Solid State for Devices

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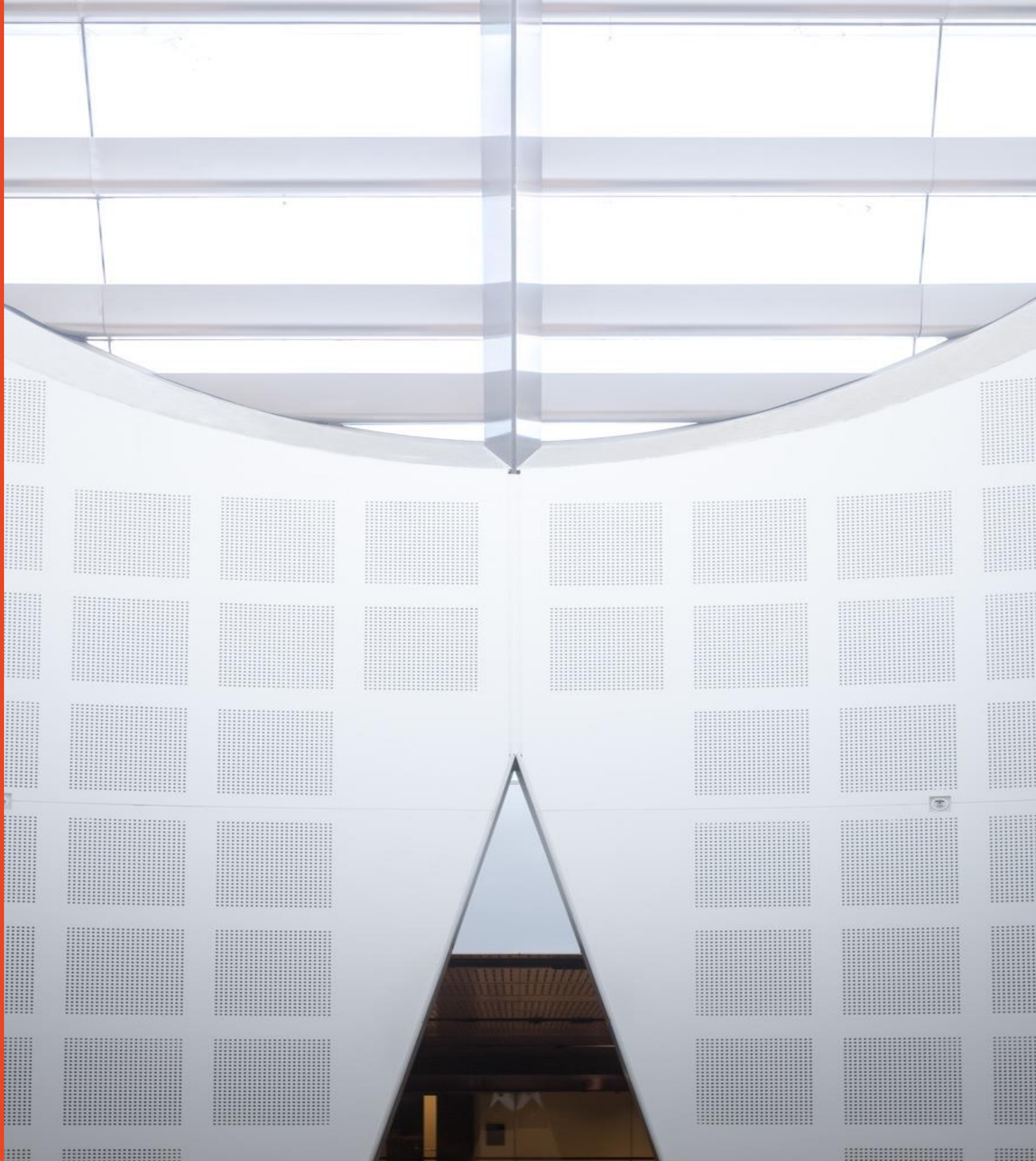


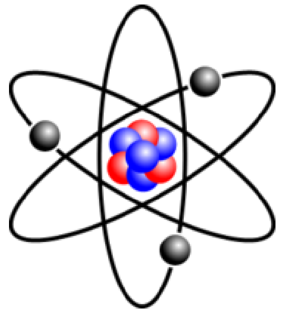
Introduction to quantum physics

- Classical Mechanics (CM) vs Quantum Mechanics (QM)
  - Black-Body
  - Photo-electric effect
  - Compton effect
- De-Broglie wavelength
- Uncertainty principle
- Quantum operators
- Schoedinger equation

Problems with Classical Mechanics

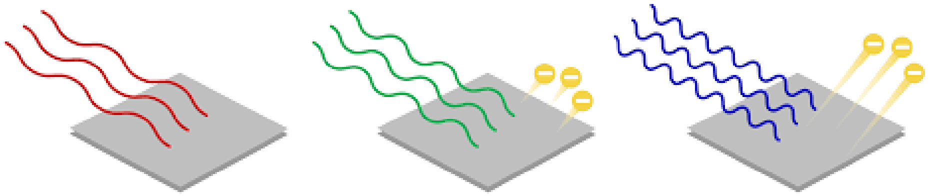
Experimental results could not be explained by classical mechanics

Stability of atom: Classical physics predicts the electron to continuously emit energy as it "orbits" around the nucleus, falling into the nucleus



Blackbody Radiation - emission of light from a body depends on the temperature of the body

Photoelectric Effect - emission of electrons from a metal surface when light shines on the metal



Classical vs Quantum Mechanics

- **Black Body Radiation**
  - **Problem:** Classical Rayleigh–Jeans law predicted the *ultraviolet catastrophe* (infinite energy at short wavelengths).

