

# 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 provides a framework to study our Universe.
- 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).
- **The purpose of this class is to teach you how to DO and USE quantum mechanics.**

# 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.

# What is Quantum Mechanics (QM)?

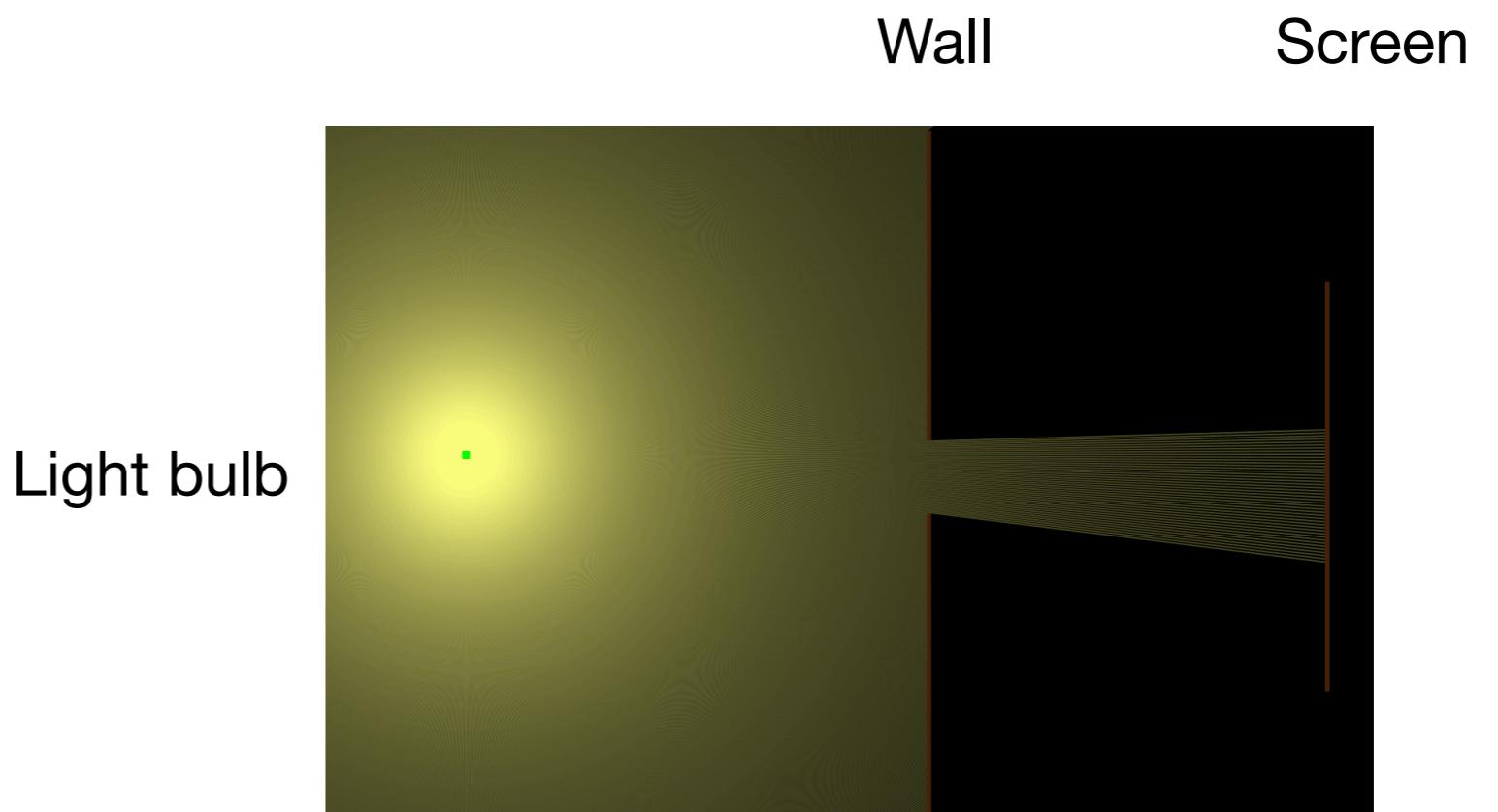
- “Don't let the mathematics (which, for us, is only a tool) interfere with the physics.”
- “QM represents an abrupt and revolutionary departure from classical ideas, calling forth a wholly new and radically counterintuitive way of thinking about the world.”
- **QM is a (mathematical) framework to do physics (at small scales).**

# Brief history of QM

**Experiments and basic ideas** 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:

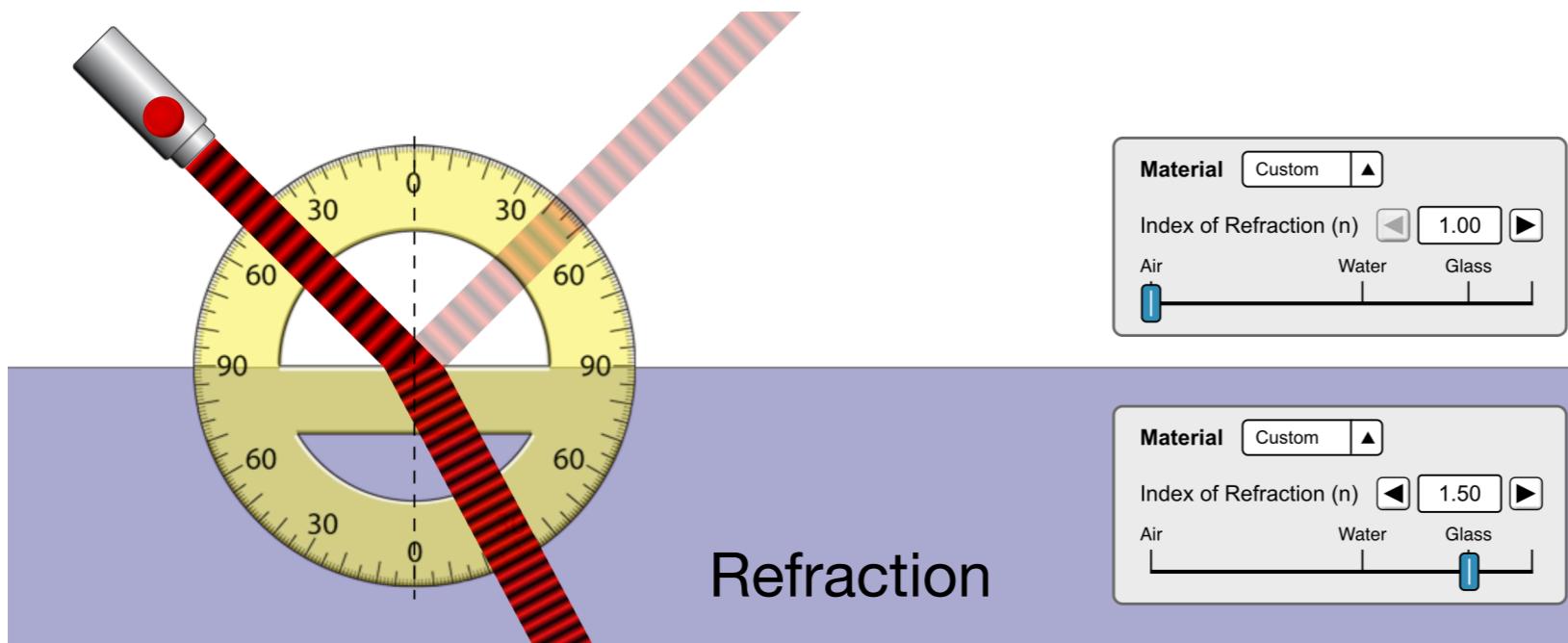
**Newton's view on light**



Applet: <https://phydemo.app/ray-optics/simulator/>

# 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.



$$\omega = \frac{ck}{n}$$

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

Applet: [https://phet.colorado.edu/sims/html/bending-light/latest/bending-light\\_en.html](https://phet.colorado.edu/sims/html/bending-light/latest/bending-light_en.html)

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

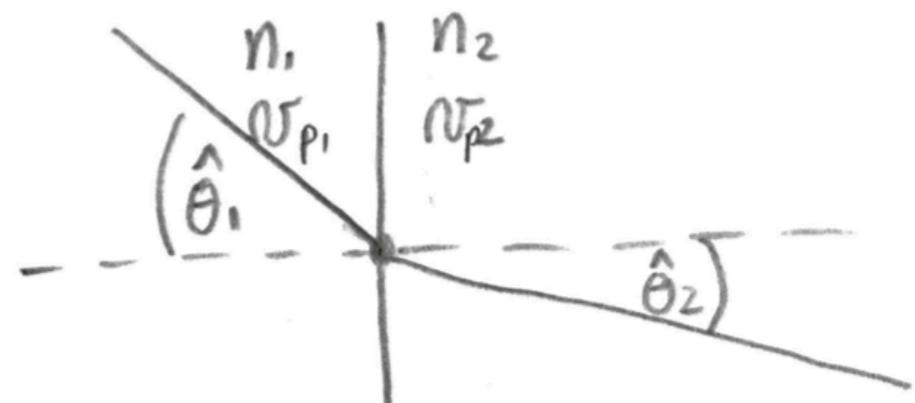
$$v_p \equiv \text{phase velocity} = \frac{\omega}{k} = \frac{\lambda}{T}$$

$\theta_1$  = incident angle

$\theta_2$  = refraction angle

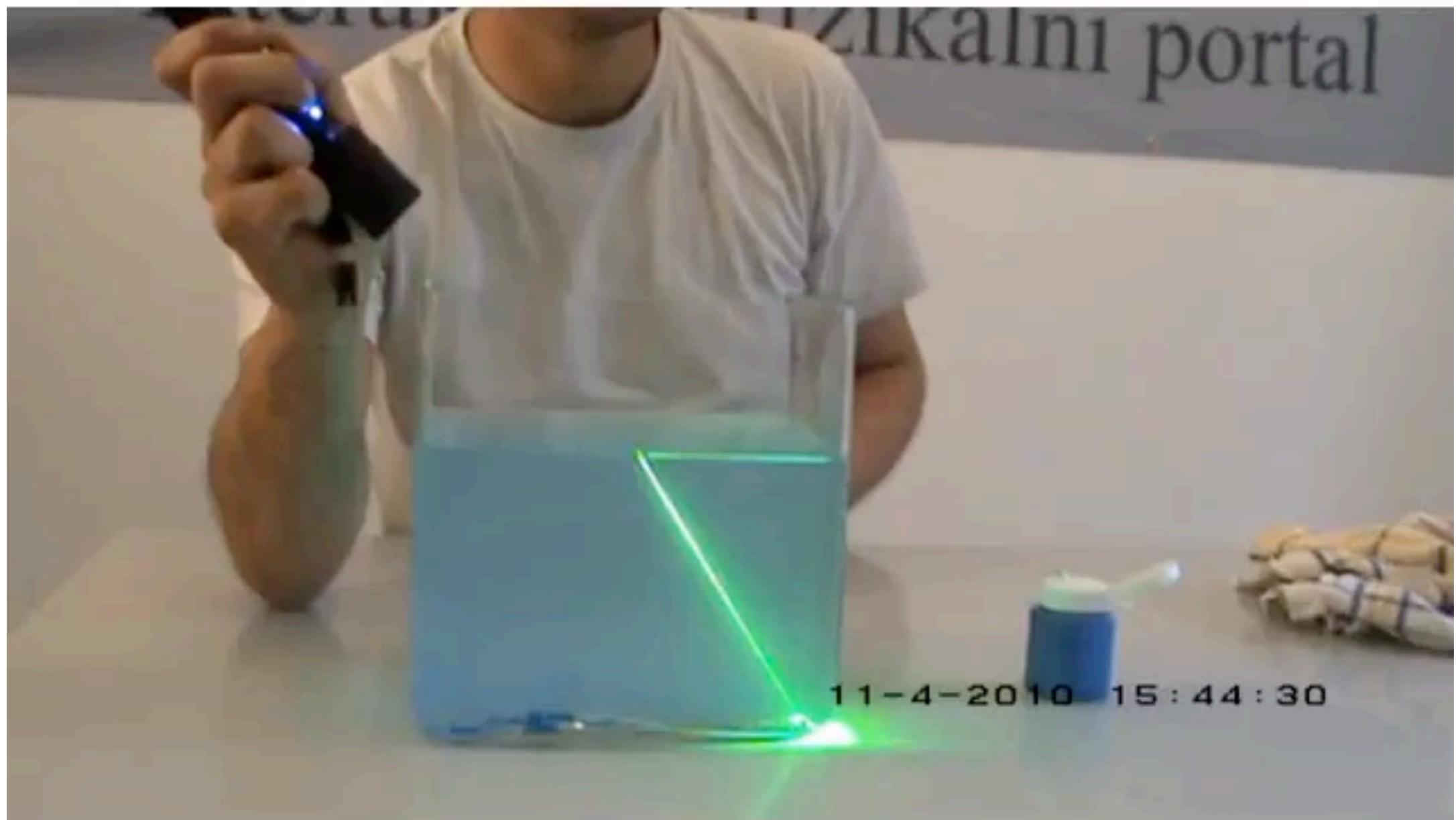
**Snell's law:**

$$\frac{\sin \theta_1}{\sin \theta_2} = \frac{v_{p,1}}{v_{p,2}} = \frac{n_2}{n_1}$$



