Quantum Materials
(UES022)

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THAPAR INSTITUTE
OF ENGINEERING & TECHNOLOGY
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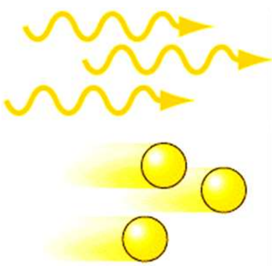
Introduction to Quantum mechanics

Newtonian mechanics

Start of thinking of science
Supposed to resolve almost all the problems

Applied to visible systems

Philosophical approach



Particles and waves

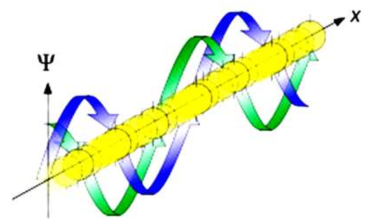
State of the particle: position and momentum

Quantum mechanics

Start of formulating science
Supposed to resolve all problems in chemistry, almost all problems of physics

Applied to all the systems.

Probabilistic approach



Dual nature

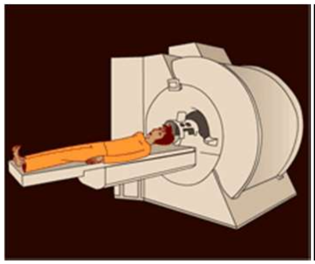
(Quantum) State of the system! wave function

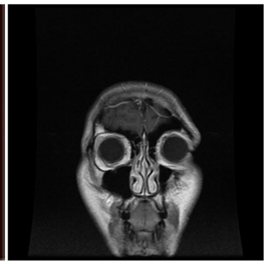
Transition from old to modern era:

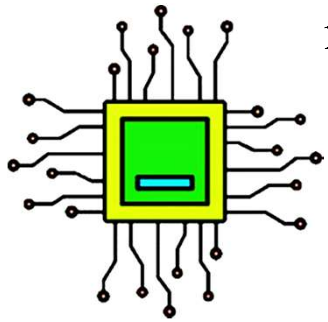
Elementary quantum mechanics

Introduction to Quantum mechanics

The beauty of the quantum theory:

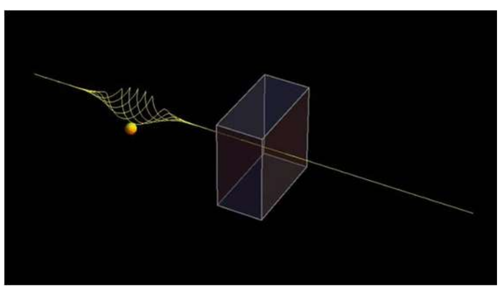




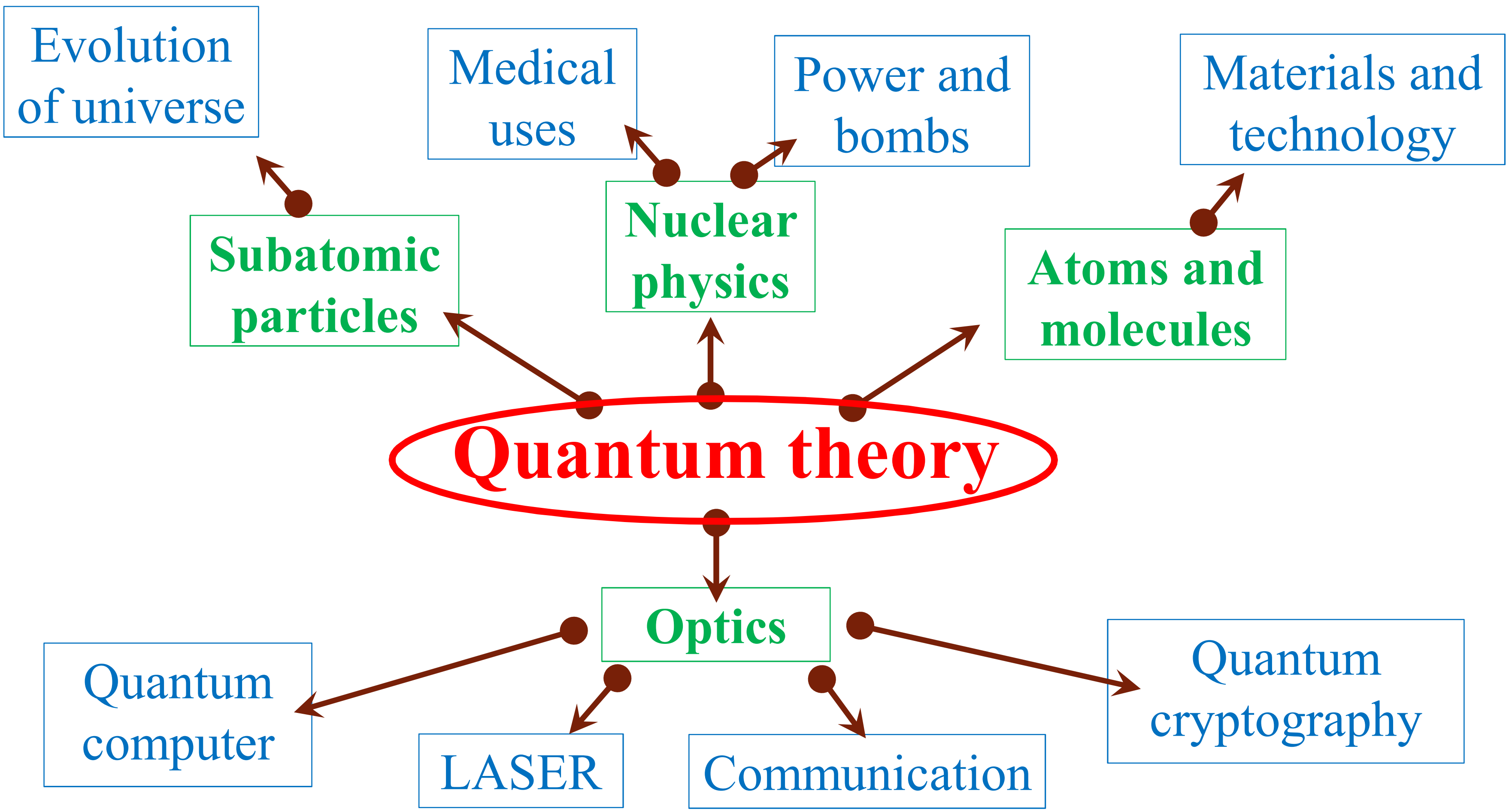


Without Quantum Mechanics, we could never have designed and built:

semiconductor devices
computers, cell phones, etc.
Lasers, CD/DVD players,
MRI technology,
Nuclear reactors,
Atomic clocks (GPS navigation)



Introduction to Quantum mechanics



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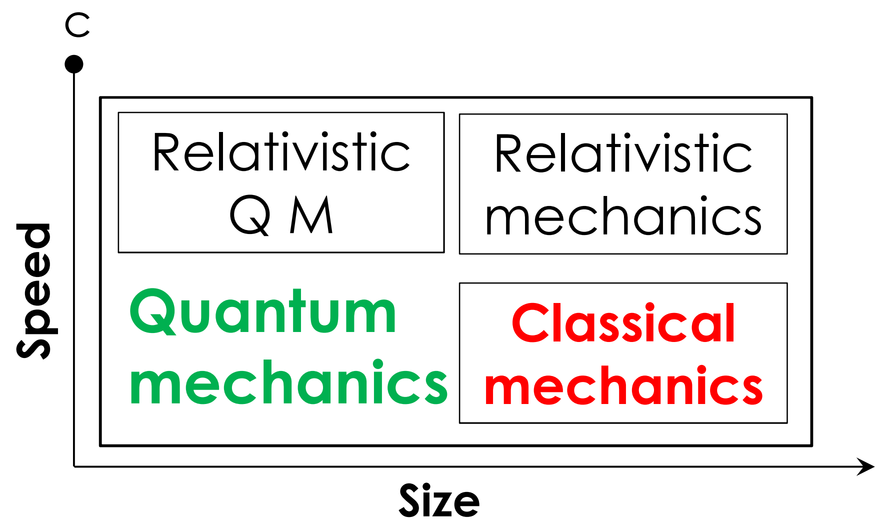
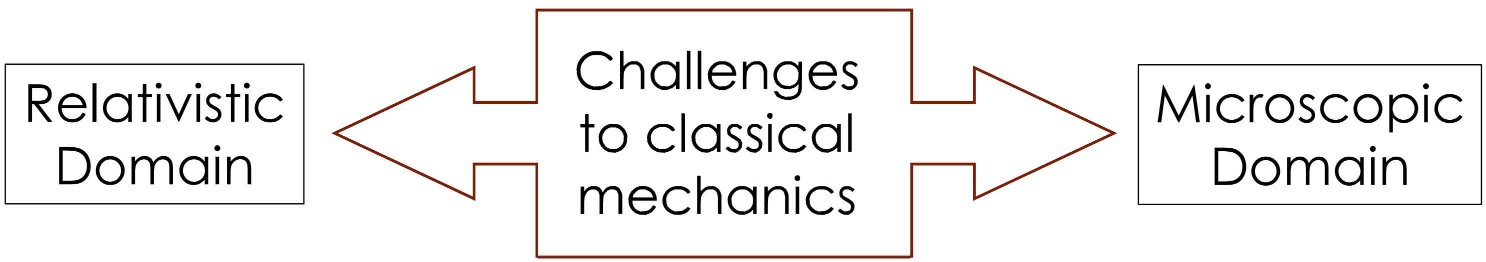
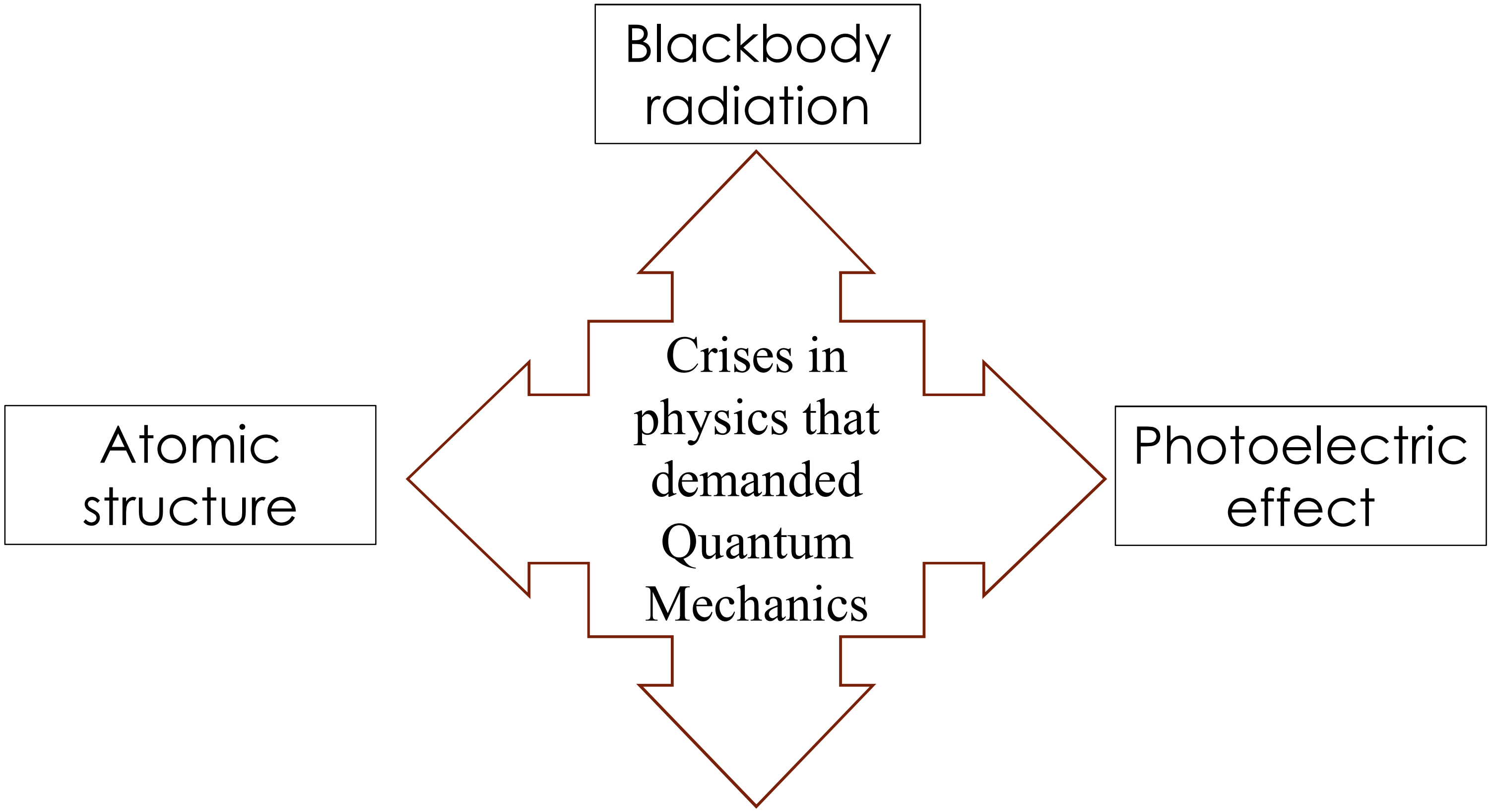




Origin of quantum mechanics

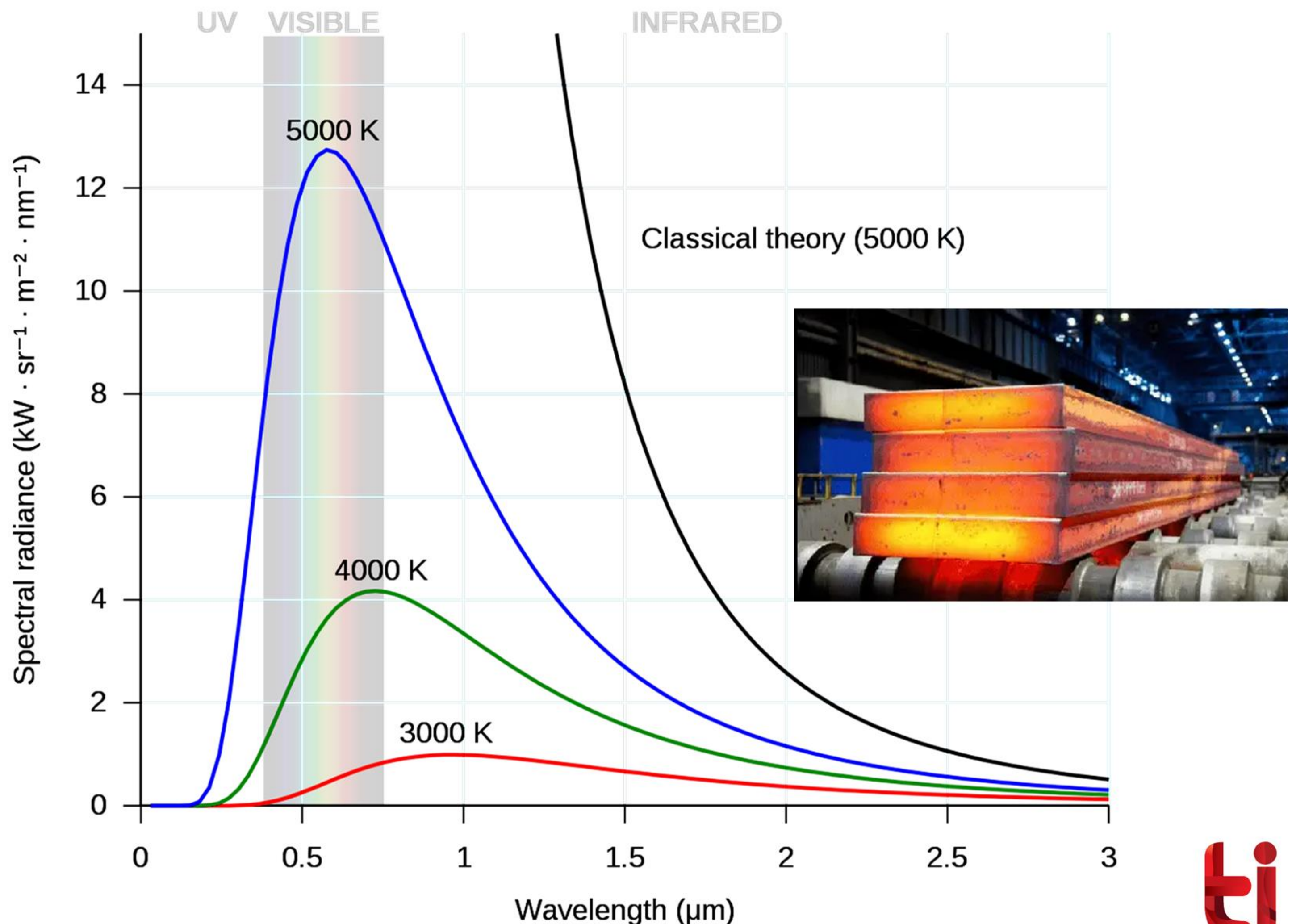


Crises in physics that demanded Q.M.