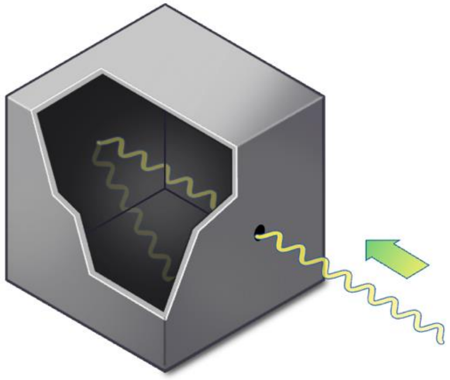
- **Photoelectric Effect**
  - **Problem:** Classical wave theory predicted that:
  - Intensity, not frequency, should control electron emission.
  - Time lag should exist for low intensities.

- **Compton Effect**
  - **Problem:** Classical wave theory of light scattering predicted no change in photon wavelength after collision with electrons.

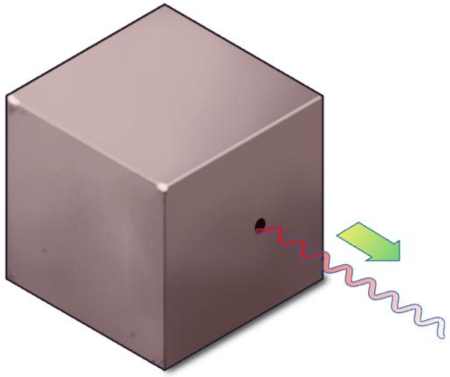
- **Davisson–Germer Experiment**
  - **Problem:** Matter was assumed to be purely particle-like.

Blackbody Radiation

Blackbody Radiator

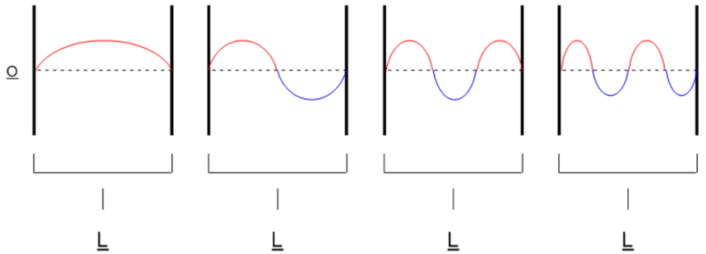


All incident radiation is absorbed



Emitted radiation is only a function of radiator's temperature (T)

$\lambda = (2L)\frac{1}{n}$



$\psi_1(x)$	$\psi_2(x)$	$\psi_3(x)$	$\psi_4(x)$
n = 1	n = 2	n = 3	n = 4
0 nodes	1 node	2 nodes	3 nodes
$\lambda = 2L$	$\lambda = L$	$\lambda = 2L/3$	$\lambda = L/2$

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

As an object is heated, it glows more brightly

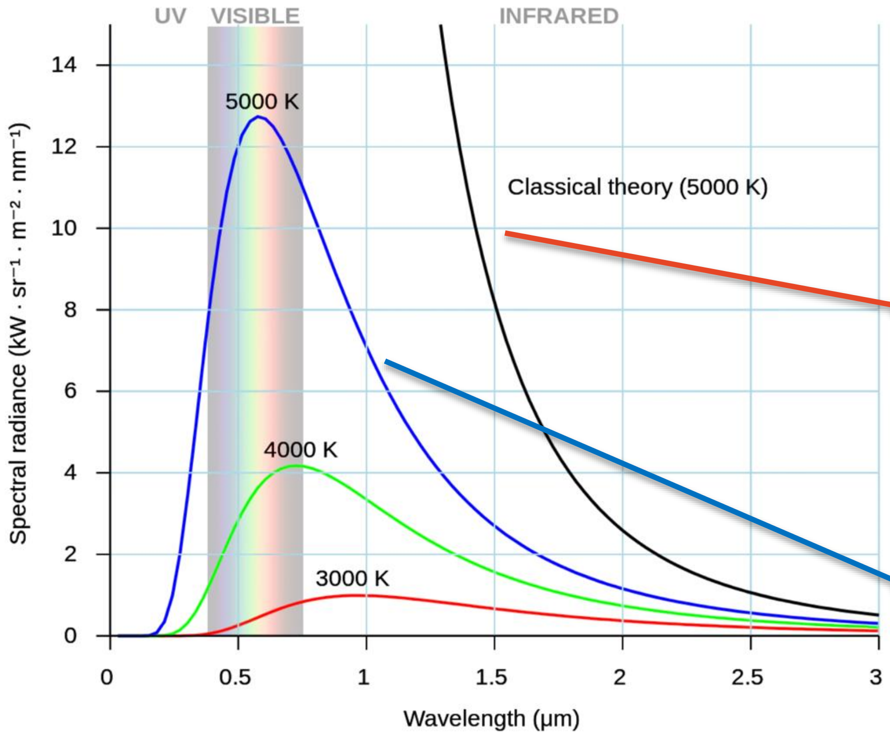
The color of light it gives off changes from red through orange and yellow toward white as it gets hotter.

The hot object is called a black body because it does not favor one wavelength over the other

The colors correspond to the range of wavelengths radiated by the body at a given temperature - black body radiation.

Blackbody Radiation

Classical physics predicts that any black body at temperature T should emit ultra-violet and even x-rays



Density of States

$$g(\nu)\,d\nu = \frac{8\pi V \nu^2}{c^3}\,d\nu.$$

Classical average energy per mode

$$\langle \epsilon \rangle_{\mathrm{cl}} = k_B T.$$

$$B_\nu^{\mathrm{RJ}}(T) = \frac{2\nu^2}{c^2} k_B T,$$

Quantum average energy per mode

$$\langle \epsilon \rangle_{\mathrm{q}} = \frac{h\nu}{e^{h\nu/(k_B T)} - 1}.$$

$$B_\nu^{\mathrm{Planck}}(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/(k_B T)} - 1},$$

CM Theoretical prediction: "Ultraviolet catastrophe"

