Quantum Materials

Introduction to Quantum Mechanics

Historical evolution from classical physics to quantum physics.

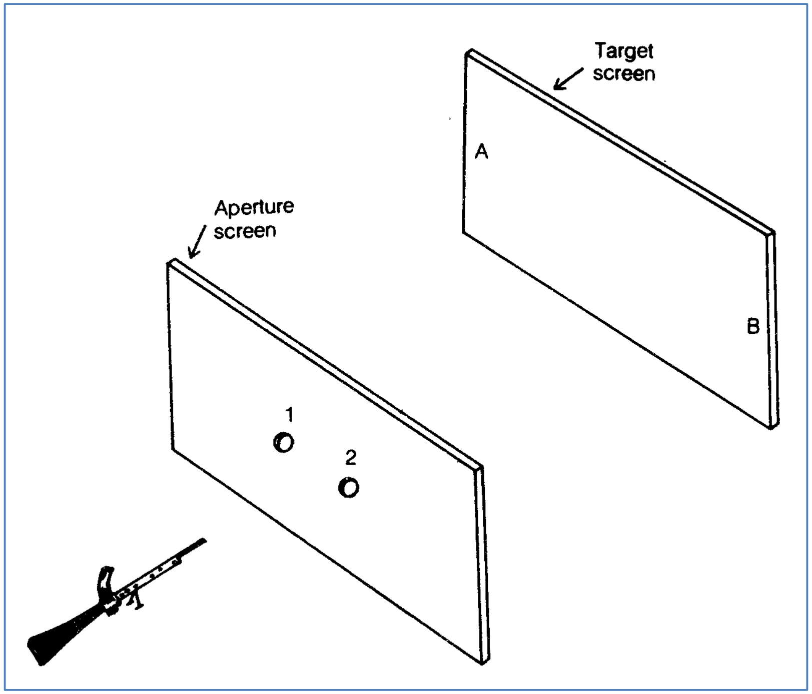
Exploration of wave-particle duality and the concept of quantum states.

Superposition and entanglement: their significance in quantum systems and potential applications.

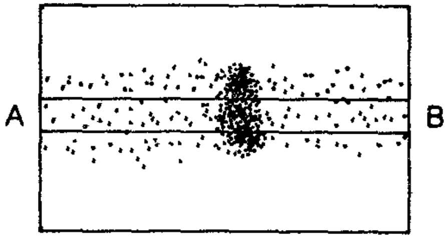
The uncertainty principle and its impact on measurement in quantum systems.

Quantum wave function, Schrödinger equation (time independent). Energy quantization: Introduction to discrete energy levels in atoms and their effects on material properties.

A simple experiment..



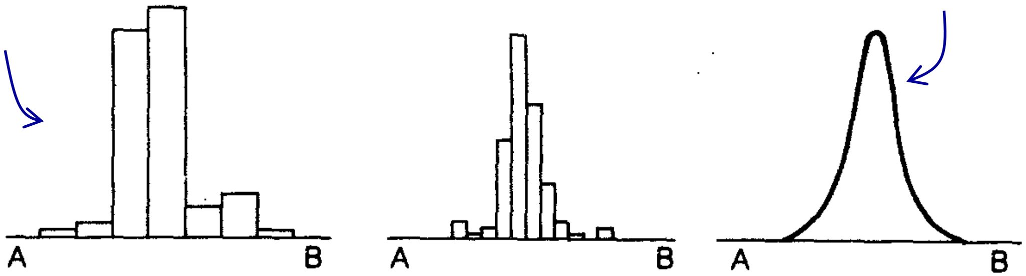
If only one aperture is open...



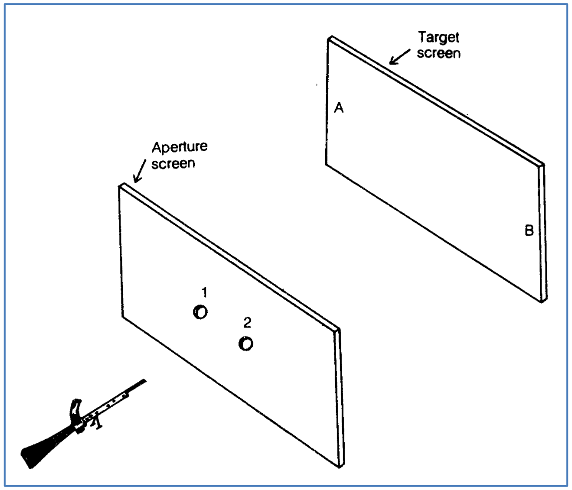
(a)

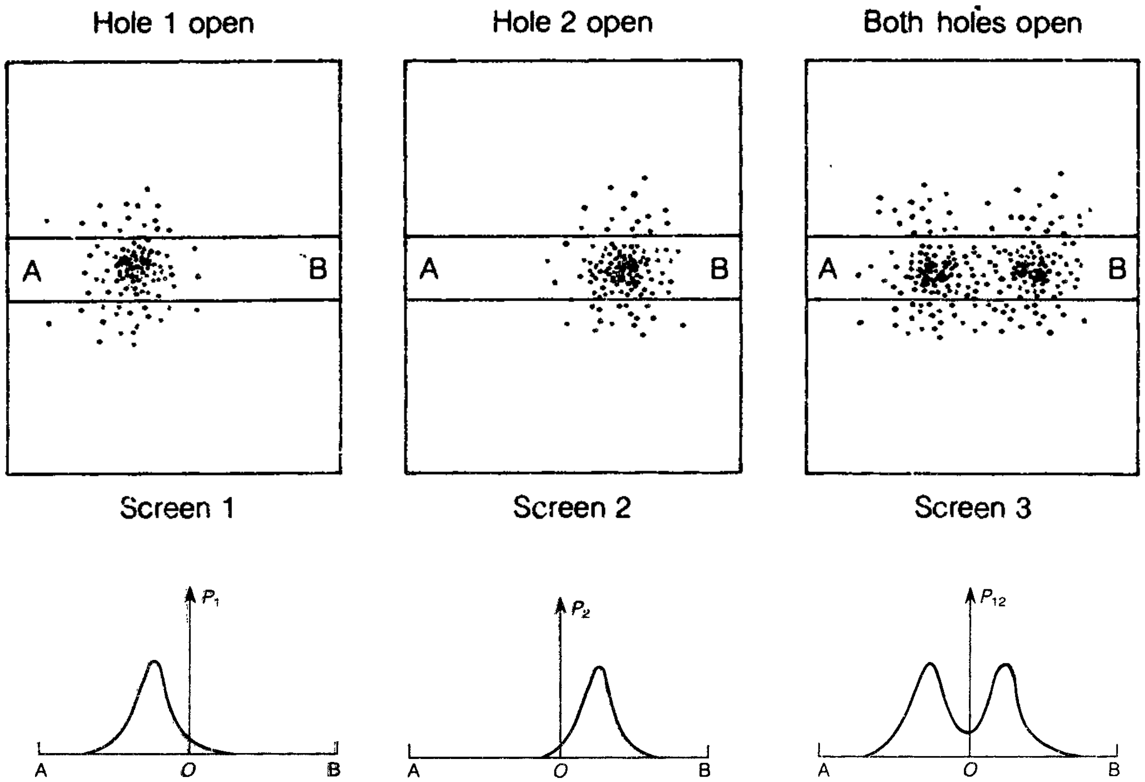
Probability distribution

Histogram



A simple experiment

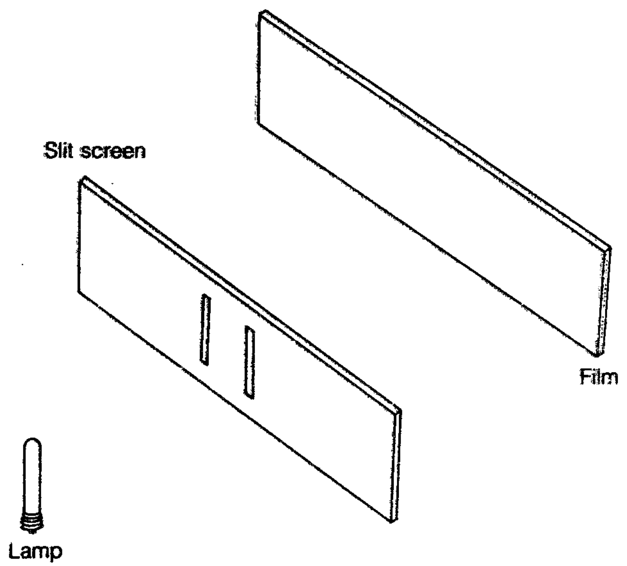




We just add probabilities!

