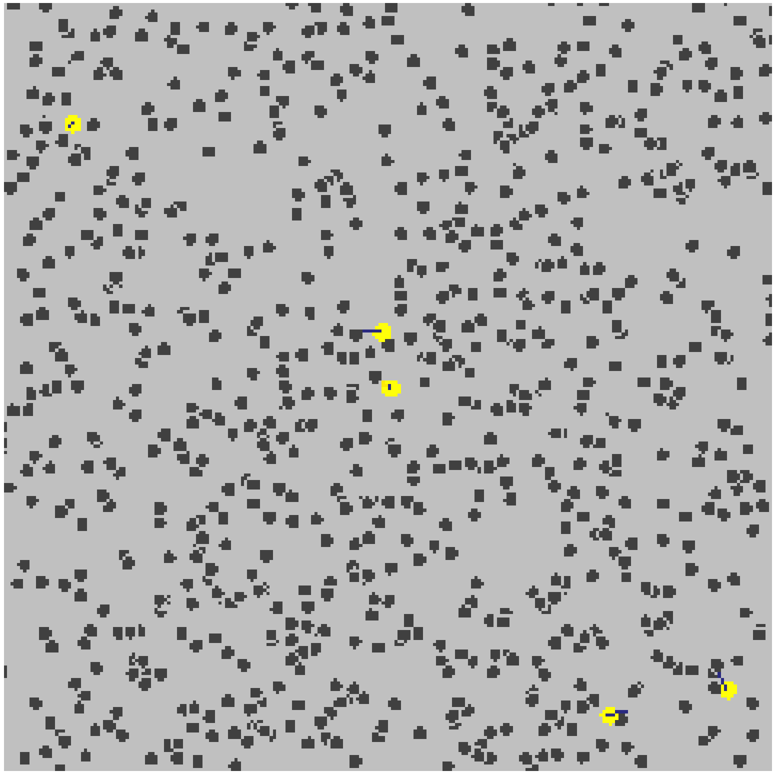
We have studied:

- Particulate Theory of Matter
- $g(r)$
- We know: Newtonian Mechanics

- Consider a single particle/sphere
- Make it very very very small!
- Shake the jar
- Do you see it where it is at every instant?

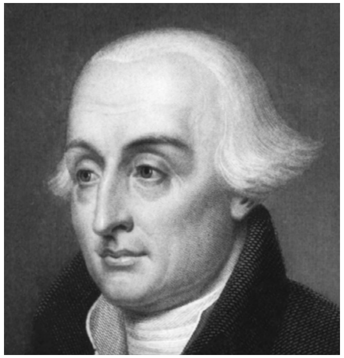
- This is what happens when you have a collection of large number of very small particles



- Still you can see them With Microscope

- Can you describe their Motion?

- First observed by Robert Brown



Prof Einstein Used
Prof. Lagrange's Math
To Solve Prof. Brown's Problem!

Lagrange's equations *(First kind)*

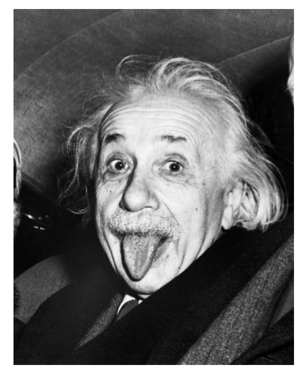
$$\frac{\partial L}{\partial \mathbf{r}_k} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\mathbf{r}}_k} + \sum_{i=1}^{C} \lambda_i \frac{\partial f_i}{\partial \mathbf{r}_k} = 0$$

L = T – V

L = Total Energy,
T = Potential Energy,
V = Kinetic Energy.

where $k = 1, 2, ..., N$ labels the particles, there is a Lagrange multiplier λ_i for each constraint equation f_i, and

$$\frac{\partial}{\partial \mathbf{r}_k} \equiv \left(\frac{\partial}{\partial x_k}, \frac{\partial}{\partial y_k}, \frac{\partial}{\partial z_k}\right), \quad \frac{\partial}{\partial \dot{\mathbf{r}}_k} \equiv \left(\frac{\partial}{\partial \dot{x}_k}, \frac{\partial}{\partial \dot{y}_k}, \frac{\partial}{\partial \dot{z}_k}\right)$$



$$\frac{\partial \rho}{\partial t} = D \cdot \frac{\partial^2 \rho}{\partial x^2},$$

Assuming that N particles start from the origin at the initial time $t = 0$, the diffusion equation has the solution

$$\rho(x,t) = \frac{N}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}.$$

- Consider this tiny marble I hold!
- I Shake the jar really fast!
- What happens?

- Particle becomes WAVY!
- How we describe such motion?

Thanks to Prof Paul A. V. M. Dirac!
Extended Prof. Einstein's Idea far!

LAGRANGIAN:

Lagrange's equations *(First kind)*

$$\frac{\partial L}{\partial \mathbf{r}_k} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\mathbf{r}}_k} + \sum_{i=1}^{C} \lambda_i \frac{\partial f_i}{\partial \mathbf{r}_k} = 0$$

L = T – V

L = Lagrangian,
T = Kinetic Energy,
V = Potential Energy.

where $k = 1, 2, ..., N$ labels the particles, there is a Lagrange multiplier λ_i for each constraint equation f_i, and

$$\frac{\partial}{\partial \mathbf{r}_k} \equiv \left(\frac{\partial}{\partial x_k}, \frac{\partial}{\partial y_k}, \frac{\partial}{\partial z_k}\right), \quad \frac{\partial}{\partial \dot{\mathbf{r}}_k} \equiv \left(\frac{\partial}{\partial \dot{x}_k}, \frac{\partial}{\partial \dot{y}_k}, \frac{\partial}{\partial \dot{z}_k}\right)$$

Concept of Path Integral connects Q-Mech with Classical Mechanics based on its Action principle using Lagrangian.

HAMILTONIAN:

H = T + V

$$\widehat{H}\psi = E.\psi$$

$$H\left|\psi(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle.$$

Path Integral Formulation

$$\hat{H} = \hat{T} + \hat{V},$$

where

$$\hat{V} = V = V(\mathbf{r}, t),$$

is the potential energy operator and

$$\hat{T} = \frac{\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}}{2m} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2,$$

is the kinetic energy operator in which m is the mass of the particle, the dot denotes the dot product of vectors, and

$$\hat{p} = -i\hbar\nabla,$$

is the momentum operator where a ∇ is the del operator. The dot product of ∇ with itself is the Laplacian ∇^2. In three dimensions using Cartesian coordinates the Laplace operator is

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

EINSTEIN'S DIFFUSION EQUATION FROM LAGRANGIAN (CLASSICAL)

$$\frac{\partial \rho}{\partial t} = D \cdot \frac{\partial^2 \rho}{\partial x^2},$$

Dirac developed the Concept of Path Integral further To connect Q-Mech with Classical Mechanics based on its Action principle using Lagrangian, shown simply Here with Brownian motion.

