Introduction to Quantum Mechanics

Lecture I

Ajay Nath

Evaluation

Mid-semester: (Completed)	30% (10% online + 10% online + 10% remote)
Continuous Evaluation:	25% (includes quizzes along with surprise tests, assignments etc.)
End-semester:	45%

Mid Semester Exam (wt. = 30%)			CA Quiz	End Semester Exam (wt. = 45%)		
Session 1 Online/	Session 2 Remote	Total Marks	Online	MCQ Online	Session 3 Remote	Total Marks
20% Third Week Sixth Week	10% 25-29 January 2021	30	10% Ninth Week	15% Twelfth Week	15% + 15% 22^{nd} -27^{th} March, 2021	ES

Syllabus

• *Introduction to Quantum Mechanics-* Failure of classical mechanics, Double-slit experiment, de Broglie's hypothesis. Uncertainty Principle, Wave-Function and Wave-Packets, Phase- and Group-velocities. Schrödinger Equation. Probabilities and Normalization. Expectation values. Eigenvalues and Eigen functions. Applications of Schrödinger Equation: Particle in a box, Finite Potential well, Harmonic oscillator, Hydrogen Atom problem.

Concepts of Modern Physics	A. Beiser, Sixth Edition.

Thermodynamics: (Prof. Sunil K Sarangi)

Temperature and Zeroth Law of Thermodynamics, Work, Heat and First Law of Thermodynamics, Ideal Gas and Heat Capacities, Second Law of Thermodynamics, Carnot Cycle, Entropy, Thermodynamic variables and energies.

Heat and Thermodynamics	M. W. Zemansky and R. H. Dittman, Seventh Edition.

The more important fundamental laws and facts of physical science have all been discovered, and these are now so firmly established that the possibility of their ever being supplanted in consequence of new discoveries is exceedingly remote. . . . Our future discoveries must be looked for in the sixth place of decimals.

Albert A. Michelson, 1894

There is nothing new to be discovered in physics now. All that remains is more and more precise measurement.

William Thomson (Lord Kelvin), 1900

Triumph of Classical Physics: The Conservation Laws

- **Conservation of energy**: The total sum of energy (in all its forms) is conserved in all interactions.
- **Conservation of linear momentum**: In the absence of external forces, linear momentum is conserved in all interactions.
- **Conservation of angular momentum**: In the absence of external torque, angular momentum is conserved in all interactions.
- **Conservation of charge**: Electric charge is conserved in all interactions.

Classical Physics of the 1890s

Mechanics

Newton's Laws of Motion

$$\vec{F} = m\vec{a} \quad \text{or} \quad \vec{F} = \frac{d\vec{p}}{dt}$$

$$\vec{F}_{21} = -\vec{F}_{12}$$

Electromagnetism

$$\oint \vec{E} \cdot d\vec{A} = \frac{q}{\varepsilon_0}$$

$$\oint \vec{B} \cdot d\vec{A} = 0$$

$$\oint \vec{E} \cdot d\vec{s} = -\frac{d\Phi_B}{dt}$$

$$\oint \vec{B} \cdot d\vec{s} = \mu_0 \varepsilon_0 \frac{d\Phi_E}{dt} + \mu_0 I$$

Thermodynamics

- **First law**: The change in the internal energy ΔU of a system is equal to the heat Q added to a system plus the work W done by the system

  $$\Delta U = Q + W$$

- **Second law**: It is not possible to convert heat completely into work without some other change taking place.
- **The "zeroth" law**: Two systems in thermal equilibrium with a third system are in thermal equilibrium with each other.
- **Third law**: It is not possible to achieve an absolute zero temperature

No idea about condensed matter, why do gold and iron have vastly different properties?? No rational way of designing materials for some specific purpose …

Waves and Particles

Two ways in which energy is transported:

Point mass interaction: transfers of momentum and kinetic energy: *particles*

Extended regions wherein energy transfers by way of vibrations are observed: *waves*

Two distinct phenomena describing physical interactions

- Both require "Newtonian mass"
- Particles in the form of point masses and waves in the form of perturbation in a mass distribution, i.e., a material medium
- The distinctions are observationally quite clear; however, not so for the case of visible light
- Thus by the 17th century begins the major disagreement concerning the nature of light

Newton promotes the corpuscular (particle) theory

- Particles of light travel in straight lines or rays
- Explains reflection and refraction

Christian Huygens promotes the wave theory

- Light propagates as a wave of concentric circles from the point of origin
- Explains reflection and refraction

The Wave Theory Advances…

- Contributions by Huygens, Young, Fresnel and **Maxwell**
- Double-slit interference patterns
- Refraction of light from air into a liquid, a spoon appears to be bend
- ***Light is an electromagnetic phenomenon***
- ***Establishes that light propagates as a wave***

- *Problem: all other waves need a medium to travel in, light also travels in a vacuum*
- Visible light covers only a small range of the total electromagnetic spectrum. All electromagnetic waves travel in a vacuum with a speed *c* given by:

$$c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}} = \lambda f$$

(where μ_0 and ε_0 are the respective permeability and permittivity of “free” space)

Electromagnetic waves can have very different wavelengths and frequencies, but they all travel with the speed of light

Unresolved Questions of 1895 and New Horizons

- The atomic theory controversy raises fundamental questions
  - Revolutionary idea, properties of matter should be due to their structure (rather than their very nature)

Three fundamental problems:

- The necessity of the existence of an “electromagnetic medium” for light waves to travel in
- The problem of observed differences in the electric and magnetic field between stationary and moving reference systems
- The failure of classical physics to explain blackbody radiation – modern physics starts from the necessity of energy in bound systems to be quantized in order for Max Planck’s theory to fit experimental data over a very large range of wavelengths

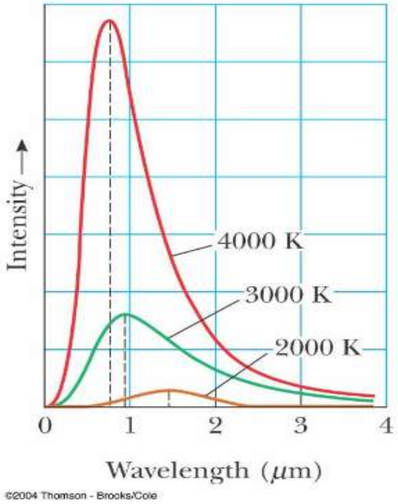
Additional discoveries that complicate classical physics interpretations

- Discovery of x-rays (1895), Discovery of radioactivity (1896), Discovery of the electron (1897), Discovery of the Zeeman effect (1897)

Blackbody Radiation Problem:

- Hot filament glows.
- Classical physics cant explain the observed wavelength distribution of EM radiation from such a hot object.
- This problem is historically the problem that leads to the rise of quantum physics during the turn of 20th century

- The intensity increases with increasing temperature
- The amount of radiation emitted increases with increasing temperature
  - The area under the curve
- The peak wavelength decreases with increasing temperature

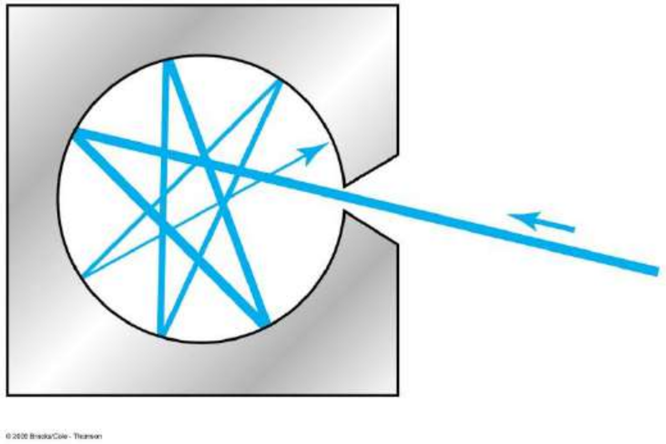


- An object at any temperature is known to emit thermal radiation
  - Characteristics depend on the temperature and surface properties
  - The thermal radiation consists of a continuous distribution of wavelengths from all portions of the em spectrum

- At room temperature, the wavelengths of the thermal radiation are mainly in the infrared region
- As the surface temperature increases, the wavelength changes
  - It will glow red and eventually white
- The basic problem was in understanding the observed distribution in the radiation emitted by a black body
  - Classical physics didn't adequately describe the observed distribution

Blackbody Radiation Problem

- When matter is heated, it emits radiation.
- A blackbody is a cavity in a material that only emits thermal radiation. Incoming radiation is absorbed in the cavity. Material is dense, so we expect a continuous spectrum



emissivity є (є = 1 for idealized black body)

- Blackbody radiation is interesting because the radiation properties of the blackbody are independent of the particular material! Physicists can study the distribution of intensity versus wavelength (or frequency) at fixed temperatures. Principle of a pyrometer to measure temperatures remotely.

Stefan-Boltzmann Law

- Empirically, total power radiated (per unit area and unit wavelength = m^{-3}) increases with temperature to power of 4: also intensity (funny symbol in Thornton-Rex)

would be very interesting to know this function (intensity as a function of λ and T)

$$R(T) = \int_0^\infty \mathcal{I}(\lambda, T)\, d\lambda = \epsilon\, \sigma T^4$$

Watt per m^2

- This is known as the **Stefan-Boltzmann law**, with the constant *σ* experimentally measured to be 5.6705 × 10^{-8} W / (m^2 · K^4), Boltzmann derived the “form” of the empirical formula from classical physics statistics, it was not understood what the constant of proportionality actually meant

- The **emissivity** ϵ (ϵ = 1 for an idealized black body) is simply the ratio of the emissive power of an object to that of an ideal blackbody and is always less than 1.

Wien’s Displacement Law

- The intensity (λ, *T*) is the total power radiated per unit area per unit wavelength at a given temperature.
- **Wien’s displacement law**: The maximum of the distribution shifts to smaller wavelengths as the temperature is increased.

$$\lambda_{\max} T = 2.898 \times 10^{-3}\ \mathrm{m \cdot K}$$

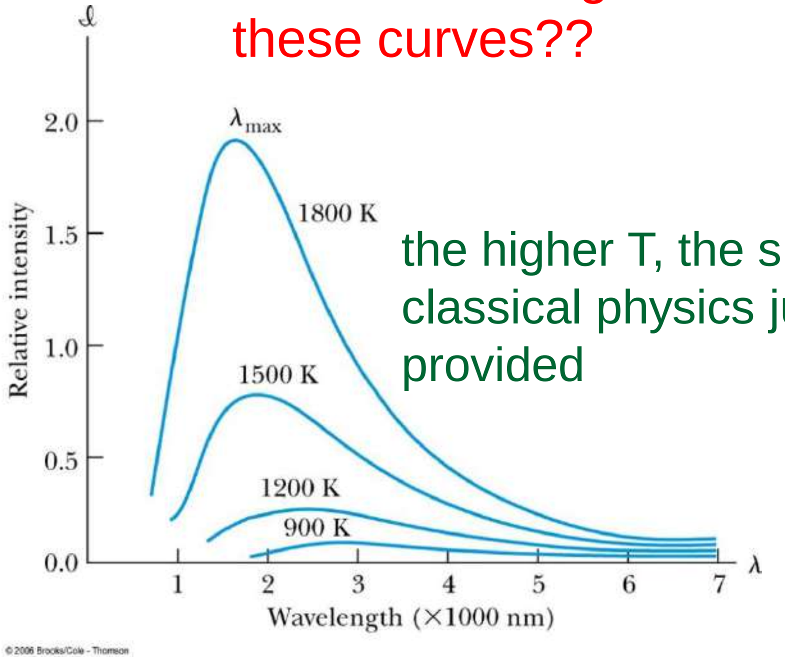
Power = Current times Voltage,
Time derivative of mechanical work, unit of watt

Energy density u(T) = $^4/_c\ \varepsilon\ \sigma\ T^4$ in Ws m^{-3}

Most interesting, what is the mathematical function that describes all of these curves??

$\mathcal{I}$

Wm^{-2}



the higher T, the shorter λ, no classical physics justification provided

Unit of intensity Watt per area

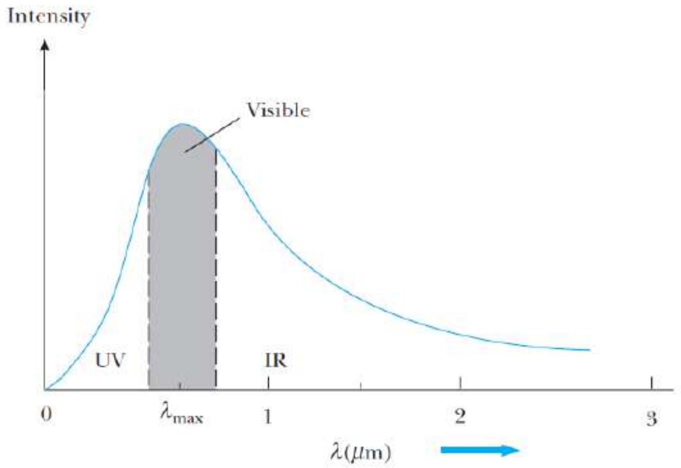


Figure 4.14 Intensity versus wavelength for a body heated to 6000 K.

So that must be approximately the black body radiation from the sun.

Why are our eyes particularly sensitive to green light of 550 nm? Because life evolved on earth receiving radiation from the sun that peaks at this particular wavelength.

https://phet.colorado.edu/sims/html/blackbody-spectrum/latest/blackbody-spectrum_en.html

Thank You

Introduction to Quantum Mechanics

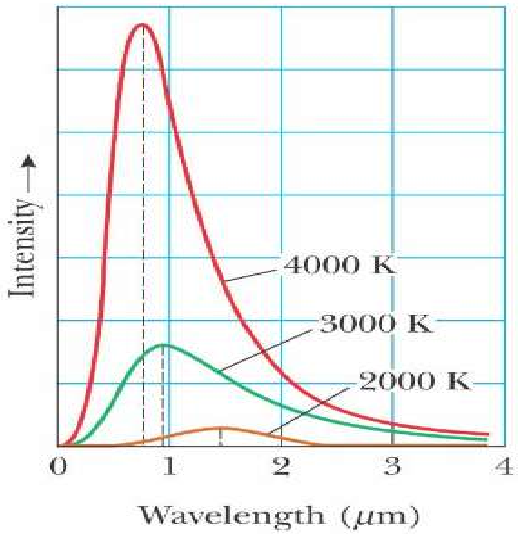
Lecture II

Ajay Nath

Blackbody Radiation Problem:

- When matter is heated, it emits radiation. A blackbody is a cavity in a material that only emits thermal radiation. Incoming radiation is absorbed in the cavity. Material is dense, so we expect a continuous spectrum.
- Blackbody radiation is interesting because the radiation properties of the blackbody are independent of the particular material! Physicists can study the distribution of intensity versus wavelength (or frequency) at fixed temperatures.

- The intensity increases with increasing temperature
- The amount of radiation emitted increases with increasing temperature
  - The area under the curve
- The peak wavelength decreases with increasing temperature



Rayleigh-Jeans Formula

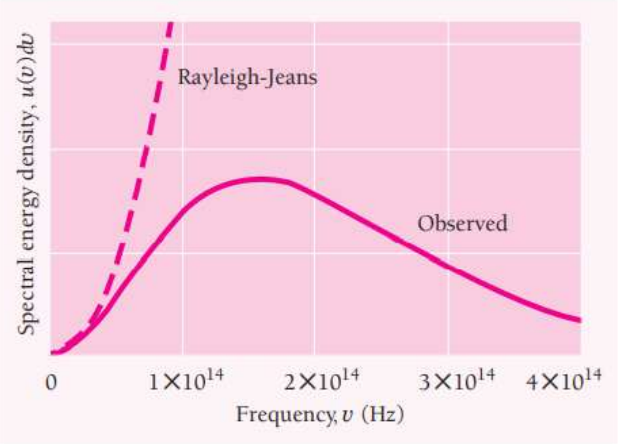
- Lord Rayleigh (John Strutt) and James Jeans used the classical theories of electromagnetism and thermodynamics to show that the blackbody spectral distribution should be, 1905

Rayleigh-Jeans formula

$$u(\nu)\,d\nu = \bar{\epsilon}G(\nu)\,d\nu = \frac{8\pi kT}{c^3}\nu^2\,d\nu$$

With k as Boltzmann constant: 1.38065 10^{-23} J/K

kT at room temperature (293 K) ≈ 25 meV



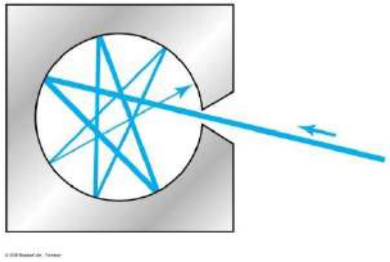
- It approaches the data at longer wavelengths, but it deviates very badly at short wavelengths. This problem for small wavelengths became known as “the ultraviolet catastrophe” and was one of the outstanding problems that classical physics could not explain around 1900s.

How Rayleigh-Jeans Formula calculated?

Consider a blackbody as a radiation-filled cavity at the temperature T. Because the cavity walls are assumed to be perfect reflectors, the radiation must consist of standing em waves.

In order for a node to occur at each wall, the path length from wall to wall, in any direction, must be an integral number *j* of half wavelengths.

If the cavity is a cube L long on each edge, this condition means that for standing waves in the *x, y,* and *z* directions respectively, the possible wavelengths are such that



$$j_x = \frac{2L}{\lambda} = 1, 2, 3, \ldots = \text{number of half-wavelengths in } x \text{ direction}$$

$$j_y = \frac{2L}{\lambda} = 1, 2, 3, \ldots = \text{number of half-wavelengths in } y \text{ direction}$$

$$j_z = \frac{2L}{\lambda} = 1, 2, 3, \ldots = \text{number of half-wavelengths in } z \text{ direction}$$

For a standing wave in any arbitrary direction, it must be true that

Standing waves in a cubic cavity

$$j_x^2 + j_y^2 + j_z^2 = \left(\frac{2L}{\lambda}\right)^2 \qquad \begin{aligned} j_x &= 0, 1, 2, \ldots \\ j_y &= 0, 1, 2, \ldots \\ j_z &= 0, 1, 2, \ldots \end{aligned}$$

To count the number of standing waves $g(\lambda)\,d\lambda$ within the cavity whose wavelengths lie between λ and $\lambda + d\lambda$, what we have to do is count the number of permissible sets of j_x, j_y, j_z values that yield wavelengths in this interval. Let us imagine a j-space whose coordinate axes are $j_x, j_y,$ *and* j_z; Fig shows part of the j_x-j_y plane of such a space. Each point in the j-space corresponds to a permissible set of j_x, j_y, j_z values and thus to a standing wave. If **j** is a vector from the origin to a particular point j_x, j_y, j_z, its magnitude is

$$j = \sqrt{j_x^2 + j_y^2 + j_z^2}$$

The total number of wavelengths between λ and $\lambda + d\lambda$ is the same as the number of points in j space whose distances from the origin lie between j and $j + dj$. The volume of a spherical shell of radius j and thickness dj is $4\pi j^2\,dj$, but we are only interested in the octant of this shell that includes non-negative values of $j_x, j_y,$ and j_z. Also, for each standing wave counted in this way, there are two perpendicular

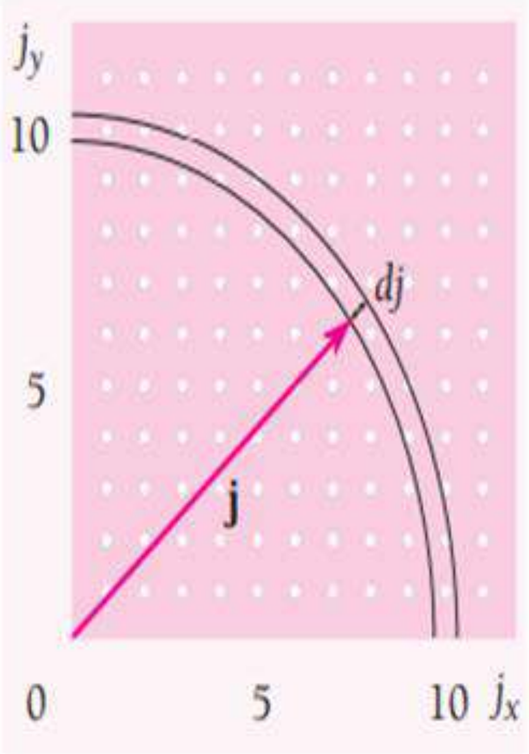


Figure Each point in j space corresponds to a possible standing wave.

directions of polarization. Hence the number of independent standing waves in the cavity is

Number of standing waves

$$g(j)\,dj = (2)(\tfrac{1}{8})(4\pi j^2\,dj) = \pi j^2\,dj$$

What we really want is the number of standing waves in the cavity as a function of their frequency ν instead of as a function of j. From Eqs. (9.31) and (9.32) we have

$$j = \frac{2L}{\lambda} = \frac{2L\nu}{c} \qquad dj = \frac{2L}{c}\,d\nu$$

and so

Number of standing waves

$$g(\nu)\,d\nu = \pi\left(\frac{2L\nu}{c}\right)^2 \frac{2L}{c}\,d\nu = \frac{8\pi L^3}{c^3}\nu^2\,d\nu$$

The cavity volume is L^3, which means that the number of independent standing waves per unit volume is

Density of standing waves in a cavity

$$G(\nu)\,d\nu = \frac{1}{L^3}\,g(\nu)\,d\nu = \frac{8\pi\nu^2\,d\nu}{c^3}$$

The next step is to find the average energy per standing wave. According to the **theorem of equipartition of energy,** a mainstay of classical physics, the average energy per degree of freedom of an entity (such as a molecule of an ideal gas) that is a member of a system of such entities in thermal equilibrium at the temperature T is $\frac{1}{2}kT$. Here k is **Boltzmann's constant:**

Boltzmann's constant $$k = 1.381 \times 10^{-23}\ \text{J/K}$$

A degree of freedom is a mode of energy possession. Thus a monatomic ideal gas molecule has three degrees of freedom, corresponding to kinetic energy of motion in three independent directions, for an average total energy of $\frac{3}{2}kT$.