Blackbody radiation:

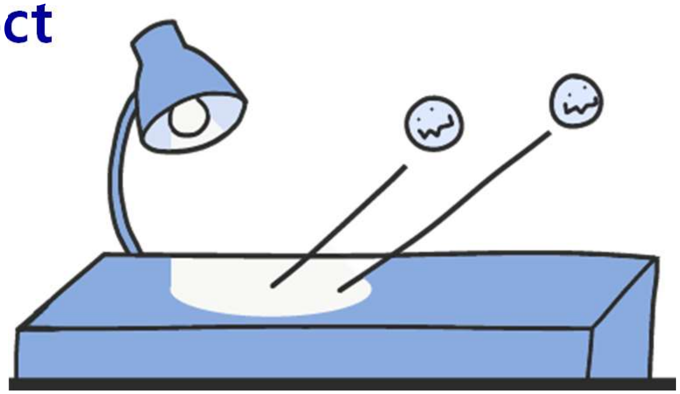
How dose the intensity of electromagnetic radiation emitted by a body depend on the frequency of the radiation and the temperature of the body?

Kirchoff (1859)



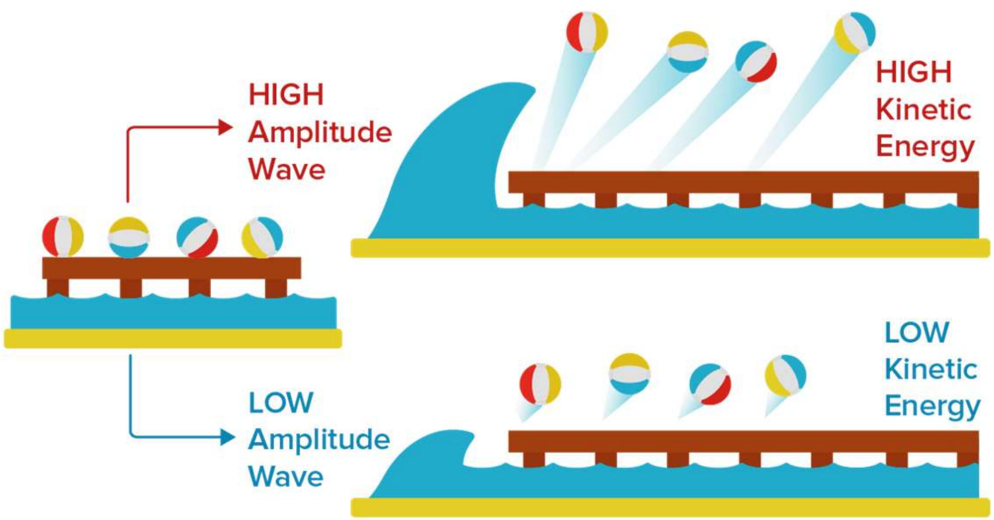
Crises in physics that demanded Q.M.

Photoelectric effect



Metals would shed electrons when certain light was incident on it.

1887, Heinrich Hertz



Wave model of light

- increasing light intensity would increase the kinetic energy of emitted photoelectrons, (Brightness should produce more electrons!)
- increasing the frequency would increase measured current.

Photoelectric effect

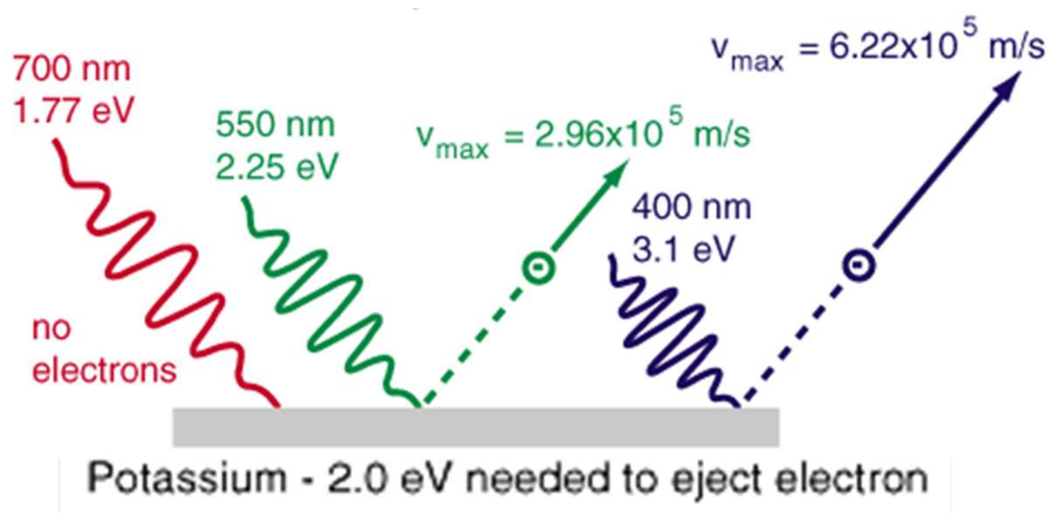
It has already been proved that light is a wave.

Solids are made by binding of atoms and atoms contain electrons.

So, why only certain light is able to generate electrons, and why not all sorts of light?

Experiments showed that

- increasing the light frequency increased the kinetic energy of the photoelectrons,
- increasing the light amplitude increased the current.



Photoelectric effect: three challenges

- There is no time interval b/w the arrival of light at a metal surface and the emission of photoelectrons. How ever, because the energy in an em wave is supposed to be spread across the wavefronts, a period of time should elapse before an individual electron accumulates enough energy to leave the metal.

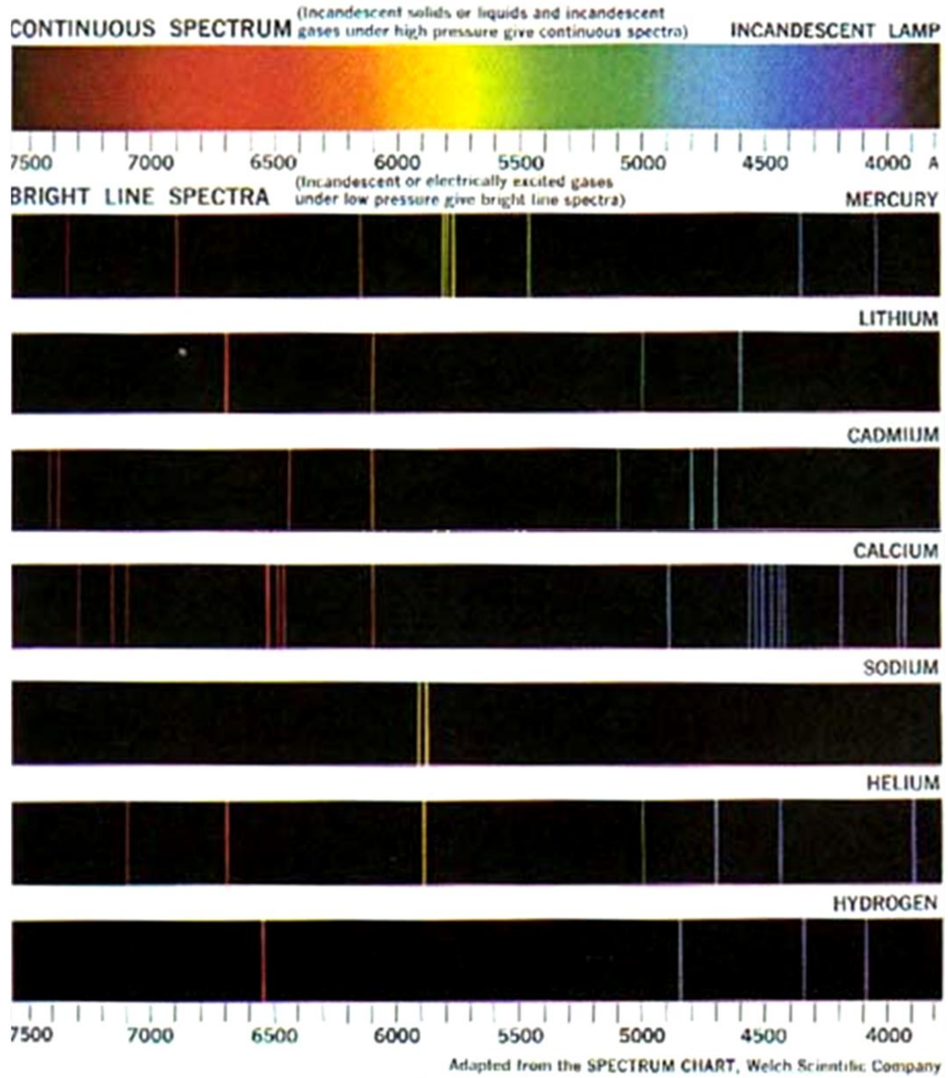
- A bright light yields more photoelectrons than a dim one of the same frequency, but the electron energies remain the same. The em theory of light, on the con trary, predicts that the more intense the light, the greater the energies of the electrons.

- The higher the frequency of the light, the more energy the photoelectrons have. At frequencies below a certain critical frequency 0, which is characteristic of each particular metal, no electrons are emitted.

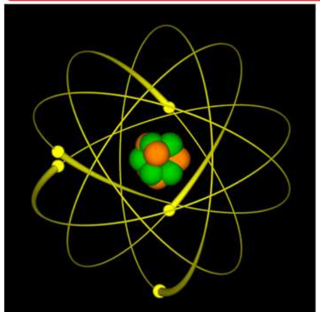
Crises in physics that demanded Q.M.

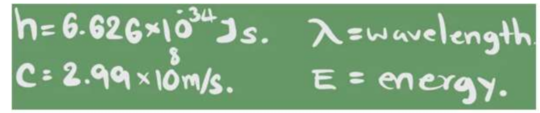
Atomic structure

Emission spectra



Origin of quantum mechanics



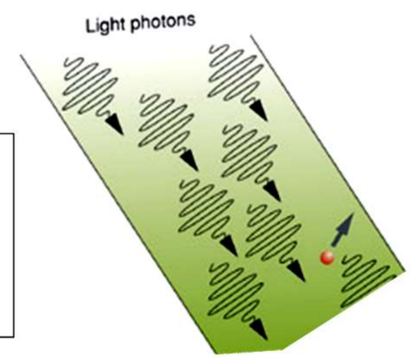


Plank: Quanta of energy (1900)

Breakthroughs in science

Bohr: Atom's discrete states (1913)

Einstein: Photon of light (1905)



Davisson, Germer: Wave behavior of electrons (1927)

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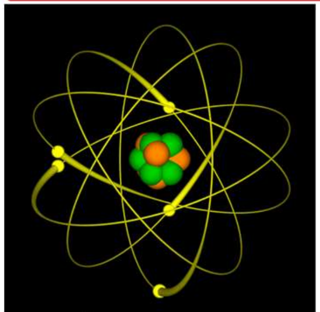

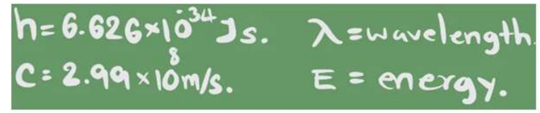

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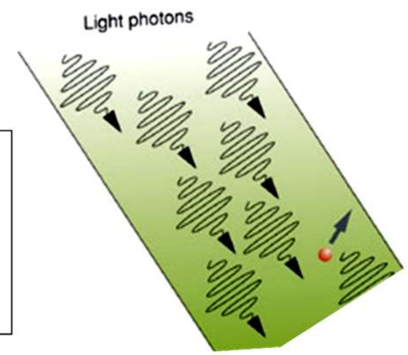

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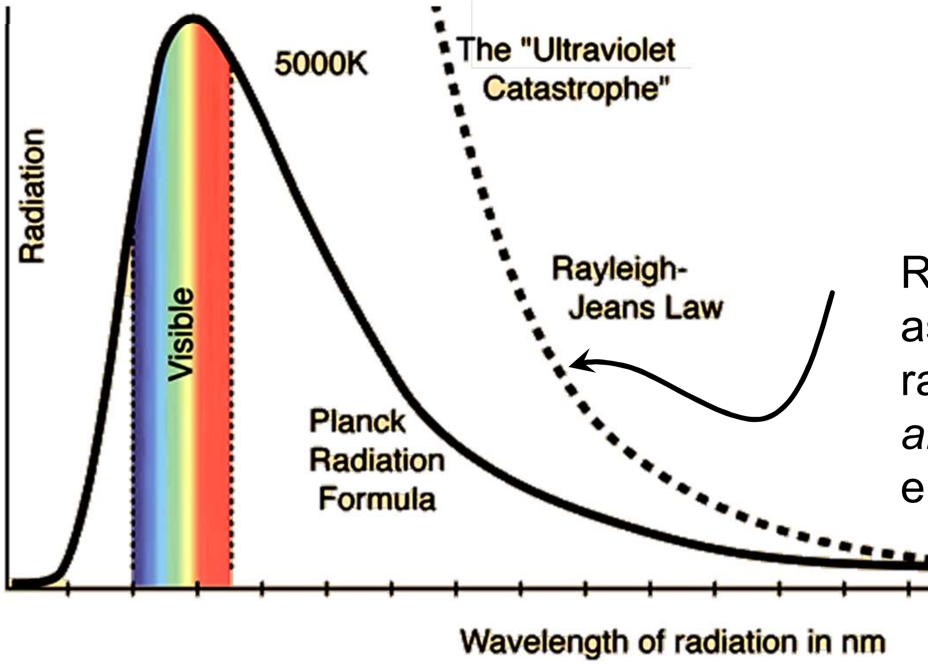
Breakthroughs in science

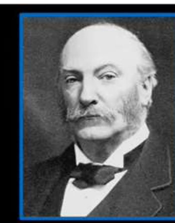
Plank's quanta of energy (1900)

Max Planck
(1858-1947)

<u>Planck's consideration</u>: the energy exchange between radiation and matter must be *discrete*.



James Jeans
(1877-1946)



John Rayleigh
(1842-1919)

Rayleigh's Classical assumption:
radiation can exchange *any* amount (continuum) of energy with matter.

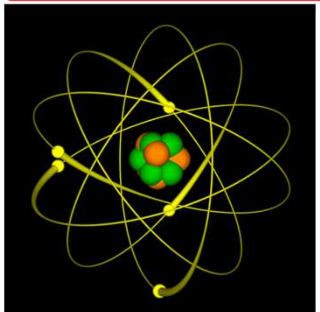
$$\langle E \rangle = k_B T$$

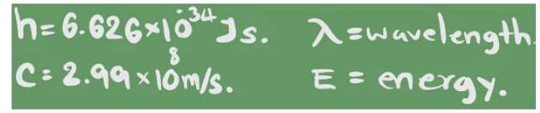
The radiation (of frequency ν) emitted by the matter (from the walls of the blackbody) must come *only* in *integer multiples* of $h\nu$.

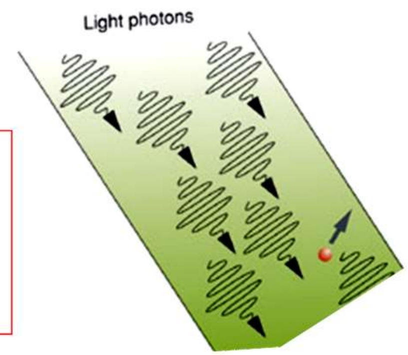
$$E_\nu = nh\nu,\ n = 1, 2, 3, 4 \ldots$$

$$\langle E \rangle = \frac{h\nu}{e^{h\nu/kT} - 1}$$

Origin of quantum mechanics







Breakthroughs in science

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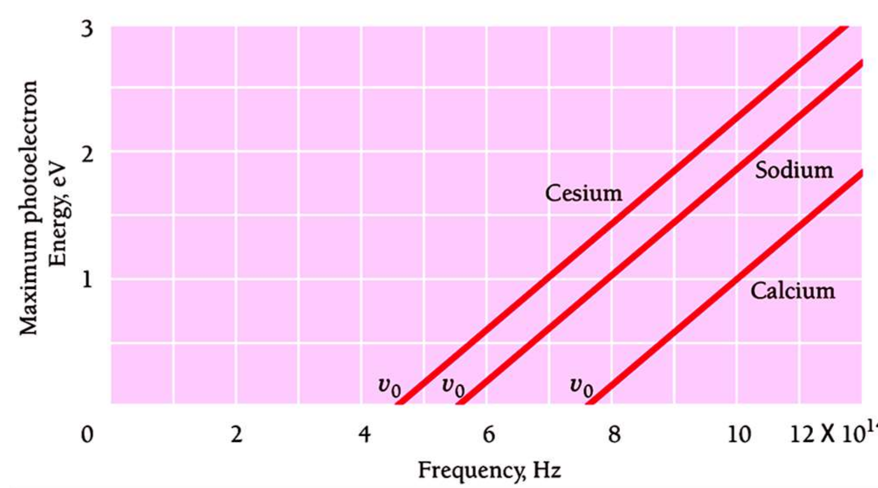
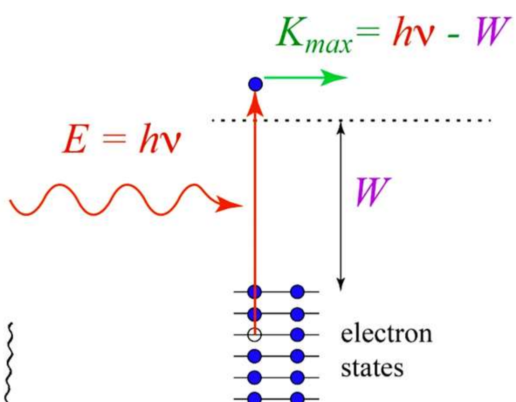
Breakthroughs in science

Einstein: Photon of light (1905)

- Einstein thought that light is equivalent to wave packets called photons – particle nature.
- Energy of each packet is $h\nu$. '*h*' is the Planck's constant.