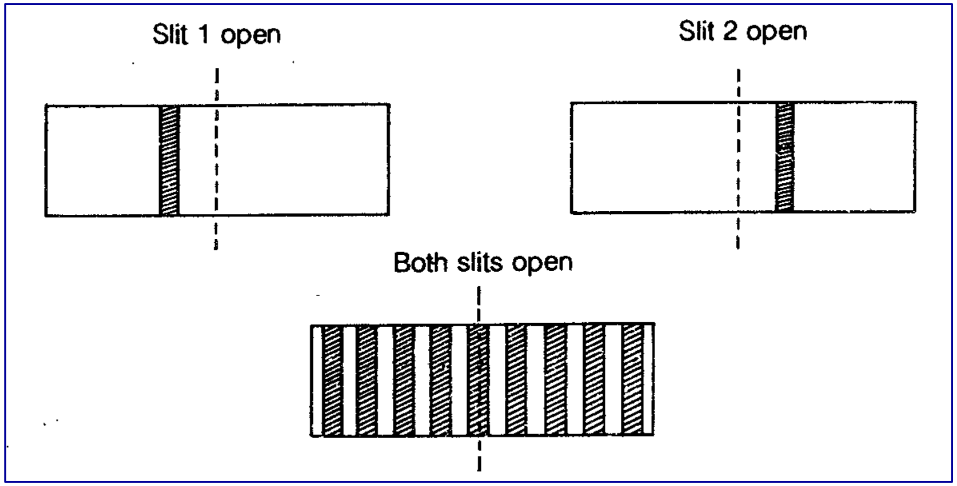
The effect with both holes open is sum of effects with each hole open alone. No interference from each other!

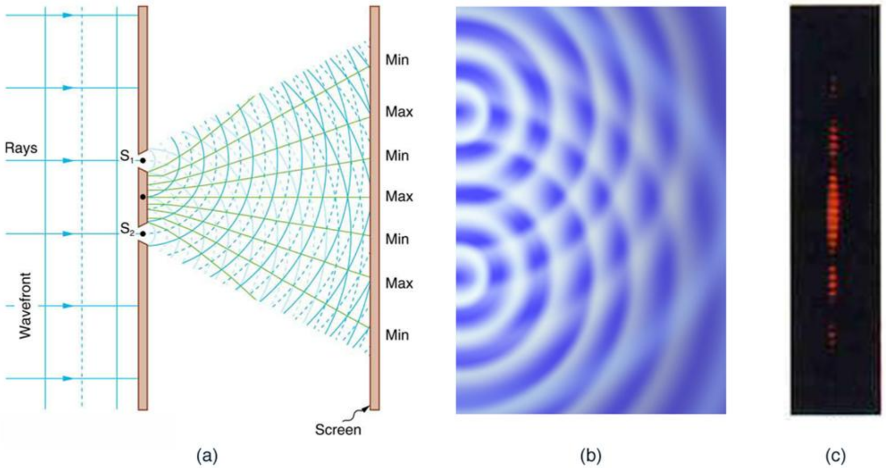
Another experiment, but with a light source



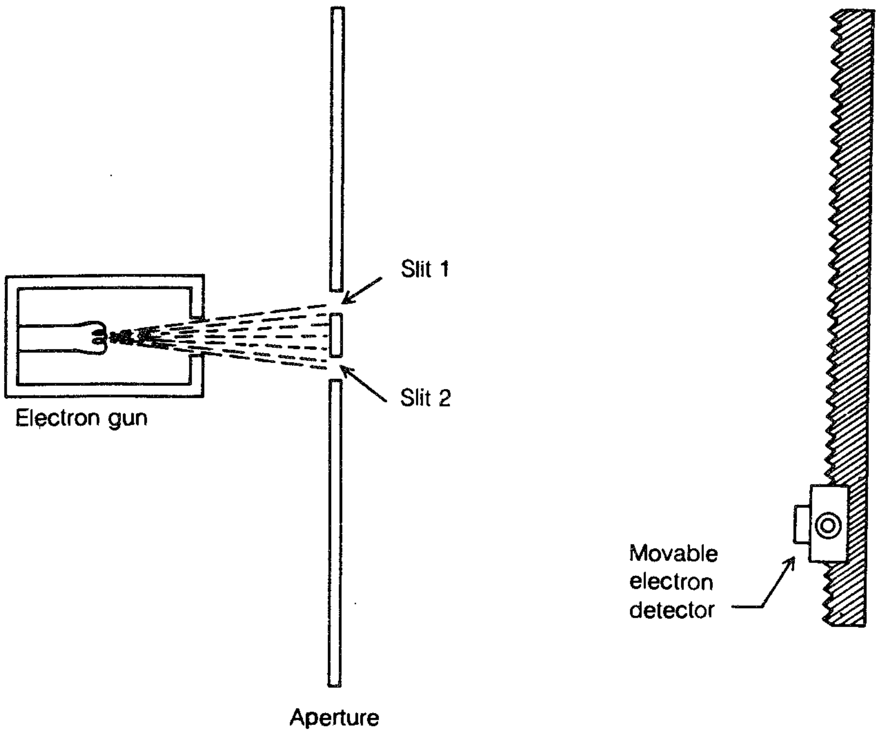
Interference pattern
Wave nature of light

With photographic plates





Another experiment, but with an electron gun

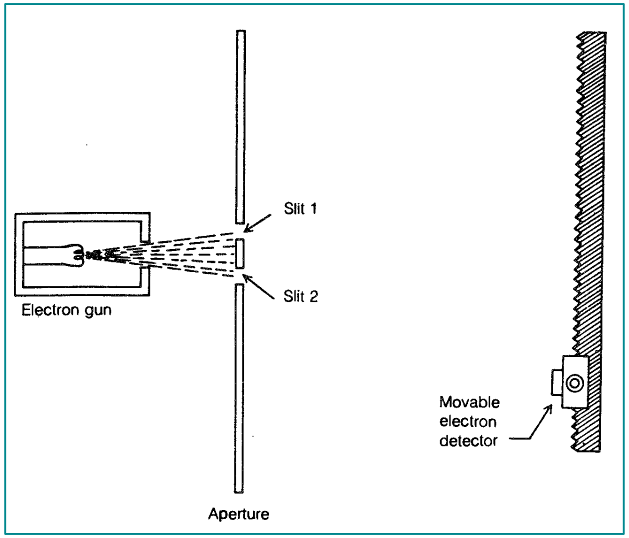


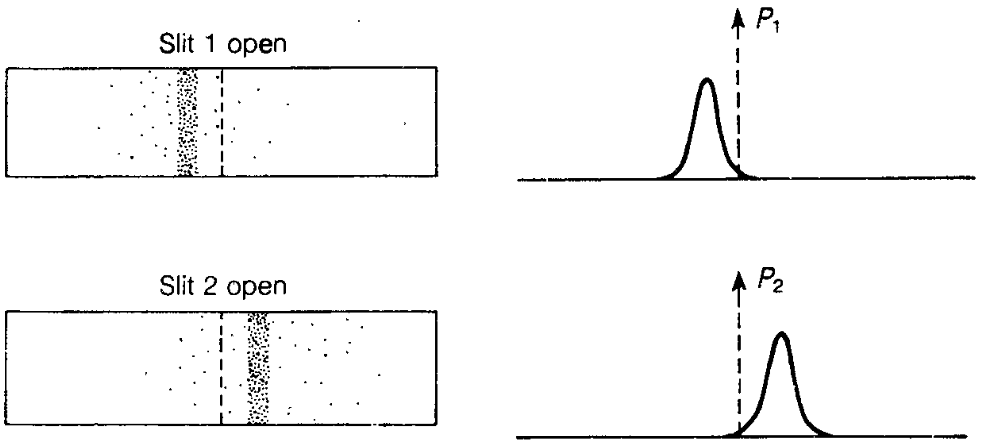
1897. J.J. Thomson discovered the electron.