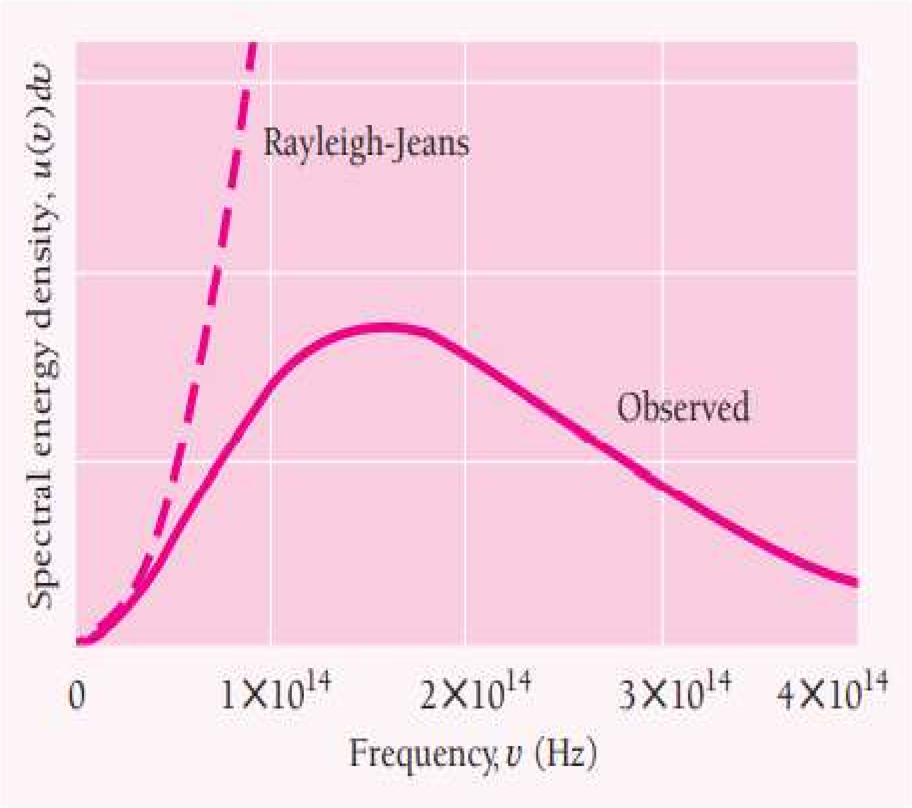
A one-dimensional harmonic oscillator has two degrees of freedom, one that corresponds to its kinetic energy and one that corresponds to its potential energy. Because each standing wave in a cavity originates in an oscillating electric charge in the cavity wall, two degrees of freedom are associated with the wave and it should have an average energy of $2(\frac{1}{2})kT$:

Classical average energy per standing wave $$\overline{\epsilon} = kT$$

The total energy $u(\nu)\,d\nu$ per unit volume in the cavity in the frequency interval from ν to $\nu + d\nu$ is therefore

Rayleigh-Jeans formula $$u(\nu)\,d\nu = \overline{\epsilon}G(\nu)\,d\nu = \frac{8\pi kT}{c^3}\nu^2\,d\nu$$

Ultraviolet Catastrophe



Planck Radiation Formula

In 1900 the German physicist Max Planck used "lucky guesswork" (as he later called it) to come up with a formula for the spectral energy density of blackbody radiation:

Planck radiation formula

$$u(\nu)\,d\nu = \frac{8\pi h}{c^3}\frac{\nu^3\,d\nu}{e^{h\nu/kT} - 1}$$

Here h is a constant whose value is

Planck's constant

$$h = 6.626 \times 10^{-34}\ \mathrm{J \cdot s}$$

At high frequencies, $h\nu \gg kT$ and $e^{h\nu/kT} \to \infty$, which means that $u(\nu)\, d\nu \to 0$ as observed. No more ultraviolet catastrophe. At low frequencies, where the Rayleigh-Jeans formula is a good approximation to the data , $h\nu \ll kT$ and $h\nu/kT \ll 1$. In general,

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

If x is small, $e^x \approx 1 + x$, and so for $h\nu/kT \ll 1$ we have

$$\frac{1}{e^{h\nu/kT} - 1} \approx \frac{1}{1 + \frac{h\nu}{kT} - 1} \approx \frac{kT}{h\nu} \qquad h\nu \ll kT$$

Thus at low frequencies Planck's formula becomes

$$u(\nu)\, d\nu \approx \frac{8\pi h}{c^3} \nu^3 \left(\frac{kT}{h\nu} \right) d\nu \approx \frac{8\pi kT}{c^3} \nu^2\, d\nu$$

which is the Rayleigh-Jeans formula. Planck's formula is clearly at least on the right track; in fact, it has turned out to be completely correct.

Thank You

Quantum Mechanics

↳ newtonian mechanics

• m → Fext
(x, t)

t,
• x,
m

(approach for day to day life)

can be determined by newton's law and laws of motion and other things

↳ but when we talk about microscopic domain, where debroglie wavelength of body will become comparable to its bodies momentum and other things, In that domain, classical mechanics fails and we have to analyse the system on the basis of quantum mechanics.

Basic core Idea of Quantum mechanics :-

"Probabilistic"
never sure that where my particle is located, there will be always uncertainty in measurement of position of body at any time t.

in b/w

0 ——— 1

↓

Location of body.

classical mechanics ⇒ 0 or 1

quantum mechanics ⇒ 0 or 1 or in b/w (0,1)

triumph of classical physics :-

- Conservation of Energy
- Conservation of linear momentum
- Conservation of Angular momentum
- Conservation of charge.

lecture 4

#

- Black body Problem :- plank's distribution law

$$\boxed{E = nh\nu}$$

- light has particle nature (photoelectric effect)

Double - slit Experiment

- used to study the effect of Interference

- $I = |E|^2$ $E \rightarrow$ Electric field

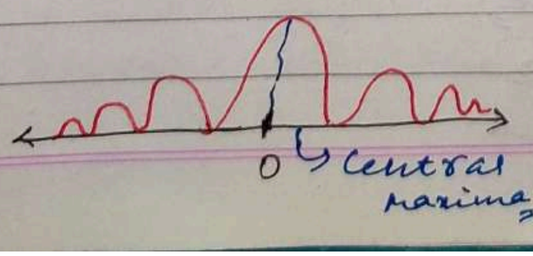
$$= |E_1 + E_2|^2 = E_1^2 + E_2^2 + 2E_1E_2$$

$$= I_1 + I_2 + 2\sqrt{I_1 \cdot I_2}$$

$(I_1 = E_1^2)$
$(I_2 = E_2^2)$

Interference $\rightarrow$ Two waves superimposes to form a Result wave of greater, lower or same Amplitude

diffraction $\rightarrow$ Bending of waves when it encounters an obstacle or opening.



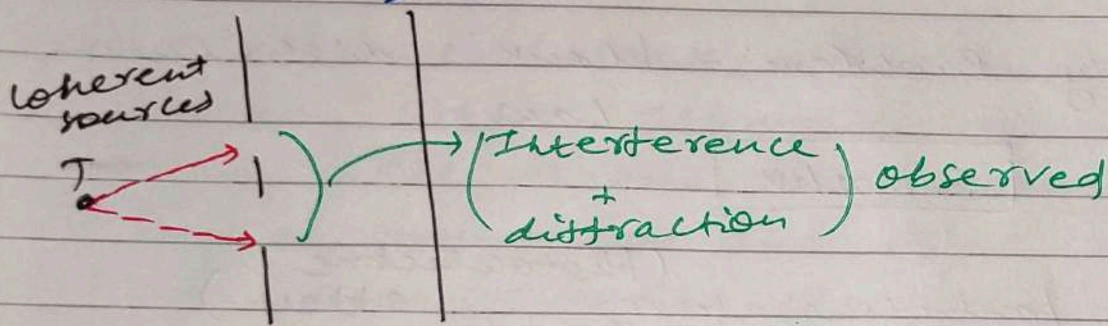
↳ Constructive Interference

$$d\sin\theta = m\lambda \quad m = 0, \pm1, \pm2, ---$$

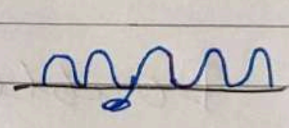
↳ Destructive Interference

$$d\sin\theta = \left(m+\frac{1}{2}\right)\lambda \quad m = 0, \pm1, \pm2, ---$$

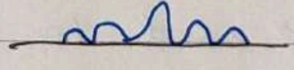
Consider light as wave:-



↳ $I = I_0 \cos^2\frac{\phi}{2}$ (Interference)



↳ $I = \frac{I_0 \sin\phi}{\phi_0}$ (diffraction)



$$\boxed{\phi = \frac{\pi a \sin\phi}{\lambda}}$$

↳ $I \propto E^2$ (wave nature)

Consider light as particle:-

↳ $E = nh\nu$

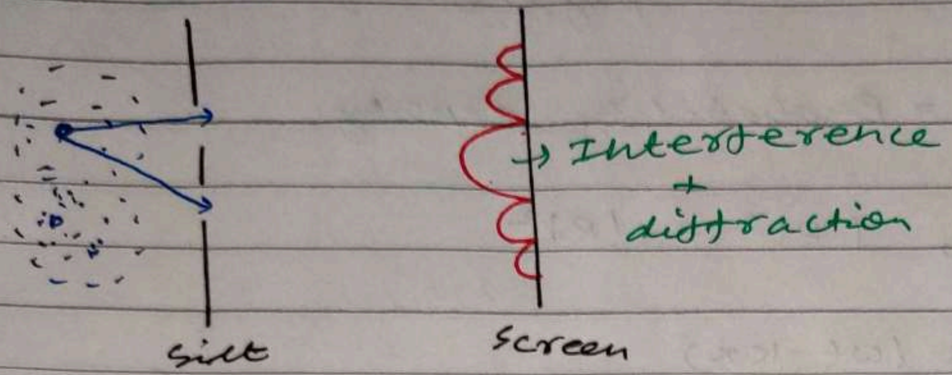
↳ no. of photons

Relation b/w light as particle and wave:-

↳ The number of photons present in the particle nature are connected with average strength of the electric field present in the wave nature.

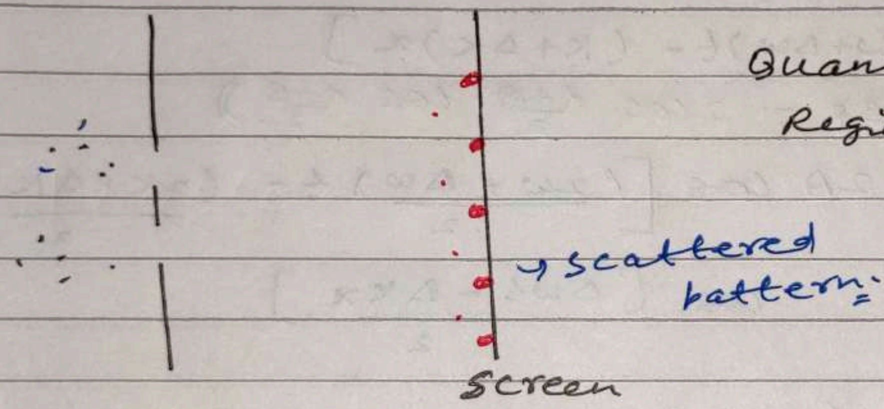
$$\boxed{N \rightarrow \bar{E}^2}$$

$n \to$ large no. of photons



Classical Regime

$n \to$ small no. of photons



Quantum Regime

↳ wave shows particle nature.

photoelectric.

↳ Debroglie hypothesis.

→ particle also shows wave nature.

$$\boxed{\lambda_B = \frac{h}{p} = \frac{h}{\gamma m v}}$$

$$\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$$

sound waves → Variation of pressure
water waves → Variation of height of water
light waves → Variation of Electric & magnetic field

matter waves → $\underbrace{\psi(x, y, z, t)}$ ← contains Real & complex

↳ no physical signidance

↳ $\psi \cdot \psi^* = |\psi|^2$ = Probability density

↳ If $\psi = Re^{i\theta}$, $|\psi|^2 = |R|^2$

$$\psi_1(x,t) = A \cos(\omega t - kx)$$

$$V = \frac{\omega}{k} = \frac{2\pi f}{2\pi/\lambda} = \lambda f = \frac{\lambda}{T}$$

$$\psi_2(x,t) = A\cos\left[(\omega+\Delta\omega)t - (k+\Delta k)x\right]$$

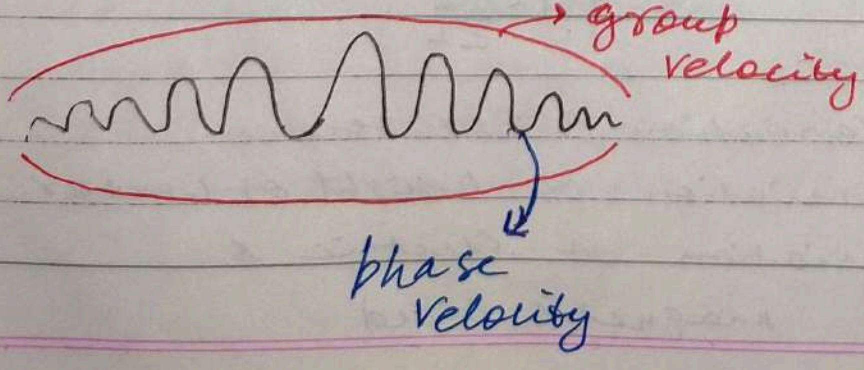
$$\left(\cos\alpha + \cos\beta = 2\cos\frac{\alpha+\beta}{2}\cos\frac{\alpha-\beta}{2}\right)$$

$$\psi = \psi_1 + \psi_2 = 2A\cos\left[\frac{(2\omega+\Delta\omega)}{2}t - \frac{(2k+\Delta k)}{2}\right] \cos\left[\frac{\Delta\omega t - \Delta k x}{2}\right]$$

$2\omega + \Delta\omega \simeq 2\omega$
$2k + \Delta k \simeq 2k$
$\left\{ \text{as } \Delta\omega > \omega, \ \Delta k > k \right\}$

$$= 2A\cos\underbrace{(\omega t - kx)}_{\text{phase velocity}} \cos\underbrace{\left(\frac{\Delta\omega t}{2} - \frac{\Delta k x}{2}\right)}_{\text{group velocity}}$$

$V_p = \frac{\omega}{k}$ $\qquad$ $V_g = \frac{\Delta\omega}{\Delta k}$



$\hookrightarrow \omega = \frac{2\pi}{T} = 2\pi\nu$

$\hookrightarrow E = h\nu = \gamma mc^2$

$\Big\} \rightarrow \nu = \frac{\gamma mc^2}{h}$

$\hookrightarrow K = \frac{2\pi}{\lambda}$

$\hookrightarrow \lambda_B = \frac{h}{p} = \frac{h}{\gamma mv}$

$\Big\} \rightarrow K = \frac{2\pi}{h}\gamma mv$

$$V_p = \frac{\omega}{K} = \frac{2\pi\gamma mc^2/h}{2\pi\gamma mv/h} = \frac{c^2}{v} \qquad \boxed{V_p = \frac{c^2}{v}}$$

$v_g = \frac{d\omega}{dK}$; $\omega(v) = \frac{2\pi mc^2}{h}\sqrt{1-\frac{v^2}{c^2}}$

$K(v) = \frac{2\pi m}{h} \frac{v}{\sqrt{1-v^2/c^2}}$

$\therefore v_g = \frac{d\omega}{dv} \cdot \frac{1}{\frac{dK}{dv}}$ $\hookrightarrow \frac{d\omega}{dv} = \frac{2\pi mc^2}{h}\left(\frac{-1}{2}\right)\frac{-2v/c^2}{\left(1-\frac{v^2}{c^2}\right)^{3/2}}$

$= \frac{2\pi m}{h} \cdot \frac{v}{(1-v^2/c^2)^{3/2}}$

$\hookrightarrow \frac{dK}{dv} = \frac{2\pi m}{h}\left[\frac{1}{\sqrt{1-v^2/c^2}} + v\left(\frac{-1}{2}\right)\frac{2v/c^2}{(1-v^2/c^2)^{3/2}}\right]$

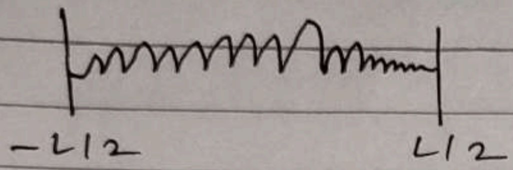
$= \frac{2\pi m}{h}\left[\frac{1-\cancel{v^2/c^2}+\cancel{v^2/c^2}}{(1-v^2/c^2)^{3/2}}\right]$

$= \frac{2\pi m}{h}$

$$\frac{d\omega}{dK} = \frac{d\omega/dv}{dK/dv} = \frac{2\pi m}{h} \cdot \frac{v}{(1-v^2/c^2)^{3/2}} \frac{h \cdot (1-v^2/c^2)^{3/2}}{2\pi m} = V$$

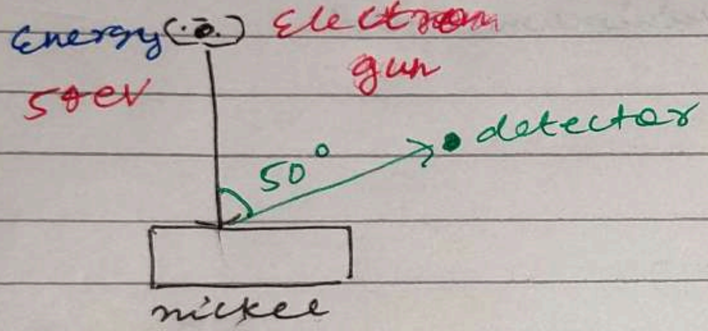
$$\boxed{V_p = \frac{c^2}{v} \quad , \quad V_g = v \quad , \quad V_p \cdot V_g = c^2}$$

#



$$\int_{-L/2}^{L/2} |\psi|^2 \cdot dx = 1$$

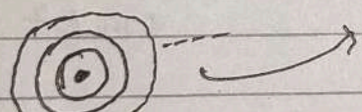
matter waves :- davisson - germer Experiment



↳ Its scattering of e⁻ particles will be independent of energy of electron gun.

↳ at 54eV at an angle of diffraction = 50°, a maximum Intensity is formed.

↳ wave characteristics.



(diffraction)

Inter Lattice distance = 0.091 nm

↳ Bragg's diffraction :- $n\lambda = 2d\sin\theta$

$\theta = 65°$, $n = 1$, $d \to$ given

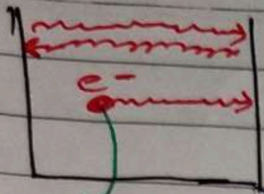
$\boxed{\hookrightarrow \lambda = 0.165\,nm}$

↳ $p = \sqrt{2m(K.E)} = \ldots$

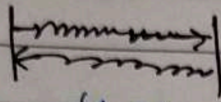
$\boxed{\lambda = \frac{h}{p} \approx 0.166\,nm.}$

↳ Validation of matter waves of particle

particle in a box



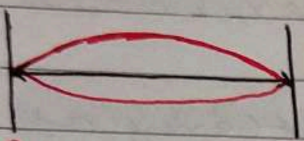
matter waves



$\rightarrow$ Energy ??

