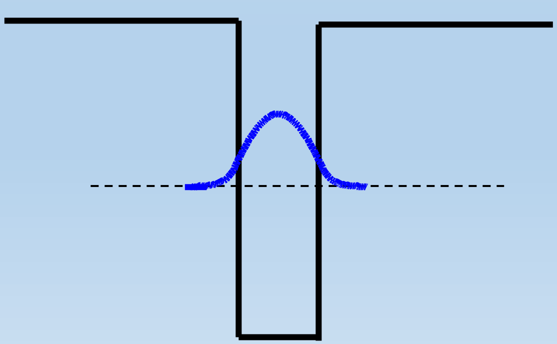
Tighter confinement → Higher energy

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

Nodes in wavefunction → Higher energy

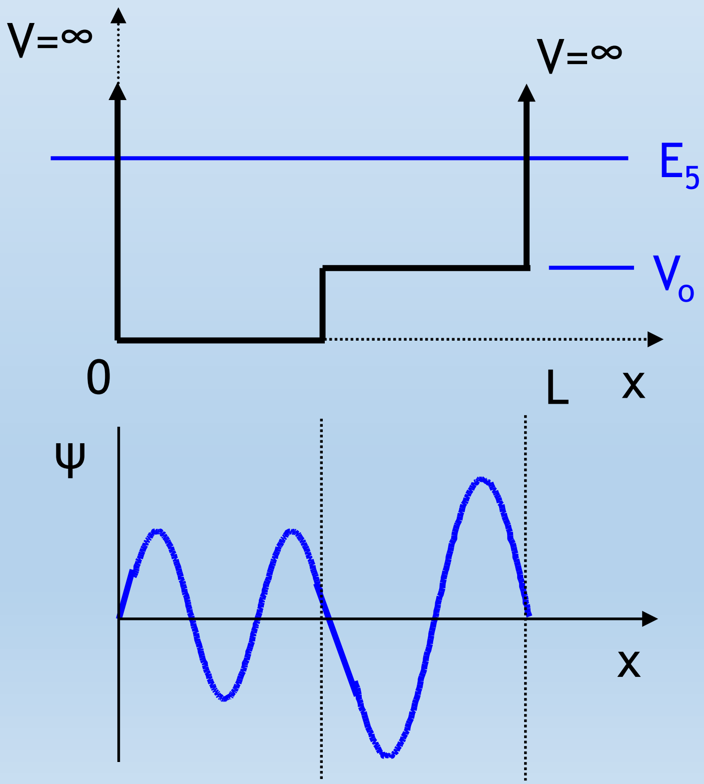
The n-th wavefunction (eigenstate) has (n-1) zero-crossings





Sketching Solutions to Schrodinger's Equation

- Estimate the wavefunction for an electron in the 5th energy level of this potential, without solving the Schrodinger Eq. Qualitatively sketch the 5th wavefunction:



Things to consider:

(1) 5th wavefunction has __ zero-crossings.

(2) Wavefunction must go to zero at <u>x = 0</u> and <u>x = L.</u>

(3) Kinetic energy is ______ on right side of well, so the curvature of ψ is _____ there (wavelength is longer).

(4) Because kinetic energy is ______ on right side of the well, the amplitude is _______ .