He made electrons fly like bullets, got them moving in curved paths.

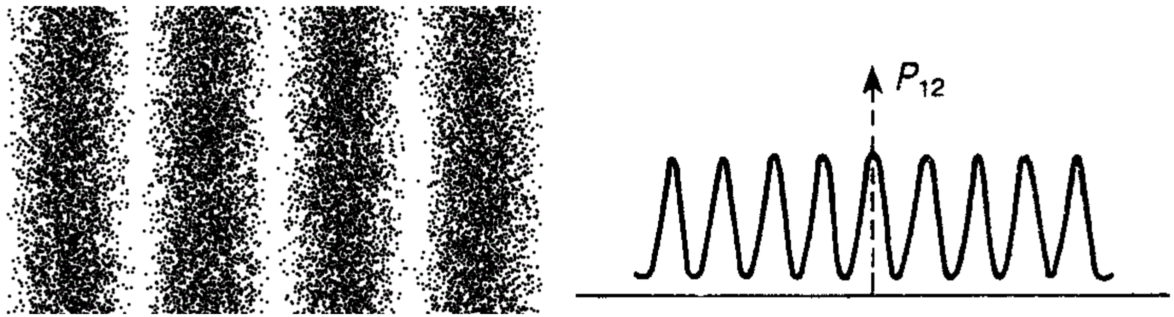
So, everyone thought it was a particle.

Another experiment, but with an electron gun





When both slit 1 and slit 2 are open….



Interference pattern of a wave!

Whether electron is a particle or a wave?

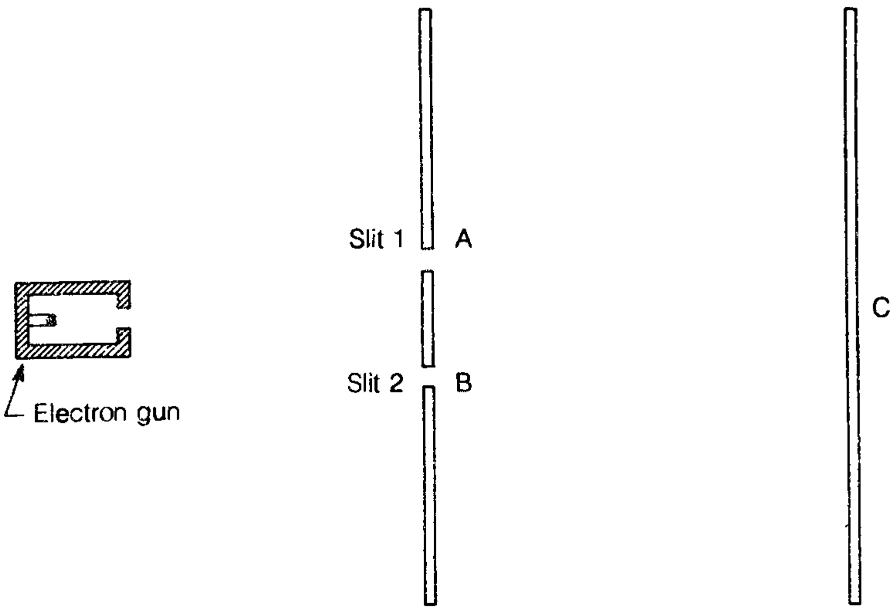
Experiment with electrons

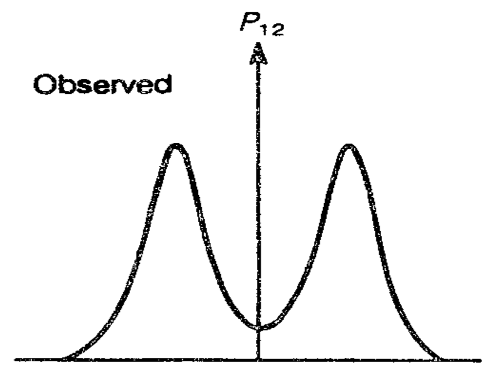
Interference occurs for light because light is a wave and the same wave goes through both the slits.

Interference also occurs in the case of electrons.

Does it mean the same electron goes through both the slits?

Does the electron secretly break up and then reassemble once it is past the slits?





A, B, C are detectors/flags to suggest us the passing/arrival of electrons.

Where is that interference pattern?

Experiment with electrons

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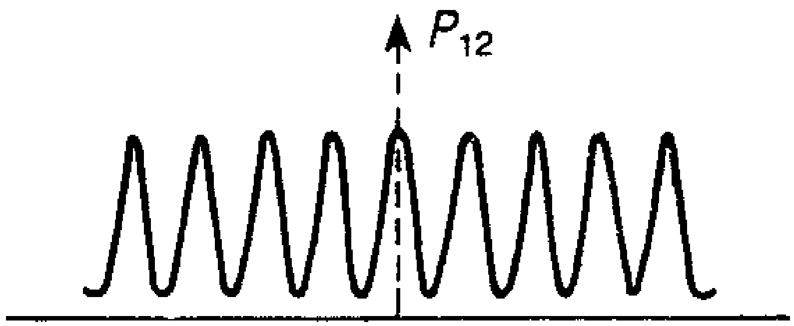
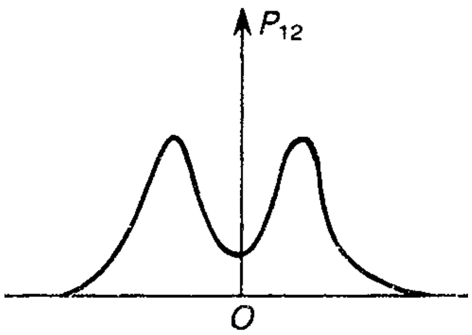


If there are no flags/observers.



If there are flags/observers.

Does it mean that presence of flags/observers changed the outcome?

Somehow, nature knows whether we have the information that "marks" which slit the electron passed through.

If the particle is marked in some fashion, you will not get an interference pattern when you look at the screen; if the particle is not marked, you will get an interference pattern.

What does it mean to observe something?

what does it all mean about the nature of reality?

Does it mean that nature is inherently non-deterministic?

Does it mean that what we keep or destroy today can affect the outcomes of events that should already be determined in the past?

That the observer plays a fundamental role in determining what is real?

It is hard to believe that nature behaves one way when you are looking and in a completely different way when you are not looking.

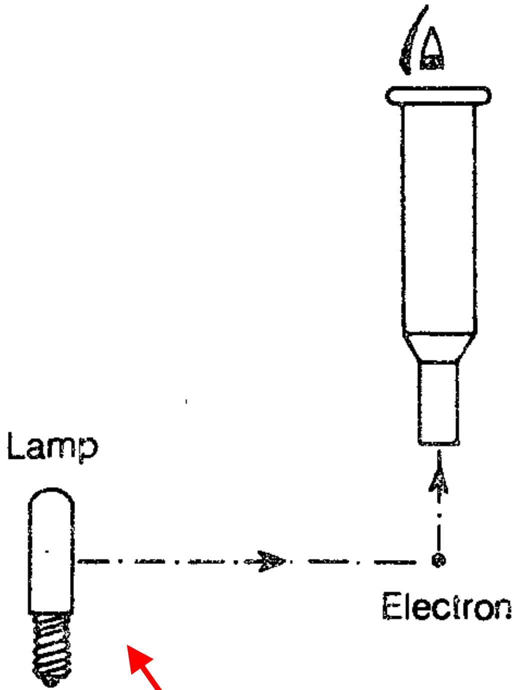
It seems that when we observe we disturb whatever we are trying to observe.

