Quantum Mechanics I

Lecture Notes by Wladimir E. Banda Barragán

School of Physical Sciences and Nanotechnology
Yachay Tech University

November 2022 - March 2023

UC1
The Schrödinger equation

UC1 contents:

- Review of quantum experiments and mathematical tools.
- The wave function and the Schrödinger equation.
- Statistical interpretation of the wave function and probability.
- Normalisation, momentum, and the uncertainty principle.

What is Quantum Mechanics (QM)?

- QM deals with small scales.
- QM can be abstract, counterintuitive and hard to grasp.
- QM is mathematically challenging.
- QM is not deterministic as it is associated with probabilities.
- Despite this, it is a linear theory, so there is harmony in the equations and there is no chaos as in Classical Mechanics (CM).

What is Quantum Mechanics (QM)?

- **Richard Feynman:** "I think I can safely say that nobody understands QM."

- "There is no general consensus as to what its fundamental principles are, how it should be taught, or what it really means."

- "QM was not created by one individual", like other theories (e.g., GR, EM).

- **<u>The purpose of this class is to teach you how to DO and USE quantum mechanics.</u>**

Reference: Griffiths 1995

What is Quantum Mechanics (QM)?

- **D. Griffiths:** “I do not believe one can intelligently discuss what quantum mechanics means until one has a firm sense of what quantum mechanics does."

- “Not only is quantum theory conceptually rich, it is also technically difficult.”

  e.g. Linear algebra, complex numbers, partial derivatives, Fourier analysis, classical mechanics, electrodynamics.

- “Using the right tool makes the job *easier,* not more difficult”

  e.g. Legendre, Hermite, and Laguerre polynomials, spherical harmonics, Bessel, Neumann, and Hankel functions, Airy functions, Hilbert spaces, Hermitian operators, Clebsch- Gordan coefficients, and Lagrange multipliers.

Reference: Griffiths 1995

What is Quantum Mechanics (QM)?

- “Don't let the mathematics (which, for us, is only a tool) interfere with the physics.”

- “QM represents an abrupt and revolutionary departure from classical ideas, calling forth a wholly new and radically counterintuitive way of thinking about the world.”

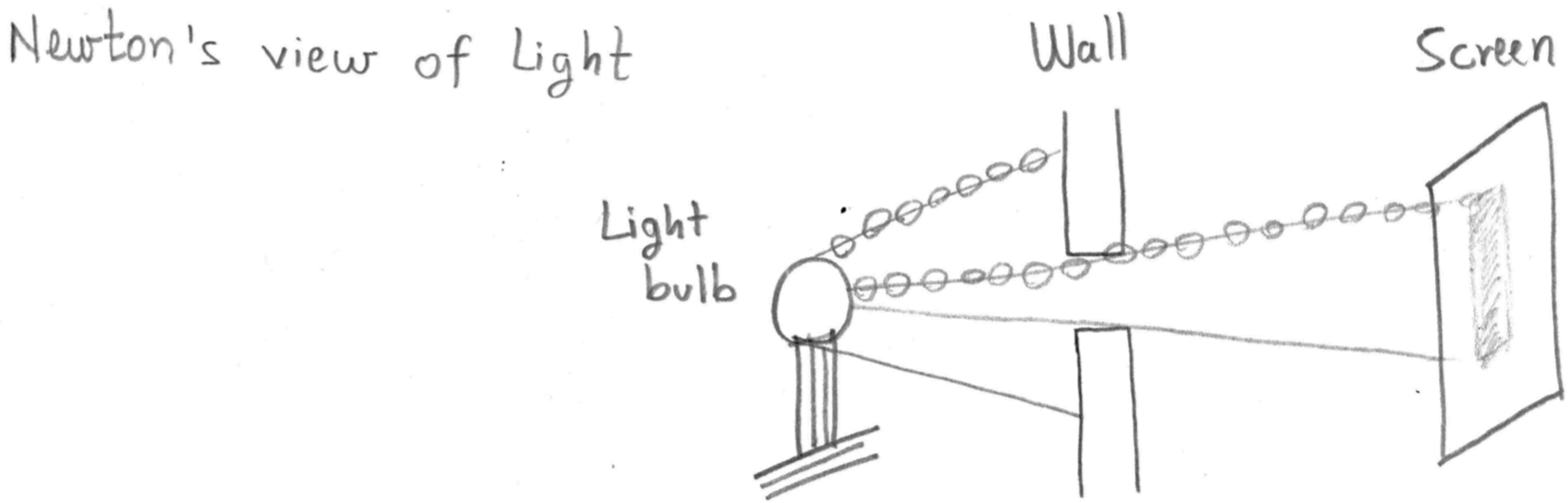
- **<u>QM is a (mathematical) framework to do physics (at small scales).</u>**

Reference: Griffiths 1995

Brief history of QM

<u>Experiments and basic ideas</u> that led to the formulation of QM:

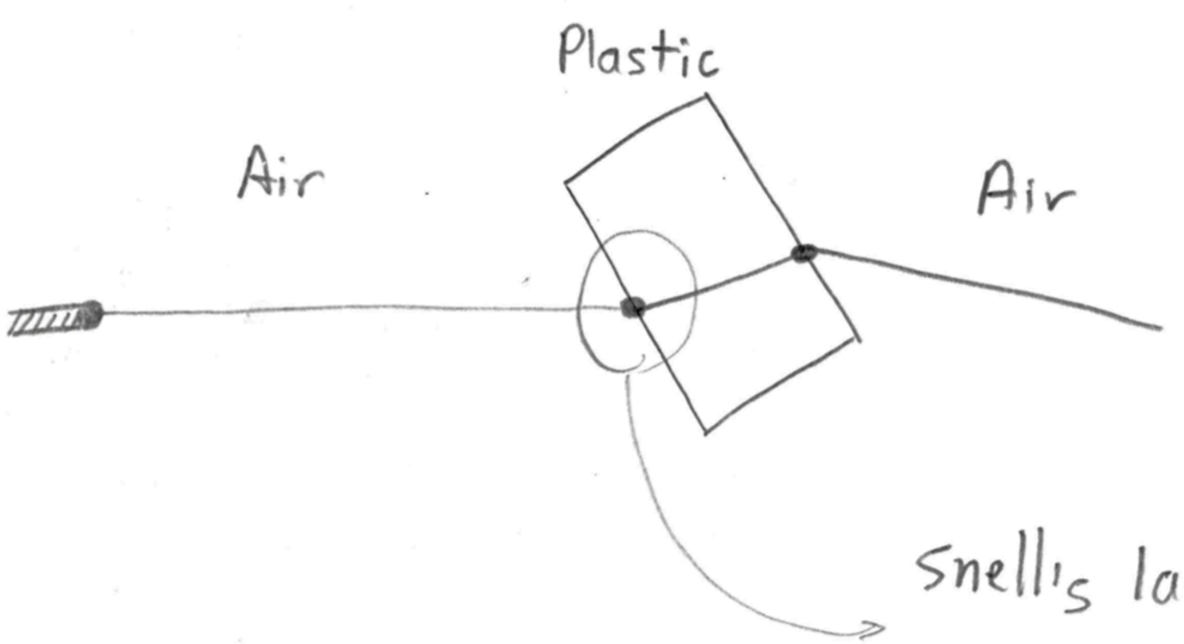
- The earliest ideas that would eventually lead to the formulation of QM emerged from trying to understand the nature of light.
- In the 1600's, I. Newton proposes light is made of a beam of particles, based on this experiment:



Brief history of QM

- Also in the **1600's,** R. Hooke proposes light is made of waves based on refraction experiments. Refraction can be explained by considering light as composed of waves.

Refraction:



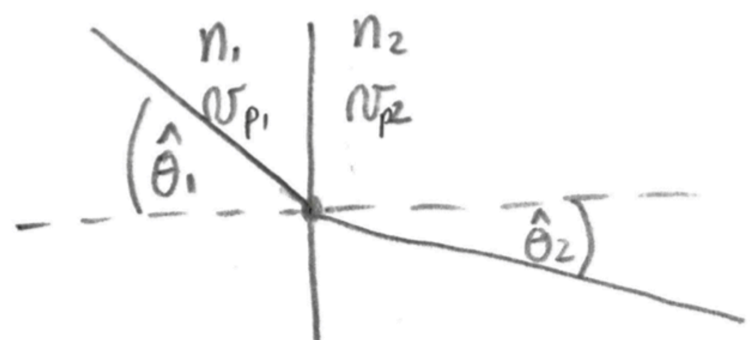
$n \equiv$ refractive indices $\equiv \frac{c}{v_p} = \frac{ck}{\omega}$

$v_p \equiv$ phase velocities $= \frac{\omega}{k} = \frac{\lambda}{T}$

$\hat{\theta}_1 \equiv$ incidence angle

$\hat{\theta}_2 \equiv$ refraction angle

Snell's law



$$\boxed{\frac{\sin \hat{\theta}_1}{\sin \hat{\theta}_2} = \frac{v_{p1}}{v_{p2}} = \frac{n_2}{n_1}}$$

$$\omega = \frac{ck}{n} \Rightarrow \frac{d\omega}{dk} = \overbrace{\frac{c}{n}}^{v_p} - \frac{c}{n^2}\frac{dn}{dk} \equiv \text{group velocity}$$

Brief history of QM

- **1800's** - Experiments on interference and diffraction probe Hooke's ideas correct.
- **1800's** - K. Maxwell compiles the EM equations. Light is EM radiation.

Gauss' law:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

Gauss' law for magnetism:

$$\nabla \cdot \mathbf{B} = 0$$

Maxwell–Faraday equation (Faraday's law of induction):

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

Maxwell–Ampère equation (circuital law):

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}$$

Reference: https://www.cantorsparadise.com/maxwells-equations-7484212839b1

Particle nature of EM radiation

- **End of 1800's** - Black-body radiation could not be explained by EM theory framework.

An object can absorb/emit radiation: $\begin{cases} \text{Absorption} \uparrow T \\ \text{Emission} \downarrow T \end{cases}$

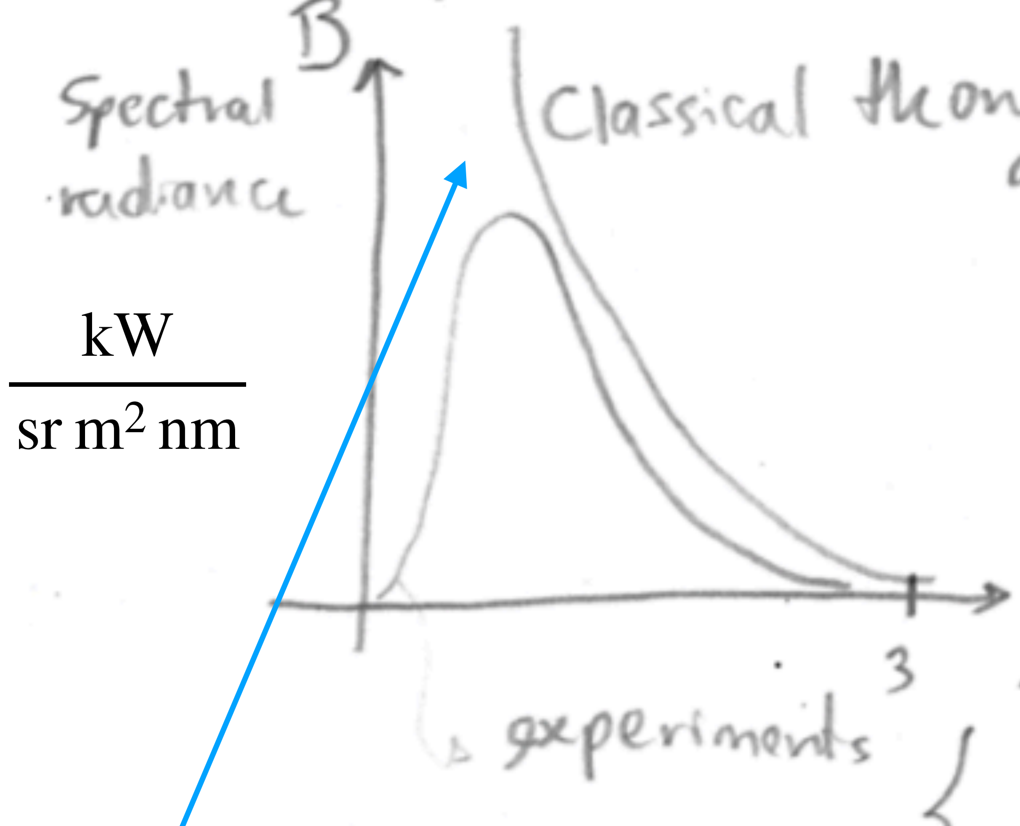
Kirchoff's law: Abs = Emission $\Rightarrow T = ct. \Leftrightarrow$ thermal eq.

Black body: Does not reflect radiation

Particle nature of EM radiation

- **End of 1800's** - Black-body radiation could not be explained by EM theory framework.

