Quantum Physics-I

Dr. Anurag Srivastava

Web address: https://profanurag.in

Email: profanurag@gmail.com

Visit me: Room-110, Block-E, IIITM Campus

Syllabus

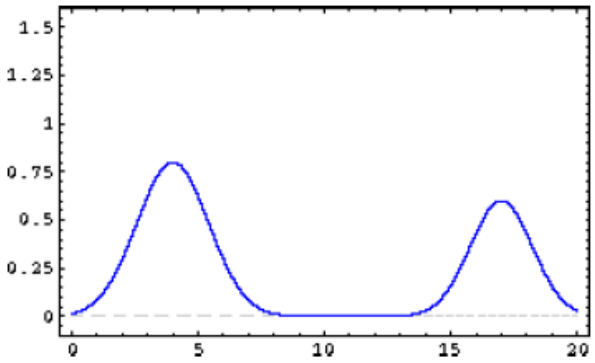
- **Electrodynamics**: Maxwell's equations: differential and integral forms, significance of Maxwell's equations, displacement current and correction in Ampere's law, electromagnetic wave propagation, transverse nature of EM waves, wave propagation in bounded system, applications.

- **Quantum Physics:** Dual nature of matter, de-Broglie Hypothesis, Heisenberg uncertainty principle and its applications, postulates of quantum mechanics, wave function & its physical significance, probability density, Schrodinger's wave equation, Eigen values & Eigen functions, Applications of Schrodinger equation.

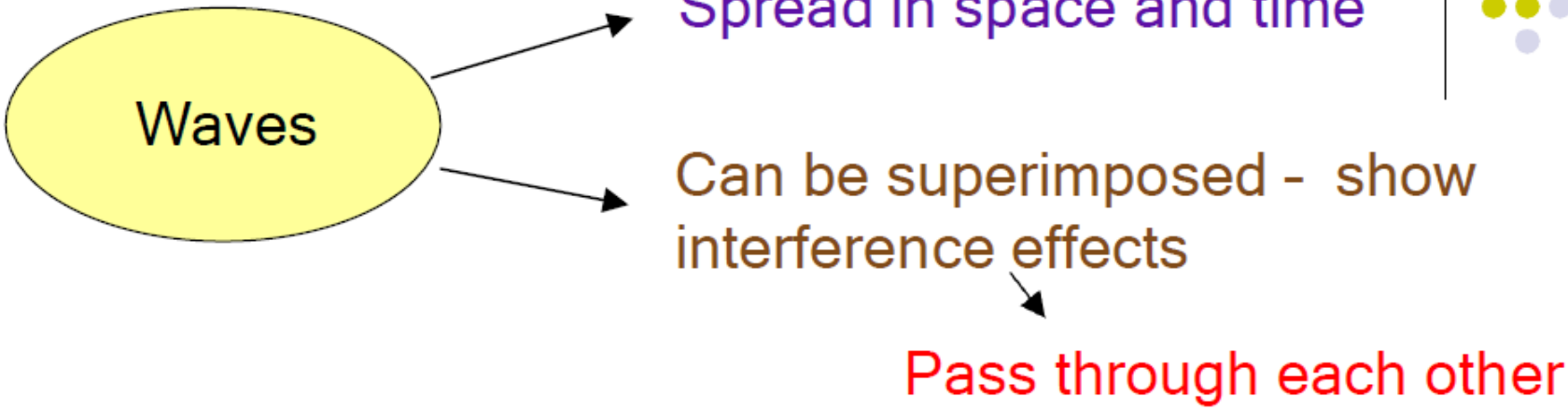
de Broglie concept of matter waves: dual nature of matter

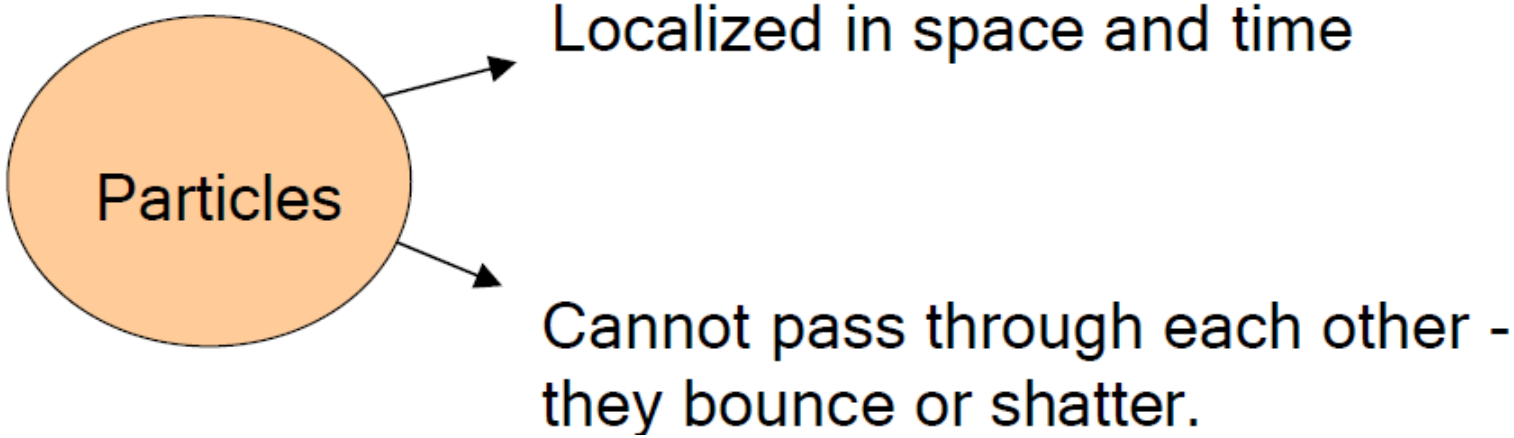
Waves and Particles Basic difference:

- Waves can pass through each other !
- As they pass through each other they can enhance or cancel each other
- Later they regain their original form !



Waves and Particles:





OUR QUANTUM WORLD

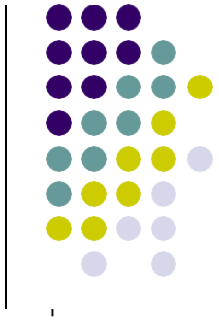


In the 20th century, study of atomic systems required a fundamental revision of these classical ideas about physical objects.

1. Light waves exhibited particle like properties -
phenomena called photo-electric effect in which light impinging on certain metals cause instantaneous emission of electrons in a billiard ball like impact.
- the basis of automatic door openers in grocery stores

2. Electrons (particles) exhibit wave like properties -
they can pass through each other !
Phenomenon of electron interference
- basis of electron microscopes

OUR QUANTUM WORLD



This quantum picture of the world is at odds with our common sense view of physical objects.
We cannot uniquely define what is a particle and what is a wave !!

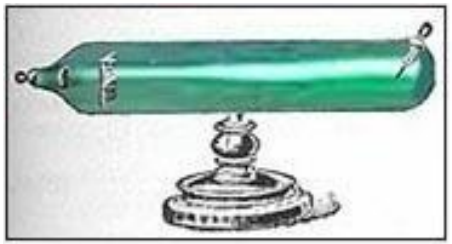
Neils Bohr and Werner Heisenberg were the architects of this quantum world view, along with Planck, Einstein, de Broglie, Schrodinger, Pauli and Dirac.

MILESTONES OF QUANTUM PHYSICS:



J.J.Thomson Established electron as a fundamental particle of nature. He measured its charge to mass ratio using a Crooke's tube.

Electric current = flow of electrons



Crooke's tube: Evacuated tube Visualization of electron beam.



Animation of electrons moving and being deflected by an electric or magnetic field.



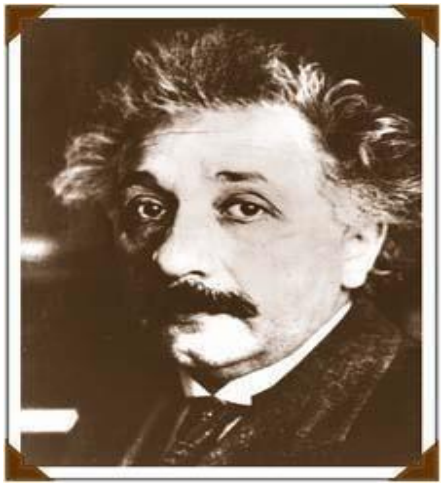
Marie Curie and Radioactivity - 1898

Discovered that certain elements ‘ spontaneously emit radiations and change into different elements.

Only woman scientist to receive two Nobel Prizes: One in chemistry and the other in physics.

Marie Curie received the Nobel Prize in Physics with her husband Pierre Curie and Henri Becquerel in 1903 , for their work on radioactivity. In 1911, she won her second Nobel Prize, this time in chemistry for her work on polonium and radium.

The Quantum of Light or the Photon



Particle nature of light was proposed by Einstein in 1905 to explain the photo-electric effect. Photo-electric effect – automatic door openers in grocery stores. Particles of light are called light quanta or photons.

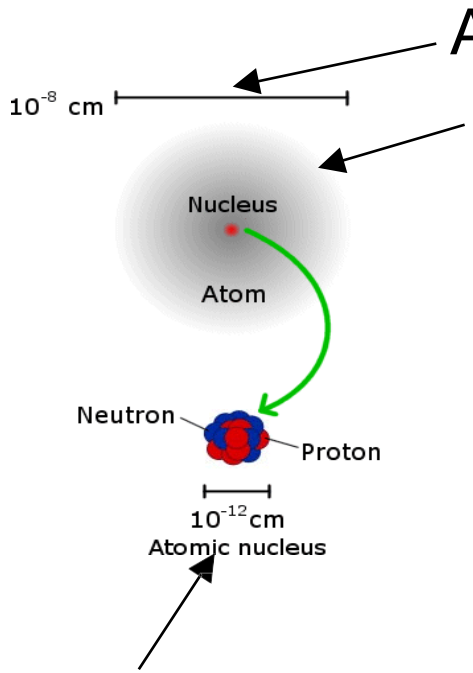
Energy of a Photon = h x frequency of light
h is a fundamental constant of nature and it is very small in size.

Packet of energy in photon is so small that we are not aware of the rain of photons of light impinging on our eyes – just as you cannot feel the impact of individual air molecules, you only feel a breeze.

Rutherford and his Nuclear Atom: 1898 -1911



Ernest Rutherford used alpha rays to discover the nucleus of the atom. The nucleus was positively charged and contained almost all of the mass of the atom. Most of the atom was empty space.



Classical physics required that this atom is unstable electrons would fall into the nucleus in 10^{-7} sec!



Planck and quantization of atomic " vibrations "

Before Einstein, Planck postulated from study of radiation from hot bodies that the radiating atoms can only radiate energy in discrete amounts – or that atoms exist only in discrete states, called Quantum states.

This was the birth of quantum physics in 1900

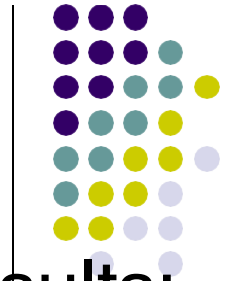
THE BOHR ATOM:


BOHR

Bohr proposed a revolutionary model:
An atom with discrete (Quantum) states
- an ad-hoc model

Bohr model explained how atoms emit light quanta and their stability. He combined the postulates of Planck and Einstein to build characteristic energy states that atoms should possess.
Model gave excellent agreement with experiment on atomic spectra.(1913)

Bohr atom



Bohr's atom model achieved three important results:

1. Atoms are stable
2. Different atoms of the same element are identical
3. Atoms regenerate if they are taken apart and then allowed to reform.

Bohr atom



BOHR

Understanding the origin of Bohr's model required an essential bold step - enter Louis de Broglie.

Wave nature of material bodies:



If light, which classically is a wave, can have particle nature As shown by Planck and Einstein,

Can material particles exhibit wave nature ?

Prince Louis de Broglie while doing his Ph.D. research said particles should have wave like properties.

Wave Nature of Matter



Louis de Broglie in 1923-24 proposed that matter particles should exhibit wave properties just as light waves exhibited particle properties. These waves have very small wavelengths in most situations so that their presence was difficult to observe

These waves were observed a few years later by Davisson and G.P. Thomson with high energy electrons. These electrons show the same pattern when scattered from crystals as X-rays of similar wave lengths.

Electron microscope picture of a fly →



A SUMMARY OF DUAL ITY OF NATURE
Wave particle duality of physical objects

LIGHT

Wave nature -EM wave

Optical microscope

Interference

Particle nature -photons

Convert light to electric current

Photo-electric effect

PARTICLES

Wave nature

Matter waves -electron microscope

Particle nature

Electric current

photon-electron collisions

Discrete (Quantum) states of confined systems, such as atoms.

Matter waves : de-Broglie concept



In 1924, Lewis de-Broglie proposed that matter has dual characteristic just like radiation. His concept about the dual nature of matter was based on the following observations:-

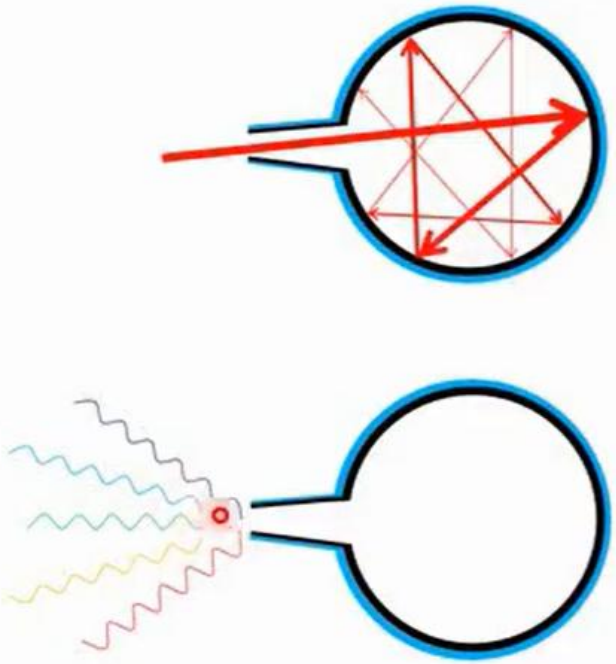
(a)The whole universe is composed of matter and electromagnetic radiations. Since both are forms of energy so can be transformed into each other.

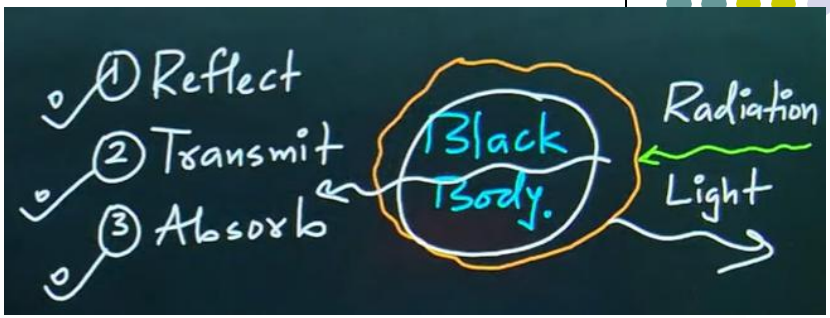
(b)The matter loves symmetry. As the radiation has dual nature, matter should also possess dual character.