↳ standing waves

$\sin(Kx - \omega t) + \sin(Kx + \omega t)$

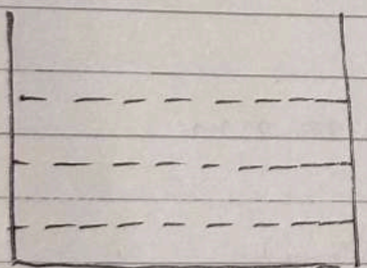
↳ 

$\frac{\lambda}{2} = L$ (minimum mode)

$n\lambda = 2L$, $n = 1, 2, ---$

$KE = \frac{1}{2} mv^2 = \frac{1}{2} \frac{(mv)^2}{m} = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$

$$\boxed{E = \frac{n^2 h^2}{8mL^2}} ; n = 1, 2, 3 --- \qquad = \frac{n^2 h^2}{8mL^2}$$



↳ for being $E = 0$, $E = \frac{1}{2} mv^2$, $m \neq 0$

not possible (E = 0)

$\lambda = \frac{h}{mv \to 0}$, $\lambda \to \infty$

Heisenburg's

uncertainity principle

$m \to$ travelling with p $\qquad \lambda_{dB} = \frac{h}{p}$

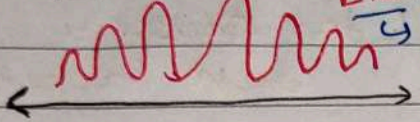
$\boxed{\bullet}$ $E \to$ quantized

↳ 1917, Heisenburg,

$\Delta\lambda \to$ small

$\Delta x =$ Large

↳ uncertainity in position

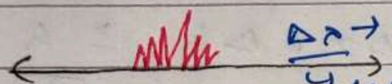


$\Delta K = \frac{2\pi}{\Delta\lambda}$

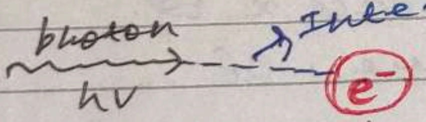
$\Delta x \to$ small

$\Delta\lambda \to$ Large

↳ uncertainity in wavelength



↳ It is impossible to measure position and momentum exactly at same time (simultaneously).



$\Delta p \approx \frac{h}{\lambda}$ $\qquad \Delta x \approx \lambda$

$\frac{h}{p}$ }

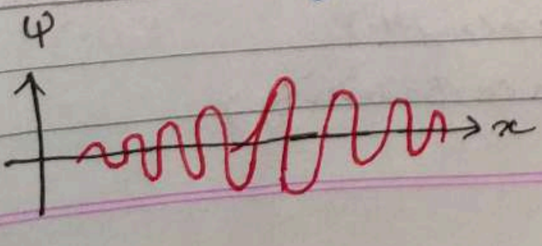
Initially having some momentum

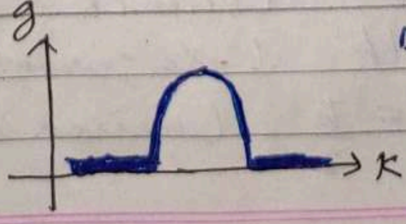
⇓

$\boxed{\Delta x \cdot \Delta p \approx h}$

↳ Heisenburg uncertainity principle

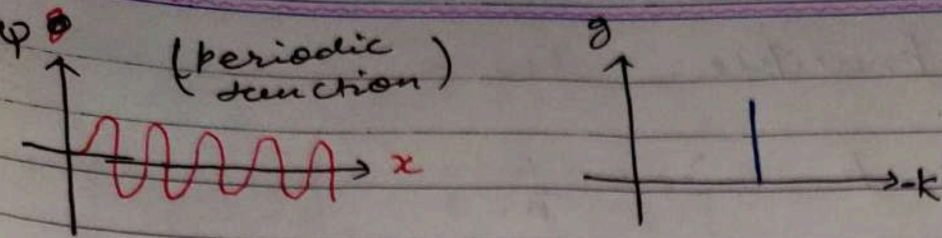
$\psi(x) = \int_0^\infty g(K) \cos Kx \cdot dx$

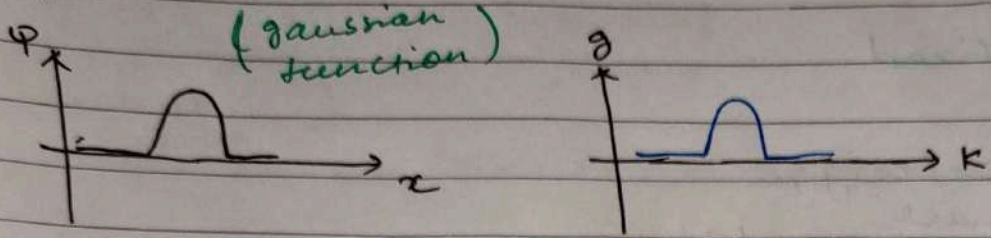




$\Delta x \to$ Small

$\Delta K \to$ Large





$$\boxed{\Delta x \cdot \Delta K = \frac{1}{2}}$$ (for gaussian wave packets)

$$K = \frac{2\pi}{\lambda} = \frac{2\pi p}{h}$$

$$\Delta p = \frac{h \Delta K}{2\pi} = \frac{h}{4\pi \cdot \Delta x} \Rightarrow \Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

$$\left(\hbar = \frac{h}{2\pi}\right) \Rightarrow \boxed{\Delta x \cdot \Delta p \geq \frac{\hbar}{2}}$$

↳ for gaussian, function, there is shape preservation ⇒ on changing space x to space k, shape remains same. If for that $\Delta p \cdot \Delta x = \frac{\hbar}{2}$,

↳ then for the other curves,

$$\Delta p \cdot \Delta x \geq \frac{h}{2}$$ (Because there shape will be different

↳ $E = nh\nu$ (planck's law)

$\lambda_{dB} = h/p$ (de-broglie wavelength)

$\Delta x \cdot \Delta p = \frac{\hbar}{2}$ (heisenberg uncertainity)

postulates of Quantum mechanics :-

$\psi(x, y, z, t) = A + iB$ } → wave function

$\psi(x, t) = \underbrace{Ae^{-i(\omega t - kx)}}_{1}$ } → $\hookrightarrow v = \frac{\omega}{k}$

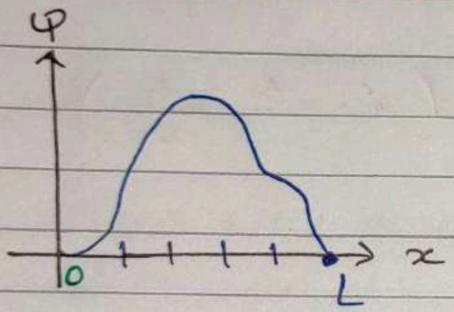
$= A[\cos(\ ) + i\sin(\ )]$

$\psi^* = A - iB$

↳ $\psi\psi^* = |\psi|^2 = A^2 + B^2$ = probability density.

ψ → not a physical meaning

$|\psi|^2$ → represent probability density



$\int_0^L |\psi|^2 \cdot dx = 1$

↳ normalization of wave function

$$\boxed{\int_{-\infty}^{\infty} |\psi|^2 \cdot dx = 1}$$

↳ ψ must be single valued.

↳ ψ must be continuous.

↳ $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial t}$ must be single valued and continuous.

↳ ψ must be Square Integrable.

} well-behaved wave function

$\psi(x, t) = Ae^{-i[\omega t - kx]}$

$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2}$ (wave equation)

LHS. $\frac{\partial^2\psi}{\partial x^2} = i^2k^2\psi = -k^2\psi$

RHS $\frac{1}{v^2}\cdot\frac{\partial^2\psi}{\partial t^2} = \frac{1}{v^2}\,-\omega^2\psi = -k^2\psi$

$\therefore$ LHS = RHS.

$\psi(x,t) = Ae^{-i[\omega t - kx]}$ ⇒ It is equation of wave.

& $\omega = 2\pi\nu$

$E = h\nu = \frac{2\pi h\nu}{2\pi} = \frac{\omega h}{2\pi} = \hbar\omega$ $\left(\because \hbar = \frac{h}{2\pi}\right)$

$$\boxed{2\pi\nu = \frac{E}{\hbar}}$$

& $k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}$ $\left(\because \hbar = \frac{h}{2\pi}\right)$

$$\boxed{k = \frac{p}{\hbar}}$$

$\psi(x,t) = Ae^{\frac{-i}{\hbar}[Et - px]}$

Energy = K.E + P.E ⇒ $\{E\psi = KE\,\psi + P.E\,\psi.\}$

$E\psi = \frac{p^2}{2m}\psi + U\psi$

$\frac{\partial^2\psi}{\partial x^2} = \left(\frac{ip}{\hbar}\right)^2\psi = -\frac{p^2}{\hbar^2}\psi$ ⇒ $\boxed{p^2\psi = -\hbar^2\cdot\frac{\partial^2\psi}{\partial x^2}}$

$\frac{\partial\psi}{\partial t} = \left(\frac{-iE}{\hbar}\right)\psi = E\psi = -\frac{\hbar}{i}\left(\frac{\partial\psi}{\partial t}\right) = i\hbar\frac{\partial\psi}{\partial t}$

$(i^2 = -1)$

↳ $$\boxed{i\hbar \cdot \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi}$$ → time dependent form of scrhodinger equation

$\psi(x,t) = Ae^{-\frac{i}{\hbar}[Et - px]}$

↓

$$i\hbar \cdot \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2} + U\psi$$

↳ $$\psi(x,t) = \underbrace{Ae^{\frac{ip}{\hbar}x}}_{\psi(x)} e^{-\frac{i}{\hbar}Et}$$

$$\psi(x,t) = \psi(x)\, e^{-\frac{i}{\hbar}Et}$$

↳ Schrodinger eqn can be written as :-

$\psi(x,t)$ / t ,

$$i\hbar \cdot \psi(x) \cdot \left(\frac{-iE}{\hbar}\right) e^{-\frac{i}{\hbar}Et}$$

$$= -\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2} \cdot e^{-\frac{i}{\hbar}Et}$$

$$+ U(x)\,\psi(x)\, e^{-\frac{iEt}{\hbar}}$$

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

↓

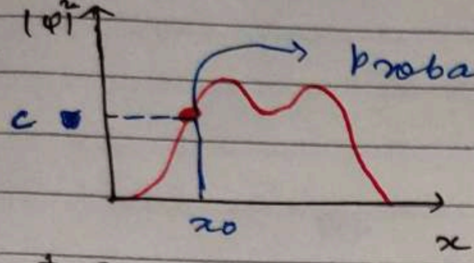
$$\boxed{\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0}$$

→ time Independent form of Schrodinger wave equation.

$\psi = Re^{-i\theta}$

$|\psi|^2 = \psi \psi^* = |\psi|^2 = |R|^2$ = probability density

#



probability of finding electron at $x_0 = c$;

$$\int_{-\infty}^{+\infty} |\psi|^2 = 1$$ } → normalization

$\psi(x,t) = Ae^{-\frac{i}{\hbar}[Et - px]}$

↳ Time-dependent form of Schrodinger wave eqⁿ:-

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

$\psi(x,t) = \psi(x)\, e^{-\frac{i}{\hbar}Et}$

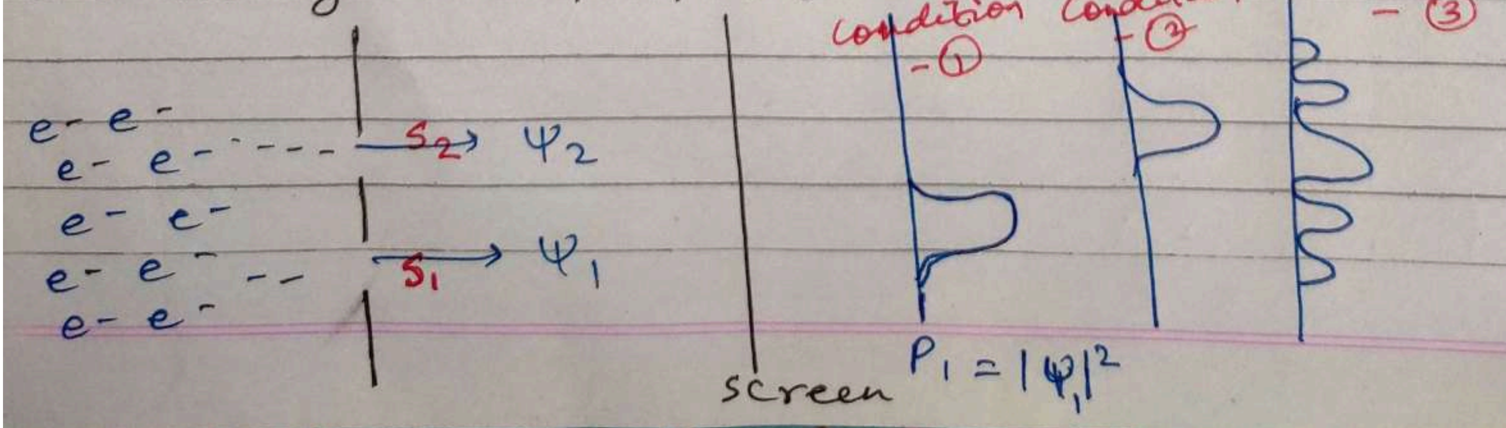
↳ time - Independent form of Schrodinger wave eqⁿ:

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi(x) = 0$$

(steady state solution of the system)

If $\psi_1(x)$, and $\psi_2(x)$ are the solⁿ (solution) of wave function then $a_1\psi_1(x) + a_2\psi_2(x)$, will also be the solⁿ of wave function;

Linearity & Superposition:-



condition 1 :- electron is allowed to pass through only slit 1.

condition 2 :- Electron is allowed to pass through only slit 2.

condition 3 :- Electron is allowed to pass through both slit 1 & 2.

$\psi = \psi_1 + \psi_2$

$$|\psi|^2 = (\psi_1+\psi_2)^* (\psi_1+\psi_2)$$
$$= \psi_1^*\psi_1 + \psi_1^*\psi_2 + \psi_2^*\psi_1 + \psi_2^*\psi_2$$
$$= |\psi_1|^2 + |\psi_2|^2 + \underbrace{\psi_1^*\psi_2 + \psi_2^*\psi_1}_{\text{Interference terms}}$$

postulates of Quantum mechanics

- $\psi \rightarrow$ Single-valued & continuous.
- $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial t} \rightarrow$ single valued & continuous.
- $\psi \rightarrow$ Square Integrable $\Rightarrow \underbrace{\int |\psi|^2 \cdot dx}_{\text{should be defined}}$

- Eigen function & Eigen value.

$\psi(x,t) = Ae^{-\frac{i}{\hbar}[Et - px]}$

$$\frac{\partial\psi}{\partial x} = \frac{ip}{\hbar}\psi \Rightarrow p\psi = \frac{\hbar}{i} \cdot \frac{\partial\psi}{\partial x} \Rightarrow \boxed{\hat{p} = \frac{\hbar}{i} \cdot \frac{\partial}{\partial x}}$$

momentum operator

$$\boxed{\hat{p}\ \psi(x,t) = a\ \psi(x,t)}$$

Eigen function

eigen value.

↳ $\frac{\partial \psi}{\partial t} = \frac{-iE}{\hbar}\psi \Rightarrow E\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = i\hbar \frac{\partial \psi}{\partial t}$

$$\boxed{\hat{E} = i\hbar \frac{\partial}{\partial t}}$$ → energy operator

Expectation value :-

$$\underset{\text{I}}{\langle x \rangle} = \frac{\int_{-\infty}^{+\infty} \psi^* x \psi \, dx}{\underbrace{\int_{-\infty}^{\infty} \psi^* \psi \cdot dx}_{\text{If it is 1}}} = \int_{-\infty}^{+\infty} \psi^* x \psi \cdot dx$$

average value of position

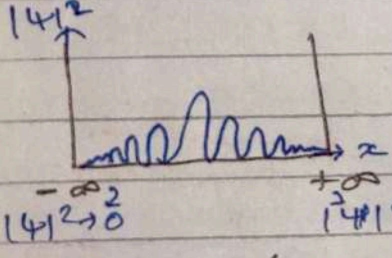
$$\langle p \rangle = \int_{-\infty}^{+\infty} \psi^* p \psi \cdot dx$$

$$= \int_{-\infty}^{+\infty} \psi^* \frac{\hbar}{i} \frac{\partial \psi}{\partial x} \cdot dx$$ → order of sequence is important

Case I

$$\langle p \rangle = -\frac{\hbar}{i} \int_{-\infty}^{+\infty} \frac{\partial}{\partial x} |\psi|^2 \cdot dx$$

$$= \frac{\hbar}{i} |\psi|^2 \Big|_{-\infty}^{+\infty} = 0$$ ✗ ~~not~~ possible



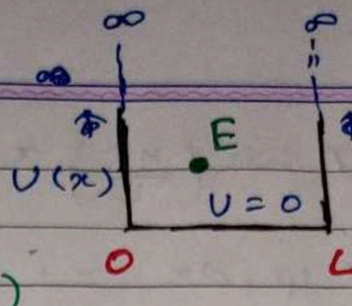
$x \to \infty^+ , \ \psi \to 0$

case-2

$$\langle p \rangle = \frac{\hbar}{i} \int \psi^* \psi \frac{\hbar}{i} \frac{\partial}{\partial x} \cdot dx$$ → meaningless

$$\boxed{\langle \hat{G} \rangle = \int_{-\infty}^{+\infty} \psi^* G \psi \cdot dx}$$ → sequence of ψ^*, G, ψ can't be changed for finding average value.

particle in a box :-



↳ ~~U(x)~~ $U = 0$ (Inside wall)

↳ find out ψ, Schrodinger eqⁿ, $\hat{\omega}\psi = a\psi$, $\langle\hat{\omega}\rangle =$

$$\Rightarrow \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - U]\psi = 0$$

(Independent Schrodinger wave eqⁿ)

$\underline{\underline{0 - L}}$: $U(x) = 0 \Rightarrow \dfrac{d^2\psi}{dx^2} + \dfrac{2m}{\hbar^2} E\psi = 0$

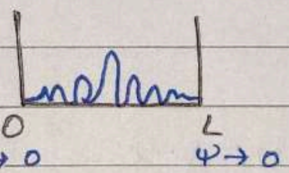
$(y'' + ay = 0 \Rightarrow y = A\cos\omega t + B\sin\omega t, \; a = \omega^2)$

$$\psi(x) = A\sin\frac{\sqrt{2mE}}{\hbar}x + B\cos\frac{\sqrt{2mE}}{\hbar}x$$

- Boundary conditions :-

↳ $x = 0$, $\psi(0) = 0$

↳ $x = L$, $\psi(L) = 0$



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

$\psi(L) = A\sin\dfrac{\sqrt{2mE}}{\hbar}L = 0$, $A \neq 0$

because we want non-trivial solution

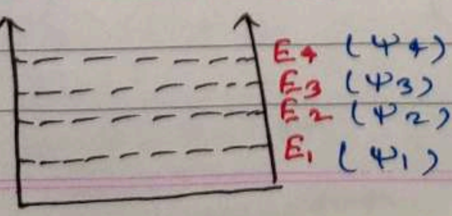
(If, $A, B = 0$, then we get trivial solⁿ.)