Quanta

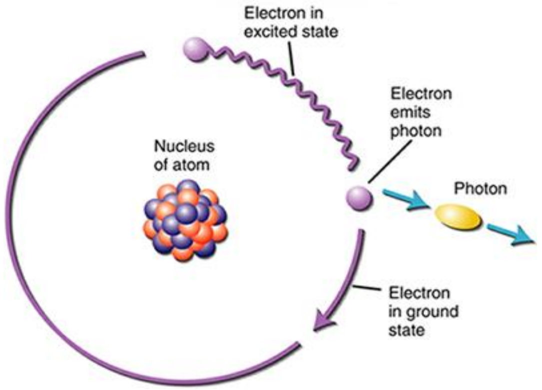
Max Planck (1900) - proposed that exchange of energy between matter and radiation occurs in packets of energy called

frequency of radiation, sometimes written as f giving expression E = hf.

$$E = h\nu$$

Quantum energy of a photon.

h = Planck's constant = 6.626×10^{-34} Joule·sec = 4.136×10^{-15} eV·s



Planck proposed: an atom oscillating at a frequency of n can exchange energy with its surroundings only in packets of magnitude given by

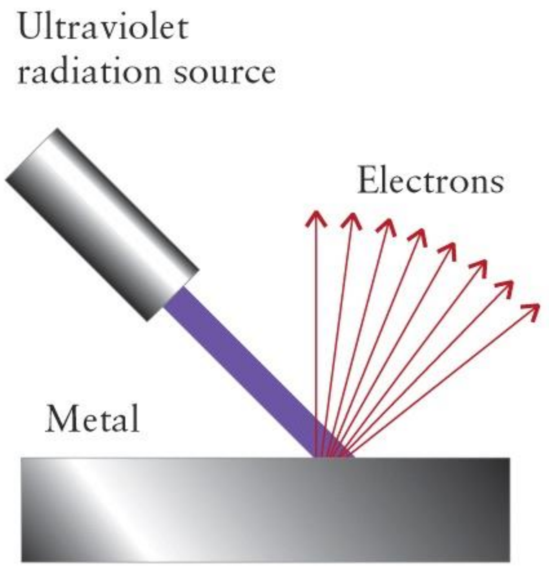
h: Planck's constant 4.136×10^{-15} eV s

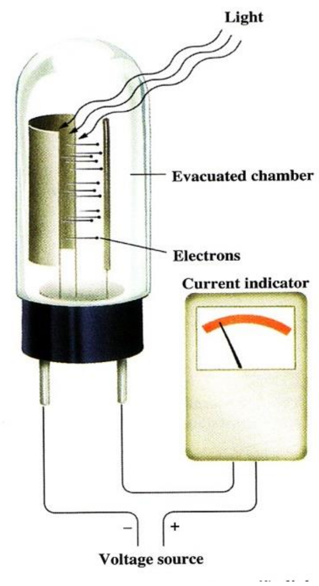
Radiation of frequency f = E / h is emitted

only if enough energy is available

Photoelectric Effect

Further evidence of Planck's work came from the photoelectric effect
ejection of electrons from a metal when its surface is illuminated with light

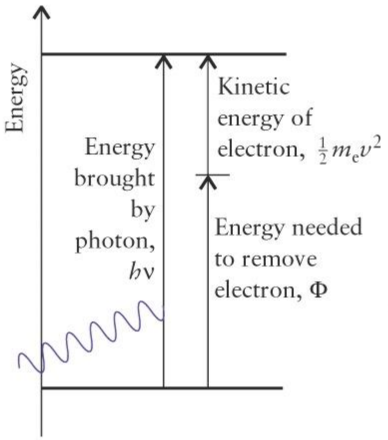


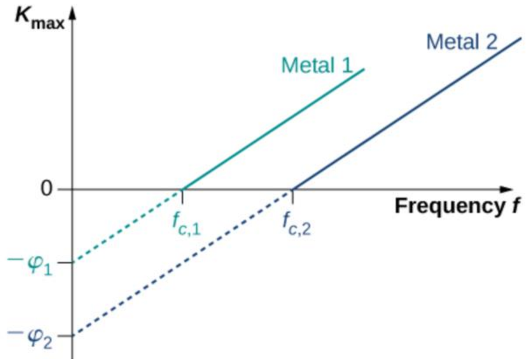


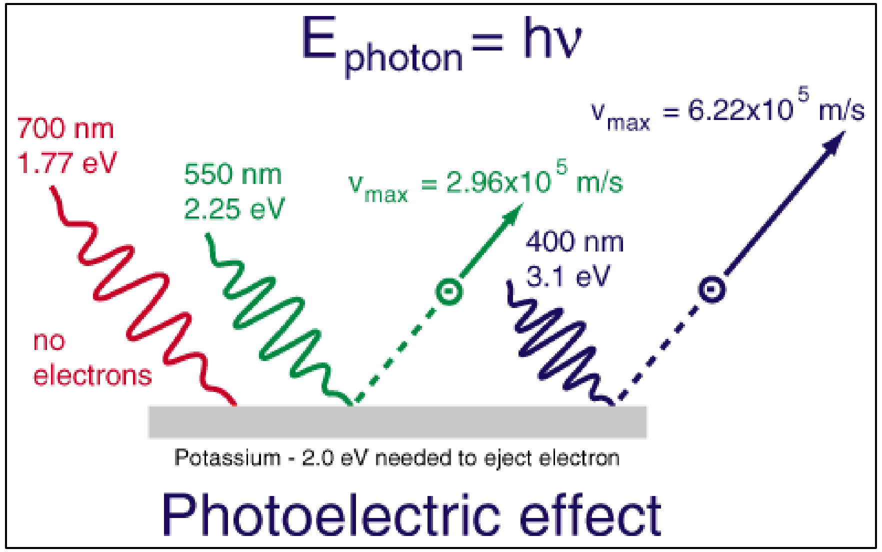
Light shining on a metal surface can eject electrons .
Key observations:
Electron emission occurs only if frequency larger threshold.
Maximum kinetic energy of electrons depends on frequency, not on light intensity.

Emission is essentially instantaneous (no time delay).
Problem: Classical wave theory predicted intensity ∝ energy, contradicting experiments

Photoelectric Effect







- Light consists of quanta (photons) with energy

$$\boxed{E_\gamma = h\nu = \hbar\omega}$$

- Each photon interacts with a single electron.
- Energy conservation:

$$h\nu = \phi + K_{\max}$$

where ϕ = work function, $K_{\max}$ = maximum kinetic energy.