Black body radiation:



UV catastrophe

$$\begin{cases} B_\lambda(T) = \dfrac{2ck_BT}{\lambda^4} \\ B_\nu(T) = \dfrac{2\nu^2 k_B T}{c^2} \end{cases}$$

Rayleigh-Jeans law

$$k_B = 1.38\times 10^{-23}\ m^2\,kg\,s^{-2}\,K^{-1}$$

$$\begin{cases} B_\lambda(T) = \dfrac{2hc^2}{\lambda^5}\dfrac{1}{e^{\frac{hc}{\lambda k_B T}}-1} \\ B_\nu(T) = \dfrac{2h\nu^3}{c^2}\dfrac{1}{e^{\frac{h\nu}{k_B T}}-1} \end{cases}$$

Particle nature of EM radiation

- **1900 -** M. Planck proposes quantisation of EM radiation

Planck: EM can only be em./abs in discrete packets:

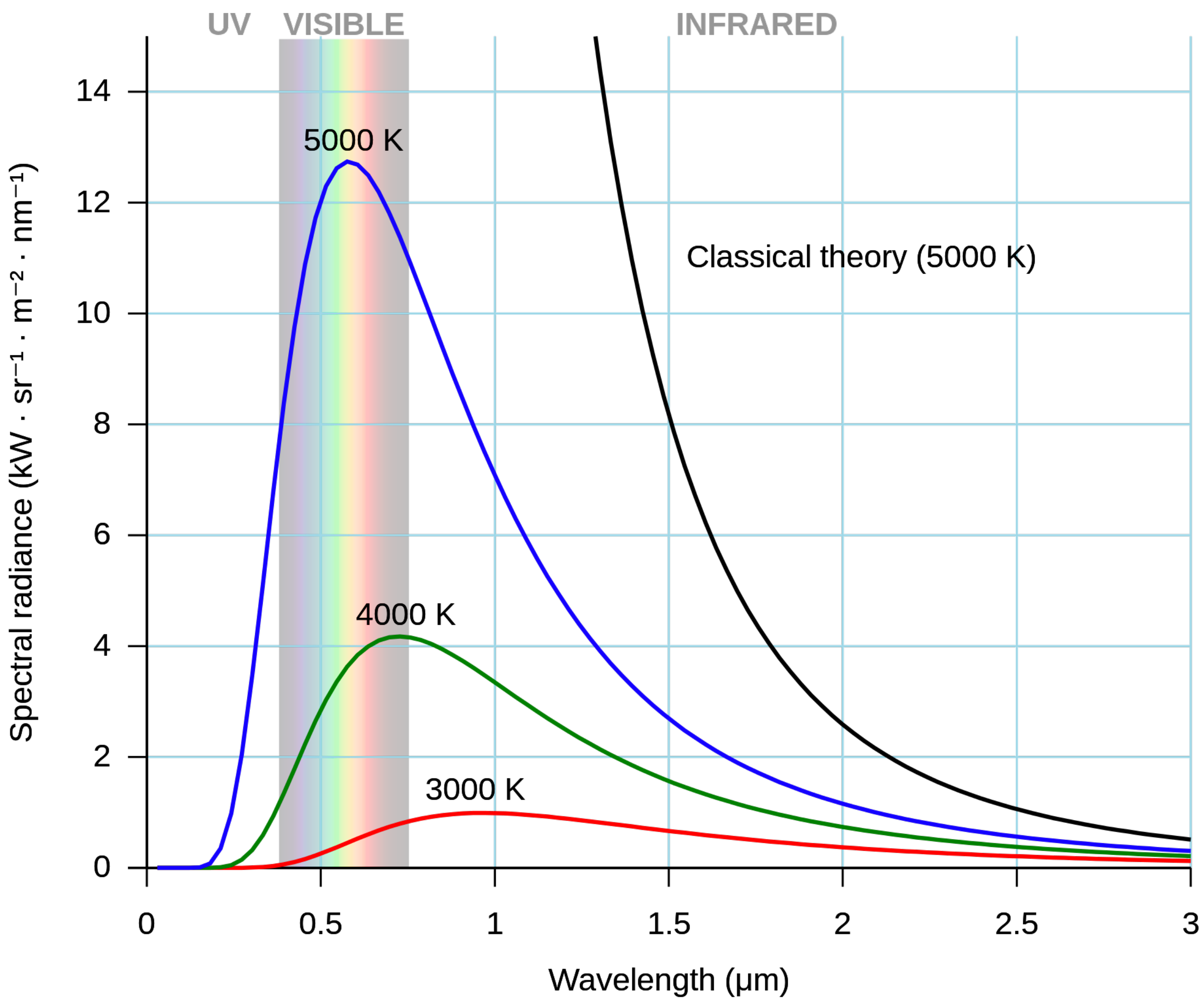
$$\boxed{E_{quanta} = h\nu = h\frac{c}{\lambda}}$$

- $E = h\nu = \hbar\omega$
- $\vec{p} = \hbar\vec{k}$

$$\hbar = \frac{h}{2\pi}$$

De Broglie relation:

$$\boxed{\lambda = \frac{2\pi}{k} = \frac{h}{p}} \Rightarrow E = pc$$



UV catastrophe

Reference: https://en.wikipedia.org/wiki/Ultraviolet_catastrophe

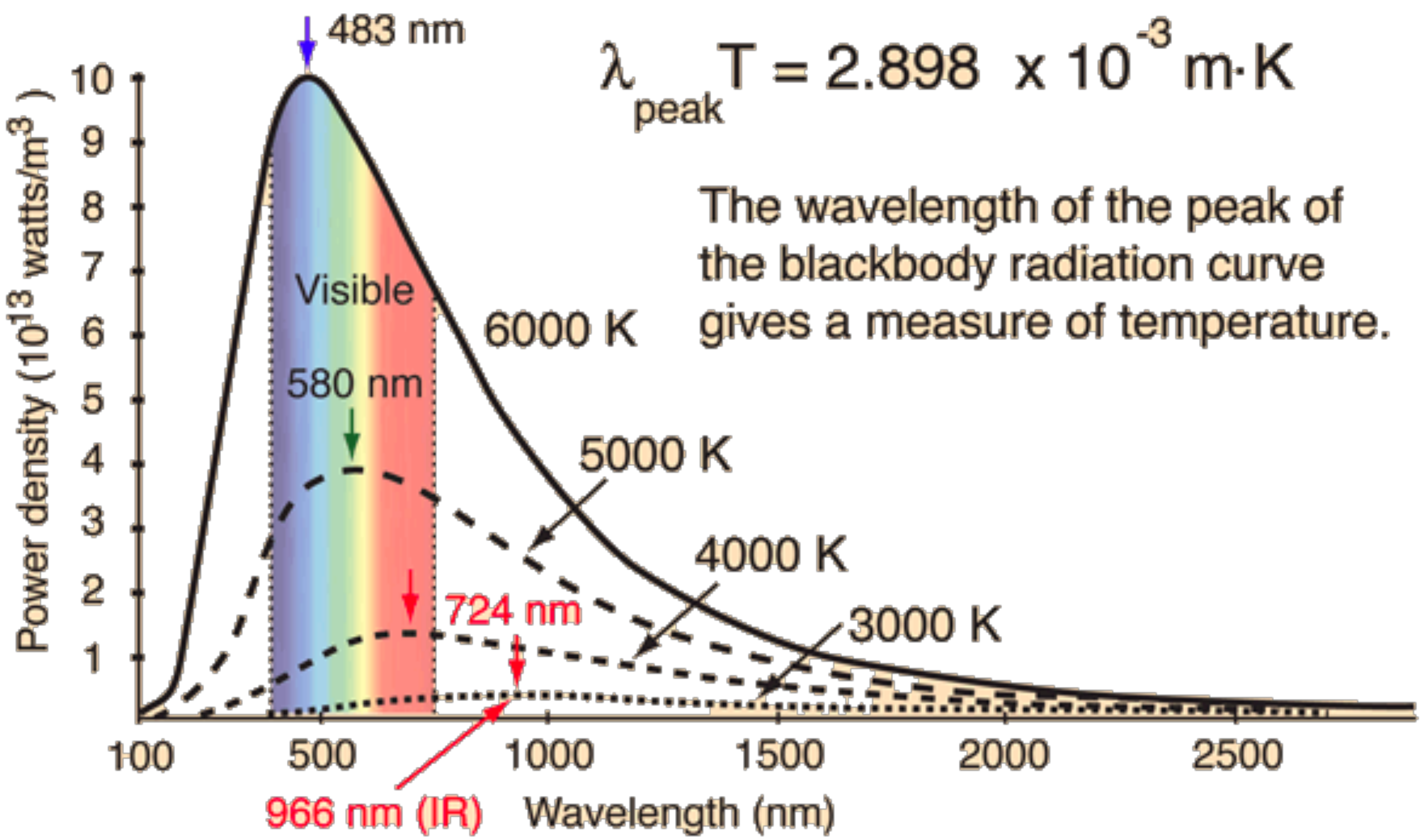
Particle nature of EM radiation

- **Wien's displacement law:**

λ at which an object emits more radiation.

$$\lambda_{\substack{max \\ peak}} = \frac{b}{T} \quad ; \quad b = 2.898 \times 10^{-3}\, mK$$

$$\nu_{peak} = \frac{\alpha}{h} kT \approx 5.879 \times 10^{10} \frac{Hz}{k} \cdot T$$



Reference: http://hyperphysics.phy-astr.gsu.edu/hbase/wien.html

Particle nature of EM radiation

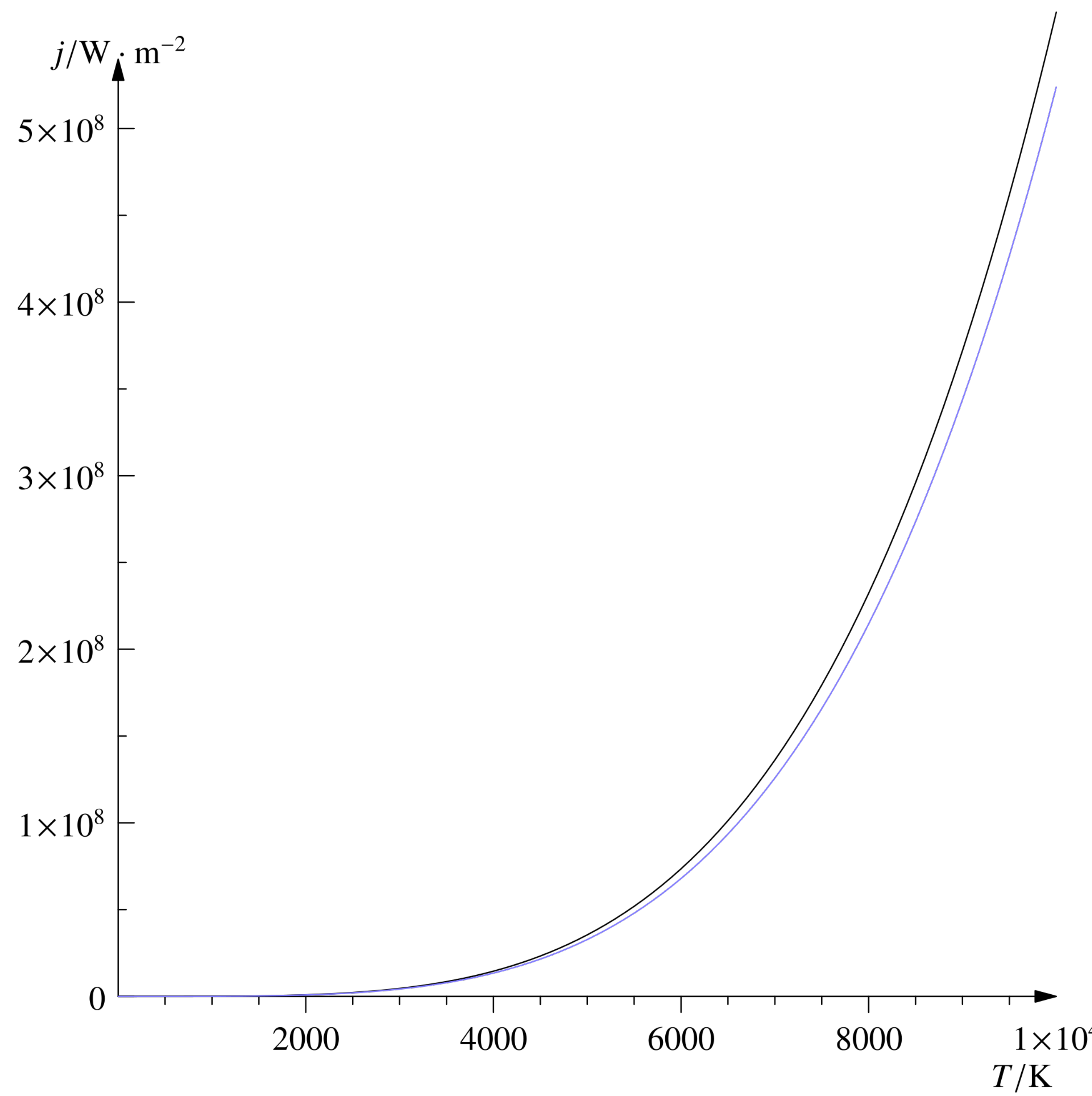
- **Stefan-Boltzmann law:**

Total radiation emitted at all λ:

$$j = \sigma T^4 \quad \left[\frac{W}{m^2}\right]$$

$$\sigma = \frac{2\pi^5 k^4}{15 c^2 h^3} = 5.67 \times 10^{-8} \frac{W}{m^2 K^4}$$

↳ SB constant



Reference: https://en.wikipedia.org/wiki/Stefan%E2%80%93Boltzmann_law

Particle nature of EM radiation

- **Planck's constant:** h

The units of h are units of angular momentum.

$$E_\gamma = h\nu$$

Units of h: $$[h] = \frac{[E]}{[\nu]} = \frac{[ML^2T^{-2}]}{[T^{-1}]} = [ML^2T^{-1}]$$

$$[h] = \underset{\text{Length}}{L} \cdot \underset{\text{Momentum}}{[MLT^{-1}]} = [r]\cdot[p] = \underset{\text{Angular momentum}}{[\ell]}$$

Example:

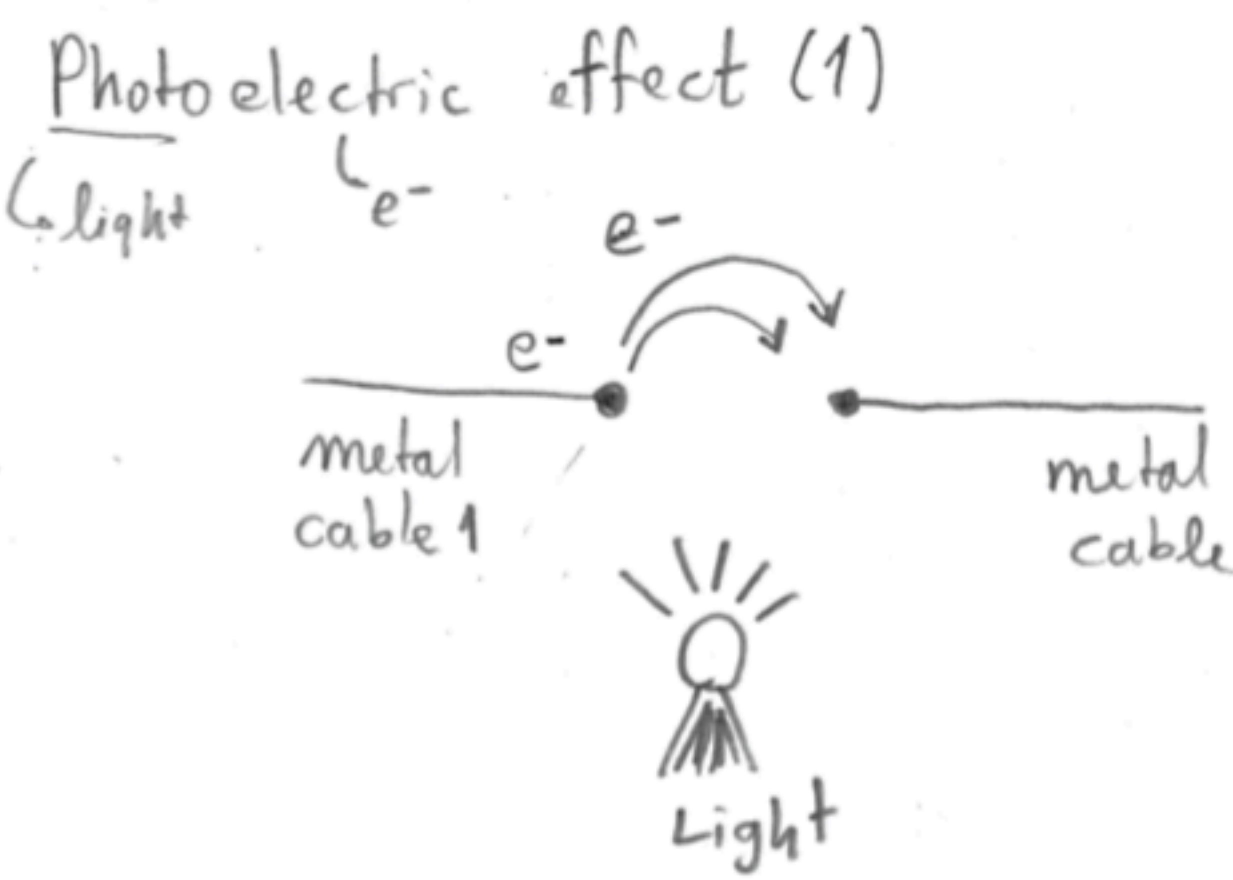
Spin 1/2 particle

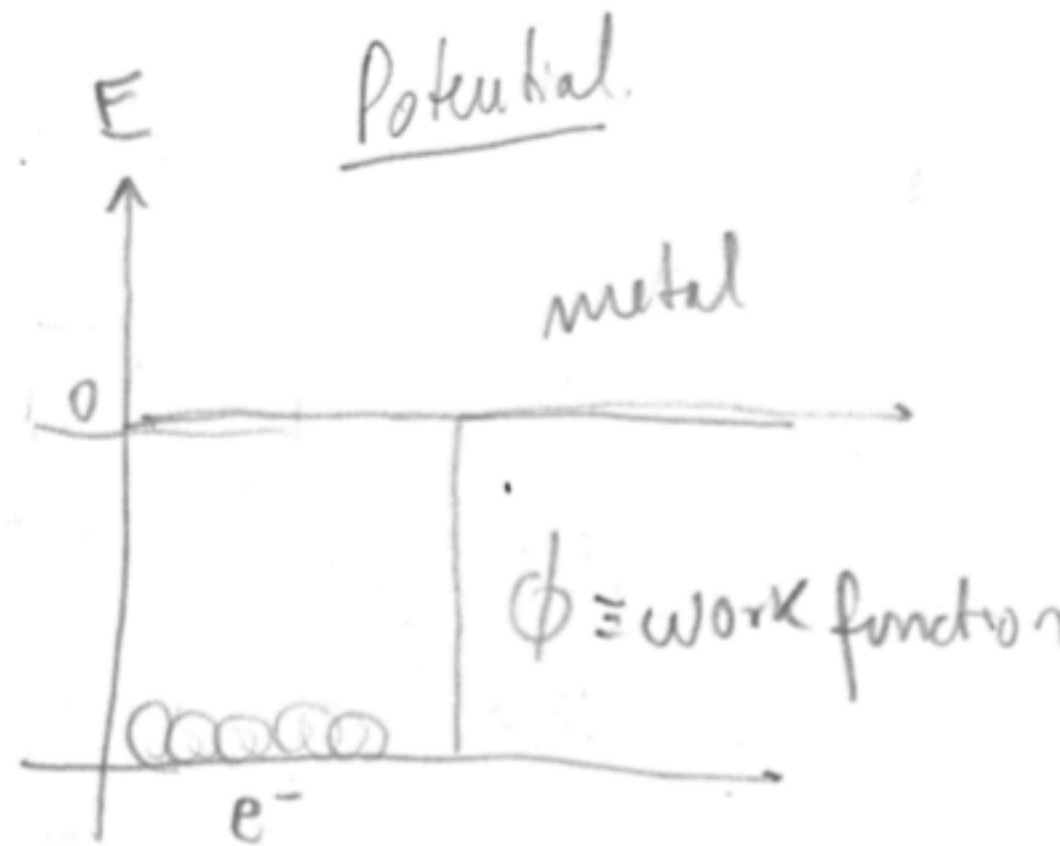
$$|\vec{s}| = \frac{1}{2}\hbar$$

The Photoelectric Effect

It is a process by which e- can be removed from a metal surface.

- **1887 -** H. Hertz discovers the Photoelectric Effect by irradiating metal plates with light.
- Irradiated polished plates emit photons called photo-electrons.





The Photoelectric Effect

- **Why does the photoelectric effect occurs?**

Classical (wave) view:

⇒ Should happen for all (any) λ

- **Did experiments agree?** No.

Photoelectric effect occurs:

Only for some λ

For other λ → no e- jump

The Photoelectric Effect

- **Einsteins' view:** photons come in packets of energy.

Einstein: Beam of light ν

Photons γ $\quad E_\gamma = h\nu$

$h \equiv$ Planck's constant $= 6.63 \times 10^{-34}\ J\cdot s$

$$E_\gamma = h\frac{c}{\lambda} = \frac{2\pi\hbar c}{\lambda}$$

$\hbar = \frac{h}{2\pi}$

$\hbar c = 200\ MeV\cdot fm \to$ fermi

$fm = 10^{-15}\ m$

$\hbar c = (197.33)$

- **Einsteins' prediction:**

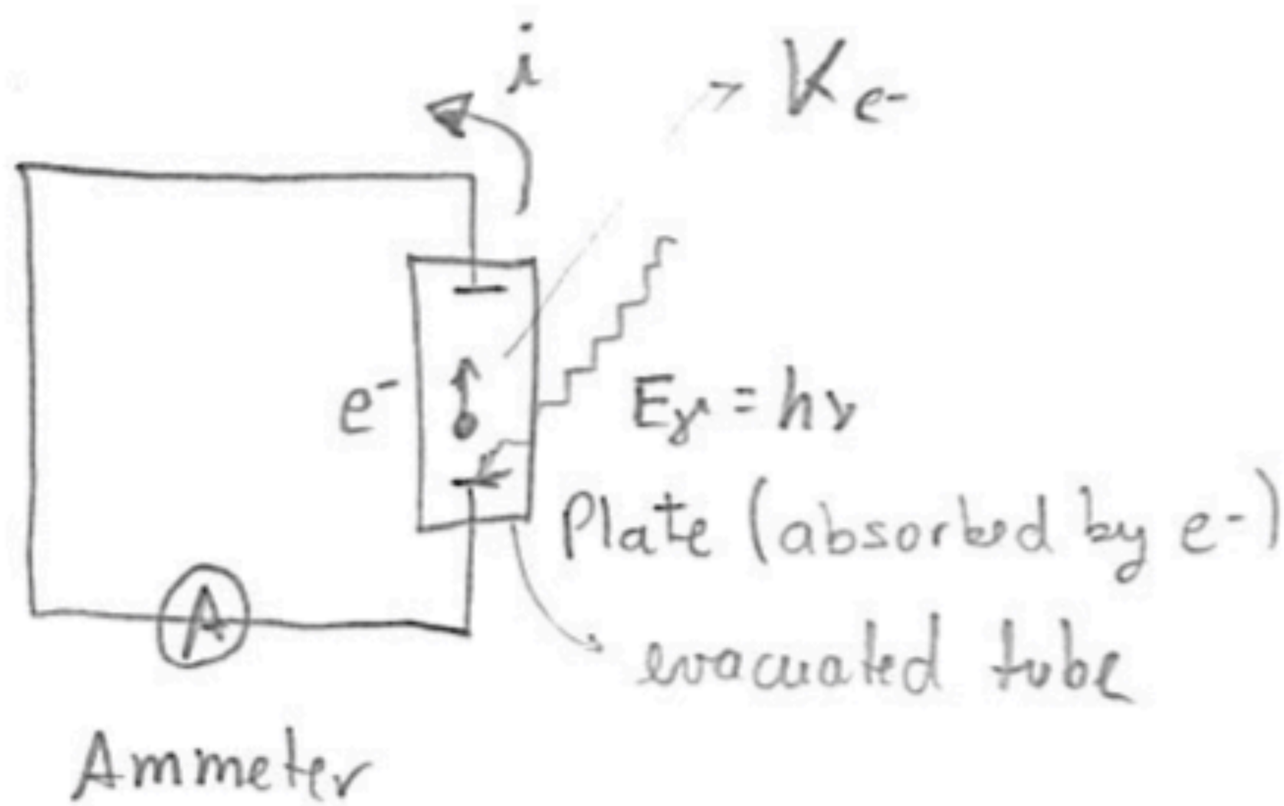
$$\underbrace{E_{e^-} = \frac{1}{2}mv^2}_{\text{Leftover energy}} = \underbrace{E_\gamma}_{\text{E given to e}^-} - \underbrace{\phi}_{\text{E needed to liberate e}^-} = h\nu - \phi$$

Einstein's prediction

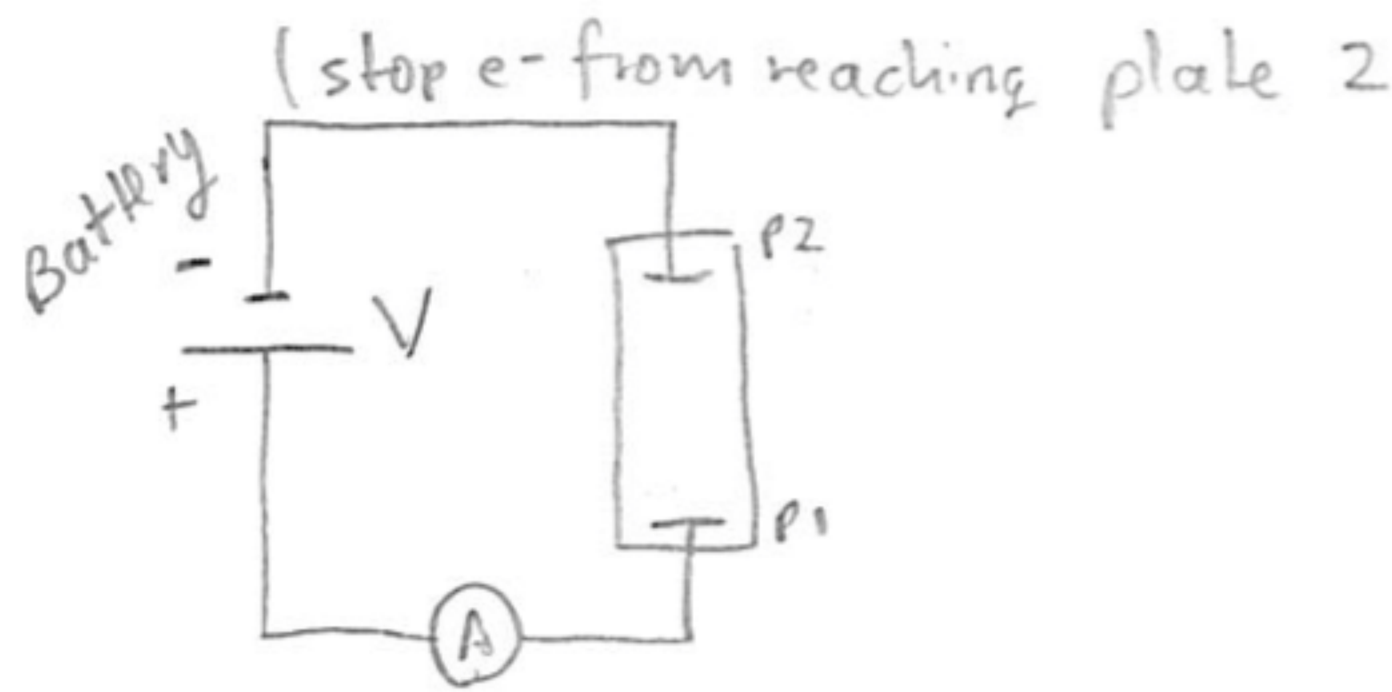
The Photoelectric Effect

- **1915 -** Millikan's experiment:

Instance 1 (no battery)



Instance 2 (battery added)

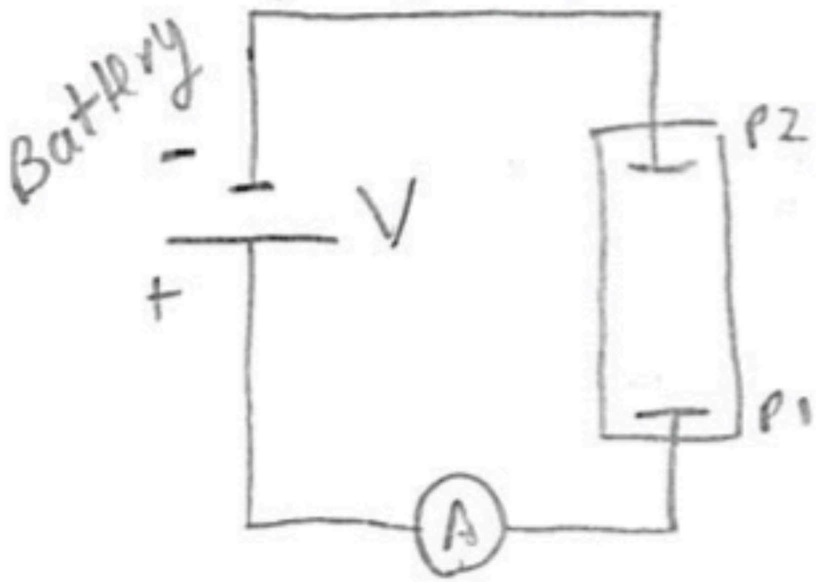


- There is a threshold frequency above which there is electric current.
- Energy to remove e- from the metal plates depends on the metal, crystalline structure on the surface of the plates.