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**

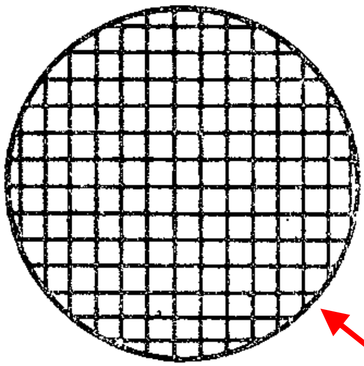
The Uncertainty Principle

1926. Werner Heisenberg

How to determine position of an electron?



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



If grid lines are closer on the graduated screen, one can read off the position of the particle more accurately.

The Uncertainty Principle

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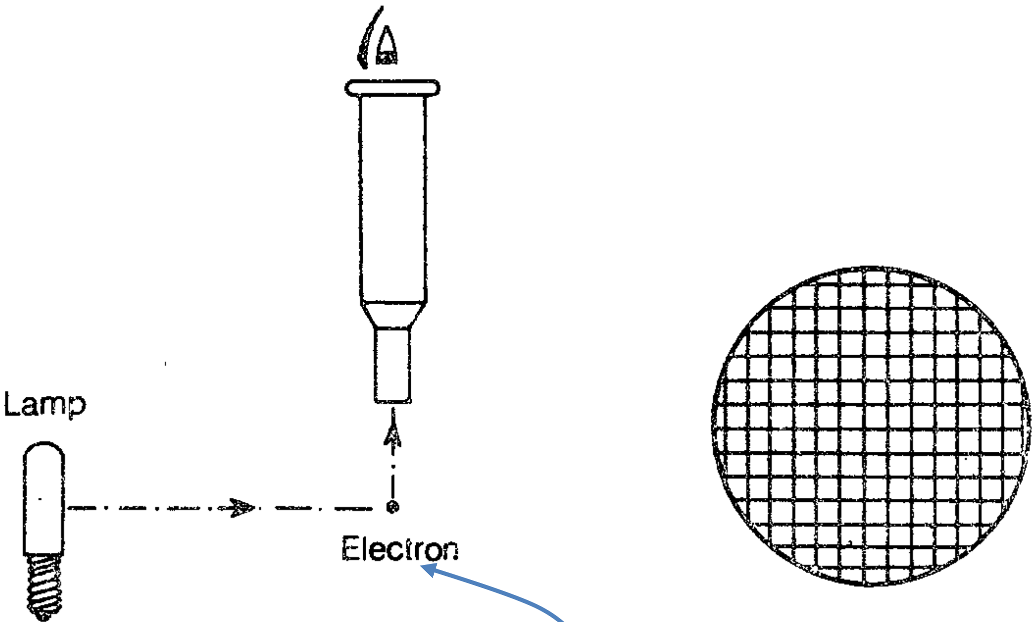
BTW, how do we see the electron or measure its position?

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



Smaller the wavelength, better is the resolution.

particle should be illuminated

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

(Light is an electromagnetic radiation, quanta of energy called photon, ~1905)

The light failing on the particle bounces off, and when it reaches our eye an image is formed.

It is from this image we get an idea of where exactly the particle is.

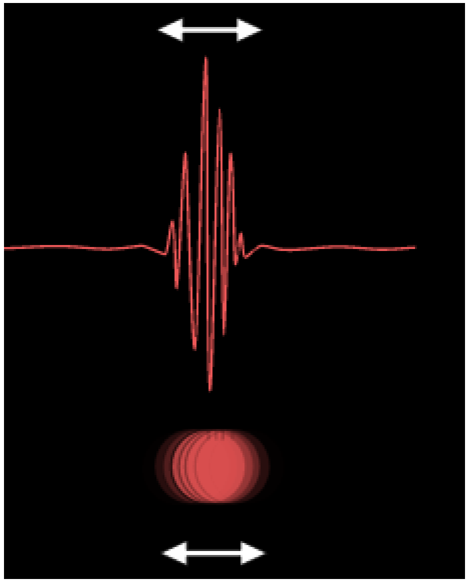
The Uncertainty Principle

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

So when we try to illuminate the electron with gamma rays, we are really bombarding it with a stream of photons (1905, Einstein).

In 1923, Compton discovered that when a photon collides with an electron, it imparts momentum besides disturbing the position.

Thus to see and measure the position of the electron we must illuminate it; but the moment we shine light on 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.

Philosophical implications…

Four important facts emerge from these experiments:

1. Classical mechanics (which works for bullets) does not work for electrons.
2. Electrons can behave like both, particles and waves. So also does light.
   Commenting on it, Feynman once observed: You had to know which experiments you were analysing in order to tell if light was waves or particles
3. The act of observation can disturb; so what you get need not be what you wanted to see.
4. To describe the electron experiment, it is necessary to associate a complex (probability) amplitude.

The Heisenberg Uncertainty Principle

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

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

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

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

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.

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

$\Delta p_y . \Delta x = 0$

$\Delta p_z . \Delta x = 0$

$\Delta p_x . \Delta y = 0$

$\Delta p_y . \Delta y \geq \hbar$

$\Delta p_z . \Delta y = 0$

$\Delta p_x . \Delta z = 0$

$\Delta p_y . \Delta z = 0$

$\Delta p_z . \Delta z \geq \hbar$

Conjugate pairs

☼Heisenberg's uncertainty principle is true for **conjugate pairs** only.

Predictions from 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 from uncertainty principle

1. Nonexistence of free electron in nucleus

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

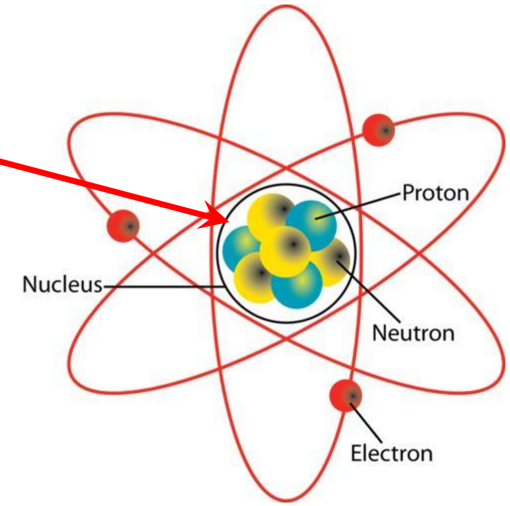
$$E^2 = p^2c^2 + m_0^2c^4$$

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

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

$$E_{min} = \frac{3.165 \times 10^{-12}\ J}{1.6 \times 10^{-19}\ C} = 19.78\ MeV$$

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:

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

$\Delta p_{min} = \hbar / \Delta x$

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

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

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

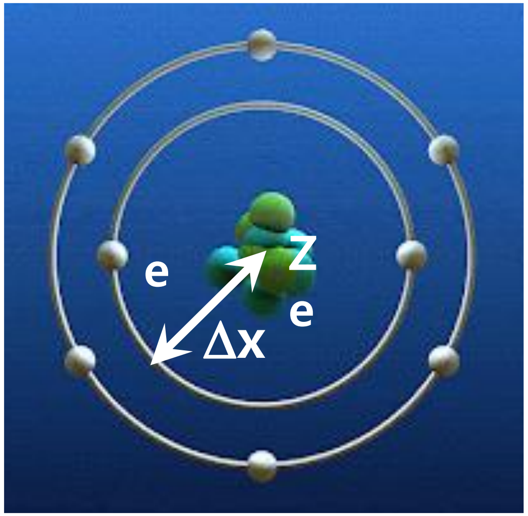
$m_0 = 9.1 \times 10^{-31}\ kg$

- 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.

Therefore electrons cannot be present within the nucleus.