Threshold frequency:

$$\nu_{\text{threshold}} = \frac{\phi}{h}$$

$$T = \frac{1}{2}mv^2 = h\nu - \Phi = h\nu - h\nu_0$$

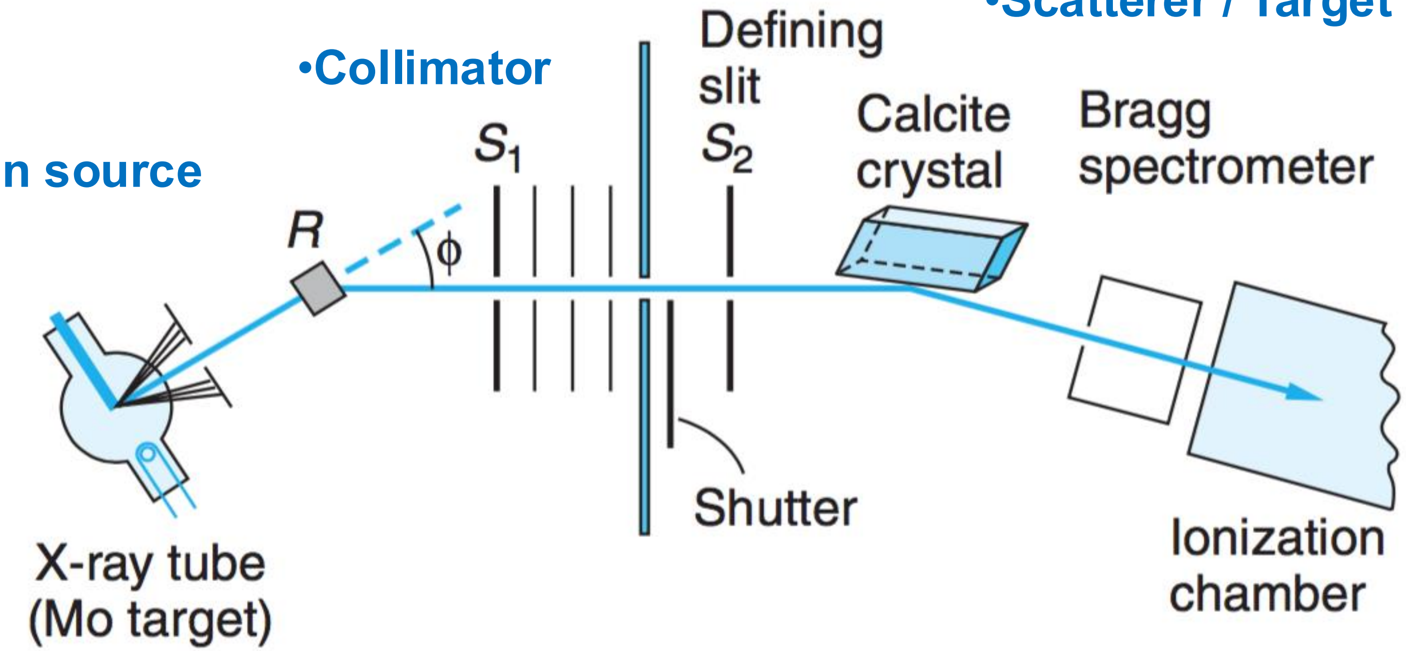
Establishing that Photon is Particle
Compton Effect (X-Ray Scattering)

In electromagnetism quanta of energy are carried by photons

Physics of semiconductors is essentially described by electrons and photons

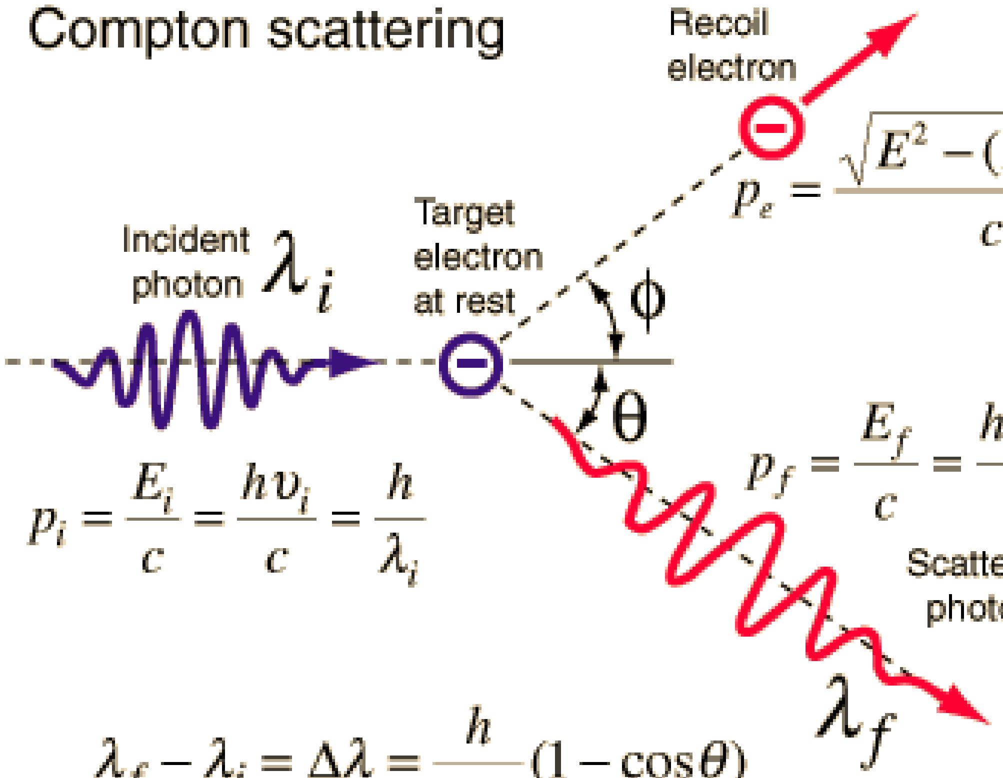
Compton effect prove the particle nature of photons