The Photoelectric Effect

- **1915 -** Millikan's experiment:

(stop e- from reaching plate 2



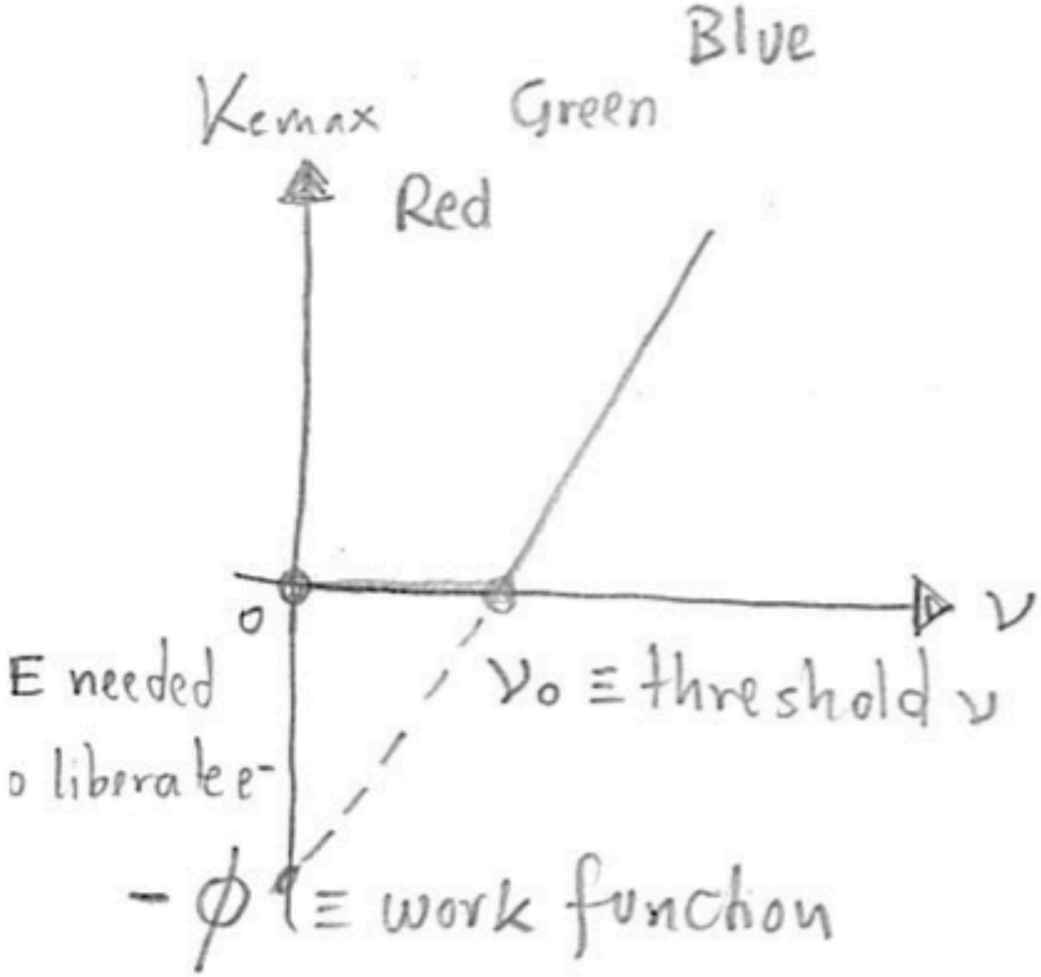
- Increase V until no e^- reach plate 2
- Stopping potential (V_s)
- $V = \frac{E_c}{q} \Rightarrow V_s = \frac{\frac{1}{2}mv^2}{e} = \frac{K_e}{e}$

$\Rightarrow K_e = eV_s \Rightarrow \boxed{K_{e\,máx} = eV_s}$

↳ only from the surface

The Photoelectric Effect

- **1915 -** Millikan's experiment:



$$E_{e^-} = \frac{1}{2}mv^2 = E_\gamma - \phi = h\nu - \phi$$

Einstein's prediction

$$\Rightarrow \boxed{\underbrace{K_{e_{max}}}_{\text{Leftover energy for e- after liberation}} = \underbrace{h\nu}_{\text{E given to e- by }\gamma} - \underbrace{\phi}_{\text{E needed to liberate e-}}}$$

$$0 = h\nu_0 - \phi$$

$$\nu_0 = \frac{\phi}{h}$$

$$\Rightarrow \boxed{\phi = \nu_0 h}$$

$$\boxed{K_{e_{max}} = h(\nu - \nu_0)}$$

Higher Intensity

- More γ do not $\uparrow$ Ke^-_{max}
- 1 γ absorbed by 1e-
- Light exists as quanta

The Photoelectric Effect

- **1915 -** Millikan's experiment conclusions:

- Millikan (1915) verifies Einstein's prediction.

- h is measured to better than 1% of its currently accepted value

h is is the slope of this linear eq:

$$K_{e_{max}} = h\nu - \phi$$

- Magnitude of the current (# of photo-e-) is proportional to light intensity.

- Energy of photo-e- is independent of light intensity

- Energy of photo-e- increases linearly with the frequency of the light.

It is NOT easy to understand the above with waves.

Light duality

- **1905** - Einstein proposes light's wave/particle duality.

  Light is made of wave-packets, bundles of energy.

  Did not say explicitly that light is a particle.

  It comes in discrete packets of energy -> **photons**

  (Lewis proposes the name photon in the 1920s)

Discovery of photons

- **Properties of photons:**
  - Photons are packets of energy.
  - Photons are the smallest pieces of light.
  - Energy = constant times a colour.
  - Charge = 0, Rest mass = 0, Spin = 1 (Right and Left)
  - Light speed c, E=pc, inability of experience time-space

Scattering experiments

- **1923** - A. Compton attributes X-ray shift to particle-like momentum to light quanta.
- **Compton scattering effect**, experiments of X-rays interacting with matter.

Compton scattering:

- X-rays shining on atoms $\left.\right\}$ X-rays: 100 eV - 100 keV; Binding e: 10 eV, 13 eV

- γ scattering on e- that are virtually free.

- Compton experiment was in disagreement with Thompson's theory of scattering.

(Classical) Thompson Scattering

- Thompson's attributes scattering to e- vibrating as a result of the incident E field.

Thompson:

EM wave $\vec{E}$ Electric

low-ν

low E

Accelerates and radiates

$$\frac{d\sigma}{d\Omega} = \underbrace{\left(\frac{e^2}{mc^2}\right)^2 \frac{1}{2}\left(1+\cos^2\hat{\theta}\right)}_{\text{units of area}}$$

Intensity of radiation as a function of Ω

- Thompson's idea seems to work at low frequencies, but not at high frequencies.
- Predicts that outgoing photons have the same energy/frequency as the ingoing photons, which is not correct.

e^- ν of $\vec{E}$ field $\Rightarrow$ $\nu_{\gamma_{out}}$ is the same

Compton Scattering

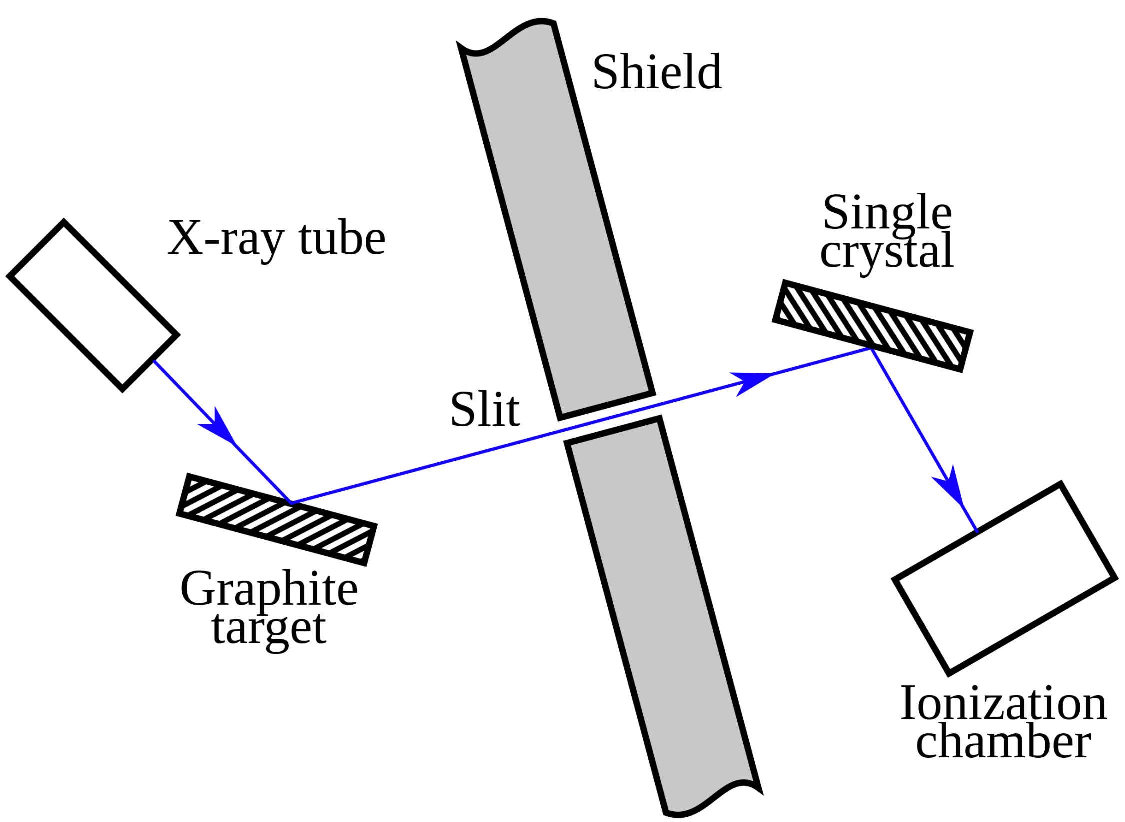
- Compton treats photons as particles:

- QM tells us a beam of monochromatic light.
↳ collection of particle-like γ

$$E_\gamma = h\nu$$

$$p_\gamma = \frac{h\nu}{c} = \frac{h}{\lambda}$$

Schematic diagram of Compton's experiment



Compton scattering occurs in the graphite target.

The slit passes X-ray photons scattered at a selected angle.

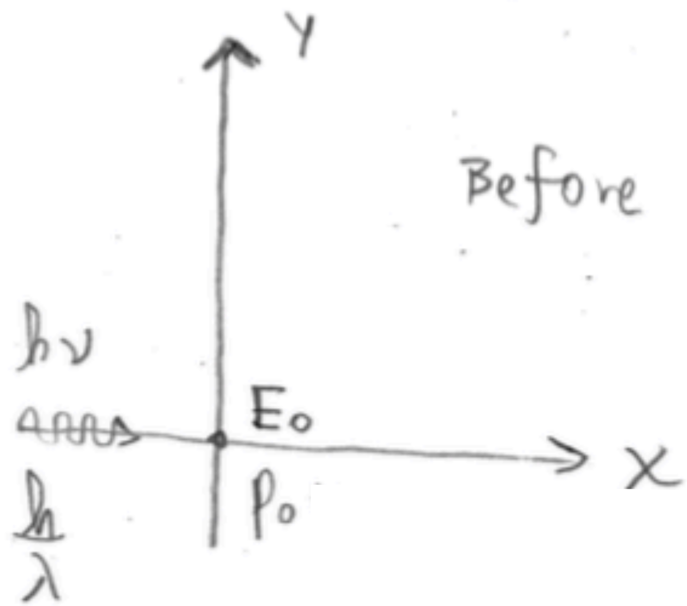
The energy of a scattered photon is measured using Bragg scattering in the crystal on the right in conjunction with the ionisation chamber.

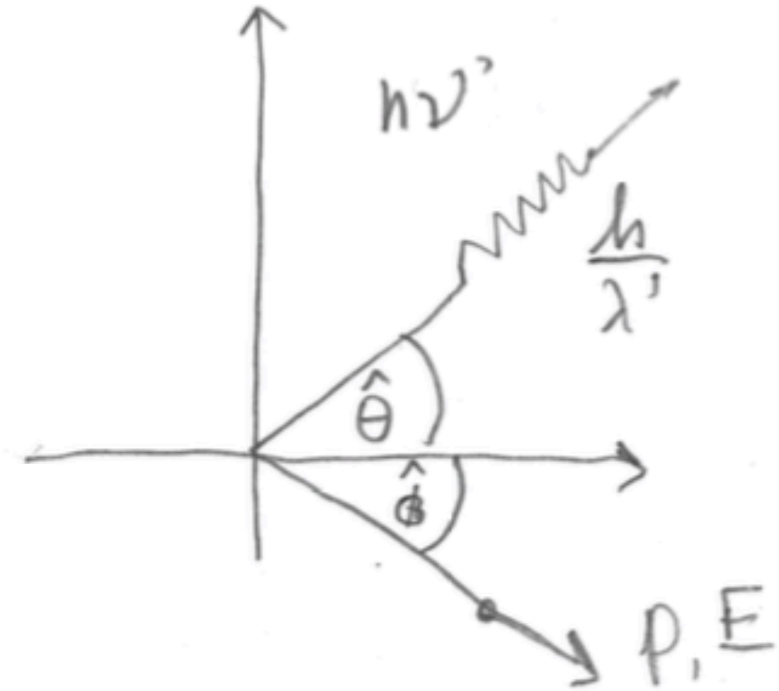
The chamber measures total energy deposited over time, not the energy of single scattered photons.