SCHROEDINGER'S DIFFUSION EQUATION FROM HAMILTONIAN (QUANTUM)

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \implies \frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}$$

ELECTRON IS A 'CLASSICAL' PARTICLE WITH 'IMAGINARY' DIFFUSION CONSTANT!

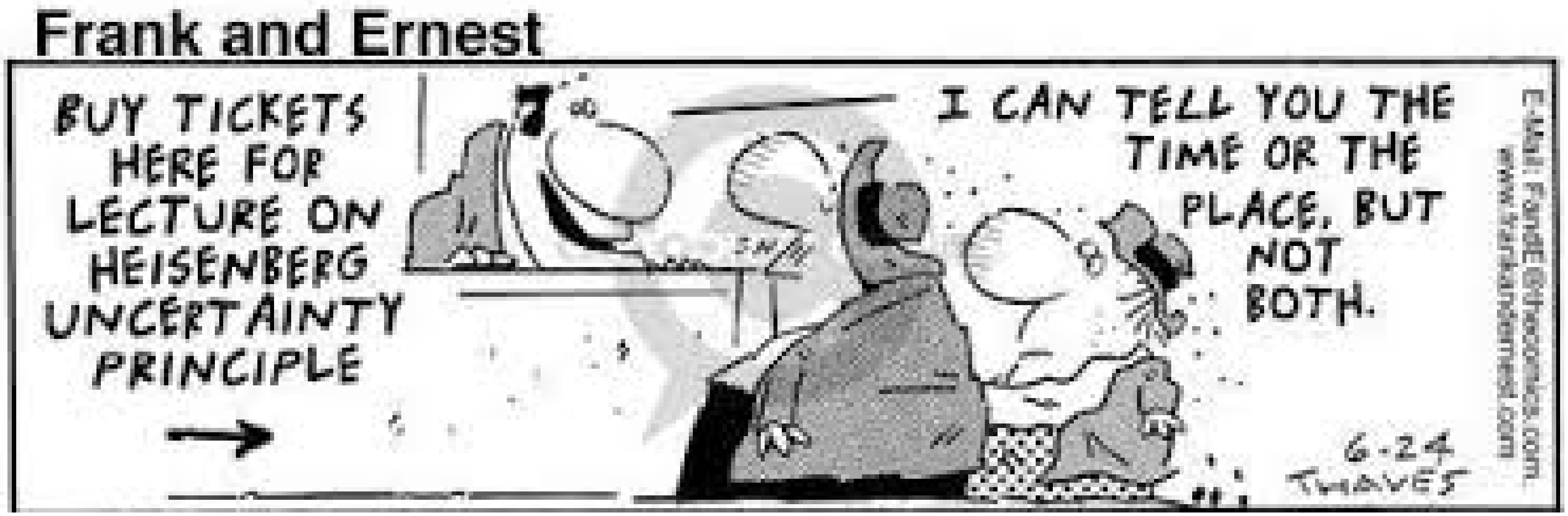
DIRAC's VIEW:

The Schrödinger equation is a diffusion equation with an imaginary diffusion constant.

DIRAC's VIEW LEADS TO:

Electrons are Particles Diffusing with Imaginary Diffusion Coefficients.

UNCERTAINTY

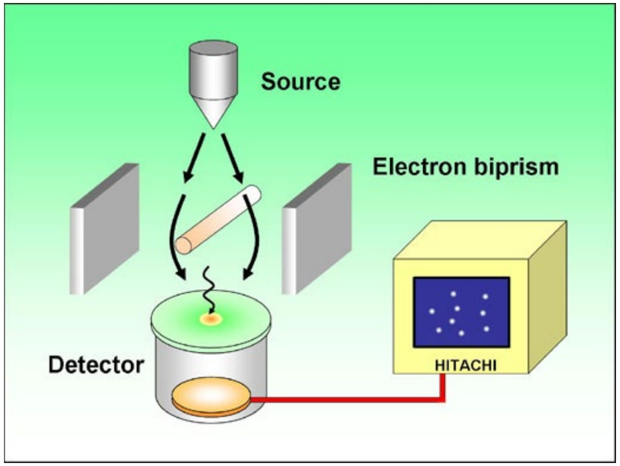


DIRAC's VIEW LEADS TO:

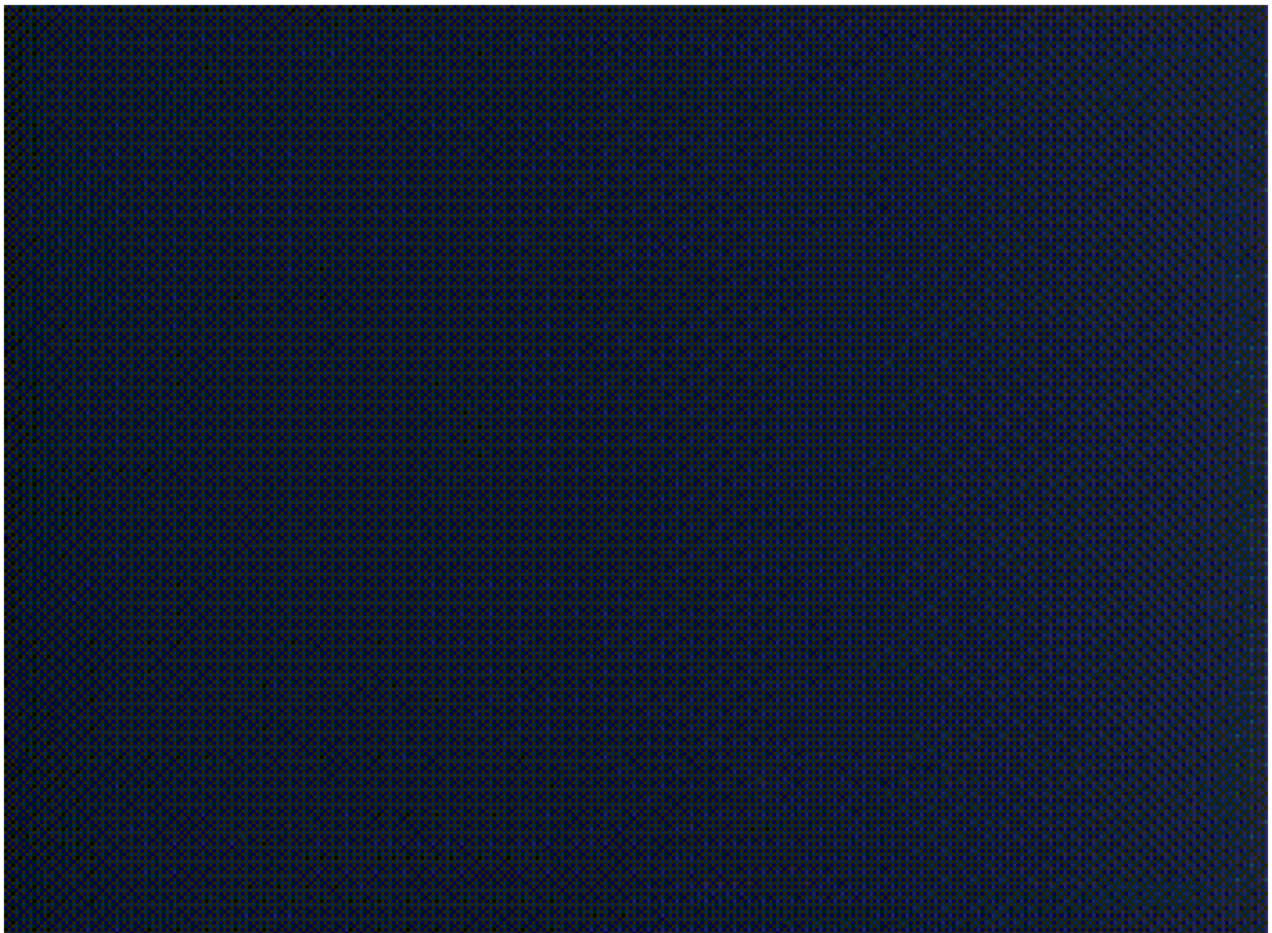
Electrons are also WAVES!

PROOF?

SHOWS INTERFERENCE



https://www.hitachi.com/rd/research/materials/quantum/doubleslit/index.html



DIRAC's VIEW EXPLAINS:

WE HAVE COME TO RECONCILE CLASSICAL AND Q-MECH BY DISCOVERING UNCERTAINTY

APPRECIATING 'CRAZY' ELECTRONS UNCERTAINTY WITH DIRAC AGAIN

SCHROEDINGER'S DIFFUSION EQUATION FROM HAMILTONIAN (QUANTUM)

UNCERTAINTY

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} \Longrightarrow \frac{\partial\rho}{\partial t} = D\frac{\partial\rho}{\partial x^2}$$

ELECTRON IS A 'CLASSICAL' PARTICLE WITH 'IMAGINARY' DIFFUSION CONSTANT!

WHO ORDERED THOSE "h"? HOW?

De Broglie: From Idea of Symmetry

Copenhagen Convention on Quantum Behavior

The moment the wavefunction is measured
The wavefunction collapses to
A Particle!

No body understands QMech!

Just describe it with Mathematics!

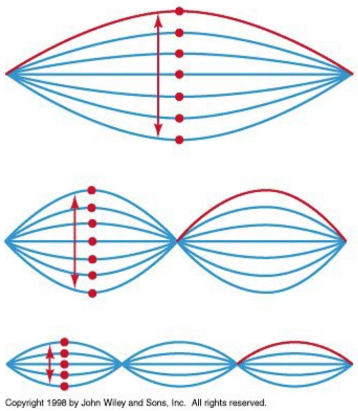
Richard Feynman on Quantum Behavior

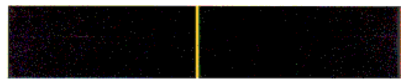
They behave in their own inimitable yet
fascinating manner, which we call
“Quantum Mechanical way“

We feel secure that Chemistry
Gives us a window to create matter
In spite of such uncertainties
of its constituents!

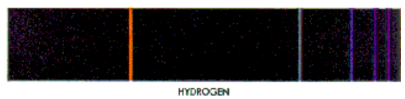
De Broglie Hypothesis: Matter Waves

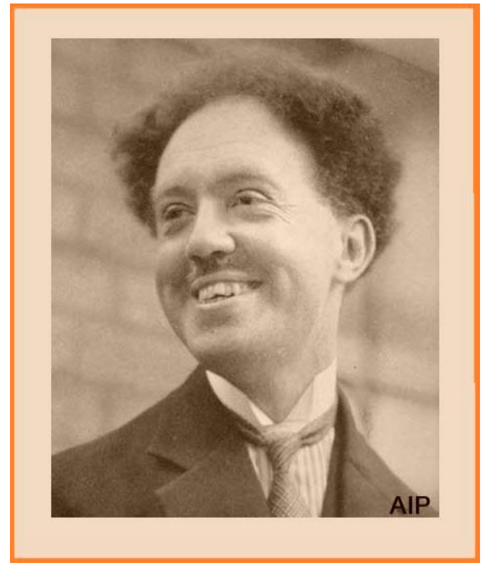
Symmetry manifests in duality of particles and waves!

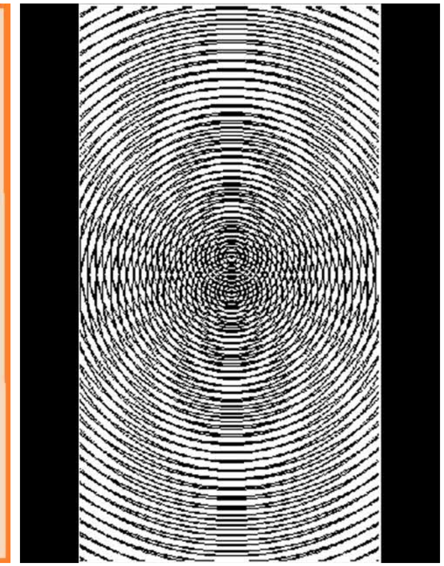




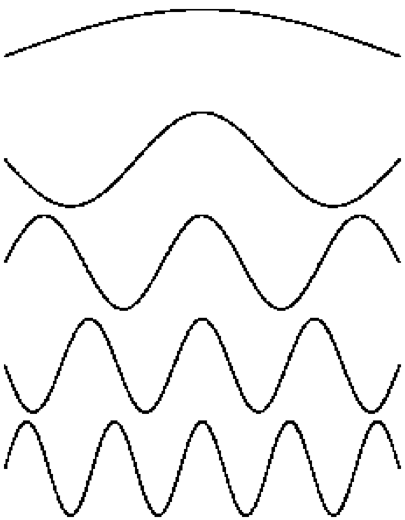
$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