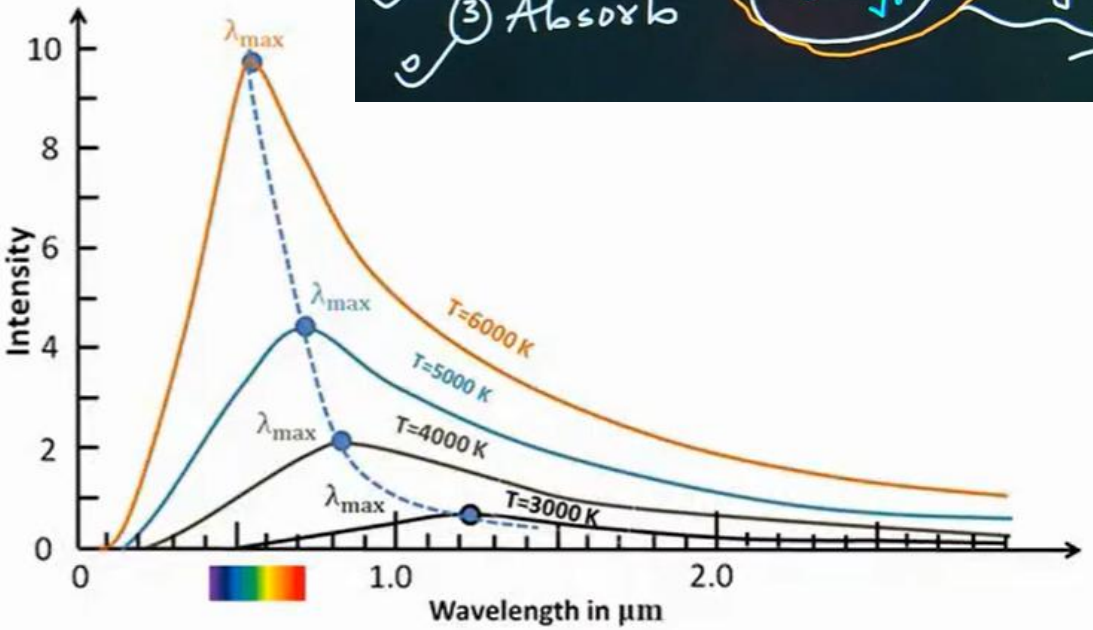
- According to the de Broglie concept of matter waves, the matter has dual nature.
- It means when the matter is moving it shows the wave properties (like interference, diffraction etc.) are associated with it and when it is in the state of rest then it shows particle properties.
- Thus the matter has dual nature. The waves associated with moving particles are matter waves or de-Broglie waves.

Quantum Physics started with Max Planck's Black Body Radiation

Black Body Radiation





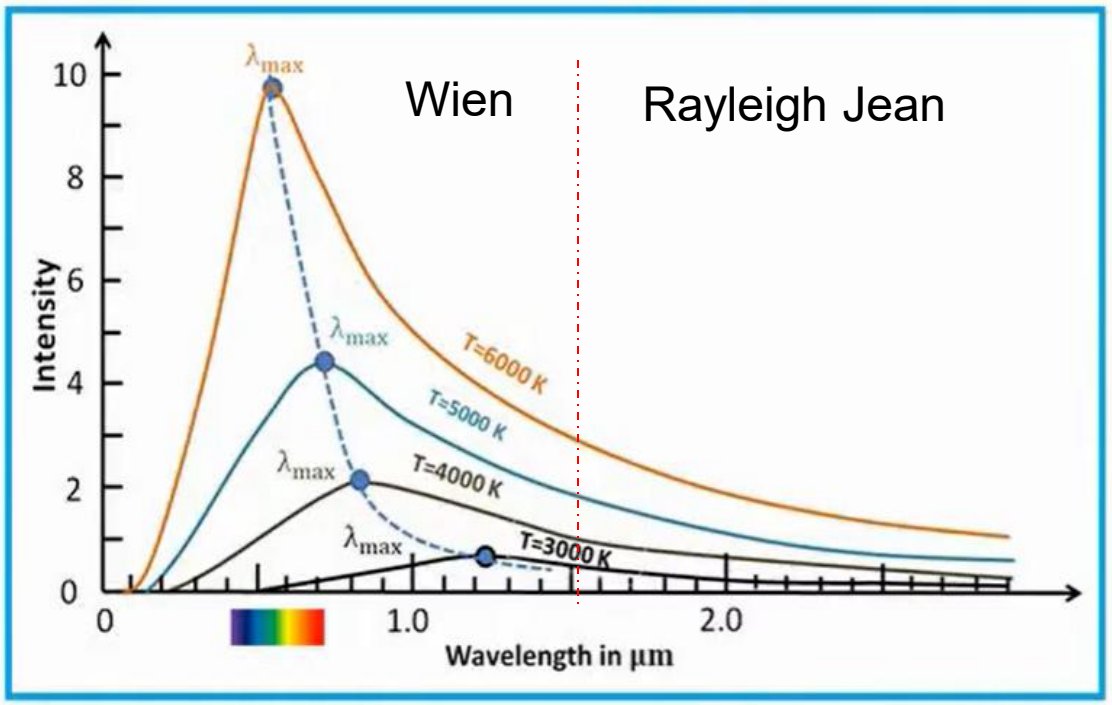


Planck's Law

1. Inside the black body, molecules vibrates and performs simple harmonic motion with all possible frequancies, called oscillators.
2. Oscillators can not emit or absorb the energy continously. But the oscillators of frequancy (ν) only can emit or absorb the energy of magnitude ($h\nu$). ← Energy per oscillator

Shift of wavelength at with temperature rise was explained by Wiens

Black Body Radiation



Wien's displacement Law

$$\lambda_{max} \propto \frac{1}{T}$$

For higher wavelength =?

Rayleigh Jean's Radiation Law gives Energy density of the radiation as -

$$\rho(\nu) = \frac{8\pi\nu^2}{c^3} kT$$

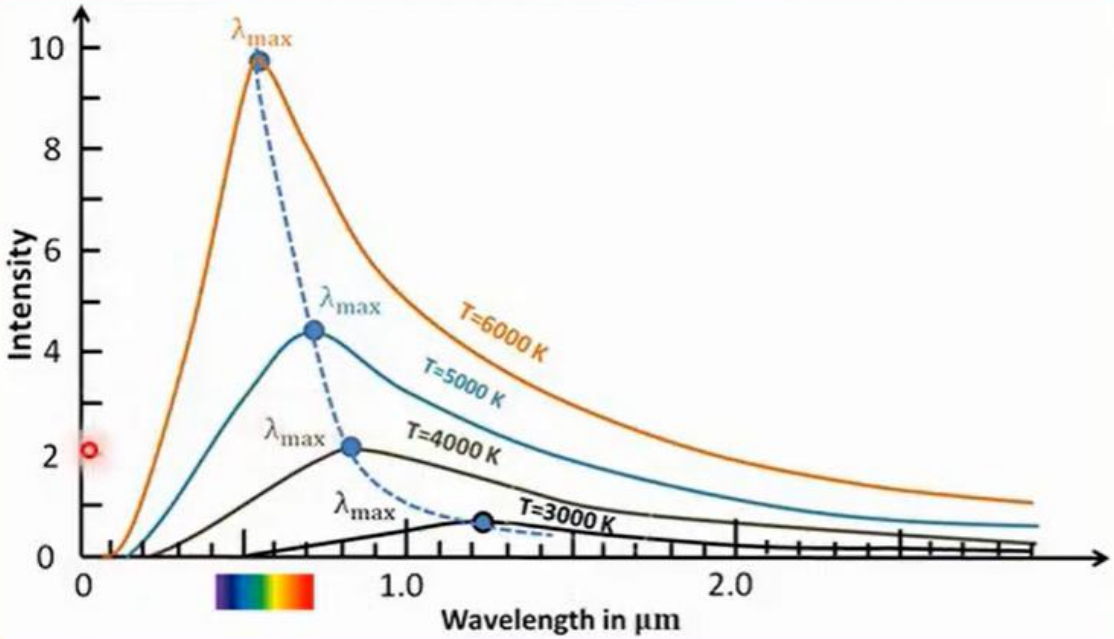
For lower wavelength =?

Complete Curve couldn't get explained by these two

Max Planck was awarded Noble Prize in 1918

Black Body Radiation

$$\rho(\nu) = \frac{8\pi\nu^2}{c^3}\,kT$$



Max Planck suggested that radiated energy must be depending on frequency of radiation and represented this energy $E = h\nu$ and replaced the average energy **kT by** $\frac{h\nu}{e^{\frac{h\nu}{kT}}-1}$

$$\therefore\ \rho(\nu) = \frac{8\pi\nu^2}{c^3}\,\frac{h\nu}{e^{\frac{h\nu}{kT}}-1}$$

$$\therefore\ \rho(\nu) = \frac{8\pi h\nu^3}{c^3}\left(\frac{1}{e^{\frac{h\nu}{kT}}-1}\right)$$

Planck's Radiation Law

- Einstein used idea of Planck to explain his photoelectric effect.
- He confirmed that light consists of discrete units of energy known as photons carrying energy - $E = h\nu$.
- **This dual nature of light is known as wave-particle duality.**

- Motion of macroscopic particles can be explained by classical theory of Mechanics.
- But it fails to explain the motion of microscopic particles like electron, proton etc.
- **Quantum mechanics** was developed from Quantum theory to explain the properties associated with such particles.

- De Broglie wave-particle duality hypothesis
- Heisenberg's Uncertainty Principle and
- Schrodinger's equation

provide base on which quantum mechanics is built .

de Broglie Hypothesis

- It states that –

  There is a wave associated with every moving particle moving with velocity v, and the wavelength of this wave is given by –

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

h = 6.626 x 10^{-34} J-s is Plank's constant

p = m v is momentum

The **de Broglie hypothesis** (proposed by Louis de Broglie in 1924) states that all moving matter—such as electrons, protons, and atoms—exhibits a dual wave-particle nature

Key Concepts

- **Wave-Particle Duality:** Just as light waves can sometimes behave like particles (photons), moving material particles act like waves.
- **Macroscopic vs. Microscopic:**
  - Everyday objects (like a baseball or car) have huge mass (m), making their de Broglie wavelength infinitesimally small and impossible to measure or observe.
  - Subatomic particles (like electrons) have tiny mass, resulting in a measurable wavelength comparable to atomic spacings.
- **Bohr's Quantized Orbits:** De Broglie explained Bohr's stable electron orbits in an atom by showing that an orbit must contain an integer number of whole matter wavelengths: $2\pi r = n\lambda$

de Broglie Hypothesis

Let us consider the case of the photon. Energy of the photon, according to Plank's theory of radiation is given by – $E = h\nu$ (1)

where h is Plank's constant and ν is frequency of radiation

If we consider a photon as a particle of mass m, its energy is given by Einstein Mass Energy relation as – $E = mc^2$ (2)

From equation (1) and (2), we get,

$$h\nu = mc^2 \quad (3)$$

As photon travels with velocity of light 'c' in free space, its momentum 'p' is given by –

$$p = mc \quad (4)$$

de Broglie Hypothesis

$E = h\nu$ (1)

$E = mc^2$ (2)

$h\nu = mc^2$ (3)

$p = mc$ (4)

Dividing equation (3) by (4) we get –

$$\frac{h\nu}{p} = \frac{mc^2}{mc} = c$$

$$\therefore \frac{h}{p} = \frac{c}{\nu} = \lambda \qquad \left(\because \frac{c}{\nu} = \lambda\right)$$

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

de Broglie assumed that this relation holds good for all material particles like electrons, neutrons etc.

de Broglie wavelength in terms of Kinetic Energy

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

de Broglie Relation

The Kinetic energy of the particle is –

$$E = \frac{1}{2}mv^2 = \frac{1}{2m}m^2v^2 = \frac{1}{2m}p^2$$

$$\therefore p^2 = 2mE$$

$$\therefore p = \sqrt{2mE}$$

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

For charged particle at potential V

$$\therefore \lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}$$

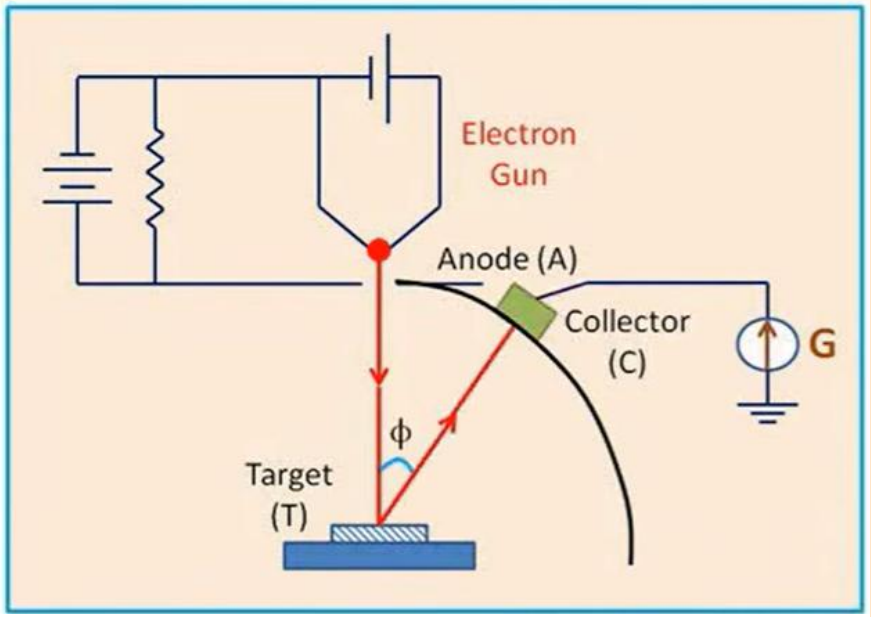
For thermal energy

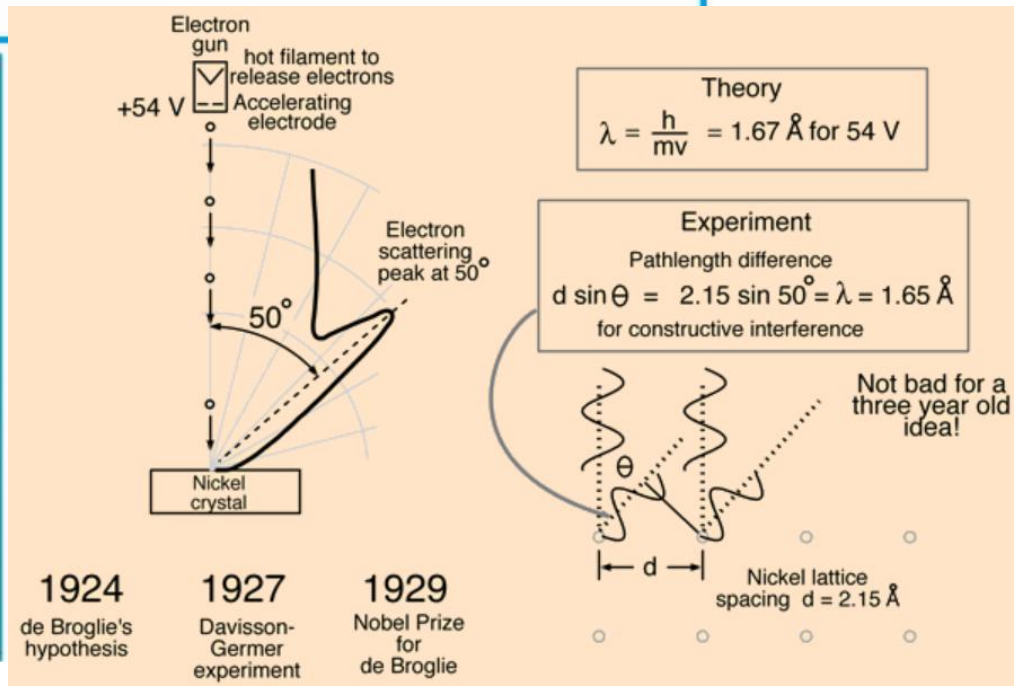
$$\therefore \lambda = \frac{h}{p} = \frac{h}{\sqrt{2mkT}}$$



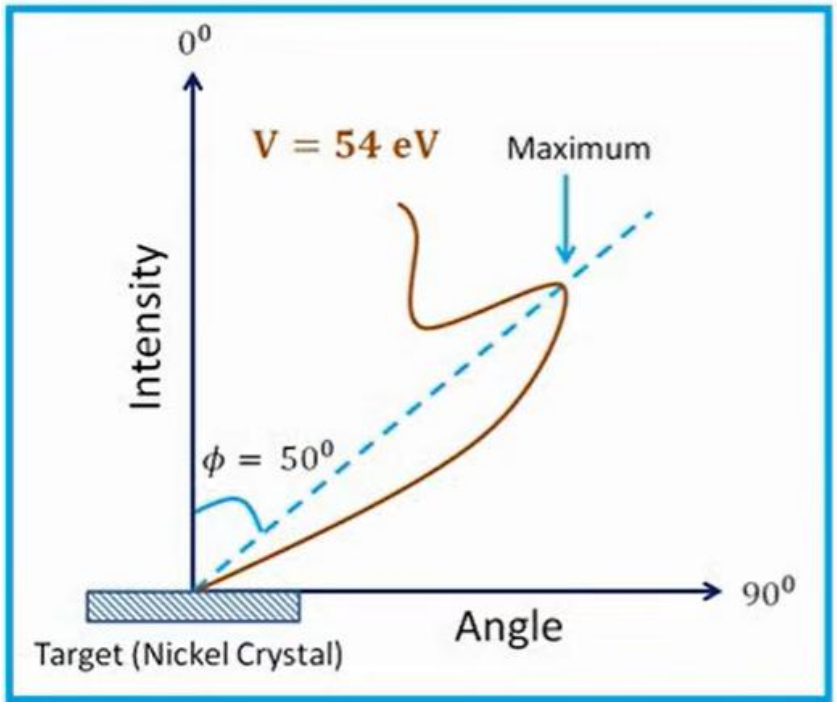
The **Davisson–Germer experiment** was conducted from 1923 to 1927 by Clinton Davisson and Lester Germer at Western Electric (later Bell Labs). Electrons, scattered by the surface of a crystal of nickel metal, displayed a diffraction pattern.