- •Scatterer / Target
- •Collimator
- •Monochromatic photon source
- •Detector mounted
- •on angular scale



Compton Effect

Measure the wavelength (or energy) of photons scattered from the target at various angles θ. One sees that the scattered photons have **longer wavelength** (lower energy) than the incident photons.



$$p_e = \frac{\sqrt{E^2 - (m_e c^2)^2}}{c}$$

$$p_i = \frac{E_i}{c} = \frac{h\upsilon_i}{c} = \frac{h}{\lambda_i}$$

$$p_f = \frac{E_f}{c} = \frac{h\upsilon_f}{c} = \frac{h}{\lambda_f}$$

$$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_0 c}(1 - \cos\theta)$$

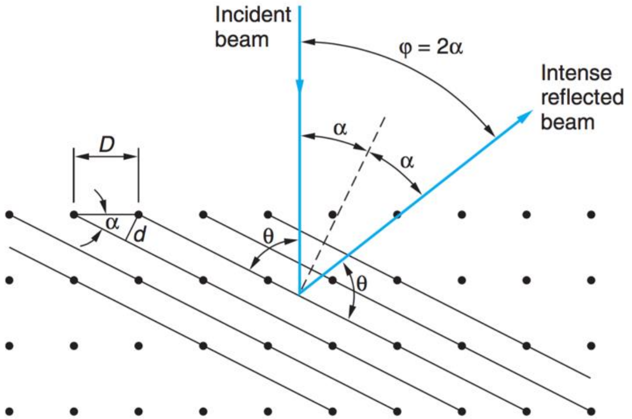
Light particles have momentum
And therefore prove particle nature of light

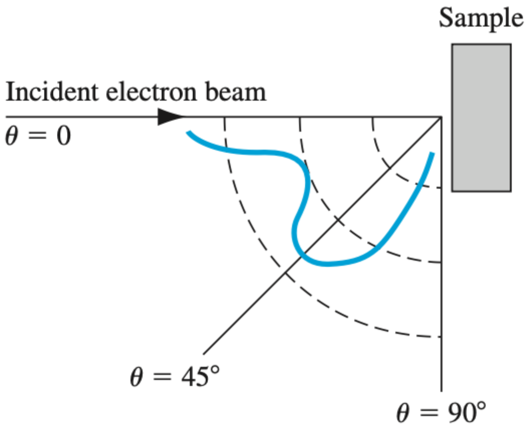
$$p = \frac{h}{\lambda}$$

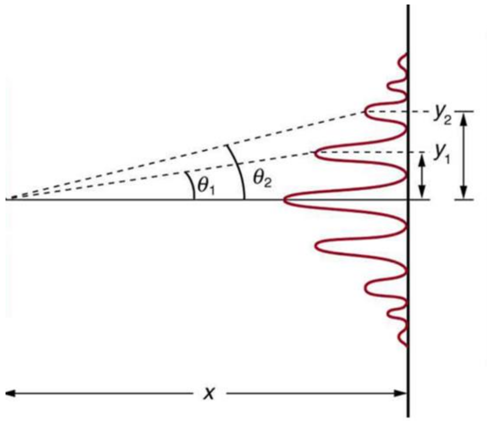
$$\boxed{p = \hbar k.}$$

The Davisson-Germer Experiment: Crystal Acts Like Thin-Film Interference

- An **electron gun** accelerated electrons with kinetic energy controlled by voltage V.
- A beam of electrons was directed onto a **nickel crystal target**.
- A movable **electron detector** measured the intensity of scattered electrons at different angles.







- Intensity of the electrons follow Bragg conditions.

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m_e eV}} \qquad \text{(de Broglie)}$$

$$2d\sin\theta = n\lambda \qquad \text{(Bragg condition)}$$

Wave nature of matter $p = \frac{h}{\lambda}$

This experiment suggests the wave nature of electrons = first evidence of wave-particle duality for classical particles

light can behave like a particle, and particles act like waves

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

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

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 !

Why use k instead of λ?
Using k is often more convenient in quantum mechanics because:

1. It appears naturally in wave equations (like the Schrödinger equation)
2. It's directly proportional to momentum ($p \propto k$)
3. It simplifies many mathematical expressions involving waves

So k is essentially a more mathematically convenient way to express the wave properties that determine a particle's momentum through its wave nature.

- Wave-like behaviour is observable when wavelength is comparable to
- system dimensions (like interatomic spacing).

Two fundamental relations

de Broglie wavelength

$$p = \frac{h}{\lambda}$$

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

Planck–Einstein relation

$$\boxed{E_\gamma = h\nu = \hbar\omega}$$

Electronic Wave-functions

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

- 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

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

Werner Heisenberg (1901–1976)

Interpretation

- Physical system can be described by a wave-functions
- In general is a functions of space and time **y** (x,t)
- The quantity **||^2** is interpreted as the **probability** that the particle can be found at a particular point *x* and a particular time *t*
- The act of measurement 'collapses' the wave function and turns it into a particle

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

Neils Bohr (1885-1962)

Momentum Operator

free-particle wave-function

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

$$\psi(x) = e^{ikx},$$

In quantum mechanics, observables correspond to operators acting on the wavefunction.

$$\frac{d}{dx}\psi(x) = ike^{ikx} = ik\psi(x).$$

$$-i\hbar\frac{d}{dx}\psi(x) = \hbar k\psi(x) = p\psi(x).$$

Momentum is naturally linked to the spatial variation of a wave

$$\hat{p}_x = -i\hbar\frac{d}{dx}, \qquad \hat{\mathbf{p}} = -i\hbar\nabla \quad \text{(3D case)}.$$

$$\psi(x) = e^{ikx}, \qquad p = \hbar k.$$

Energy Operator

free-particle wavefunction

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

$$\psi(t) = e^{-iEt/\hbar}.$$

In quantum mechanics, observables correspond to operators acting on the wavefunction.

$$\frac{d}{dt}\psi(t) = -\frac{iE}{\hbar}\psi(t) \quad \Rightarrow \quad i\hbar\frac{\partial}{\partial t}\psi(t) = E\psi(t).$$

Energy is naturally linked to the time variation of a wave

$$\hat{E} = i\hbar\frac{\partial}{\partial t}.$$

Kinetic Energy

Classically $T = p^2/2m$. In quantum mechanics:

$$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2.$$

Plane wave check

For $\psi(x) = e^{ikx}$:

$$\nabla^2\psi = -k^2\psi \quad \Rightarrow \quad \hat{T}\psi = \frac{\hbar^2 k^2}{2m}\psi,$$

matching the classical $E = p^2/2m$.