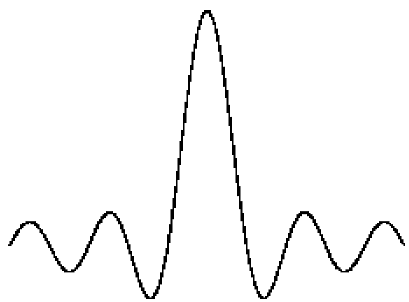






1892-1987





Electron-wave moving @ 10^6 m/s

$$\lambda = \frac{h}{mv} = \frac{6.6\text{x}10^{-34}\ \text{kg m}^2\ \text{s}^{2-}\ \text{s}}{9.1\text{x}10^{-31}\ \text{Kg} \times 1\text{x}10^6\ \text{m/s}} = 7 \times 10^{-10} m = 7\ \text{Å}$$

Compare the electron's λ to the diameter of atoms: 0.5 to 4 Å

What did the fitting coefficient 'h' do?

Helped explaining 3 problems:

1. **Black Body Radiation**
2. **Nature of light**
3. **Structure of Atoms**

What did we learn so far?

1. We learnt how Matter came into being.

2. To understand that becoming we learnt that Symmetry, Energy and Conservation are threaded and encrypted in Noether's Theorem.

3. We further learnt that Matter is particulate (Made of Particles) and as they are threaded with rules of Symmetry and Energy, so structure is a function of energy and numbers.

Consequence: g(r)

What did we learn so far?

4. g(r) takes care of the state of matter.

5. Matter shows phases, which can be understood with g (r).

6. We learnt how particulate matter's structure in various phases can be determined by bouncing waves of light on its surface and how there g (r) helps.

7. We then saw what happens when these particles change size and their interactions change (different liquids).

What did we learn so far?

8. We visited critical phenomenon.

9. We saw criticality and its possibility for making of new materials in the light of g (r).

10. We learnt that how particle's motion can become 'fuzzy' as they become smaller.

11. We learnt how Einstein described that motion exactly using same type of functions as we use to explain planetary motions in a way. (Use of Lagrangian)

What did we learn so far?

12. We even reduced the size of those particles.

13. We then learnt how Dirac related the Brownian Motion with 'wavy'motion of electrons.

13. We learnt Schroedinger Equation and came to the idea of 'Particles diffusing with imaginary diffusion coefficients' using Dirac's formalism.

What did we learn so far?

14. Such an idea quantitatively led us to 'see' that both classical and quantum behaviour are 'operationally similar' but changes with introduction of 'h'.

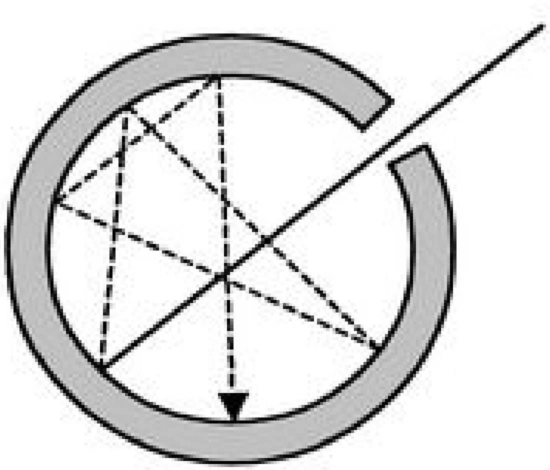
13. 'h' takes care of uncertainties.

14. Consequence of uncertainties are:.

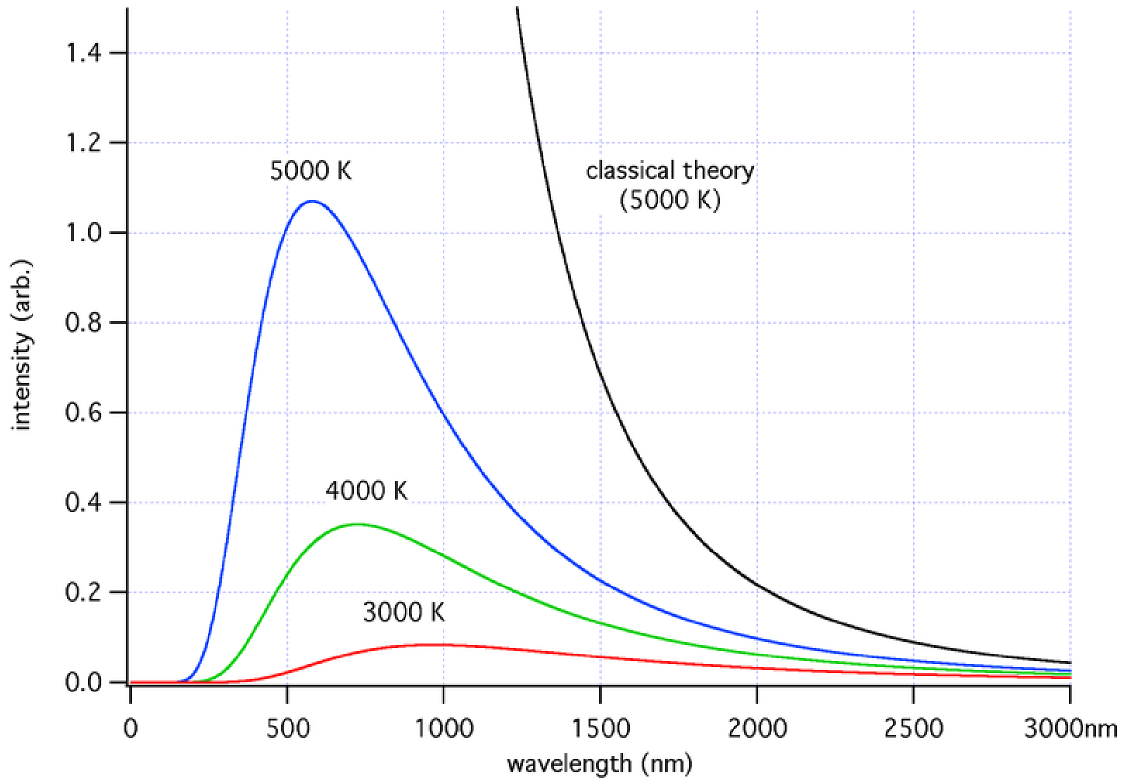
15. Electrons are Dualistic: wave/particle.