# 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.



Video: <https://www.youtube.com/watch?v=m9cUy6B--xc>

# 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:**

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

**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  
(circuitual law):**

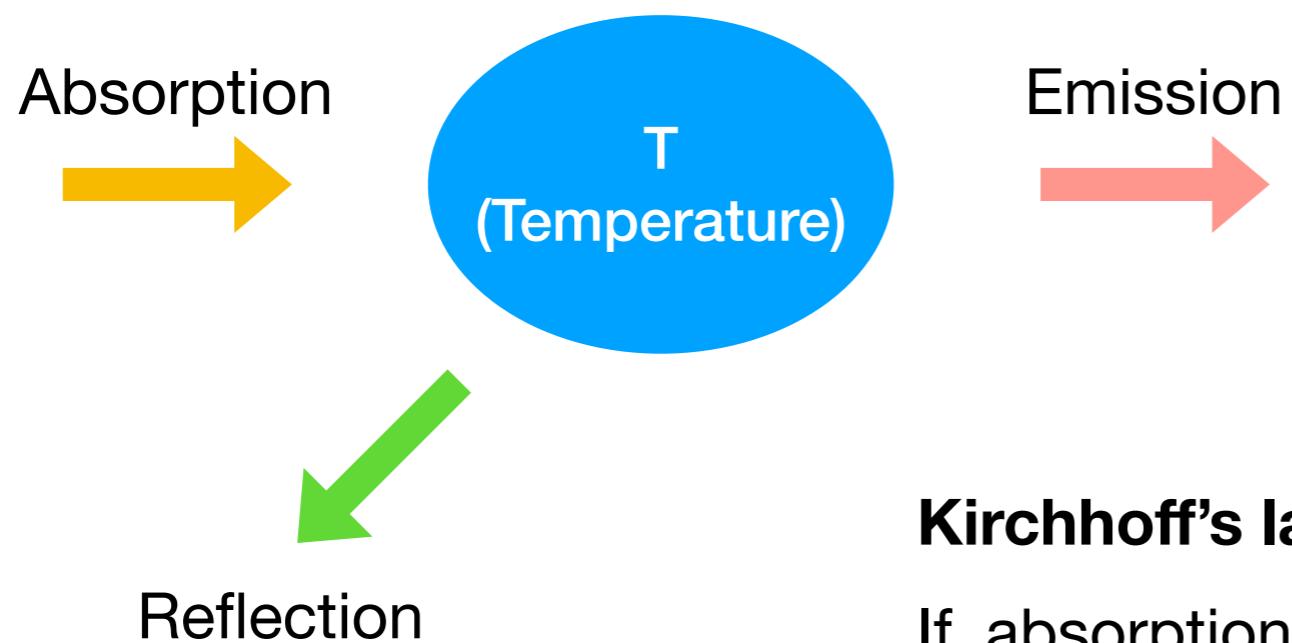
$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}$$

# Particle nature of EM radiation

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

An object can absorb, reflect and emit radiation:

- When it absorbs radiation, its temperature goes up.
- When it emits radiation, its temperature goes down.



## Kirchhoff's law:

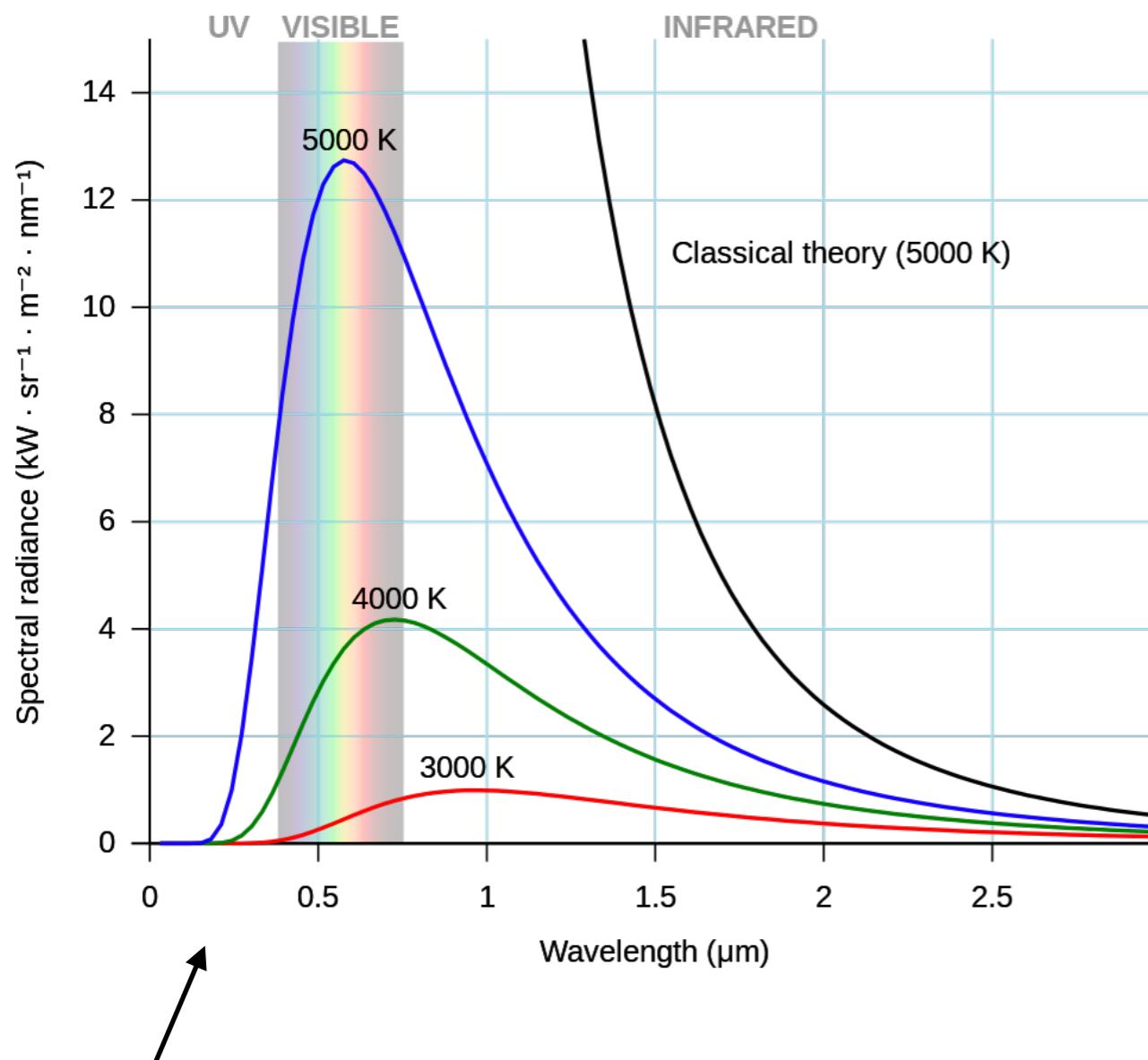
If absorption = emission, then the temperature of the object remains constant (thermal equilibrium).

A **black body** is an object that does NOT reflect any 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**

**Rayleigh-Jeans (classical) law:**

$$B_\lambda(T) = \frac{2 c k_B T}{\lambda^4}$$

$$B_\nu(T) = \frac{2 \nu^2 k_B T}{c^2}$$

$k_B \equiv 1.38 \times 10^{-23} \text{ J K}^{-1} \equiv$  Boltzmann constant

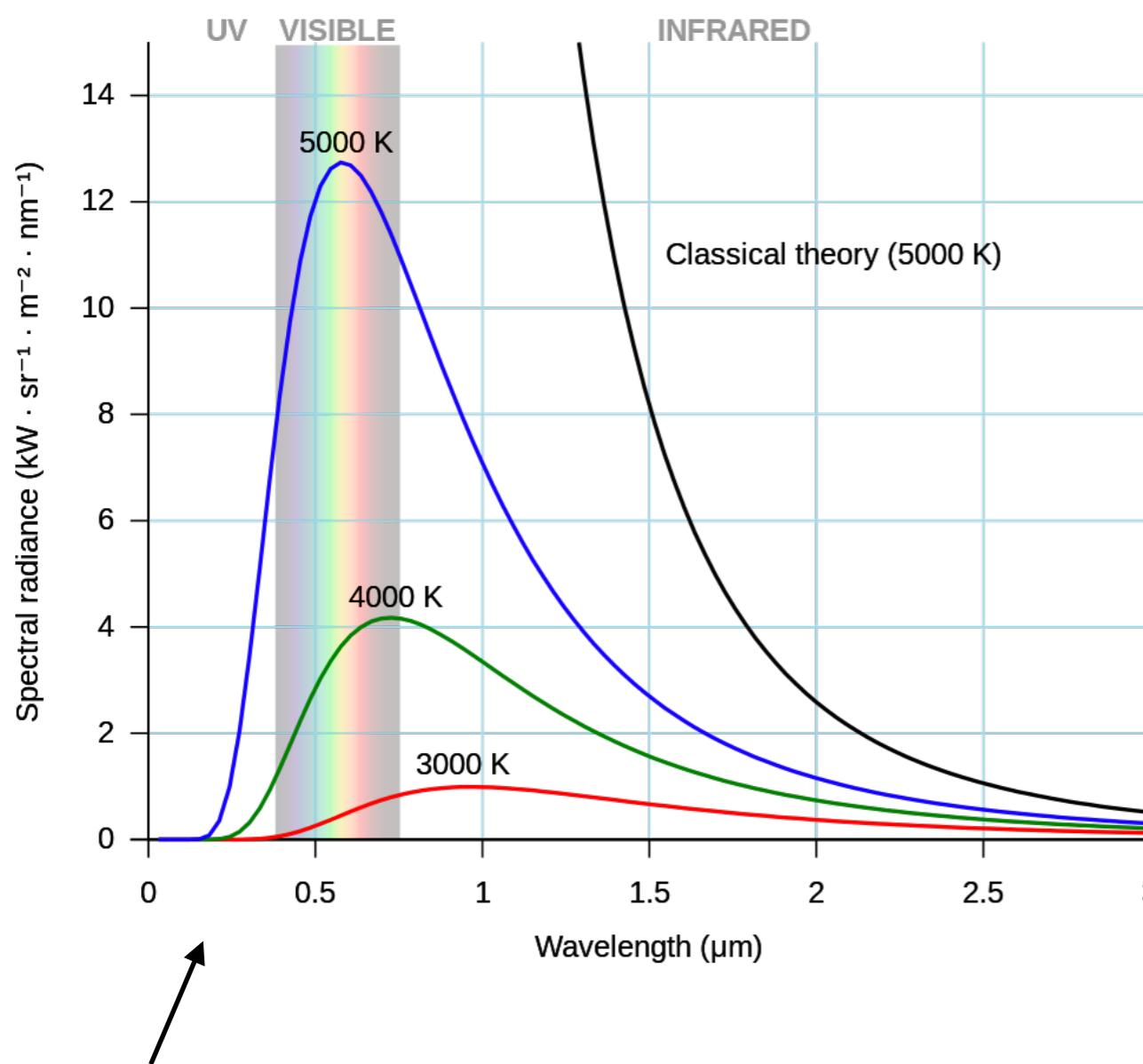
**Planck (quantum) law:**

$$B_\lambda(T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{hcl/(\lambda k_B T)} - 1}$$

$$B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/(k_B T)} - 1}$$

# Particle nature of EM radiation

- 1900 - M. Planck proposes quantisation of EM radiation
- Energy is not emitted or absorbed continuously, but rather in discrete packets or "quanta."