LIGHT IS A
particle!

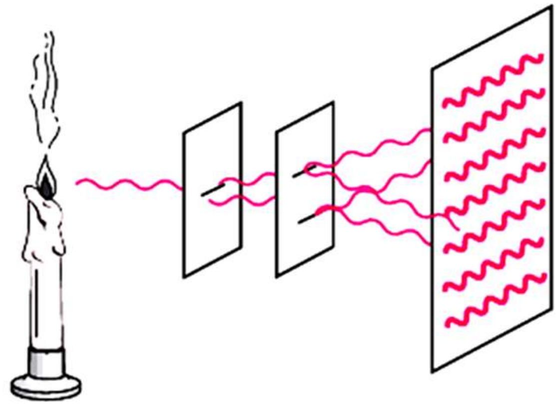
When a photon of frequency ν is incident on a metal, it is entirely absorbed by the electron near the surface.

If $h\nu$ is larger than the metal's *work function W,* the electron will then be knocked out of the metal. Hence no electron can be emitted from the metal's surface unless $h\nu > W$.

Breakthroughs in science

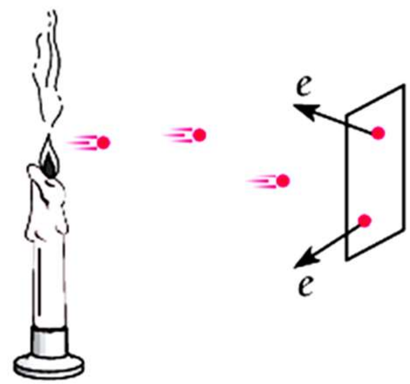
Light: wave or particle?

(a) The wave theory of light explains diffraction and interference.



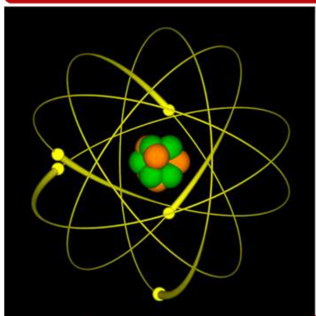
(a)

(b) The quantum theory explains the photoelectric effect, which the wave theory cannot account for.



(b)

Origin of quantum mechanics



Bohr: Atom's discrete states (1913)

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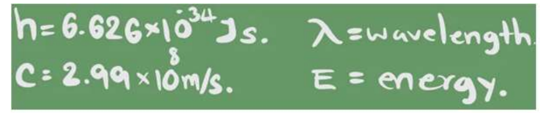

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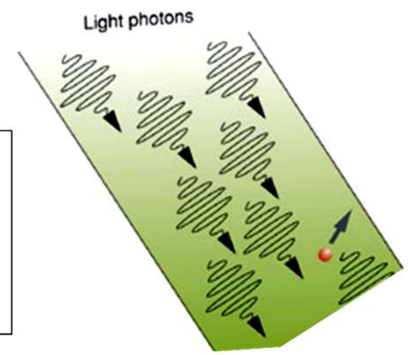

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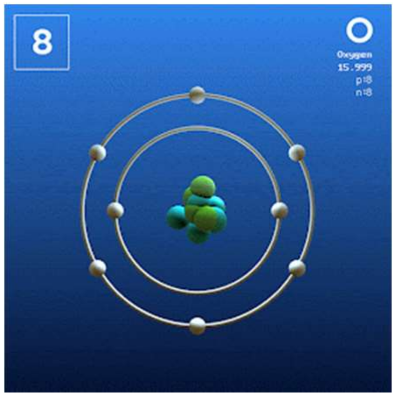
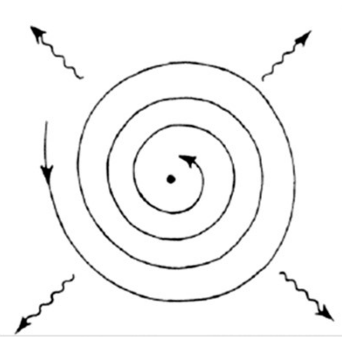
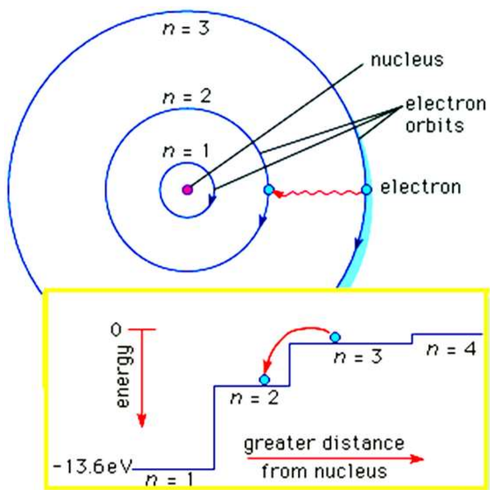
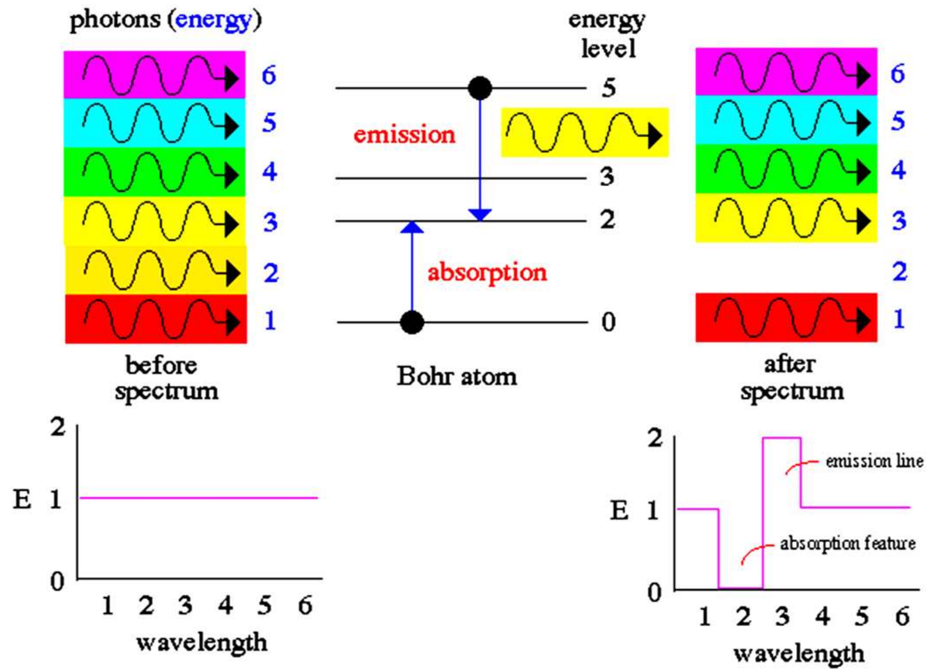
Bohr: Atom’s discrete states (1911)





?



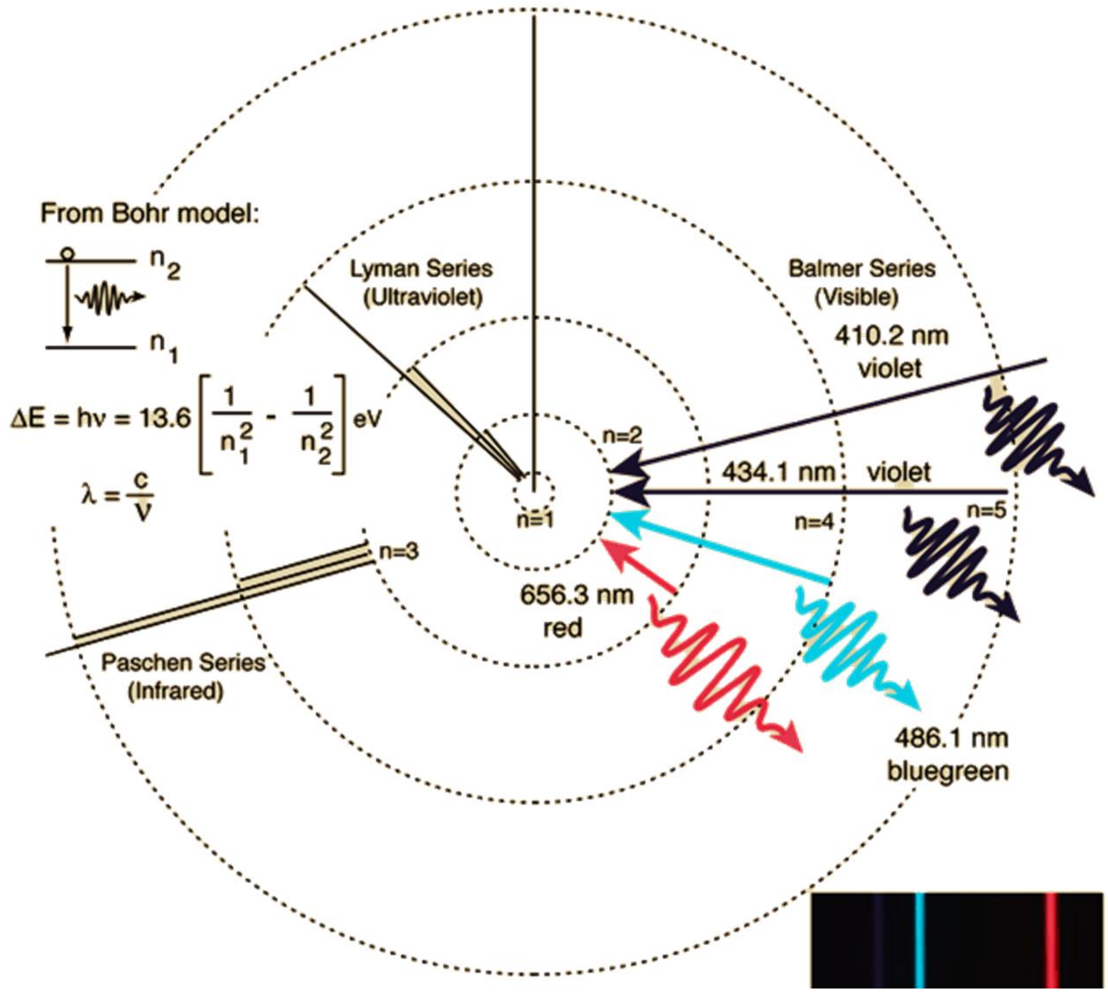


If an electron jumps one orbit closer to the nucleus, it must emit energy equal to the difference of the energies of the two orbits.

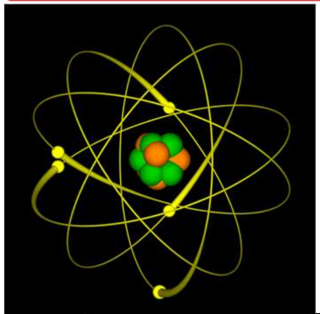
Conversely, when the electron jumps to a larger orbit, it must absorb a quantum of light equal in energy to the difference in orbits.

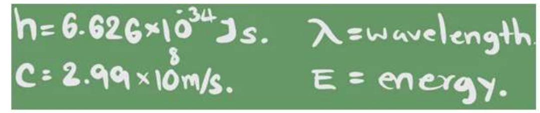
Breakthroughs in science

Bohr: Atom's discrete states (1911)



Origin of quantum mechanics





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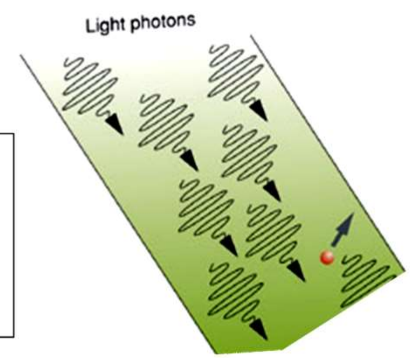

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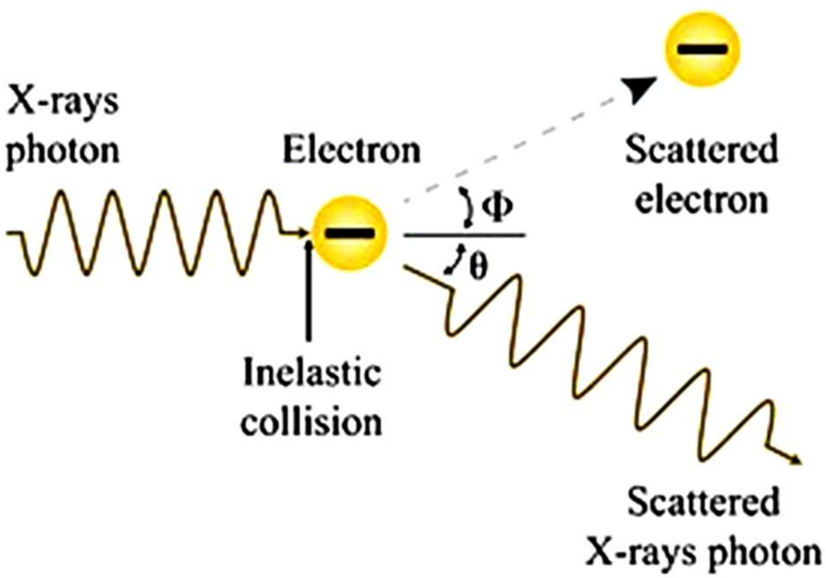
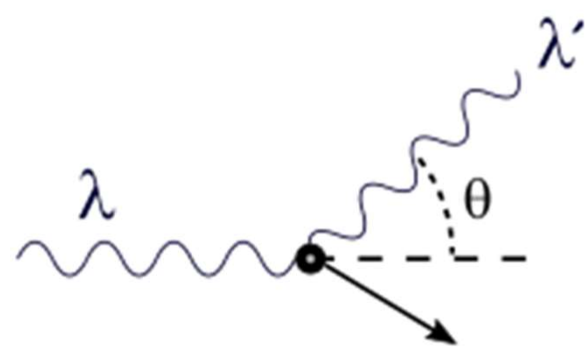
When a high frequency photon hits electrons, it gets scattered. There is a decrease in the energy of the photon. The lost energy from the photon is transferred to the recoiling electrons.

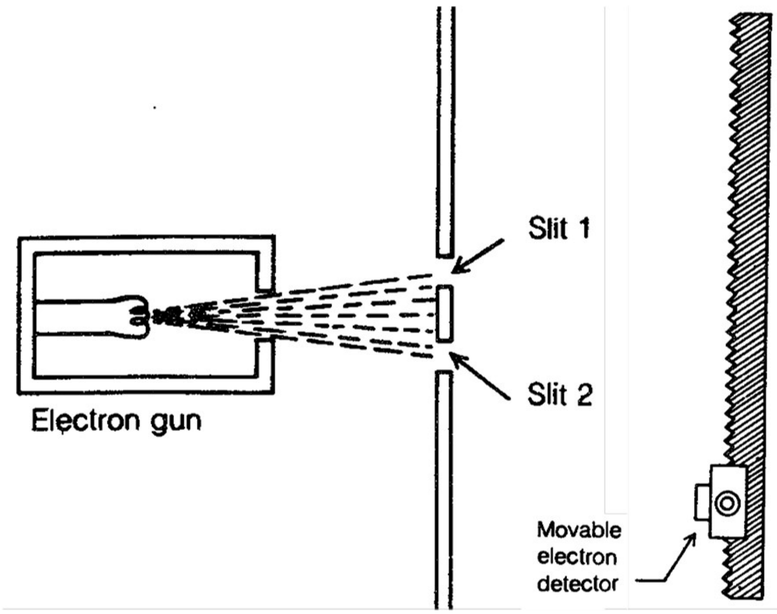


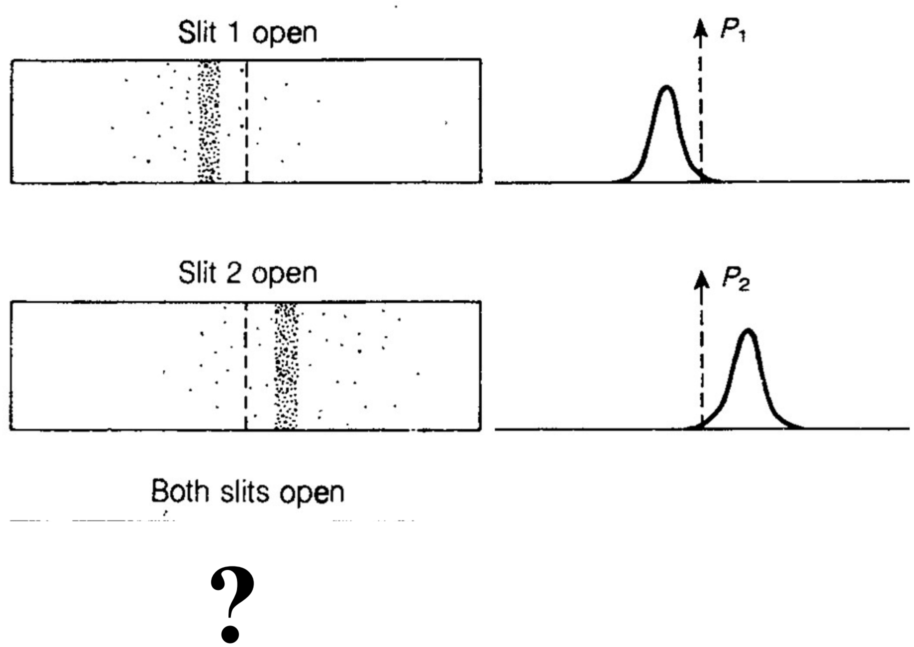


$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta),$$

Breakthroughs in science

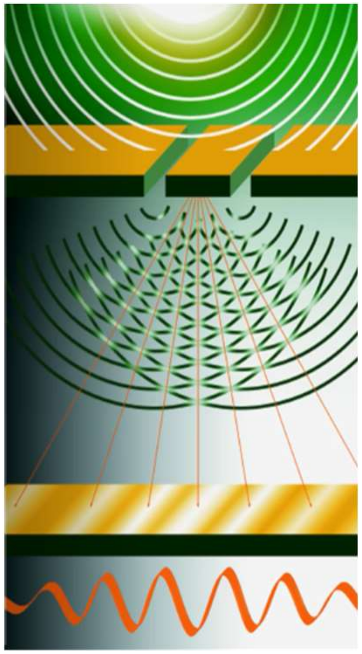
Double slit experiment with electron beam (1923)