Thus the appearance of the **second derivative** in the Schrdinger equation is a direct consequence of kinetic energy being quadratic in momentum.

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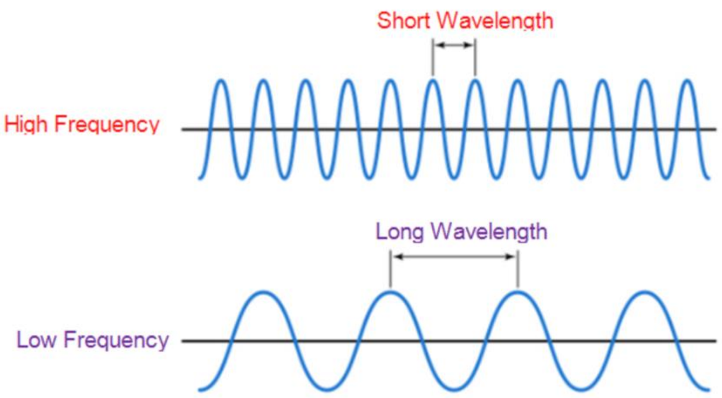
Heisenberg’s Uncertainty Principle

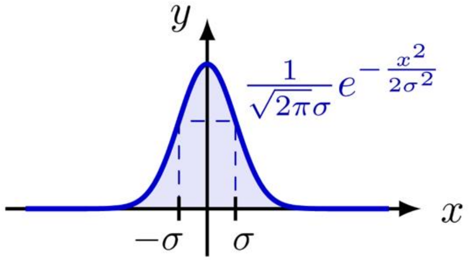
Free wave has perfectly defined momentum p = hk but is completely delocalised in space is completely delocalized in space

$$\psi(x) = e^{ikx},$$



A wave that is localized in space is described by superposition of many plane waves:

$$\psi(x) = \int \tilde{\psi}(k) e^{ikx}\, dk.$$



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.**

Classical to Quantum operators

– Classical momentum takes a different form in QM

$$E = \frac{1}{2}mv^2 + V \qquad E = \frac{p^2}{2m} + V$$

$$p = mv$$

$$p = -i\hbar\frac{\partial}{\partial x} \qquad p^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

Important Concepts/equations

$$E = h\nu$$

$$\nu = c/\lambda$$

$$\Delta x \Delta p \geq \hbar \qquad \Delta E \Delta t \geq \hbar$$

$$\lambda = h/p = h/mv$$

- Wave equation
- Hamiltonian Operator
- Wave-function interpretation
- Boundaries conditions

Hamiltonian

From Planck and de Broglie we have

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

A plane wave takes the form

$$\psi(\vec{r}, t) = e^{i(\vec{k}\cdot\vec{r} - \omega t)}.$$

Applying the quantum operators

$$\hat{p} = -i\hbar\nabla, \qquad \hat{E} = i\hbar\frac{\partial}{\partial t},$$

yields eigenvalues p and E.

In classical mechanics, the Hamiltonian H represents the total energy. In quantum mechanics it becomes an operator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{r}, t).$$

Since energy is the generator of time evolution, the dynamics of the state are given by

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t) = \hat{H}\psi(\vec{r}, t),$$

which is the **time-dependent Schrdinger equation**.

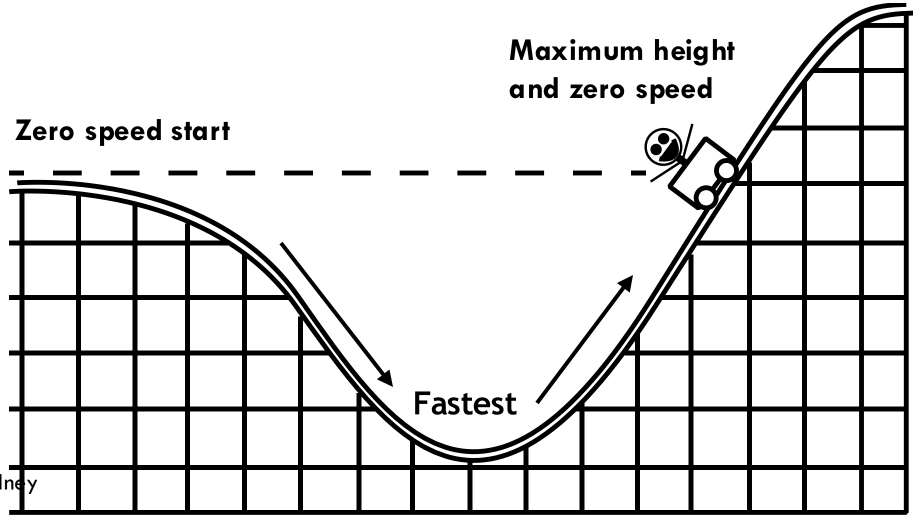
Schrödinger Equation

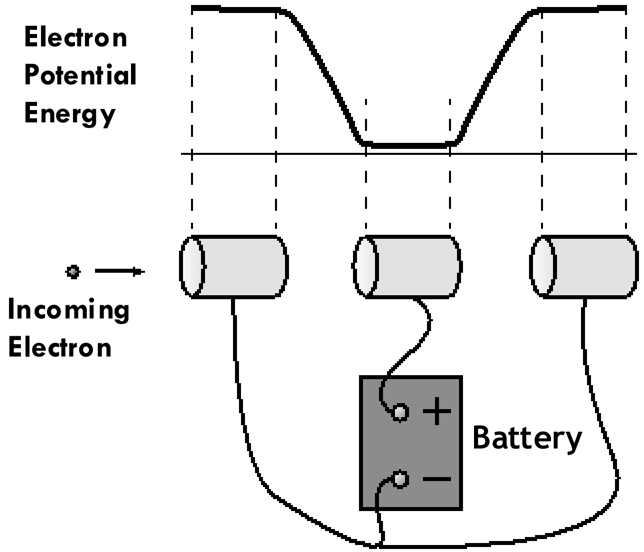
$$E = T + V$$

$$\underbrace{i\hbar\frac{\partial\Psi}{\partial t}}_{\text{Total E term}} = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}}_{\text{K.E. term}} + \underbrace{V(x,t)\Psi}_{\text{P.E. term}}$$