Experimental Verification of de Broglie Hypothesis (Davisson and Germer Experiment)





Experimental Verification of de Broglie Hypothesis (Davisson and Germer Experiment)

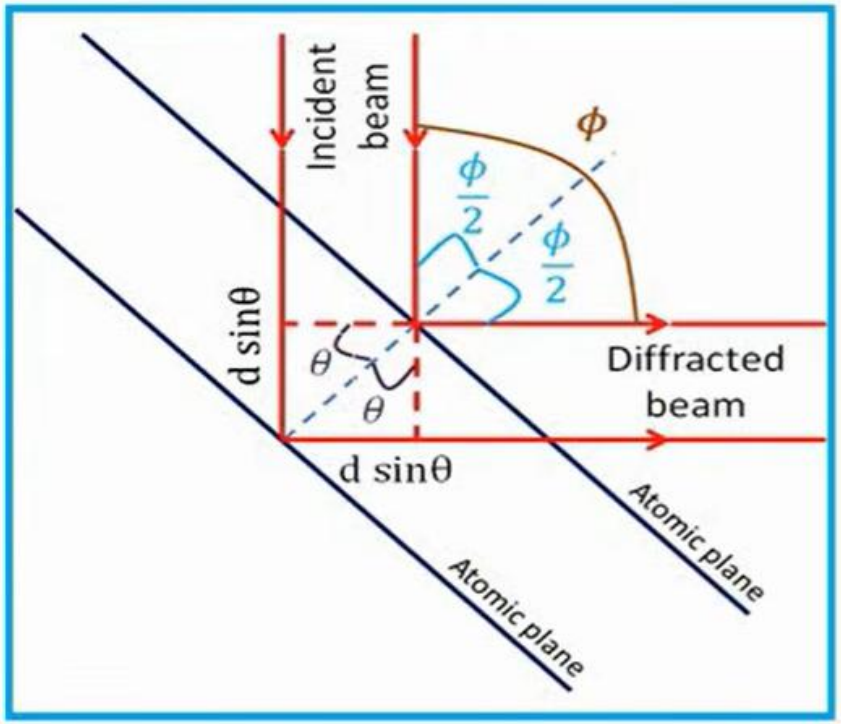


$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}$$

$$\therefore \lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 54}}$$

$$\therefore \lambda = 1.67 \times 10^{-10} \text{m} = 1.67\ \text{A}^0$$

Experimental Verification of de Broglie Hypothesis (Davisson and Germer Experiment)



From Bragg's diffraction law, we have

$$2\,d\sin\theta = n\lambda$$

$$\therefore \lambda = \frac{2\,d\sin\theta}{n}$$

$$\therefore \lambda = \frac{2 \times 9.086 \times 10^{-11} \times \sin 65}{1}$$

$$\therefore \lambda = 1.65 \times 10^{-10}\,\mathrm{m} = 1.65\,\mathrm{A}^0$$

This value matches with the wavelength calculated using de Broglie relation.

Properties of Matter Waves

- Waves associated with moving particles are called matter waves.
- Wavelength of matter wave is give by $\lambda = \frac{h}{p} = \frac{h}{mv}$
- Matter waves are not electromagnetic waves and can be associated with any particle whether charged or uncharged
- Matter waves can propagate in a vacuum, hence they are not mechanical wave.
- Phase velocity of matter wave $v_p = \frac{c^2}{v} > c$

A bullet of mass 40 gm and an electron both travel with the velocity of 1100 m/s. What wavelengths can be associated with them? Why the wave nature of bullet can not be revealed using diffraction effect?

i) For electron, Given : $h = 6.63 \times 10^{-34}\ J - s$, $m = 9.1 \times 10^{-31} kg$,

$e = 1.6 \times 10^{-19} C$ $v = 1100 \frac{m}{s}$, $\lambda = ?$

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 1100} = 6.623 \times 10^{-7} m = 6623\ A^0$$

ii) For bullet, Given : $h = 6.63 \times 10^{-34}\ J - s$, $m = 40\ gm = 40 \times 10^{-3}\ kg$,

$v = 1100 \frac{m}{s}$, $\lambda = ?$

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{40 \times 10^{-3} \times 1100} = 1.507 \times 10^{-35} m$$

As the wavelength associated with bullet is of the order of 10^{-35}m, to reveal the wave nature of wave associated with bullet, a diffraction grating having width of the slit of the order of 10^{-35}m is needed. Such diffraction grating is not available. So the wave nature of the bullet can not be revealed.

Calculate the de Broglie wavelength of the proton moving with a velocity equal to $\frac{1}{20}$ th of velocity of light. Mass of proton is 1.6×10^{-27} kg.

Given : $h = 6.63 \times 10^{-34} J - s$, $m = 1.6 \times 10^{-27} kg$

$v = \frac{1}{20} \times 3 \times 10^{8}$ m/s, $\lambda = ?$

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{1.6 \times 10^{-27} \times \frac{1}{20} \times 3 \times 10^{8}}$$

$$= 2.763 \times 10^{-14} m$$

Calculate the wavelength of the wave associated with a neutron moving with energy 0.025eV. Mass of neutron is 1.676 x 10^{-27} kg.

Given : $h = 6.63 \times 10^{-34} J - s,$ $m = 1.676 \times 10^{-27} kg$

$E = 0.025\ eV = 0.025 \times 1.6 \times 10^{-19}\ J$

$\lambda = ?$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.676 \times 10^{-27} \times 0.025 \times 1.6 \times 10^{-19}}}$$

$$= 1.811 \times 10^{-10} m$$

Calculate de Broglie wavelength associated with an α – particle accelerated by a potential difference of 100 kV. Mass of α – particle is 6.68×10^{-27}kg.

Given : $h = 6.63 \times 10^{-34}$J – s, $m = 6.68 \times 10^{-27}$kg,

$q = 2e = 2 \times 1.6 \times 10^{-19}$C, $V = 100 \times 10^{3}$ volts,

$\lambda = ?$

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mqV}} = \frac{6.63\times10^{-34}}{\sqrt{2\times6.68\times10^{-27}\times2\times1.6\times10^{-19}\times100\times10^{3}}}$$

$$= 3.206 \times 10^{-14}\text{m}$$

An electron beam is accelerated from rest through a potential difference of 200 V.

i) Calculate the associated wavelength.

ii) This beam is passed through a diffraction grating of spacing 3 A^0. At what angle deviating from the incident direction will be the first maximum observed?

i) Given : $h = 6.63 \times 10^{-34}\ J-s$, $m = 9.1 \times 10^{-31} kg$, $e = 1.6 \times 10^{-19} C$

$V = 200$ volts, $\lambda = ?$

$$\lambda = \frac{h}{\sqrt{2meV}} = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 200}}$$

$$= 8.688 \times 10^{-11} m = \mathbf{0.8688\ A^0}$$

ii) $d = 3 \times 10^{-10} m$, order $n = 1$ $\theta = ?$

$$2d\sin\theta = n\lambda$$

$$\therefore\ \theta = \sin^{-1}\left(\frac{n\lambda}{2d}\right) = \sin^{-1}\left(\frac{1 \times 8.688 \times 10^{-11}}{2 \times 3 \times 10^{-10}}\right) = \mathbf{8.32^0}$$

Find the energy of neutron in units of electron volt whose de Broglie wavelength is $1A^0$.
Given – mass of neutron = $1.674 \times 10^{-27} kg$

Given : $h = 6.63 \times 10^{-34}\ J - s$, $m = 1.674 \times 10^{-27} kg$

$\lambda = 1\ A^0 = 10^{-10} m$, $E = ?$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \qquad \therefore E = \frac{h^2}{2m\lambda^2} = \frac{(6.63 \times 10^{-34})^2}{2 \times 1.674 \times 10^{-27} \times (10^{-10})^2}$$

$$= 1.313 \times 10^{-20}\ J = \frac{1.313 \times 10^{-20}}{1.6 \times 10^{-19}} = \mathbf{0.082\ eV}$$

An electron and photon each have a wavelength of 2 A^0. What are their momentum and energy? Mass of electron $= 9.1 \times 10^{-31}$kg, Planck's constant $= 6.63 \times 10^{-34}$J − s

Given: Mass of electron $= 9.1 \times 10^{-31}$kg, Planck's constant $= 6.63 \times 10^{-34}$J.s, $\lambda = 2 \times 10^{-10}$m

For an electron,

$$\text{momentum, } p = \frac{h}{\lambda} = \frac{6.63\times10^{-34}}{2\times10^{-10}} = 3.315 \times 10^{-24} \frac{\text{kg-m}}{\text{s}}$$

$$\text{Energy, } E = \frac{p^2}{2m} = \frac{(3.315\times10^{-24})^2}{2\times9.1\times10^{-31}} = 6.038\times 10^{-18}\text{J}$$

For a photon,

$$\text{momentum, } p = \frac{h}{\lambda} = \frac{6.63\times10^{-34}}{2\times10^{-10}} = 3.315 \times 10^{-24} \frac{\text{kg-m}}{\text{s}}$$

$$\text{Energy, } E = h\nu = \frac{hc}{\lambda} = \frac{6.63\times10^{-34}\times3\times10^{8}}{2\times10^{-10}} = 9.945\times 10^{-16}\text{J}$$

Matter waves, confirmed again and again

1927

G. P. Thomson

Electrons through thin metal films give diffraction rings.

1930

Estermann and Stern

Helium atoms diffract from a lithium fluoride crystal.

1961

Jönsson

A true double-slit experiment with electrons.

1989

Tonomura

Electrons sent one at a time still build up interference fringes.

1999

Arndt, Zeilinger et al.

Diffraction of C_{60} molecules, each of 60 carbon atoms.

Nobel

1929 and 1937

de Broglie (1929); Davisson and G. P. Thomson (1937).

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- Phase velocity of matter wave $v_p = \frac{c^2}{v} > c$

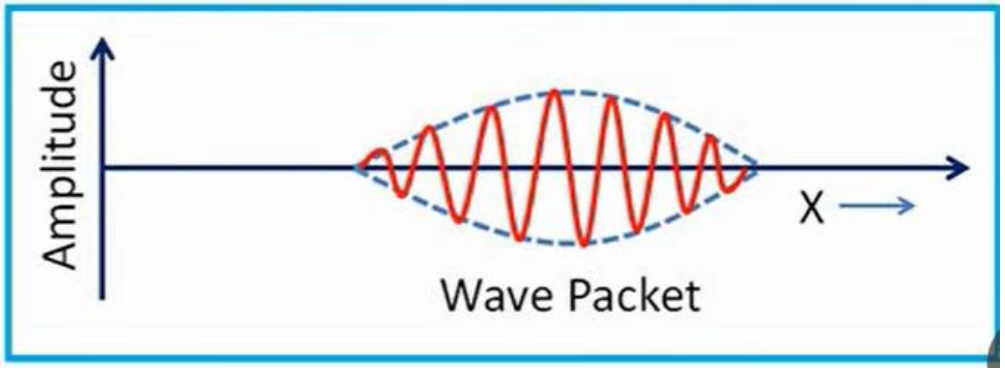
Which type of wave associated with matter?

- Single Monochromatic wave?
  - Location of the particle?



  - Phase velocity $v_p = \nu\lambda = \frac{h\nu\lambda}{h} = \frac{h\nu}{h/\lambda} = \frac{E}{p} = \frac{mc^2}{mv} = \frac{c^2}{v}$

- Schrodinger's solution
  - Group of waves
  - Wave packet



Schrodinger suggested that it is not single monochromatic wave is associated with particle, rather it is a group of wave associated with particle

Phase velocity and group velocity describe how waves and their energy travel through a medium

The **phase velocity** is the velocity with which a particular phase of the wave propagates in the medium.

Let the equation of the wave travelling in x-direction with vibrations in y-direction is –

$$y = A\sin(\omega t - kx) \quad (1)$$

Where A is amplitude of vibration,

$k = \frac{2\pi}{\lambda}$ is propagation constant,

$\omega = 2\pi\nu$ is the angular frequency

$$\therefore \lambda = \frac{2\pi}{k} \text{ and } \nu = \frac{\omega}{2\pi} \quad (2)$$

Phase velocity,

$$v_p = \nu\lambda = \frac{\omega}{2\pi} \times \frac{2\pi}{k} = \frac{\omega}{k} \quad (3)$$

From (2)

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/mv} = \frac{2\pi mv}{h} \quad (4)$$

As from de Broglie relation says $\lambda = \frac{h}{mv}$

Phase Velocity

$$y = A\sin(\omega t - kx) \quad (1)$$

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$$v_p = \nu\lambda = \frac{\omega}{2\pi} \times \frac{2\pi}{k} = \frac{\omega}{k} \quad (3)$$

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Now, let us equate energy $E = h\nu$ with energy $E = mc^2$

$$h\nu = mc^2 \Rightarrow \nu = \frac{mc^2}{h}$$

From (2) $\omega = 2\pi\nu = \frac{2\pi mc^2}{h}$ (5)

Phase velocity,

$$v_p = \frac{\omega}{k} = \frac{\frac{2\pi mc^2}{h}}{\frac{2\pi mv}{h}} = \frac{c^2}{v} \quad (6)$$

Feature	Phase Velocity (v_p)	Group Velocity (v_g)
What it measures	Speed of individual wave crests/troughs.	Speed of the collective wave packet/envelope.
Formula	$v_p = \frac{\omega}{k}$	$v_g = \frac{d\omega}{dk}$
Physical meaning	Represents pure phase propagation speed.	Represents the speed of energy, information, or particle velocity.
Relativity limit	Can exceed the speed of light (c) in certain media.	Cannot exceed c when transmitting information or energy.

The relation between the two velocities depends entirely on how the medium affects different wave frequencies. This relationship is written as:

$$v_g = v_p + k\frac{dv_p}{dk}$$

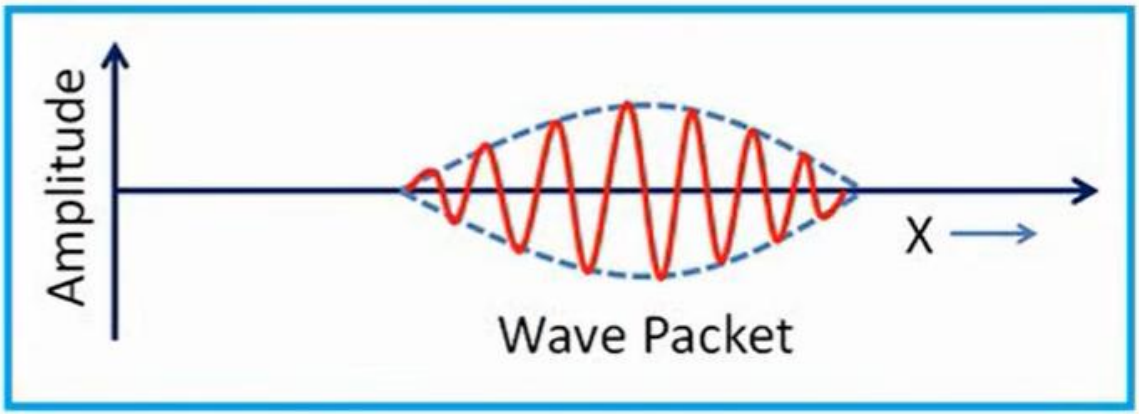
Alternatively, expressed in terms of wavelength (λ), it is written as:

$$v_g = v_p - \lambda\frac{dv_p}{d\lambda}$$

Schrodinger's solution

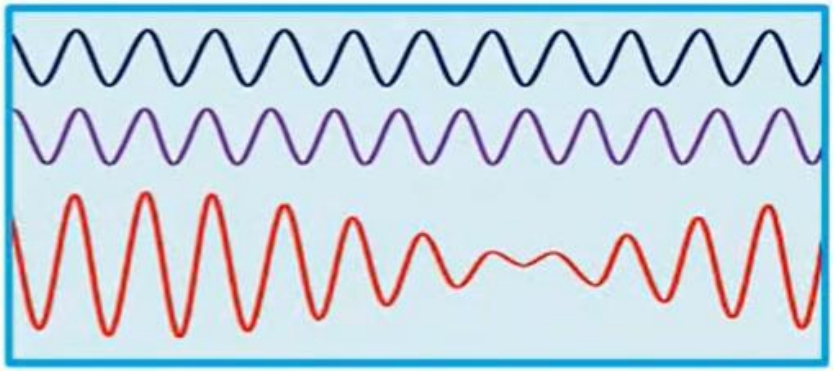
– Group of waves

– Wave packet



- ✓ The phases and amplitude of the waves in group are such that they undergo constructive interference only over a small region where the particle may be located.
- ✓ Outside this region, destructive interference occurs and amplitude is zero.
- ✓ Velocity with which this wave packet moves is called as group velocity. This group velocity is equal to the velocity of particle.