**UV catastrophe**

$$E_{\text{quanta}} = h\nu = h\frac{c}{\lambda} = \hbar\omega$$

$$\vec{p}_{\text{quanta}} = \hbar\vec{k}$$

$$\hbar = \frac{h}{2\pi} \equiv \text{reduced Planck constant}$$

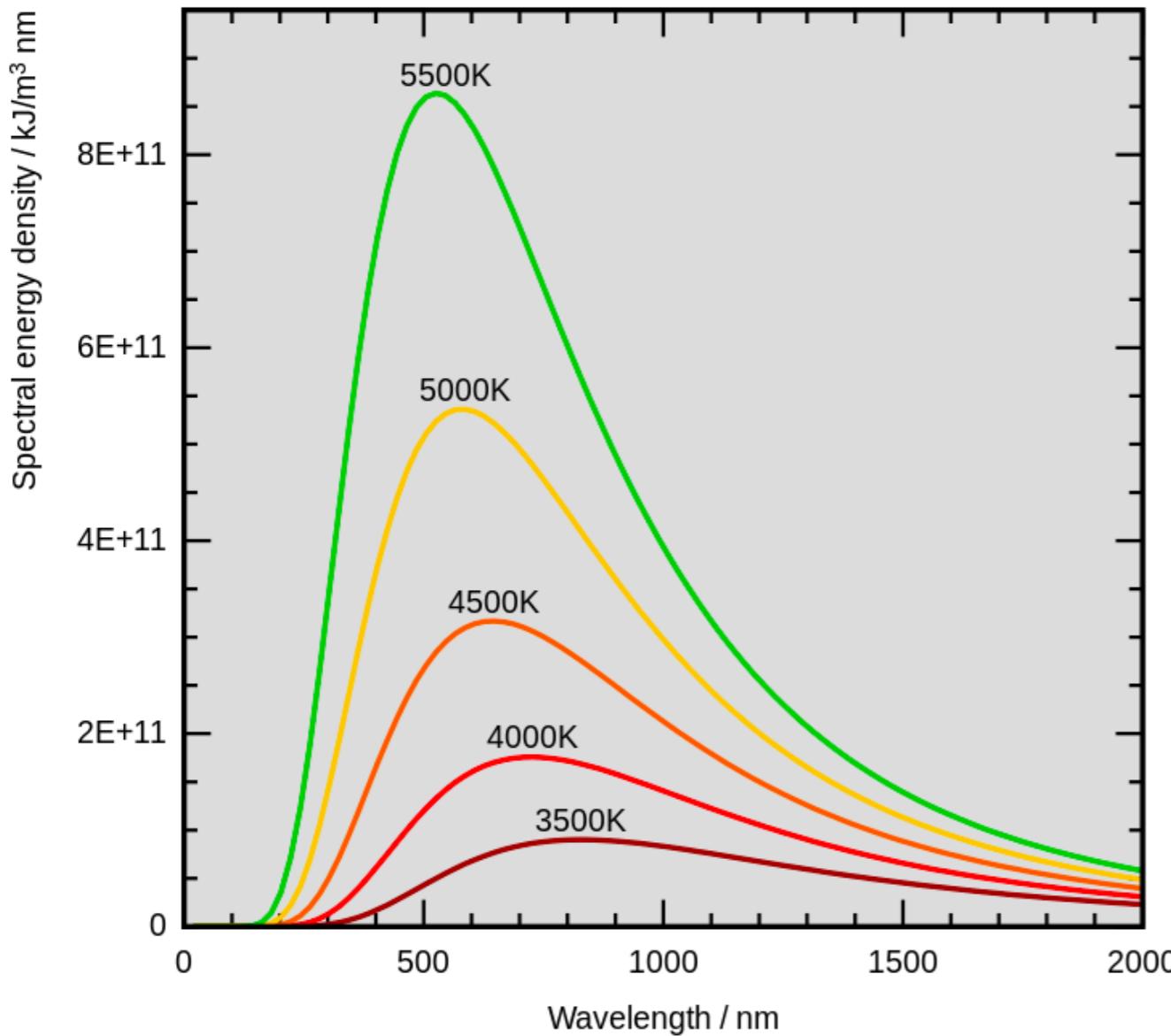
**De Broglie relation:**

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

# Particle nature of EM radiation

- **Wien's displacement law:**

The wavelength at which the spectral radiance of a black body peaks gives a measurement of the temperature.



$$\lambda_{\text{peak}} = \frac{b}{T}$$

$$b = 2.898 \times 10^{-3} \text{ m K}$$

$$\nu_{\text{peak}} = \frac{\alpha}{h} k_B T$$

$$\frac{\alpha}{h} k_B = 5.879 \times 10^{10} \text{ Hz K}^{-1}$$

# Particle nature of EM radiation

- **Stefan-Boltzmann law:**

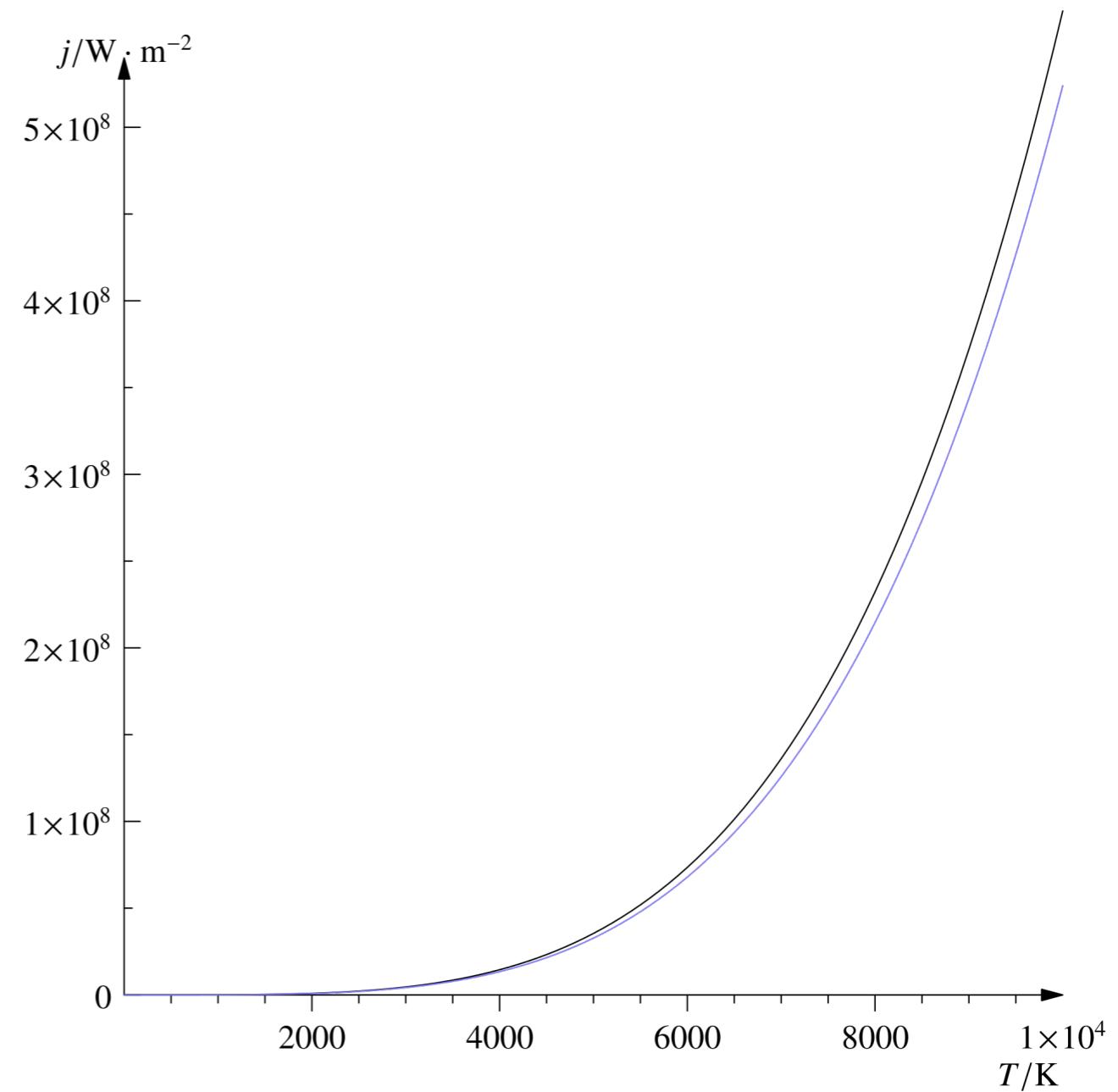
The total radiation emitted at all wavelengths is:

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

Where the Stefan-Boltzmann constant is:

$$\sigma = 5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$$

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



# Particle nature of EM radiation

- Planck's constant:  $h$

The units of  $h$  are units of angular momentum.

$$E_\gamma = h\nu$$

# Dimensional analysis of the Planck constant:

$$[h] = \frac{[E_\gamma]}{[\nu]} = \frac{[ML^2 T^{-2}]}{[T^{-1}]} = [ML^2 T^{-1}]$$

$$[h] = [L] [MLT^{-1}] = [\vec{r}] [\vec{p}] = [\vec{L}]$$

## Length x Momentum

# Angular momentum

## **Example:**

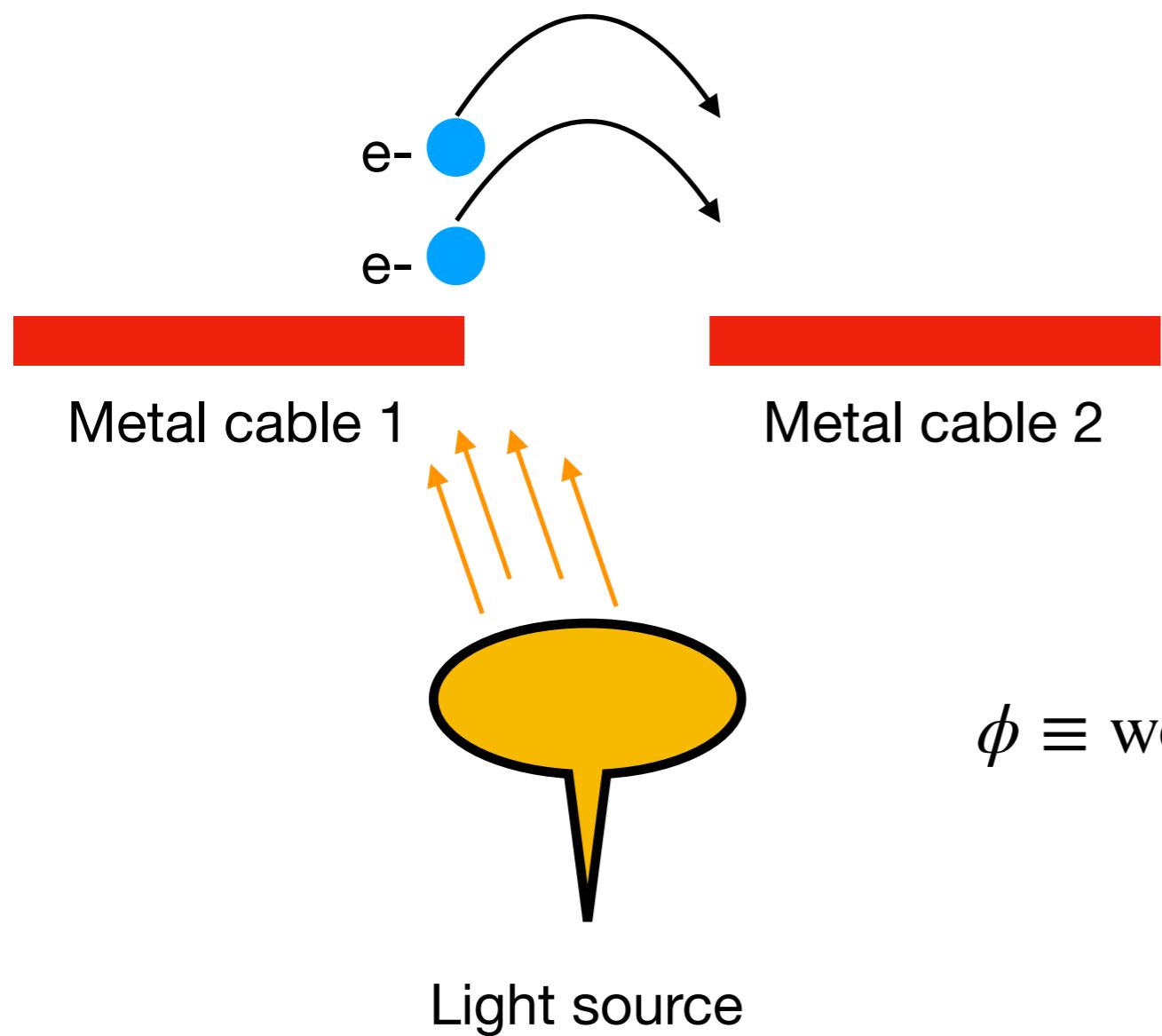
# Spin 1/2 particle

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

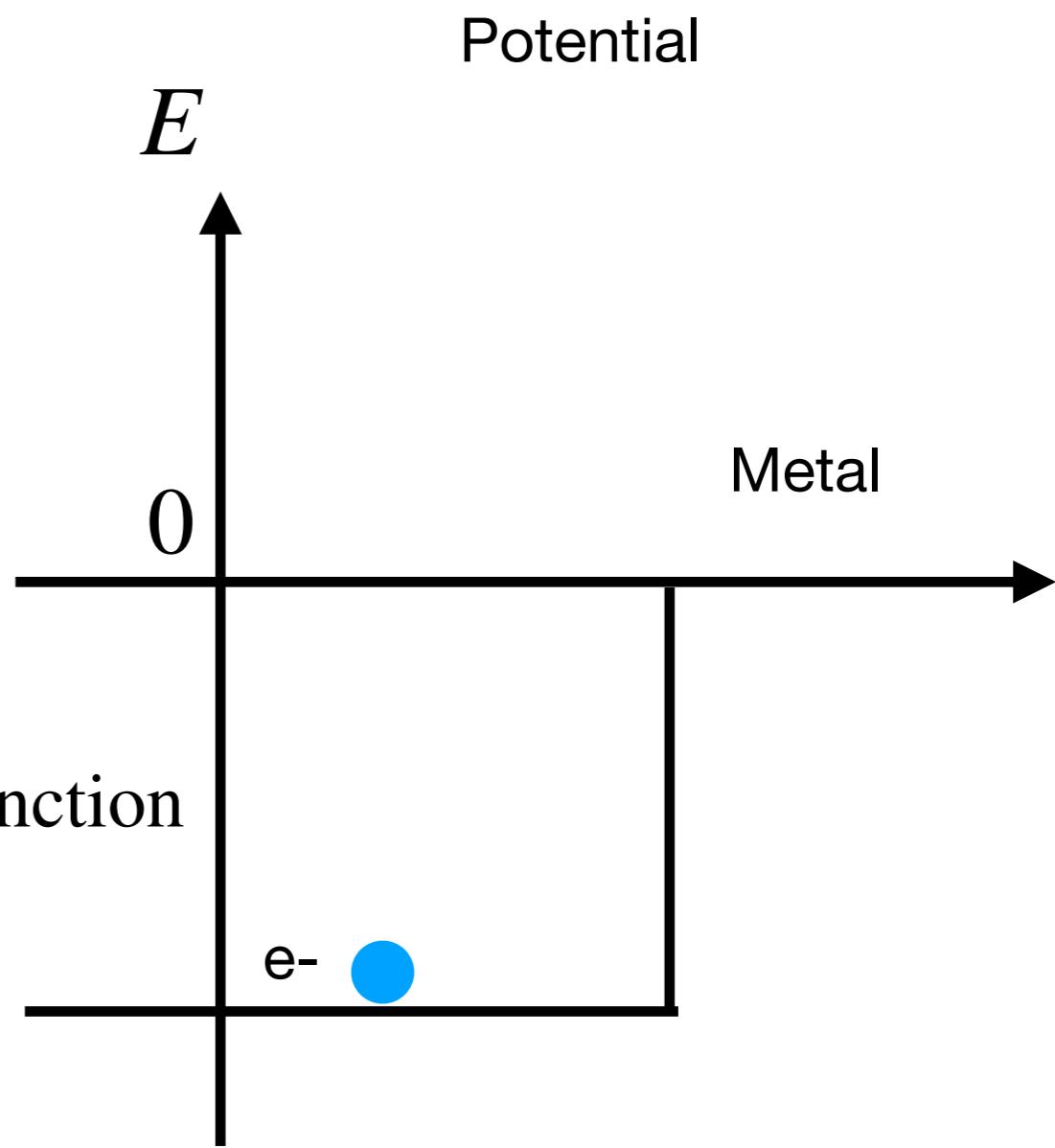
# The Photoelectric Effect

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  $e^-$  called photo-electrons.
- Photo  $\rightarrow$  light, electric  $\rightarrow$  electron