Predictions from uncertainty principle

2. Estimate of radius of Bohr's first orbit



$$\Delta p_x . \Delta x \geq \hbar \qquad \Delta p_x = \frac{\hbar}{\Delta x}$$

Kinetic energy of electron

$$K = \frac{p^2}{2m} \qquad \Delta K = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2m(\Delta x)^2}$$

Potential energy of electron

$$V = \frac{(Ze)(-e)}{4\pi\varepsilon_0\, x} \qquad \Delta V = \frac{(Ze)(-e)}{4\pi\varepsilon_0\, \Delta x}$$

Uncertainty in total energy of electron

$$\Delta E = \frac{\hbar^2}{2m(\Delta x)^2} - \frac{Ze^2}{4\pi\varepsilon_0\, \Delta x}$$

Uncertainty in total energy of electron will be minimum if

$$\frac{\partial(\ E)}{\partial(\Delta x)} = 0$$

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

Bohr's first orbit

Predictions from uncertainty principle

3. Zero point energy of simple harmonic oscillators

Total energy of oscillator at displacement x

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

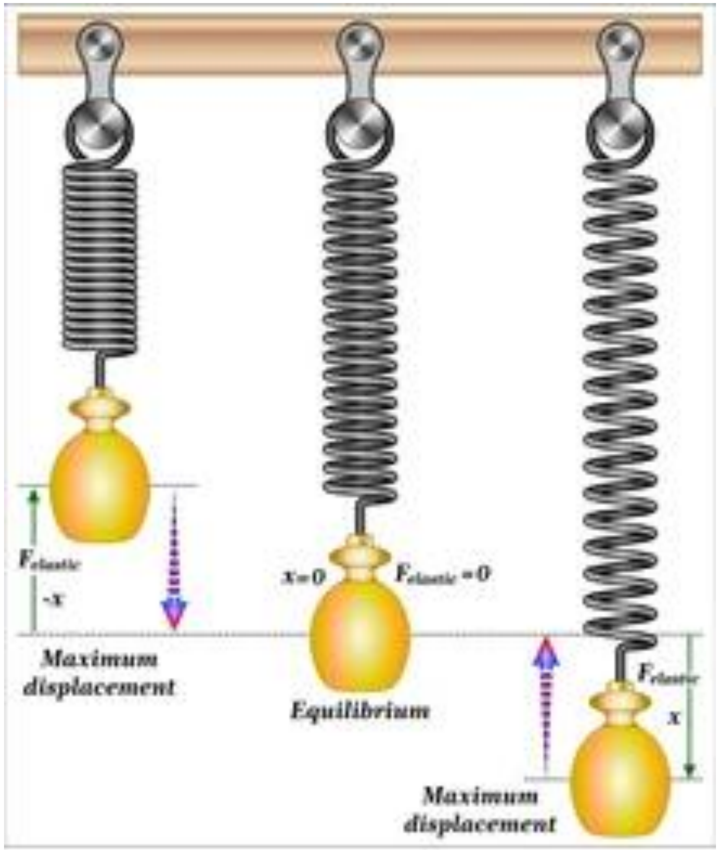
$x_{max} = a$ $\qquad (\Delta x)_{max} = 2a$ $\qquad (\Delta p_x)_{min} = \frac{\hbar}{2a}$

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

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

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

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



Predictions from uncertainty principle

3. Zero point energy of simple harmonic oscillators

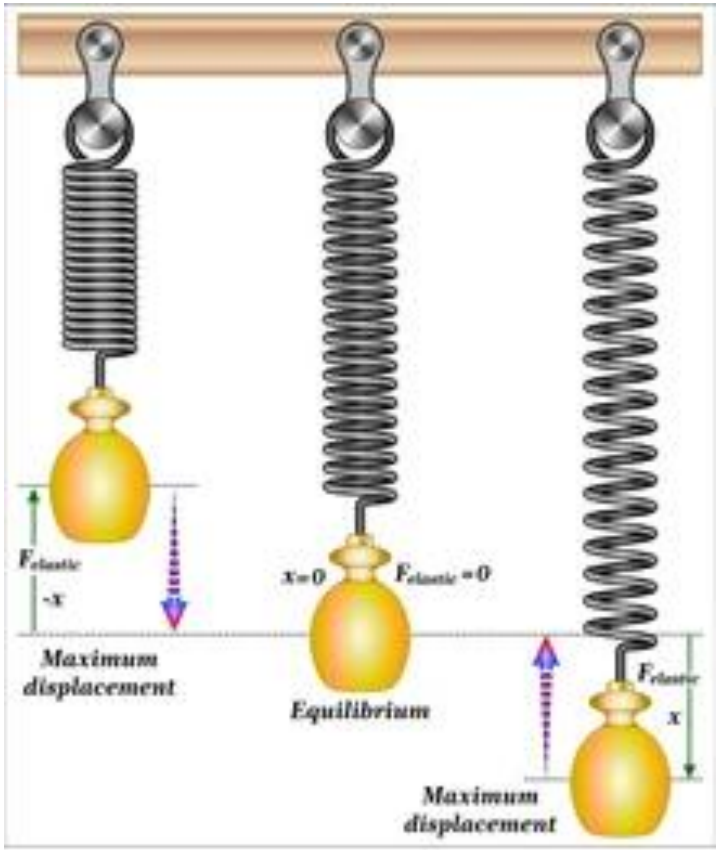
$$E = \frac{\hbar^2}{8ma^2} + \frac{m\omega^2 a^2}{2}$$

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

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

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

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

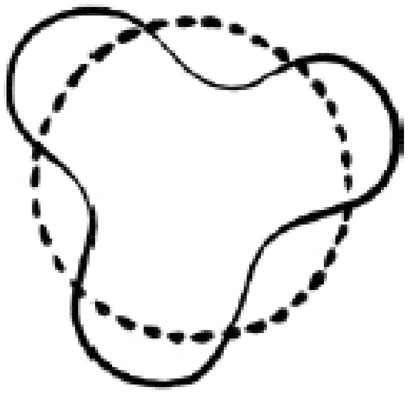


Wave-particle duality

Matter can behave both like particles as well as waves.

Louis de Broglie was the first to draw attention to this possibility.

If a particle of mass *m* moves with a velocity *v* then it behaves like a wave having a wavelength $\lambda = h/(mv)$.



Such a matter wave is referred to as a de Broglie wave, and λ = de Broglie wavelength.

This discovery was the starting point of what might be called the wave theory of matter.

The curious fact that matter can exhibit wave-like properties (or should this rather be waves acting like particles?) is now referred to as the wave particle duality.

Louis de Broglie: Noble prize in Physics, 1929

Wave-particle duality

Is he Bruce Wayne or Batman? Well, he's both. It really depends on when you ask the question.

Breakthroughs – Evolution of Quantum Mechanics

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(1900)
Planck: quanta of energy

(1905)
Einstein: Photoelectric effect (Photon of light)

(1913)
Bohr: Atom's discrete state

(1923)
Compton: Particle behavior of radiation;
de Broglie: dual nature;
Heisenberg: Uncertainty principle;
Davisson-Germer: Wave behavior of electrons

Radiation from a hot body

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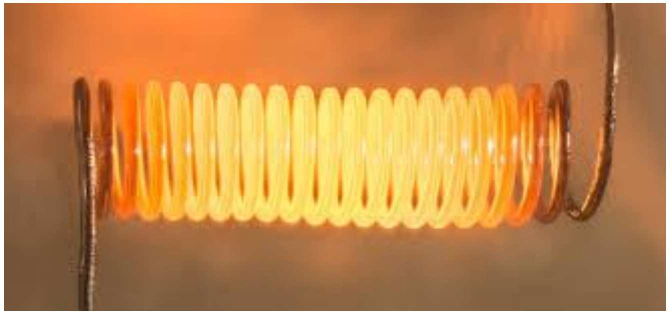