Group Velocity



Let us consider two waves represented by -

$$y_1 = A\sin(\omega t - kx)$$

$$y_2 = A\sin[(\omega + d\omega)t - (k + dk)x]$$

The resultant displacement y an any time t is $y = y_1 + y_2$

$$y = 2A\sin\left(\frac{2\omega + d\omega}{2}t - \frac{2k + dk}{2}x\right)\cos\left(\frac{d\omega}{2}t - \frac{dk}{2}x\right)$$

The sine term represents a wave of angular frequency ω and propagation constant k

The Cosine term modulates this wave with angular frequency $\frac{d\omega}{2}$ to produce wave-group travelling with velocity $v_g = \frac{d\omega}{dk}$

Group Velocity

We know - $\lambda = \frac{2\pi}{k}$ and $\nu = \frac{\omega}{2\pi}$ (1)

Group velocity $v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$ (2)

$h\nu = mc^2$ ⇒ $\nu = \frac{mc^2}{h}$

$\omega = 2\pi\nu = \frac{2\pi mc^2}{h}$

Putting $m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$ (Relativistic mass)

$\omega = 2\pi\nu = \frac{2\pi c^2}{h}\frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$

$\therefore \frac{d\omega}{dv} = \frac{2\pi m_0}{h} v\left(1-\frac{v^2}{c^2}\right)^{-3/2}$ (3)

$k = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h} = \frac{2\pi v}{h}\frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$

$\therefore \frac{dk}{dv} = \frac{2\pi m_0}{h}\left(1-\frac{v^2}{c^2}\right)^{-3/2}$ (4)

Group Velocity

We know - $\lambda = \frac{2\pi}{k}$ and $\nu = \frac{\omega}{2\pi}$ (1)

Group velocity $v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$ (2)

$$\therefore \frac{d\omega}{dv} = \frac{2\pi m_0}{h} v \left(1 - \frac{v^2}{c^2}\right)^{-3/2} \quad (3)$$

$$\therefore \frac{dk}{dv} = \frac{2\pi m_0}{h} \left(1 - \frac{v^2}{c^2}\right)^{-3/2} \quad (4)$$

From (2) (3) and (4)

Group velocity

$$v_g = \frac{d\omega/dv}{dk/dv} = \frac{\frac{2\pi m_0}{h} v \left(1 - \frac{v^2}{c^2}\right)^{-3/2}}{\frac{2\pi m_0}{h} \left(1 - \frac{v^2}{c^2}\right)^{-3/2}}$$

$$\therefore v_g = v$$

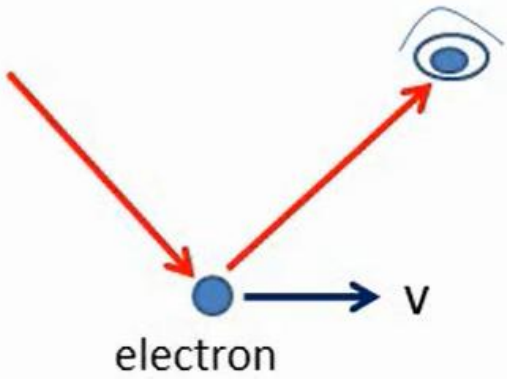
Thus, group velocity associated with the wave packet is equal to the velocity of the particle.



The **Heisenberg Uncertainty Principle** states that it is fundamentally impossible to simultaneously measure both the exact position (Δ x) and the exact momentum (Δ p) of a particle with absolute precision. Formulated by German physicist Werner Heisenberg in 1927, this law establishes that the more precisely one property is determined, the less precisely the other can be known.

Heisenberg Uncertainty Principle

- If we are finding position of an moving electron, a photon must be seen by us after collision with the electron.
- But then the velocity and hence momentum of the electron will change due to collision.
- This will cause error or uncertainty in the measurement of momentum.
- If we try to determine momentum accurately, error or uncertainty in position is introduced.
- Thus, It is not possible to measure the position and momentum of an electron simultaneously and accurately.



Heisenberg Uncertainty Principle



- If the width of the wave packet is small as shown in fig. (a) then the particle can be located somewhat accurately, but the determination of wavelength (And hence the momentum) becomes a problem.
- If width of the wave packet is more (fig.(b)), then wavelength measurement (and hence determination of momentum) is accurate. However, position of the particle cannot be determined accurately.

The Mathematical Formula

The relation between the uncertainty of position and momentum is expressed by the inequality:

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

Where:

- **Δ x**: The uncertainty in position.
- **Δ p**: The uncertainty in momentum (mass × velocity).
- **h**: Planck's constant (6.626×10^{-34} J·s).
- **$\hbar$** (h-bar): The reduced Planck's constant (h / 2π).

A similar trade-off also exists for other conjugate variables, most notably **Energy (Δ E) and Time (Δ t)**:

Heisenberg Uncertainty Principle

It is impossible to determine simultaneously, the position and momentum of the moving particle accurately. In any simultaneous determination of position and momentum of the particle, the product of uncertainties is equal to or greater than $\frac{\hbar}{2}$ i.e. $\frac{h}{4\pi}$

$$\Delta x \ \Delta p_x \geq \frac{h}{4\pi}$$

where Δx is uncertainty in measurement of position and

Δp_x is uncertainty in measurement of momentum along X-axis

Wavelength versus Size

With a visible light microscope, we are limited to being able to resolve objects which are at least about $0.5*10^{-6}$ m = 0.5 μm = 500 nm in size.

This is because visible light, with a wavelength of ~500 nm cannot resolve objects whose size is smaller than it's wavelength.

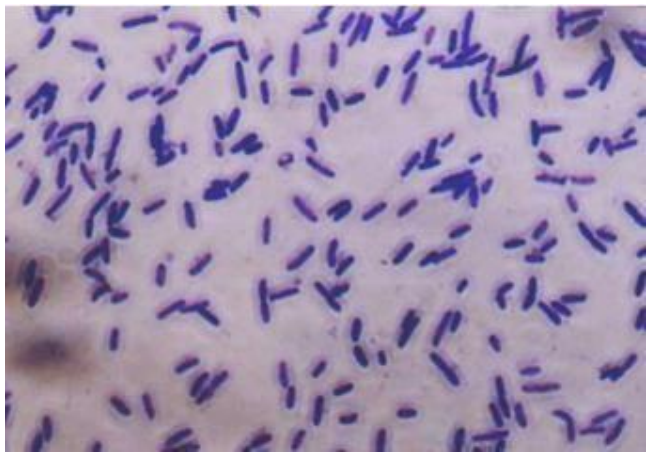


Image is in the public domain

Bacteria, as viewed using visible light

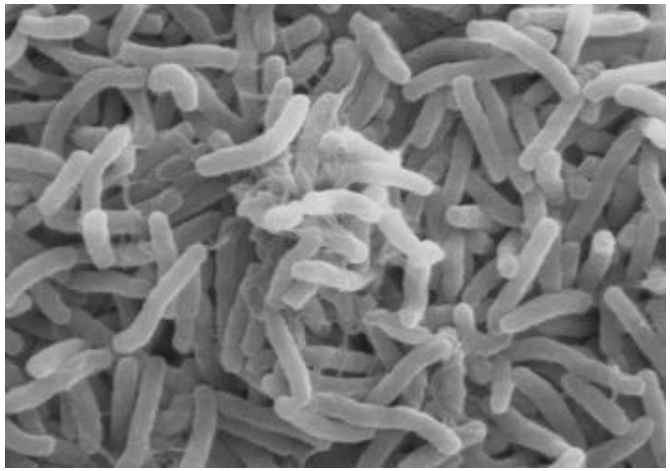


Image is in the public domain

Bacteria, as viewed using electrons!

Electron Microscope

The electron microscope is a device which uses the wave behavior of electrons to make images which are otherwise too small for visible light!

This image was taken with a Scanning Electron Microscope (SEM).

SEM can resolve features as small as 5 nm. This is about 100 times better than can be done with visible light microscopes!

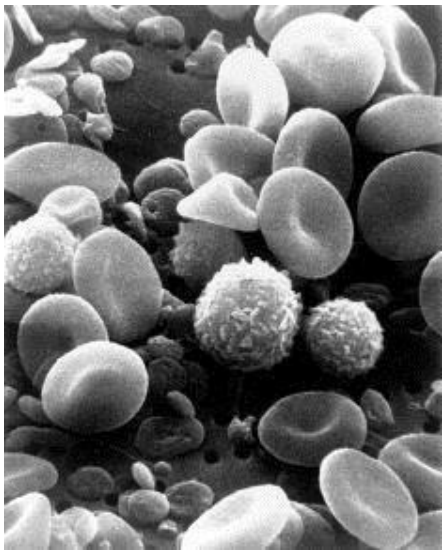
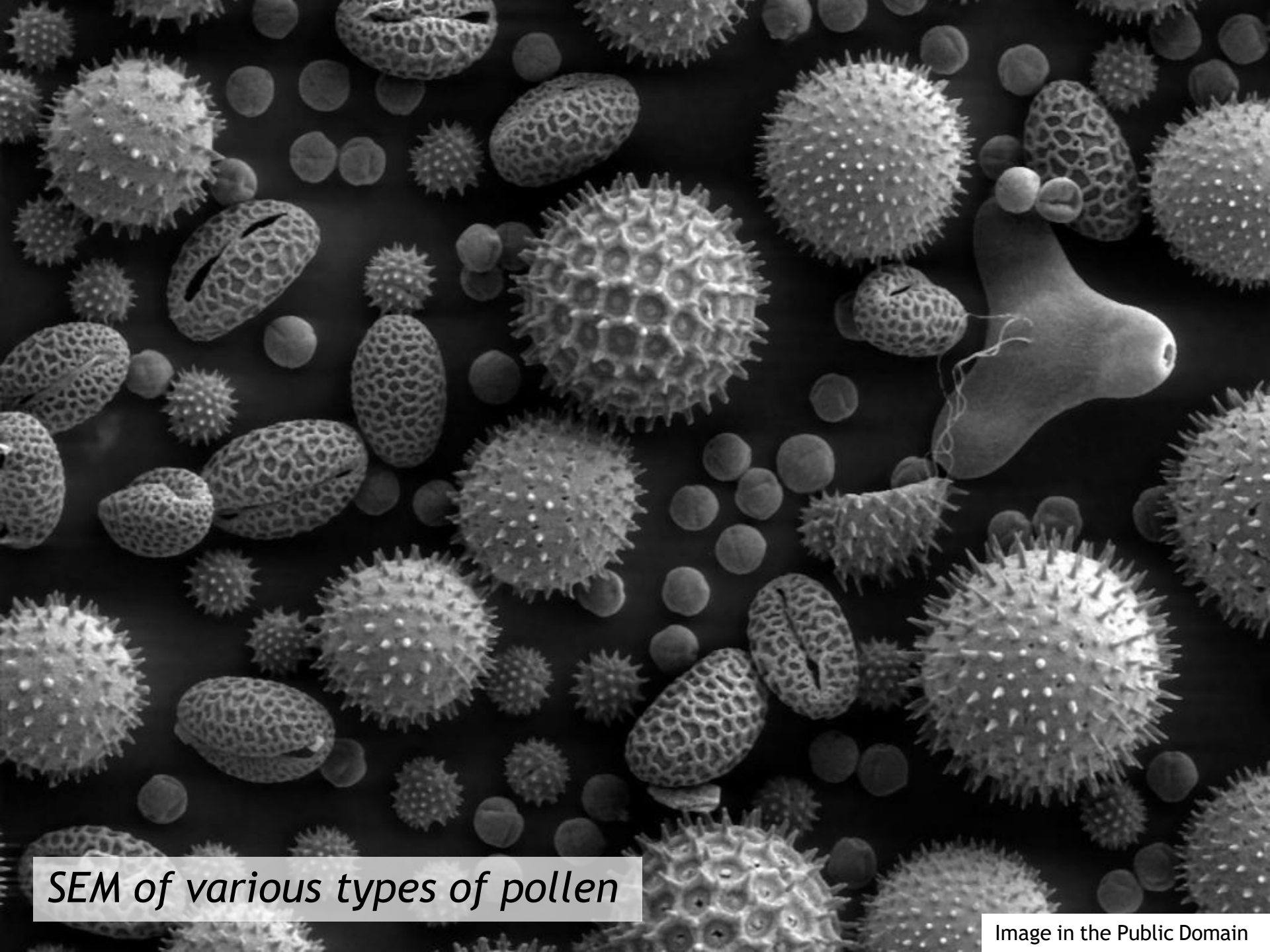


Image in the Public Domain

IMPORTANT POINT:

High energy particles can be used to reveal the structure of matter !



SEM of various types of pollen

Image in the Public Domain



SEM of an ant head

Image in the Public Domain

Summary

- Light is made up of photons, but in macroscopic situations it is often fine to treat it as a wave.
- Photons carry both energy & momentum.

$$E = hc/\lambda \qquad p = E/c = h/\lambda$$

- Matter also exhibits wave properties. For an object of mass *m*, and velocity, v, the object has a wavelength, $\lambda = h / mv$
- One can probe 'see' the fine details of matter by using high energy particles (they have a small wavelength !)

wave packet, phase velocity and group velocity

Heisenberg uncertainty principle (HUP)

Properties of Matter Waves

- Waves associated with moving particles are called matter waves.
- Wavelength of matter wave is give by $\lambda = \frac{h}{p} = \frac{h}{mv}$
- Matter waves are not electromagnetic waves and can be associated with any particle whether charged or uncharged
- Matter waves can propagate in a vacuum, hence they are not mechanical wave.
- Phase velocity of matter wave $v_p = \frac{c^2}{v} > c$

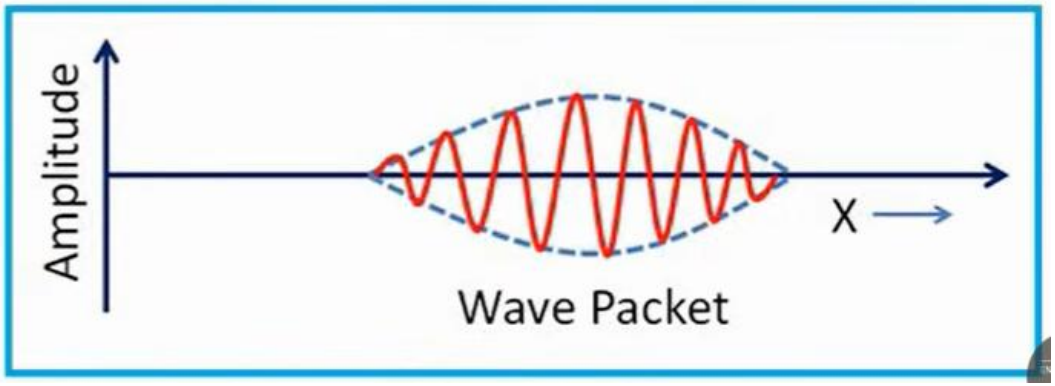
Which type of wave associated with matter?

- Single Monochromatic wave?
  - Location of the particle?



  - Phase velocity $v_p = \nu\lambda = \frac{h\nu\lambda}{h} = \frac{h\nu}{h/\lambda} = \frac{E}{p} = \frac{mc^2}{mv} = \frac{c^2}{v}$

- Schrodinger's solution
  - Group of waves
  - Wave packet



The **phase velocity** is the velocity with which a particular phase of the wave propagates in the medium.