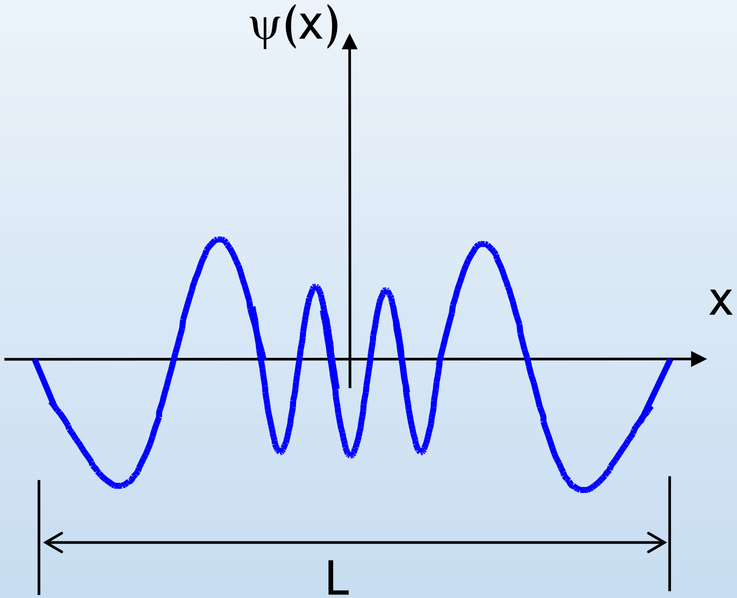
Solutions to Schrodinger's Equation

In what energy level is the particle? n = …

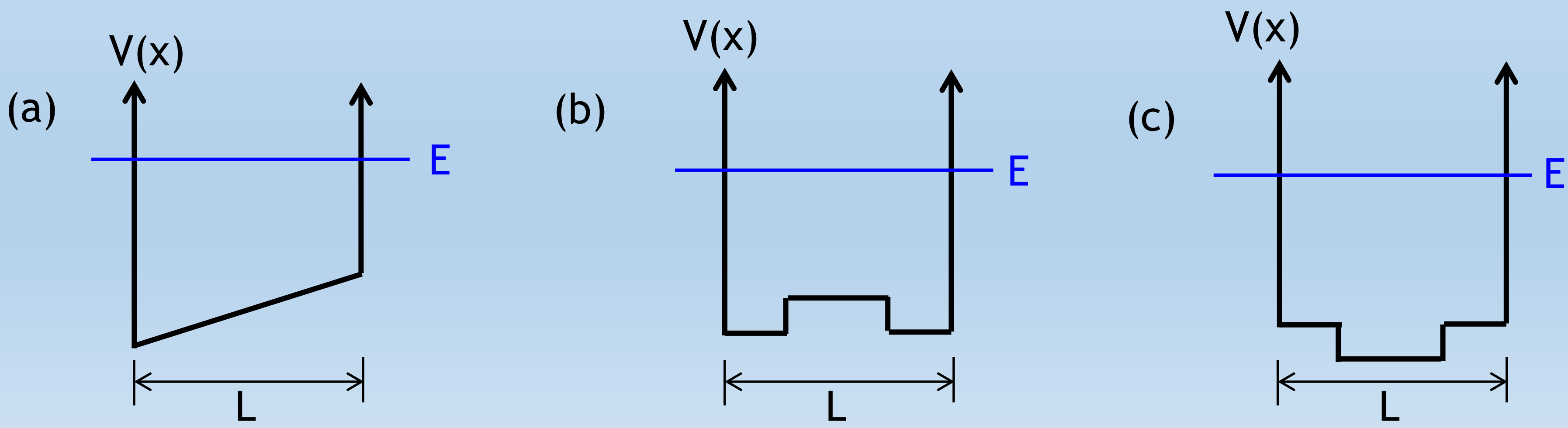
(a) 7

(b) 8

(c) 9

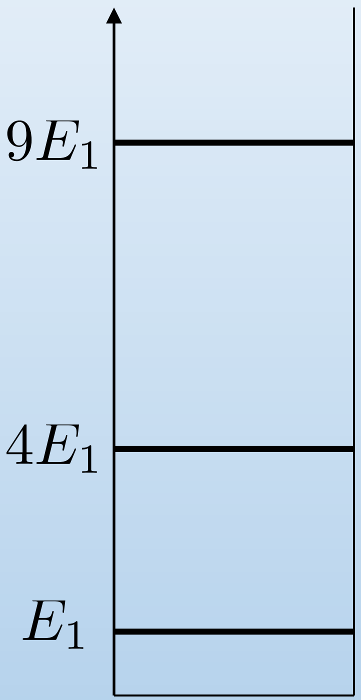


What is the approximate shape of the potential V(x) in which this particle is confined?

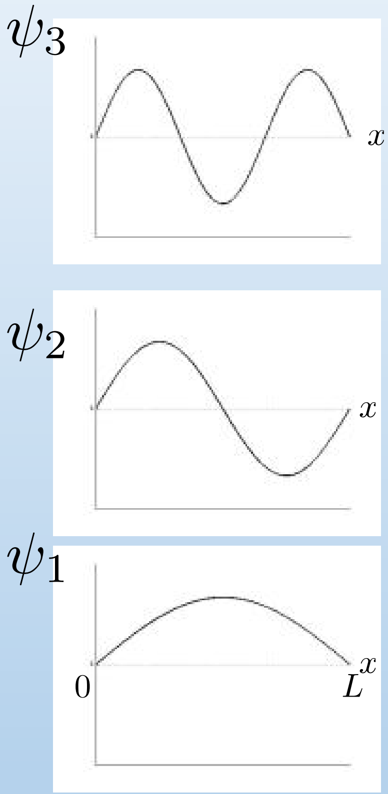


Key Takeaways

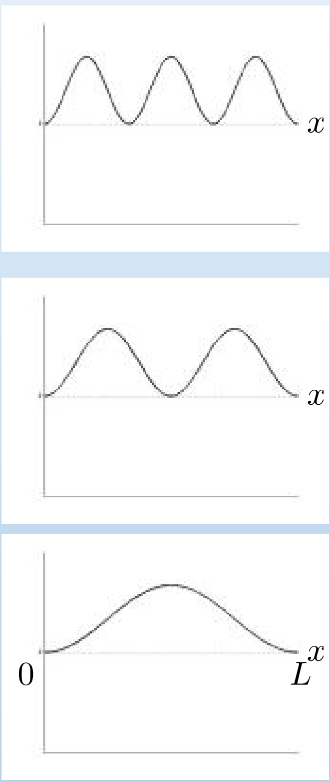
EIGENENERGIES for 1-D BOX



EIGENSTATES for 1-D BOX



PROBABILITY DENSITIES



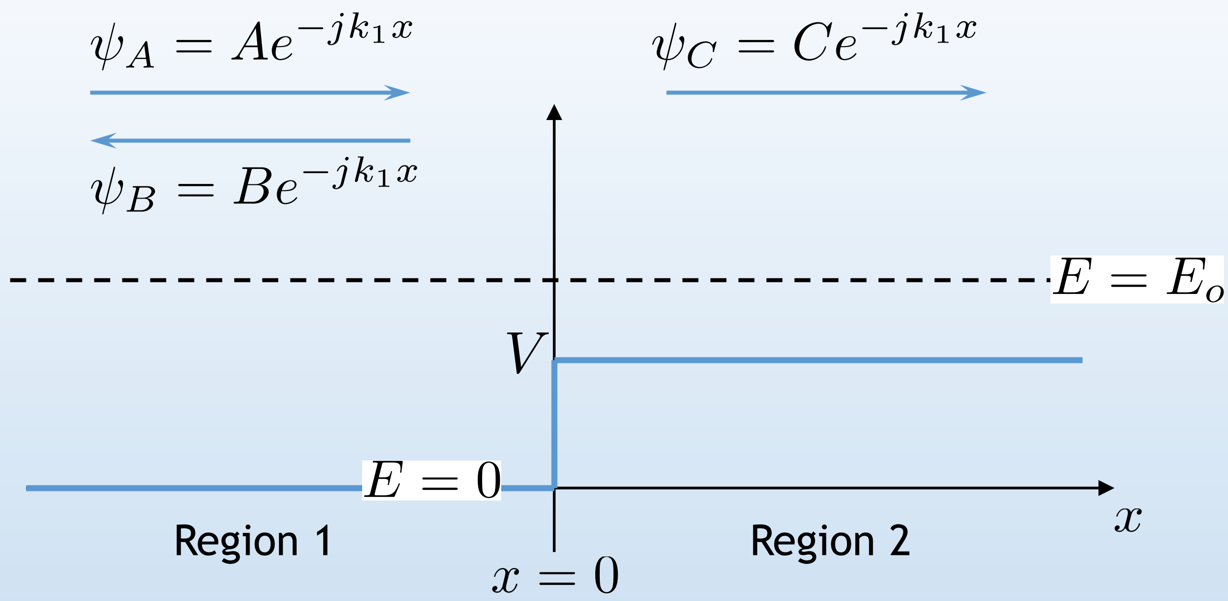
$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

When drawing a wavefunction by inspection:

1. The wavefunction of the **n**th Energy level has **n**-1 zero crossings
2. Higher kinetic energy means higher curvature and lower amplitude.
3. Exponential decay occurs when the Kinetic energy is “smaller” than the Potential energy.