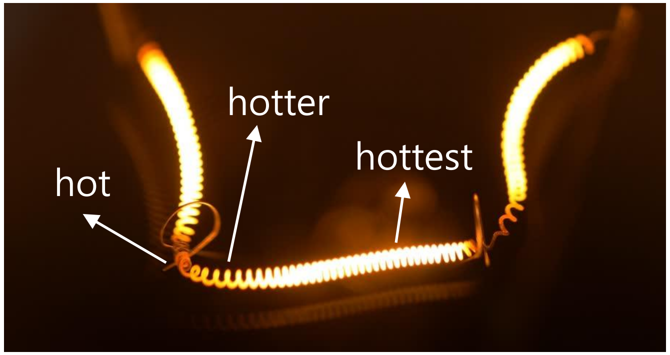

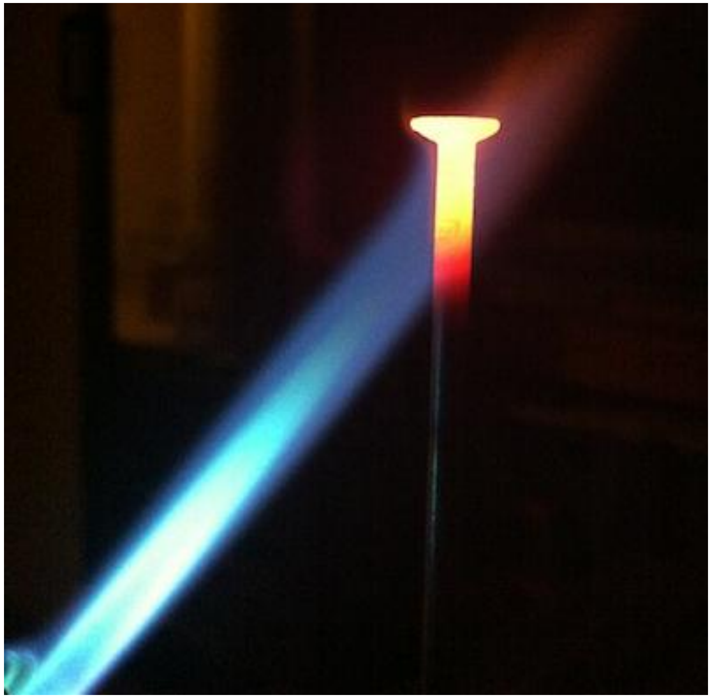

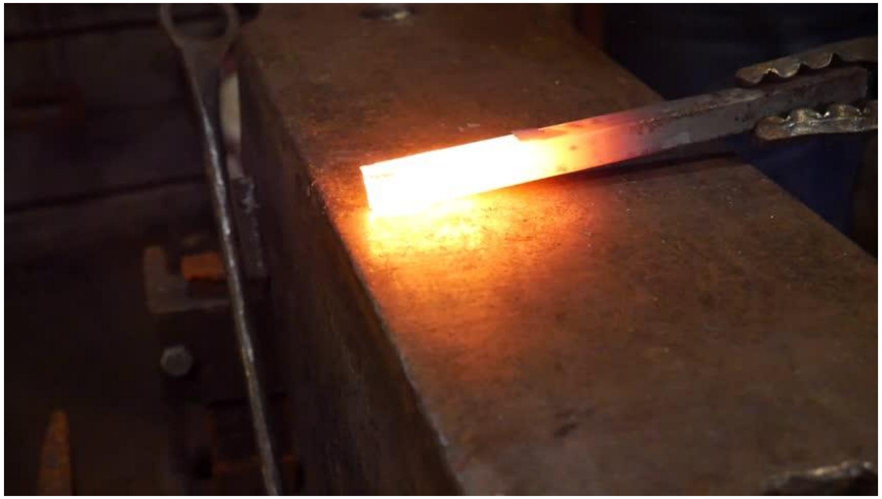

Radiation from a hot body

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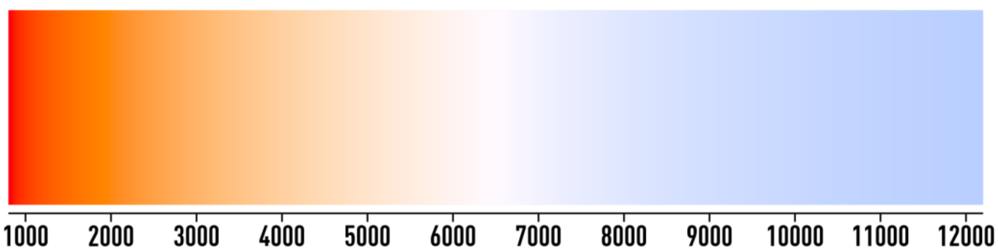
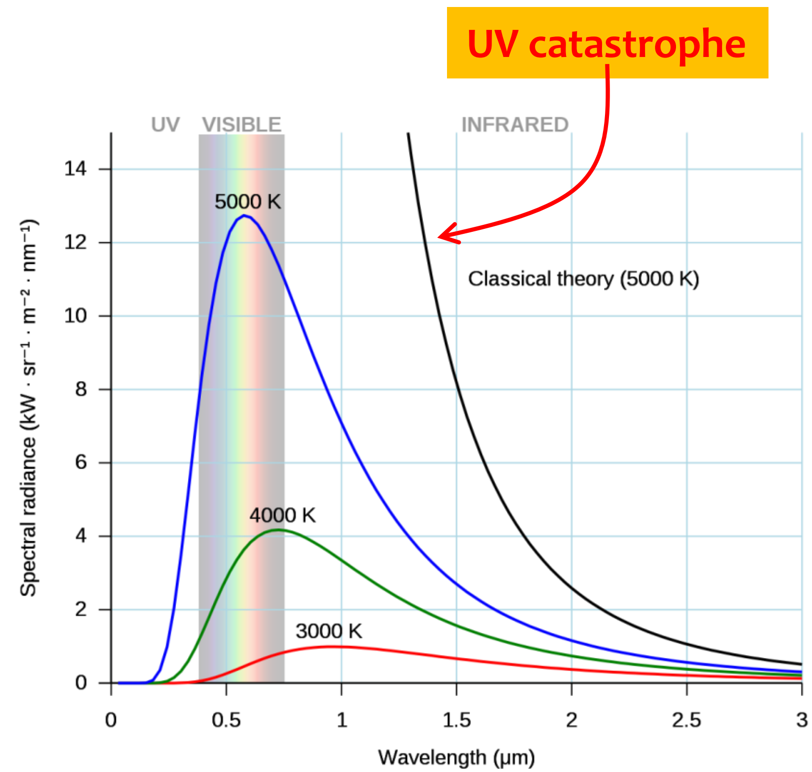
“How does the intensity of the electromagnetic radiation emitted by a body depend on the frequency of the radiation (i.e., the color of the light) and the temperature of the body?” **1859, Kirchoff**





Radiation from a hot body - Planck's Law

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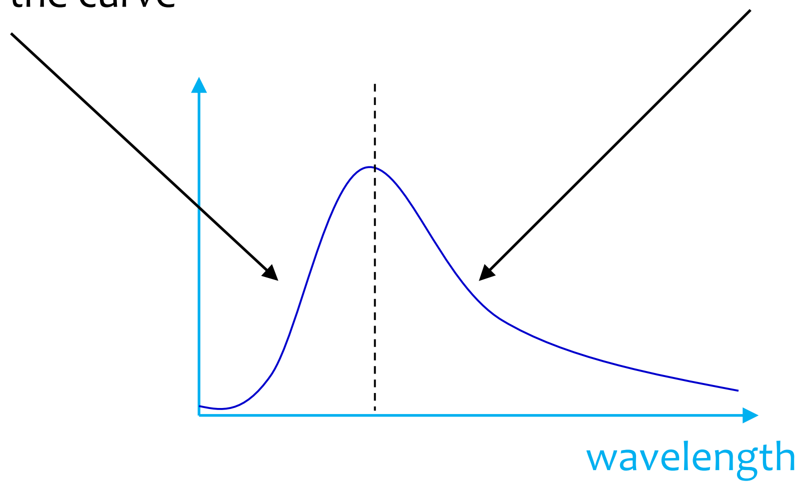
Wilhelm Wien
Explained left hand side of the curve

Lord John Rayleigh & *Sir* James Jeans
Explained the right hand side of the curve

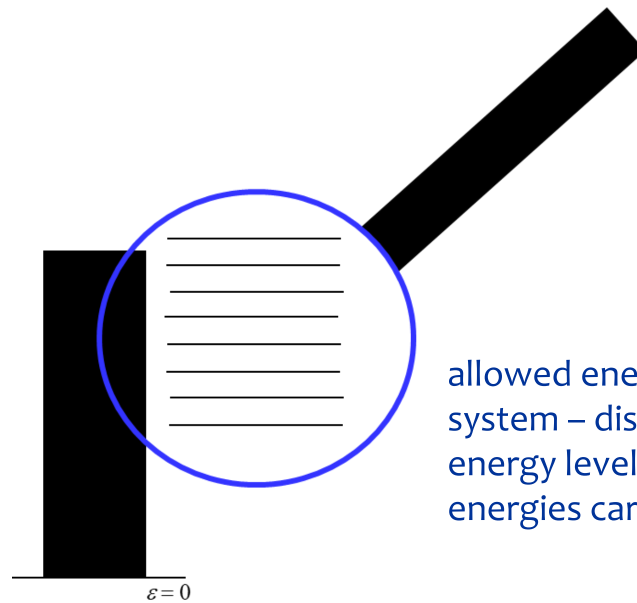


In 1900, Max Planck heuristically derived a formula for the observed spectrum.