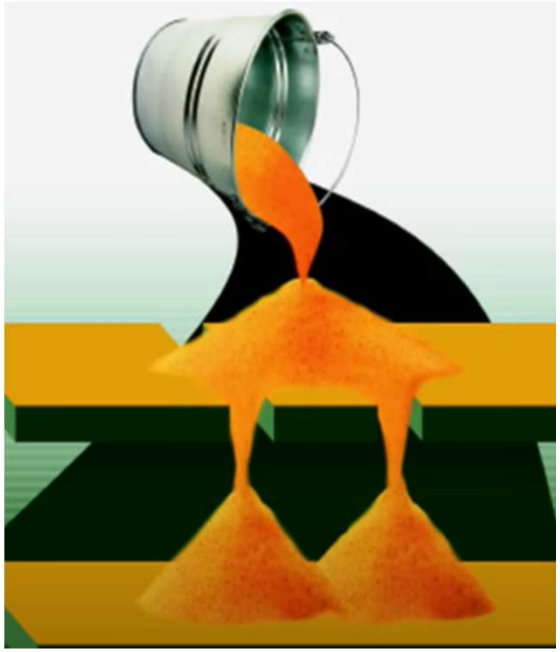




Breakthroughs in science

Double slit experiment with wave and with particles





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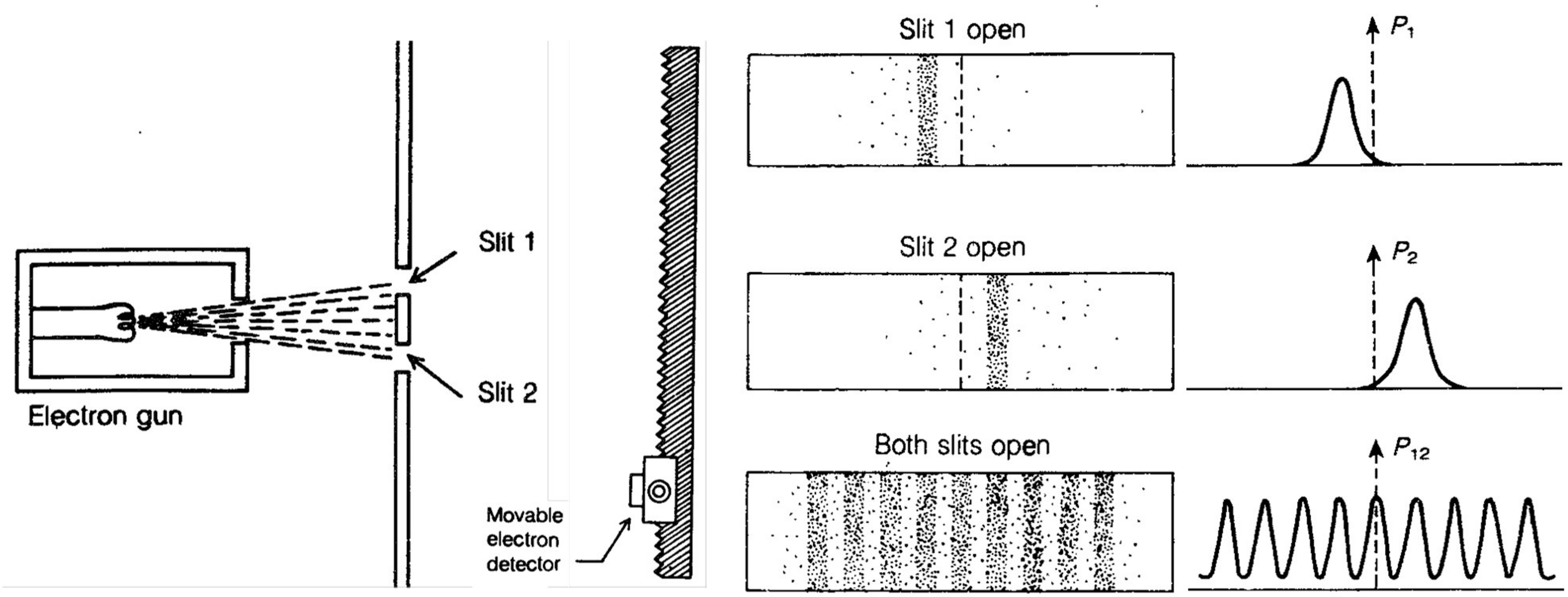
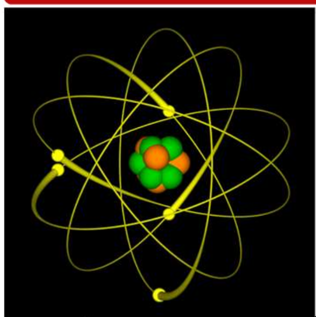


Interference pattern of a wave!

Wave behavior of the electron?

Origin of quantum mechanics



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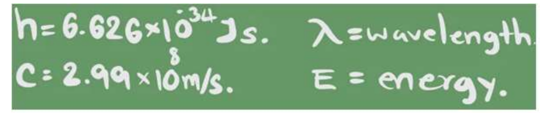

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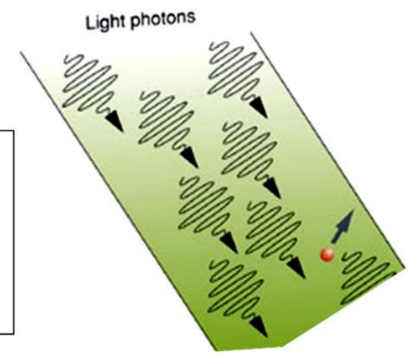

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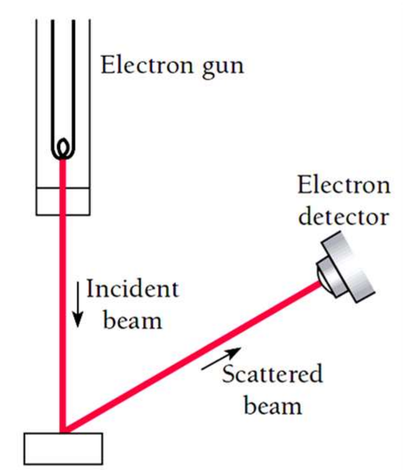
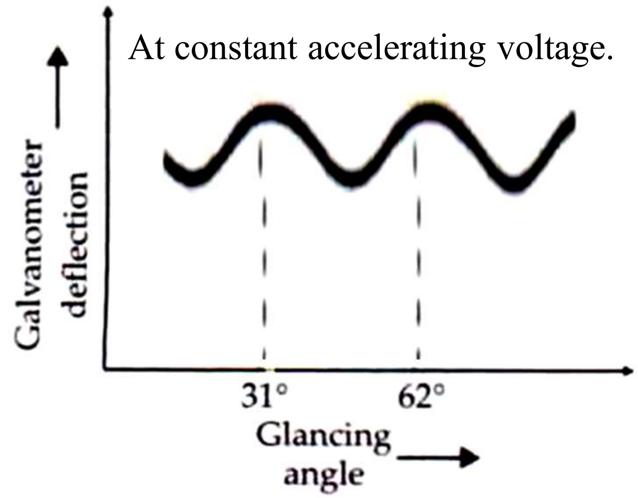
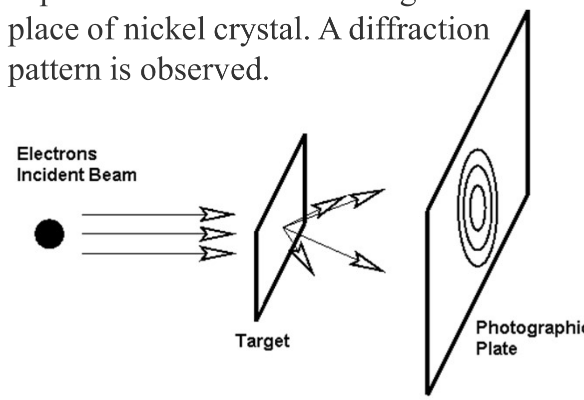
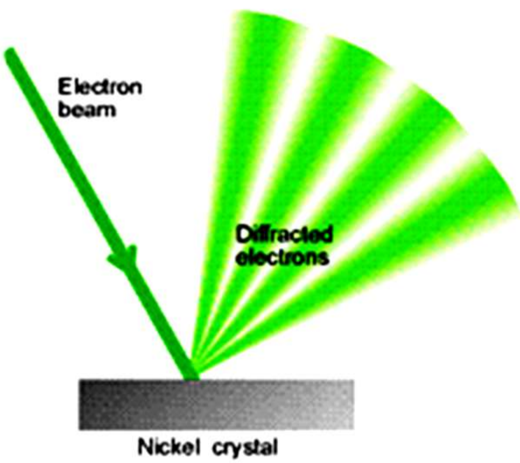




G.P. Thomson in 1928 performed experiments with thin foil of gold in place of nickel crystal. A diffraction pattern is observed.





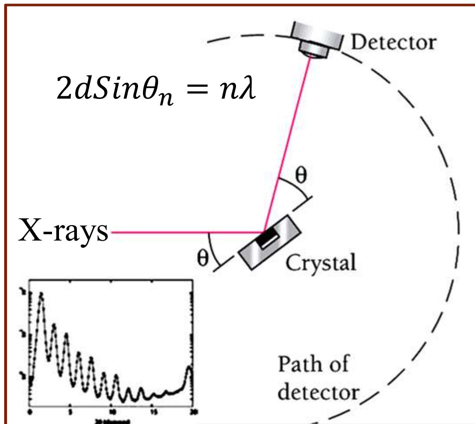
$$2dSin\theta_n = n\lambda$$

$$2dSin\theta_{n+1} = (n+1)\lambda$$

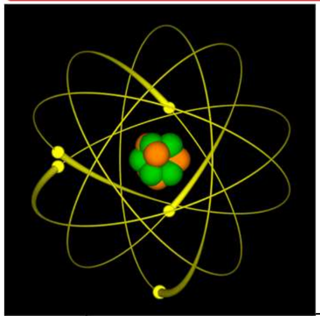
$$2d(Sin\theta_{n+1} - Sin\theta_n) = \lambda$$

$$2 \times 2.15 \times (Sin62° - Sin31°) = \lambda$$

$$\lambda = 0.158 \text{ nm}$$



Origin of quantum mechanics



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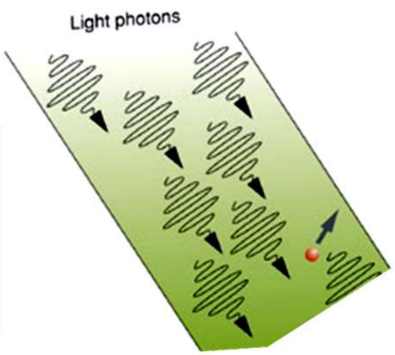
Bohr: Atom's discrete states (1913)

Breakthroughs in science

Einstein: Photon of light (1905)



Davisson, Germer: Wave behavior of electrons (1927)

De Broglie: Dual nature (1923)

Compton: Particle behavior of radiation (1923)

Heisenberg: Uncertainty in measurements (1923)

Breakthroughs in science

Particle-like wave	Plank's quanta
	Photoelectric effect
	Compton scattering
Wave-like particle	Double slit experiment
	Davisson & Germer exp.
	Thomson's gold foil exp.

De Broglie: Dual nature

The wavelength of a particle

de Broglie wavelength

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

Matter waves

Wave-particle duality

The momentum of a wave

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

Breakthroughs in science

De Broglie: Dual nature (1923)

A photon

$E = h\nu$

Planck's quanta

$E = \mathrm{m}c^2$

As a particle of mass 'm'

$$h\nu = \mathrm{m}c^2 = hc/\lambda$$

$$\boldsymbol{\lambda} = h/mc = \boldsymbol{h/p}$$

- *For a cricket ball of mass 160 gm and velocity of 150 km/h is* ***λ=0.98X10^-34 m***.
- *For an electron accelerated by applied potential of 1 volt is* ***λ=1.228 nm.***

Pilot waves

Probability waves

Mechanical waves?

Electromagnetic waves?

Electron in potential V

$$E_K = \frac{1}{2}mv^2 = \frac{p^2}{2m} = eV$$

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

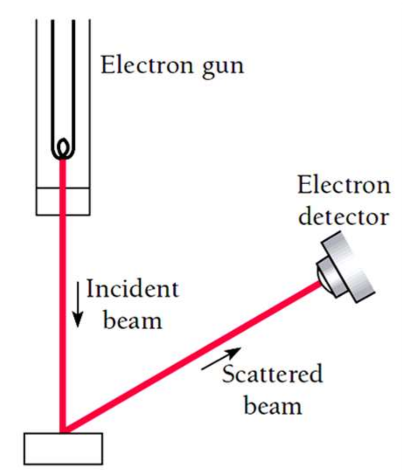
$$p = \sqrt{2meV}$$

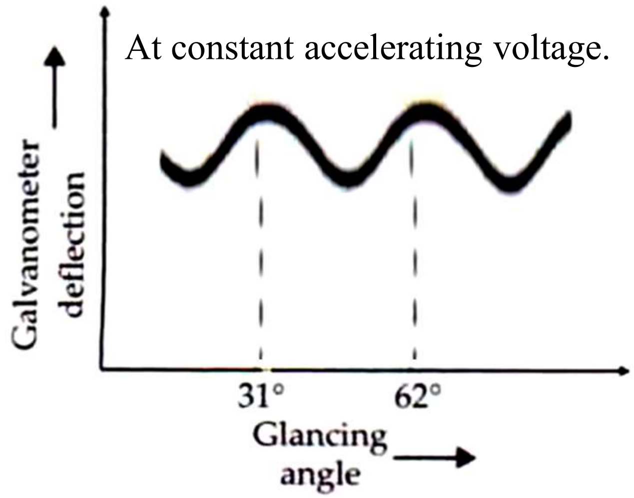
$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}$$

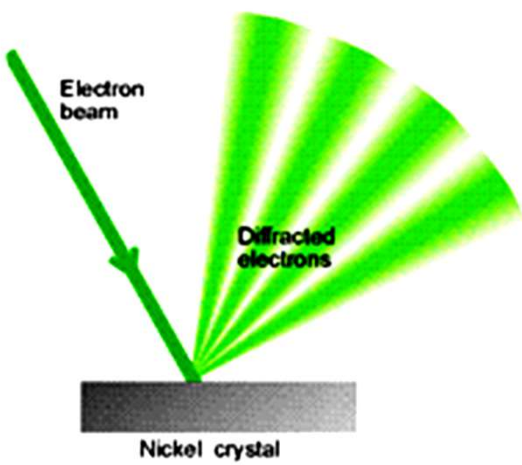
$$\lambda = \frac{1.228}{\sqrt{V}}\ nm$$

Breakthroughs in science

Davisson, Germer: Wave behavior of electrons (1927)







$$2dSin\theta_n = n\lambda$$

$$2dSin\theta_{n+1} = (n+1)\lambda$$

$$2d(Sin\theta_{n+1} - Sin\theta_n) = \lambda$$

$$2 \times 2.15 \times (Sin62° - Sin31°) = \lambda$$

$$\lambda = 0.158 \text{ nm}$$

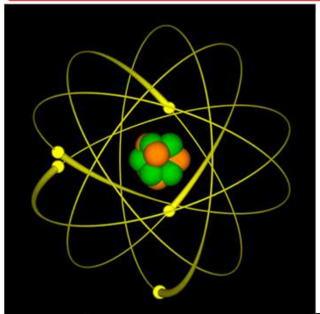
V = 60 V

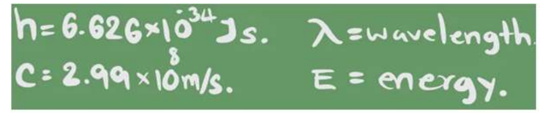
$$\lambda = \frac{1.228}{\sqrt{V}}\ nm$$

$$\lambda = \frac{1.228}{\sqrt{60}}\ nm$$

$$\lambda = 0.155\ nm$$

Origin of quantum mechanics





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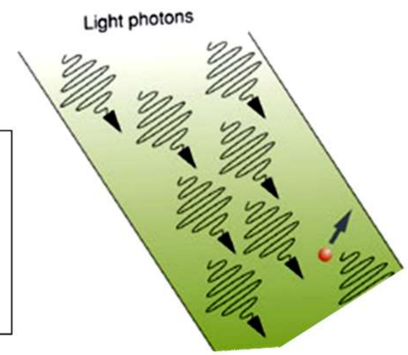