Reference: https://en.wikipedia.org/wiki/Compton_scattering

Compton Scattering

- Compton Scattering: collision of γ with charged particle





Compton shift:

$$\boxed{\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0 c}\left(1 - \cos\hat{\theta}\right)}$$

Compton wavelength of the charged particle (e.g. e-)

QM predicts that ν decreases
λ increases

$\hat{\theta}$ is the scattering $\measuredangle$.

γ loses energy $\lambda' > \lambda$

Photons are particles

1916: quanta of E, p

$$\left.\begin{aligned} E &= \frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}} \\ \vec{p} &= \frac{m\vec{v}}{\sqrt{1-\frac{v^2}{c^2}}} \end{aligned}\right\} \quad E^2 - p^2c^2 = m^2c^4$$

Non-relativistic case:

$$E = \frac{1}{2}mv^2, \quad \vec{p} = m\vec{v} \Rightarrow E = \frac{p^2}{2m}$$

Photon: $m_\gamma = 0$, $E_\gamma = p_\gamma c \quad \Rightarrow p_\gamma = \frac{E_\gamma}{c} = \frac{h\nu_\gamma}{c} = \frac{h}{\lambda_\gamma}$

↳ looks like a particle.

De Broglie and Compton wavelengths

de Broglie wavelength:

$$\boxed{\lambda = \frac{h}{p}} = \lambda_{dB}$$

m → Rest energy : mc^2

↳ not moving → $\gamma = mc^2$ → natural length

Compton wavelength:

$$\boxed{\lambda_c = \frac{h}{mc}}$$ → Compton λ of a particle of mass "m".

↳ Length associated to any particle of mass "m".

De Broglie and Compton wavelengths

The rest energy of the particle is: $E = mc^2$

What is the λ of a γ whose energy is the rest mass of a particle?

$$mc^2 = E_\gamma = h\nu = h\frac{c}{\lambda} \Rightarrow \lambda_c = \frac{h}{mc}$$

The Compton λ is the λ of light that has that rest energy.

If we have an e^- with a Compton λ_e and we shine on it a γ with that size, that γ is carrying the same energy as the rest energy of the e^-.

Experimental implication $\rightarrow$ particle creation
particle destruction

It's difficult to isolate particles in sizes smaller than their λ_c.

De Broglie and Compton wavelengths

Definitions:

1. de Broglie λ: the length/size at which the wavelike nature of particles become apparent.
2. Compton λ: the length/size at which the concept of a single pointlike particle breaks down completely.

See: https://asafpeer2.ph.biu.ac.il/wp-content/uploads/2020/08/Introduction_QFT.pdf

De Broglie's proposal: matter waves

de Broglie relations (1924)

↳ De Broglie's proposal.

- γ are particles — definite amount of E, packets, cannot be broken. & momentum p
- γ is also a wave — interferes / described by waves, ν

therefore ⟹ this could be a more general property.

Is this universal?

de Broglie:

↳ All "matter particles" behave as waves, not just the γ's.

↳ There is a wave associated to a matter particle.

De Broglie's proposal: matter waves

QM: probability amplitude to be somewhere
probability waves

Matter waves are introduced:

↳ Matter waves → probability amplitudes. $\mathbb{C}$#'s
↳ Associate to a particle a wave that depends on the momentum.

For a particle of momentum p, we associate a plane wave $\boxed{\lambda = \frac{h}{p}}$ which is the de Broglie λ.

QM arises as a theory

- **1925** - Schrödinger/Heisenberg wrote the governing equations of QM.
- QM is almost a 100 years old!

What is QM?

QM is a framework to do physics.

Quantum physics

- QM replaces classical mechanics CM. CM is a good approximation but it is not accurate when describing some experiments.
- **Quantum physics:** principles of QM applied to physical phenomena.
- **Branches of QM:**
  - **QED:** QM + EM
  - **QCD:** QM + Strong interaction
  - **Quantum optics:** QM + photons
  - **Quantum gravity:** QM + gravitation -> String theory (QM of gravity)

Mathematical tools for QM

- **Is QM a linear theory?**
- Why do we need complex numbers?

linear theory:

$$\left.\begin{array}{l}\text{Solution 1}\\ \text{Solution 2}\end{array}\right\} \Rightarrow \text{New Solution 3}$$

We can create linear combinations of known solutions to get new solutions.

Linear Operators

- L.u =0
- L = linear operator, u = unknown
- Several operators applied to the same unknown: L1.u=0, L2.u=0
- Same operator applied to different unknowns: L(u1,u2,u3) =0

Properties of linear operators:

- Scale a solution: L(au) = a Lu
- Combine solutions: L(u1+u2) = L(u1) + L(u2)

EM theory is linear

Example: EM

$\frac{q}{V}$

$\frac{q}{A \cdot t}$

$(\vec{E}, \vec{B}, \rho, \vec{J})$ is a solution

$\overset{L}{\Rightarrow} (\alpha\vec{E}, \alpha\vec{B}, \alpha\rho, \alpha\vec{J})$ is also a solution, $\alpha \in \mathbb{R}$

$$\left.\begin{array}{l}(E_1, B_1, \rho_1, J_1) \\ (E_2, B_2, \rho_2, J_2)\end{array}\right\} \text{ are solutions:}$$

$\overset{L}{\Rightarrow} (E_1+E_2, B_1+B_2, \rho_1+\rho_2+ J_1+J_2)$ is a sln.

EM is linear

Linear theory: Maxwell’s theory of EM

- 2 1D plane waves propagating (do not touch each other, without affecting each other).
- 3rd solution, 2 plane waves propagate simultaneously.
- EM waves are all around - superposition, do not interfere with each other.
- E, B, charge density, current J (charge per unit area per unit time).
- Scale by #: Linearity x alpha (sln) is also a solution, alpha belong to R
- Sln1 + sln2 = sln

Is QM a linear theory?

<u>Linear equation</u>:

$$L \quad u = 0$$

Linear operator (eq) — unknown (variable)

Properties:
$$\begin{cases} L(\alpha u) = \alpha L u \\ L(u_1 + u_2) = L u_1 + L u_2 \end{cases}$$

Linear combinations:

$$L(\alpha u_1 + \beta u_2) = L(\alpha u_1) + L(\beta u_2) = \alpha L u_1 + \beta L u_2$$

If $u_1, u_2 \equiv$ sln $\Rightarrow$ $\alpha u_1 + \beta u_2 \Rightarrow$ sln

Linear vs. Non-linear Theories

linear & non-linear theories:

L $\left\{ \begin{array}{l} \text{EM} \\ \text{QM} \end{array} \right.$

much simpler

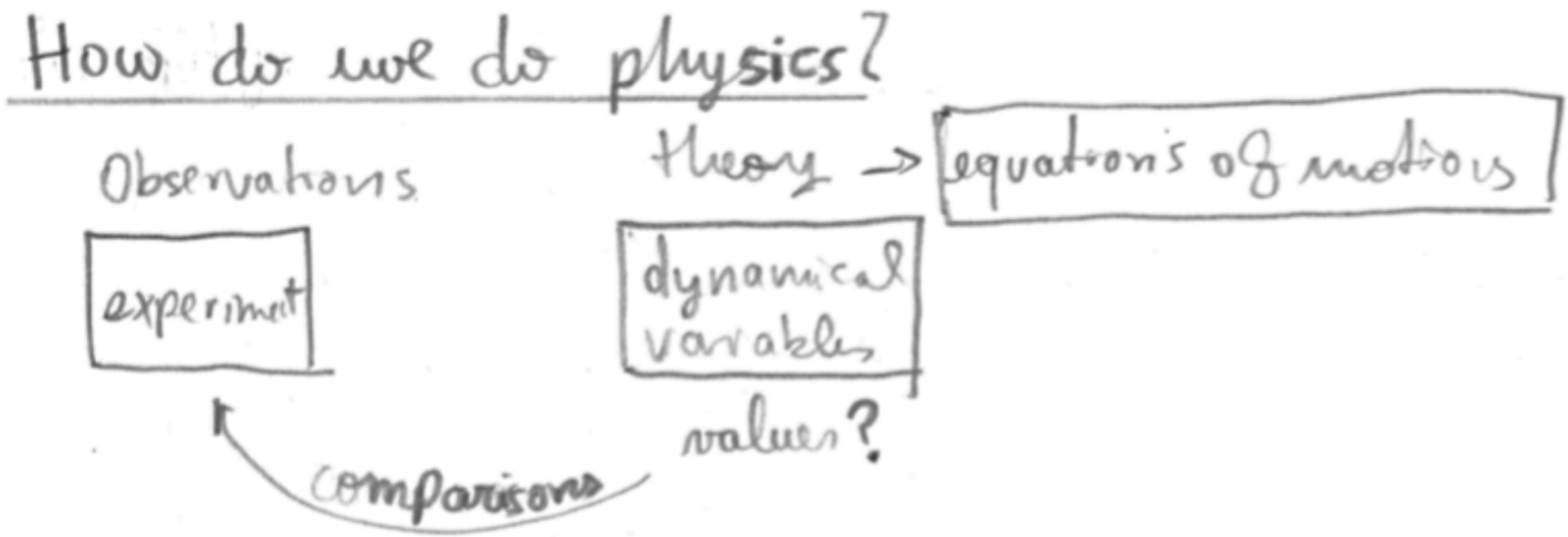
NL $\left\{ \begin{array}{l} \text{G.R.} \\ \text{C.M. e.g. 3-body problem} \end{array} \right.$

very non-linear

QM is linear!

How do we do physics? Scientific method

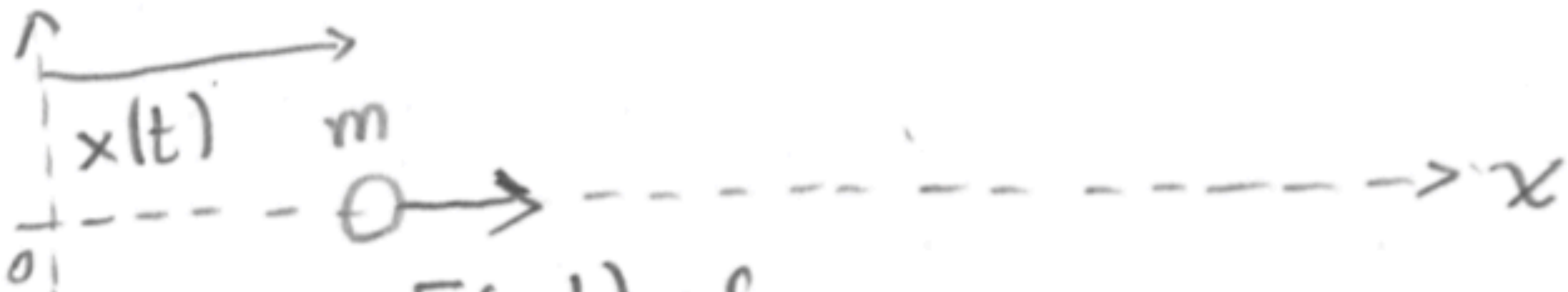
- Observations/experiments <-> dynamical variables (theory)
- Equations of motion solve for dynamical variables.



How do we do physics? Scientific method

- Motion of classical particles

In classical mechanics: 1D motion (non relativistic $v \ll c$)



$F(x,t) \equiv$ force

$$\left.\begin{array}{l} x(t) = ? \rightarrow v_x = \dfrac{dx}{dt} \rightarrow a_x = \dfrac{dv_x}{dt} = \dfrac{d^2x}{dt^2} \\ \vec{p}_x = m\vec{v}_x \\ T = \dfrac{1}{2} m v_x^2 \end{array}\right\} \underline{\underline{\text{dynamical variables}}}$$

How do we determine $x(t)$?

How do we do physics? Scientific method

- Motion of classical particles

Theory: Newton's 2nd law $F = ma = -\frac{\partial V}{\partial x}$ (conservative system)

$V \equiv$ potential energy function

$$\Rightarrow \boxed{m \frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}}$$

If we know the initial conditions, eg $x(t=0)$, $v(t=0)$

$\Rightarrow x(t)$ ✓

e.g. elastic potential energy:

$$V = \frac{1}{2}kx^2 \Rightarrow \frac{\partial V}{\partial x} = kx$$

How do we do physics? Scientific method

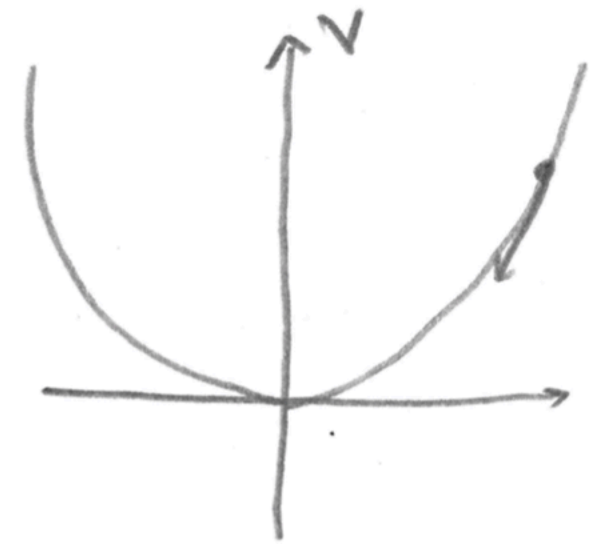
- Motion of classical particles

Motion in 1D: dynamical variable $x(t)$)

$$m\ddot{x} = -\frac{\partial V}{\partial x}$$

↳ derivatives are linear

non-linear



e.g. elastic potential energy:

$$V = \frac{1}{2}kx^2 \Rightarrow \frac{\partial V}{\partial x} = kx$$

$$\Rightarrow m\ddot{x} = -kx$$

$$\Rightarrow \boxed{m\ddot{x} + kx = 0}$$ ODE

Solution is:

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

$$\omega = \sqrt{\frac{k}{m}}$$ (Angular frequency)

How do we do quantum mechanics?

- Motion in quantum mechanics:

sai

QM is linear: dynamical variable Ψ (wavefunction)

↳ describes dynamics of the Q system

- The equation of motion is Schrödinger's equation:

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

Schrödinger's equation.

↳ Hamiltonian, linear operator.