16. Light is also dualistic: wavy and particle like.

Classical EM theory can not explain Blackbody Radiation



Sun, stars…hot iron rod

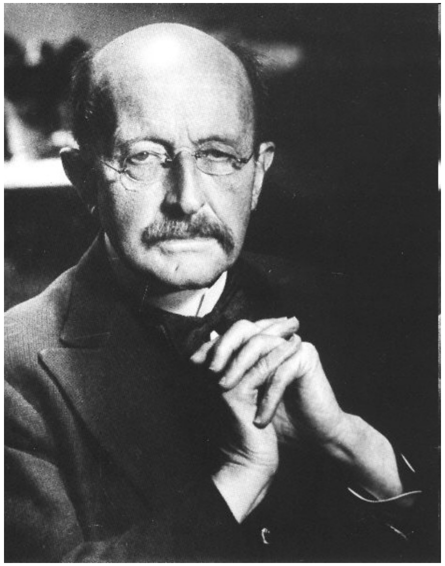


Theories based on classical physics unable to explain temperature dependence of emitted radiation (radiant energy density)

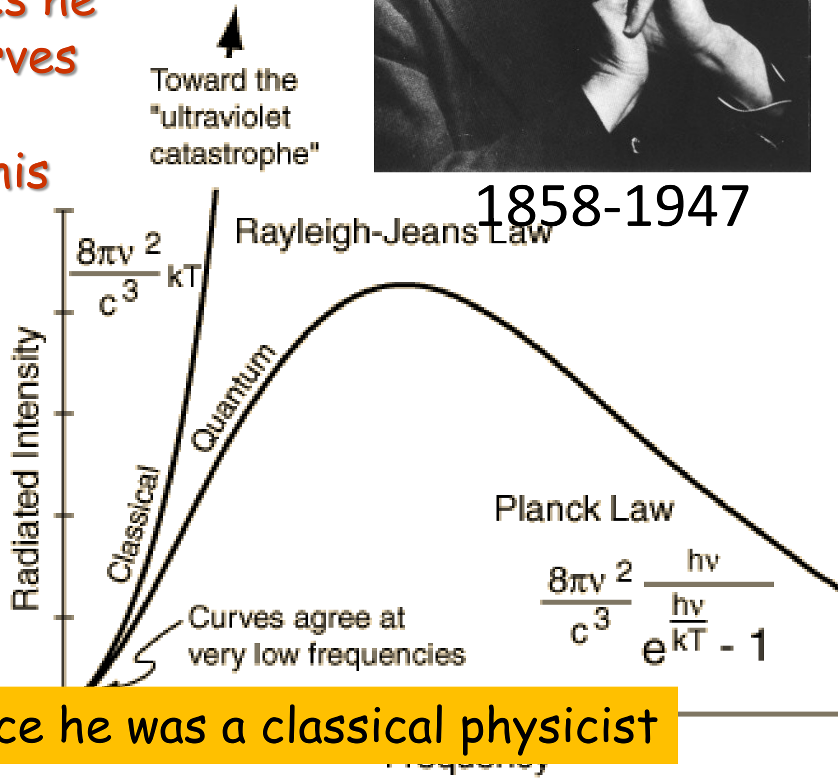
Max Planck assumed energies of oscillators are discontinuous

Assumption:

- Presence of electronic oscillators in these materials which must be giving of radiation
- *Energy of electronic oscillators were discrete; Proportional to integral multiple of frequencies*
- Proposed that this radiation was being emitted in quanta or chunks
- Using this idea and some statistical mechanics he was able to calculate the shapes of these curves
- To get the intensity correct he had to use scaling factors in front of the frequency of his oscillators -the Plank's constant.



1858-1947



E = Energy of electronic oscillators
v = frequency of electronic oscillators
h = Planck's constant = 6.626 x e^{-34} joule-sec
<u>Note</u>: h came in as a fitting parameter

$$E_{Osc} = nh\nu$$

Planck never believed his theory was right, since he was a classical physicist

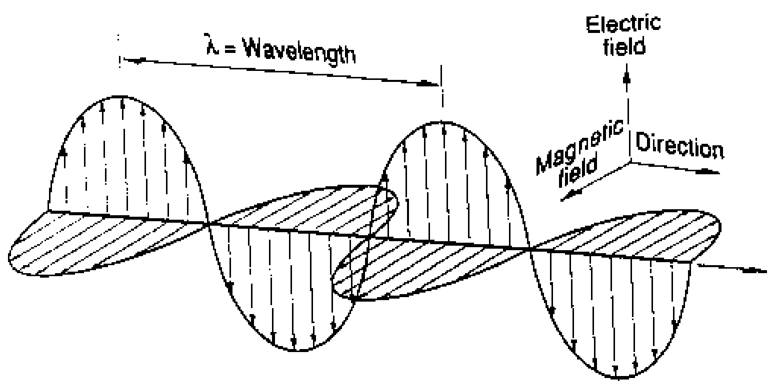
What did the fitting coefficient 'h' do?

Helped explaining 3 problems:

1. Black Body Radiation
2. Nature of light
3. Structure of Atoms

We move to explain Nature of light.