Let the equation of the wave travelling in x-direction with vibrations in y-direction is –

$$y = A\sin(\omega t - kx) \quad (1)$$

Where A is amplitude of vibration,

$k = \frac{2\pi}{\lambda}$ is propagation constant,

$\omega = 2\pi\nu$ is the angular frequency

$$\therefore \lambda = \frac{2\pi}{k} \text{ and } \nu = \frac{\omega}{2\pi} \quad (2)$$

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Phase Velocity

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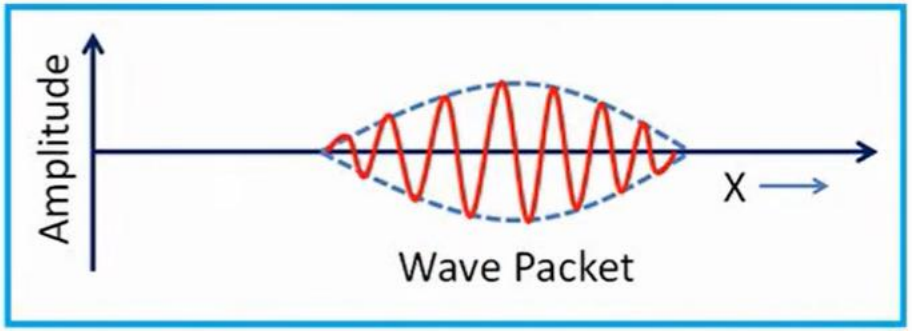
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Schrodinger's solution

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All physical theories on one slide

Inverse speed of light, 1/c

Special relativity, $E = mc^2$

Einstein's general relativity

$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = \frac{8\pi G}{c^4} T_{\mu\nu}$

Quantum field theory (Feynman, Dirac, Schwinger,...)



Planck's constant, $\hbar$



Non-relativistic quantum mechanics, (Bohr, Heisenberg, Schrödinger,...)

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

Classical mechanics

$\vec{F} = m\vec{a} \leftarrow \delta S = 0$

Newtonian gravity

$F_g = G \frac{m_1 m_2}{r^2}$

Gravity constant, G

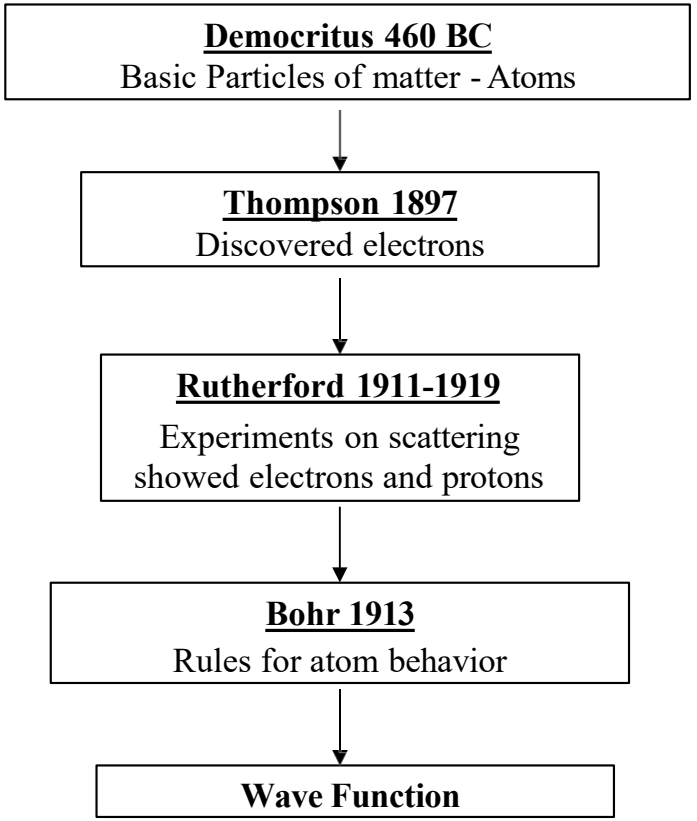
Where did Quantum Mechanics Come From?



- The development of quantum mechanics is strongly tied to the evolving understanding of the nature of matter over many centuries.
- It required a definitive understanding that atoms are composed of separate particles, nuclei and electrons.
- It also required experimental determination of a number of behaviors that were unexplained at the time.

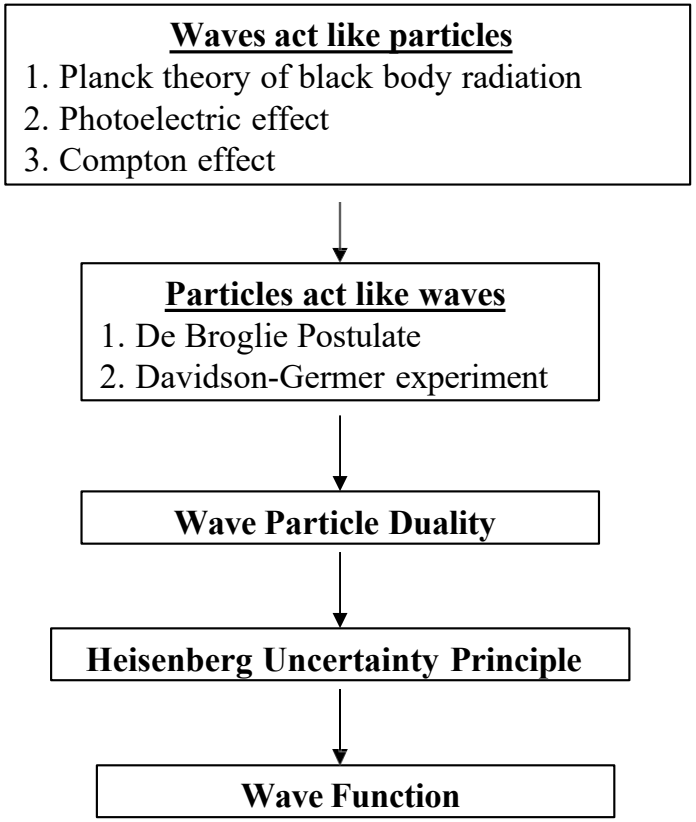
History of Atoms

- The existence of atoms was first proposed in 460 BC.
- But not begun to be understood until the late 19th century.



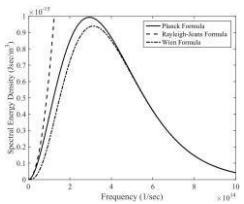
Historical Development of Quantum Mechanics

- Quantum mechanics arose out of a number of important experimental and conceptual advances.



Wave-Particle Duality - Electromagnetic radiation behaves like particles

1)Black Body Radiation (Planck 1900) - Oscillators absorb and emit at discrete energies.





$$\varepsilon_n = nh\nu$$

2)Photoelectric Effect (Einstein 1904) - Only the concept of photons, discrete packets of radiation, explain experimental observations.



$$\varepsilon = h\nu$$

3)Compton Effect (1923) - Photons scatter like particles with momentum



$$p = h/\lambda$$

Particle-Wave Duality - Particles can display wave-like behavior.

1) DeBroglie Postulate (1924) - Particles can behave like waves.



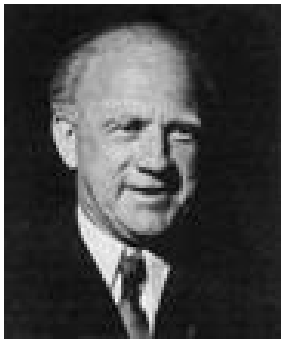
$$\lambda = h/p$$

2) Davisson-Germer Experiment (1927) - Electrons diffracted like waves.

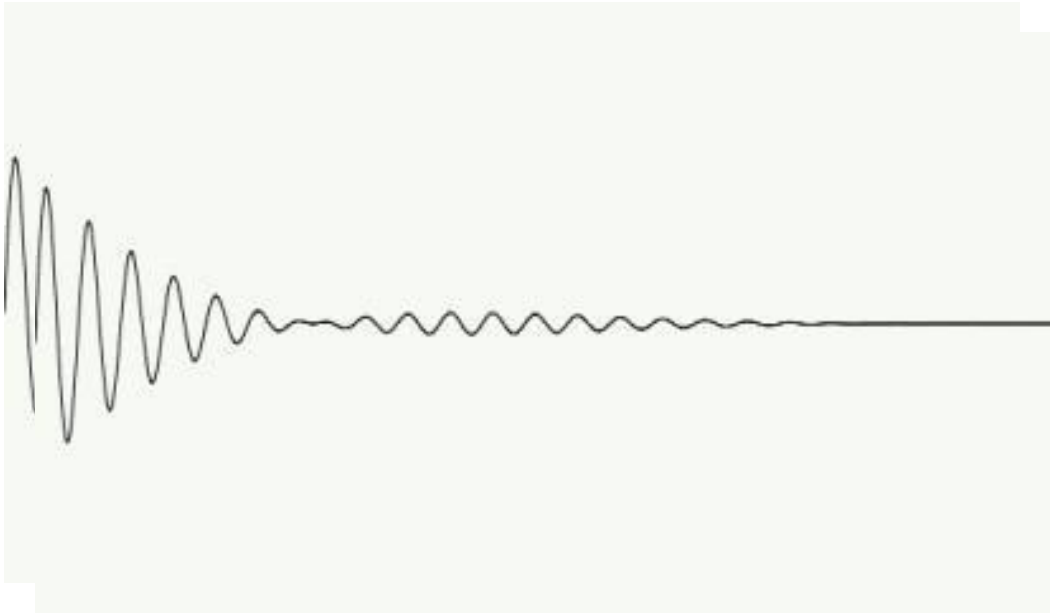


Heisenberg Uncertainty Principle (1927)

Suggested how to deal with duality. Since we can't know everything about a particle, we must content ourselves with a statistical approach. We will describe behavior in terms of a ***wave function***.



Why Would This Work?



http://en.wikipedia.org/wiki/Wave_packet

Schrodinger (1924)

- Used De Broglie's electron wave postulate to develop a wave equation that represents mathematically the distribution of a charge of an electron distributed through space, being spherically symmetric or prominent in certain directions, i.e. directed valence bands, which gave the correct values for spectral lines of the hydrogen atom.



Finding the Wave Function

- We will obtain the wave function by solving Schrodinger's wave equation.
- Schrodinger obtained the equation by starting with the equation for the total energy of a particle and applying the operators for each term.



Energy of a Particle

- The total energy of a particle is the sum of its kinetic and potential energies.
- We can write the kinetic energy as

$$\text{K.E.} = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

- The form of the potential energy will depend on the nature of the particle. For now we will call it $V(x,t)$ as it may be a function of both space and time.

Hamiltonian

- In classical mechanics, the sum of the potential and kinetic energy is called the Hamiltonian.

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

- Substituting the operators for p and ε,

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

Why Schrodinger chose this form

- He needed a linear equation to describe the propagation of wave packets,
- He wanted the equation to be symmetric with the classical conservation of energy statement.

What does the Wave Equation Describe?

- It describes the time dependent, transient behavior (motion) of any collection of quantum particles subject to body forces, including internal motion, collisions and chemical reactions.

Analytic Solutions of the Wave Equation we will Explore:



- Separate time dependence from stationary behavior

- Two Particle Systems
- Particle in a box
- Rigid Rotator
- Harmonic Oscillator
- Hydrogenic Atom

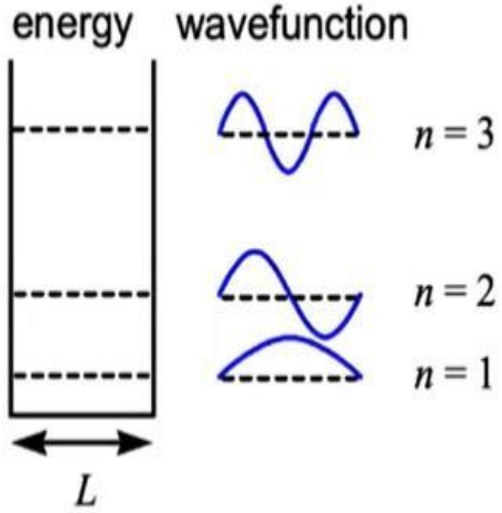
We will also explore using numerical methods for real systems.

Eigenvalues and eigenfunctions

- A general eigenvalue equation: $\mathbf{A}\vec{\mathbf{x}} = \lambda\vec{\mathbf{x}}$
  - Only the operator $\mathbf{A}$ is given and both the eigenvalue and eigenvector (or eigenfunction) need to be found.
- Eigensolutions consist of
  - a specific set of allowed values of a parameter (here energy): *eigenvalues*
  - and a particular solution associated with each eigenvalue: *eigenfunctions*.
- It is possible to have more than one eigenfunction with a given eigenvalue,
  - a phenomenon known as degeneracy.
  - The number of such states with the same eigenvalue is called the degeneracy.

Symmetry property of eigenfunctions - parity

- All eigenfunctions of the infinite potential well have definite "parity",
  - Symmetry about the center of the well.
- The lowest (n = 1) eigenfunction is symmetric about the center of the well, and
  - is said to have "even parity".
- The second (n = 2) eigenfunction is anti-symmetric about the center of the well, and
  - is said to have "odd parity".
- Parity is the result of symmetric potential, and
  - is one of the most important characteristics of quantum states.



Fourier series

- Notice the eigenfunctions of the infinite potential well problem form the basis of Fourier series.
- That is, any arbitrary function, $f(z)$, can be expressed as,

$$f(z) = \sum_{n=1}^{\infty} c_n \psi_n(z) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi z}{L}\right)$$

- A set of functions that can be used to represent a function is called
  - a *basis set* or just *basis*.
- When a basis set can represent any function within the given domain, it is said to be "complete" or
  - a complete basis set.

Orthogonality

- In addition to being "complete", our eigenfunctions are also orthogonal to one another.
- Orthogonality between functions is defined as

$$\int_{-\infty}^{\infty} g^*(z) f(z) dz = 0$$

- In the case of infinite potential well problem, it is easy to show

$$\int_0^L \psi_m^*(z) \psi_n(z) dz = 0 \qquad \text{for } m \neq n$$

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

Orthonormality

- Furthermore, from the normalization condition, we have

$$\int_0^L |\psi_n(z)|^2 dz = 1$$

- Thus, we can write in general,

$$\int_0^L \psi_m^*(z)\psi_n(z)dz = \delta_{mn}$$

  - This condition is called orthonormality.

Expansion coefficient

- The orthogonality (and orthonormality) of a set of functions makes it very easy to evaluate the expansion coefficients.
- Consider a function $f(x)$ which can be expressed by a linear combination of orthonormal basis set,

$$f(z) = \sum_n c_n \psi_n(z)$$

- Then, to find the coefficient c_m, we simply evaluate,

$$\int \psi_m^*(z) f(z) dz = \sum_n c_n \int \psi_m^*(z) \psi_n(z) dz$$

$$= \sum_n c_n \delta_{mn} = c_m$$

Completeness

- The solutions (eigenfunctions) of time-independent Schrödinger's equation have some important mathematical properties.
- First, they form a **complete set**, which means
  - Any arbitrary function can be expressed as a linear combination of the eigenfunctions.

$$\phi(z) = \sum_n a_n \psi_n(z)$$

- When a set of functions is used to represent a function as above,
  - the set is called a **basis** and
  - the set of coefficients is **representation**.
- In the example of infinite potential well, it is clear the eigenfunctions form a complete basis set, as they are the harmonics of Fourier series.

Orthogonality

- In addition to being complete, the eigenfunctions (solutions of time-independent Schrödinger's equation) are orthogonal to one another.
- In order to define orthogonality, we must first define inner product.
- The inner product of functions is defined as

$$\int_{-\infty}^{\infty} f^*(z)g(z)dz$$

- When the inner product is zero, the two functions are said to be orthogonal to each other.
- If all eigenfunctions $\psi_n(z)$ are normalized, they are called orthonormal.

$$\int_{-\infty}^{\infty} \psi_m^*(z)\psi_n(z)dz = \delta_{mn}$$

Expansion coefficient

- When using the eigenfunctions as orthonormal basis set to represent a function,

$$\phi(z) = \sum_n a_n \psi_n(z)$$

- The expansion coefficient, a_n, can be found by

$$\int_{-\infty}^{\infty} \psi_m^*(z)\phi(z)dz = \int_{-\infty}^{\infty} \psi_m^*(z)\left[\sum_n a_n\psi_n(z)\right]dz = \sum_n a_n \int_{-\infty}^{\infty} \psi_m^*(z)\psi_n(z)dz = \sum_n a_n\delta_{mn} = a_m$$

- Note that this is perfectly analogous to geometrical vector, $\vec{r} = a\hat{x} + b\hat{y} + c\hat{z}$
  - whose x-component can be found by

$$\hat{x}\cdot\vec{r} = a\hat{x}\cdot\hat{x} + b\hat{x}\cdot\hat{y} + c\hat{x}\cdot\hat{z} = a$$

  - thanks to the orthonormality of the unit vectors, $\hat{x}$, $\hat{y}$, $\hat{z}$.