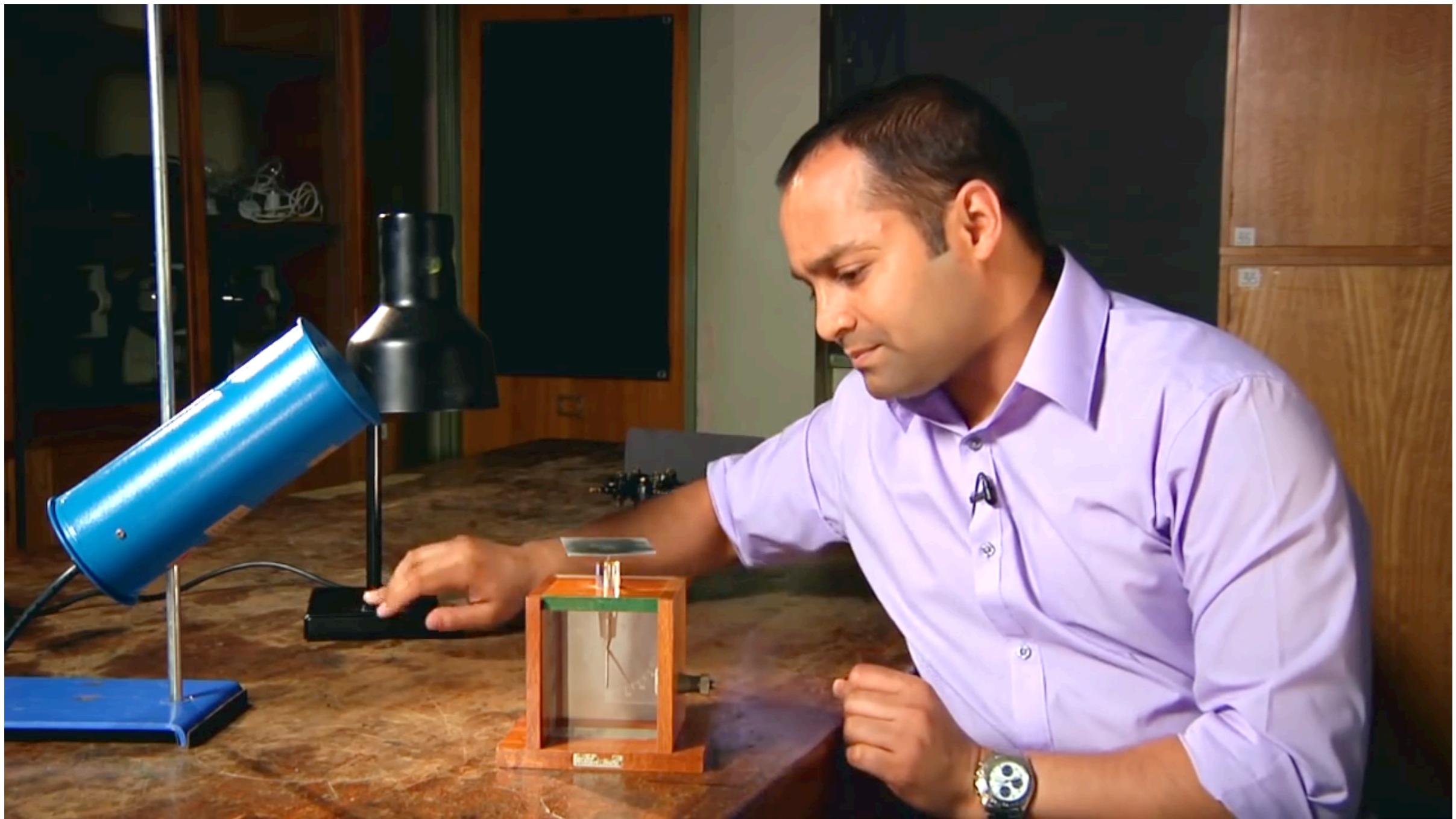


$$\phi \equiv \text{work function}$$



# The Photoelectric Effect

The gold leaf electroscope.



Video: <https://www.youtube.com/watch?v=v-1zjdUTu0o>

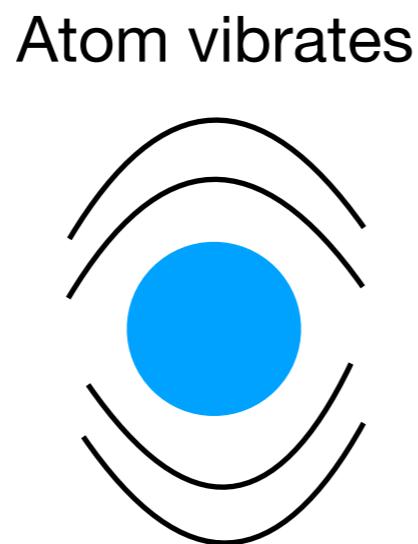
# The Photoelectric Effect

- Why does the photoelectric effect occurs?

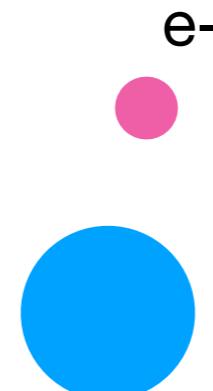
Classical (wave) view:



Light waves



Atom vibrates



Vibrating atom  
releases e-

e-

However, this should  
happen for all  $\lambda$ .

- Did experiments agree?

No.

Photoelectric effect occurs only for some  $\lambda$ , for others there is no e- jump.

# The Photoelectric Effect

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

Photons ( $\gamma$ ) composed beams of light and have energy:

$$E_\gamma = h\nu$$

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

where  $h = 6.63 \times 10^{-34} \text{ J s} \equiv$  the Planck constant.

$$\hbar c \equiv 197.33 \text{ MeV fm}$$

where fm  $\equiv 10^{-15} \text{ m} \equiv 1 \text{ fermi}$

- **Einstiens' prediction:** using these ideas:

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

↓  
Leftover  
energy

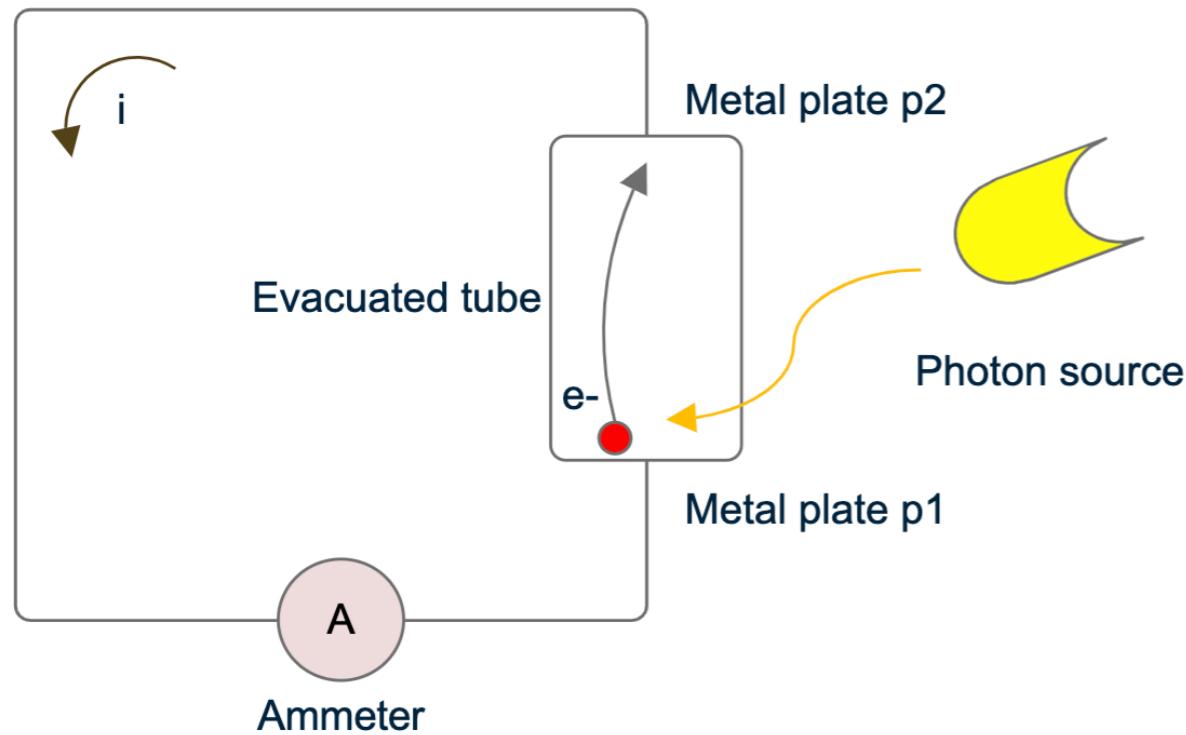
Energy given  
to the e-

Energy needed  
to liberate the e-

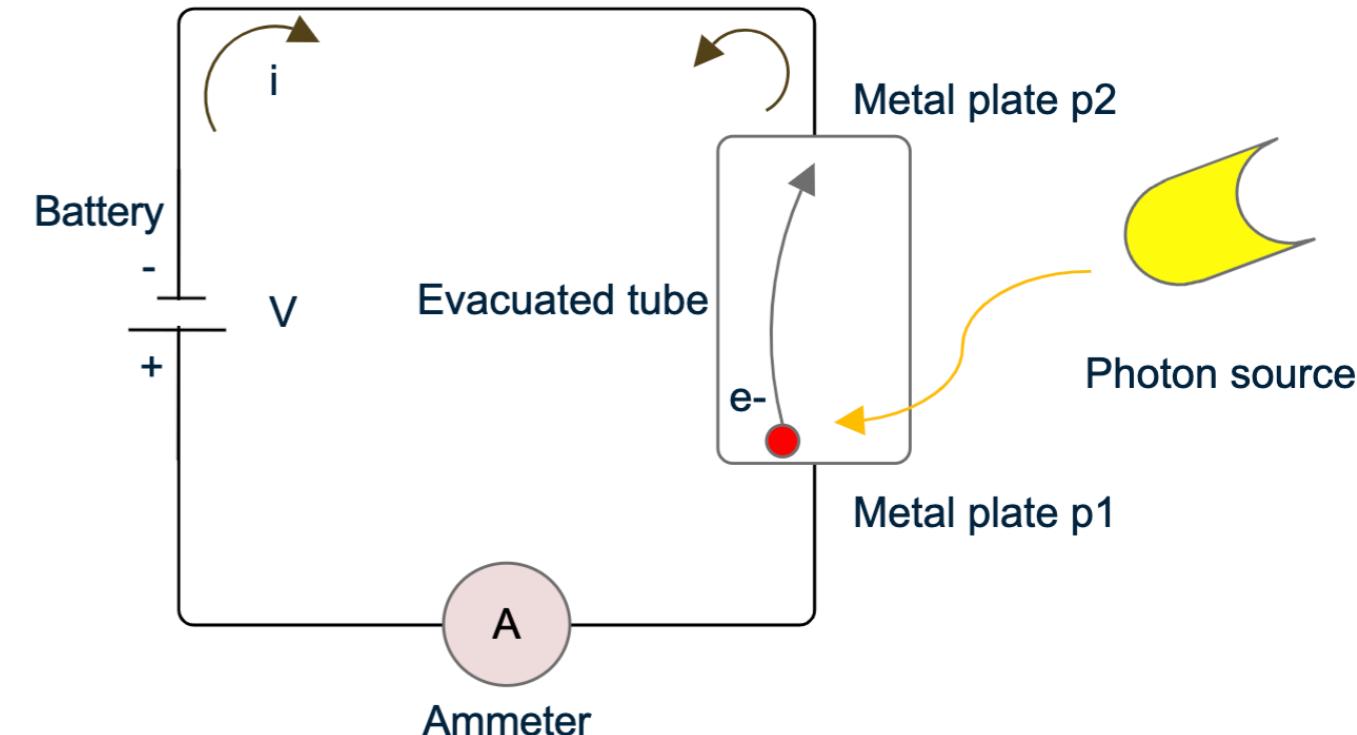
# The Photoelectric Effect

- 1915 - Millikan's experiment:

**Instance 1** (no battery)



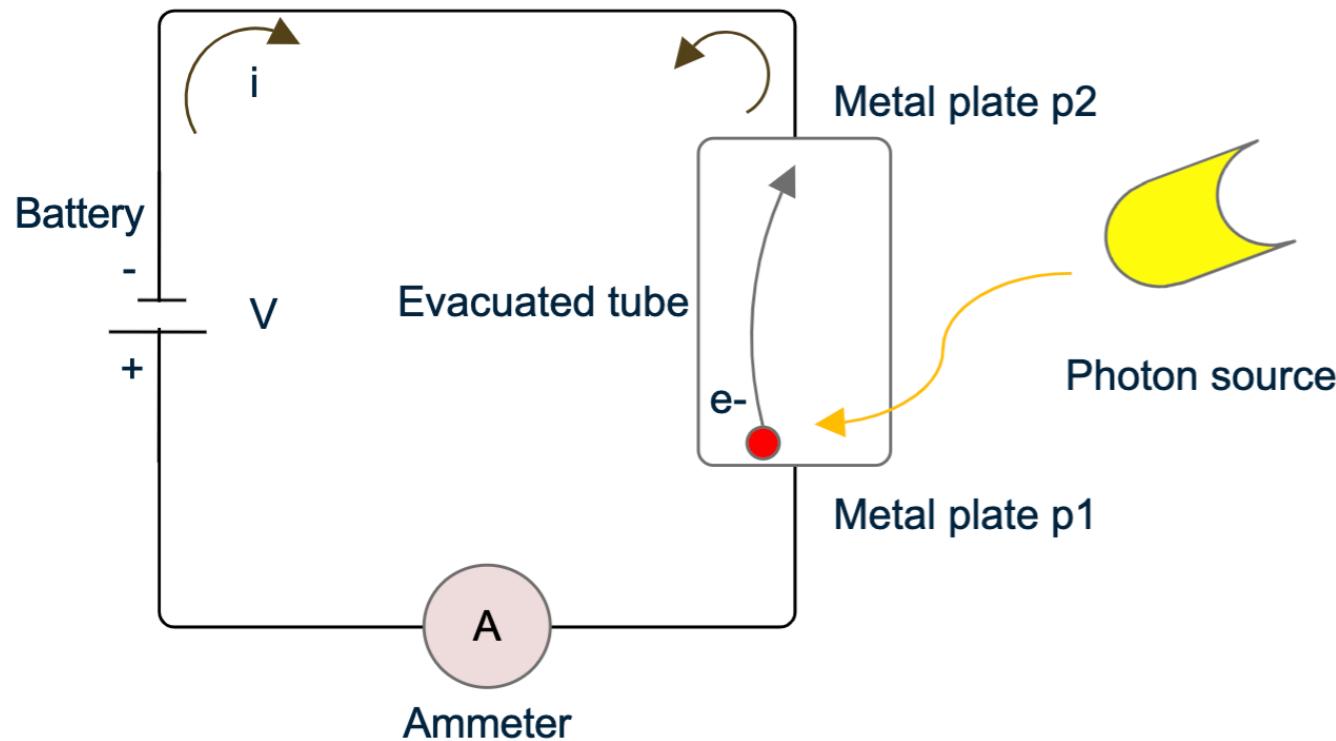
**Instance 2** (battery added)



- The goal of the battery is to stop an  $e^-$  from reaching plate p2.
- 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:



$$V_s = \frac{K_{e^-}}{e} = \frac{\frac{1}{2}mv^2}{e}$$

$$\Rightarrow K_{e^-} = e V_s$$

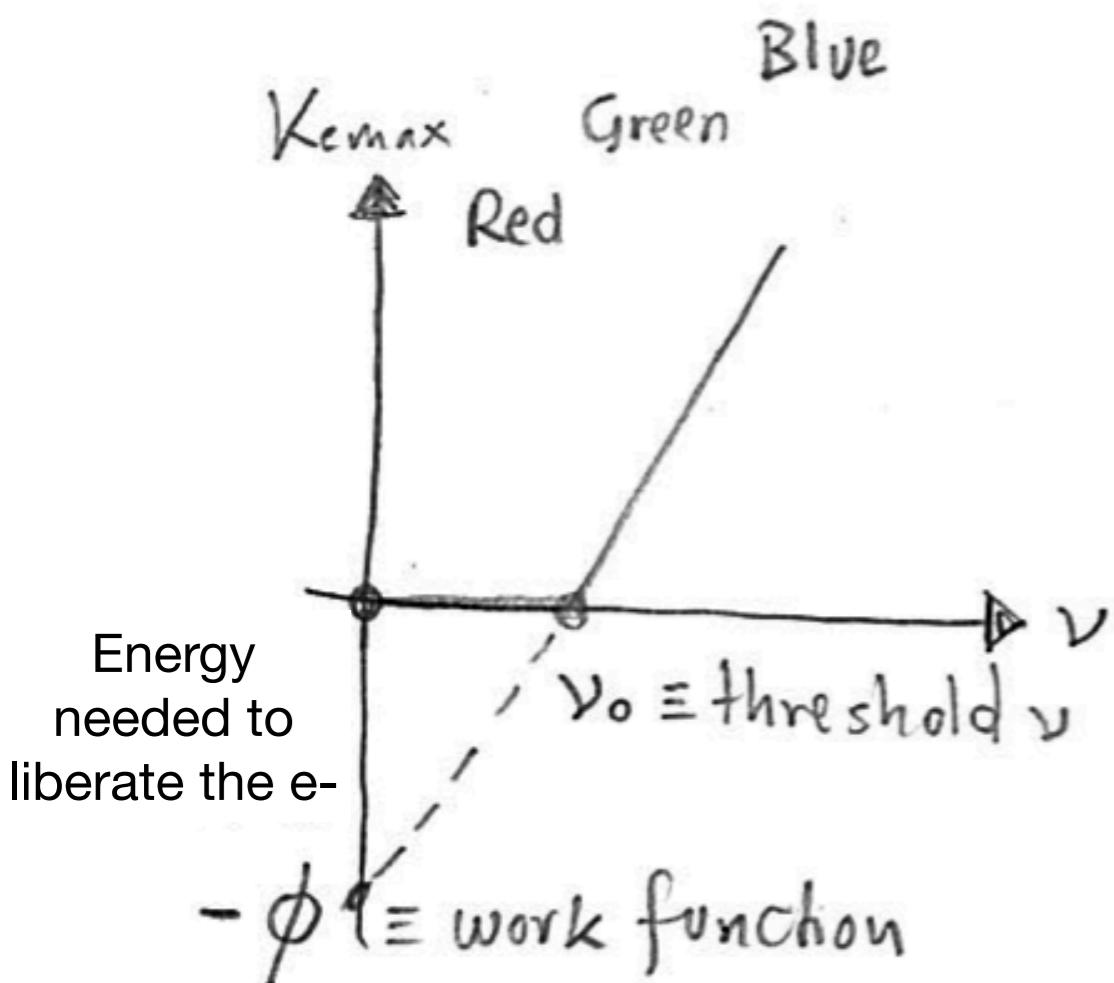
$$\Rightarrow K_{e^-} = e V_s = h\nu - \phi$$

- We increase the potential until no  $e^-$  reaches plate  $p_2$ .
- We call such potential the stopping potential,  $V_s$ .
- $e^-$  are only removed from the metal surface.

**Applet:** <https://applets.kcvs.ca/photoelectricEffect/PhotoElectric.html>

# The Photoelectric Effect

- 1915 - Millikan's experiment:



**$h$**  is the slope of this linear eq:

$$K_{e-,max} = h\nu - \phi$$

Einstein's prediction:

$$K_{e-,max} = e V_s = h\nu - \phi$$

Leftover energy  
after liberation

Energy given  
to the e-

Energy needed  
to liberate the e-

We recognise the equation of a line above.

The threshold frequency,  $\nu_0$ , can be estimated from:

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

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

$$\Rightarrow K_{e-,max} = h\nu - \phi = h(\nu - \nu_0)$$

# The Photoelectric Effect

- 1915 - Millikan's experiment conclusions:
  - Millikan verifies Einstein's prediction.
  - The Planck constant,  $h$ , is measured to better than 1% of its currently accepted value.
  - 1 photon is absorbed by 1e-.
  - Magnitude of the current (# of photo-e-) is proportional to light intensity.
  - Energy of photo-e- is independent of light intensity. More photons does not translate into higher kinetic energies.
  - Energy of photo-e- increases linearly with the frequency of the light.

**It is NOT easy to understand the above with waves.**

- **Light exists in quanta, not as a continuum.**

# 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)

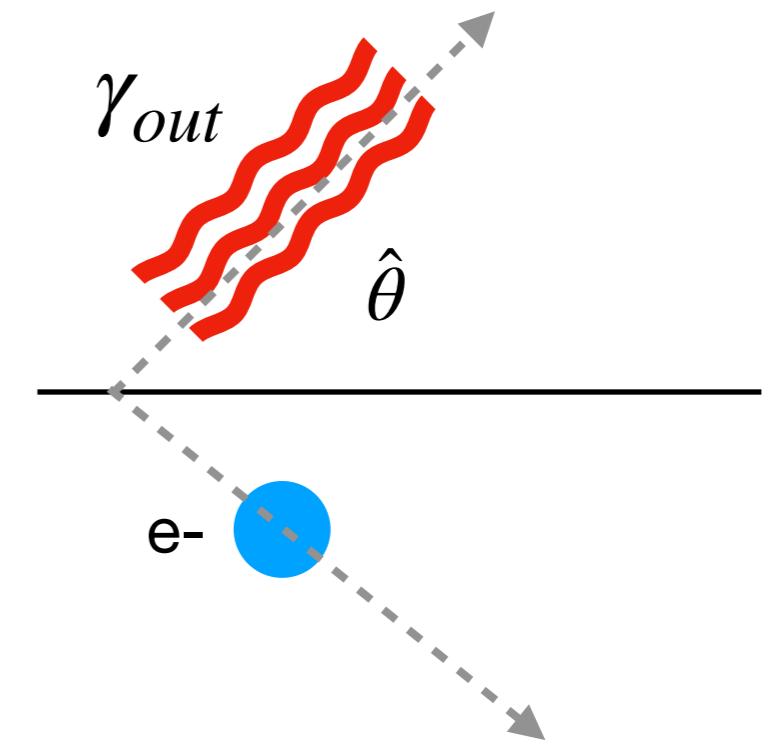
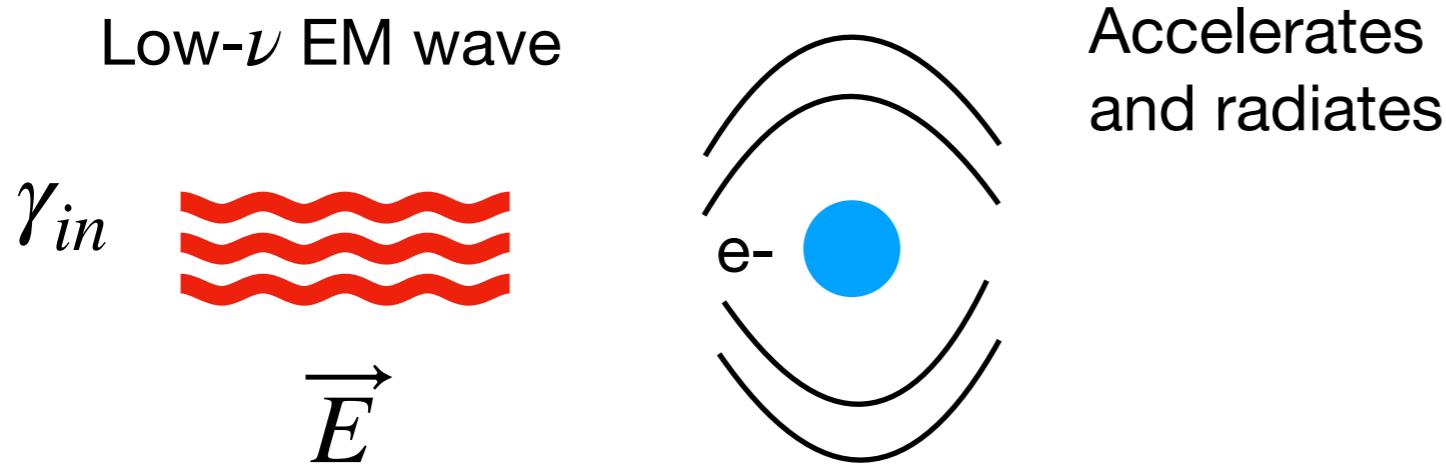
## Discovery of photons

- **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

# (Classical) Thomson Scattering

- Thomson's attributes scattering to e- vibrating as a result of the incident  $\vec{E}$  field.



The intensity of radiation as a function of  $\Omega$

$$\frac{d\sigma_t}{d\Omega} = \left( \frac{e^2}{4\pi\epsilon_0 mc^2} \right)^2 \frac{1 + \cos^2 \theta}{2}$$

- Thomson'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.