Light is EM Radiation: Waves

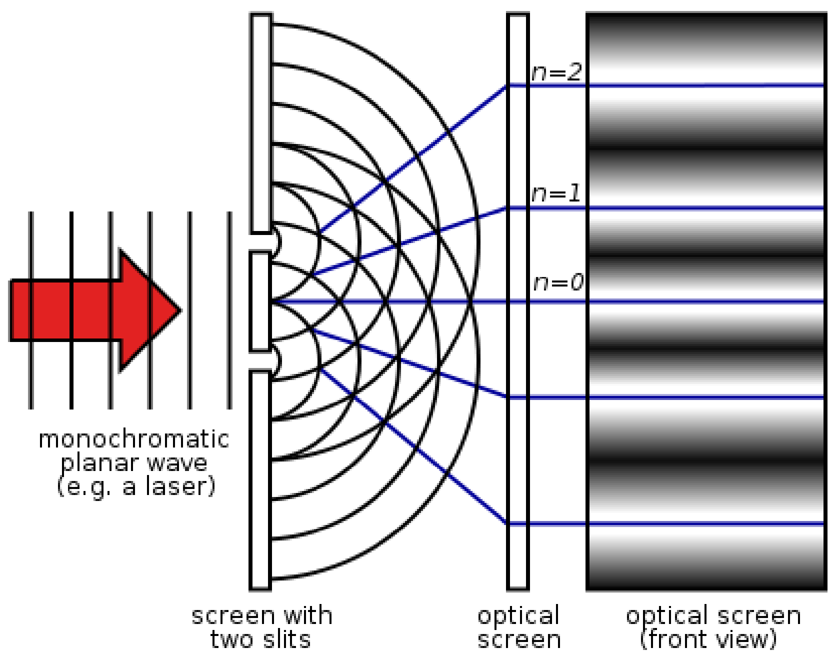


$$E = E_m Sin(kx - \omega t)$$

$$B = B_m Sin(kx - \omega t)$$

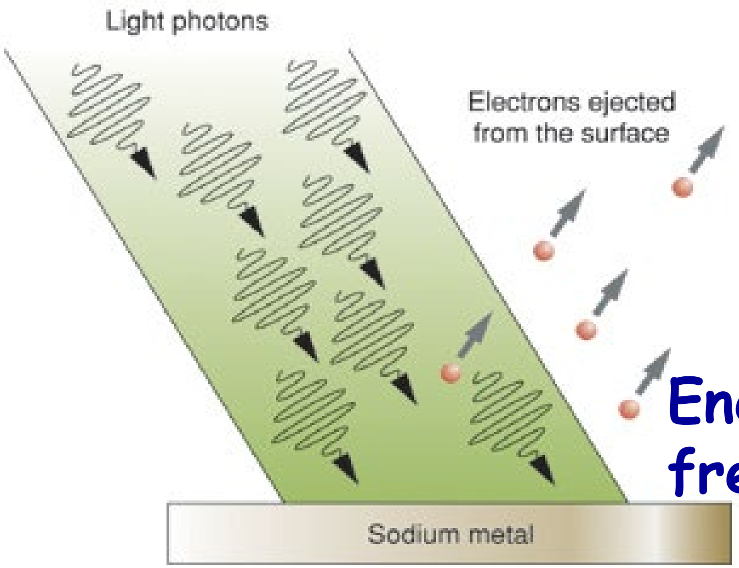
$$\frac{E_m}{B_m} = c \sim 3\times 10^{10}\, cm/\sec$$

Diffraction or Interference Pattern can be possible only if light is a wave



Einstein: light behaves like particles

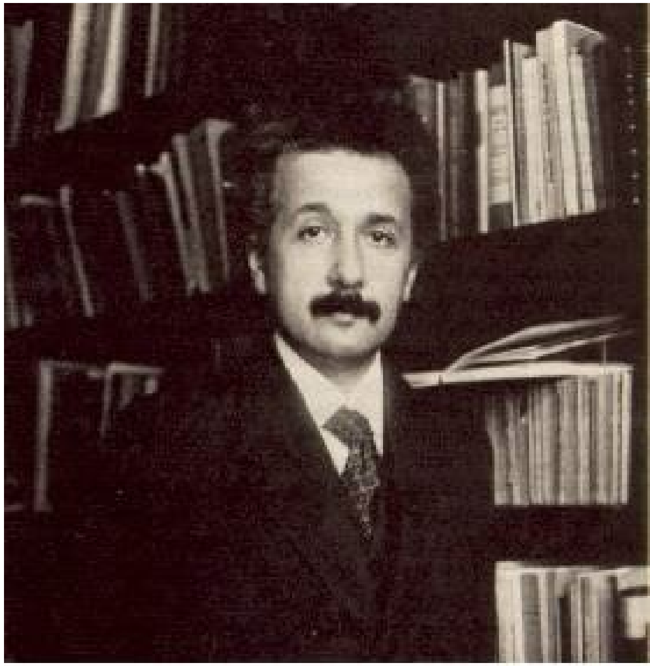
Embracing Planck's idea that $\Delta E = h\nu$, Einstein further proposed radiation itself existed as small packets of energy (Quanta), known as PHOTONS



$$E_P \propto \nu$$

$$E_P = h\nu$$

Energy of photon is frequency dependent



Albert Einstein

$$E_P = h\nu = KE_M + \phi = \frac{1}{2}mv^2 + \phi$$

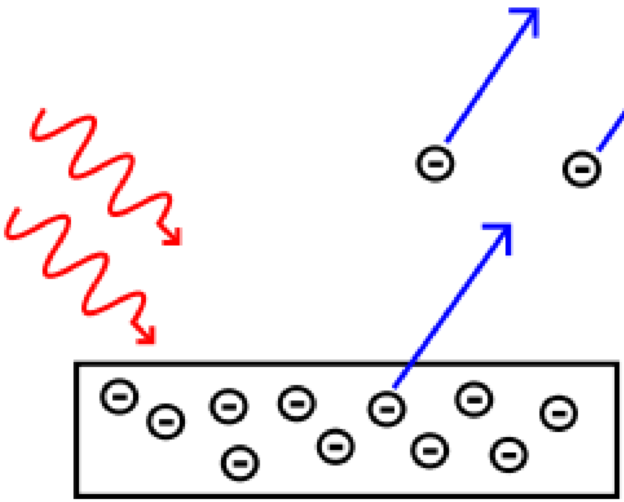
$$\phi = \text{ Energy to remove e' from surface}$$

$$KE_M = h\nu - \phi_0 \geq 0$$

1879-1955; Nobel prize For explanation of Photoelectric effect

Photoelectric Effect

Photodetectors, Photovoltaics, Elevator sensor, smoke detectors



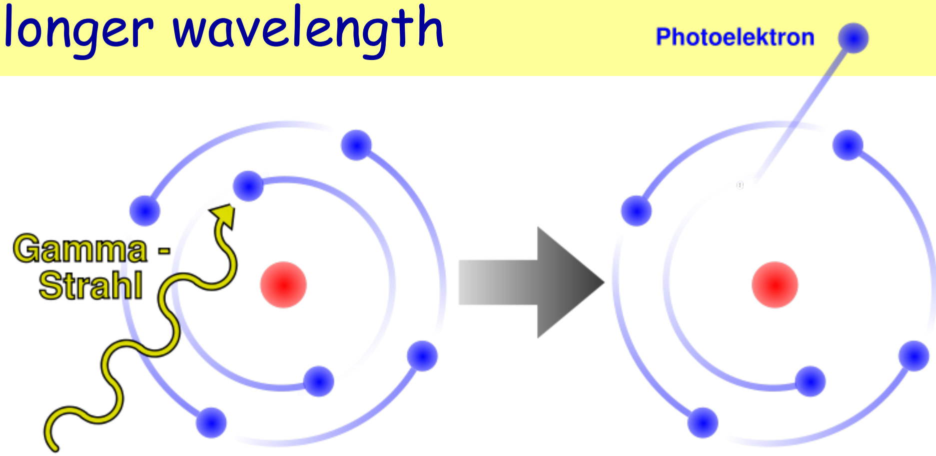
- Classical physics predicted that kinetic energy would not change with the frequency of light
- In addition it predicted that KE should be dependent on the Intensity of light.