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

$$L\Psi = 0$$

$$L \equiv i\hbar \frac{\partial}{\partial t} - \hat{H}$$ is linear.

How do we do quantum mechanics?

- Schrödinger's equation: $i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$

$i = \sqrt{-1}$

$\hbar \equiv$ Planck's constant $= \frac{h}{2\pi} = 1.054573 \times 10^{-34}$ J·s

- QM is linear, so in some sense it is simpler than CM.

- We can scale solutions, and add/combine solutions to create superpositions, which become new solutions.

Q physical systems $\begin{cases} \Psi \to \text{wave function} \\ \hat{H} \to \text{we need to find it} \end{cases}$

How do we do quantum mechanics?

In 1D: $\psi(x,t)$

3D: $\psi(\vec{r},t)$

Schrödinger did not give a physical interpretation for Ψ

Initially ψ did not have a physical interpretation

Max Born $\rightarrow$ probabilities.

Motion in 1D : $\hat{H} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi}$$

Schrödinger Eq.

Initial conditions : $\psi(x,0) \Rightarrow \psi(x,t)$

The necessity of complex numbers

- Why do we need complex numbers?

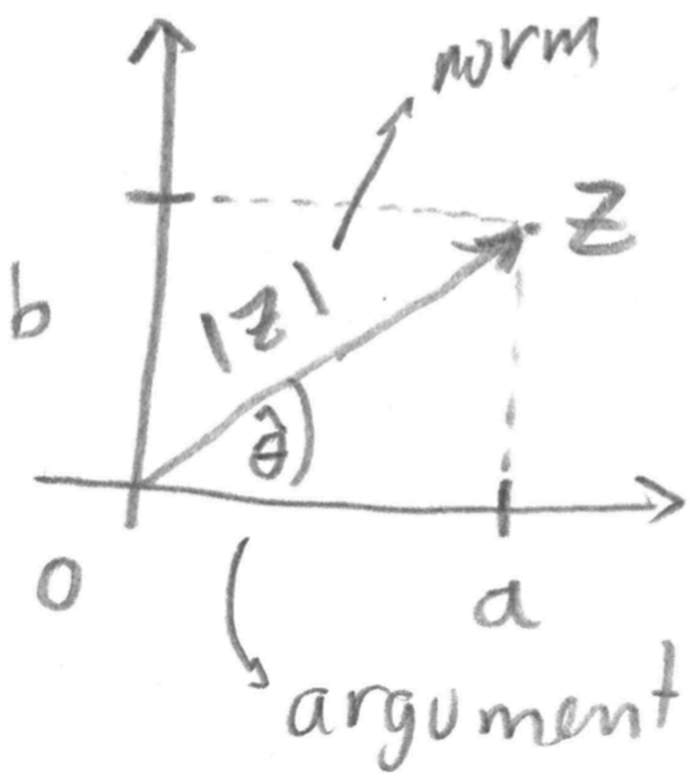
Complex numbers: $x^2 = 1 \Rightarrow x = \sqrt{-1}$

$i = \sqrt{-1}$

$\boxed{z = a + ib}$; $a, b \in \mathbb{R}$

$z \in \mathbb{C}$

$$\begin{cases} Re(z) = a \\ Im(z) = b \end{cases}$$



The necessity of complex numbers

- Why do we need complex numbers?

Complex conjugate of z:

$\boxed{z^* = a - ib}$ $(\bar{z}, \hat{z})$

Norm of a complex #: $\in \mathbb{R}$

$|z| = \sqrt{a^2+b^2}$, $|z|^2 = a^2+b^2 = z z^*$

Summation:

$(a+bi) + (c+di) = (a+c) + (b+d)i$

Multiplication:

$(a+bi)(c+di) = (ac-bd) + (bc+ad)i$

The necessity of complex numbers

- Why do we need complex numbers?

In polar coordinates:

$$a = |z| \cos \hat{\theta} \qquad b = |z| \sin \hat{\theta} \quad \Rightarrow \quad z = |z|(\cos \hat{\theta} + i \sin \hat{\theta}) = |z| e^{i\theta}$$

Identity: $e^{i\hat{\theta}} = \cos \hat{\theta} + i \sin \hat{\theta}$ (Euler formula)

$$e^{-i\theta} = \cos \hat{\theta} - i \operatorname{sen} \hat{\theta}$$

$$\boxed{\text{In QM } \psi \in \mathbb{C}}$$

We need $\mathbb{C}$ numbers.

- The wave function, Ψ, has to be a complex number to satisfy Schrödinger equation.

The necessity of complex numbers

- What about measurement?

What we measure are $\mathbb{R}$ #'s, we cannot measure $\mathbb{C}$ #'s

$\mathbb{C}$ # are not auxiliary

$\psi \in \mathbb{C}$, physical interpretation ??

$|\psi^2| \sim$ probabilities (Max Born)

$|\psi^2| \equiv$ norm $\in \mathbb{R}$

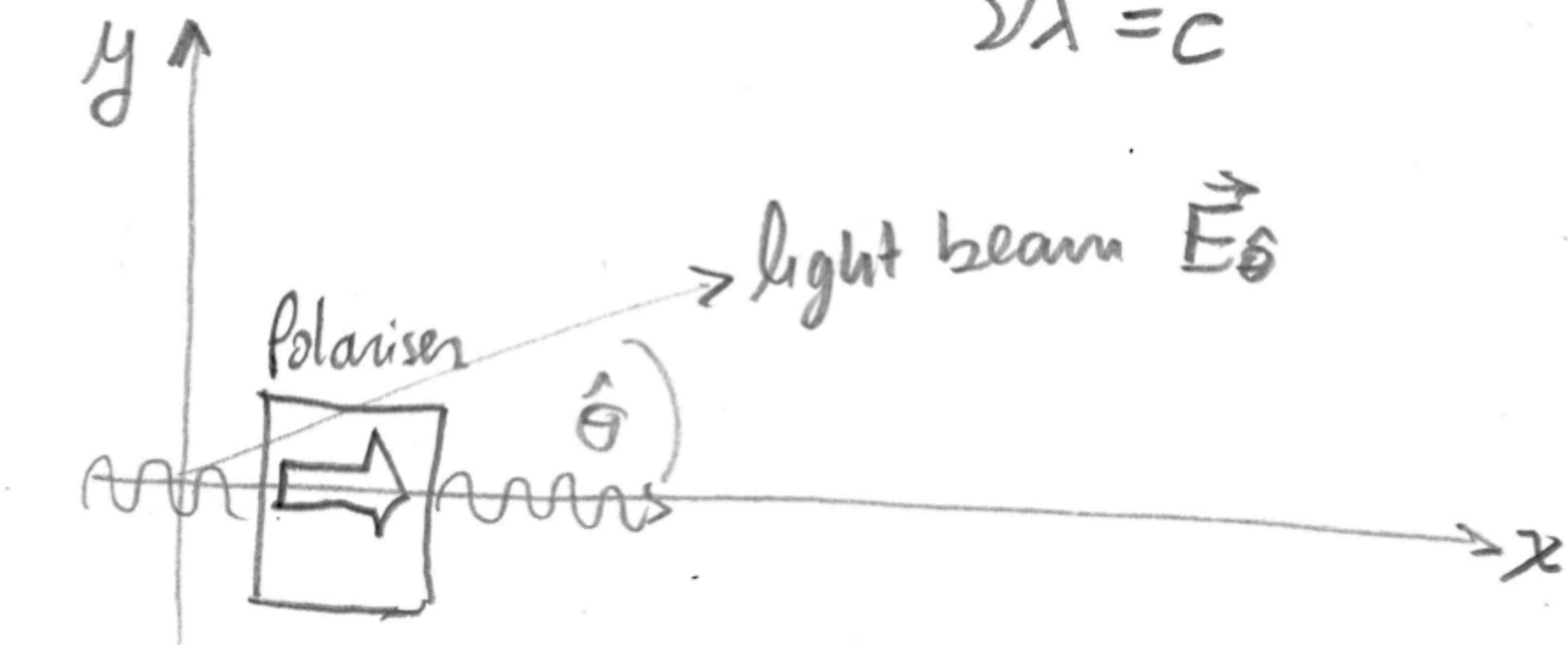
- Max Born proposes that Ψ is related to probabilities.

The loss of determinism

- **Classical Particles:** object with zero size with certain velocity at certain position.
- **Quantum Particles:** indivisible amount of energy that propagates.

γ: waves/particles ; $E = h\nu$

$\nu\lambda = c$



Same light, same energy. The colour does not change.

$$\vec{E}_\theta = E_0 \cos\hat{\theta}\, \hat{e}_x + E_0 \sin\hat{\theta}\, \hat{e}_y$$

Electric field before the polariser.

The loss of determinism

After the polariser:

$$\vec{E} = E_0 \cos\hat{\theta}\, \hat{e}_x \Rightarrow \left(\frac{E}{E_0}\right)^2 = \left(\cos^2\hat{\theta}\right)$$

magnitude of E field

fraction of $\vec{E}$ that goes thru.

γ

Now we send γ one by one.

In CM: identical γ should either get absorbed or go thru.

In QM: identical γ sometimes go thru / sometimes they don't

$\Rightarrow$ We lose predictability / we lose determinism

The loss of determinism

- A γ either gets thru or not.
- We can only predict probabilities.

wavefunction / states / vectors

- ψ of a γ polarised in the x direction; Dirac's notation

$$\underbrace{|\gamma; x>}_{\text{vector}}$$

vector
wavefunction
represents a possible state

$|\gamma; y>$ polarised along y.

The loss of determinism

Photon state before the polariser:

$$\boxed{|\gamma;\theta> = |\gamma;x> \cos\hat{\theta} + |\gamma;y> \sin\hat{\theta}}$$ superposition

Photon state after the polariser:

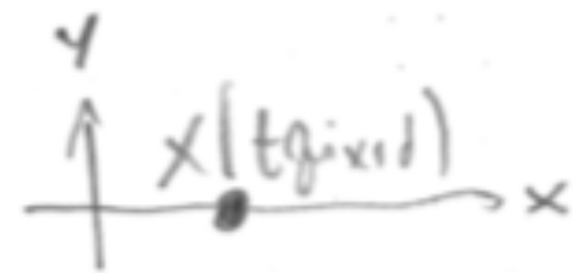
$|\gamma;x>$ when it goes thru, the whole γ goes thru.

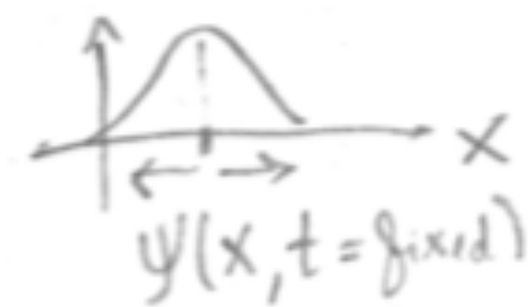
Einstein's view:

γ has a hidden property we don't know about. (hidden variable theory). Bell inequality shows that this is not the explanation.
Hidden variables would satisfy an inequality.
↳ did not hold experimentally.

The statistical interpretation

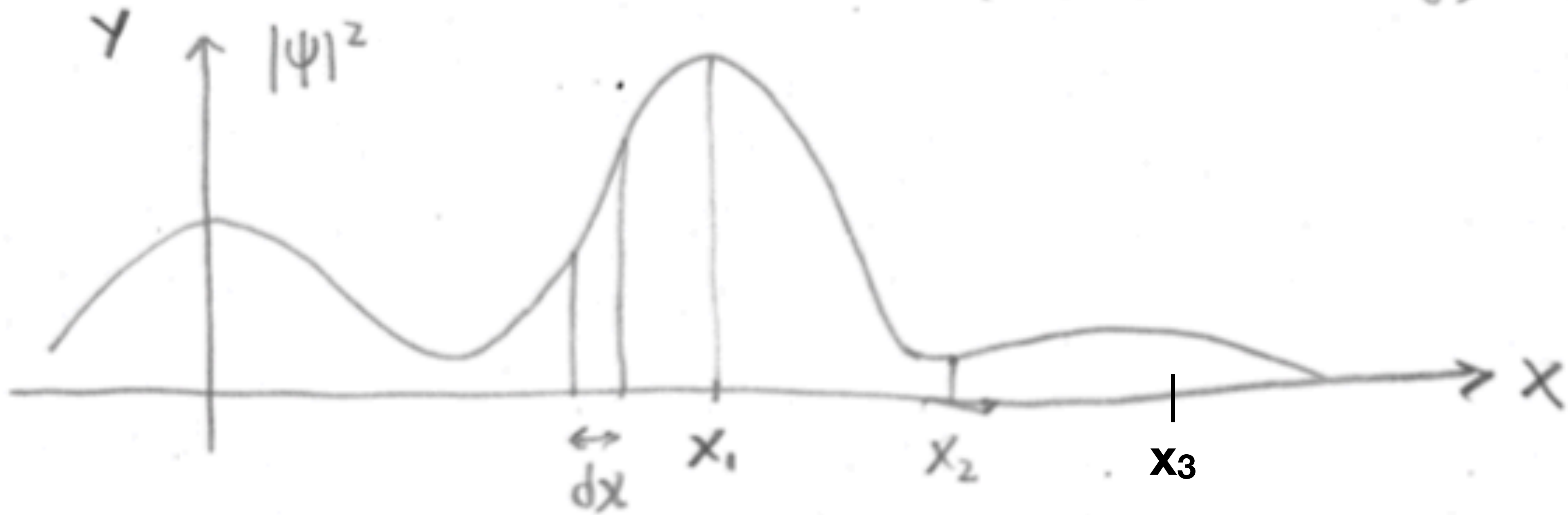
- What is the wave function ?
  - ⊛ light
  - ⊛ matter
- Particle → located at a point $x(t)$
- wave function → spread out in space $\Psi(x,t)$
- How can Ψ describe the state of a particle ?
  ↳ Born's statistical interpretation of Ψ





Born's statistical interpretation

$|\Psi(x,t)|^2 dx \equiv$ probability of finding the particle between x & $(x+dx)$ at time t,



- Likely to find the particle in x_1
- Unlikely to find the particle in x_2

This interpretation introduces indeterminacy.