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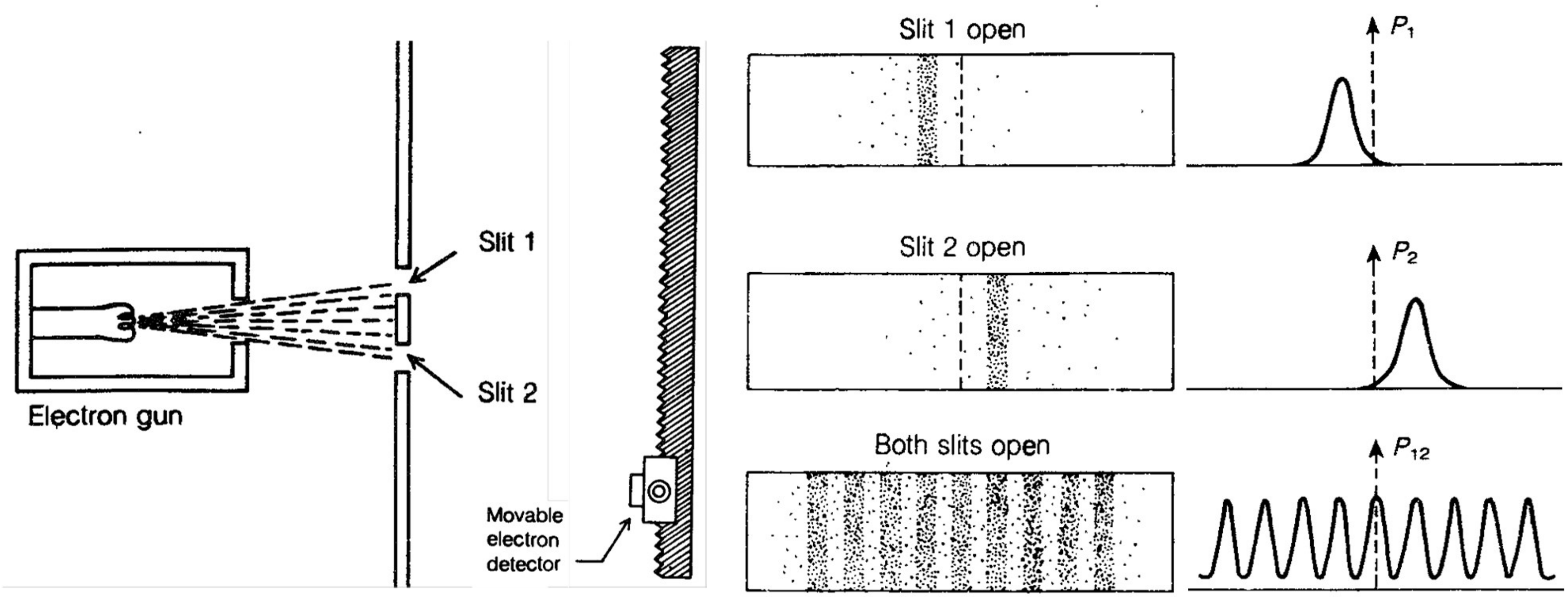
Breakthroughs in science

Heisenberg: Uncertain measurements (1923)

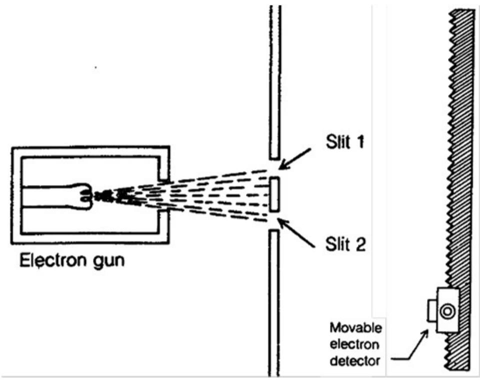


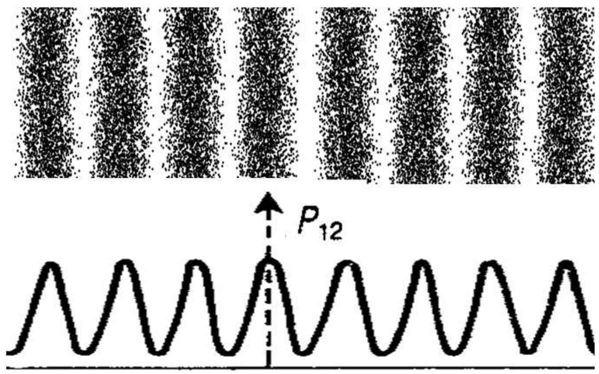
Interference pattern of a wave!

Whether electron is a particle or a wave?

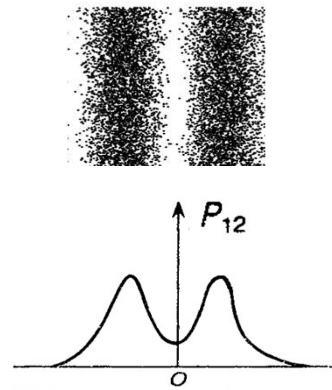
Breakthroughs in science

Heisenberg: Uncertain measurements (1923)

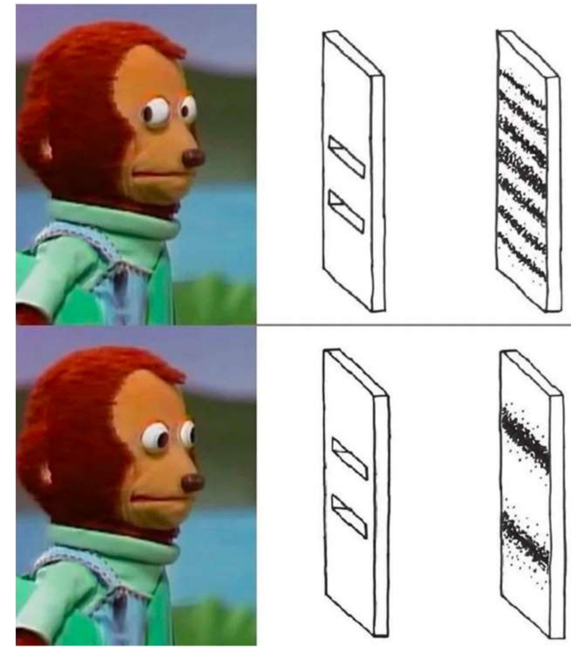




If there is no observer.



If there are observers.

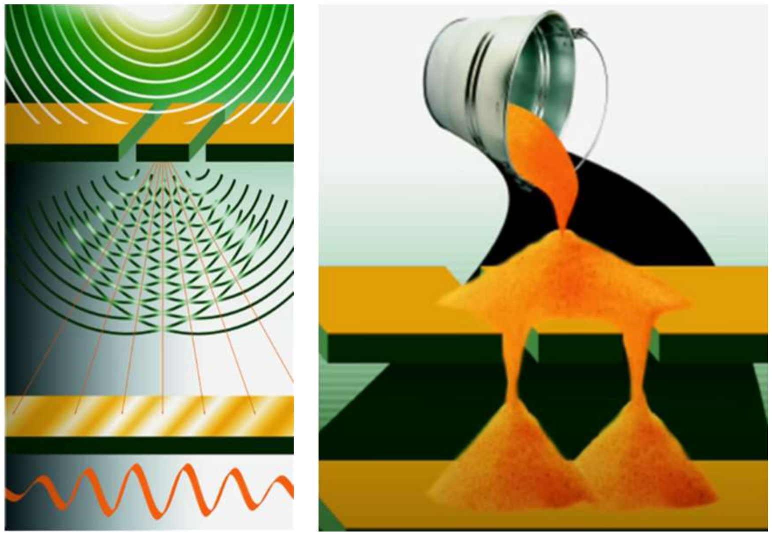


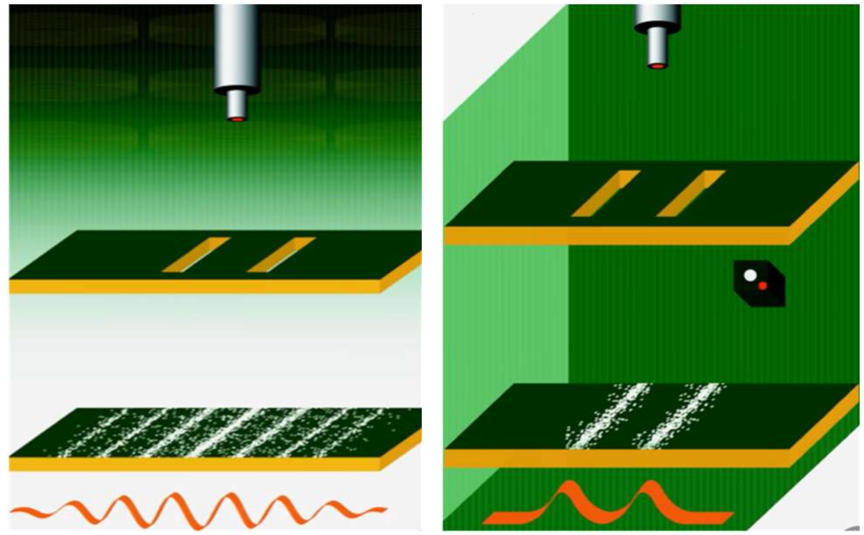
- Somehow, nature knows whether we have the information of which slit the electron passed through.
- If the particle is marked in some fashion, you will not get an interference pattern at the screen.

Does it mean that presence of observers disturbed the outcome?

Breakthroughs in science

Heisenberg: Uncertain measurements (1923)





- Nature behaves one way when you are looking and in a completely different way when you are not looking.
- It seems that when we observe we disturb whatever we are trying to observe.

Heisenberg: Uncertain measurements (1923)

This is a very strange result, since it seems to indicate that the observation plays a decisive role in the event and that reality varies, depending upon whether we observe it or not.
- **Heisenberg**

What does it mean to observe something?

How clearly we can see depends on the wavelength of the illuminating light.

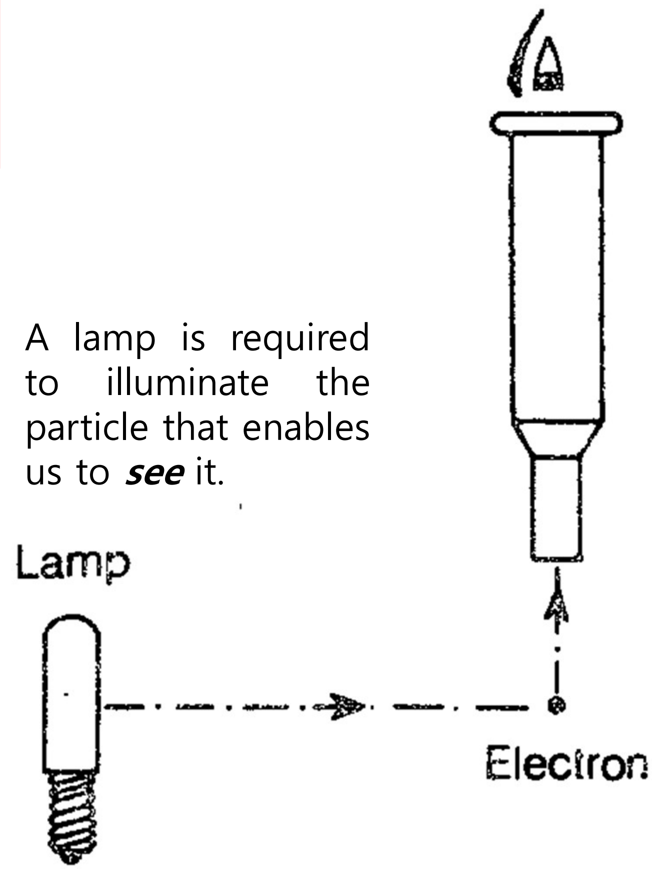
Smaller the wavelength, better is the resolution.

Hence to see the electron, we should use gamma rays (extremely small wavelength).

The light failing on the particle bounces off, and reaches our eye to form an image.

From this image we get idea of particle's position.

A lamp is required to illuminate the particle that enables us to ***see*** it.



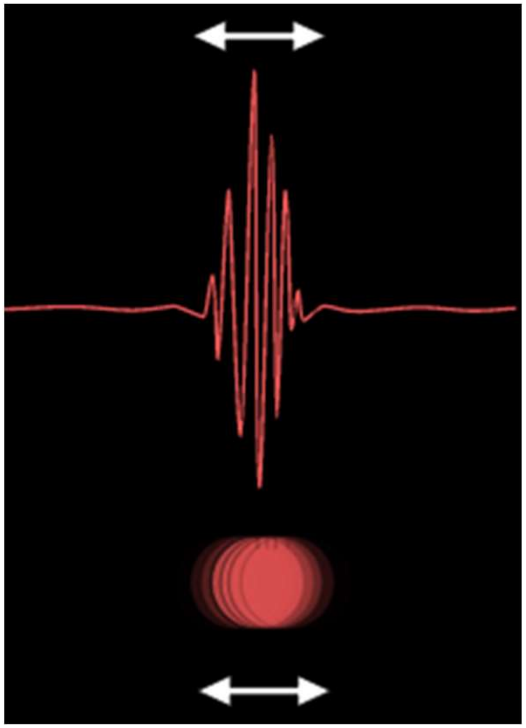
Heisenberg: Uncertain measurements (1923)

The Uncertainty in measurement

There is a serious problem with the gamma-ray microscope.

When we illuminate the electron with gamma rays, we are really bombarding it with a stream of photons, which impart momentum (Compton scattering) and disturb the position of electron.

Thus to measure the position of electron we must illuminate it; but the moment we shine the election it is disturbed and moves away from the position it was originally in.



Heisenberg's conclusion:

One cannot simultaneously measure with infinite precision, both the position and the momentum of a particle.

The Heisenberg Uncertainty Principle

It is impossible to simultaneously describe with absolute accuracy the position and momentum of a particle

$$\Delta p_x . \Delta x \geq \hbar/2$$

It is impossible to simultaneously describe with absolute accuracy the energy of a particle and the instant of time the particle has this energy

$$\Delta E . \Delta t \geq \hbar/2$$

When the Heisenberg uncertainty principle is applied to electrons it states that we can not determine the exact position of an electron. Instead, we could determine the probability of finding an electron at a particular position.

$$\Delta p_x . \Delta x \geq \hbar/2$$
$$\Delta p_y . \Delta x = 0$$
$$\Delta p_z . \Delta x = 0$$

$$\Delta p_x . \Delta y = 0$$
$$\Delta p_y . \Delta y \geq \hbar/2$$
$$\Delta p_z . \Delta y = 0$$

$$\Delta p_x . \Delta z = 0$$
$$\Delta p_y . \Delta z = 0$$
$$\Delta p_z . \Delta z \geq \hbar/2$$

<u>Conjugate pairs</u>

☼Heisenberg's uncertainty principle is true for **<u>conjugate pairs</u>** only.

Predictions or results of uncertainty principle:

1. Nonexistence of free electron in nucleus
2. Estimate of radius of Bohr's first orbit
3. Zero point energy of simple harmonic oscillators

Predictions or results of uncertainty principle:

1. Nonexistence of free electron in nucleus

According to theory of relativity, energy of a particle is given by the relation

$$E^2 = p^2c^2 + m_0^2c^4$$

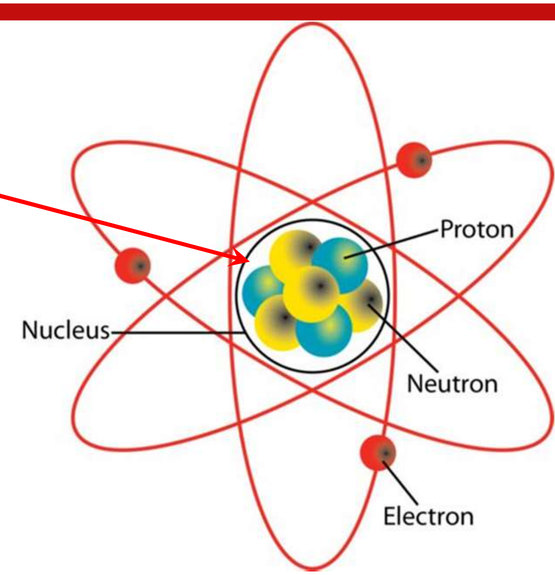
$$E_{min}^2 = p_{min}^2c^2 + m_0^2c^4$$

$$E_{min} = 3.165 \times 10^{-12}\, J$$

$$E_{min} = \frac{3.165 \times 10^{-12}\, J}{1.6 \times 10^{-1}\quad C} = 19.78\, MeV$$

- Thus, if a free electron exists in the nucleus it must have a minimum energy of about 20 MeV.
- The maximum K.E. of a β-particle, emitted from radioactive nuclei is of the order of 4 MeV.