A Simple Potential Step

CASE I : $E_o > V$

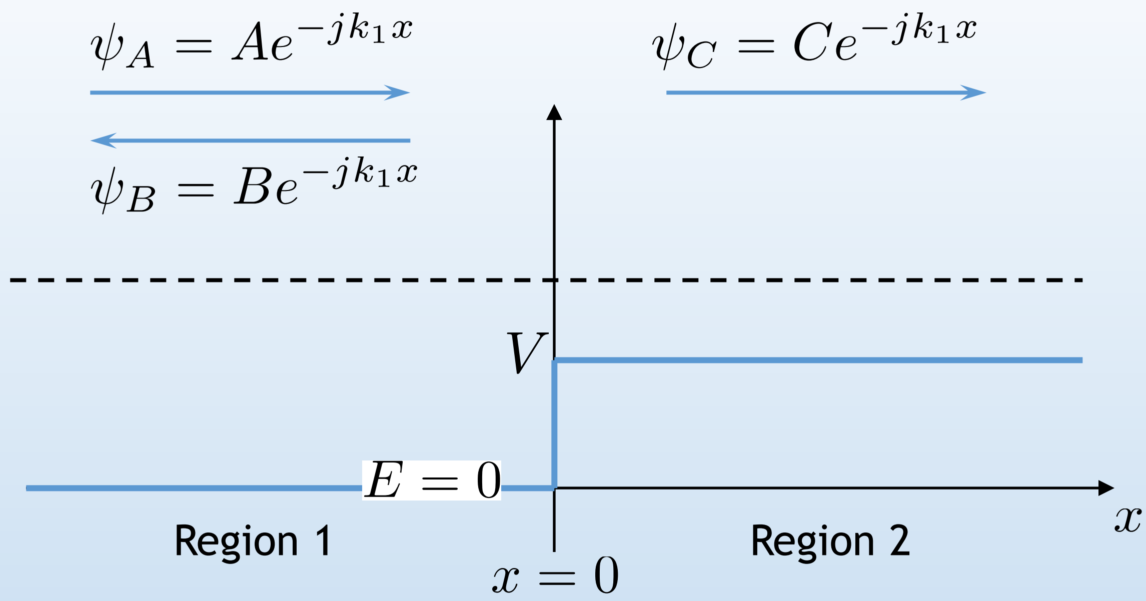


In Region 1: $$E_o \psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \quad \Rightarrow \quad k_1^2 = \frac{2mE_o}{\hbar^2}$$

In Region 2: $$\left(E_o - V\right)\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \quad \Rightarrow \quad k_2^2 = \frac{2m\left(E_o - V\right)}{\hbar^2}$$

A Simple Potential Step

CASE I : $E_o > V$



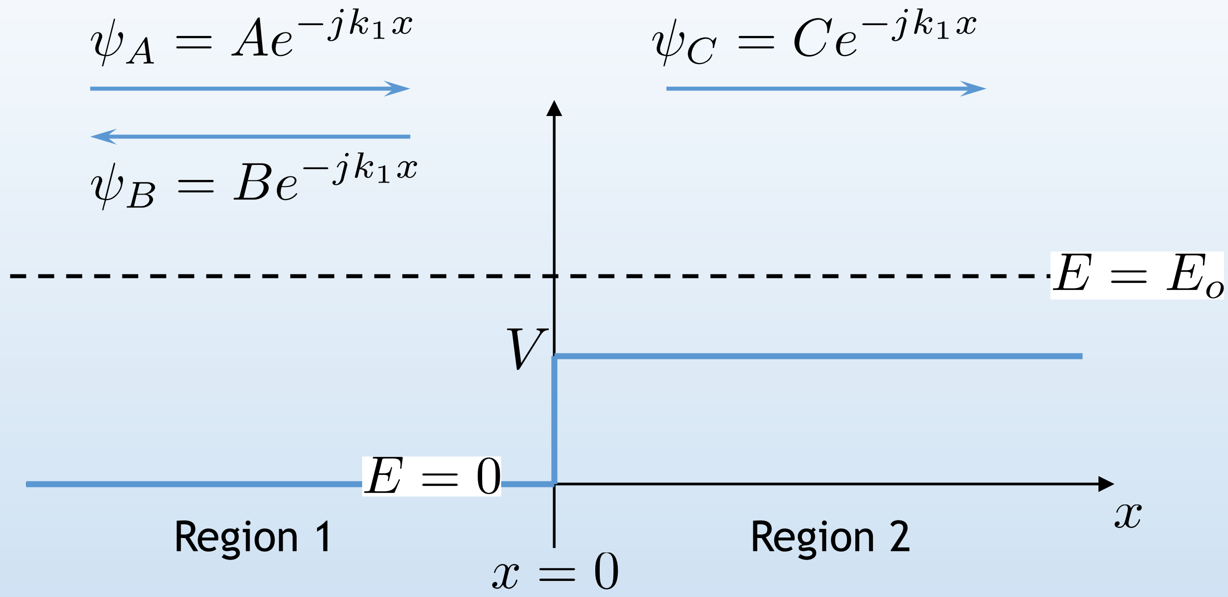
$$\psi_1 = Ae^{-jk_1x} + Be^{jk_1x} \qquad \psi_2 = Ce^{-jk_2x}$$