$(\sin n\pi = 0; \; n = 1, 2, ---)$

$$\frac{\sqrt{2mE}}{\hbar} \cdot L = n\pi$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$$

→ Energy is Quantized. ; $n = 1, 2, ----$



$$\psi(x) = A \sin\left(\frac{n\pi}{L}\right) x$$

$$\Rightarrow \int_{-\infty}^{+\infty} \psi^* \psi \cdot dx = 1 \quad \text{(normalization condition)}$$

$$\Rightarrow A^2 \int_0^L \sin^2\left(\frac{n\pi}{L}\right) x \cdot dx = 1$$

$$\Rightarrow A^2 \cdot \frac{L}{2} = 1 \Rightarrow A^2 = \frac{2}{L}$$

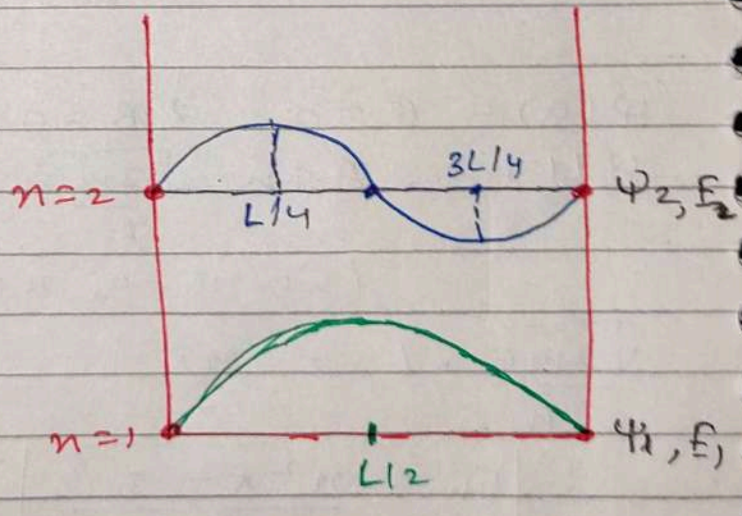
$$\Rightarrow A = \sqrt{\frac{2}{L}}$$

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

$$\boxed{p = \sqrt{2mE} = \frac{n\pi}{L} \hbar}$$

wave function :-

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right) x$$



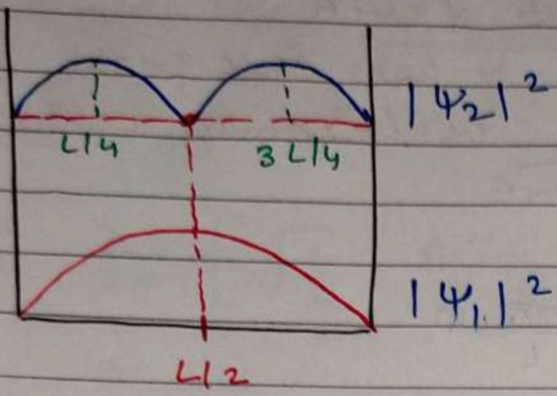
$n=1$,

$$\psi_1 = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}\right) x$$

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

$n=2$ $\quad \psi_2 = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi}{L}\right) x$

$$E_2 = \frac{4\pi^2 \hbar^2}{2mL^2}$$



momentum operator ($\hat{p}$) $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$

$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right)x$ ($\psi = \psi^*$) → In this case.

$\langle \hat{p} \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{p} \psi \cdot dx$ → Expectation value of momentum

$$\langle \hat{p} \rangle = \int_0^L \underbrace{\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right)x}_{\psi^*} \underbrace{\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\right]}_{\hat{p}} \underbrace{\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right)x}_{\psi} \cdot dx$$

$$= \frac{2}{L} \cdot \frac{n\pi}{L} \cdot \frac{\hbar}{i} \underbrace{\int_0^L \sin\left(\frac{n\pi}{L}\right)x \cdot \cos\left(\frac{n\pi}{L}\right)x\, dx}_{\frac{L}{n\pi} \sin^2\left(\frac{n\pi}{L}\right)x}$$

$$\Rightarrow \frac{\hbar}{i} \cdot \frac{2n\pi}{L^2} \cdot \frac{L}{n\pi} \underbrace{\sin^2\left(\frac{n\pi}{L}\right)x}_{\substack{x \to L,\ f(x) \to 0 \\ x \to 0,\ f(x) \to 0}} \Big|_0^L$$

$$\underbrace{\langle \hat{p} \rangle = 0}_{\text{Expectation value of momentum}} = \text{zero}.$$

Q. $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \rightarrow p = \sqrt{2mE}$

↳ how this term is becoming zero

$\frac{p^2}{2m} = E \Rightarrow p = \pm\sqrt{2mE}$

$$p_{av} = \pm \frac{n\pi}{L}\hbar$$

$p_{av} = \frac{p^+ + p^-}{2} = 0$

↳ particle in a box is doing back-forth motion due to which average momentum is zero.

momentum wave functions: $\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right)x$

$\hat{O}\psi_n = a\psi_n$

$\hat{p}\psi_n = p_n\psi_n$ $\qquad \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$

$\frac{\hbar}{i}\frac{\partial}{\partial x}\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}\right)x \Rightarrow \frac{\hbar}{i}\sqrt{\frac{2}{L}}\frac{n\pi}{L}\cos\left(\frac{n\pi}{L}\right)x$

$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$

$$\psi_n = \sqrt{\frac{2}{L}}\left[\underbrace{\frac{e^{i\cdot\frac{n\pi x}{L}}}{2i}}_{1} - \underbrace{\frac{e^{-\frac{in\pi x}{L}}}{2i}}_{2}\right]$$

1 carries the Information of wave moving in forward direction

2 carries the Information of wave moving in backward direction.

$\psi_n^+ = \sqrt{\frac{2}{L}}\frac{e^{\frac{in\pi x}{L}}}{2i}$ $\qquad \psi_n^- = -\sqrt{\frac{2}{L}}\frac{e^{-\frac{in\pi x}{L}}}{2i}$

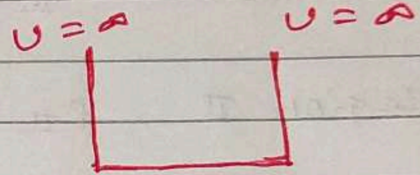
$\hookrightarrow \psi_n = \psi_n^+ + \psi_n^-$

$$\hat{p}\, \psi_n^+ = p_n^+\, \psi_n^+$$

$$\frac{\hbar}{i} \frac{\partial}{\partial x} \left[\sqrt{\frac{2}{L}} \frac{e^{\frac{in\pi}{L}x}}{2i} \right] \Rightarrow \frac{\hbar}{i} \sqrt{\frac{2}{L}} \frac{in\pi}{L} \cdot \underbrace{\frac{e^{\frac{in\pi}{L}x}}{2i}}_{\psi_n^+}$$

$$\boxed{\begin{array}{l} p_n^+ \rightarrow \text{Eigen value} = \dfrac{n\pi\hbar}{L} \\ p_n^- \rightarrow \text{Eigen value} = -\dfrac{n\pi\hbar}{L} \end{array}}$$

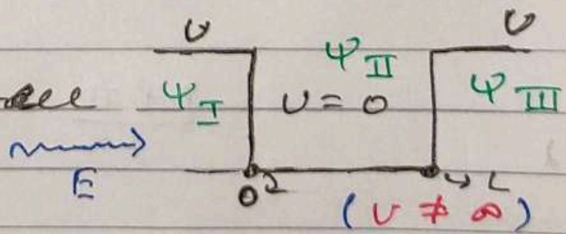
particle in a box (Ideal case)



- Energy is Quantized
- wave function is quanted
- $E_n = \dfrac{n^2 \pi^2 h^2}{2mL^2}$
- $\langle p \rangle = 0$
- momentum $\psi_n^+ = \sqrt{\dfrac{2}{L}} \dfrac{e^{\frac{in\pi x}{L}}}{2i}$

$$\psi_n^- = -\sqrt{\frac{2}{L}} \frac{e^{-\frac{in\pi x}{L}}}{2i}$$

particle in a potential well (Practical case)



region I.

$$\frac{d^2\psi_I}{dx^2} + \frac{2m}{\hbar}[E-U]\psi_I = 0$$

region II $\dfrac{d^2\psi_{II}}{dx^2} + \dfrac{2m}{\hbar^2} E\psi_{II} = 0$

region III $\dfrac{d^2\psi_{III}}{dx^2} + \dfrac{2m}{\hbar^2}[E-U]\psi_{III} = 0$

Region I.

$$\alpha^2 = \frac{2m}{\hbar}[E-U]$$

$$-\alpha^2 = \frac{2m}{\hbar}[U-E]$$

$$\psi_1(x) = Ce^{\alpha x} + De^{-\alpha x}$$

Region III

$$\psi_{III}(x) = Fe^{\alpha x} + Ge^{-\alpha x}$$

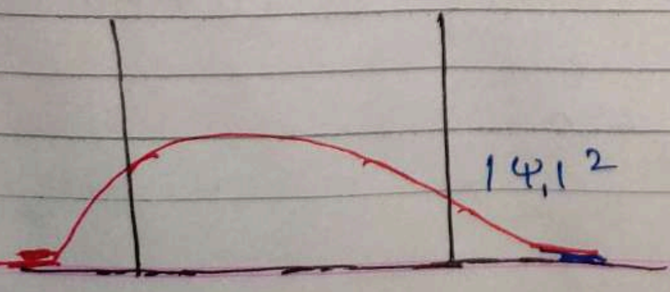
Region II

$$\psi_{II}(x) = A\sin\sqrt{\frac{2mE}{\hbar}}\,x + B\cos\sqrt{\frac{2mE}{\hbar}}\,x$$

- Boundary conditions:

at $x=0$,
$$\left.\begin{aligned}\psi_I(0) &= \psi_{II}(0)\\ \frac{\partial\psi_I(0)}{\partial x} &= \frac{\partial\psi_{II}(0)}{\partial x}\end{aligned}\right\} \rightarrow 2\text{ conditions}$$

at $x=L$,
$$\left.\begin{aligned}\psi_{II}(L) &= \psi_{III}(L)\\ \frac{\partial\psi_{II}(L)}{\partial x} &= \frac{\partial\psi_{III}(L)}{\partial x}\end{aligned}\right\} \rightarrow 2\text{ conditions.}$$



$\Rightarrow$ λ has Increased

$\mapsto$ p decreased

$\mapsto$ E decreased.

Reflection and Transmission at a Potential Step

<u>Outline</u>

- Review: Particle in a 1-D Box
- Reflection and Transmission - Potential Step
- Reflection from a Potential Barrier
- Tunneling

Schrodinger: A Wave Equation for Electrons

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

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

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

..The Free-Particle Schrodinger Wave Equation !

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

Schrodinger Equation and Energy Conservation

The Schrodinger Wave Equation

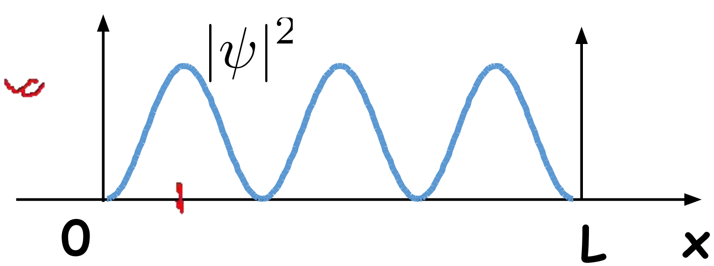
$$\psi''(x) + \frac{2m}{\hbar^2}[E - V]\psi = 0$$

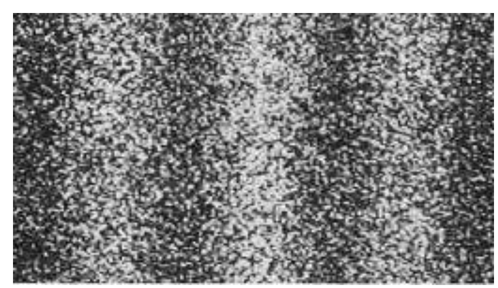
$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x)$$

The quantity **P(x)** is interpreted as the probability that the particle can be found at a particular point *x* (within interval dx)

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

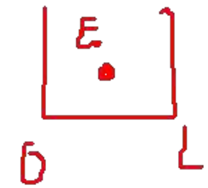
n=3





Schrodinger Equation and Particle in a Box

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



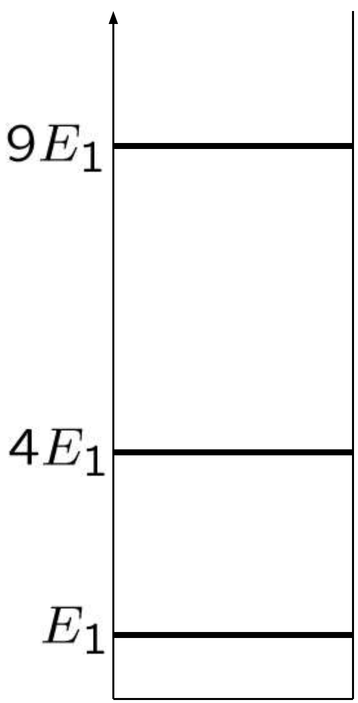
$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

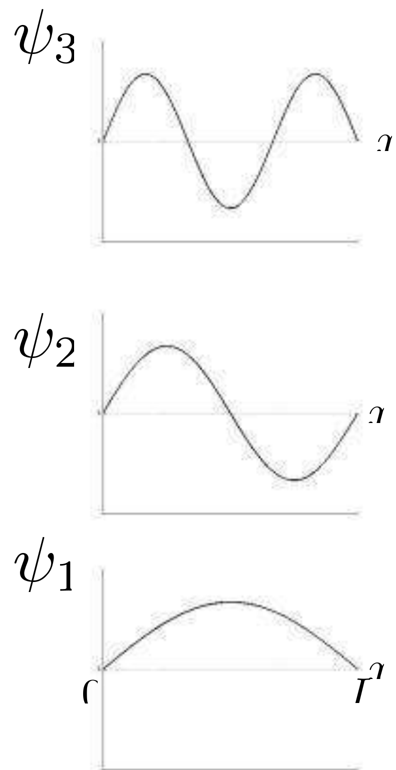
$$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \qquad P(x) = |\psi(x)|^2\,dx$$

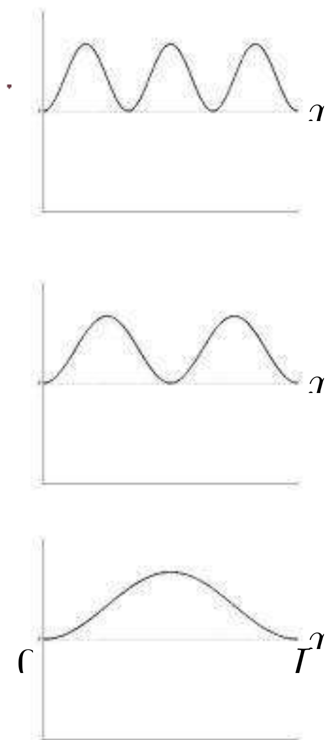
EIGENENERGIES for 1-D BOX

EIGENSTATES for 1-D BOX

PROBABILITY DENSITIES







Solutions to Schrodinger's Equation

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

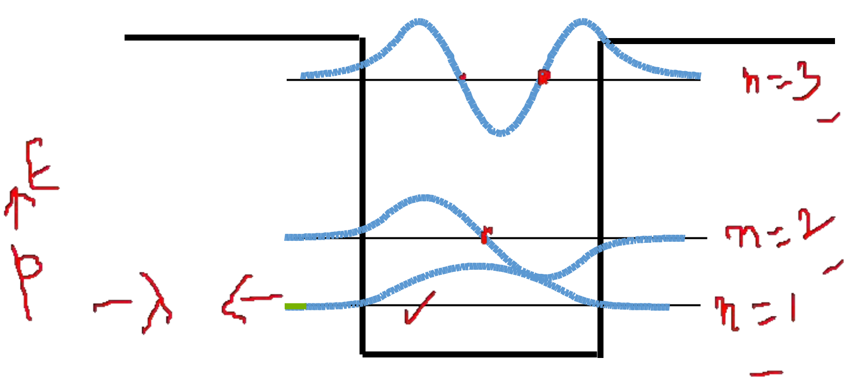
The kinetic energy of the electron is related to the curvature of the wavefunction

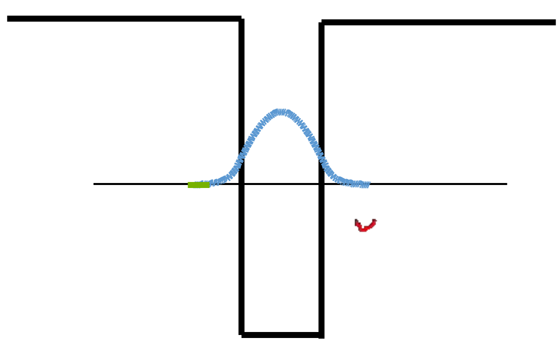
Tighter confinement → Higher energy

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

Nodes in wavefunction → Higher energy

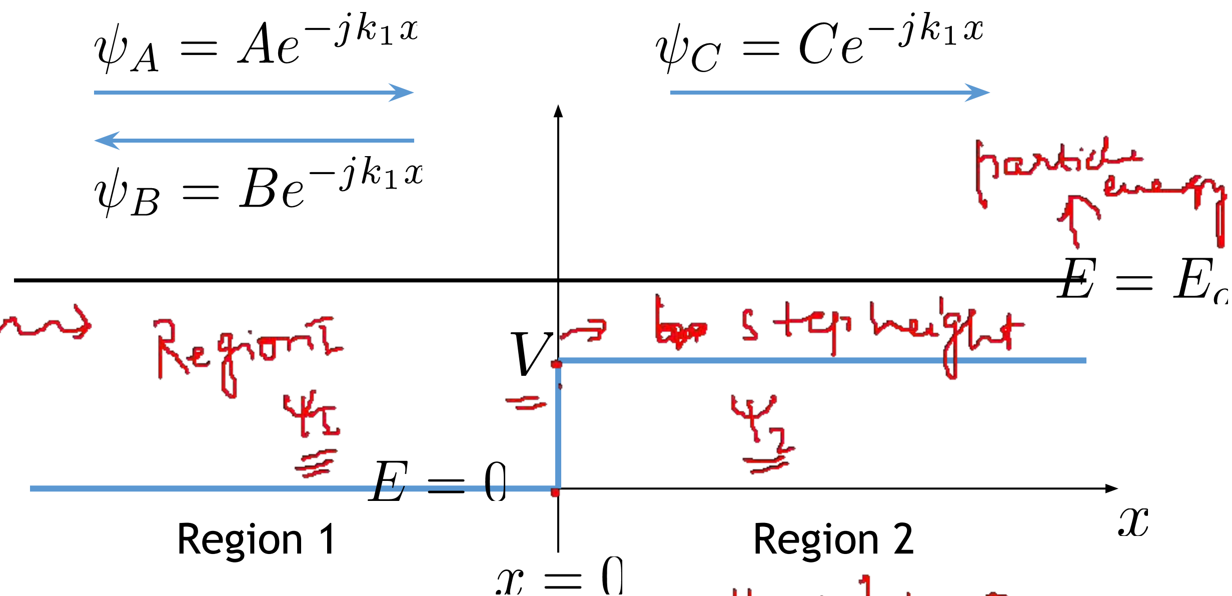
The n-th wavefunction (eigenstate) has (n-1) zero-crossings

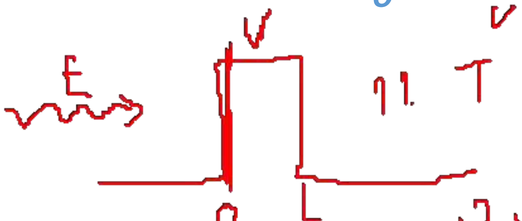




A Simple Potential Step

CASE I : $E_o > V$





$F = -kx$

$\ddot{x} + \frac{k}{m}x = 0$

ω_0

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V]\psi = 0 \qquad (V \to 0)$$

$\psi'' + k_1^2\psi = 0$

$\psi = A\sin k_1x + B\cos k_1x$

$\psi = Ae^{jk_1x}$

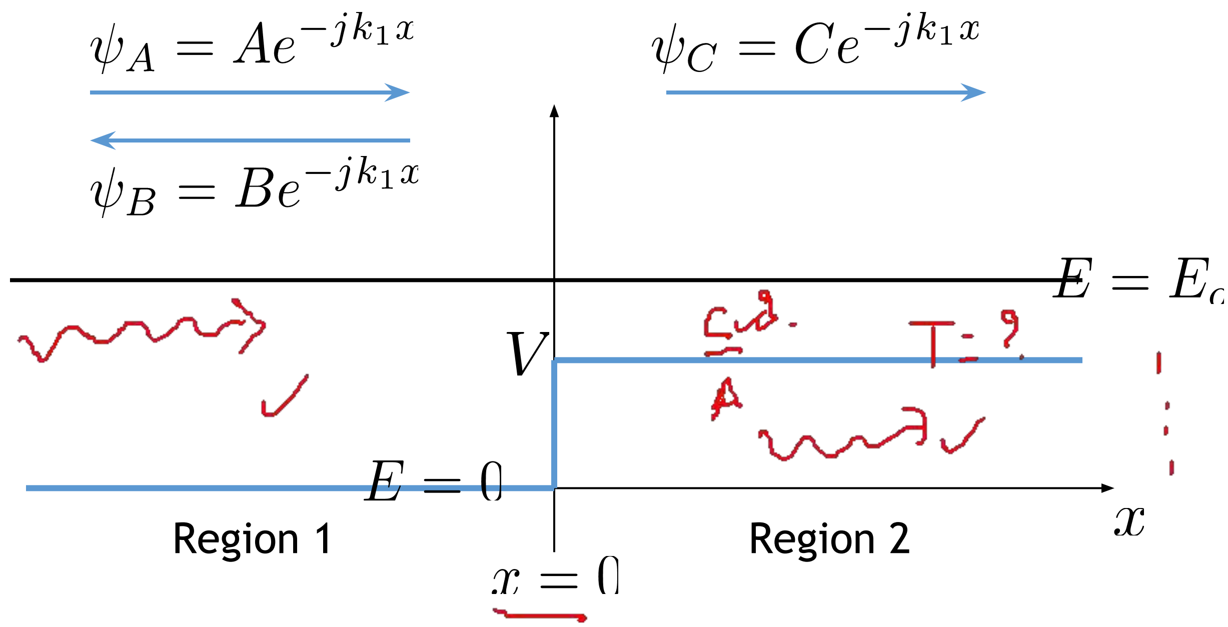
In Region 1: $\rightarrow$ $$E_o\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \Rightarrow \boxed{k_1^2 = \frac{2mE_o}{\hbar^2}}$$