Diameter of nucleus
~10^{-14} m



Maximum uncertainty in position of electron, if it is inside the nucleus:

$\Delta x_{max} = 10^{-14}$ m

Minimum uncertainty in momentum of electron, if it is inside the nucleus:

$$\Delta p_x . \Delta x \geq \hbar$$

$\Delta p_{min} = \hbar / \Delta x$ $\quad \Delta p_{min} = 1.055 \times 10^{-34}\, Js/10^{-14}$ m

$\Delta p_{min} = 1.055 \times 10^{-20}\, kg\, m/s$

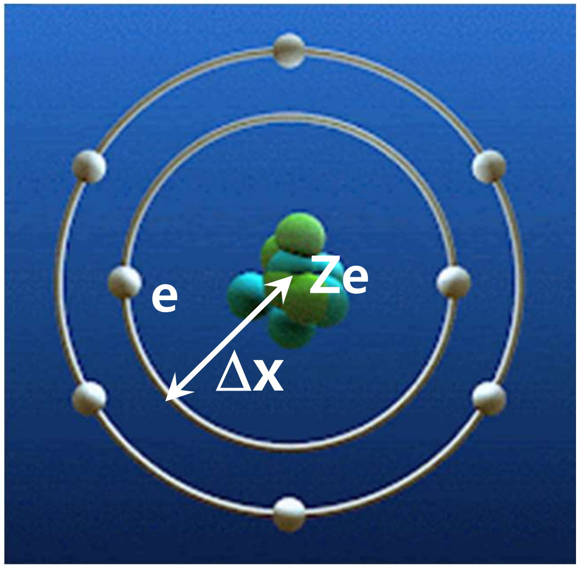
$p_{min} = 1.055 \times 10^{-20}\, kg\, m/s$

$m_0 = 9.1 \times 10^{-31}\, kg$

Therefore electrons cannot be present within the nucleus.

Predictions or results of uncertainty principle:

2. Estimate of radius of Bohr's first orbit



Kinetic energy of electron $K = \dfrac{p^2}{2m}$ $\qquad \Delta K = \dfrac{(\Delta p)^2}{2m} = \dfrac{\hbar^2}{2m(\Delta x)^2}$

$\Delta p_x . \Delta x \geq \hbar$

$\Delta p_x = \dfrac{\hbar}{\Delta x}$

Potential energy of electron $V = \dfrac{(Ze)(-e)}{4\pi\varepsilon_0\, x}$ $\qquad \Delta V = \dfrac{(Ze)(-e)}{4\pi\varepsilon_0\, \Delta x}$

Uncertainty in total energy of electron $\Delta E = \dfrac{\hbar^2}{2m(\Delta x)^2} - \dfrac{Ze^2}{4\pi\varepsilon_0\, \Delta x}$

Uncertainty in total energy of electron will be minimum if $\dfrac{\partial(\Delta E)}{\partial(\Delta x)} = 0$

$$-\frac{\hbar^2}{m(\Delta x)^3} + \frac{Ze^2}{4\pi\varepsilon_0(\Delta x)^2} = 0 \qquad \Delta x = \frac{4\pi\varepsilon_0\hbar^2}{mZe^2} \qquad \Delta x = \frac{\varepsilon_0 h^2}{\pi m Z e^2}$$

Bohr's first orbit

Predictions or results of uncertainty principle:

3. Zero point energy of simple harmonic oscillators

Total energy of oscillator at displacement x

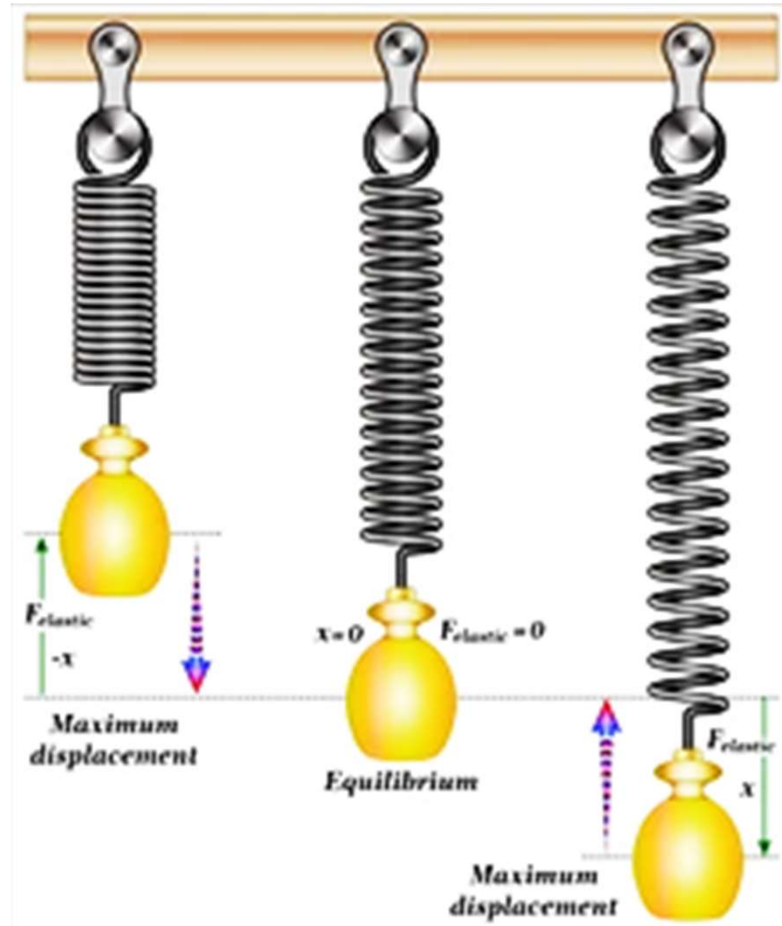
$$E = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$$

$x_{max} = a$ $\quad (\Delta x)_{max} = 2a \quad (\Delta p_x)_{mi} = \frac{\hbar}{2a}$

$$p_{mi} = \frac{\hbar}{2a}$$

$$E = K_{min} + V_{max} = \frac{p_{min}^2}{2m} + \frac{m\omega^2 x_{max}^2}{2} = \frac{\hbar^2}{8ma^2} + \frac{m\omega^2 a^2}{2}$$

Value of 'a' at which total energy is minimum?
Is it 0?



Predictions or results of uncertainty principle:

3. Zero point energy of simple harmonic oscillators

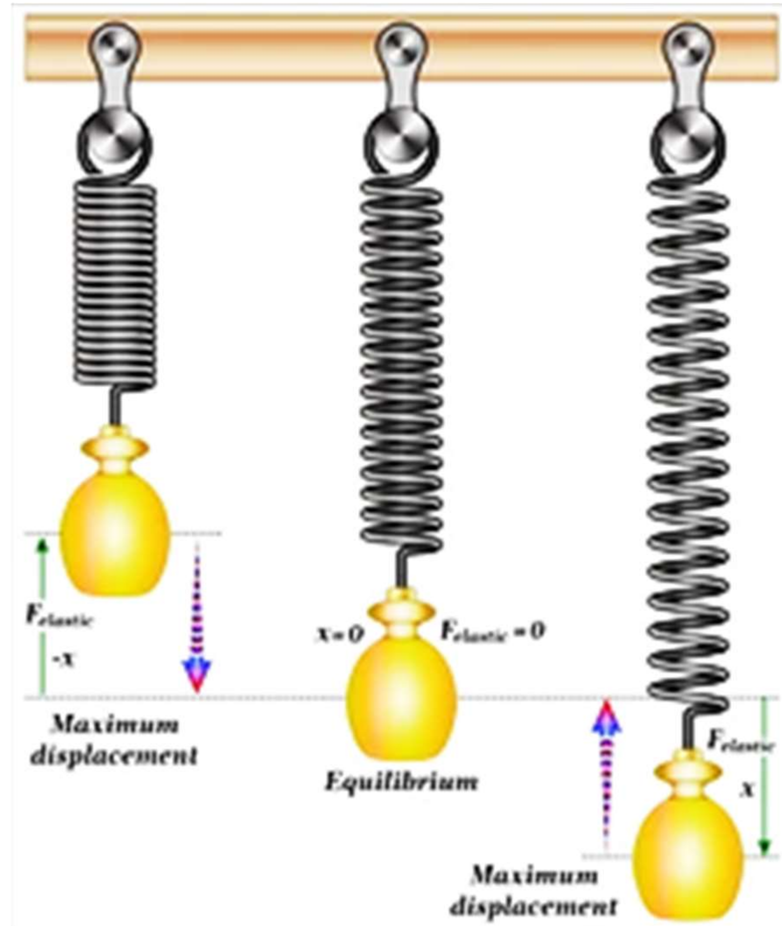
$$E = \frac{\hbar^2}{8ma^2} + \frac{m\omega^2 a^2}{2}$$

Let at a='A' at which total energy is minimum?

$$\left(\frac{\partial E}{\partial a}\right)_{a=A} = 0 \qquad \rightarrow A^2 = \frac{\hbar}{2m\omega}$$

$$E = \frac{\hbar^2 2m\omega}{8m\hbar} + \frac{m\omega^2}{2}\frac{\hbar}{2m\omega}$$

$$E = \frac{1}{2}\hbar\omega = \frac{1}{2}h\nu$$



Dual nature and uncertainty principle

1. Find the de Broglie wavelengths of (*a*) a 46-g golf ball with a velocity of 30 m/s, and (*b*) an electron with a velocity of 10^7 m/s.
2. Calculate the de-Broglie wavelength associated with proton of kinetic energy 100 eV. (Mass of proton = 1.6725×10^{-27} kg).
3. Thermal speed of hydrogen molecule at 0° C is ~ 1.84×10^3 m/s. Find its de-Broglie wavelength.
4. Call a photon and an electron of the same energy have the same wavelength?
5. Calculate the de-Broglie wavelength of (a) an electron accelerated by a potential difference of 10,000 V; and (b) an electron moving with a velocity of 0.01 c, where c is the speed of light.
6. Find the momentum of a proton whose de Broglie wavelength is 1 fm.
7. An electron has a de-Broglie wavelength of 4 pm. Find its kinetic energy and velocity.

Given h =6.63×10^{-34} Js

Dual nature and uncertainty principle

8. An electron initially at rest is accelerated through a potential difference of 4900 V. Compute its (i) momentum, (ii) the de-Broglie wavelength, and (iii) the magnitude of wave propagation vector of the electron.
9. The average period that takes between the excitation of an atom and the time it radiates is 10^{-8} s. Find the width of excited energy level of the atom.
10. The speed of an electron revolving around the nucleus in K-cell is of the order of 3×10^6 m/s. Find the smallest possible uncertainty in position of this electron.
11. A microscope, using photons, is employed to locate an electron in an atom within a distance of 0.02 nm. What is the uncertainty in the momentum of the electron located in this way?
12. Show that if the uncertainty in the location of the particle is equal to de-Broglie wavelength the uncertainty in its velocity is equal to its velocity.

Given $h = 6.63 \times 10^{-34}$ Js

Formulating

Quantum mechanics

Formulation of Quantum mechanics

Dual nature of matter $\lambda = \frac{h}{p}$ *Matter waves*

Uncertainty Principle $\Delta p_x . \Delta x \geq \hbar/2$

How will you define a system?

State of a system is not defined classically but it requires a mathematical expression named as **wave function $\boldsymbol{\psi(r, t)}$**.

We shell call this state of a system, the **quantum state**. It is so formulated that all information about the system is contained in ψ.

Any variation in property/behaviour of the system will be reflected in ψ.

Formulation of Quantum mechanics

Wave function

While ψ itself has no physical interpretation, its square $\boldsymbol{\psi^2}$ at a particular place at any time is the **probability of finding** the particle there at that time.

The problem of quantum mechanics is to determine ψ for a body when its motion is limited by the action of external forces.

Probability cannot be negative

Quantum physics is probabilistic in nature.

- ψ may be any function, real or complex, akin to the behavior of the real physical system.

If ψ is a complex function then $\boldsymbol{\psi^2 = \psi^*\psi}$

$\boldsymbol{\psi^*}$ is complex conjugate of $\boldsymbol{\psi}$

Formulation of Quantum mechanics

$\psi \rightarrow 0$

at r = ∞.

ψ
Finite,
continuous,
Single valued

well behaved wave function

$d\psi/dr$
Finite,
continuous,
Single valued

$$\int_{-\infty}^{+\infty} \psi^2 dV = 1$$

Normalization

Formulation of Quantum mechanics

Extraction of information

- Applying certain operations/instruction on wave function ψ, information/observable can be extracted.
- These ***information specific*** operations are called the **operator** for a given observable.

$$\boxed{\hat{p}_x \equiv \left(-i\hbar\frac{\partial}{\partial x}\right),\ \hat{E} \equiv \left(i\hbar\frac{\partial}{\partial t}\right)}$$

How to use an operator

Eigen value equation $\hat{O}\,\psi(r,t) = O.\psi(r,t)$

Average measurement

expectation value

$$\int_{-\infty}^{+\infty} \psi^* \hat{O} \psi dV$$

Formulation Quantum mechanics

Construction of wave function

Schrodinger equation

A basic physical principle that cannot be derived from anything else

It is a basic principle in itself

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

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

Postulates of quantum mechanics

Set rules to find the solution of the problem in quantum mechanics.

Postulates 1: State of a physical system: Wave function

Postulates 2: Operator corresponding to a classical observable

$$\boxed{\hat{p}_x \equiv \left(-i\hbar\frac{\partial}{\partial x}\right),\ \hat{E} \equiv \left(i\hbar\frac{\partial}{\partial t}\right)}$$

Postulates 3: Measurement of physical quantity: eigen value equation

$$\hat{O}\,\psi(r,t) = O.\psi(r,t)$$

Postulates 4: Probabilistic measurement: expectation value

$$\boxed{\int_{-\infty}^{+\infty} \psi^* \hat{O} \psi dV}$$

Postulates 5: Evolution of wave function (The Schrodinger equation)

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

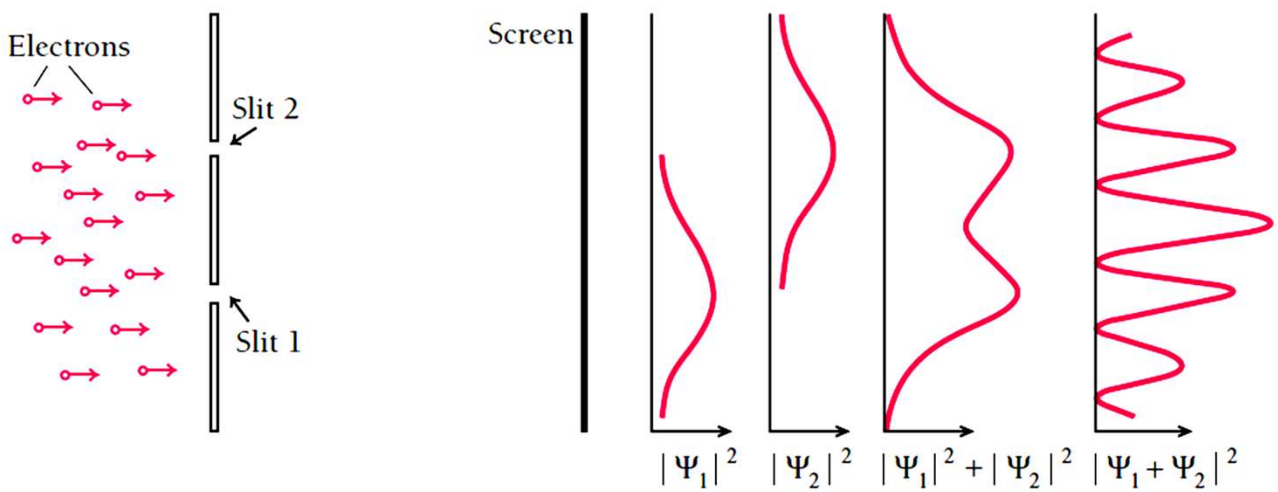
Formulation of Quantum mechanics

Wave function

Schrodinger equation may have a number of solutions as the wave function. Which solution is of our use?

Superposition is the characteristic property of the waves so as of a wave function of the quantum state of a quantum system.

A linear combination of solutions of Schrödinger's equation for a given system is also a solution!



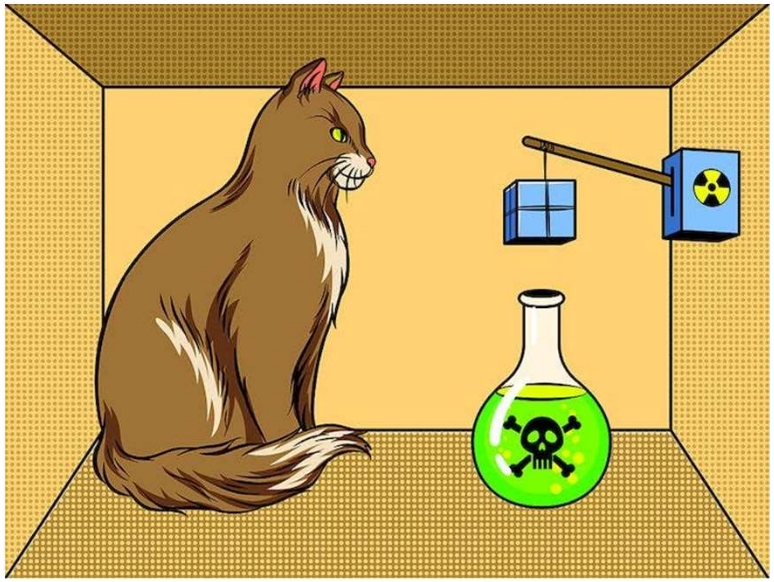
$$\psi = a\psi_1 + b\psi_2$$

It is wave function, not the probability, which add.