He explained both parts of the curve!

Radiation from a hot body - Planck's Law

- Planck argued that radiations come from atomic oscillations.
- These atomic oscillators have some fixed (discreet) energy related to their frequency of oscillation.
    - Energy of the oscillators is quantized.
    - Each discreet energy value corresponds to a **quantum state.**
- These oscillators can absorb or emit energy and jump from one quantum state to another.



allowed energies in quantised system – discrete (such as energy levels in an atom, energies carried by a photon)

allowed energies in classical system – continuous (such as an harmonic oscillator, energy carried by a wave; total mechanical energy of an orbiting planet, etc.)

Can convictions change?

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- Can one's convictions change? or should you change?
  - Planck changed!
- He was responding to a theoretical challenge issued by Kirchhoff many years ago in 1860 to find the function of temperature and wavelength for the observed spectrum of radiating bodies.
- Planck was not looking for a revolution. He was a counter-revolutionary!

- One of his motivations in studying the thermodynamics of electromagnetic radiation was to rebut the statistical theories of Boltzmann.
- Planck had never been convinced by the atomistic and discrete approach which Boltzmann had used in context of entropy and 2nd law of thermodynamics.
- With the continuum of light radiation he thought he had the perfect system that would show how entropy behaved in a continuous manner, without the need for discrete quantities.
- Therefore, Planck's original intentions were to use blackbody radiation to argue against Boltzmann - to set back the clock.

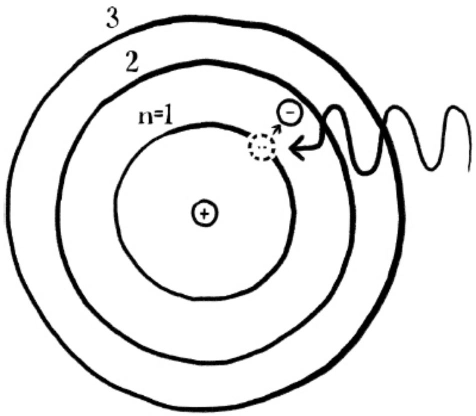
https://galileo-unbound.blog/tag/black-body/

Implication of Planck's Law

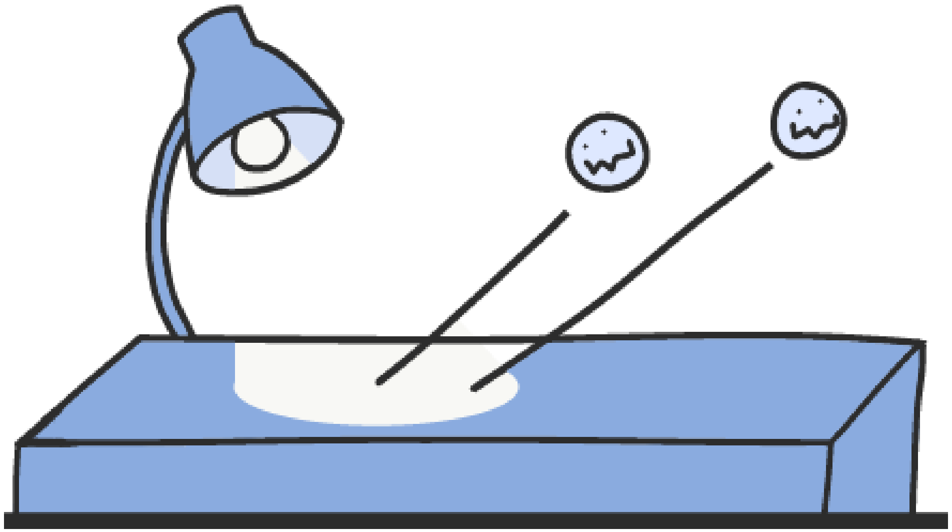
"According to the assumption to be contemplated here, when a light ray is spreading from a point, the energy is not distributed continuously over ever-increasing spaces, but consists of a finite number of 'energy quanta' that are localized in points in space, move without dividing, and can be absorbed or generated only as a whole.“ 1905, Einstein, Photoelectric effect

1913, Bohr explained the spectral lines of the hydrogen atom, again by using quantization.

These energy quanta later came to be called "photons", a term introduced by Gilbert N. Lewis in 1926.



Photoelectric effect



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

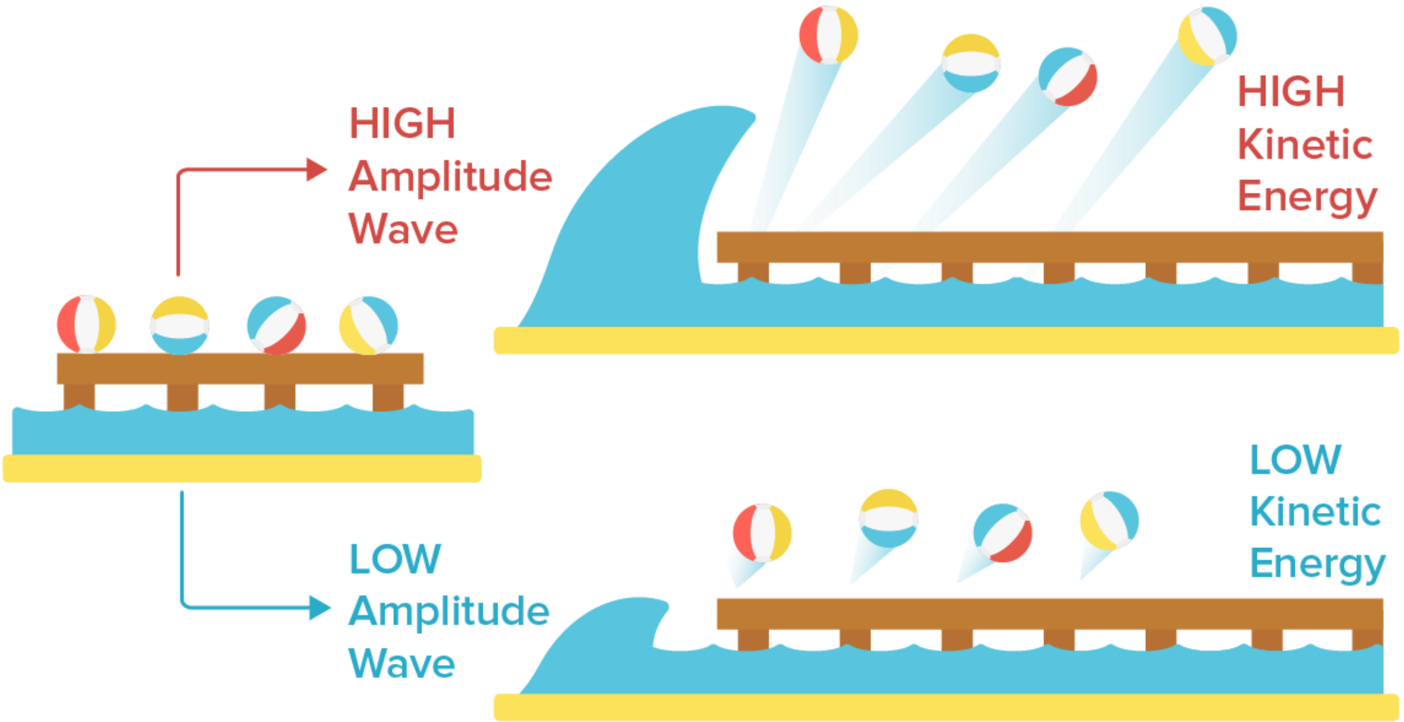
1887, Heinrich Hertz

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?