$Ae^{i\omega_0 x} + Be^{-i\omega_0 x}$

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

$\hookrightarrow \frac{d^2\psi}{dx^2} + k_2^2\psi = 0$

A Simple Potential Step



CASE I : $E_o > V$

$\frac{B}{A}$, $\frac{C}{A}$

$$\psi_1 = Ae^{-jk_1x} + Be^{jk_1x}$$

R

$$\psi_2 = Ce^{-jk_2x} \cancel{+De^{jk_2x}}$$

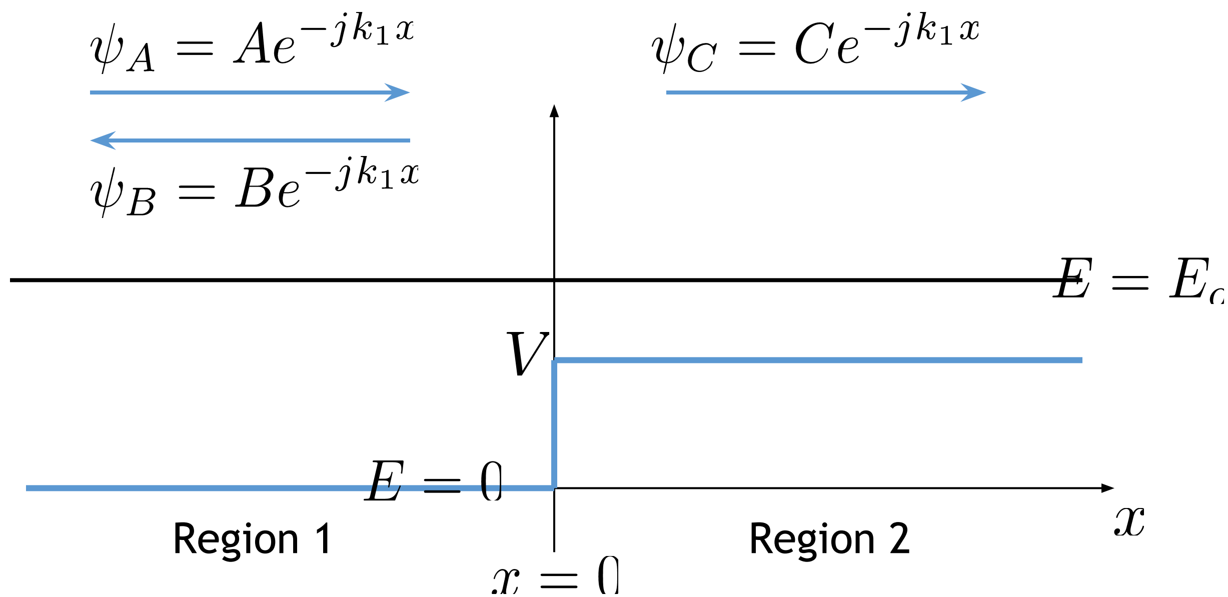
Boundary Condn

① ψ is continuous: $\psi_1(0) = \psi_2(0)$ ➡ $A + B = C$

$+jk_1 A \mp jk_1 B = +jk_2 C$

② $\frac{\partial \psi}{\partial x}$ 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 : $E_o > V$

$$K_1 = \frac{2mE_0}{\hbar^2}, \quad K_2 = \frac{2m}{\hbar^2}\left[E_0 - V\right] \quad 2A = \left(1 + \frac{K_2}{K_1}\right)C$$

$$A + B = C$$

$$1 + \frac{B}{A} = \frac{C}{A}$$

$$A - B = \frac{k_2}{k_1}C$$

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

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

Quantum Electron Currents

$p = \hbar k$

Given an electron of mass m

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

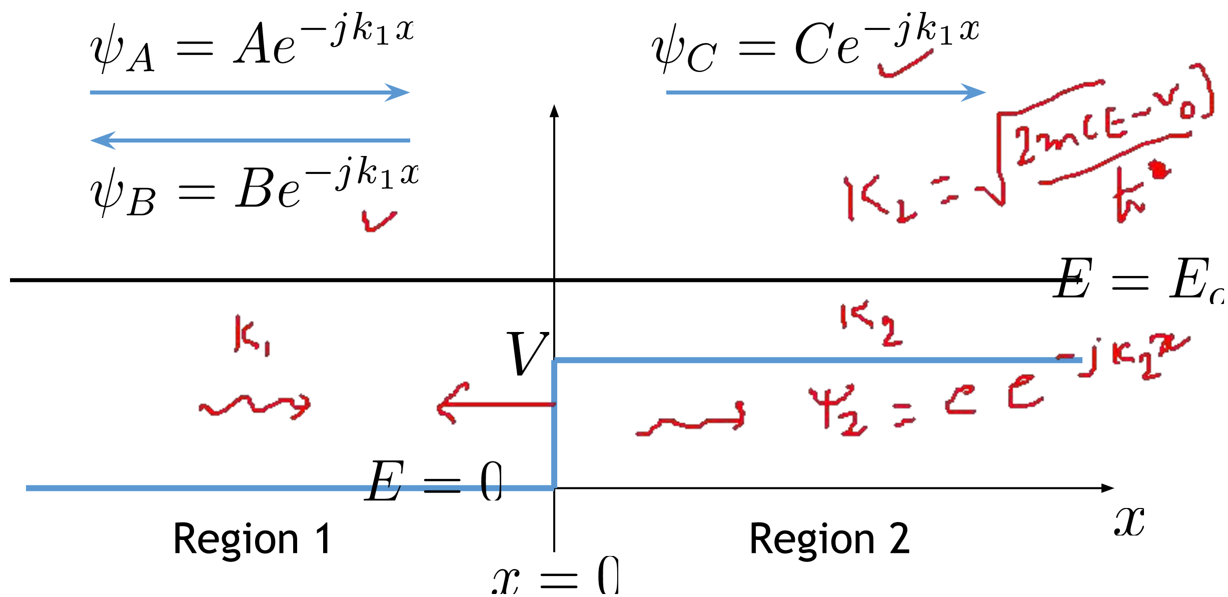
and moving with momentum $<p>$ corresponding to $<v> = \hbar k/m$

… 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 : $E_o > V$



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

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

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

A Simple Potential Step

$$\psi_A = Ae^{-jk_1x}$$

$$\psi_B = Be^{-jk_1x}$$

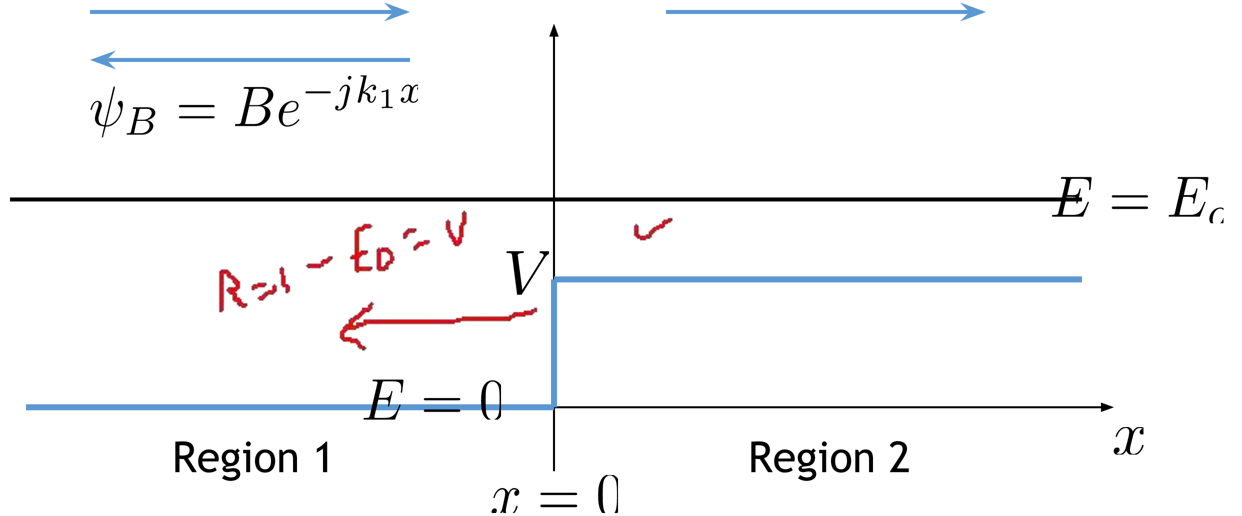
$$\psi_C = Ce^{-jk_1x}$$

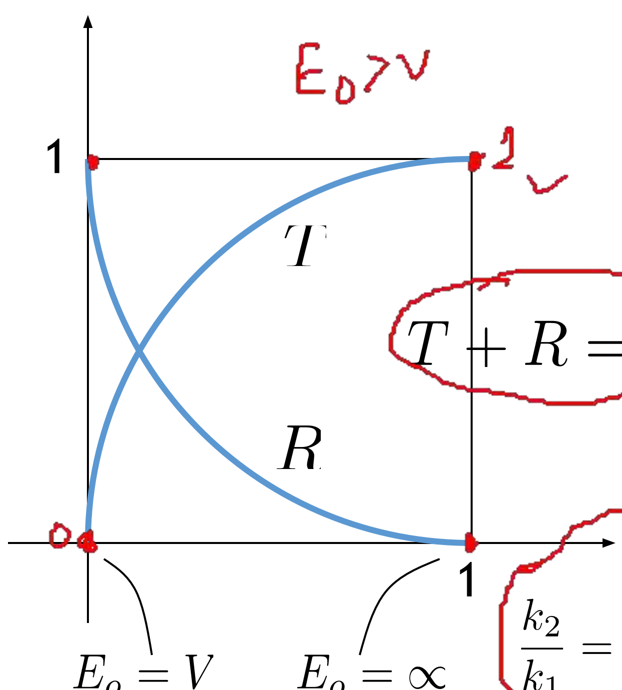
CASE I : $E_o > V$

$$k_2^2 = \frac{2m}{\hbar^2}(E_0 - V_0)$$

$$k_1^2 = \frac{2mE_0}{\hbar^2}$$

$$= \left(1 - \frac{V}{E_0}\right)$$





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

$$1 - \frac{k_2}{k_1}$$

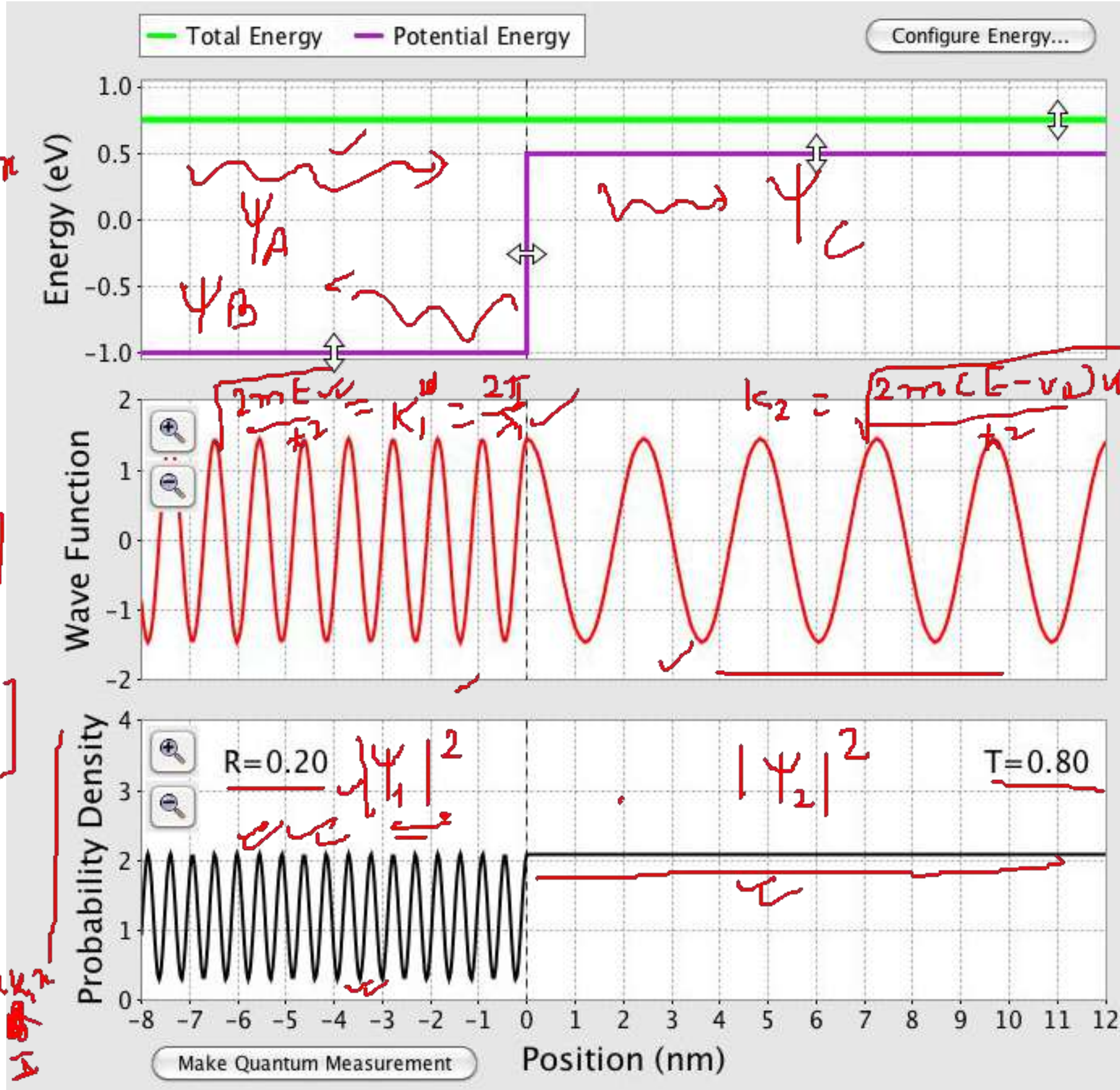
$$\text{Reflection} = R = \left|\frac{B}{A}\right|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2$$

$$1 + \frac{k_2}{k_1}$$

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

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

$$1 + \frac{k_2}{k_1}$$



$\psi_1 = Ae^{-jk_1x} + Be^{jk_1x}$

$|\psi_1|^2 = \psi_1^* \psi_1$

$= [Ae^{jk_1x} + Be^{-jk_1x}][Ae^{-jk_1x} + Be^{jk_1x}]$

$= |A|^2 + |B|^2 + 2AB\cos 2k_1x$

$\psi_2 = Ce^{-jk_2x}$

$|\psi_2|^2 = \psi_2^* \psi_2$

$= Ce^{jk_2x} \cdot Ce^{-jk_2x}$

$= |C|^2$

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

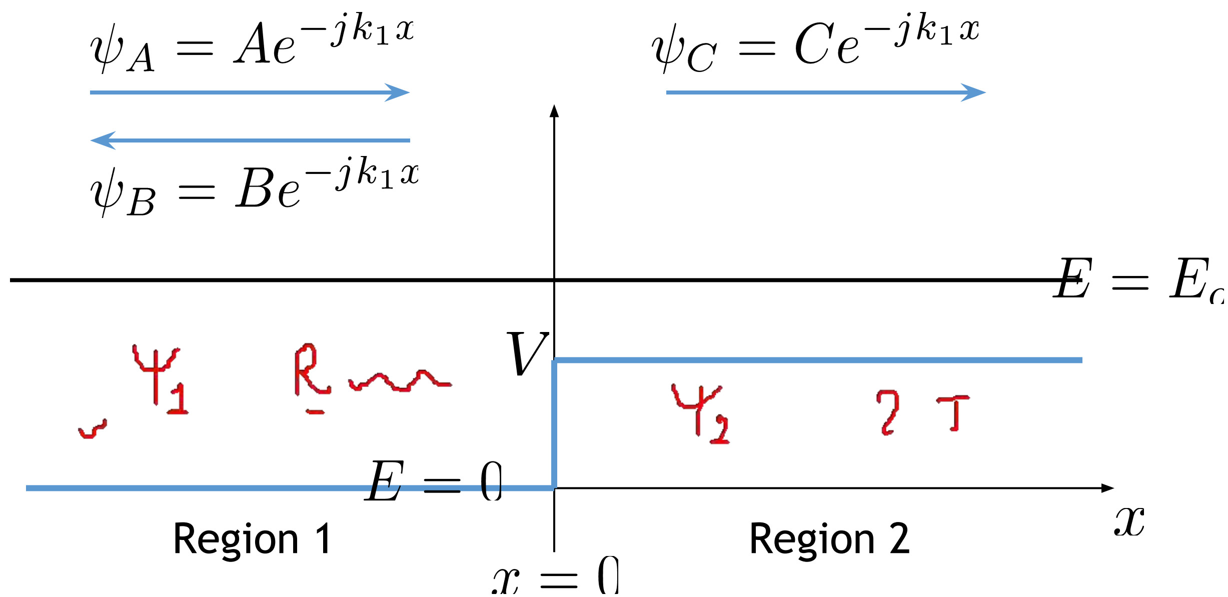
Reflection and Transmission at a Potential Step

Outline

- Review: Reflection and Transmission - Potential Step
- Reflection from a Potential Barrier
- Tunneling

A Simple Potential Step

CASE I : $E_o > V$



In Region 1:

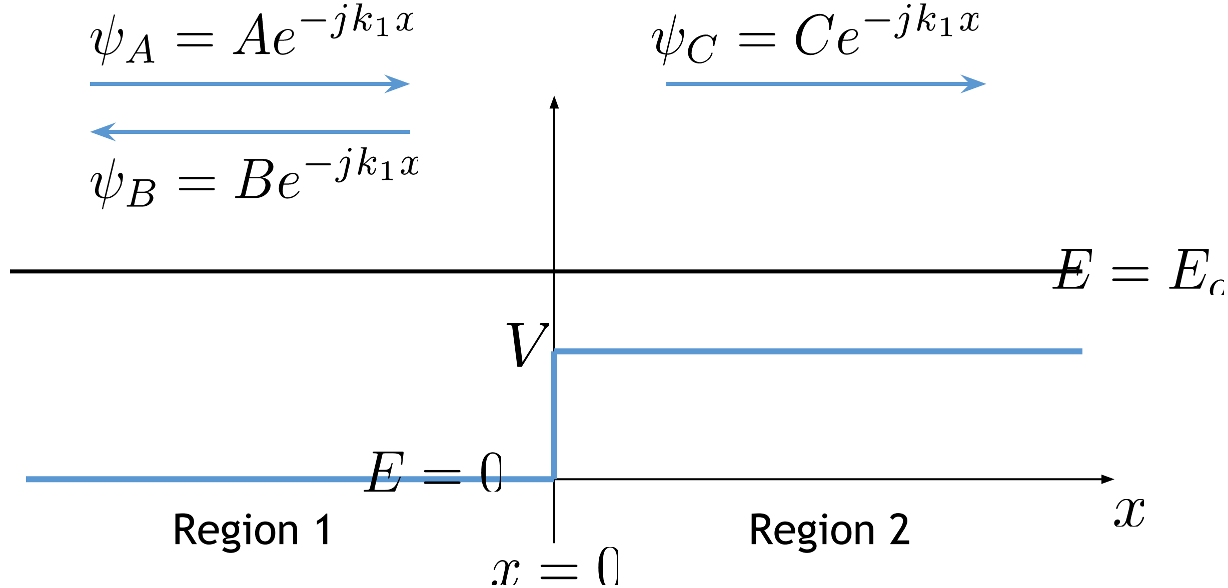
$$E_o\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \quad \Rightarrow \quad k_1^2 = \frac{2mE_o}{\hbar^2}$$

In Region 2:

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

A Simple Potential Step

CASE I : $E_o > V$



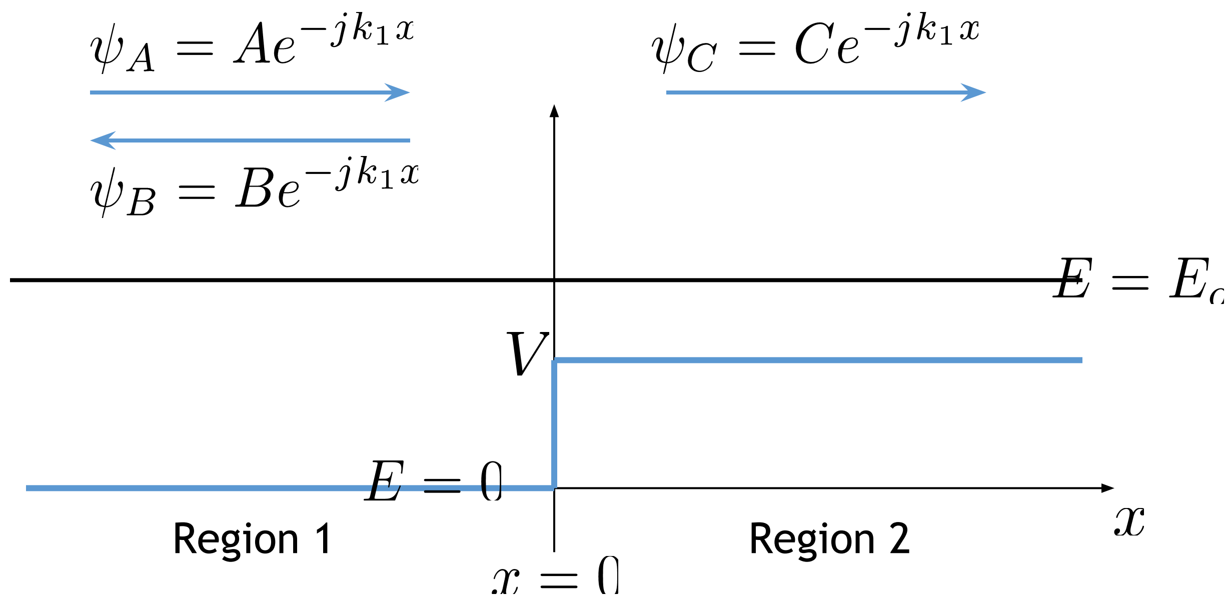
$$\psi_1 = Ae^{-jk_1x} + Be^{jk_1x} \qquad \psi_2 = Ce^{-jk_2x}$$

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

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

A Simple Potential Step

CASE I : $E_o > V$



$$A + B = C$$

$$A - B = \frac{k_2}{k_1}C$$

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

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

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

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

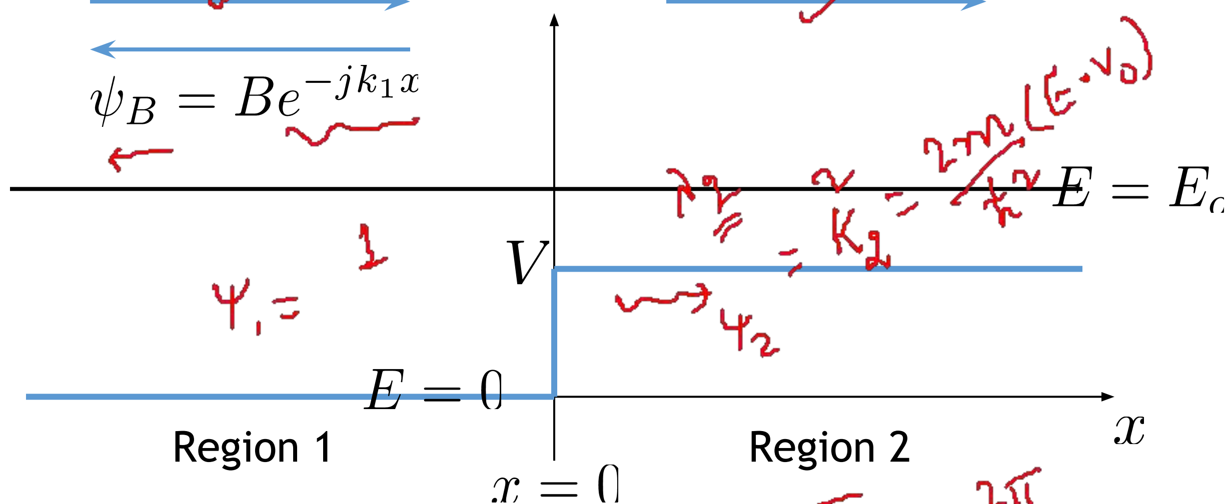
A Simple Potential Step

CASE I : $E_o > V$

$\psi_A = Ae^{-jk_1x}$

$\psi_B = Be^{-jk_1x}$

$\psi_C = Ce^{-jk_1x}$



$\psi_B^* \psi_B$

$k_2^2 = \frac{2m(E-V_0)}{\hbar^2}$

$k_1 = \frac{\sqrt{2mE}}{\hbar} = \frac{2\pi}{\lambda_1}$

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

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

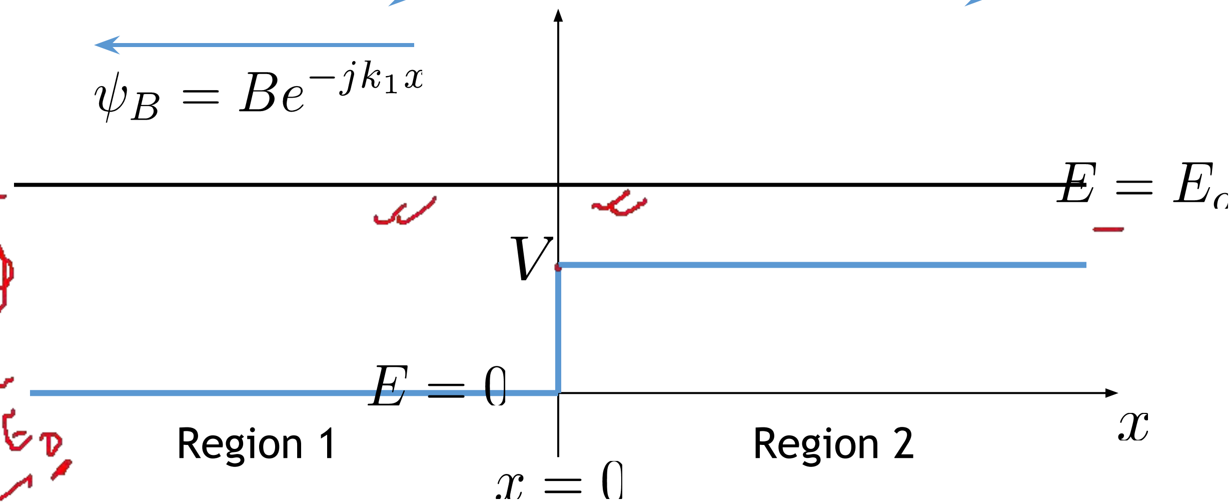
$$\frac{B}{A} = \frac{1 - k_2/k_1}{1 + k_2/k_1} \qquad \frac{C}{A} = \frac{2}{1 + k_2/k_1}$$

A Simple Potential Step

$$\psi_A = Ae^{-jk_1x}$$

$$\psi_B = Be^{-jk_1x}$$

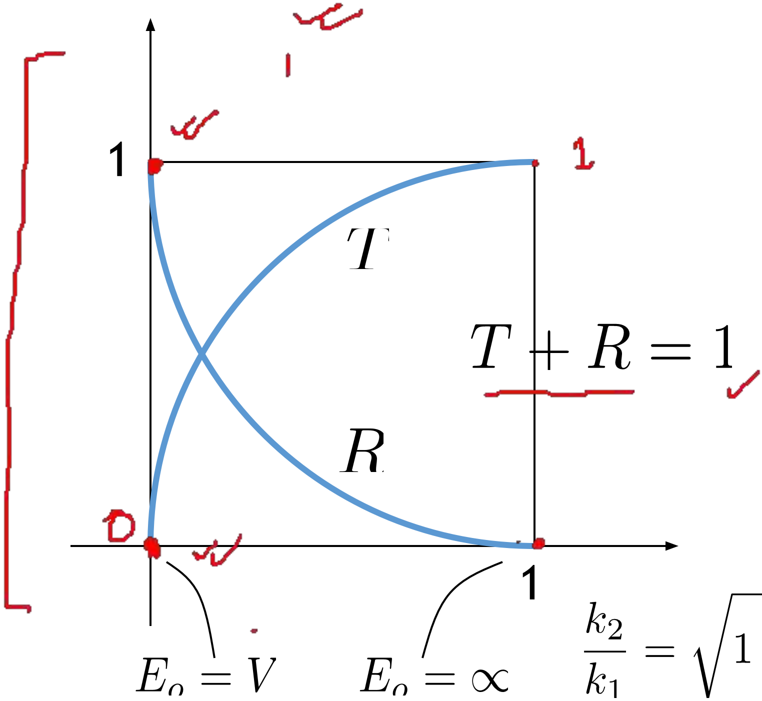
$$\psi_C = Ce^{-jk_1x}$$



CASE I : $E_o > V$

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

$$k_1 = \frac{\sqrt{2mE_o}}{\hbar}$$



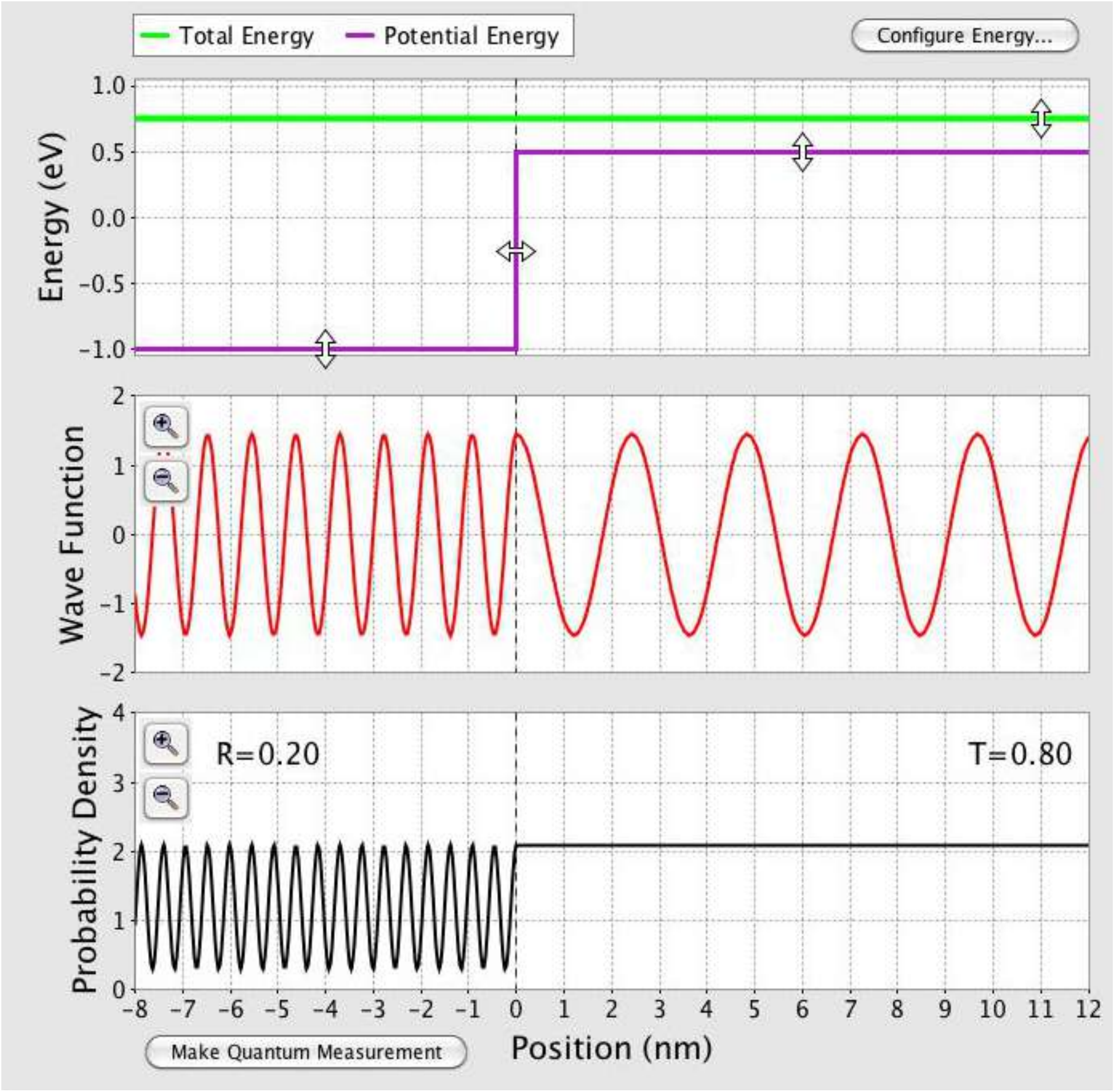
$$\frac{k_2}{k_1} = \sqrt{1 - \frac{V}{E_o}}$$

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

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

$$\frac{\left|1 - \frac{k_2}{k_1}\right|^2}{\left|1 + \frac{k_2}{k_1}\right|}$$

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



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

A Simple Potential Step

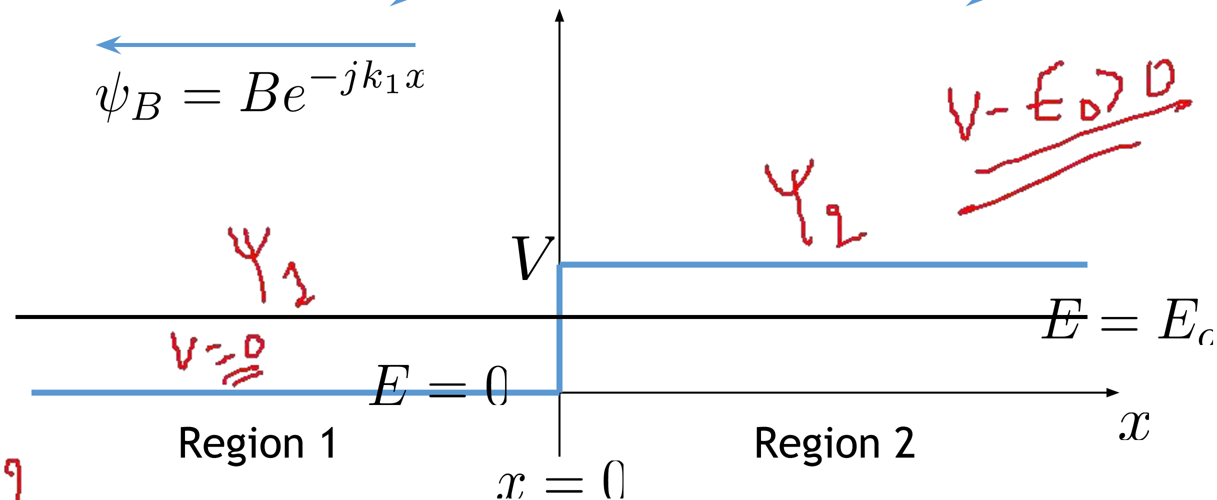
$$\psi_A = Ae^{-jk_1x}$$

$$\psi_B = Be^{-jk_1x}$$

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

CASE II : $E_o < V$

$T = 0$ → ??



$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0 \rightarrow \psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$$

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

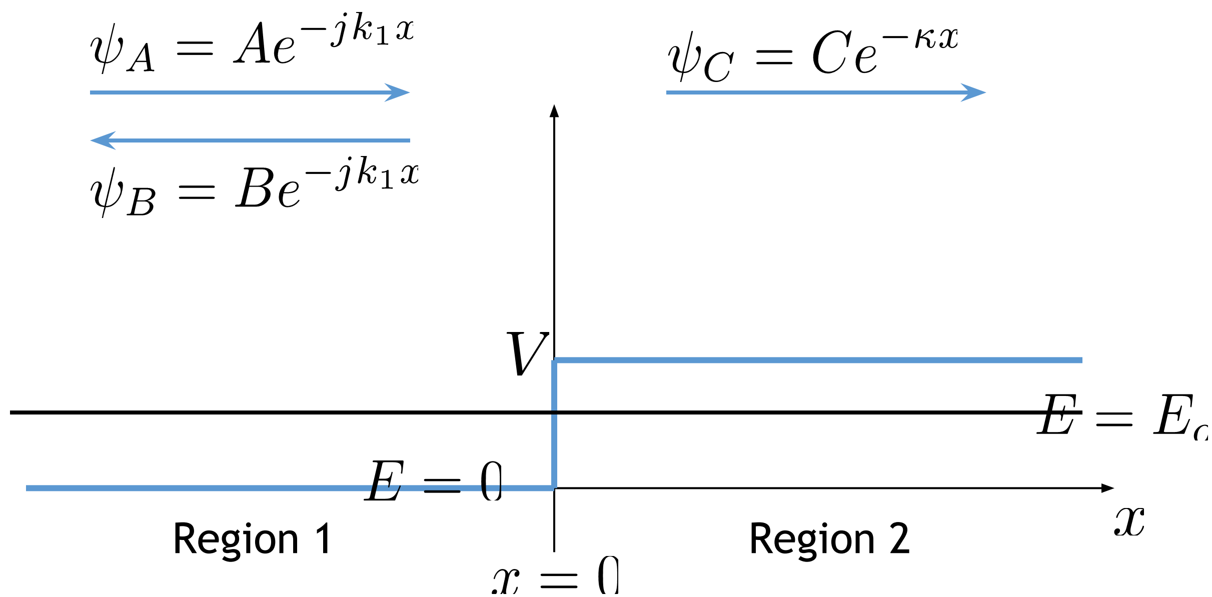
$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}[E - V_0]\psi_2 = 0$$

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

$$\psi'' - \kappa^2\psi = 0 \longrightarrow \psi_2$$

A Simple Potential Step

CASE II : $E_o < V$



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

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

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

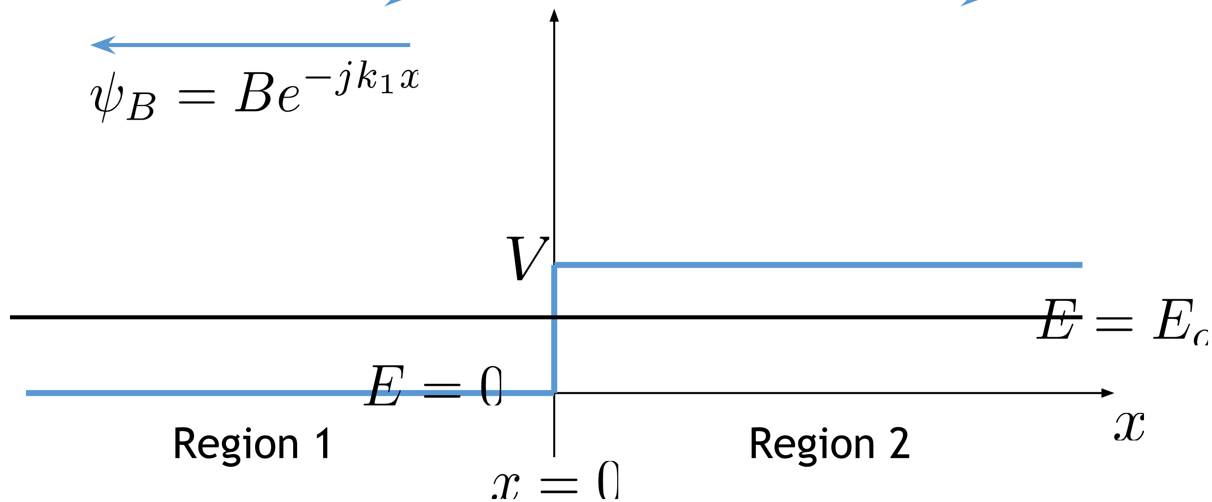
A Simple Potential Step

CASE II : E_o < V

$$\psi_A = Ae^{-jk_1x}$$

$$\psi_B = Be^{-jk_1x}$$

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



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

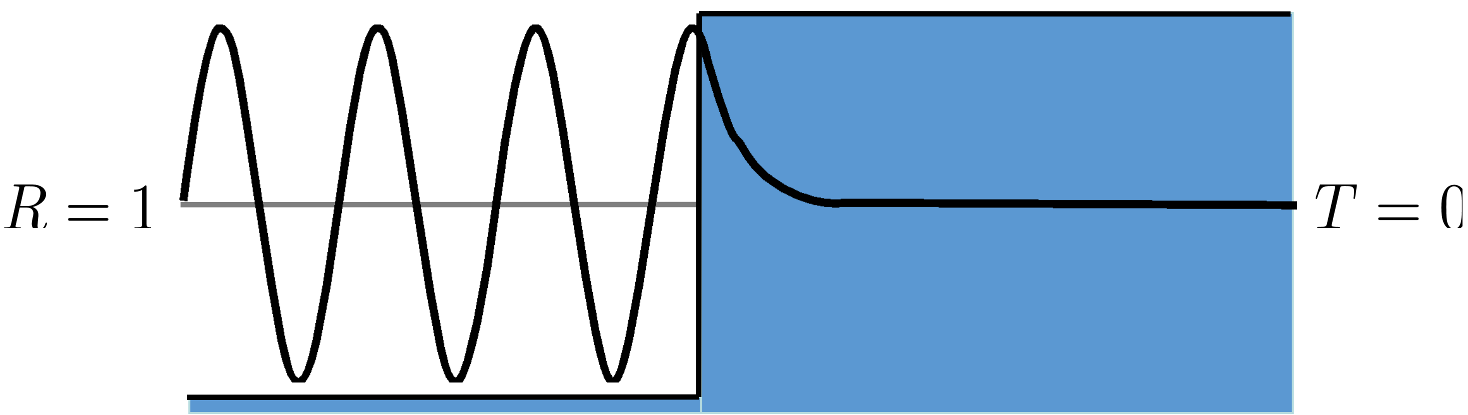
$$\frac{B}{A} = \frac{1 + j\kappa/k_1}{1 - j\kappa/k_1} \qquad \frac{C}{A} = \frac{2}{1 - j\kappa/k_1}$$