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

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





The Hamiltonian operator

Time-dependent
Schrödinger equation

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

Can think of the RHS of the Schrödinger equation as a ***differential operator that represents the energy of the particle.***

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$$

This operator is called the *Hamiltonian* of the particle, and usually given the symbol $\hat{H}$

$$\left[\underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\text{Kinetic energy operator}} + \underbrace{V(x,t)}_{\text{Potential energy operator}}\right]\Psi \equiv \hat{H}\Psi$$

Hence there is an alternative (shorthand) form for the time-dependent Schrödinger equation:

Hamiltonian is a linear differential operator.
Schrödinger equation is a linear homogeneous partial differential equation

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

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

If $V(\vec{r})$ is independent of t, separation of variables $\psi(\vec{r},t) = \phi(\vec{r})e^{-iEt/\hbar}$ gives

Let's assume that we can write the wave-function as

$$\Psi(x,t) = \psi(x)\phi(t)$$

Space and time can be separated as independent variables

Let's rewrite the fundamental equation with this assumption
(Valid when the potential energy term does NOT depend on time)

$$\Psi(x,t) = \psi(x)\phi(t)$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}$$

Each side of the equation is a function of a different variable

Each side must be equal to a constant

Time dependent term

$$\phi(t) = e^{-i(\eta/\hbar)t}$$

$$\eta = E$$

$$\phi(t) = e^{-i(E/\hbar)t}$$

$$\boxed{\phi(t) = e^{-i\omega t}}$$

$$E = \omega\hbar$$

Indicate the evolution in time of the total wave-function

- The exponential $e^{-iEt/\hbar}$ is a **phase factor** of unit modulus.
- Its probability is always 1 — it does not affect measurable probabilities.
- This is why stationary states are called “stationary”: their probability density is independent of time, even though the phase evolves.

From time-Dependent Schrodinger Wave Equation

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

To time-Independent Schrodinger Wave Equation

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

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = E$$

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

Time independent wave-function

- In one space dimension, the time-independent Schrödinger equation is an **ordinary differential equ**ation (not a partial differential equation)

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

- **The time-independent Schrödinger equation is an eigenvalue equation** for the Hamiltonian operator:

$$\hat{H}\psi=E\psi$$

Operator × function = number × function

(Compare Matrix × vector = number × vector)

- We will consistently use uppercase Ψ(x,t) for the full wavefunction (TDSE), and lowercase ψ(x) for the spatial part of the wavefunction when time and space have been separated (TISE)

Interpretation of $|\psi|^2$ and consequences

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

$$\left|\Psi(x,t)\right|^2 = \Psi(x,t)\Psi^*(x,t) = 1$$

$$\left|\psi(x)\right|^2 = 1$$

$$p = -i\hbar\frac{\partial}{\partial x}$$

$$p = -i\hbar\frac{\partial}{\partial x}$$

– Probability density is independent from time component

Boundaries conditions

- The probability of a wavefunction to be somewhere in the space must be certain (**Normalisation Condition**)

- Also, **wave-function must be finite and continuous**

- **The derivative must be finite and continuous**

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$$

$$p = -i\hbar \frac{\partial}{\partial x}$$

$$p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

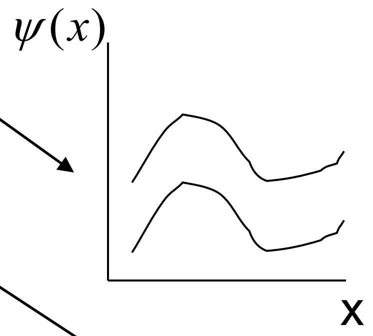
ψ **boundaries conditions** to fully determine the wavefunction in a given state

Boundary conditions for the wavefunction

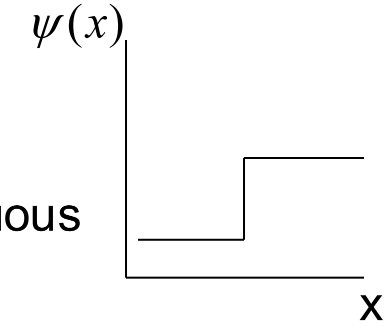
The wavefunction must:

Examples of unsuitable wavefunctions

1. Be a continuous and single-valued function of both *x* and *t* (in order that the probability density is uniquely defined)