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

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

A Simple Potential Step

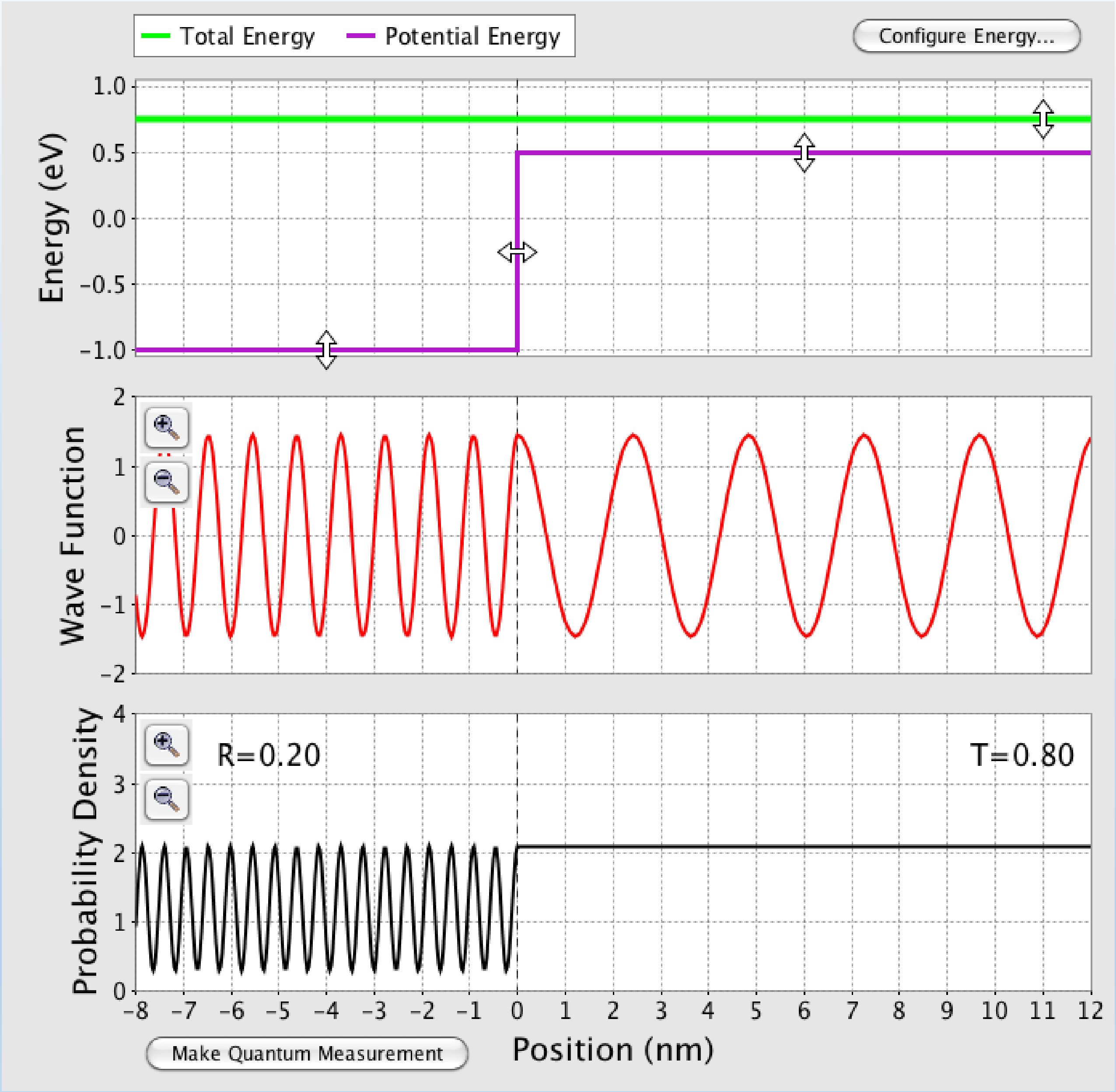
CASE I : E_o > V



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

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

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



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 $\rho = q\,|\psi(x)|^2$

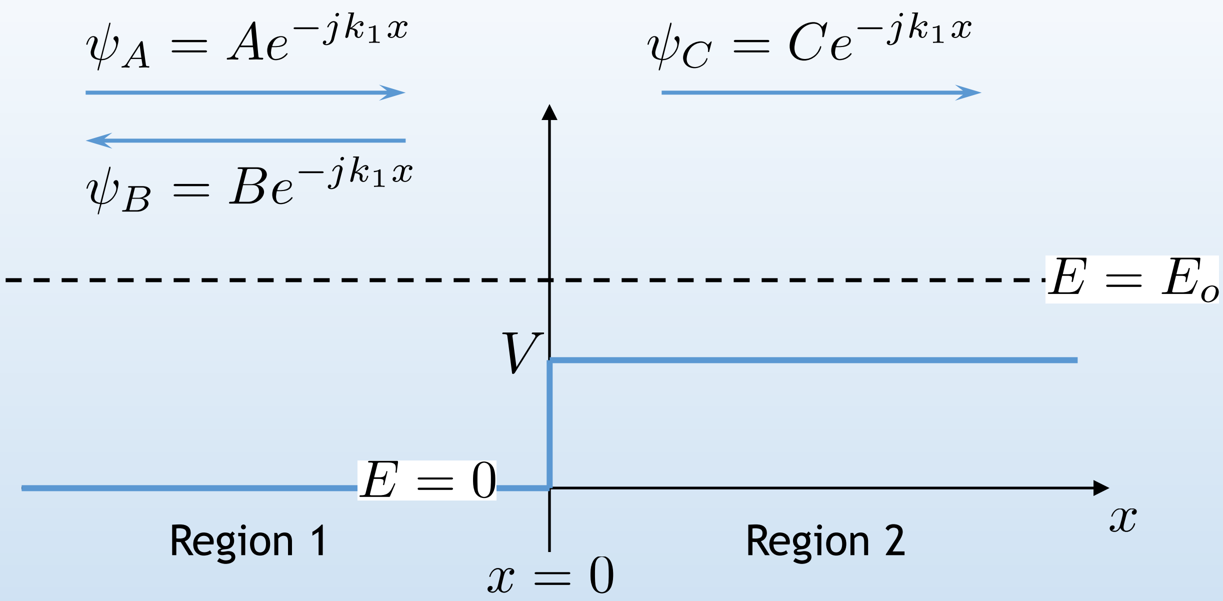
and moving with momentum $< p >$ corresponding to $< v >= \hbar k/m$

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

$$\boxed{J = \rho v = q\,|\psi|^2\,(\hbar k/m)}$$

A Simple Potential Step

CASE I : $E_o > V$

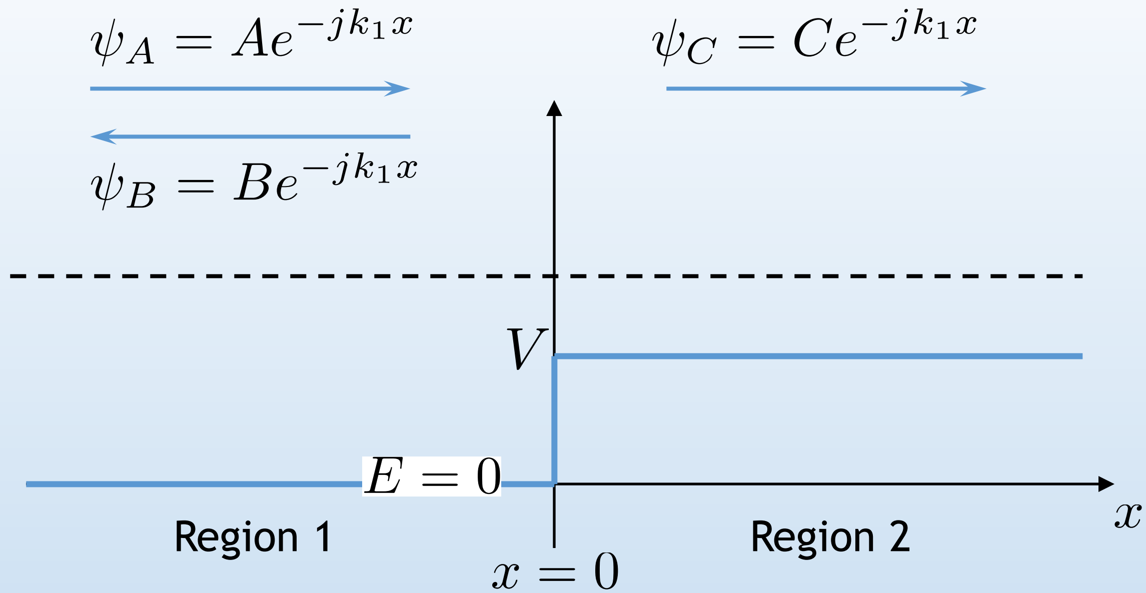


$$\text{Reflection} = R = \frac{J_{reflected}}{J_{incident}} = \frac{J_B}{J_A} = \frac{|\psi_B|^2(\hbar k_1/m)}{|\psi_A|^2(\hbar k_1/m)} = \left|\frac{B}{A}\right|^2$$