Experimental Observations

1. Increasing intensity of light increases number of photoelectrons, but not their max. kinetic energy (KE_{MAX})!

2. Light below a certain wavelength will not cause ejection of electrons, no matter how high it's intensity!

3. Extremely weak violet light ejects few electrons! But their KE_{Max} >> KE_{Max} of electrons ejected by intense light of longer wavelength



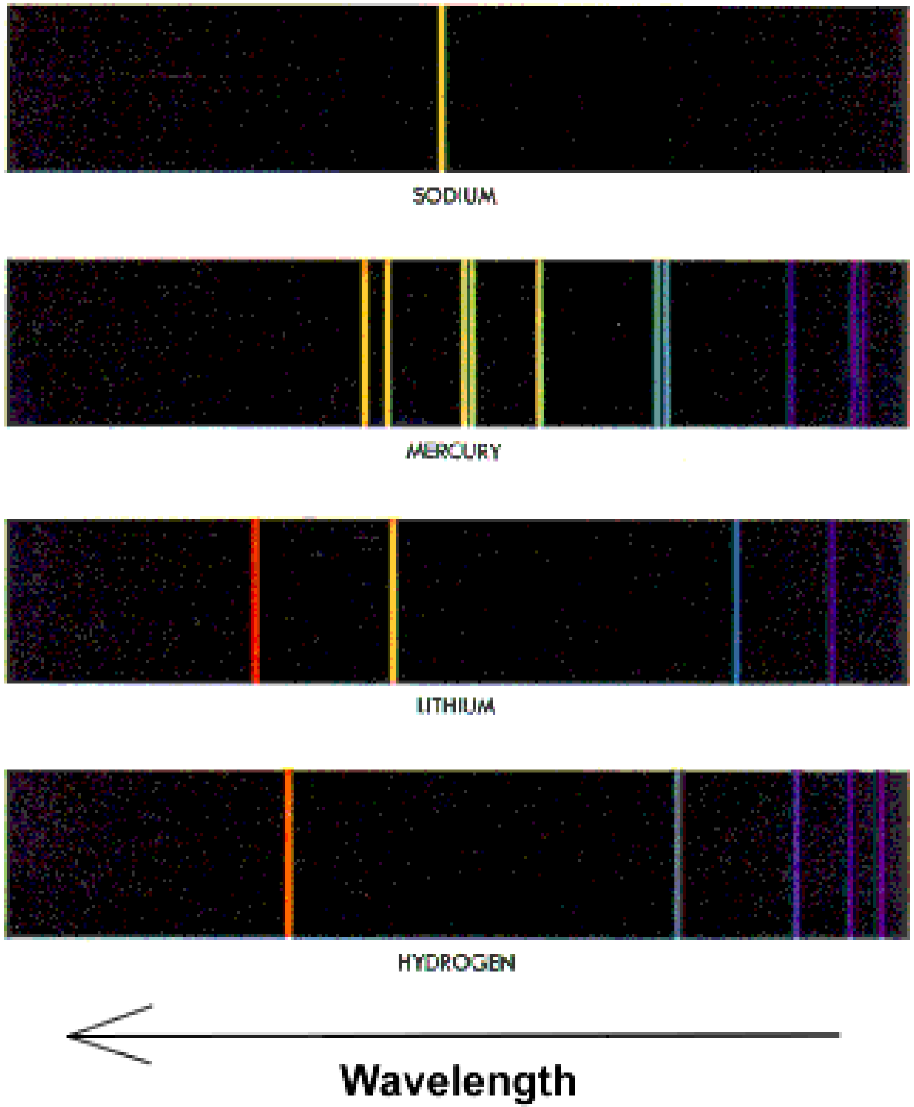
What did the fitting coefficient 'h' do?

Helped explaining 3 problems:

1. Black Body Radiation
2. Nature of light
3. **Structure of Atoms**

On structure of Atoms.

Line Spectra of Atoms



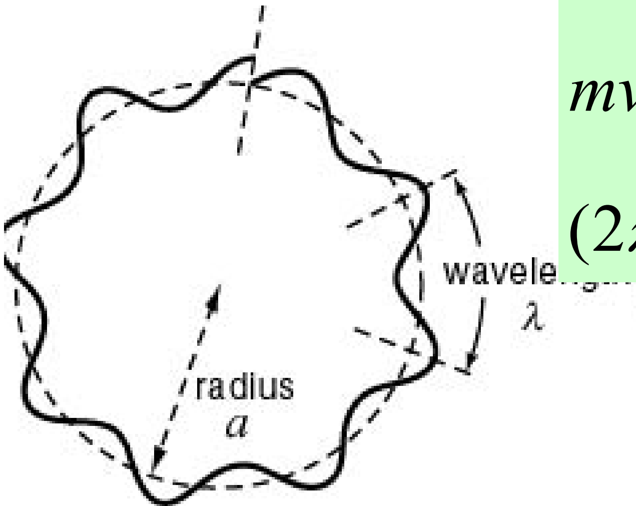
1854-1919

Rydberg's formula:

$$\bar{\nu} = \frac{\nu}{c} = \frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right); \quad n_1 > n_2$$