# Scattering experiments

## 1923 - Compton scattering:

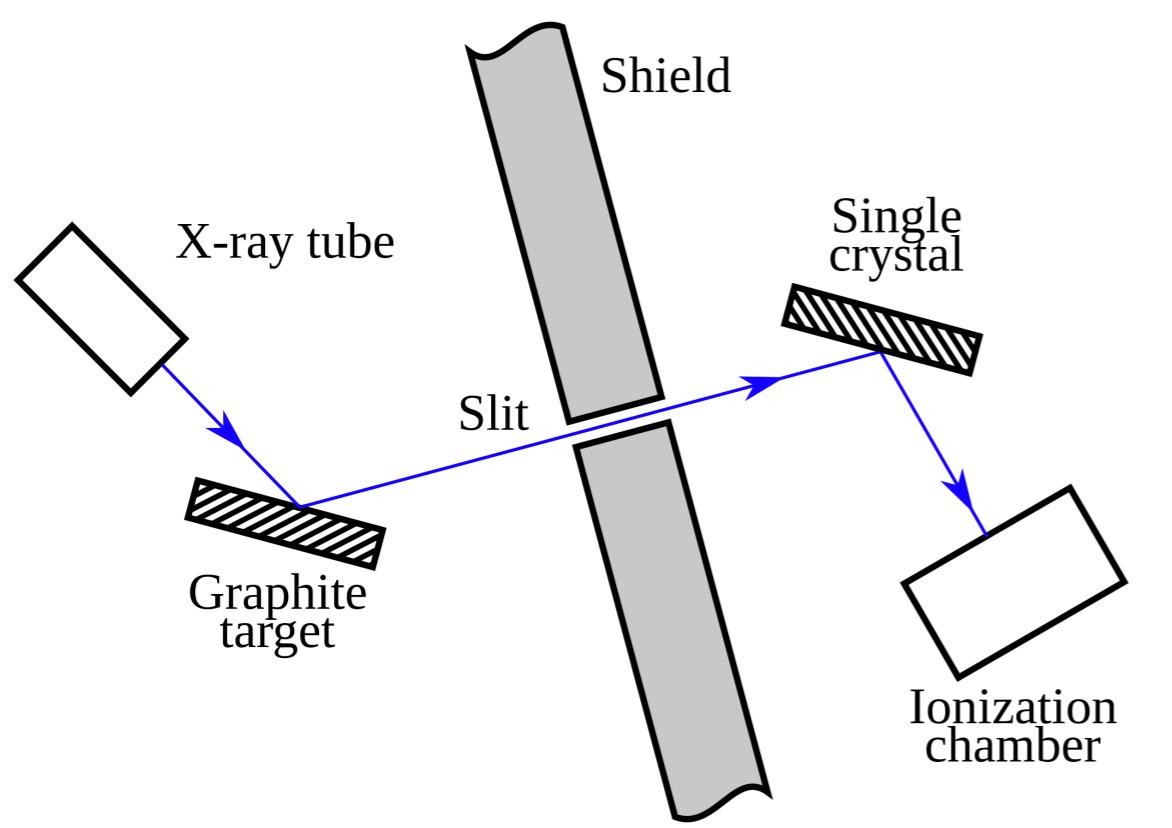
- Compton shows that Thomson's idea only works for low frequencies.
- Compton attributes the observed X-ray shift of particle-like momentum to light quanta.
- **Compton scattering effect**, experiments of X-rays interacting with matter.
- Compton studied X-rays shining on atoms. He used X-rays as they are highly energetic:
  - X-rays:  $100\text{ eV} - 100\text{ keV}$
  - Binding energy of  $e^-$  to atoms:  $10\text{ eV} - 13\text{ eV}$
- $\gamma$  scattering on  $e^-$  that are virtually free.
- Compton experiment was in disagreement with Thompson's theory of scattering.

# Compton Scattering

- Compton treats photons as particles.
- QM tells us a beam of monochromatic light is a collection of particle-like  $\gamma$ .

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

## 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.

# Compton Scattering

- Compton treats photons as particles:

Schematic diagram of Compton's experiment

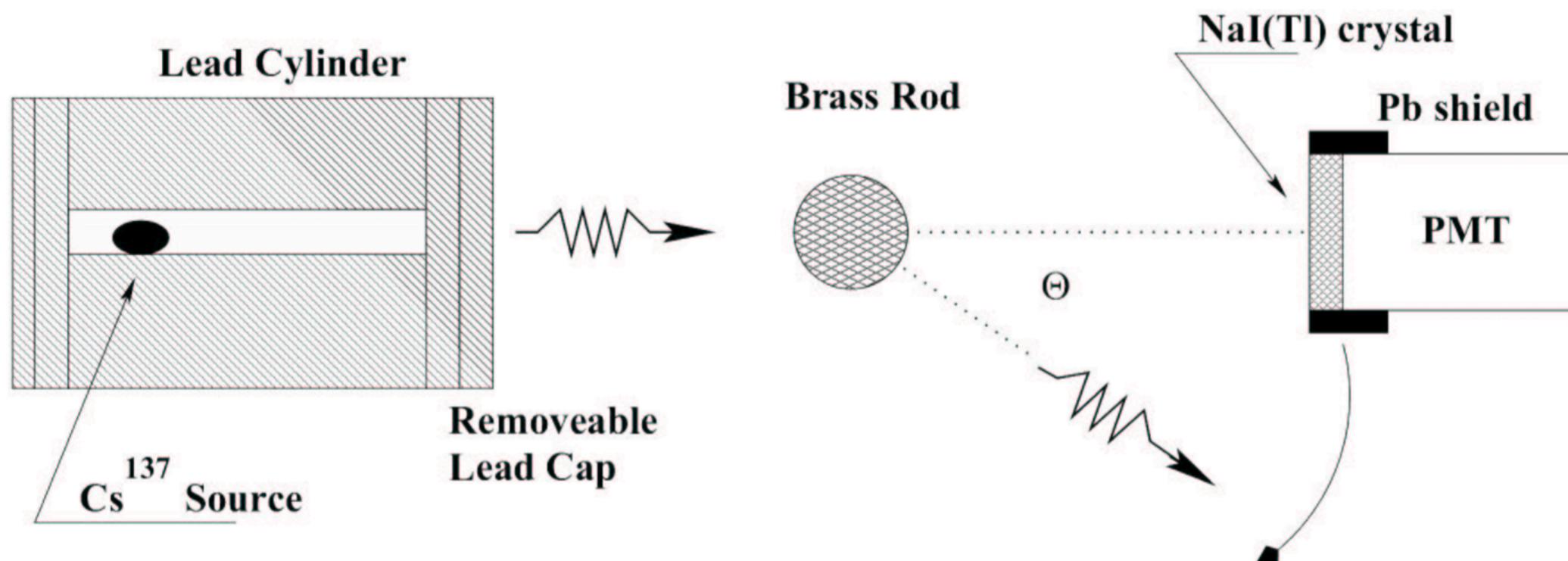


Figure 2: A schematic diagram of the experimental apparatus.

# Compton Scattering

- Compton treats photons as particles:

Schematic diagram of Compton's experiment

Decay Scheme of  $\text{Cs}^{137}$

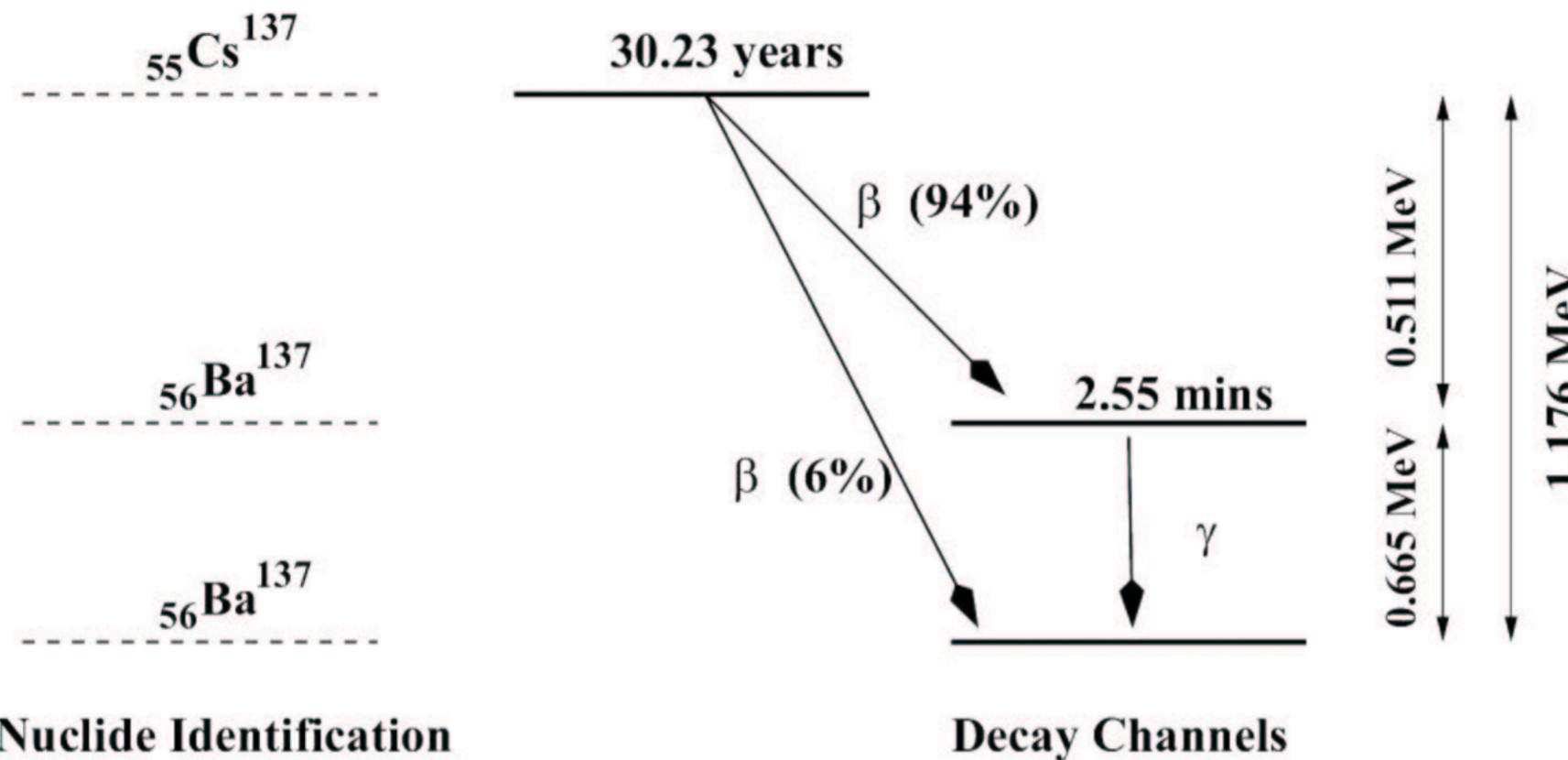
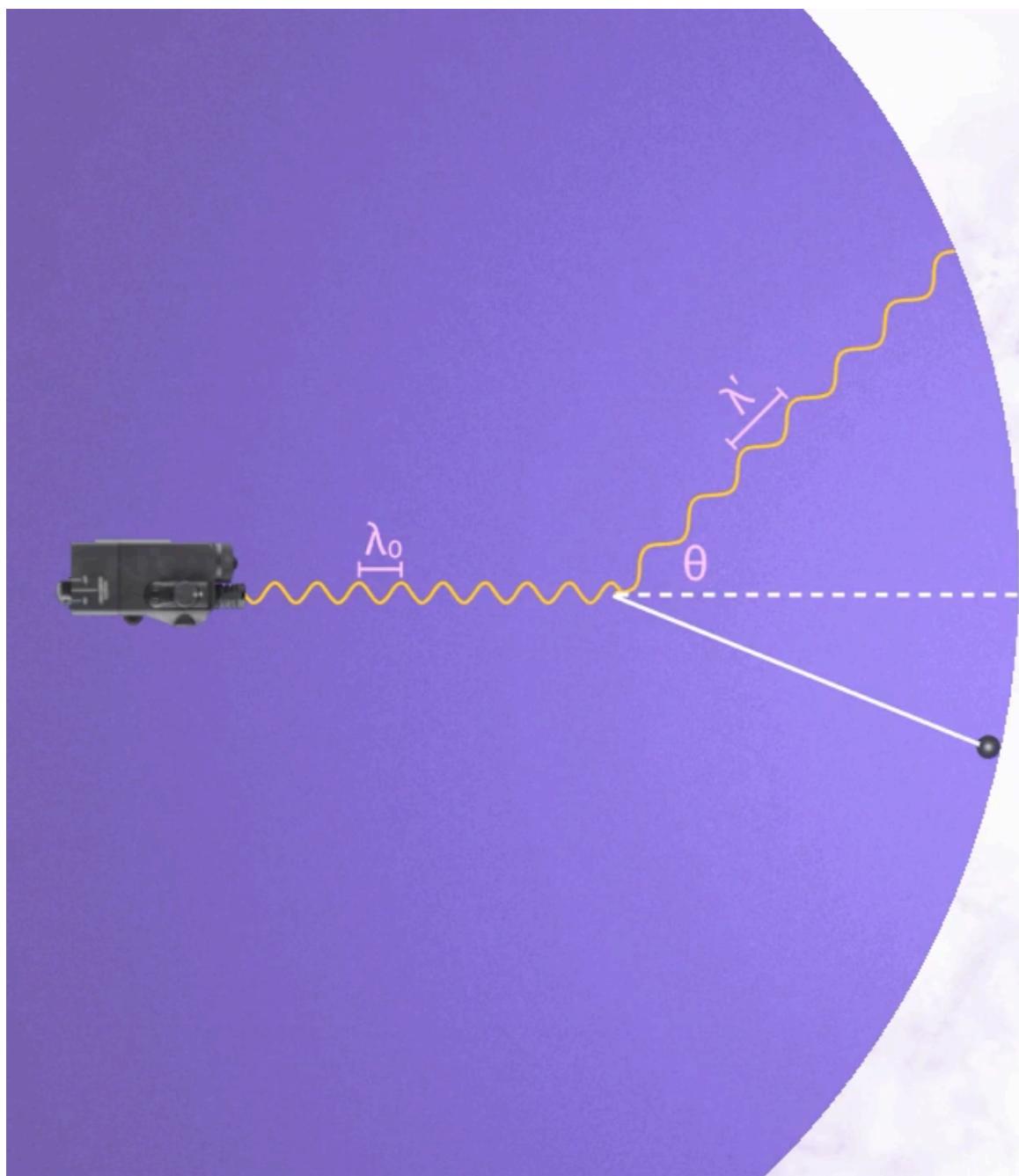


Figure 3: A schematic of the energy decay scheme of  $\text{Cs}^{137}$ .