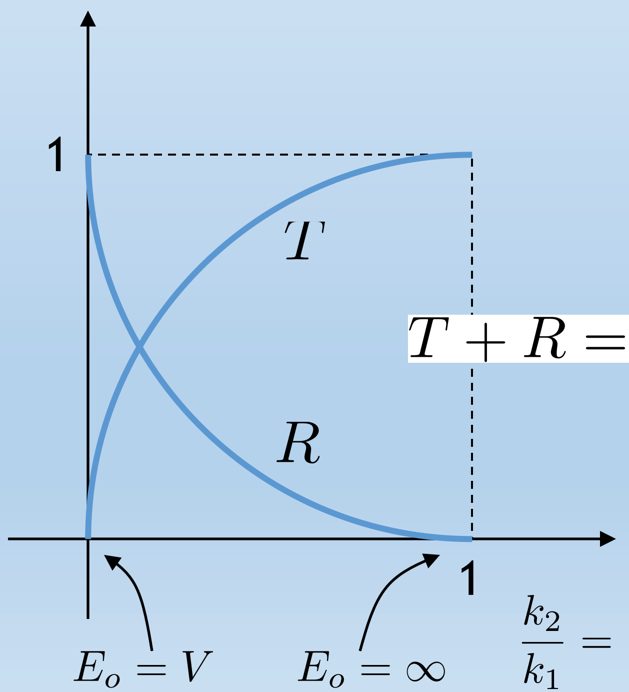
$$\text{Transmission} = T = \frac{J_{transmitted}}{J_{incident}} = \frac{J_C}{J_A} = \frac{|\psi_C|^2(\hbar k_2/m)}{|\psi_A|^2(\hbar k_1/m)} = \left|\frac{C}{A}\right|^2 \frac{k_2}{k_1}$$

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

A Simple Potential Step



CASE I : E_o > V



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

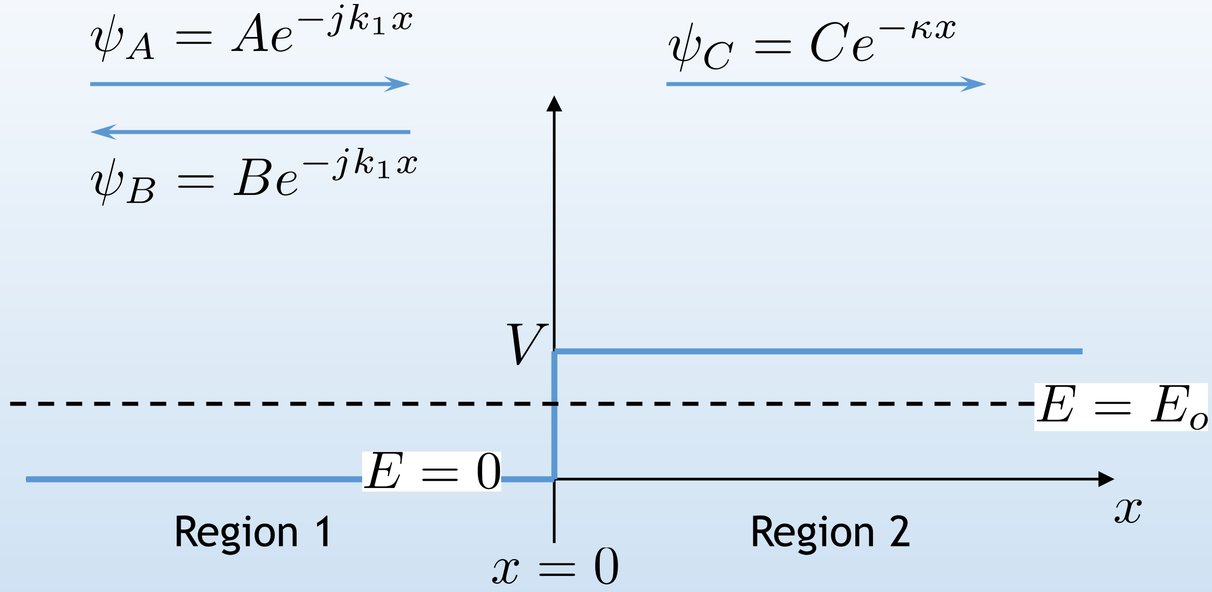
$$\text{Reflection} = R = \left|\frac{B}{A}\right|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2$$

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

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

A Simple Potential Step

CASE II : $E_o < V$

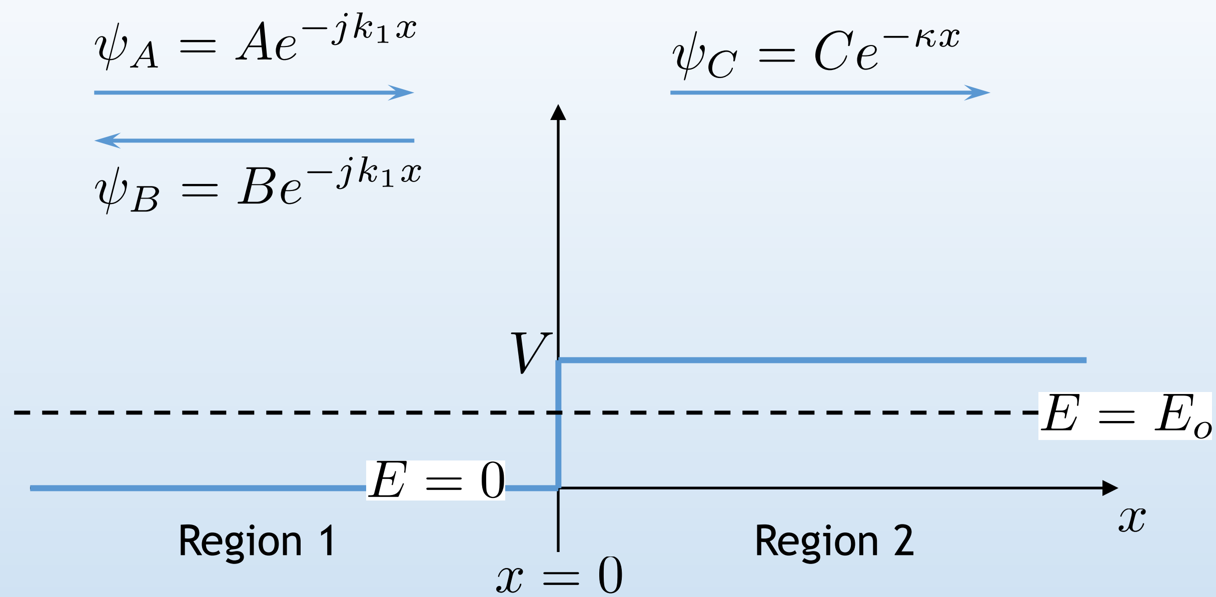


In Region 1: $$E_o\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \quad \Rightarrow \quad k_1^2 = \frac{2mE_o}{\hbar^2}$$