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

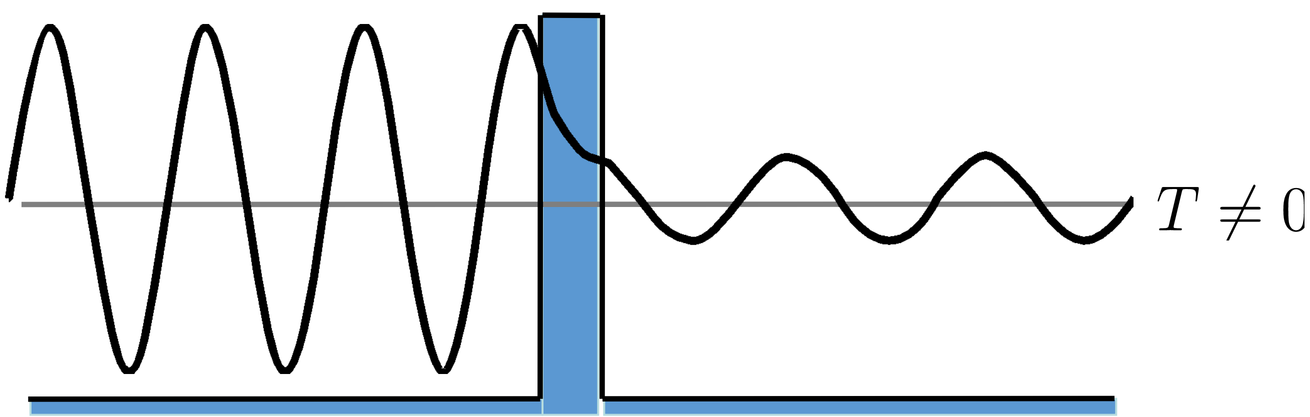
Total reflection □ Transmission must be zero

Quantum Tunneling Through a Thin Potential Barrier

Total Reflection at Boundary



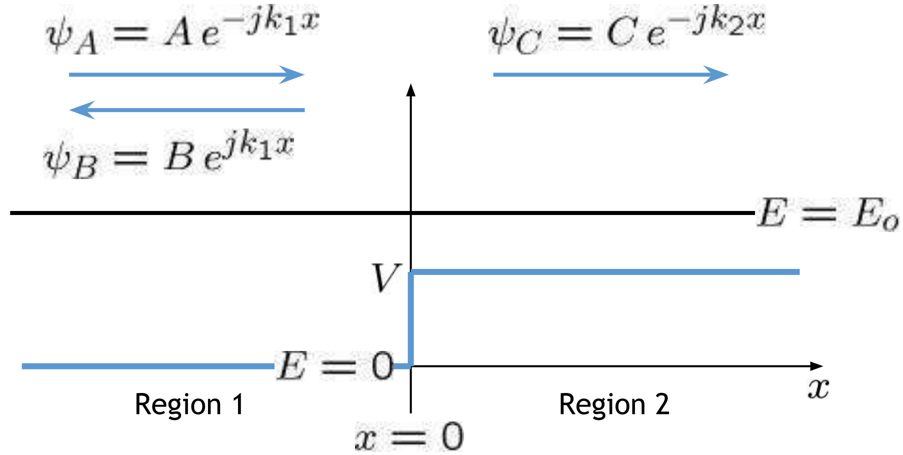
Frustrated Total Reflection (Tunneling)



KEY TAKEAWAYS

A Simple Potential Step

CASE I : $E_o > V$



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

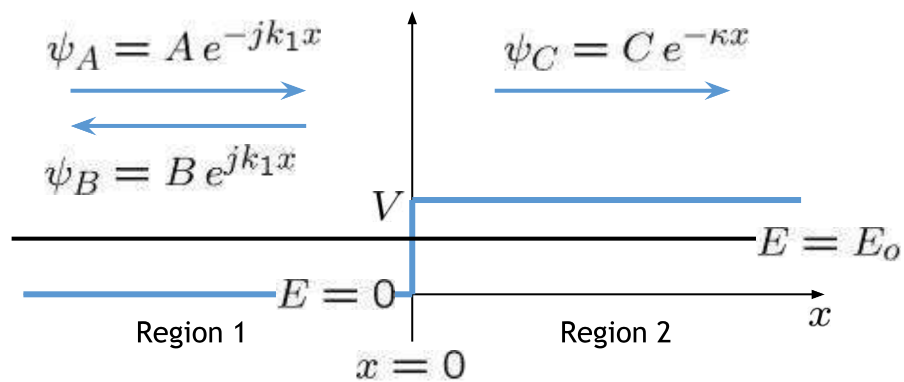
$$Transmission = T = 1 - R = \frac{4\,k_1 k_2}{|k_1 + k_2|^2}$$

PARTIAL REFLECTION

$$\psi_1 = A\,e^{-jk_1x} + B\,e^{jk_1x} \qquad \psi_2 = C\,e^{-jk_2x}$$

$$k_1^2 = \frac{2m\,E_o}{\hbar^2} \qquad k_2^2 = \frac{2m\,(E_o - V)}{\hbar^2}$$

CASE II : $E_o < V$



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

$$T = 0$$

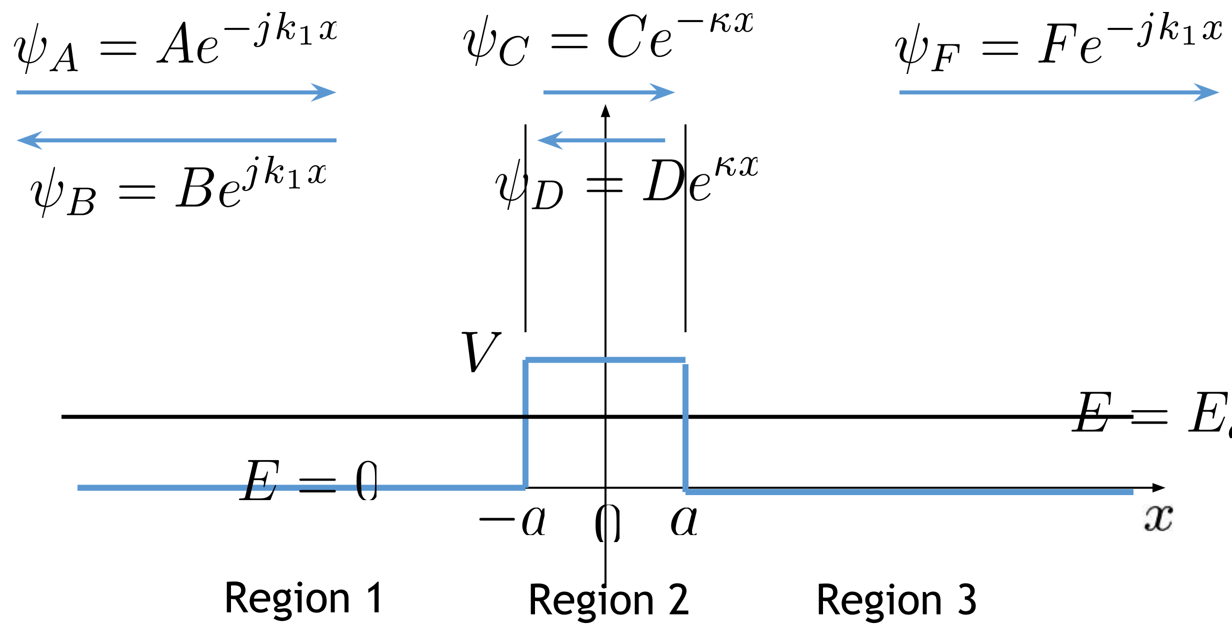
TOTAL REFLECTION

$$\psi_1 = A\,e^{-jk_1x} + B\,e^{jk_1x} \qquad \psi_2 = C\,e^{-\kappa x}$$

$$k_1^2 = \frac{2m\,E_o}{\hbar^2} \qquad \kappa^2 = \frac{2m\,(V - E_o)}{\hbar^2}$$

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:

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

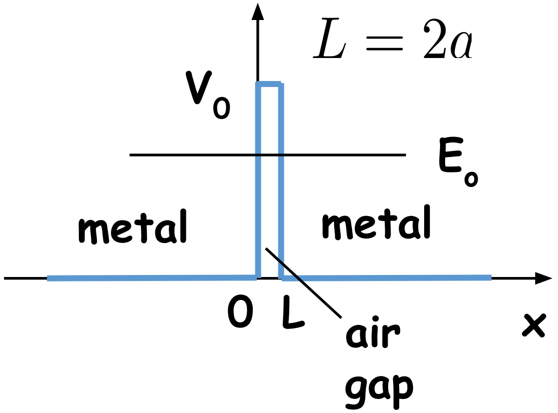
for $E_o < V$:

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

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?



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

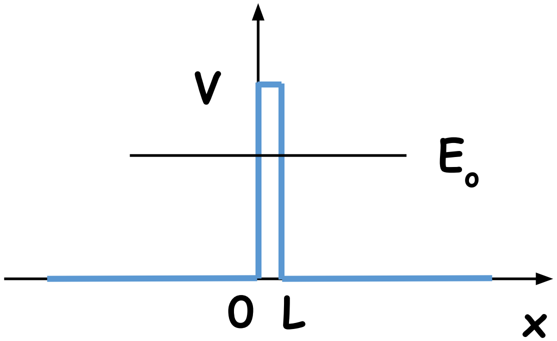
$$\kappa = \sqrt{\frac{2m_e}{\hbar^2}(V - E_o)} = 2\pi\sqrt{\frac{2m_e}{h^2}(V - E_o)} = 2\pi\sqrt{\frac{6\text{eV}}{1.505\text{eV-nm}^2}} \approx 12.6 \text{ nm}^{-1}$$

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

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?

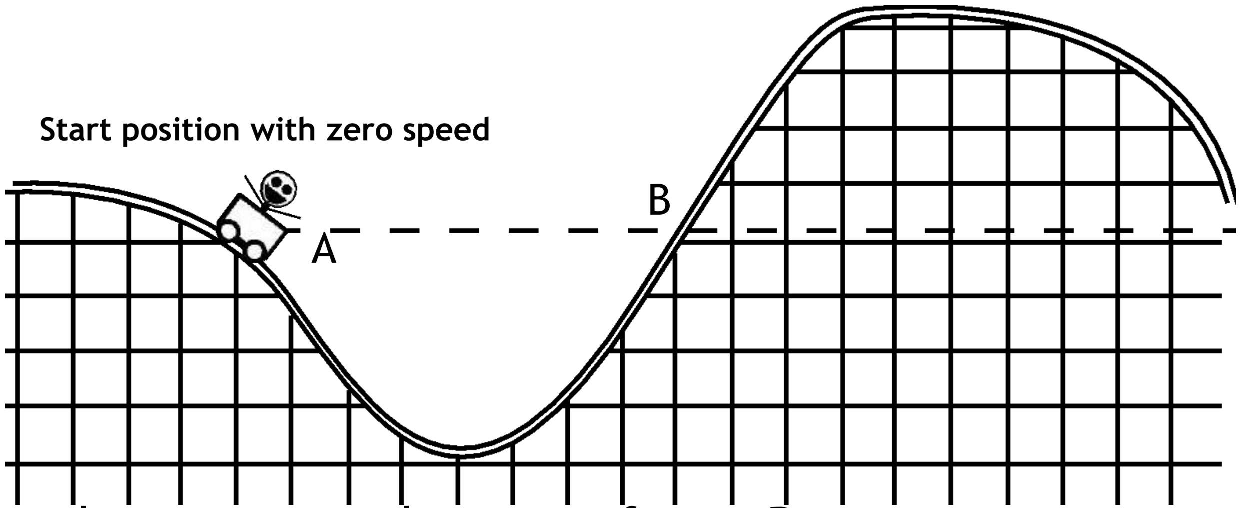
   a. decrease the height of the barrier
   b. decrease the width of the barrier
   c. decrease the mass of the particle

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

Imagine the Roller Coaster ...



- Normally, the car can only get as far as B, before it falls back again
- But a fluctuation in energy could get it over the barrier to E!
- A particle 'borrows' an energy *ΔE* to get over a barrier
- Does not violate the uncertainty principle, provided this energy is repaid within a certain time *Δt*

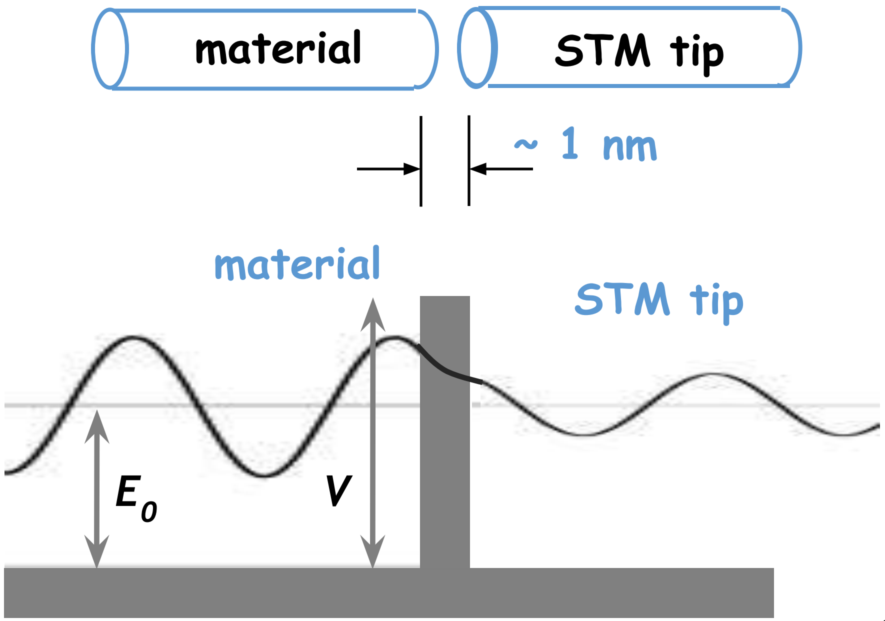
$$\Delta E \Delta t \geq \frac{h}{4\pi}$$

Application of Tunneling:

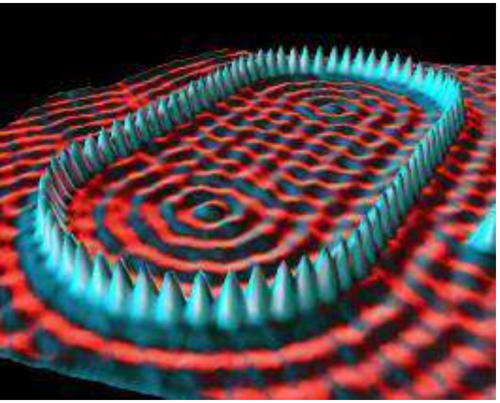
Scanning Tunneling Microscopy (STM)

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:



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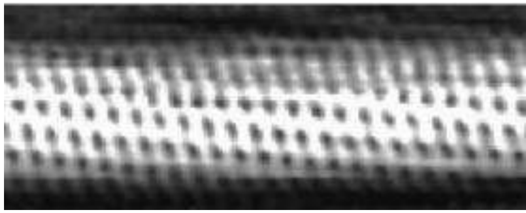
STM images

Single walled carbon nanotube:



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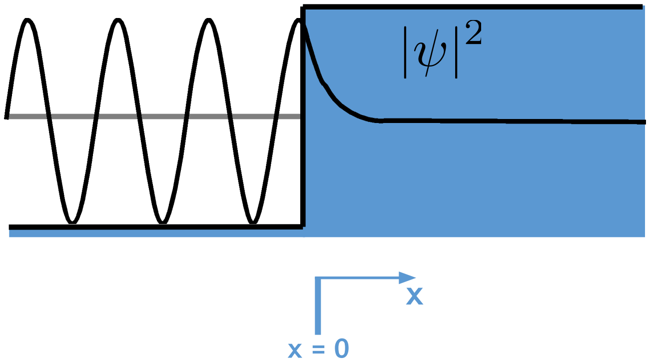
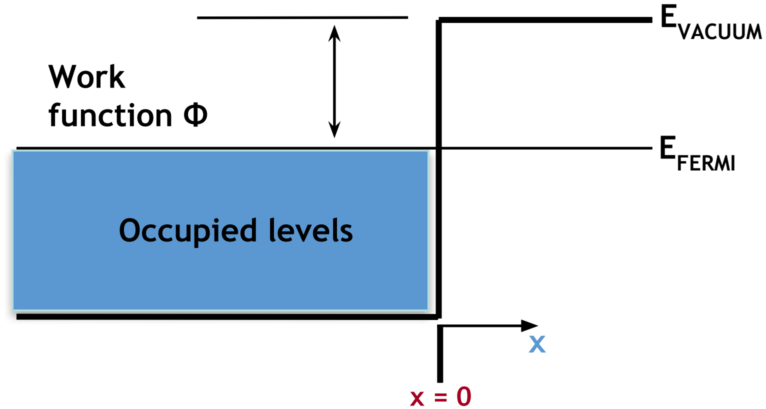
Leaky Particles

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



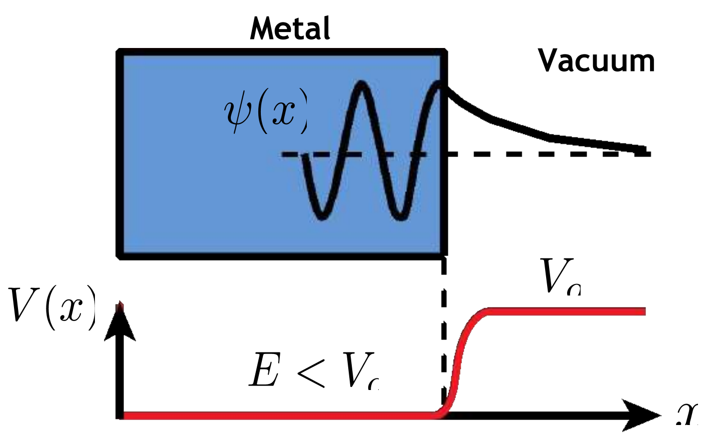


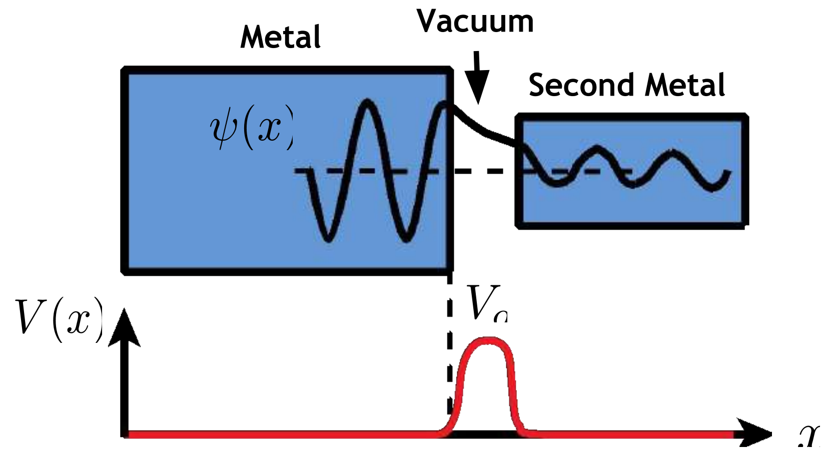
Assume that the work function (i.e., the energy difference between the most energetic conduction electrons and the potential barrier at the surface) of a certain metal is $\Phi = 5$ eV. Estimate the distance x outside the surface of the metal at which the electron probability density drops to 1/1000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