Function as a vector

- The analogy between functions and geometric vectors is in fact almost perfect.
- It is easily visualized a column vector can be constructed by collecting all coefficients in the linear expansion

$$\phi(z) = \sum_n a_n \psi_n(z) \quad \Rightarrow \quad \phi = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{bmatrix}$$

  - Here the eigenfunctions serve as the unit vectors and coefficients as the coordinates in geometric vector case.
  - Only that the vector is infinite dimensional.

Hilbert space

- The set of square integrable functions form a vector space called **Hilbert space** with the following properties.

1. Addition and scalar multiplication,

$$f(z)+g(z)=g(z)+f(z) \qquad f(z)+\{g(z)+h(z)\}=\{f(z)+g(z)\}+h(z)$$

$$c\{f(z)+g(z)\}=cf(z)+cg(z)$$

2. Inner product,

$$c\int_{-\infty}^{\infty} f^*(z)g(z)dz=\int_{-\infty}^{\infty}\{cf^*(z)\}g(z)dz$$

$$\int_{-\infty}^{\infty} f^*(z)\{g(z)+h(z)\}dz=\int_{-\infty}^{\infty} f^*(z)g(z)dz+\int_{-\infty}^{\infty} f^*(z)h(z)dz$$



Hilbert space

3. Finite norm $\int_{-\infty}^{\infty} |f(z)|^2 dz$

4. Completeness
   - Any vector in the space can be represented to an arbitrary degree of accuracy as a linear combination of the basis vectors.



Linear operators

- A linear operator transforms a function in Hilbert space into another function in the same Hilbert space,
  - Both of which can be represented by linear combinations of basis functions.

$$\hat{A}f = g \quad \text{where} \quad f = \sum_n a_n \psi_n \qquad g = \sum_n b_n \psi_n$$

- If we represent the functions f and g as vectors, it is easy to see that the linear operator $\hat{A}$ will be represented by a matrix.

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- If we represent the functions f and g as vectors, it is easy to see that the linear operator $\hat{A}$ will be represented by a matrix.
- Using the orthonormality of basis functions, we can show the matrix elements are given as,

$$A_{mn} = \int_{-\infty}^{\infty} \psi_m^*(z) \hat{A} \psi_n(z) dz$$

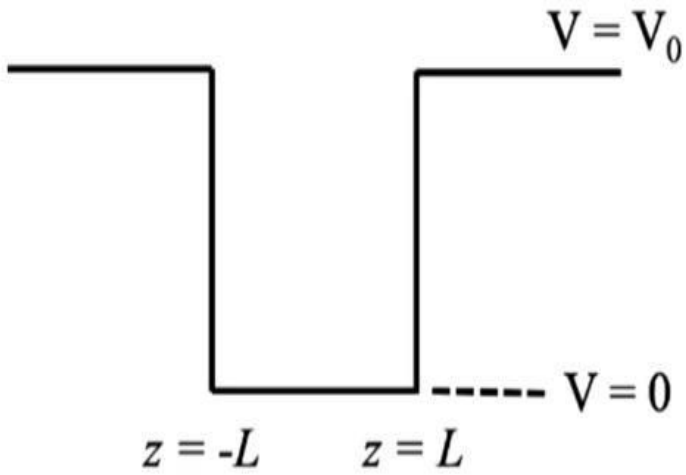
Additional notes

- The solutions of time-independent Schrödinger's equation describe the quantum state of a given problem.
  - Energy eigenstate or steady state
- Since they form a complete basis set,
  - They can be used to represent functions and operators.
  - In this case, they are simply mathematical tools,
  - not necessarily related to the original physical problem described by the time-independent Schrödinger's equation.
- There are many choices of basis functions
  - Which may not be necessarily related to any form of Schrödinger's equation.

Finite potential well

- The potential is given as,

$$V(z) = \begin{cases} 0, & -L \le z \le L \\ V_0, & \text{otherwise} \end{cases}$$



- A more realistic case than infinite potential well.
- Assume bound state: $0 < E < V_0$
- One should expect the solutions should approach those of infinite well,
  - as V_0 is increased or
  - L is decreased.

Finite potential well

- Write down the Schrödinger equation:
  - In region I where $-L \le z \le L$,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2} = E\psi(z) \quad \Rightarrow \quad \frac{d^2\psi(z)}{dz^2} + k^2\psi(z) = 0 \quad \text{where} \quad k = \sqrt{\frac{2mE}{\hbar^2}} \qquad (1)$$

  - In region II ($z \le -L$) and III ($z \ge L$),

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

$$\Rightarrow \quad \frac{d^2\psi(z)}{dz^2} - k_0^2\psi(z) = 0 \quad \text{where} \quad k_0 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \qquad (2)$$



Boundary conditions

- If V is finite everywhere and we are seeking solutions with finite E,
  - then the second derivative must be finite.

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

Finite potential well

- Solutions of equation (1) for region I ($-L \leq z \leq L$)

$$\psi_I(z) = Ae^{ikz} + Be^{-ikz}$$

- Solving equation (2) for regions II ($z \leq -L$) and III ($z \geq L$),

$$\psi_{II}(z) = Ce^{k_0 z} + De^{-k_0 z}$$

$$\psi_{III}(z) = Fe^{k_0 z} + Ge^{-k_0 z}$$

- Apply boundary conditions to determine constants, A ~ G.

Boundary conditions

- If V is finite everywhere and we are seeking solutions with finite E,
  - then the second derivative must be finite.

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

- In order for the second derivative to be finite,
  - the first derivative, $\frac{d\psi}{dz}$, must be finite and continuous.
- In order for the first derivative to be finite,
  - the wavefunction, ψ, itself must be finite and continuous.

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  - the wavefunction, ψ, itself must be finite and continuous.

Finite potential well

- General solutions:

$$\psi_I(z) = Ae^{ikz} + Be^{-ikz} \qquad -L \le z \le L$$

$$\psi_{II}(z) = Ce^{k_0 z} + De^{-k_0 z} \qquad z \le -L$$

$$\psi_{III}(z) = Fe^{k_0 z} + Ge^{-k_0 z} \qquad z \ge L$$

- First, the wavefunction must be finite everywhere.
  - Thus, $D = F = 0$.

$$\Rightarrow \quad \psi_{II}(z) = Ce^{k_0 z} \quad \text{and} \quad \psi_{III}(z) = Ge^{-k_0 z}$$

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  - Thus, $D = F = 0$.

$$\Rightarrow \quad \psi_{II}(z) = Ce^{k_0 z} \quad \text{and} \quad \psi_{III}(z) = Ge^{-k_0 z}$$

- Next, impose continuity of ψ and $\dfrac{d\psi}{dz}$ at $z = \pm L$.

Finite potential well

- At $z = -L$: $Ce^{-k_0 L} = Ae^{-ikL} + Be^{+ikL}$ (1)

  $k_0 Ce^{-k_0 L} = ikAe^{-ikL} - ikBe^{+ikL}$ (2)

- At $z = +L$: $Ge^{-k_0 L} = Ae^{ikL} + Be^{-ikL}$ (3)

  $-k_0 Ge^{-k_0 L} = ikAe^{ikL} - ikBe^{-ikL}$ (4)

- Add (1) and (3), $(C+G)e^{-k_0 L} = 2(A+B)\cos(kL)$ (5)
- Subtract (4) from (2), $(C+G)k_0 e^{-k_0 L} = 2(A+B)k\sin(kL)$ (6)
- If C ≠ -G and A ≠ -B, we can divide (6) by (5) to obtain,

$$\tan(kL) = \frac{k_0}{k} \quad (7)$$

Finite potential well

- Alternatively, subtract (1) from (3), $(G-C)e^{-k_0 L} = 2i(A-B)\sin(kL)$ (8)
- And add (2) and (4), $-(G-C)k_0 e^{-k_0 L} = 2i(A-B)k\cos(kL)$ (9)
- If $C \neq G$ and $A \neq B$, we can divide (9) by (8) to obtain,

$$\cot(kL) = -\frac{k_0}{k} \qquad (10)$$

- Note that equations (7) and (10) are contradictory to each other.
  - Thus, one can only have $C = G$ and $A = B$, in which case equation (7) applies.
    - Symmetric or even parity solution
  - Or $C = -G$ and $A = -B$,in which case equation (10) applies.
    - Anti-symmetric or odd parity solution

Finite potential well

- Values of k and k_0, and thus the allowed values of energy E are determined from equations (7) and (10) numerically or graphically.
- Define $\eta = kL$ and $\xi = k_0 L$ and from the definitions of k and k_0, we find

$$\xi^2 + \eta^2 = \frac{2mV_0L^2}{\hbar^2}$$

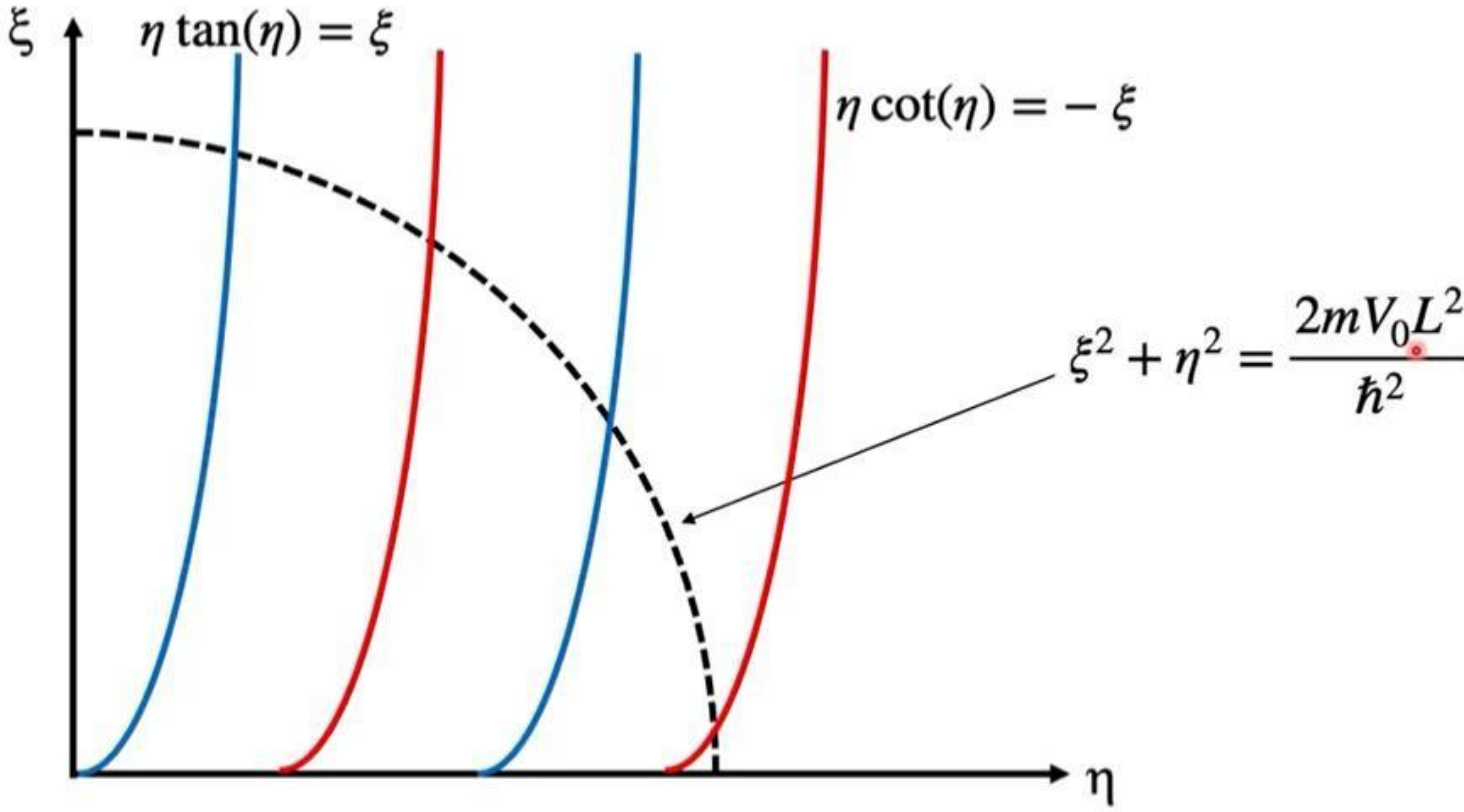
- Equations (7) and (10) are rewritten as

$$\eta \tan(\eta) = \xi$$

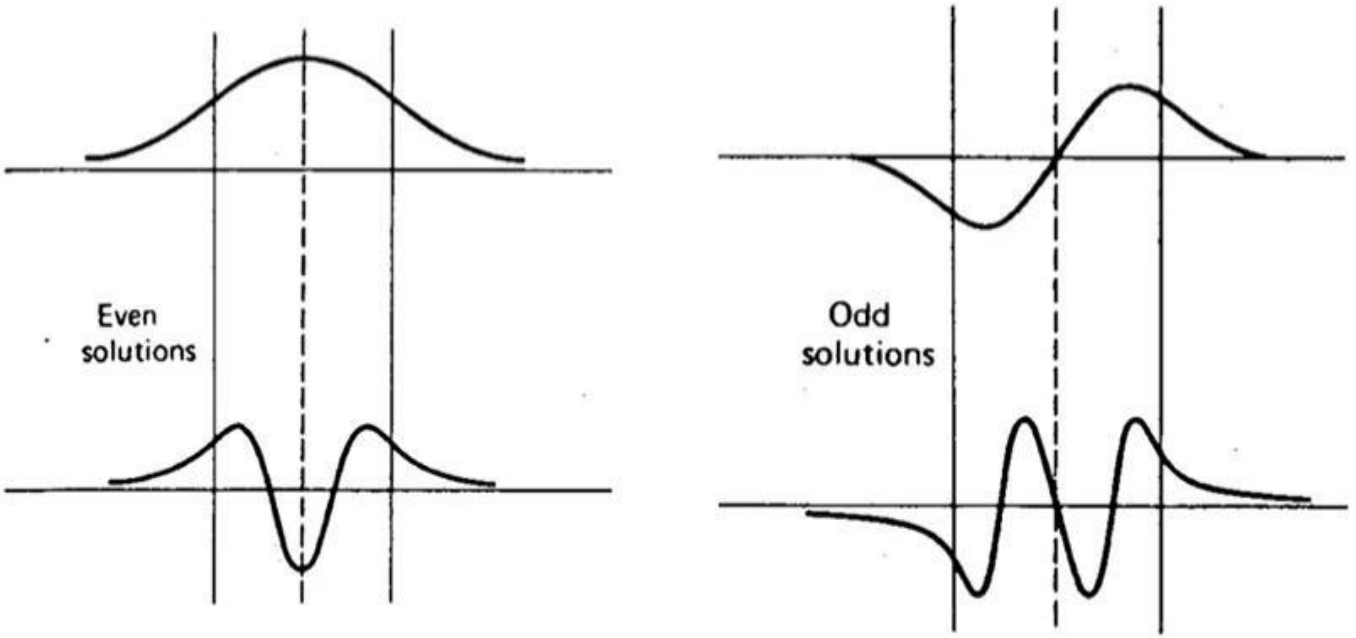
$$\eta \cot(\eta) = -\xi$$

- Now plot the above three equations and find intersections.

Graphical solution



Wavefunctions



- There is a non-zero probability that the particle is inside the barrier region.

Classical harmonic oscillator

- Consider a mass, m, attached to a spring whose restoring force, F, is proportional to displacement, z,

$$F = -kz$$

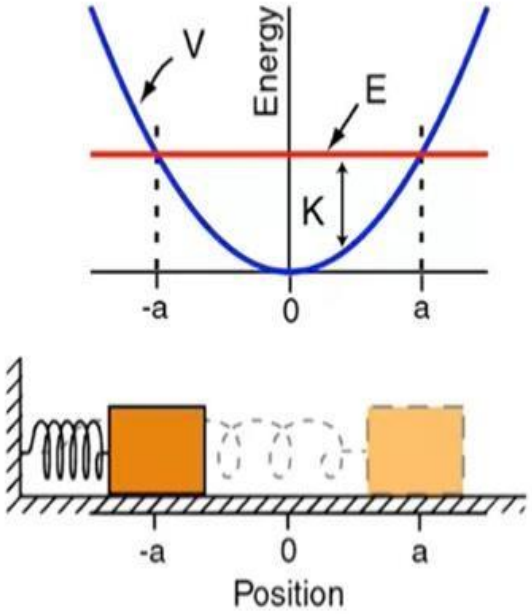
  - where k is the spring constant.