Views on determinism

- Even if I know Ψ of a particle
  I cannot predict with certainty the outcome of an experiment to measure its position

QM offers statistical information about the possible results.

- Experiment: I measure the position of the particle
  the particle shows up at point x_3

Views on determinism

* Where was the particle before?

① Realist view: it was at x_3, QM is incomplete, there are hidden var.

② Orthodox view: it was nowhere, measurement made it take a stand; observations produce a measurement; Copenhagen interpretation

③ Agnostic view: let's not worry about where the particle was.

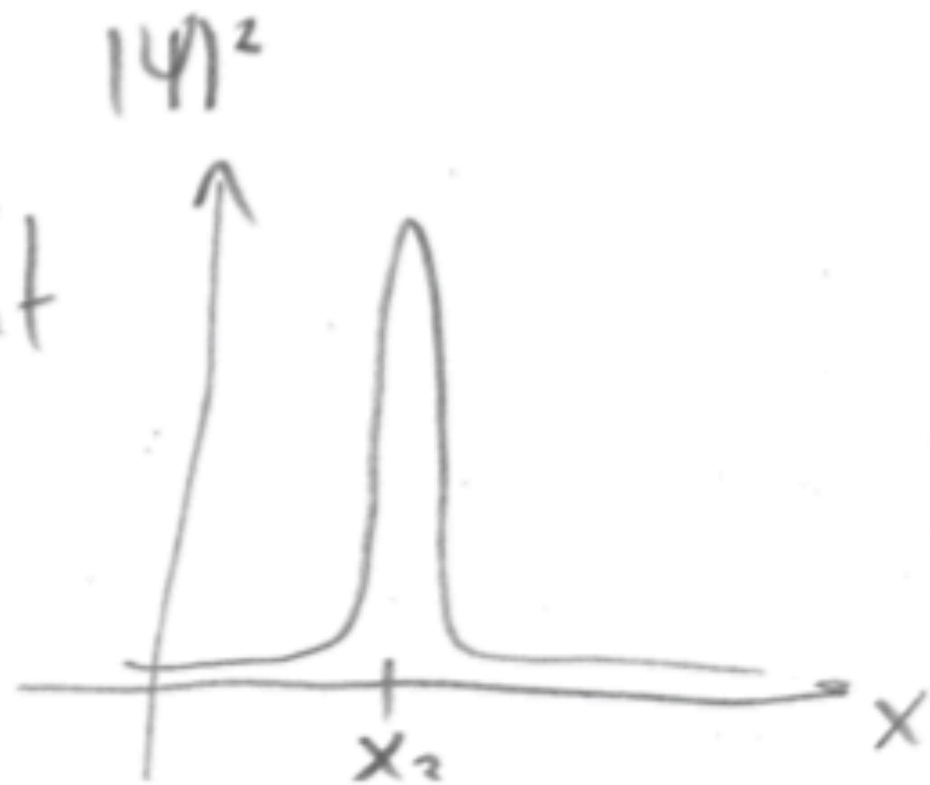
Bell's theorem (1964): If there are hidden variables, they would satisfy an inequality. They don't!

Orthodox view wins: wave function collapse

- A particle does not have a precise position before measurement.
- The measurement process insists on a particular #
  creates the result
- Limited by weighting of Ψ

Second measurement?

- Must return the same value
- Measurement alters the Ψ
- The Ψ collapses upon measurement



Processes in Quantum Mechanics

In QM; there are two physical processes:

1. Ordinary: Ψ evolves according to S. eq.
2. Measurement: Ψ collapses

To do: Add sketch on experiment on 1 particle and on identical particles to illustrate point.

Processes in Quantum Mechanics

Linear polarisation of EM waves:

Also explained by Ψ collapse.

$$|\psi\rangle \stackrel{\text{def}}{=} \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} = \begin{pmatrix} \cos\hat\theta\, e^{i\alpha_x} \\ \sin\hat\theta\, e^{i\alpha_y} \end{pmatrix} \equiv \text{Jones vector}$$

The wave is linearly polarised if $\alpha_x = \alpha_y = \alpha$

Unit vectors:

$|x\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$|y\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\Rightarrow |\psi\rangle = \begin{pmatrix} \cos\hat\theta \\ \sin\hat\theta \end{pmatrix} e^{i\alpha}$$

$$\Rightarrow |\psi\rangle = \overbrace{\cos\hat\theta\, e^{i\alpha}}^{\alpha} |x\rangle + \overbrace{\sin\hat\theta\, e^{i\alpha}}^{\beta} |y\rangle$$

$$\Rightarrow \boxed{|\psi\rangle = \psi_x |x\rangle + \psi_y |y\rangle}$$ Superposition (1γ)

Imagine we have a polariser only $\psi_x|x\rangle$ goes thru.

$|\gamma, \hat\theta\rangle = \cos\hat\theta\, |\gamma, x\rangle + \sin\hat\theta\, |\gamma, y\rangle$ Before

$|\gamma, x\rangle$ After

Quantum Superposition

In C.M.: $\left.\begin{array}{l}\vec{E}_1\\ \vec{E}_2\end{array}\right\} \Rightarrow \underbrace{\vec{E}}_{\text{physical state}} = \vec{E}_1 + \vec{E}_2$ (Superposition in C.M.)

In Q.M.: $\begin{array}{l}|\psi_1\rangle\\ |\psi_2\rangle\end{array}$ are two states $\xrightarrow[\text{same property}]{\text{measurement}}$ $\begin{array}{l}|\psi_1\rangle \to a\\ |\psi_2\rangle \to b\end{array}$ always!

Superposition:

$$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle, \quad \alpha, \beta \in \mathbb{C} \rightarrow \Big\} \text{ either } a \text{ or } b$$

What happens if you measure the same property?

- No certain answer
- No intermediate answer
- α, β affect the probabilities with which we obtain a or b.

$$\text{Probability}(a) \sim |\alpha|^2$$
$$\text{Probability}(b) \sim |\beta|^2$$

Quantum Superposition

Superposition:

$$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle, \quad \alpha, \beta \in \mathbb{C} \rightarrow \Big\{ \text{either } a \text{ or } b$$

Actual probabilities:

$$P(a) = \frac{|\alpha|^2}{|\alpha|^2 + |\beta|^2}$$

$$P(b) = \frac{|\beta|^2}{|\alpha|^2 + |\beta|^2}$$

Experiment:

If a, then repeated experiments $a \xRightarrow[\text{measurement}]{\text{After}} |\psi\rangle = |\psi_1\rangle$

$b \Rightarrow |\psi\rangle = |\psi_2\rangle$

Principle of Physical Equivalence

What happens if we superpose a state with itself?

$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_1\rangle$

$\Rightarrow |\psi\rangle = (\alpha+\beta)|\psi_1\rangle$ The # in front changes, but not the physics.

In general two states: $\alpha|\psi_1\rangle$, $(\alpha+\beta)|\psi_1\rangle$
represent the same physics for any
$\alpha, \beta \in \mathbb{C}$ not zero.

Physical equivalence:

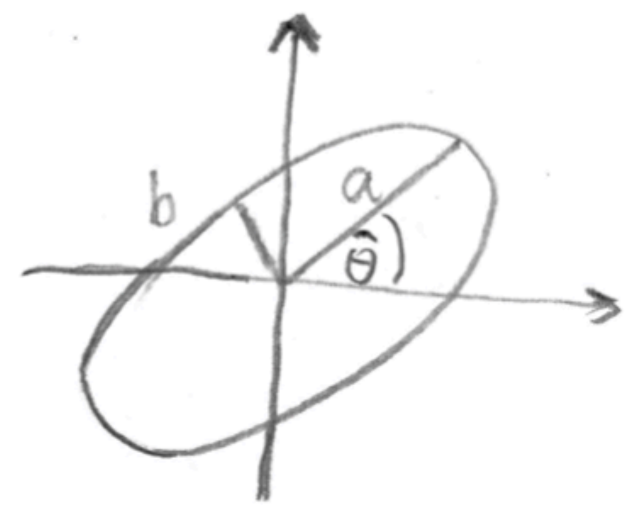
$$\alpha|\psi_1\rangle \cong (\alpha+\beta)|\psi_1\rangle \cong -|\psi_1\rangle \cong 2|\psi_1\rangle$$

This means:

- We conveniently choose a normalised state.
- The overall factor in front of the wave function does not matter.

Principle of Physical Equivalence

Example:
polarisation



Free parameters

$\frac{a}{b} \in \mathbb{R}$ ✓

$\hat{\theta} \in \mathbb{R}$

$|\psi\rangle = \alpha\,|\psi_x\rangle + \beta\,|\psi_y\rangle$

$\alpha, \beta \in \mathbb{C} \Rightarrow \begin{cases} \alpha = a + bi \\ \beta = c + di \end{cases}$

$\Rightarrow$ 4 $\mathbb{R}$ parameters (a, b, c, d)

But thanks to physical equivalence:

$|\psi\rangle = |\psi_x\rangle + \frac{\beta}{\alpha}\,|\psi_y\rangle$

$\Rightarrow \frac{\beta}{\alpha} \in \mathbb{C} \Rightarrow \frac{\beta}{\alpha} = p + qi$

$\Rightarrow$ 2 $\mathbb{R}$ parameters ✓

Probabilities

- Probability plays a key role in QM.
- Sample of N elements with a property j

$N(j) \equiv \#$ of elements of j property

$\rightarrow$ Histogram (Distro)

- Total # of elements:

$$N = \sum_{j}^{\infty} N(j)$$

Probabilities

① What is the probability that an element would be a specific j?

$$P(j) = \frac{N(j)}{N}$$

$$P(j_1 \vee j_2) = P(j_1) + P(j_2)$$

⇒ the sum of all P is 1

$$\sum_{j=1}^{\infty} P(j) = 1$$

② What is the most probable value?

It is j for which $P(j)$ is a maximum.

Probabilities

3) What is the median j?
It is j such that the P of getting a smaller result is the same as getting a larger result.

4) What is the average / mean?

$$\langle j \rangle = \frac{\sum j N(j)}{N} = \sum_{j}^{\infty} j P(j)$$

In QM, we are interested in average values.
$\langle j \rangle$ is called the expectation value

Probabilities

(5) What is the average of the square of values?

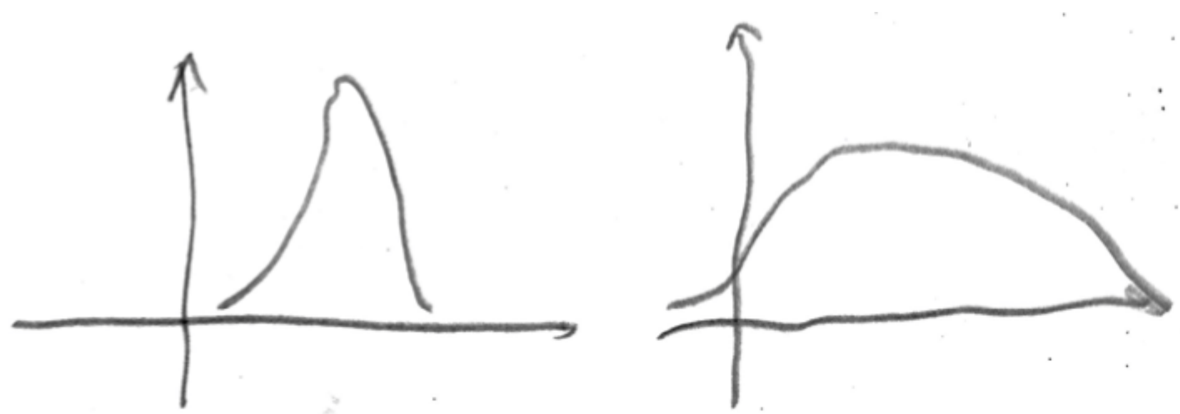
$$\langle j^2 \rangle = \frac{\sum_{j}^{\infty} j^2 N(j)}{N} = \sum_{j}^{\infty} j^2 P(j)$$

Therefore, in general:

$$\langle f(j) \rangle = \sum_{j}^{\infty} f(j) P(j)$$

In general, $\langle j^2 \rangle \neq \langle j \rangle^2$

(6) How do we quantify the spread?



Probabilities

⑥ How do we quantify the spread?

constant. } does not change when changing j

* $\Delta j = j - \langle j \rangle$

$$\langle \Delta j \rangle = \sum (j - \langle j \rangle) P(j) = \sum j P(j) - \langle j \rangle \sum P(j)$$

$$= \langle j \rangle - \langle j \rangle = 0$$

* $(\Delta j)^2 = (j - \langle j \rangle)^2$

$$\langle (\Delta j)^2 \rangle = \sigma^2 \equiv \text{variance}$$

$$\sigma = \sqrt{\langle \Delta j^2 \rangle} \equiv \text{std. deviation}$$

$$\sigma^2 = \langle j^2 \rangle - \langle j \rangle^2$$

$$\Rightarrow \langle j^2 \rangle \geq \langle j \rangle^2$$

= for distros with no spread.

Continuous functions

7) What about continuous distros?

The $P(j) = 0$ precisely j

- It is only sensible to speak about the P that j lies in some interval. (infinitesimal interval)
- The P is $\propto$ to the length of this interval.

$$P(x) = \rho(x)\, dx$$

$\rho(x) \equiv$ probability density

- The prob that "x" lies between "a" ^ "b":

$$P_{ab} = \int_a^b \rho(x)\, dx$$

Continuous functions

Same rules as for discrete distros:

$$\int_{-\infty}^{+\infty} \rho(x)\,dx = 1$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x\,\rho(x)\,dx$$

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x)\,\rho(x)\,dx$$

$$\sigma^2 = \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

Normalisation

$$\underbrace{|\Psi(x,t)|^2}\, dx = \left\{ \begin{array}{l} \text{P of finding a particle} \\ \text{between } x \wedge x+dx \text{ at time } t. \end{array} \right.$$

Probability density for finding the particle at x at t.

The particle has to be somewhere:

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \, dx = 1 \qquad (*)$$

compatible
Is this consistent with Sch. eq?

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

If $\Psi(x,t)$ is a solution, so is $A\Psi(x,t)$, where $A \in \mathbb{C}$

Normalisation

Is ⊛ satisfied? We must pick A so that ⊛ is satisfied.