# Compton Scattering

- Compton treats photons as particles:



$$\Delta\lambda = \lambda_c (1 - \cos \theta)$$

$\lambda_0$  The initial wavelength

$\lambda'$  The wavelength of scattered light

$\theta$  The scattering angle

$\lambda_c$  The Compton wavelength  $2.426 \times 10^{-12}$  m

$\Delta\lambda$  Pergeseran Compton

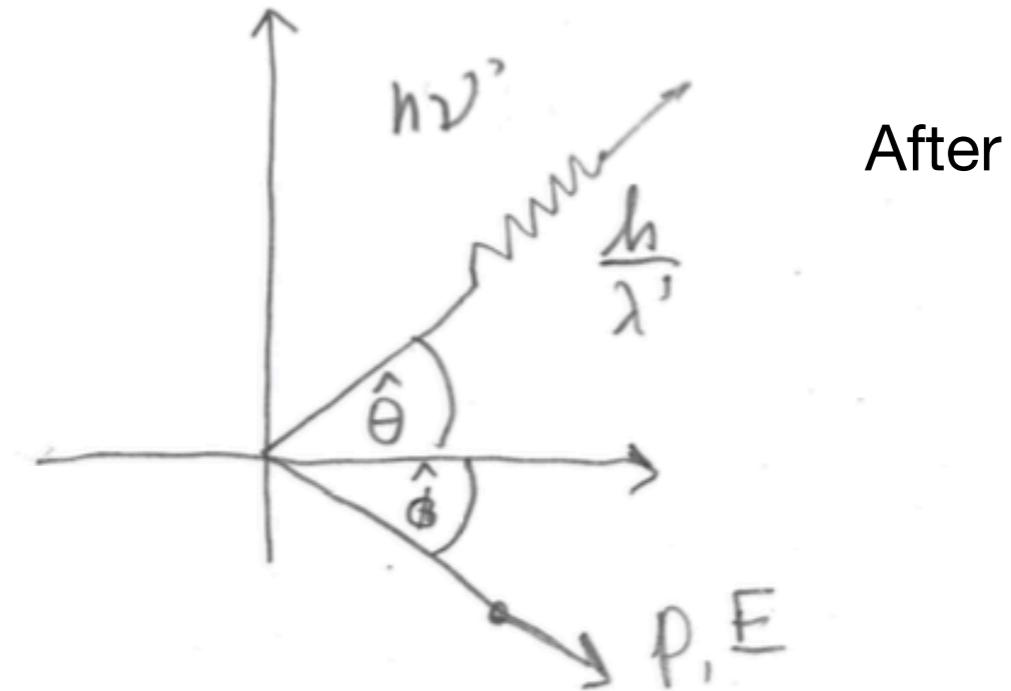
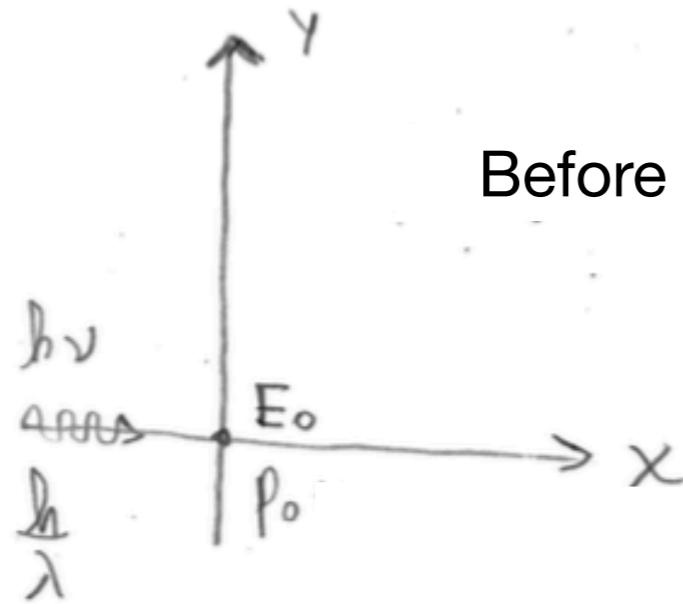
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# Compton Scattering

- **Compton scattering:** collision of  $\gamma$ 's with charged particles.



Compton shift:

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



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

QM correctly predicts that the  $\nu$  decreases (or  $\lambda$  increases) after the collision.

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

Photons ( $\gamma$ 's) lose energy:  $\lambda' > \lambda$

# Photons are particles

- 1916: photons are quanta of energy ( $E$ ) and momentum ( $p$ ).

$$E = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}} \Rightarrow E^2 - p^2 c^2 = m^2 c^4$$
$$\vec{p} = \frac{m \vec{v}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

- In QM1, we study non-relativistic cases only:

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad \text{where : } \vec{p} = m\vec{v}$$

- A photon is massless:  $m_\gamma = 0, E_\gamma = p_\gamma c$

$$p_\gamma = \frac{E_\gamma}{c} = \frac{h\nu_\gamma}{c} = \frac{h}{\lambda_\gamma}$$

# 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  $\lambda$  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  $\lambda$  of a  $\gamma$  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  $\lambda$  is the  $\lambda$  of light that has that rest energy.

If we have an  $e^-$  with a Compton  $\lambda_e$  and we shine on it a  $\gamma$  with that size, that  $\gamma$  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  $\lambda_c$ .

# De Broglie and Compton wavelengths

## Definitions:

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

# De Broglie's proposal: matter waves

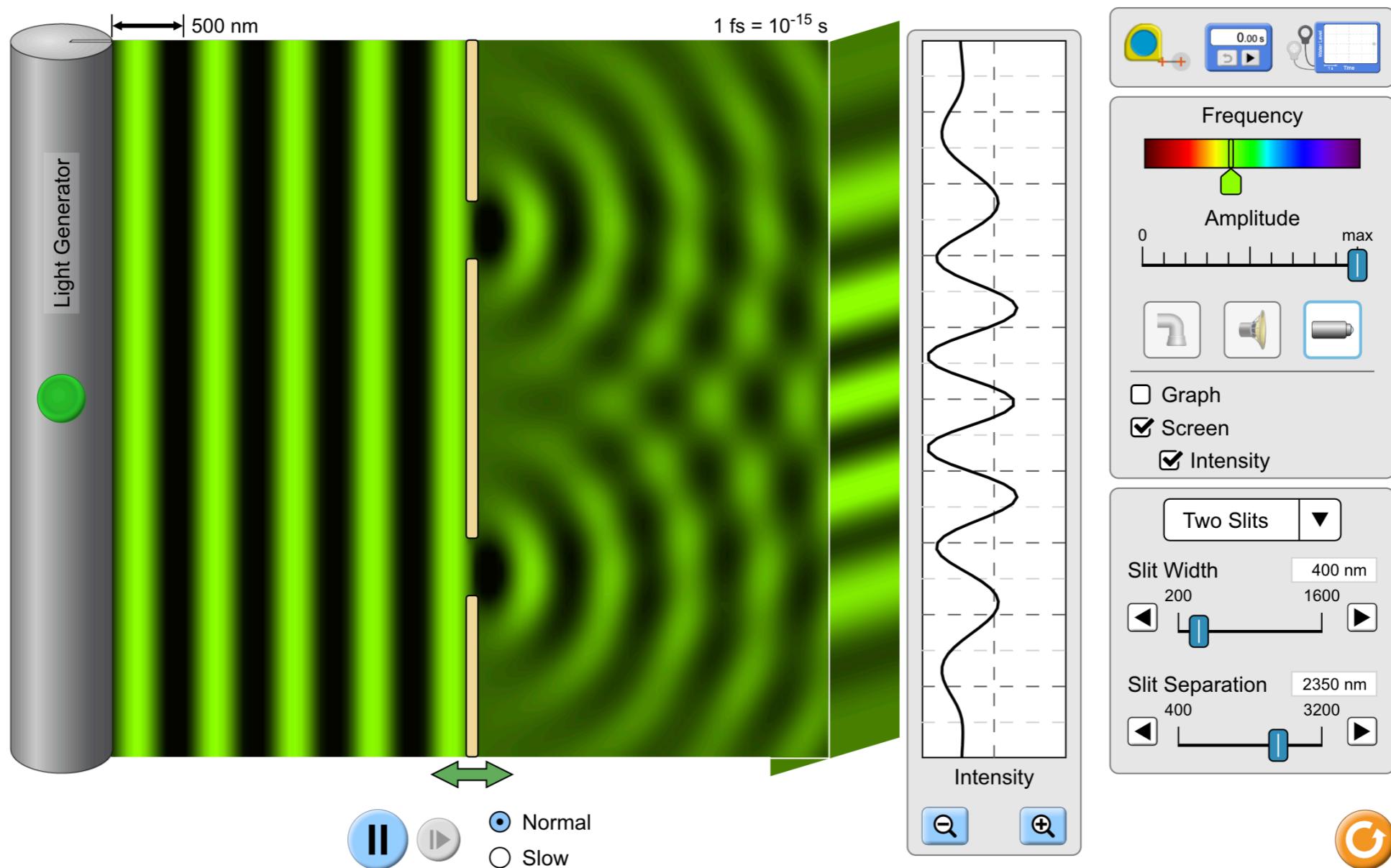
- de Broglie's equation for  $\lambda_{db}$  is proposed in 1924.
- **de Broglie's proposal:**
- Photons are particles and also waves, is this universal? **de Broglie says YES.**
- Particles have definite amounts of  $E$  and momentum  $\vec{p}$ , i.e. they are packets that cannot be broken.
- Waves, on the other hand, can interfere.
- **de Broglie proposes that this is a more general property of matter.**
- All matter particles behave as waves, nos just photons.
- There is a wave associated to every matter particle.

# De Broglie's proposal: matter waves

- QM then studies these “**matter waves**”.
- Matter waves are introduced, but new math/physics is needed.
- QM introduces probability waves to describe them.
- Matter waves are described as probability amplitudes with Complex numbers.
- We associate to a particle a wave that depends on momentum.
- For a particle of momentum,  $\vec{p}$ , we associate a plane wave with  $\lambda = \frac{h}{p}$ , where  $\lambda = \lambda_{\text{db}}$  is the de Broglie wavelength.