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

A Simple Potential Step

CASE II : E_o < V



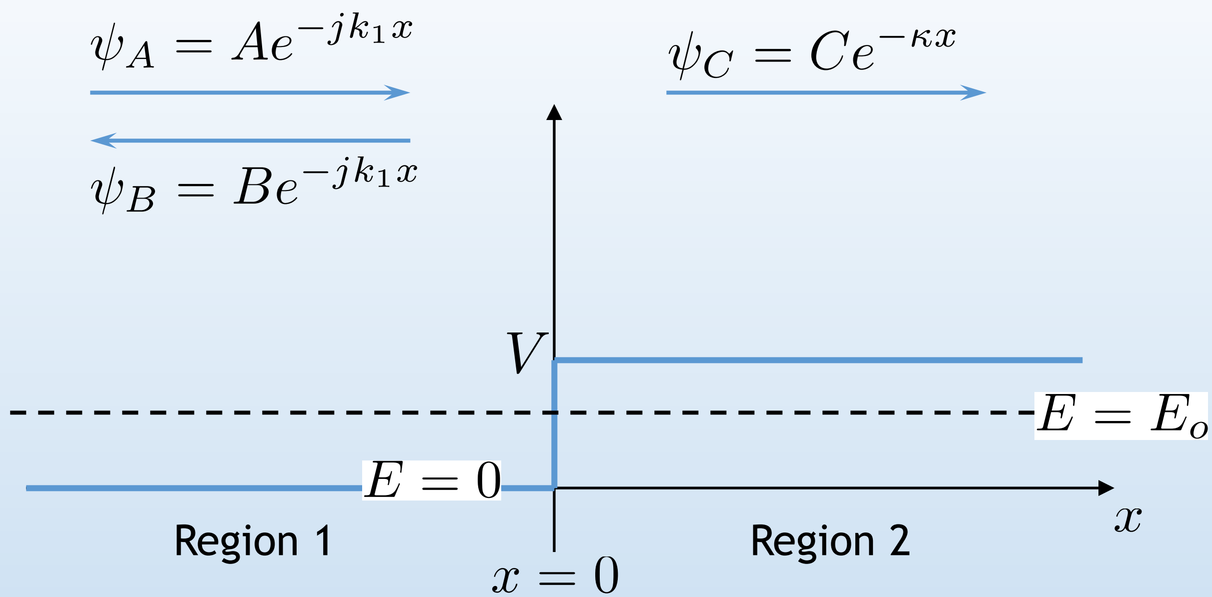
$$\psi_1 = Ae^{-jk_1x} + Be^{jk_1x} \qquad\qquad \psi_2 = Ce^{-\kappa x}$$

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

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

A Simple Potential Step

CASE II : $E_o < V$



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

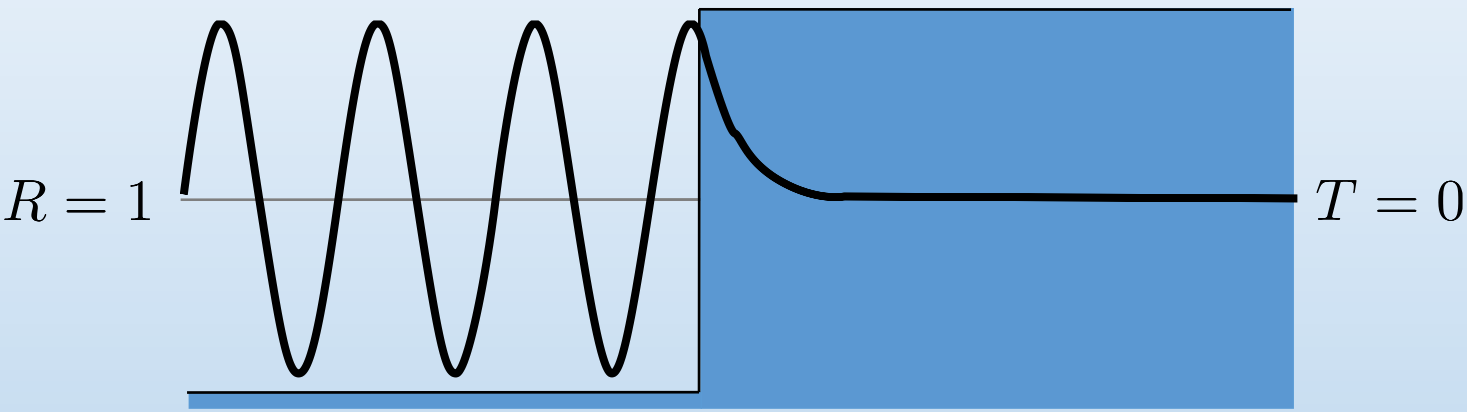
$$\frac{B}{A} = \frac{1 + j\kappa/k_1}{1 - j\kappa/k_1} \qquad \frac{C}{A} = \frac{2}{1 - j\kappa/k_1}$$