Formulation of Quantum mechanics

Superposition of Wave function

Schrodinger's cat



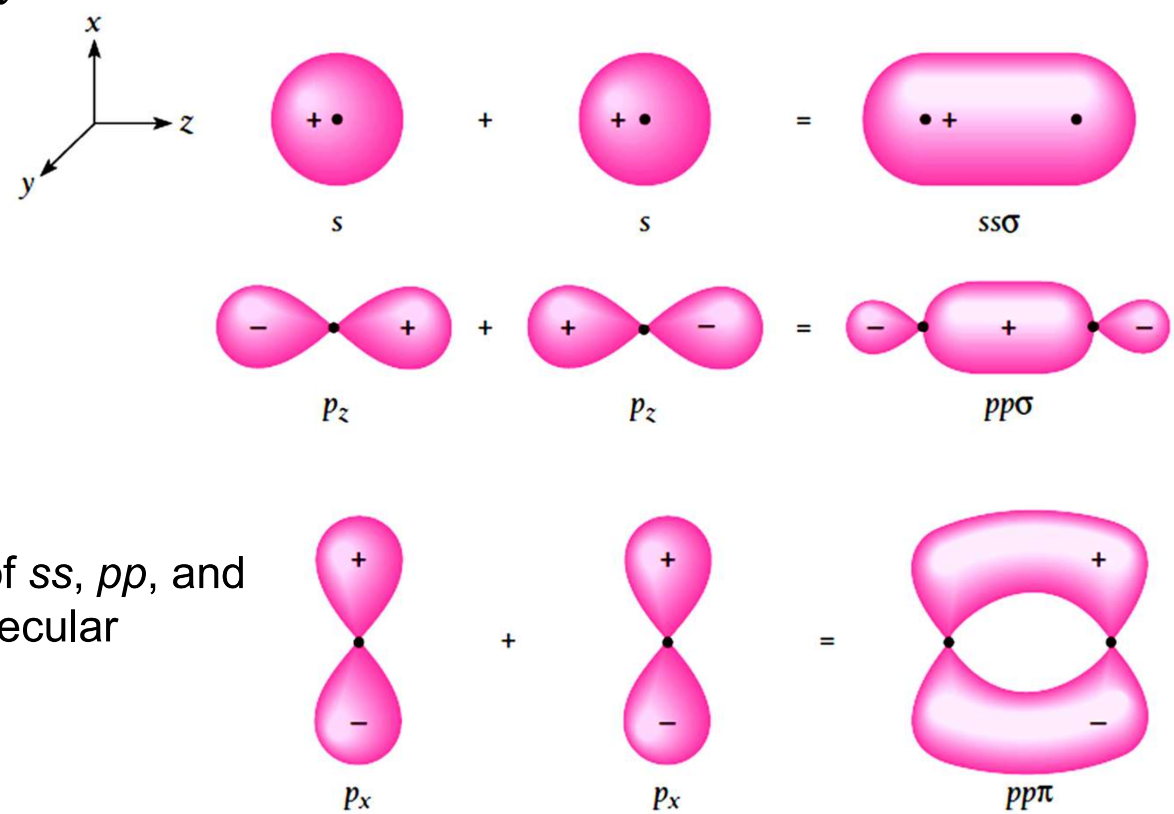
$$\psi_{cat} = a\psi_{cat}^{alive} + b\psi_{cat}^{dead}$$

On opening the box ψ_{cat} will collapse to either ψ_{cat}^{alive} or ψ_{cat}^{dead}.

Quantum mechanics: **Application**

Superposition of Wave function

linear combination of solutions of Schrödinger's equation for a given system is also a solution!



The formation of *ss*, *pp*, and *pp* bonding molecular orbitals.

Quantum mechanics: **Application**

Superposition of Wave function

For an electron there are two quantum states, i.e., spin-up and spin-down states represented by $\psi^{\downarrow}$ and $\psi^{\uparrow}$.

For electron A $\quad \psi_A^{\uparrow}$ and $\psi_A^{\downarrow}$

For electron B $\quad \psi_B^{\uparrow}$ and $\psi_B^{\downarrow}$

for the requirement of Pauli exclusion principle.

For the combination the quantum state will be the linear combination:

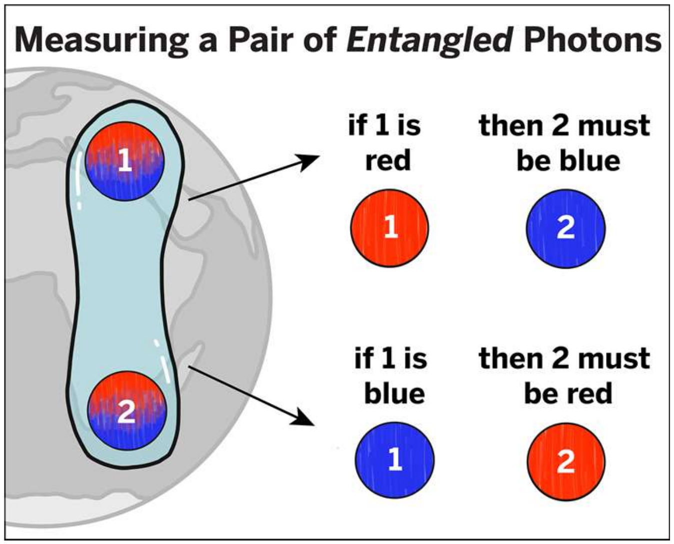
$$\psi_{AB} = \frac{1}{\sqrt{2}}\left(\psi_A^{\uparrow}\psi_B^{\downarrow} \pm \psi_A^{\downarrow}\psi_B^{\uparrow}\right)$$

Entangled-state of two quantum particles

These two electrons are related with each other via some condition, they are entangled.

Quantum mechanics: Quantum Entanglement

Spooky Science



Quantum entanglement is the phenomenon of a group of particles being generated, interacting, or sharing spatial proximity in such a way that the quantum state of each particle of the group cannot be described independently, including when the particles are separated by a large distance.

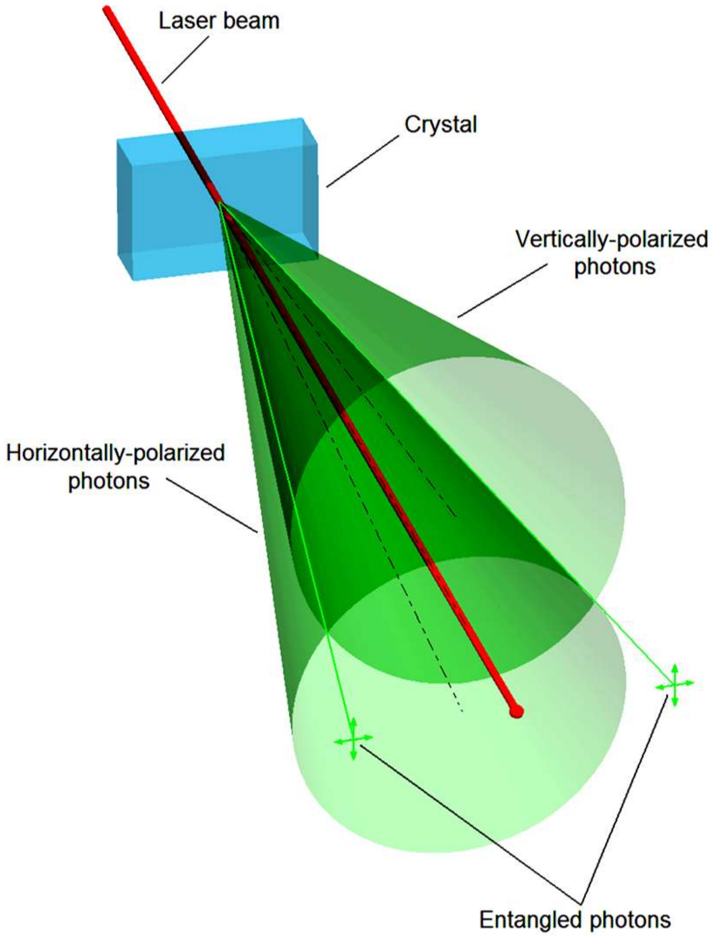
Key Characteristics:

Non-locality: Particles seem "connected" over large distances.

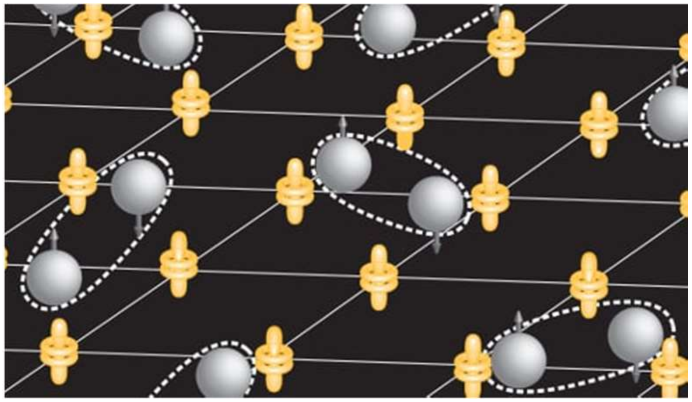
Quantum Correlation: Measurement of one particle affects the state of the other.

Quantum mechanics: Quantum Entanglement

Entangled State of Two Particles: Where can I find them?



- **Superconductors:** Cooper pair.
- **Superconducting qubits:** IBM's or Google's quantum computers.
- **Trapped Ions or Atoms:** Using electromagnetic traps, individual ions or atoms can be entangled by controlled laser interactions.
- **Beam Splitters:** Entangled photon pairs can also be generated using beam splitters and polarizers.



Quantum mechanics: Quantum Entanglement

Entangled vs. Non-Entangled

Aspect	Entangled State	Non-Entangled State
Definition	Quantum correlation between particles.	Particles behave independently.
Mathematical Form	Cannot be separated into individual particle states.	Can be written as a product of states.
Measurement Effect	Measurement of one instantly affects the other.	Measurement of one does not affect the other.

1. **Quantum Cryptography**: Secure communication via Quantum Key Distribution (QKD).
2. **Quantum Computing**: Entangled qubits perform computations faster than classical bits.
3. **Quantum Teleportation**: Transfer quantum states over large distances.
4. **Quantum Networking**: Basis for a future quantum internet.

Quantum mechanics: **Application**

1) <u>Free particle</u>

- Unrestricted particle that may have any energy.
- Unrestricted particle that may be anywhere in space.
- A wave is associated with particle.

Wave function

No restriction = no force = no potential

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

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

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0$$

Since k may have any value

The particle may have continuous energy.

$\psi(x) = Ae^{i(kx)}$ or $Be^{-i(kx)}$

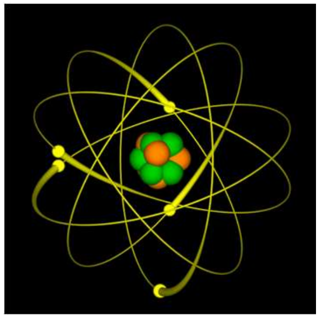
There is no discreetness in behavior of free particle.

Lets introduce restriction in motion.

Quantum mechanics: **Application**

2) Particle in a box

Particle's motion is restricted



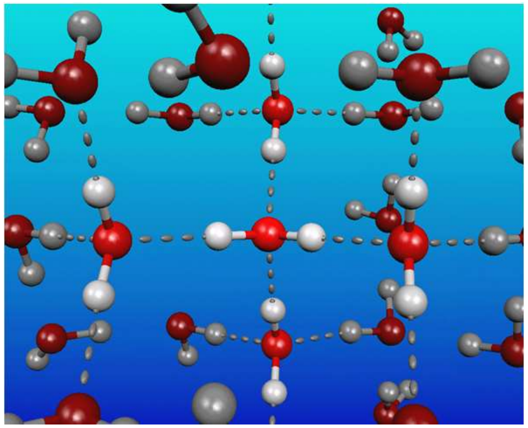
Electrons in Atoms

Electrons in Atoms: Electrons are often modeled as particles in a box when considering their behavior in atoms. The potential well created by the nucleus confines the electrons, leading to quantized energy levels.

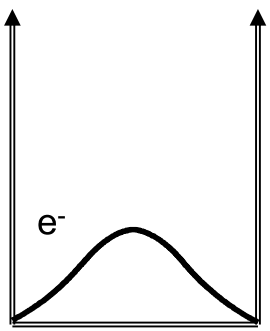
Quantum Dots: These are semiconductor particles that confine electrons in three dimensions, effectively creating a "box" for the electrons. The size of the quantum dot determines the energy levels and the properties of the material, which can be used in applications like lasers and displays.

Molecular Vibration: The atoms in a molecule can be thought of as confined to specific vibrational energy levels, leading to quantized vibrational states.

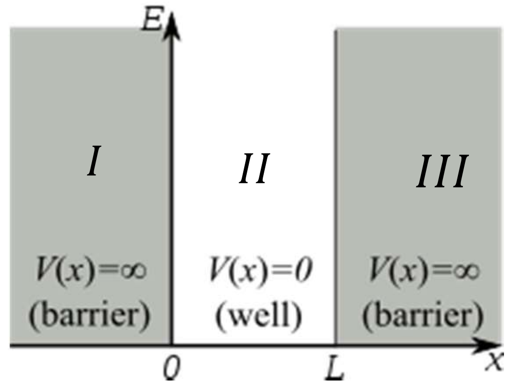
Optical Cavities: In lasers, light can be confined in a cavity, leading to quantized modes of light. The behavior of photons in these cavities can be analogous to particles in a box.



2) Particle in a box



$$\psi_I(x) = 0$$
$$\psi_{III}(x) = 0$$



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

$$\psi_{II}(x) \neq 0$$

Boundary conditions

$$\psi_{x=0} = 0$$

$$\psi_{x=L} = 0$$

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

$$\int_{-\infty}^{0} |\psi_I(x)|^2 dx + \int_{0}^{L} |\psi_{II}(x)|^2 dx + \int_{L}^{+\infty} |\psi_{III}(x)|^2 dx = 1$$

$$\int_{x=0}^{x=L} |\psi_{II}(x)|^2 dx = 1$$

2) Particle in a box

$$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2mE}{\hbar^2}\psi(x)=0$$

$$\frac{\partial^2\psi_{II}(x)}{\partial x^2}+k^2\psi_{II}(x)=0$$

$$k^2=\frac{2mE}{\hbar^2} \qquad E=\frac{\hbar^2k^2}{2m}$$

$$\psi_{II}(x)=A.Sin(kx)+B.Cos(kx)$$

$$\psi_{x=0}=0=0+B$$

$$\psi_{x=L}=0=A.Sin(kL)$$

$$Sin(kL)=Sin(n\pi) \qquad k=\frac{n\pi}{L},\ \ n=0,\pm1,\pm2,\ldots$$

- But if n=0, $\psi_{II}=0$ $\qquad n=\pm1,\pm2,\ldots$

$$\psi_{II}(x)=ASin\left(\frac{n\pi x}{L}\right)$$

$$\psi_n(x)=ASin\left(\frac{n\pi x}{L}\right)$$

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

$$\boxed{E\neq0}$$

2) Particle in a box

$$\psi_n(x) = ASin\left(\frac{n\pi x}{L}\right)$$

$$\int_{x=0}^{x=L} |\psi_{II}(x)|^2 dx = 1$$

$$\int_{x=0}^{x=L} \left|ASin\left(\frac{n\pi x}{L}\right)\right|^2 dx = 1$$

$$\frac{A^2}{2}\int_{x=0}^{x=L} \left[1 - Cos\left(\frac{2n\pi x}{L}\right)\right] dx = 1$$

$$\frac{A^2}{2}\left[x - \frac{L}{2n\pi} Sin\left(\frac{2n\pi x}{L}\right)\right]_0^L = 1$$

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

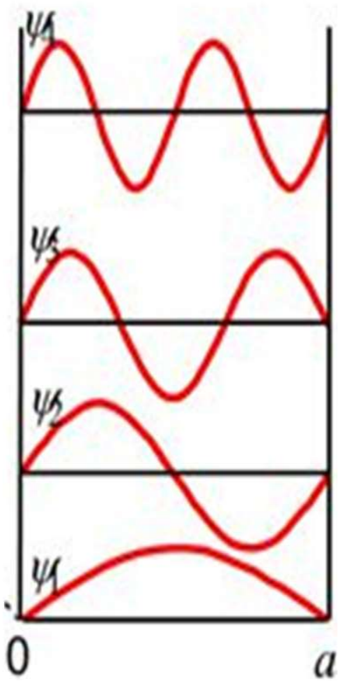
$$A = \sqrt{\frac{2}{L}}$$

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

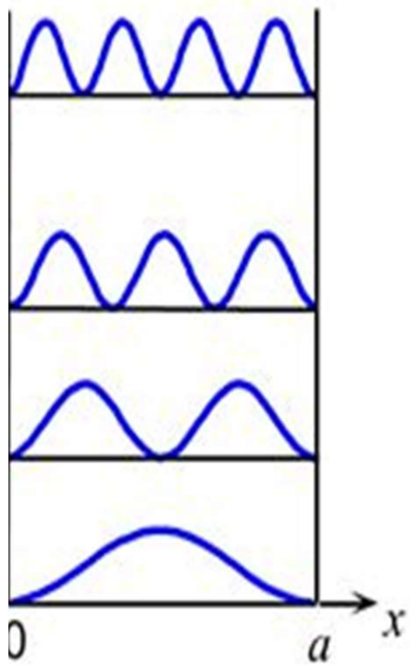
$$\boxed{E = \frac{\hbar^2\pi^2}{2mL^2} n^2}$$

2) Particle in a box

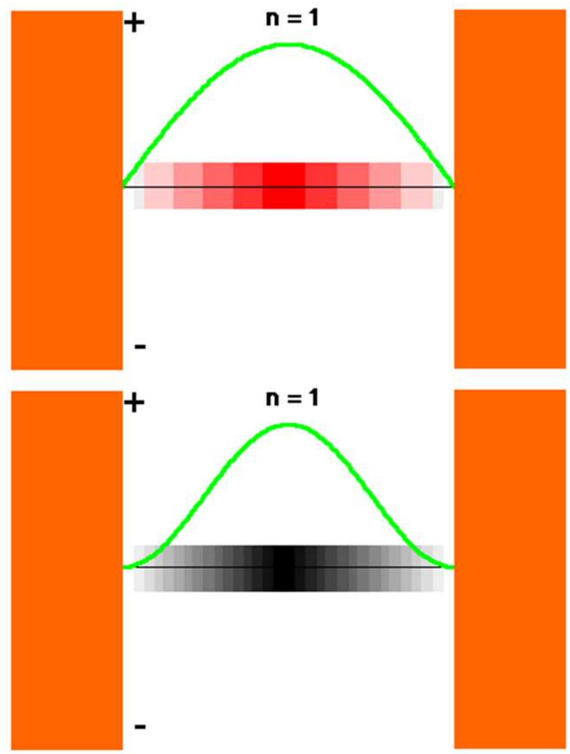
$$\psi_n(x,t) = \sqrt{\frac{2}{L}}\, Sin\left(\frac{n\pi x}{L}\right) \qquad E_n = \left(\frac{\hbar^2\pi^2}{2mL^2}\right)n^2 \quad n = 1,2,3,4,\ldots..$$



Wave functions



Probabilities



Zero point energy of a bound particle

Why not n = 0???