↳ This process is called normalisation of Ψ.

In some cases: $\left.\begin{array}{l}\int |\Psi(x,t)|^2\,dx \to \infty \\ \Psi(x,t) = 0\end{array}\right\}$ we have non-normalizable solutions

↳ cannot represent particles, must be rejected.

Physical states correspond to square-integrable slns.

Sch. eq automatically preserves the normalization of the Ψ.

Proof:

$$\underbrace{\frac{d}{dt}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\,dx}_{\mathcal{F}(t)} = \int_{-\infty}^{+\infty} \frac{\partial}{\partial t} \underbrace{|\Psi(x,t)|^2}_{\mathcal{G}(x,t)}\,dx \qquad (**)$$

Normalisation

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial t}(\psi^* \psi) = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}$$

Remember:

$$\frac{-1}{\sqrt{-1}} = \sqrt{-1}$$

$$-\frac{1}{i} = i$$

$$\xRightarrow{\text{S.Eq}} \begin{cases} \dfrac{\partial \psi}{\partial t} = \dfrac{i\hbar}{2m}\dfrac{\partial^2 \psi}{\partial x^2} - \dfrac{i}{\hbar} V\psi \\[2ex] \dfrac{\partial \psi^*}{\partial t} = -\dfrac{i\hbar}{2m}\dfrac{\partial^2 \psi^*}{\partial x^2} + \dfrac{i}{\hbar} V\psi^* \end{cases}$$

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

$$\Rightarrow \frac{\partial}{\partial t}|\psi|^2 = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi\right)$$

$$= \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\right]$$

Normalisation

$$\Rightarrow (**) \Rightarrow \frac{d}{dt}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = \left[\frac{i\hbar}{2m}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\right]_{-\infty}^{+\infty}$$

$\Psi(x,t) \to 0$ when $x \to \pm\infty$

$$\Rightarrow \frac{d}{dt}\underbrace{\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx}_{\text{constant}} = 0$$

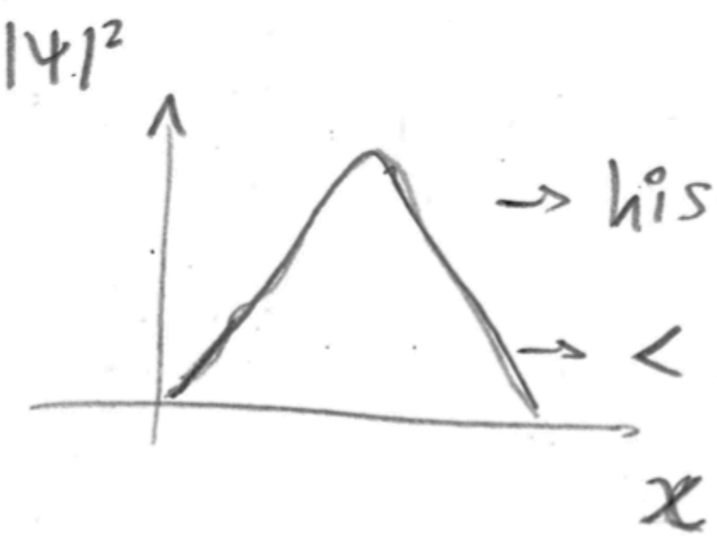
constant $\Rightarrow$ normalisation is preserved!

Expectation values

For a particle in state Ψ, the expectation value of position "x" is:

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \, |\Psi(x,t)|^2 \, dx$$

- This is **not** the average of the results you'll get when measuring x of one particle over and over again.
- 1st measurement → Ψ collapses → same result.
- $\langle x \rangle$ is the $\langle \rangle$ of measurements performed on particles all in the state Ψ (ensemble of particles)



→ histogram – $|\Psi|^2$

→ $\langle \ \rangle$ → $\langle x \rangle$

Expectation values

Velocity of the expectation value of x:

$\Psi(x,t) \rightarrow \langle x \rangle_t$ changes with time.

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{+\infty} x \frac{\partial}{\partial t} |\Psi|^2 \, dx$$ $\neq$ velocity of the particle

$$\Rightarrow \frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{m} \int \Psi^* \frac{\partial \Psi}{\partial x} \, dx$$ $\Rightarrow \langle v \rangle$ from Ψ.

Expectation value of the velocity:

$$\boxed{\langle v \rangle = \frac{d\langle x\rangle}{dt}}$$

Expectation values

Momentum : $p = mv$

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = -i\hbar \int \Psi^* \frac{\partial \Psi}{\partial x} dx$$

Operators : provides an instruction to do something to the function that follows.

Derivatives

Multipliers.

operator x

Position operator: $\langle x \rangle = \int \Psi^* (x) \Psi \, dx$

operator p

$$\langle p \rangle = \int \Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi \, dx$$

⇒ to calculate expectation values : $\Psi^* \, op. \, \Psi$

Expectation values

What about other dynamical variables?

* Kinetic energy: $T = \frac{1}{2} m v^2 = \frac{p^2}{2m}$

* Angular momentum: $\vec{L} = \vec{r} \times m\vec{v} = \vec{r} \times \vec{p}$

In general:

$$\boxed{\langle Q(x,p) \rangle = \int \Psi^* Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi \, dx}$$

expectation value of any dyn. var. for a particle in state Ψ.

Example:

$$\langle T \rangle = \int \Psi^* \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \Psi \, dx$$

The Ehrenfest Theorem

The Ehrenfest theorem:

$$\int u\,dv = uv - \int v\,du$$

$$\int \psi^* \frac{\partial}{\partial x}\frac{\partial^2 \psi}{\partial x^2} = \psi^* \frac{\partial^2 \psi}{\partial x^2} - \int \frac{\partial^2 \psi}{\partial x^2}\frac{\partial \psi^*}{\partial x}$$

Expectation values obey classical laws.

① $\langle p \rangle = m \dfrac{d\langle x \rangle}{dt}$

② $\dfrac{d\langle p \rangle}{dt} = \left\langle -\dfrac{\partial V}{\partial x} \right\rangle$

Let's prove that ② holds. $\langle p \rangle = \int \psi^* \left(-i\hbar \dfrac{\partial}{\partial x}\right) \psi \, dx$

$$\Rightarrow \frac{d\langle p \rangle}{dt} = -i\hbar \int \frac{\partial}{\partial t}\left(\psi^* \frac{\partial \psi}{\partial x}\right) dx$$

$$\Rightarrow \frac{d\langle p \rangle}{dt} = -i\hbar \int \left[\frac{\partial \psi^*}{\partial t}\frac{\partial \psi}{\partial x} + \psi^* \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial t}\right)\right] dx \qquad ①$$

The Ehrenfest Theorem

Remember: (Sch. eq)

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

$$\Rightarrow \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^* \quad (3)$$

(2) ∧ (3) in (1):

$$\Rightarrow \frac{d\langle p\rangle}{dt} = -i\hbar \int \left\{ \left[-\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^* \right] \frac{\partial \Psi}{\partial x} + \Psi^* \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi \right] \right\} dx$$

$$-i\hbar \int \left\{ \frac{i\hbar}{2m}\left[\Psi^* \frac{\partial^3 \Psi}{\partial x^3} - \frac{\partial^2 \Psi^*}{\partial x^2}\frac{\partial \Psi}{\partial x} \right] + \frac{i}{\hbar}\left[V\Psi^* \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial}{\partial x}(V\Psi) \right] \right\} dx$$

$$I_1 = \frac{i\hbar}{2m}\int \left(\Psi^* \frac{\partial^3 \Psi}{\partial x^3} - \frac{\partial^2 \Psi^*}{\partial x^2}\frac{\partial \Psi}{\partial x} \right) dx$$

$$I_1 = \frac{i\hbar}{2m}\int \Psi^* \frac{\partial^3 \Psi}{\partial x^3}\, dx - \frac{i\hbar}{2m}\underbrace{\int \frac{\partial^2 \Psi^*}{\partial x^2}\frac{\partial \Psi}{\partial x}\, dx}_{I_2}$$

The Ehrenfest Theorem

$$I_2 = \int \overset{dv}{\frac{\partial^2\psi^*}{\partial x^2}}\,\overset{u}{\frac{\partial\psi}{\partial x}}\,dx = \cancelto{0}{\left[\overset{v}{\frac{\partial\psi^*}{\partial x}}\,\overset{u}{\frac{\partial\psi}{\partial x}}\right]_{-\infty}^{+\infty}} - \int \overset{v}{\frac{\partial\psi^*}{\partial x}}\,\overset{du}{\frac{\partial^2\psi}{\partial x^2}}\,dx$$

$$I_2 = -\int \overset{dv}{\frac{\partial\psi^*}{\partial x}}\,\overset{u}{\frac{\partial^2\psi}{\partial x^2}}\,dx$$

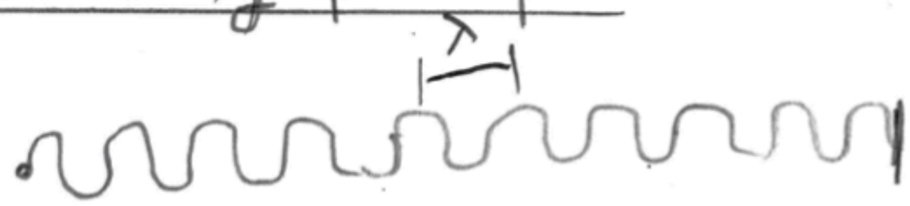
$$= -\cancelto{0}{\left[\psi^*\frac{\partial^2\psi}{\partial x^2}\right]_{-\infty}^{+\infty}} + \int \psi^*\frac{\partial^3\psi}{\partial x^3}\,dx$$

$$\Rightarrow I_2 = \int \psi^*\frac{\partial^3\psi}{\partial x^3}\,dx$$

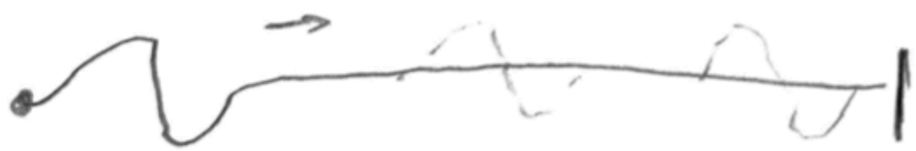
$$\Rightarrow I_1 = \frac{i\hbar}{2m}\int \psi^*\frac{\partial^3\psi}{\partial x^3}\,dx - \frac{i\hbar}{2m}\int \psi^*\frac{\partial^3\psi}{\partial x^3}\,dx = 0$$

The Uncertainty Principle

The uncertainty principle:

(1) 

Where is the wave? ✗ ill-defined $\vec{r}$
What is the λ? ✓ well defined λ.

(2) 

Where is the wave? ✓
What is the λ? ✗

- The more precise the wave position is, the less precise is its λ, and viceversa.
- Also, applies to waves in QM.

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda} \qquad \text{(de Broglie formula)}$$

- λ of ψ.

⇒ a spread in λ → a spread in p.

Heisenberg's Uncertainty Principle

$$\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$$

$\sigma_x \equiv$ stdev of x
$\sigma_p \equiv$ stdev of p

* Position measurements
* Momentum measurements

} precise answers

* Measurements on identical systems do not yield consistent results

* Q system where x measurements by making Ψ a localized spike, p measurements will be widely scattered.

* " " p measurements Ψ a long sine wave, x " " "

* No limit on how big σ_x, σ_p can be.

General QM problem

Time-dependent Schrödinger equation:

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

Separation of variables, assuming V=V(x).

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

We obtain 2 ODEs:

(wiggle factor)

1. $$\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi,$$ $$\varphi(t) = e^{-iEt/\hbar}.$$

Time-independent Schrödinger equation:

2. $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi.$$ To solve it we need V(x).

Separable Solutions:

- They are stationary states.

- Every expectation value is constant in time

- They are states of definite total energy, i.e., every measurement of the total energy is certain to return the value E.

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = E^2 - E^2 = 0.$$

- The general solution is a linear combination of separable solutions, i.e., there is a different wave function for each allowed energy:

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}.$$

General Solution:

- The strategy is first to solve the time-*in*dependent Schrödinger equation.

- This yields, in general, an infinite set of solutions, $\{\psi_n(x)\}$, each with its own associated energy, $\{E_n\}$.

- To fit $\psi(x, 0)$ you write down the general linear combination of these solutions:

$$\Psi(x, 0) = \sum_{n=1}^{\infty} c_n \, \psi_n(x);$$

- Construct global solution from the stationary states:

$$\boxed{\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} = \sum_{n=1}^{\infty} c_n \Psi_n(x, t).}$$

- Coefficients:

$\lvert c_n \rvert^2$	is the *probability* that a measurement of the energy would return the value E_n.

Bound states versus scattering states

Bound states are *normalisable*, and labeled by a *discrete index n*

Scattering states are *non-normalisable*, and labeled by a *continuous variable k*.

$$\begin{cases} E < V(-\infty) \text{ and } V(+\infty) \Rightarrow & \text{bound state,} \\ E > V(-\infty) \text{ or } V(+\infty) \quad \Rightarrow & \text{scattering state.} \end{cases}$$

$$\begin{cases} E < 0 \Rightarrow & \text{bound state,} \\ E > 0 \Rightarrow & \text{scattering state.} \end{cases}$$

Time-independent Schrödinger equation

Time-independent Schrödinger equation:

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

To solve it we need V(x).

Steps:

1. Define and sketch V(x).
2. Divide the problem into regions of interest.
3. Analyse the expected type of solutions (e.g. bound states or scattering states)
4. Divide the problem based on the energy of the particle.
5. Re-write Schrödinger equation for each region.
6. Define an appropriate and real wavenumber.
7. Solve the resulting ODE.
8. Analyse the asymptotic behaviour of the ODE solutions, remove diverging terms.
9. Analyse boundary conditions (usually two: ψ(x) and ψ'(x) have to be continuous).
10. Find energies and normalise the solution.
11. Append the wiggle factor and construct a general solution.

UC1
The Schrödinger equation

UC1 contents:

- **Review of** quantum experiments and **mathematical tools.**
- The wave function and the Schrödinger equation.
- Statistical interpretation of the wave function and probability.
- Normalisation, momentum, and the uncertainty principle.