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

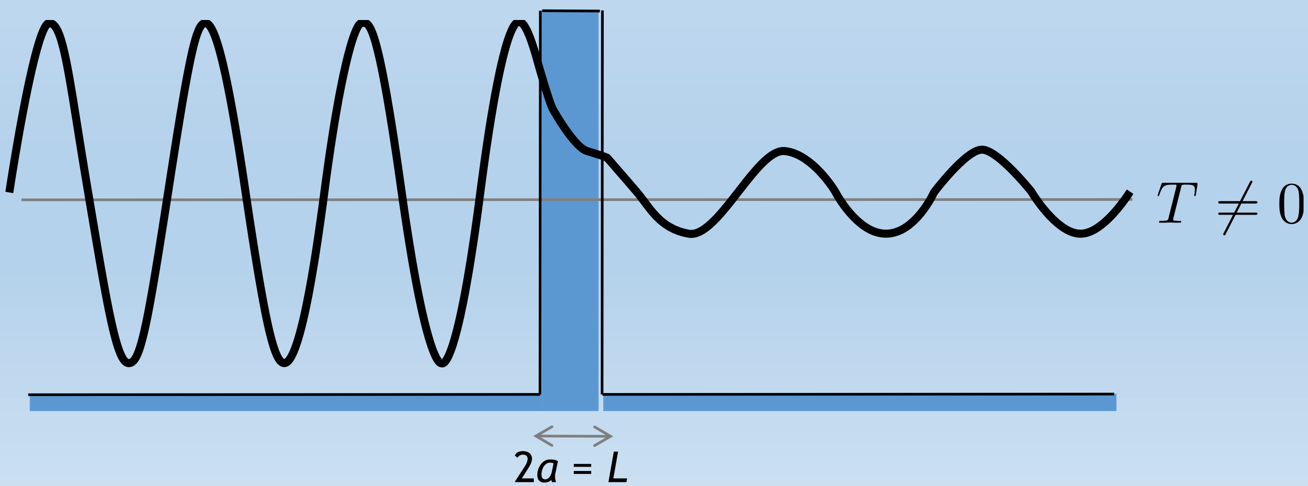
Total reflection → Transmission must be zero

Quantum Tunneling Through a Thin Potential Barrier

Total Reflection at Boundary

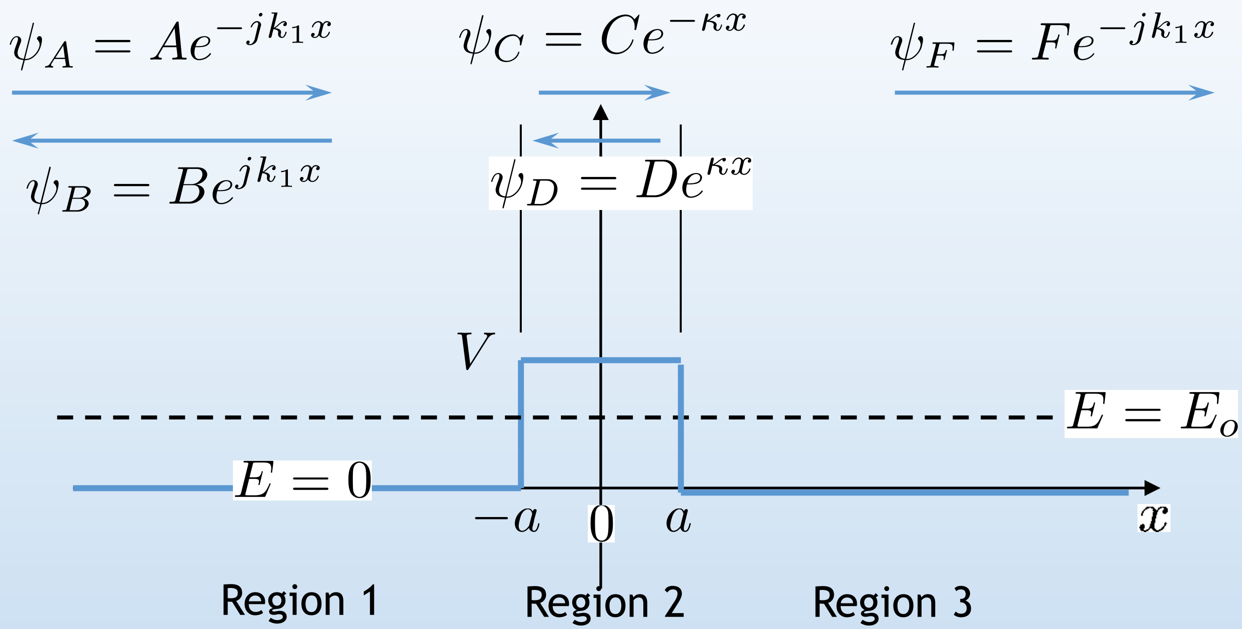


Frustrated Total Reflection (Tunneling)



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:

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

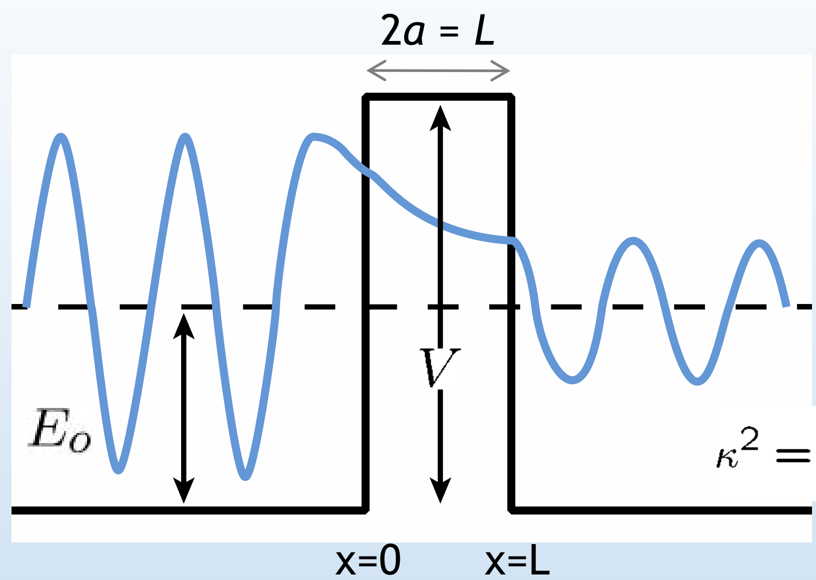
for $E_o < V$:

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

A Rectangular Potential Step

Real part of Ψ for $E_o < V$, shows hyperbolic (exponential) decay in the barrier domain and decrease in amplitude of the transmitted wave.