$R_H = 109677.57\ cm^{-1}$

Explanation of atomic spectra



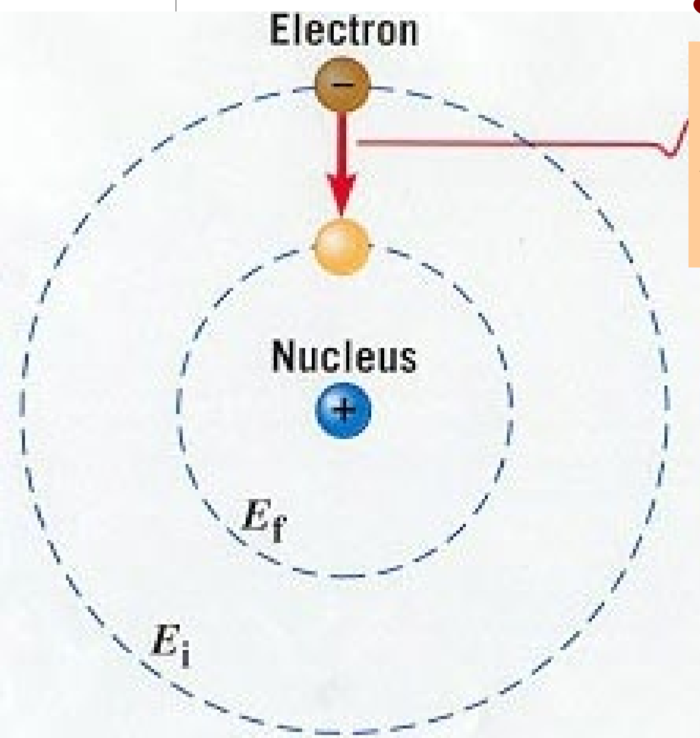
$$mvr = \frac{nh}{2\pi} \qquad n=1,2,3,\ldots$$

$$(2\pi r = n\lambda\ )$$

Quantization of Angular momentum

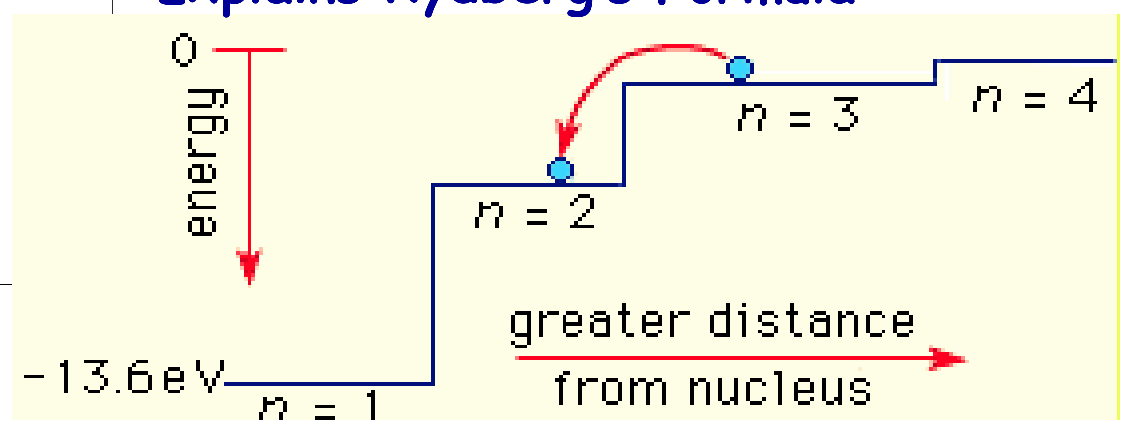
$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2} \cdot \frac{1}{n^2}$$

Spectral Transitions: $\Delta E = hc/\lambda$

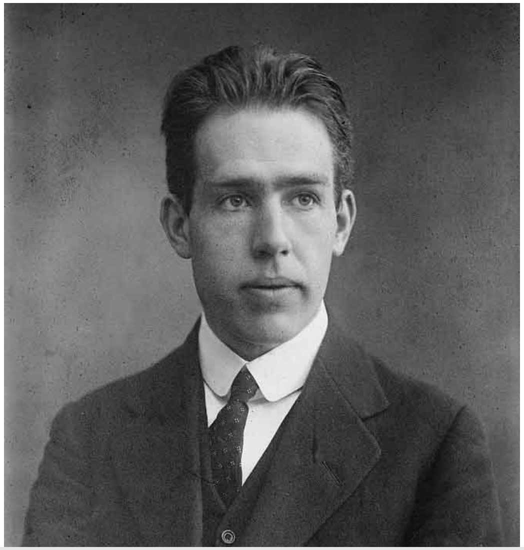


$$\Delta E = \frac{m_e e^4}{8\varepsilon^2 h^2}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right) = h\nu \quad n_i, n_f = 1, 2, 3, \ldots$$

Explains Rydberg's Formula



Bohr's Phenomenological Model
(Rutherford-Planck-Einstein-Bohr Model)



1885-1962

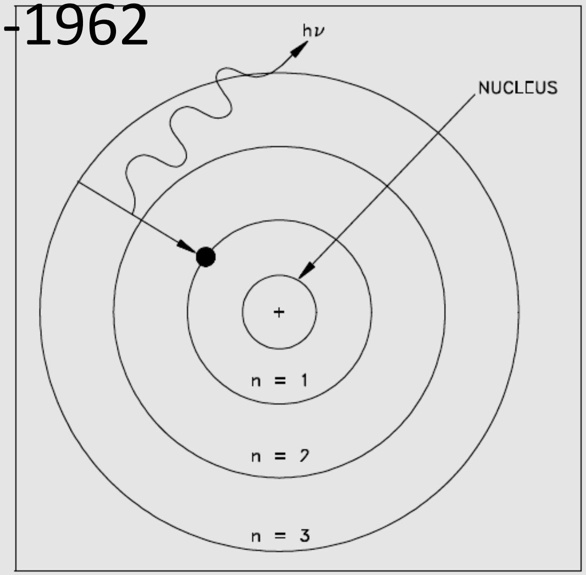


Figure 1 Bohr's Model of the Hydrogen Atom

- Electrons rotate in circular orbits around a central massive nucleus (+ve), and obey laws of classical mechanics.
- Allowed orbits are those for which the electron's angular momentum $m_e vr = n\, h/2\pi$, n=1,2,3,4,……
- Only certain discrete energy values: "Stationary States" - Atom in such a state does not emit EM radiation (light)
- Transition from a stationary state (E_a) to another (E_b), atom emits or absorbs EM radiation (light)

What did we learn today?

1. Learnt Electrons are 'Crazy', at times they are waves and when we 'see' those waves they become particles.

2. Learnt Light too is 'Crazy', at times they are waves and when we 'see' those waves they become particles.

3. Electrons 'make' Atoms and they are 'wavy And particle-like'