1. If a particle has zero energy, it will be at rest inside the well violating Heisenberg's uncertainty principle.

2. Confinement of the particle to a limited region in space requires: i.e., $\Delta x_{\mathbf{maximum}} \sim L$ which leads to $\Delta p_{\mathbf{minimum}} \sim h/2L$, causing **minimum** kinetic energy of the system $E = \frac{\hbar^2\pi^2}{2mL^2}$.

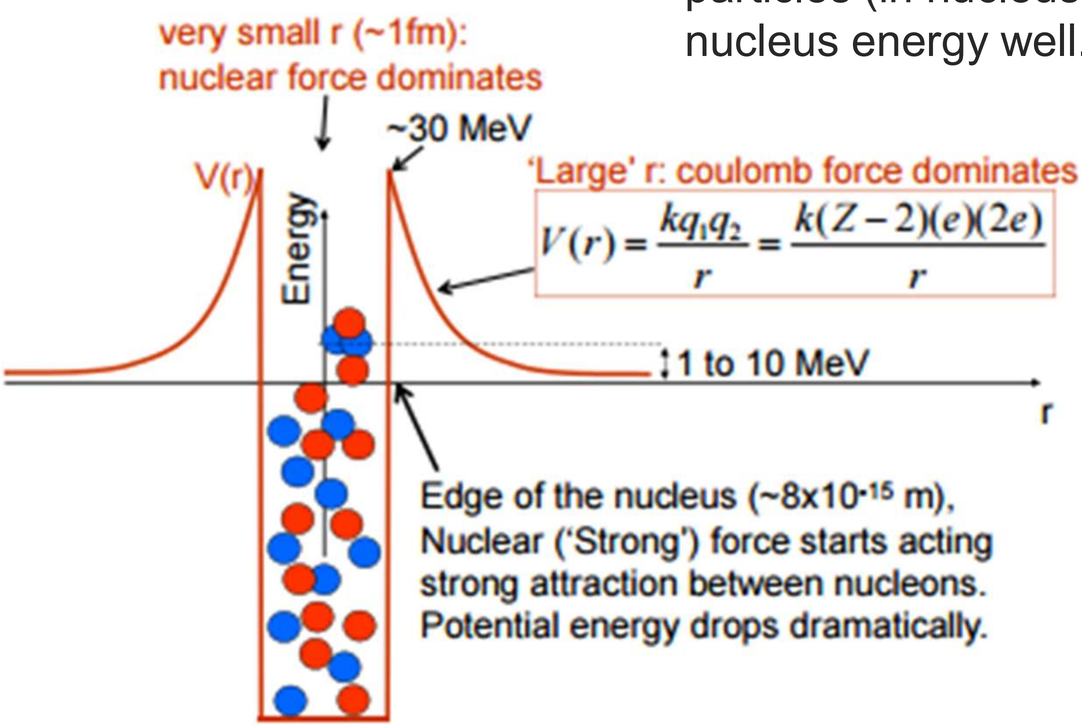
The zero-point energy reflects the **necessity of a minimum motion** of a particle due to localization.
The zero-point energy occurs in all bound state potentials.

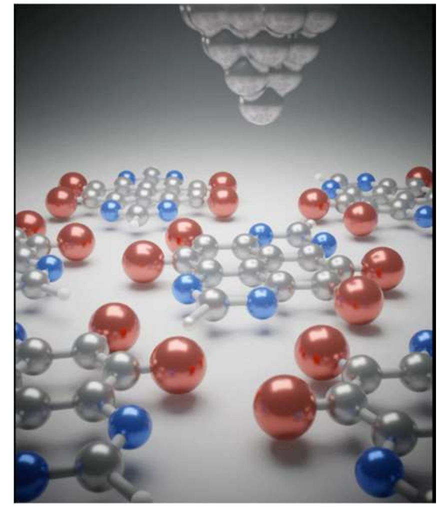
Physical consequences in microscopic world
Without zero-point motion, atoms would not be stable, for the electrons would fall into the nuclei.
Zero-point energy prevents helium from freezing at very low temperatures.

Quantum mechanics: **Application**

3) Particle encountering a potential barrier

•**Radioactive decay:** Heisenberg Uncertainty results in the probability of particles (in nucleus) coming outside the nucleus energy well.

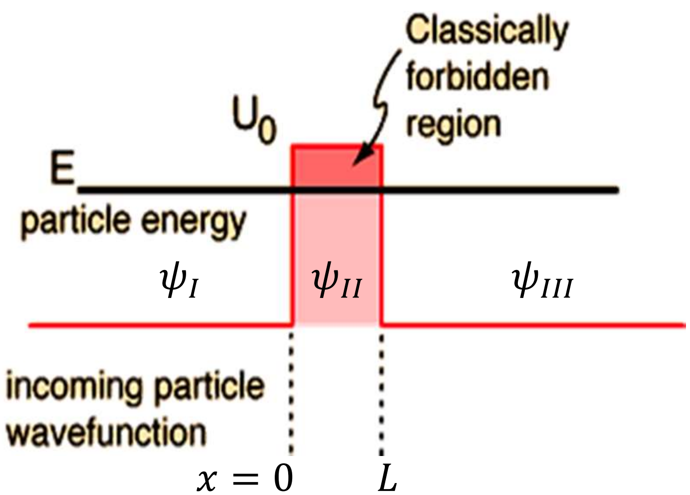




Semiconductors: Tunneling is essential in tunnel diodes and transistors.

- **Nuclear Fusion**: Tunneling allows particles to overcome repulsive forces in nuclear reactions.
- **Scanning Tunneling Microscopy (STM)**: Utilizes tunneling to image surfaces at the atomic level.

3) Particle encountering a potential barrier



$$\boldsymbol{V} = \begin{cases} 0 & x \le 0 \\ U_0 & 0 < x < L \\ 0 & x \ge L \end{cases}$$

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

$$\frac{\partial^2 \psi_I(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi_I(x) = 0$$

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} + \frac{2m(E-U_0)}{\hbar^2}\psi_{II}(x) = 0$$

$$\frac{\partial^2 \psi_{III}(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi_{III}(x) = 0$$

$$k_1^2 = \frac{2mE}{\hbar^2}, \qquad k_2^2 = \frac{2m(U_0-E)}{\hbar^2}$$

3) <u>Particle encountering a potential barrier</u>

$$\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\frac{\partial^2\psi_I(x)}{\partial x^2} + k_1^2\psi_I(x) = 0$$

$$\psi_{II} = Ce^{k_2x} + De^{-k_2x}$$

$$\frac{\partial^2\psi_{II}(x)}{\partial x^2} - k_2^2\psi_{II}(x) = 0$$

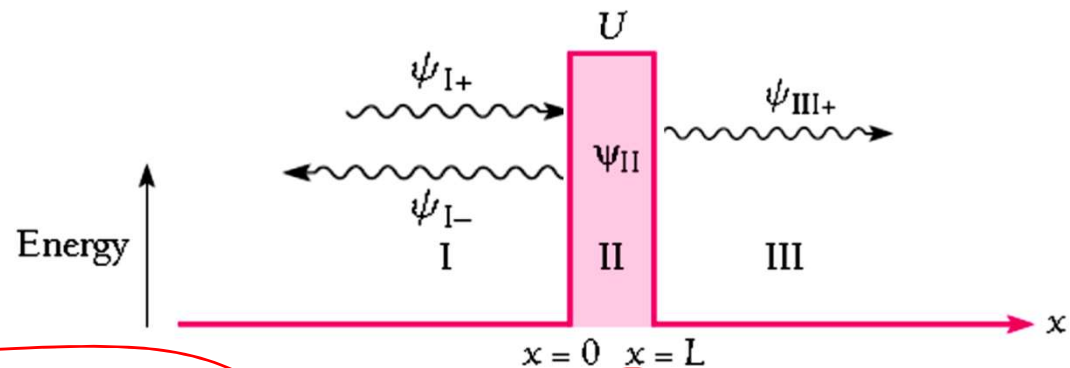
$$\psi_{III} = Fe^{ik_1x} + Ge^{-ik_1x}$$

$$\frac{\partial^2\psi_{III}(x)}{\partial x^2} + k_1^2\psi_{III}(x) = 0$$

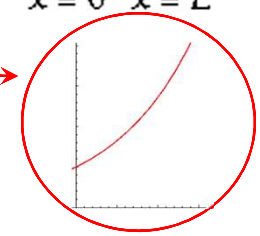
$$k_1^2 = \frac{2mE}{\hbar^2}, \quad k_2^2 = \frac{2m(U_0 - E)}{\hbar^2}$$

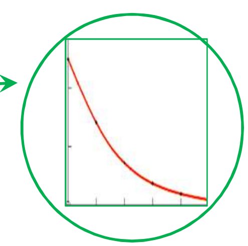
3) Particle encountering a potential barrier

$$\psi_I = \underbrace{Ae^{ik_1x}}_{\psi_{I+}} + \underbrace{Be^{-ik_1x}}_{\psi_{I-}}$$



$$\psi_{II} = \cancel{Ce^{k_2x}} + De^{-k_2x}$$





$$\psi_{III} = \underbrace{Fe^{ik_1x}}_{\psi_{III+}} + \underbrace{\cancel{Ge^{-ik_1x}}}_{\psi_{III-}}$$

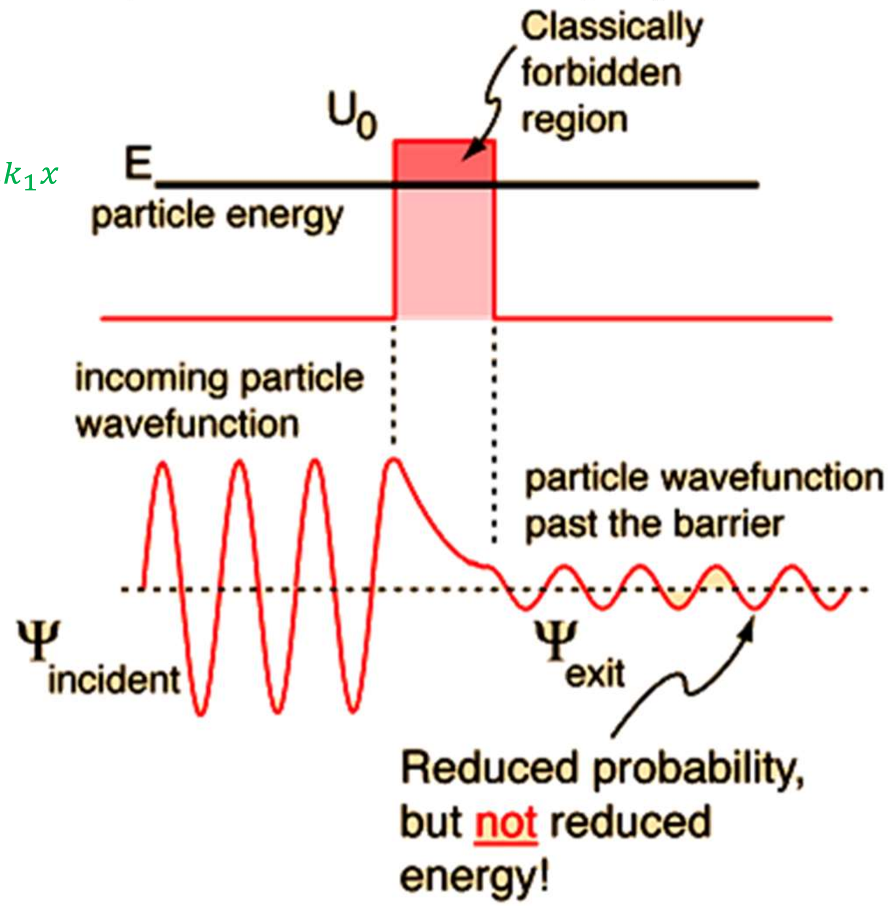
Quantum mechanics: **Application**

3) Particle encountering a potential barrier

$\psi_i = Ae^{ik_1x} + Be^{-ik_1x}$

$\psi_b = De^{-k_2x}$

$\psi_o = Fe^{ik_1x}$



Quantum mechanical tunneling

$$T = 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right)e^{-2k_2L}$$

$$T \approx e^{-2k_2L}$$

$$k_2 = \frac{1}{\hbar}\sqrt{2m(U_0 - E)}$$

1. Is ψ a well behaved wavefunction if

(a) $\psi = A\ Sinx$, (b) $\psi = N\ Tanx$,

(c) $\psi = B\ \exp(kx)$, (d) $\psi = A\ \exp(ikx)$,

(e) $\psi = A\ Sinx + B\ \exp(ikx)$?

2. Is $\psi = A\ Sin(k_1 x)Sin(k_2 y)Sin(k_3 z)$ an eigenfunction of Laplacian operator? If yes find the eigenvalue of the operator.

3. Find the uncertainty in momentum of a particle for which $\psi(x,t) = A\exp[i(ax - bt)]$. Uncertainty in momentum is given by $\Delta p_x = \sqrt{\langle p_x^2\rangle - \langle p_x\rangle^2}$.

4. A particle limited to the x axis has the wave function ψ=ax between x=0 and x=1; ψ=0 elsewhere. Normalize the wave function. (i) Find probability to find the particle between x =0.45 and x=0.55. (ii) Find expectation value x of the particle's position. (iii) Can you find particle's momentum using momentum operator?

5. For a particle trapped in an infinite square well of width L, what is (i) the probability that it is found between 0.4 L and 0.5 L, (ii) the expectation value of its position?

6. A small 0.40-kg cart is moving back and forth along an air track between two bumpers located 2.0 m apart. We assume no friction; collisions with the bumpers are perfectly elastic so that between the bumpers, the car maintains a constant speed of 0.50 m/s. Treating the cart as a quantum particle, estimate the value of the principal quantum number that corresponds to its classical energy.

7. For an electron in one dimensional infinite potential well of width 0.1 nm calculate (i) separation between two lowest energy levels, (ii) frequency and wavelength of photon corresponding to the transition between these two levels, and (iii) region of electromagnetic spectrum in this frequency.

8. An electron in one dimensional infinite potential well makes transition from third excited state to first excited state. If the frequency of emitted photon is 3.43×10^{14} Hz, what is the width of the well?

9. Electrons with energies of 1.0 eV and 2.0 eV are incident on a barrier 10.0 eV high and 0.50 nm wide. (a) Find the ratio of their transmission probabilities. (b) How are these affected if the barrier is doubled in width?

10. Electrons with energies of 0.400 eV are incident on a barrier 3.00 eV high and 0.100 nm wide. Find the approximate probability for these electrons to penetrate the barrier.

11. A beam of electrons is incident on a barrier 6.00 eV high and 0.2 nm wide. Find the energy they should have if 1 percent of them are to get through the barrier.

12. For a quantum particle at ground state $\psi(x) = \exp(-a^2x^2)$, with energy eigen value $a^2\hbar^2/m$. Find the potential in which the particle moves.

13. For a particle bound by 1-D potential show that $\frac{d}{dt}\int_{-\infty}^{+\infty} \psi^*(x,t)\,\psi(x,t)dx = 0.$

14. Show that wavefunctions for different energy states of a particle in square well potential are orthogonal. (Wavefunctions are said to be orthogonal if $\int_{-\infty}^{+\infty} \psi_n\psi_m\,dx = 0$).

15. A 1 eV electron got trapped inside a metal surface. If potential barrier is 4 eV and width of barrier is 0.2 nm, calculate its transmission probability.

16. An alpha particle of 2MeV energy, is trapped in a nucleus of radius 1.4 fm. What is the probability that it will escape from nucleus? Potential barrier at surface of nucleus is 4 MeV and mass of alpha particle is 6.64×10^{-27} kg.

17. An electron in ground state of a 1-D infinite potential well with L = 0.1 nm. Find the force that the electron exerts on the wall during an impact on the wall.