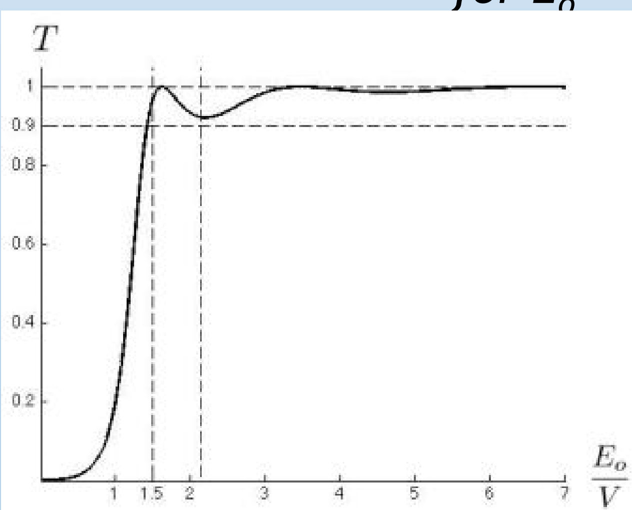
$E = 0$



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

for $E_o < V$:

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



Transmission Coefficient versus E_o/V for barrier with $2m(2a)^2V/\hbar = 16$

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

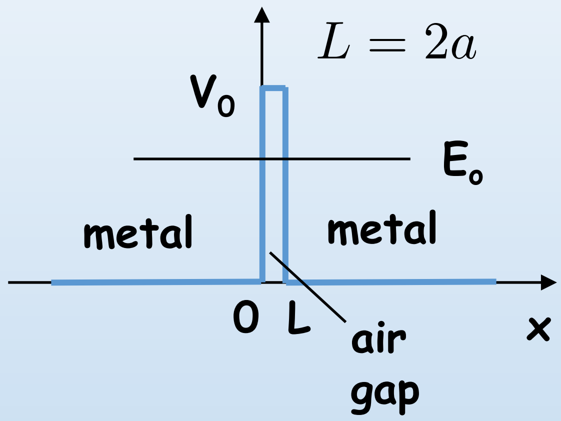
$$T = \left|\frac{F}{A}\right|^2 \approx \frac{1}{1 + \frac{1}{4}\frac{V^2}{E_o(V-E_o)}}e^{-4\kappa a}$$

Tunneling Applet: http://www.colorado.edu/physics/phet/dev/quantum-tunneling/1.07.00/

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?



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

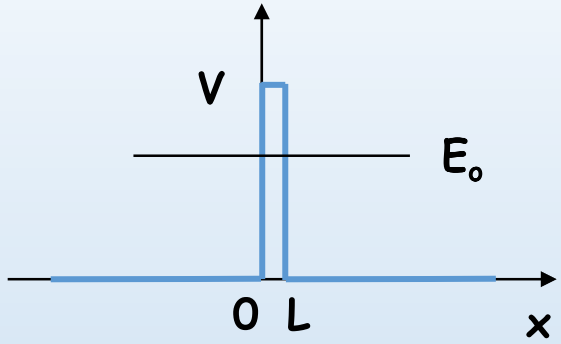
$$\kappa = \sqrt{\frac{2m_e}{\hbar^2}(V - E_o)} = 2\pi\sqrt{\frac{2m_e}{h^2}(V - E_o)} = 2\pi\sqrt{\frac{6\text{eV}}{1.505\text{eV-nm}^2}} \approx 12.6 \text{ nm}^{-1}$$

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

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"?

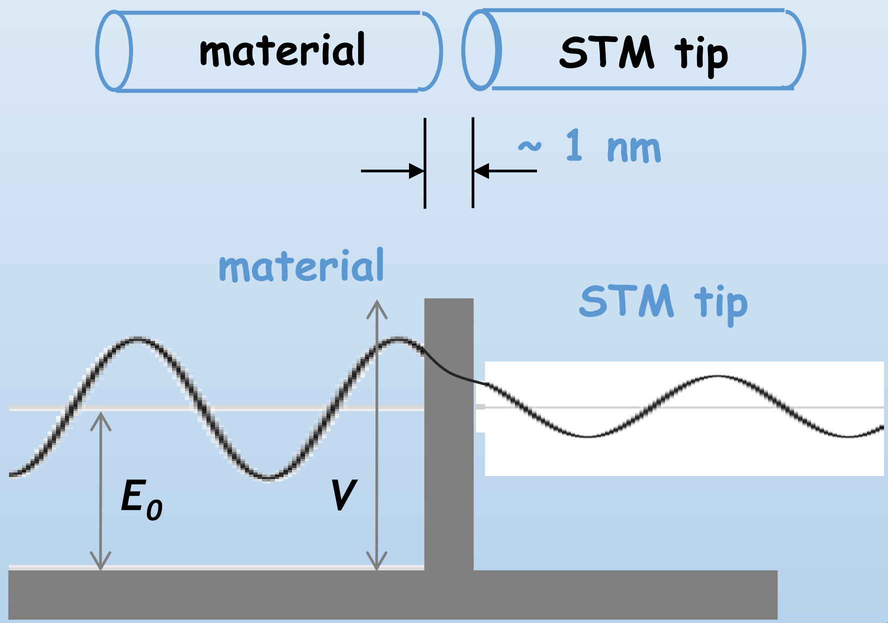
a. < initial energy
b. = initial energy
c. > initial energy

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

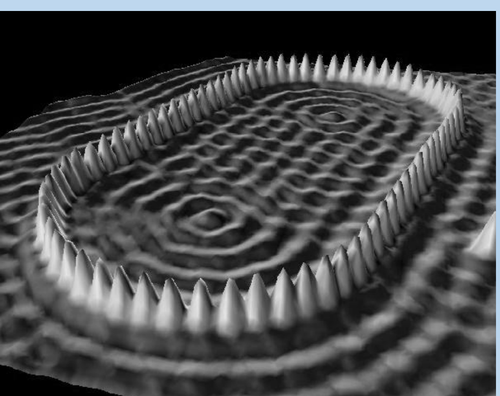
Application of Tunneling:
Scanning Tunneling Microscopy (STM)

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:

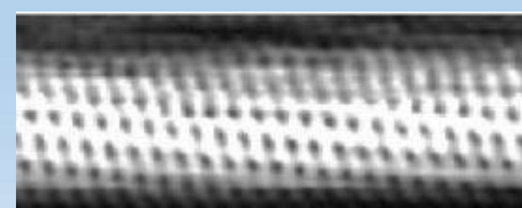


Image is in the public domain

Reflection of EM Waves and QM Waves

$$P = \hbar\omega \times \frac{\text{photons}}{\text{s cm}^2}$$

$$P = \frac{|E|^2}{\eta}$$

$$R = \frac{P_{reflected}}{P_{incident}} = \left|\frac{E_o^r}{E_o^i}\right|^2$$

Then for optical material when $\mu=\mu_0$:

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

$$= \left|\frac{n_1 + n_2}{n_1 + n_2}\right|^2$$

= probability of a particular photon being reflected

$$J = q \times \frac{\text{electrons}}{\text{s cm}^2}$$

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

$$R = \frac{J_{reflected}}{J_{incident}} = \frac{|\psi_B|^2}{|\psi_A|^2}$$

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

= probability of a particular electron being reflected