Photoelectric effect



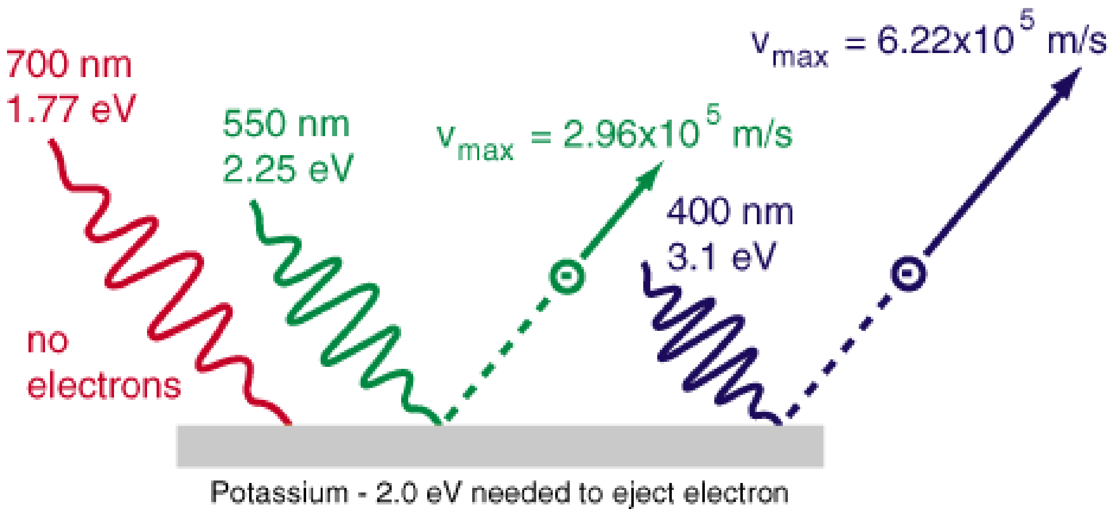
Wave model of light failed to explain it!

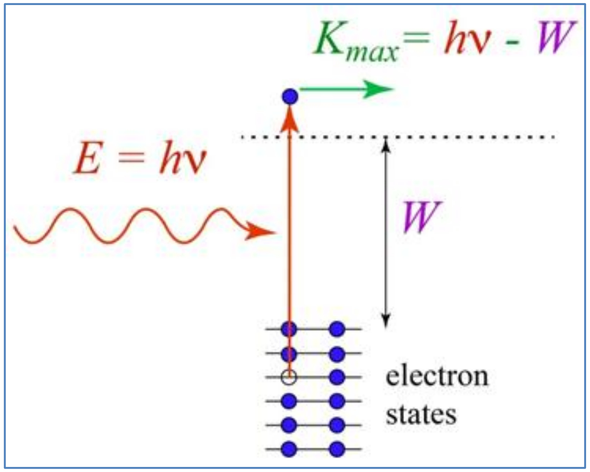
- increasing light amplitude (intensity) would increase the kinetic energy of emitted photoelectrons, (Brightness should produce more electrons!)
- increasing the frequency would increase measured current.

Photoelectric effect

Experiments showed that

- increasing the light frequency increased the kinetic energy of the photoelectrons (no of emitted electrons remained same, but energy of electrons increased)
- increasing the light amplitude increased the current (more no of electrons emitted).





- Einstein thought that light is equivalent to wave packets – particle nature.
- Energy of each packet is directly proportional to frequency of the light, and proportionality constant is the Planck's constant.

Noble prizes in physics

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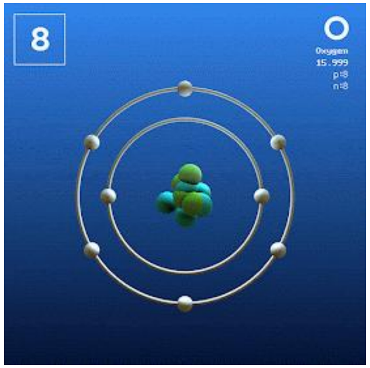
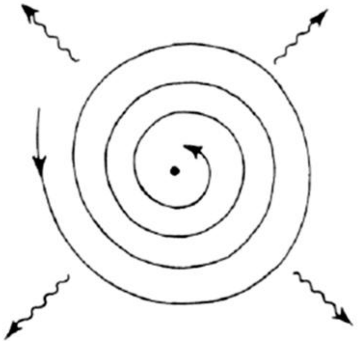
1918	Max Planck	“in recognition of the services he rendered to the advancement of Physics by his discovery of energy quanta”
1921	Albert Einstein	“for his services to Theoretical Physics, and especially for his discovery of the law of the photoelectric effect”
1922	Niels Bohr	“for his services in the investigation of the structure of atoms and of the radiation emanating from them”
1923	Robert Andrews Millikan	“for his work on the elementary charge of electricity and on the photoelectric effect”
1929	Louis-Victor de Broglie	“for his discovery of the wave nature of electrons”
1932	Werner Heisenberg	“for the creation of quantum mechanics, the application of which has, inter alia, led to the discovery of the allotropic forms of hydrogen”

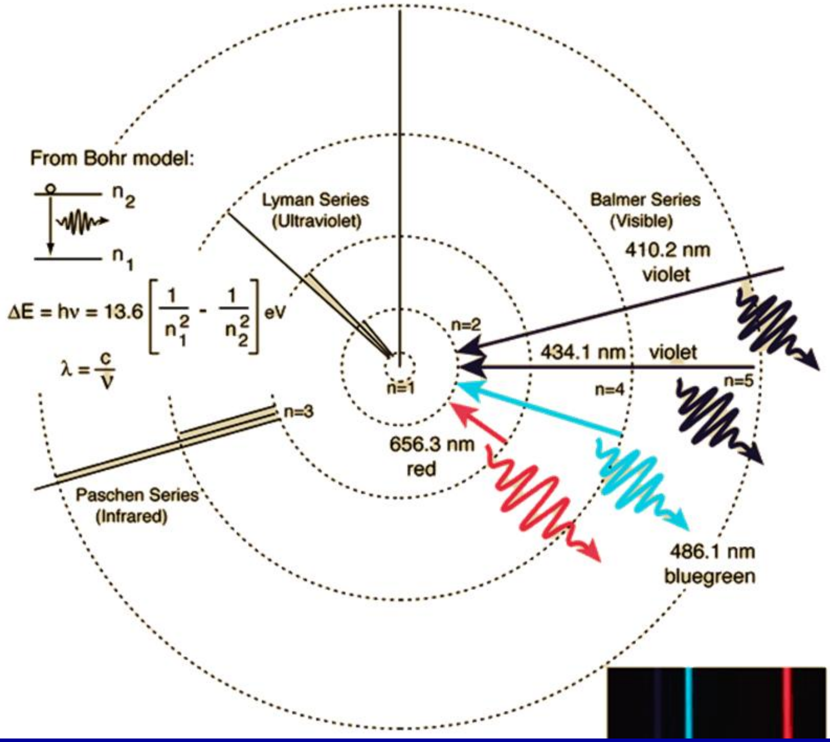
Bohr’s theory of discrete energy state



Prediction of classical theory of orbiting charged particle!



- Angular momentum is quantized. Electrons have discrete energies.
- 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.



Evolution of Quantum Mechanics

Home Assignment

Compton: Particle behavior of radiation;
de Broglie: Dual nature of matter;
Heisenberg: Uncertainty principle;
Davisson-Germer: Wave behavior of electrons