- Newton's equation of motion is,

$$m\frac{d^2z}{dt^2} = -kz$$

- The solution is a sinusoidal function, e.g. $\sin(\omega t)$, with angular frequency,

$$\omega = \sqrt{\frac{k}{m}}$$



Quantum mechanical harmonic oscillator

- To write down the Schrödinger equation, first derive potential energy, V(z).

$$V(z) = -\int F(z)dz = \frac{1}{2}kz^2 = \frac{1}{2}m\omega^2 z^2$$

- The Schrödinger equation now becomes,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2} + \frac{1}{2}m\omega^2 z^2\psi = E\psi$$

- For mathematical convenience, define dimensionless quantity, $\xi = \sqrt{\frac{m\omega}{\hbar}}z$
- And rewrite the Schrödinger equation as,

$$\frac{d^2\psi}{d\xi^2} - \xi^2\psi = -\frac{2E}{\hbar\omega}\psi$$

Hermite differential equation

- Seek for solutions of the form,

$$\psi_n(\xi) = A_n H_n(\xi)\exp(-\xi^2/2)$$

- Substituting this function in the Schrödinger equation yield,

$$\frac{d^2H_n(\xi)}{d\xi^2} - 2\xi\frac{dH_n(\xi)}{d\xi} + \left(\frac{2E}{\hbar\omega} - 1\right)H_n(\xi) = 0$$

- This equation is called Hermite differential equation for which
  - solutions can be found, provided

$$\left(\frac{2E}{\hbar\omega} - 1\right) = 2n \quad \text{or} \quad E = \left(n + \frac{1}{2}\right)\hbar\omega$$

  - where $n = 0, 1, 2, \ldots$

Hermite polynomial

- Solutions of Hermite differential equation are Hermite polynomials.

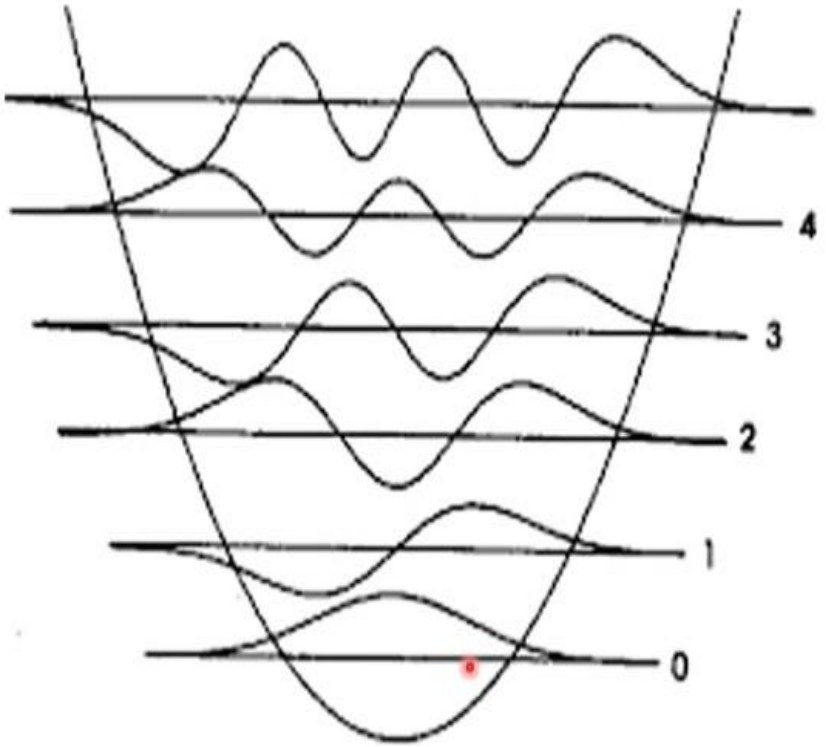
$$H_0(x) = 1,$$
$$H_1(x) = 2x,$$
$$H_2(x) = 4x^2 - 2,$$
$$H_3(x) = 8x^3 - 12x,$$
$$H_4(x) = 16x^4 - 48x^2 + 12,$$
$$H_5(x) = 32x^5 - 160x^3 + 120x,$$

- The remaining constant A_n is found by the normalization condition, $A_n = \sqrt{\frac{1}{\sqrt{\pi}\,2^n n!}}$
- The final solution can now be written as,

$$\psi_n(z) = \sqrt{\frac{1}{2^n n!}\sqrt{\frac{m\omega}{\pi\hbar}}}\exp\left(-\frac{m\omega}{2\hbar}z^2\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}z\right)$$

Quantum mechanical harmonic oscillator

- Energy levels
  - Equally spaced
  - Zero-point energy
- Wavefunctions
  - Gaussian function modulated by Hermite polynomial
  - Have definite parity
    - due to symmetric potential



Stationary state

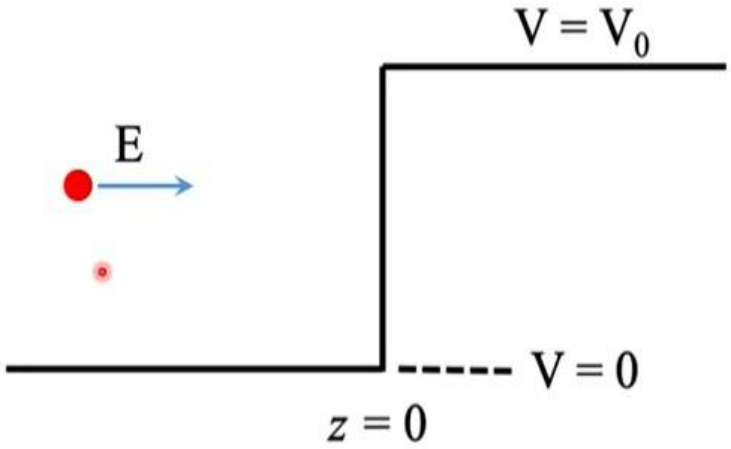
- We obtained the solution of harmonic oscillator problem by solving time-independent Schrödinger equation.
- Therefore, our solutions do not involve any time dependence and thus do not exhibit actual oscillation.
- Solutions of time-independent Schrödinger equation represent "stationary" states.
- The stationary solutions of the harmonic oscillator problem do not represent the classical oscillator.
- Classical oscillator can, however, be represented by a linear combination of stationary solutions or eigenfunctions.
- Actual harmonic oscillation can then be recovered by time-dependent Schrödinger equation.

Potential step

- The potential is given as,

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

- A particle with energy E is incident from the left.
- The energy E is assumed to be greater than zero,
  - Can be smaller or larger than V_0.



Schrödinger equation

- Write down the time-independent Schrödinger equation:
- In region I where $z < 0$,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2} = E\psi(z) \quad \Rightarrow \quad \frac{d^2\psi(z)}{dz^2} + k_0^2\psi(z) = 0 \quad \text{where} \quad k_0 = \sqrt{\frac{2mE}{\hbar^2}} \qquad (1)$$

- In region II where $z > 0$,

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

$$\Rightarrow \quad \frac{d^2\psi(z)}{dz^2} + k^2\psi(z) = 0 \quad \text{where} \quad k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \qquad (2)$$

Solutions

- Solutions of equation (1) for region I ($z < 0$)

$$\psi_I(z) = Ae^{ik_0 z} + Be^{-ik_0 z} \qquad (3)$$

- Solving equation (2) for regions II ($z > 0$)

$$\psi_{II}(z) = Ce^{ikz} + De^{-ikz} \qquad (4)$$

- With the time-dependence of $\exp(-i\omega t)$ implied,
  - the terms, $\exp(ik_0 z)$ and $\exp(ikz)$, represent right-propagating wave, while
  - the terms, $\exp(-ik_0 z)$ and $\exp(-ikz)$, represent left-propagating wave.
- Since the particle is incident from the left,
  - There should not be any left-propagating wave in region II.

$$\Rightarrow \quad D = 0 \quad \Rightarrow \quad \psi_{II}(z) = Ce^{ikz} \qquad (5)$$

Solutions

- Now require continuity of ψ and $d\psi/dz$ at $z = 0$:

$$A + B = C \qquad (6)$$

$$k_0 A - k_0 B = kC \qquad (7)$$

- Which yields,

$$\frac{B}{A} = \frac{k_0 - k}{k_0 + k} \quad \text{and} \quad \frac{C}{A} = \frac{2k_0}{k_0 + k} \qquad (8)$$

- The solutions are now written as,

$$\psi_I(z) = A\left[e^{ik_0 z} + \frac{k_0 - k}{k_0 + k} e^{-ik_0 z}\right] \qquad z < 0 \qquad (9)$$

$$\psi_{II}(z) = A\frac{2k_0}{k_0 + k} e^{ikz} \qquad z > 0 \qquad (10)$$

$E > V_0$

- In this case, both k_0 and k are real and positive with $k_0 > k$.

$$k_0 = \sqrt{\frac{2mE}{\hbar^2}} \qquad k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

$E > V_0$

- In this case, both k_0 and k are real and positive with $k_0 > k$.
- The right-propagating wave, $\exp(ik_0z)$, in region I represents the incident wave.
- The left-propagating wave, $\exp(-ik_0z)$, in region I represents the reflected wave.
- The right-propagating wave, $\exp(ikz)$, in region II represents the transmitted wave.
- Define reflection and transmission coefficients as

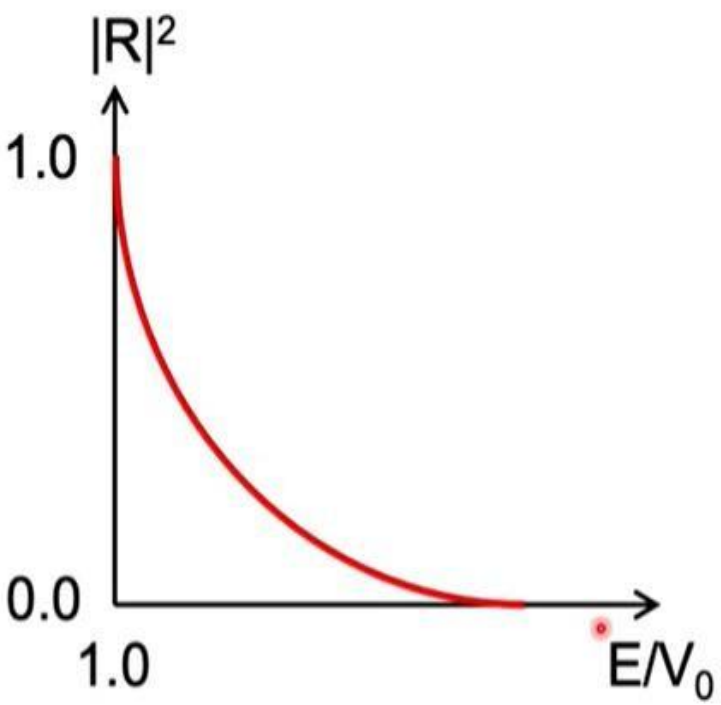
$$R \equiv \frac{B}{A} = \frac{k_0 - k}{k_0 + k} \qquad T \equiv \frac{C}{A} = \frac{2k_0}{k_0 + k}$$

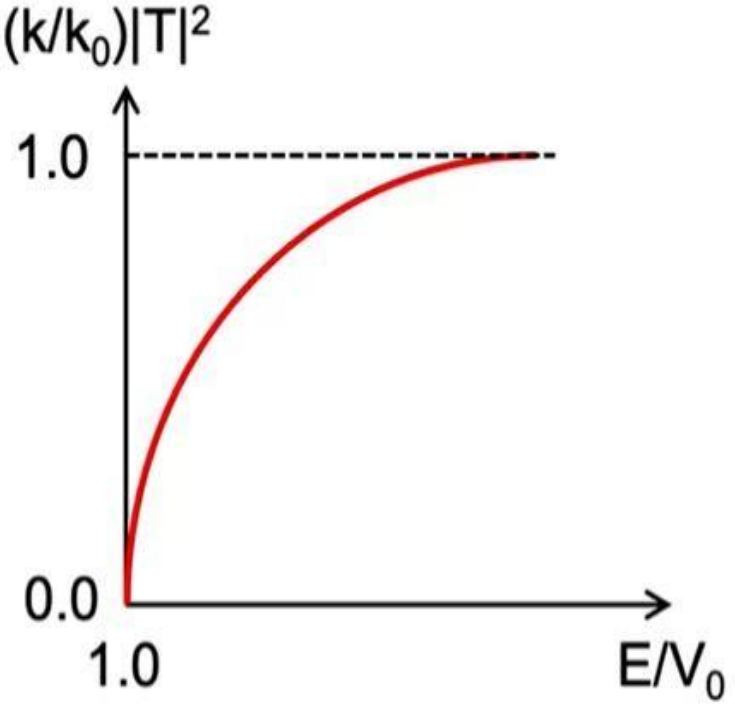
- Total reflection and transmission probabilities are given as,

$$P_{refl} = |R|^2 = \left(\frac{k_0 - k}{k_0 + k}\right)^2 \qquad P_{trans} = 1 - |R|^2 = \frac{4kk_0}{(k_0 + k)^2} = \frac{k}{k_0}|T|^2$$

$E > V_0$

- Since the probability is proportional to $|\psi|^2$, the probabilities of reflection and transmission are given by $|R|^2$ and $|T|^2$, respectively.





$E < V_0$

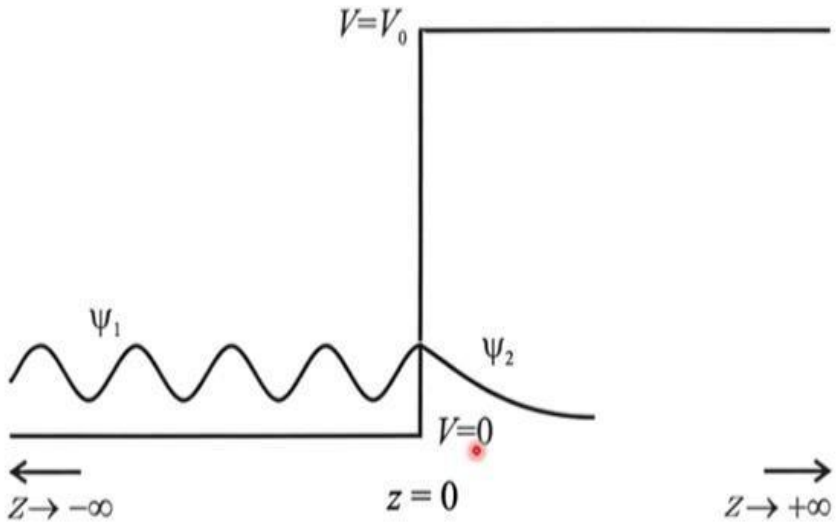
- In this case, k is imaginary, $k = i\kappa$, where

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

- The reflection coefficient becomes,

$$R = \frac{k_0 - i\kappa}{k_0 + i\kappa} \quad \text{and} \quad |R|^2 = 1$$

- The transmitted wave in region II becomes evanescent, $\exp(-\kappa z)$.
  - Penetration into the barrier
  - Non-classical behavior

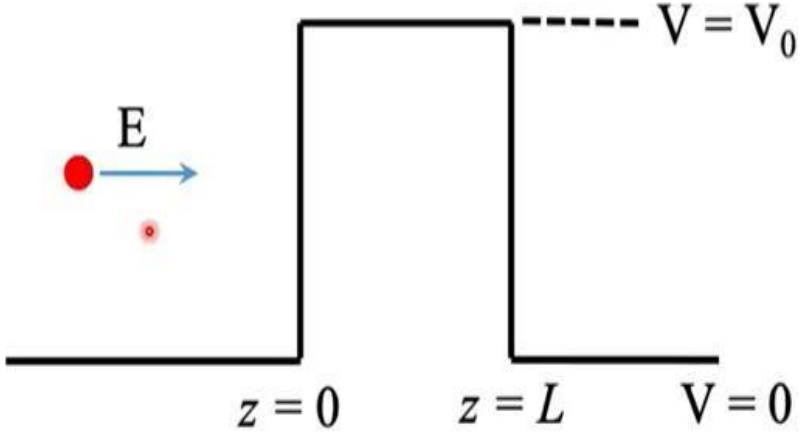


Potential barrier

- Potential is given as,

$$V(z) = \begin{cases} V_0, & 0 \le z \le L \\ 0, & \text{otherwise} \end{cases}$$

- A particle with energy E is incident from the left.
- The energy E is assumed to be greater than zero,
  - Can be smaller or larger than V_0.