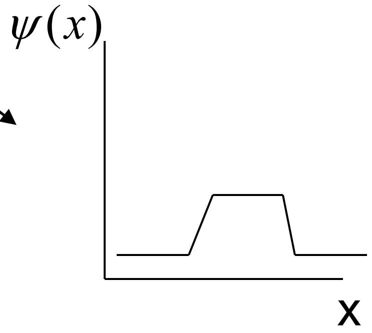


Not single valued



Discontinuous

2. Have a continuous first derivative (except at points where the potential is infinite)



Gradient discontinuous

3. Have a finite normalization integral (so we can define a normalized probability)

Free electrons

Schrodinger equation: $-\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$

Solution: $\psi(x) = Ae^{ikx} = A(\cos kx + i\sin kx)$

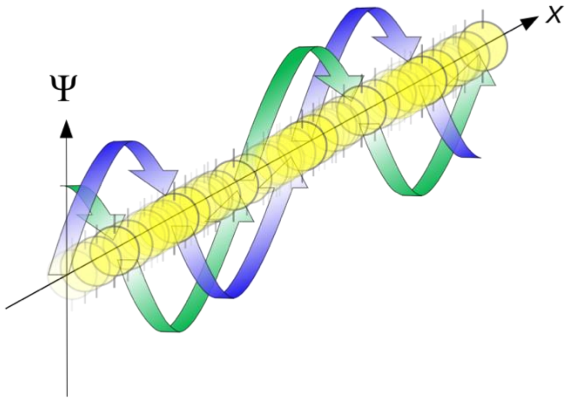
Different k →different quantum states

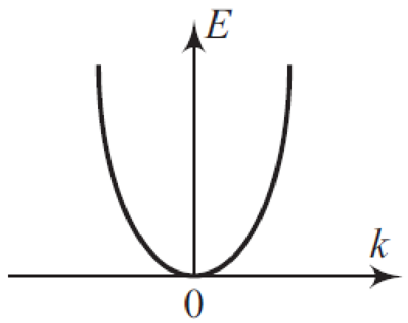
Probability: $|\psi(x)|^2 = A^2$

Wave vector: $k = \frac{2\pi}{\lambda}$

Momentum: $p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda} = \hbar k$ de Broglie Relation

Energy (Kinetic) : $E = \frac{p^2}{2m}$ $E = \frac{\hbar^2 k^2}{2m}$





Energy-Momentum (E-k/p) Diagram:

$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m}$ $\frac{1}{\hbar}\frac{dE}{dk} = v$ vs. Band Diagram

Infinite Potential Well

Schrodinger equation (1D): $-\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$

In both regions I and III: $\psi(x) = 0$

In region II: $-\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$

Solution: $\psi(x) = A_1 e^{ikx} + A_2 e^{-ikx}$

$= (A_1 + A_2)coskx + i\,(A_1 - A_2)sinkx$

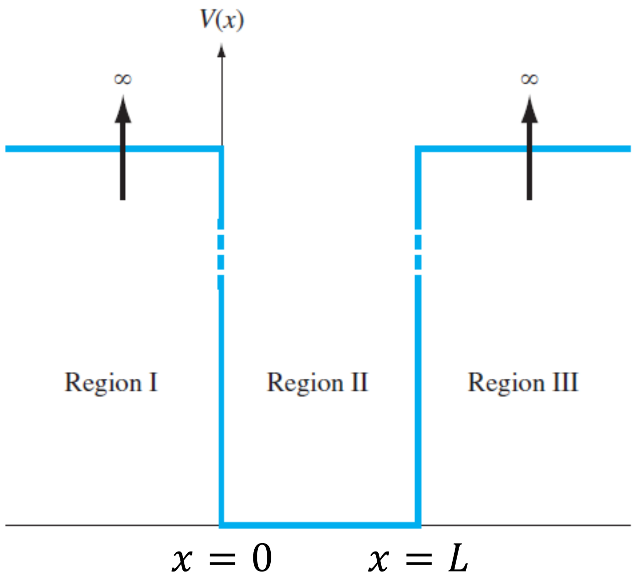
boundary condition: $\psi(x=0) = \psi(x=L) = 0$

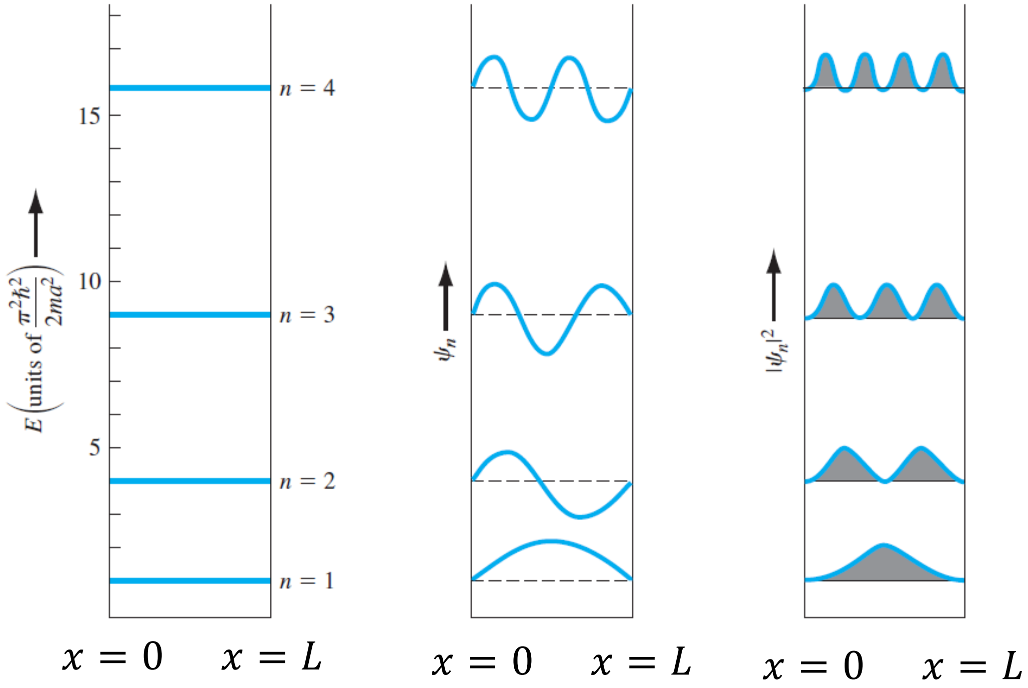
So: $A_1 + A_2 = 0;\ k = \frac{n\pi}{L};\ \psi(x) = 2iA_1 sin\frac{n\pi}{L}x$

Probability in region II: $\int_0^L \psi(x)\psi^*(x)dx = 1$

So: $A_1 = \sqrt{\frac{1}{2L}};\ \psi(x) = \sqrt{\frac{2}{L}}sin\frac{n\pi}{L}x$, where n=1, 2, 3, . . .

$E = \frac{\hbar^2 k^2}{2m} \Longrightarrow E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$, where n=1, 2, 3, . . .





discrete, quantum confinement