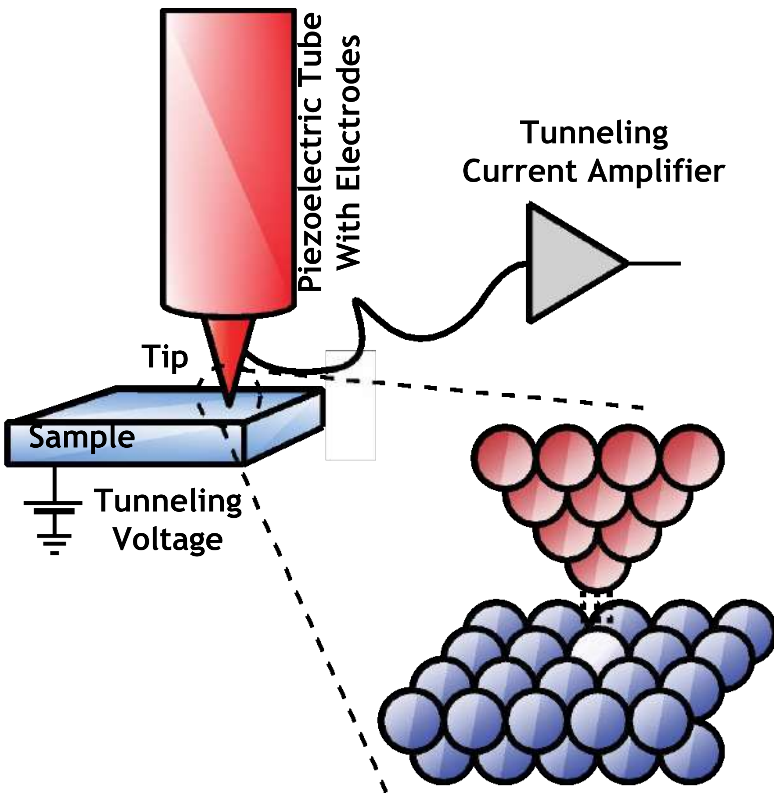
$$\boxed{\frac{|\psi(x)|^2}{|\psi(0)|^2} = e^{-2\kappa x} \approx \frac{1}{1000}} \longrightarrow \boxed{x = -\frac{1}{2\kappa}\ln\left(\frac{1}{1000}\right) \approx 0.3 \text{ nm}}$$

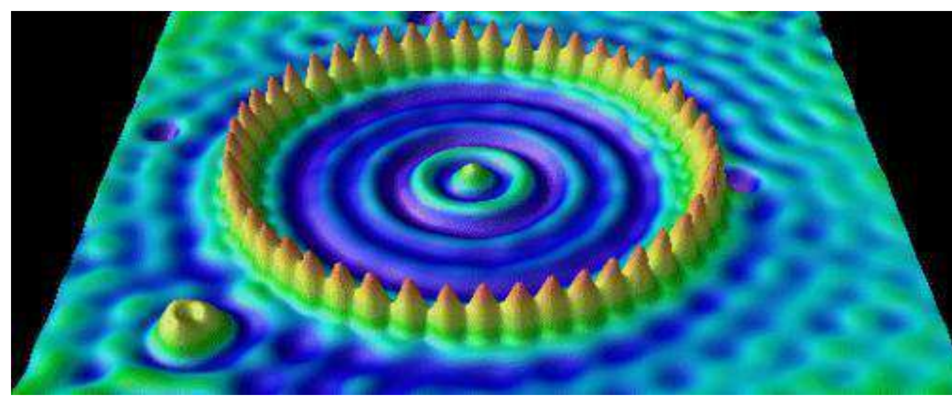
using $$\kappa = \sqrt{\frac{2m_e}{\hbar^2}(V_o - E)} = 2\pi\sqrt{\frac{2m_e}{h^2}\Phi} = 2\pi\sqrt{\frac{5 \text{ eV}}{1.505 \text{ eV}\cdot\text{nm}^2}} = 11.5 \text{ nm}^{-1}$$

Application: Scanning Tunneling Microscopy









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Application of Tunneling:

Scanning Tunneling Microscopy (STM)

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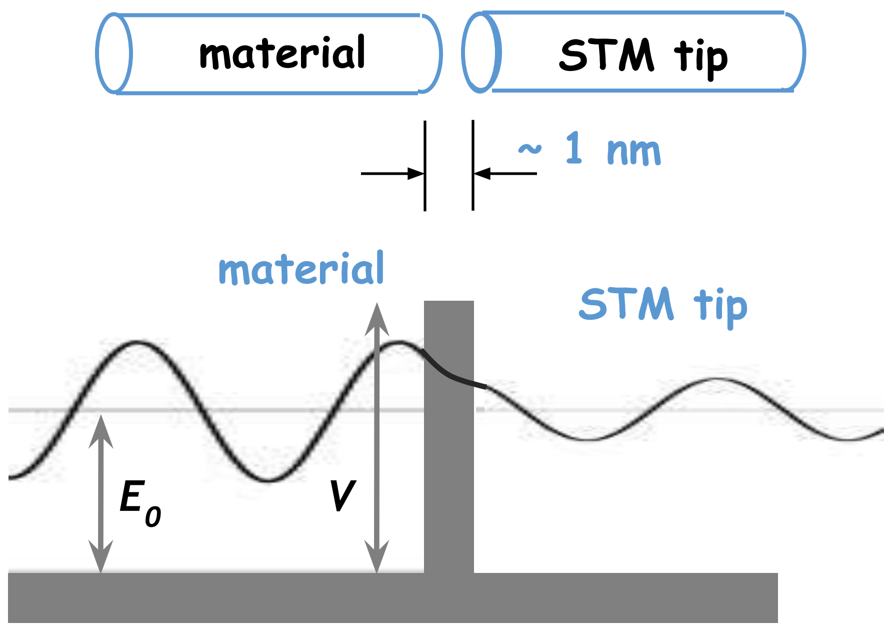
One can exploit this to measure the electron density on a material's surface:



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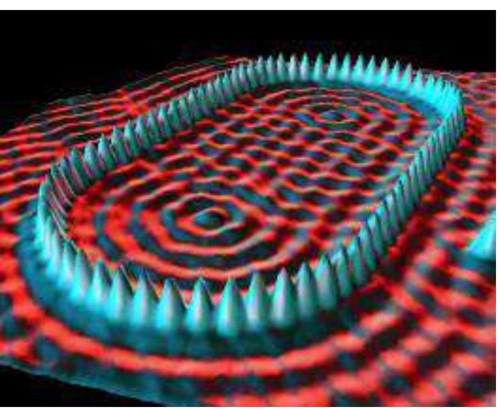

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STM images

DNA Double Helix:

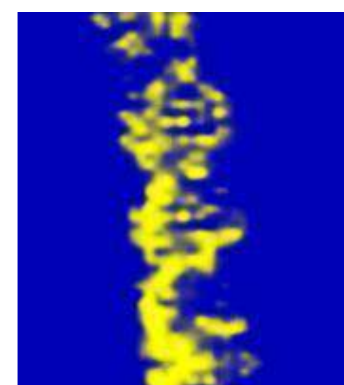
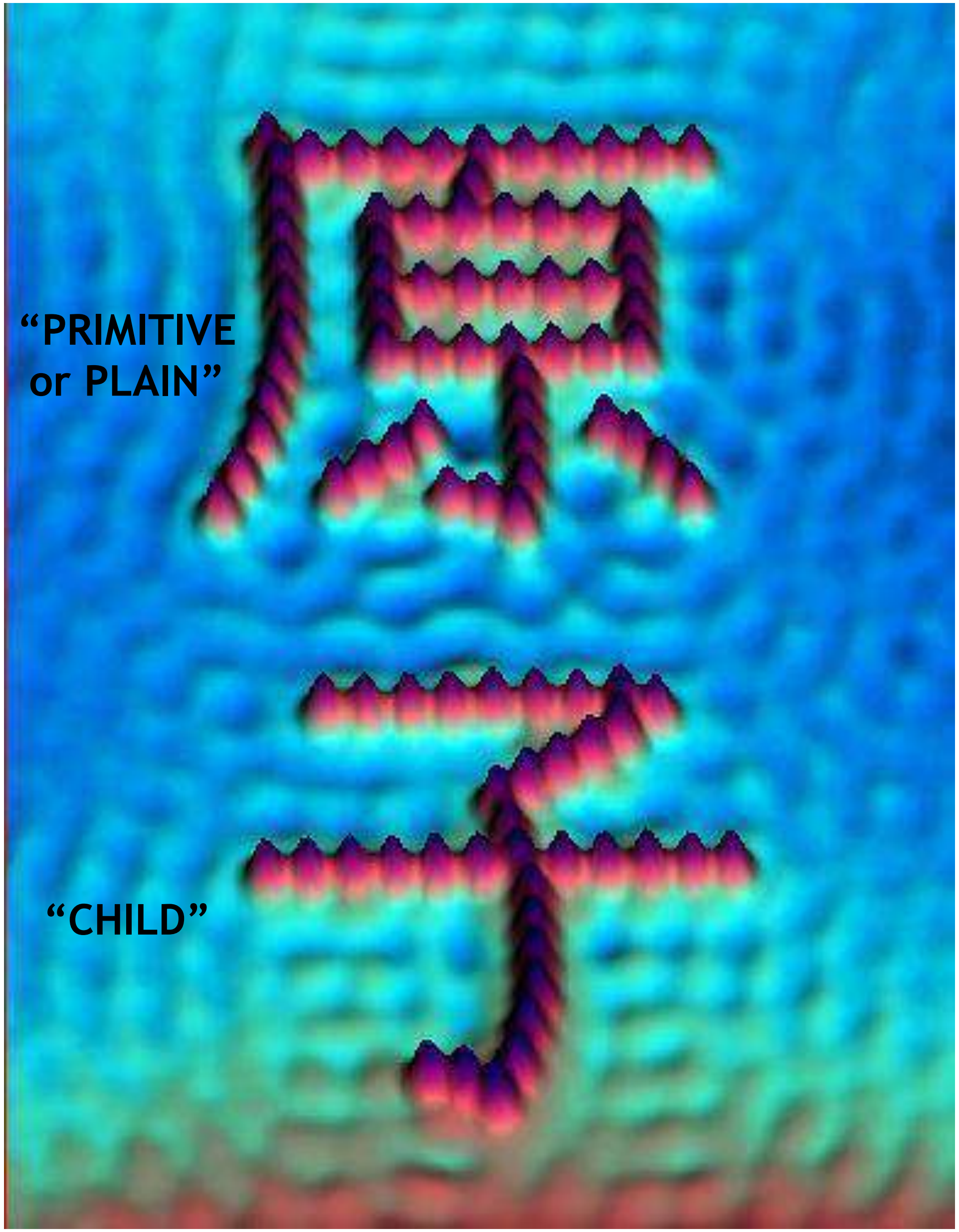
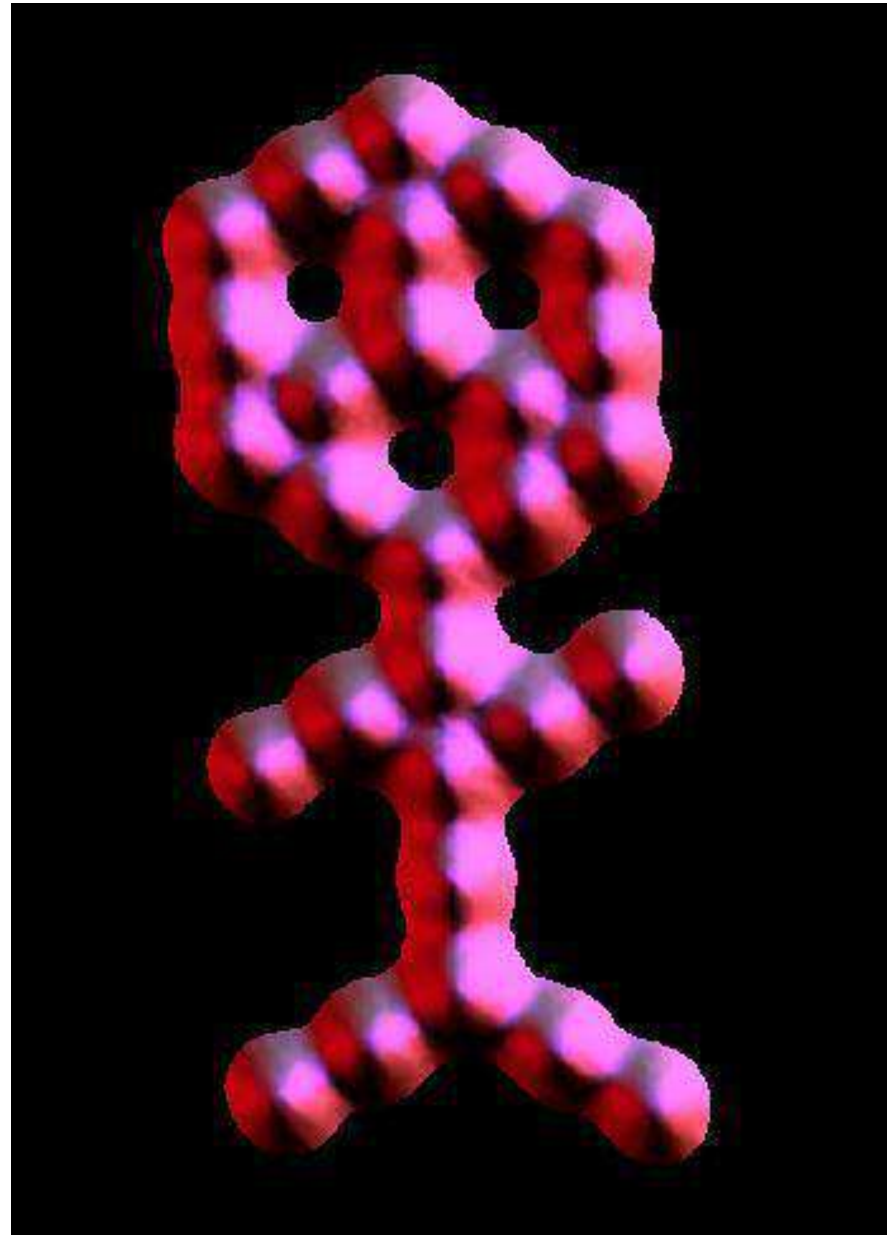


Image by Wolfgang Schonert of GSI Biophysics Research Group





= “ATOM”

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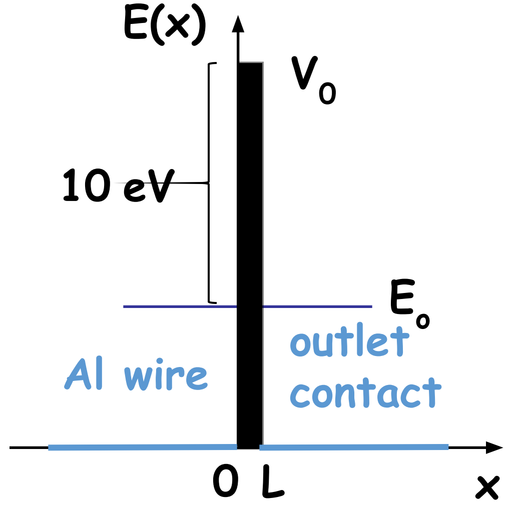
Example: Al wire contacts



"Everyday" problem:

You're putting the electrical wiring in your new house, and you're considering using Aluminum wiring, which is cheap and a good conductor. However, you also know that aluminum tends to form an oxide surface layer (Al_2O_3) which can be as much as several nanometers thick.

This oxide layer could cause a problem in making electrical contacts with outlets, for example, since it presents a barrier of roughly <u>10 eV</u> to the flow of electrons in and out of the Al wire.

Your requirement is that your transmission coefficient across any contact must be $T > 10^{-10}$, or else the resistance will be too high for the high currents you're using, causing a fire risk.

<u>Should you use aluminum wiring or not?</u>

<u>Compute L:</u>

$$T \approx e^{-2\kappa L} \approx 10^{-10} \Rightarrow \boxed{L \approx -\frac{1}{2\kappa}\ln(10^{-10}) \approx 0.72\ \text{nm}}$$

$$\kappa = \sqrt{\frac{2m_e}{\hbar^2}(V_o - E)} = 2\pi\sqrt{\frac{2m_e}{h^2}(V_o - E)} = 2\pi\sqrt{\frac{10\ \text{eV}}{1.505\ \text{eV}\cdot\text{nm}^2}} = 16\ \text{nm}^{-1}$$

Oxide is thicker than this, so go with Cu wiring! (Al wiring in houses is illegal for this reason)

Quantum Harmonic Oscillator

Solution of Schrödinger's equation for SHO

The classical 1-dim simple harmonic oscillator (SHO) of mass m and spring constant k is described by *Hooke's law* and the equation of motion is,

$$F = -kx = m\frac{d^2x}{dt^2} \Rightarrow x = A\,e^{ikx} + B\,e^{-ikx}. \tag{1}$$

The potential energy of such a SHO is,

$$V(x) = \frac{1}{2}k\,x^2 \equiv \frac{1}{2}m\omega^2x^2 \tag{2}$$

where ω is the angular frequency of the oscillator, $\omega = \sqrt{k/m}$. The quantum problem is to solve the Schrödinger equation for the potential (2). The time-independent Schrödinger equation for SHO is,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\,\psi. \tag{3}$$

$$\xi = \alpha x \quad \rightarrow \quad \frac{d}{dx} = \alpha \frac{d}{d\xi} \quad \text{and} \quad \frac{d^2}{dx^2} = \alpha^2 \frac{d^2}{d\xi^2}.$$

The Schrödinger equation (3) becomes,

$$\frac{d^2\psi(\xi)}{d\xi^2} + \frac{2mE}{\hbar^2\alpha^2}\,\psi(\xi) - \frac{m^2\omega^2}{\hbar^2\alpha^4}\,\xi^2\,\psi(\xi) \;=\; 0.$$

The SHO Schrödinger equation can be written in terms of dimensionless varible by making the coefficient of ξ^2 unity and introducing a dimensionless number ϵ,

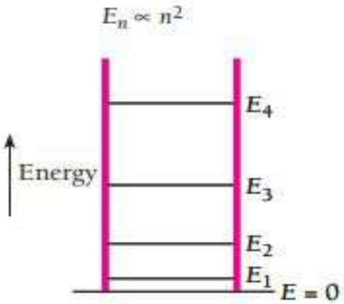
$$\frac{m^2\omega^2}{\hbar^2\alpha^4} = 1 \quad \Rightarrow \quad \alpha^2 = \frac{m\omega}{\hbar} \quad \text{therefore, } \xi = \sqrt{\frac{m\omega}{\hbar}}\,x, \tag{4}$$

$$\epsilon = \frac{2mE}{\hbar^2\alpha^2} = \frac{2E}{\hbar\omega} \tag{5}$$

Hence, the equation (3) in terms of dimensionless variable becomes,

$$\frac{d^2\psi}{d\xi^2} + (\epsilon - \xi^2)\,\psi \;=\; 0. \tag{6}$$

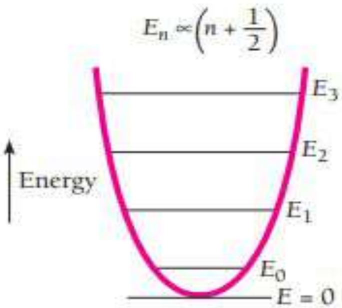
$$\boxed{\epsilon = 2n+1 = \frac{2E}{\hbar\omega} \quad \Rightarrow \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0,\,1,\,2,\,3,\,\ldots}$$



The general formula for the *n*th wave function is

Harmonic oscillator

$$\psi_n = \left(\frac{2m\nu}{\hbar}\right)^{1/4}(2^n n!)^{-1/2}H_n(y)e^{-y^2/2}$$



Some Hermite Polynomials

n	$H_n(y)$	α_n	E_n
0	1	1	$\frac{1}{2}h\nu$
1	$2y$	3	$\frac{3}{2}h\nu$
2	$4y^2 - 2$	5	$\frac{5}{2}h\nu$
3	$8y^3 - 12y$	7	$\frac{7}{2}h\nu$
4	$16y^4 - 48y^2 + 12$	9	$\frac{9}{2}h\nu$
5	$32y^5 - 160y^3 + 120y$	11	$\frac{11}{2}h\nu$