Potential barrier

- Similarly to the potential step problem, solve the time-independent Schrödinger equation to obtain,

$$\psi_I(z) = e^{ik_0 z} + Re^{-ik_0 z} \qquad z < 0$$

$$\psi_{II}(z) = Ae^{ikz} + Be^{-ikz} \qquad 0 < z < L$$

$$\psi_{III}(z) = Te^{ik_0 z} \qquad z > L$$

  - where $k_0 = \sqrt{\frac{2mE}{\hbar^2}}$ $\qquad k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$

- Here, we normalized all coefficients with respect to the incident wave amplitude and
- Left-propagating wave in region III is omitted.

Potential barrier

- Now require continuity of ψ and $d\psi/dz$
  - at $z = 0$: $1 + R = A + B$

    $ik_0(1 - R) = ik(A - B)$

    at $z = L$: $Te^{ik_0 L} = Ae^{ikL} + Be^{-ikL}$

    $ik_0 Te^{ik_0 L} = ik(Ae^{ikL} - Be^{-ikL})$
- Solve for constants:

$$R = \frac{(1-\mu^2)\sin kL}{(1+\mu^2)\sin kL + 2i\mu\cos kL}$$

$$T = e^{-ik_0 L}\frac{2i\mu}{(1+\mu^2)\sin kL + 2i\mu\cos kL}$$

$$A = e^{-ikL}\frac{-i(1+\mu)}{(1+\mu^2)\sin kL + 2i\mu\cos kL}$$

$$B = e^{ikL}\frac{-i(1-\mu)}{(1+\mu^2)\sin kL + 2i\mu\cos kL}$$

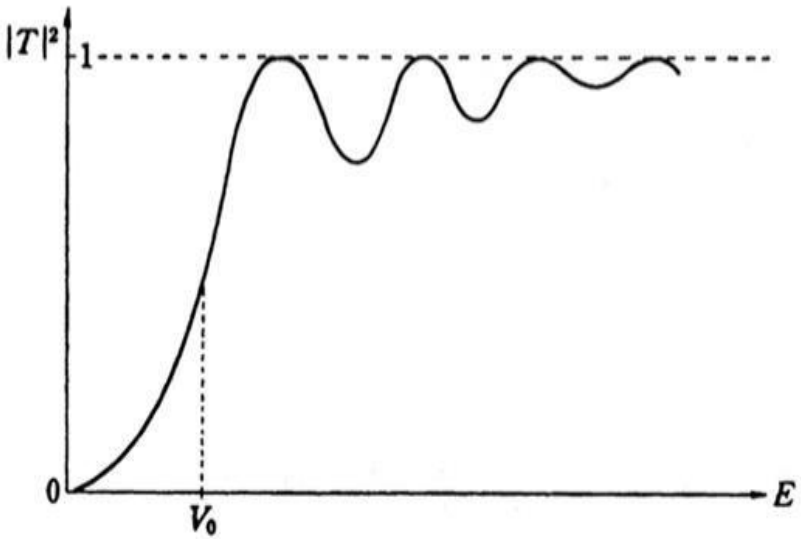
where $\mu = \frac{k}{k_0} = \sqrt{1 - \frac{V_0}{E}}$

Potential barrier

- For $E < V_0$: both k and μ are imaginary
  - $|T|^2 > 0$ always: tunneling
  - $|T|^2$ increases monotonically with increasing E
  - Evanescent waves inside the barrier
- For $E > V_0$: both k and μ are real
  - $|T|^2$ oscillates and reaches unity at

$$E = V_0 + \frac{n^2\pi^2\hbar^2}{2mL^2}$$

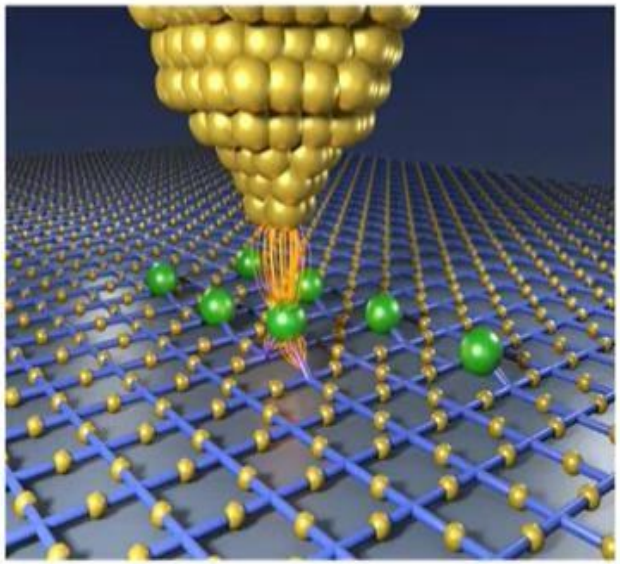
  - Resonant tunneling
  - Applies for negative V_0 too.



Scanning tunneling microscope

- Electron mass = 9.1 X 10^{-31} kg
- Barrier height = 5 eV (typical metal work function)
- Barrier thickness = 0.5 nm (separation between metal surface and probe tip)
- Assuming an electron kinetic energy of 1 eV,

→ T ~ 1 X 10^{-4}



http://www.desy.de/information__services/press/press_releases/2012/pr_120112/index_eng.html

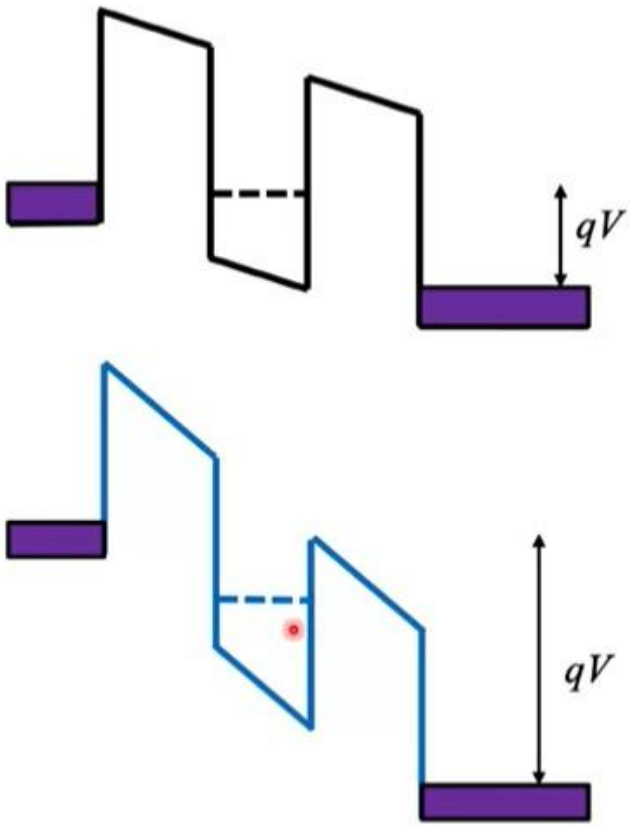
- Kinetic energy = 3000 J (or 1.9 X 10^{22} eV)
  - Person (mass = 60 kg) running at a speed of 10 m/s
- Approximate the Flatirons with a rectangular barrier
  - Barrier height ~ 4.7 x 10^{5} J (or 2.9 X 10^{24} eV)
    - Gravitational potential energy for a 800 m high peak
  - Barrier width = 5 km

→ $T = 10^{-10\text{^}75}$



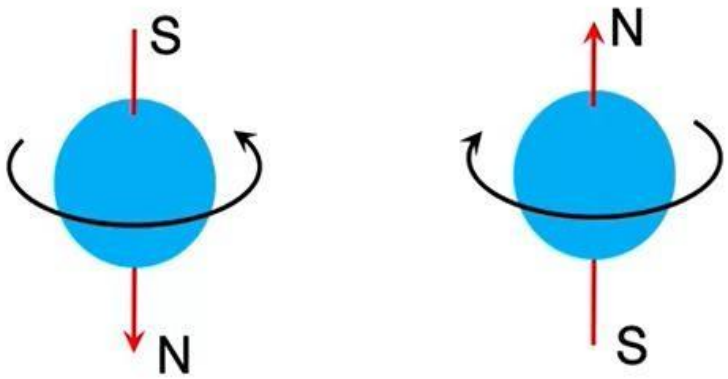
Resonant tunnel diode

- A semiconductor heterostructure with double barriers.
- When the allowed energy level within the finite quantum well is aligned with the input electron energy level,
  - High tunneling probability and thus high current.
  - Resonant tunneling
- When it is misaligned,
  - Low current
- Produces negative differential resistance



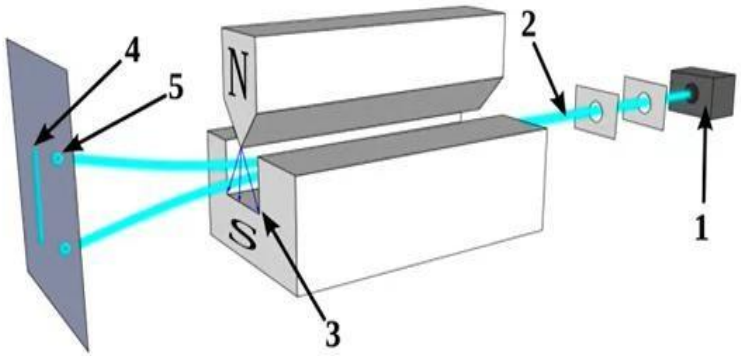
Electron spin

- Electron (and many other elementary particles) has intrinsic angular momentum.
  - That is, angular momentum that does not depend on its motion.
  - Called “spin”.
- Just like orbital angular momentum, spin produces magnetic moment.
- As a result, electron interacts with magnetic field.



Stern-Gerlach experiment

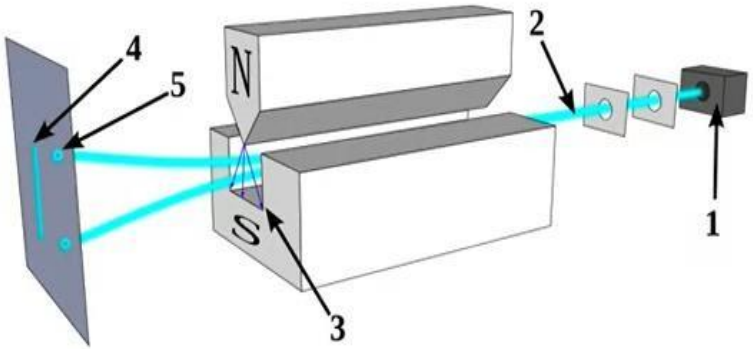
- In Stern-Gerlach experiment, electrons are sent through a region with non-uniform magnetic field.
  - Magnetic field is stronger near the top (N) magnet than near the bottom (S) magnet.
- If electron spin is up (N down), then electron is pushed upward.
  - And vice versa.
- If electron spin is horizontally aligned, electron will not be pushed up- or down-ward.



https://en.wikipedia.org/wiki/Stern%E2%80%93Gerlach_experiment

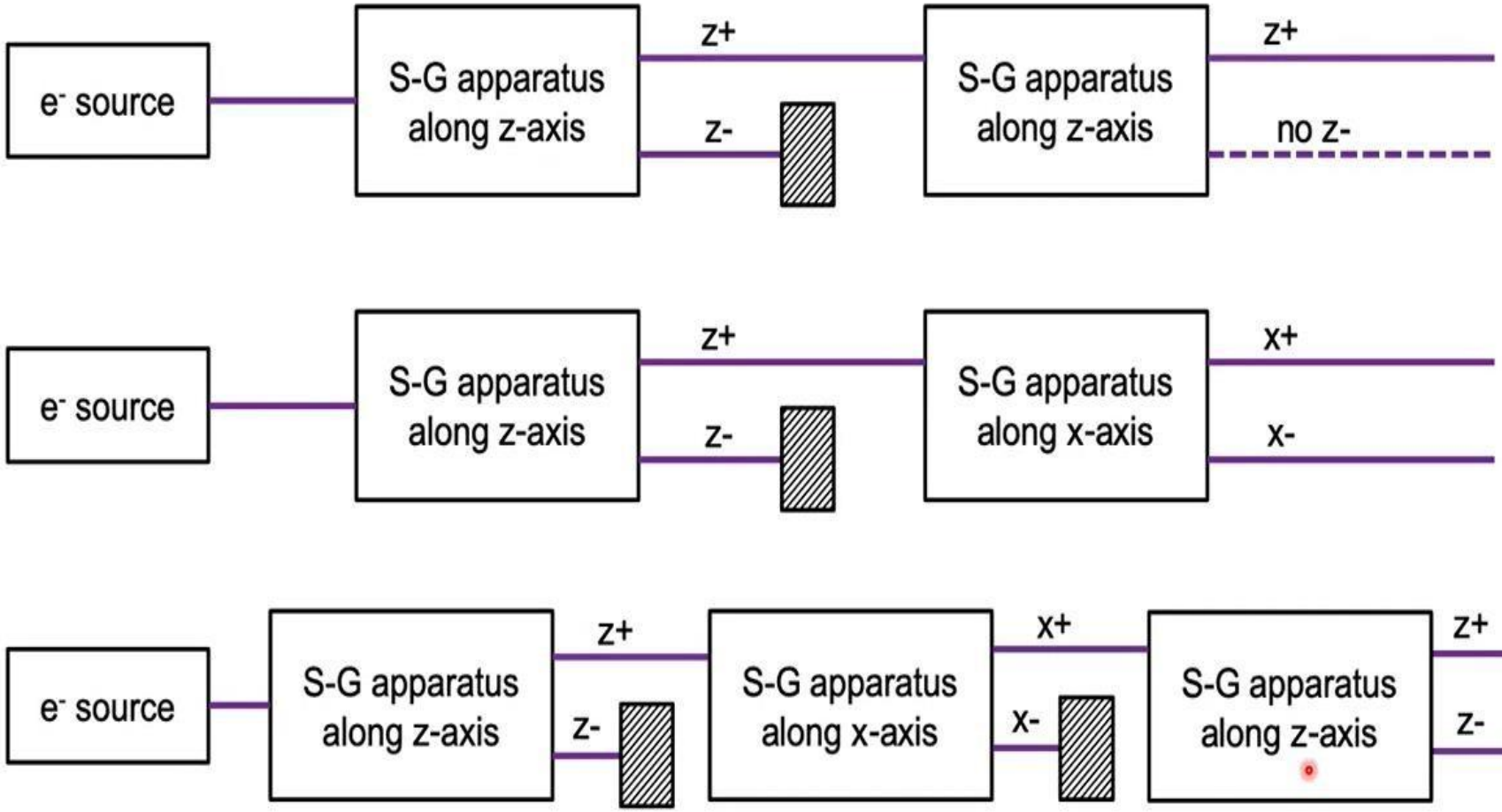
Stern-Gerlach experiment

- If electrons are produced thermally by a hot cathode (or oven),
  - Spins should be randomly oriented.
  - We expect a continuous distribution of electrons on the screen (4 in the figure).
- But in actual experiments, we observe only two spots (5 in the figure).
  - Electron spin is either up or down.
- Even when we rotate the magnets,
  - Still two dots on the screen, rotated the same way as the magnets.



https://en.wikipedia.org/wiki/Stern%E2%80%93Gerlach_experiment

Sequential S-G experiments



Measurement

- In quantum mechanics, when we make a measurement,
  - we "collapse" the state of the system into one of the allowed states.
  - In the case of S-G experiment, they are "spin up" or "spin down" states.
- A measurable quantity is represented by an operator.
- And the allowed states are the eigenstates of the operator.
- For example, time-independent Schrödinger equation is an eigenvalue equation.

$$\hat{H}\Psi = E\Psi \quad \text{where} \quad \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$$

  - Solutions are eigenvalues (allowed values of E) and the corresponding wavefunctions (eigenfunctions).

Measurement

- Suppose we measured energy of a quantum system and
  - obtained a certain value, E_n.
- The operator for energy is the Hamiltonian, $\hat{H}$.
- Quantum mechanical explanation of what actually happened is
  - the quantum system has "collapsed" into the eigenstate of $\hat{H}$ operator corresponding to the eigenvalue E_n.
- The probability of measuring E_n depends on the initial state.
- The result of the measurement cannot be predicted precisely and
  - can only be described by probability,
  - unless the initial state is one of the eigenstates of the operator representing the quantity being measured.



THANKS