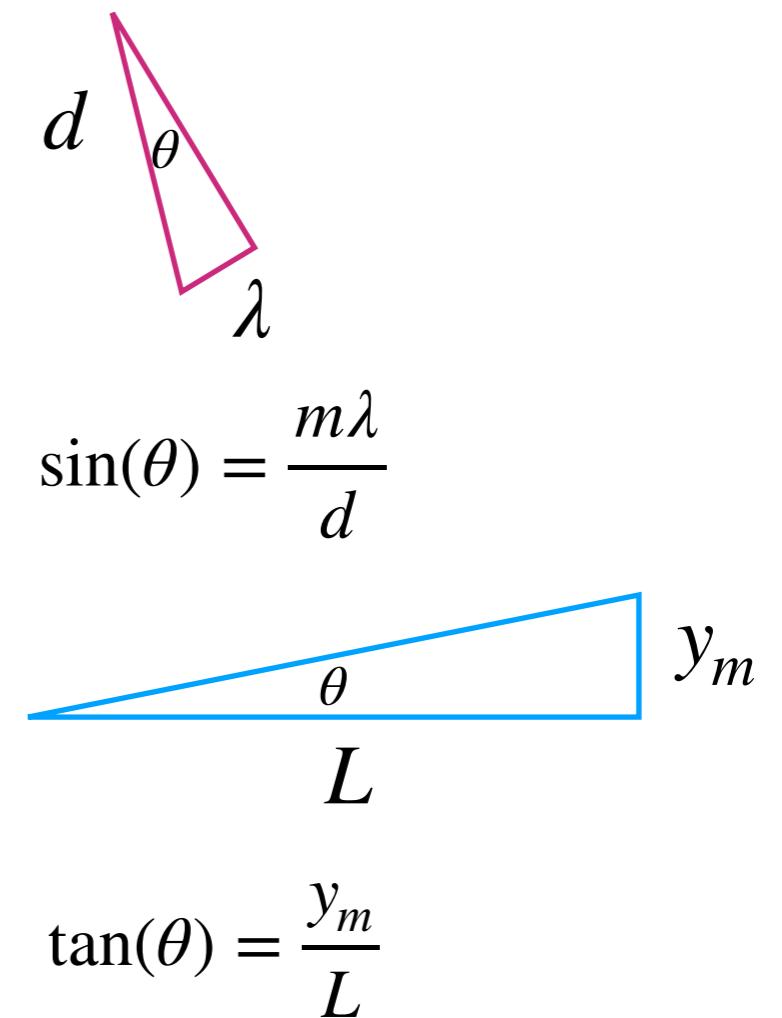
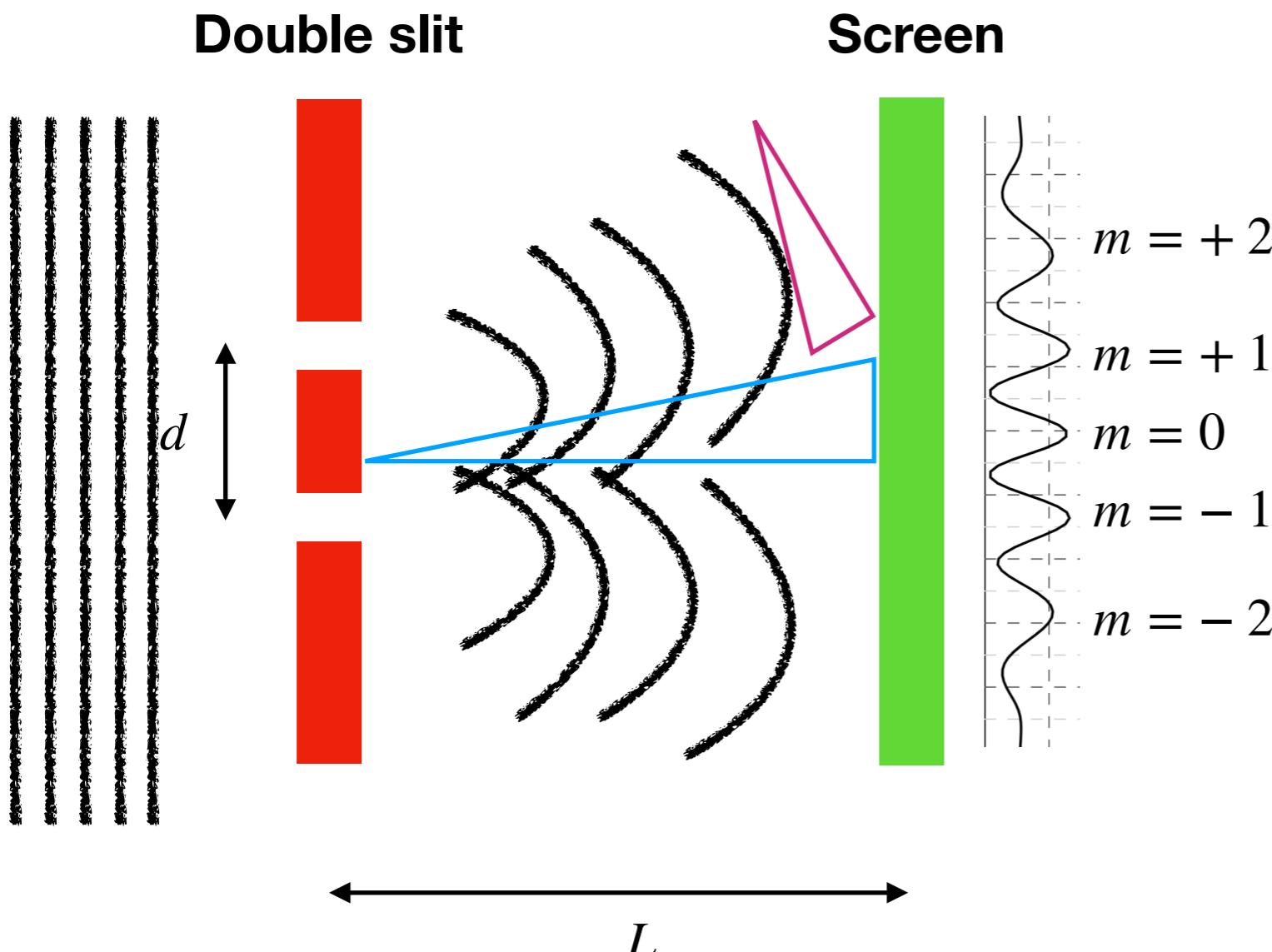
# Young's double slit experiment

- One experiment that shows the duality of photons and matter particles in Young's diffraction experiment with double slits.



# Young's double slit experiment

- A pattern with several fringes form on the screen as a result of wave interference.
- The middle fringes are brighter than the ones farther away from the centre.



For small angles:

$$\sin(\theta) \approx \theta$$

$$\Rightarrow y_m d = L m \lambda$$

$$\tan(\theta) \approx \theta$$

# 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

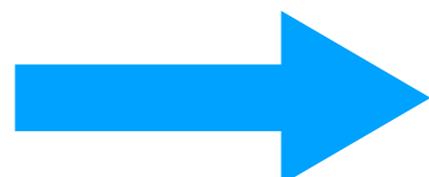
- QM replaces classical mechanics CM. CM is a good approximation, but it is not accurate when describing some experiments at small scales.
- **Quantum physics:** principles of QM applied to physical phenomena.
- **Branches of QM:**
  - **QED:** QM + EM
  - **QCD:** QM + Strong interaction
  - **Quantum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

# Mathematical tools for QM

- **Two important aspects of QM that we need to address are:**
  1. Is QM a linear theory?
  2. Why do we need complex numbers?

The answer to question 1 is yes. QM is a linear theory, i.e., we can create linear combinations of known solutions to get new solutions:

Solution 1



Solution 2

Solution 3 = linear combination  
of solutions 1 and 2

# Linear Operators

- In QM, we will find linear equations like this one:  $L \cdot u = 0$ , where:  
 $L$  = linear operator (matrix),  $u$  = unknown (vector).
- Several operators can be applied to the same unknown:  $L_1 \cdot u = 0$ , and  $L_2 \cdot u = 0$ .
- The same operator can be applied to different unknowns:  $L \cdot (u_1, u_2, u_3) = 0$ .

## Fundamental properties of linear operators:

- We can scale a solution:  $L \cdot (\alpha u) = \alpha L \cdot (u)$
- We can combine solutions:  $L \cdot (u_1 + u_2) = L \cdot (u_1) + L \cdot (u_2)$
- Therefore, we can have a general case:  $L \cdot (\alpha u_1 + \beta u_2) = \alpha L \cdot (u_1) + \beta L \cdot (u_2)$ ,  
which implies that  $(\alpha u_1 + \beta u_2)$  is also a solution.

# Electromagnetic (EM) theory is also linear

- Imagine we have a solution to Maxwell's equations of the form:  $(\vec{E}, \vec{B}, \rho, \vec{J})$ , where  $\rho$  is the charge density (charge per unit volume) and  $\vec{J}$  is the current density (charge per unit area per unit time), then thanks to linearity, we can say that  $(\alpha \vec{E}, \alpha \vec{B}, \alpha \rho, \alpha \vec{J})$  is also a solution, where  $\alpha \in \mathbb{R}$ .
- Now imagine we have 2 solutions to Maxwell's equations of the form:  $(\vec{E}_1, \vec{B}_1, \rho_1, \vec{J}_1)$  and  $(\vec{E}_2, \vec{B}_2, \rho_2, \vec{J}_2)$ , then thanks to linearity, we can say that  $(\vec{E}_1 + \vec{E}_2, \vec{B}_1 + \vec{B}_2, \rho_1 + \rho_2, \vec{J}_1 + \vec{J}_2)$  is also a solution.
- The above makes sense as we have e.g. two 1D plane waves propagating without affecting each other (they do not touch each other).
- The 3rd solution implies we have 2 plane waves propagate simultaneously.
- EM waves are all around in superposition, they do not interfere with each other.

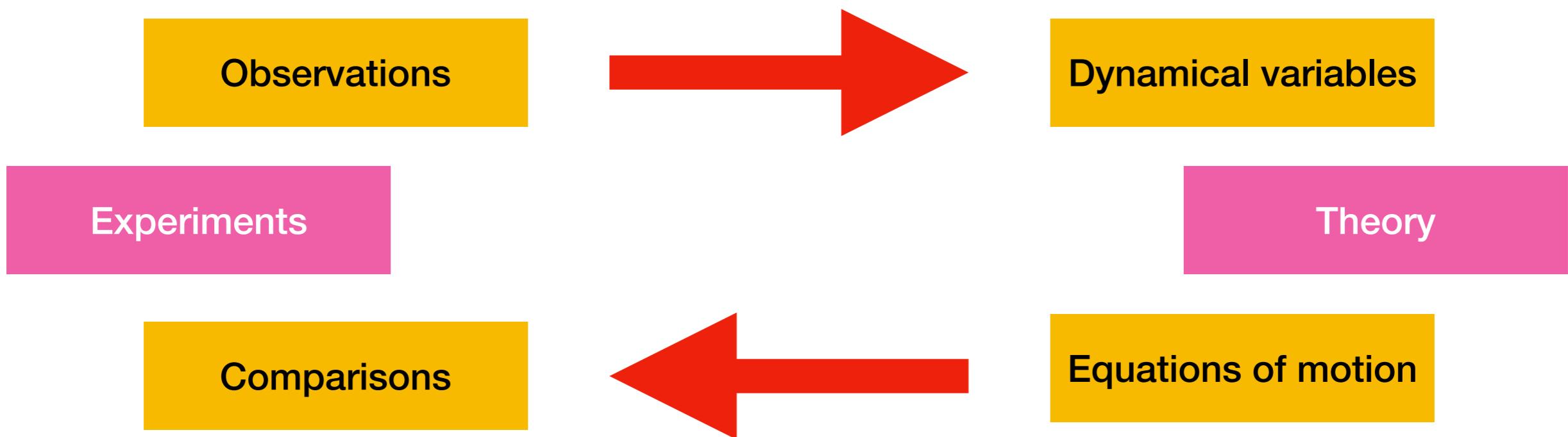
# Linear vs. Non-linear Theories in Physics

- In physics, we have linear and non-linear theories:
  1. **Linear theories:** EM and QM (we can combine solutions)
    - In some sense linear theories are much simpler.
    - We can use linear algebra and the fundamental properties of linear equations.
  2. **Non-linear theories:** CM and GR (we canNOT combine solutions)
    - Examples on non-linearity: the 3-body problem, turbulence in fluids, chaos always emerges in CM/GR.

**QM is fortunately linear!**

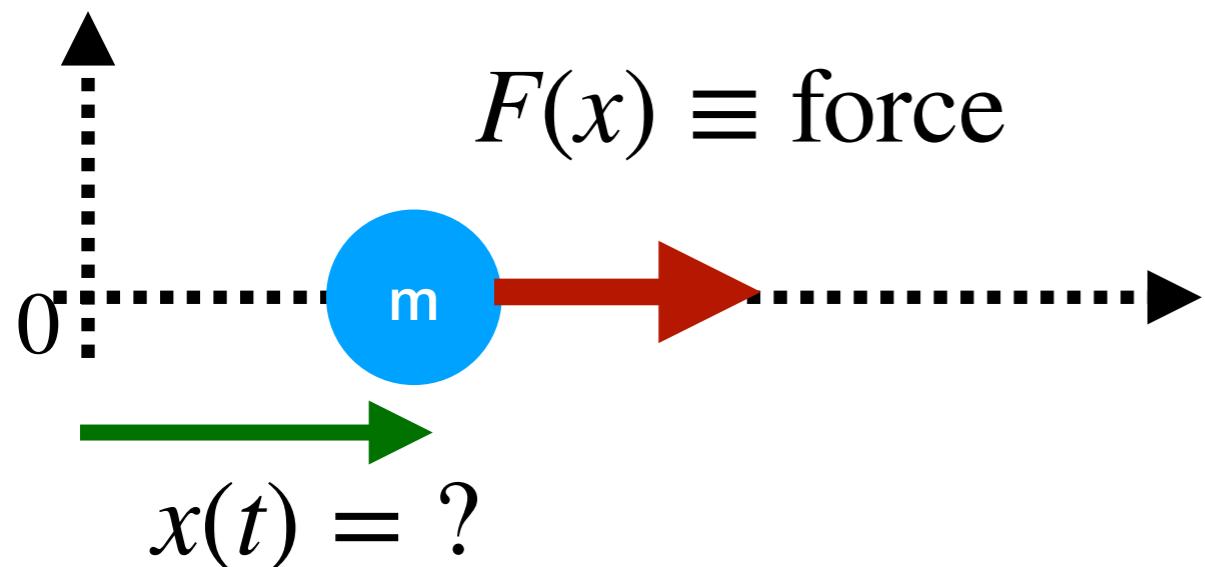
# How do we do physics? The scientific method

- In physics, as in any other branch of science, we use the scientific method to make progress.
- There are two important components: **experiments and theory**. They work TOGETHER, not separately.
- Observations and experiments allow us to find good sets of dynamical variables. A good theory provides equations of motion to solve for such dynamical variables and compare to experiments.



# How do we do physics? CM particle

- In CM, we study the 1D motion of classical (non-relativistic) particles using the scientific method, i.e. experimenting, setting dynamical variables, and using Newton's laws as equations of motion.
- Imagine we study the motion of a particle under the influence of a force,  $F(x)$ , associated with a parabolic potential,  $V(x) = \frac{1}{2}kx^2$ .



**Dynamical variables:**

$x(t) \equiv \text{position}$

$v_x = \dot{x} \equiv \text{velocity}$

$a_x = \ddot{v}_x = \ddot{x} \equiv \text{acceleration}$

$p_x = m v_x \equiv \text{momentum}$

$T = \frac{1}{2}mv_x^2 \equiv \text{kinetic energy}$

# How do we do physics? CM particle

- To determine  $x(t)$ , we need an equation of motion.
- We use Newton's second law:  $F = m\ddot{x} = -\frac{\partial V}{\partial x}$  (for a conservative system).
- For a parabolic (elastic) potential:  $V(x) = \frac{1}{2}kx^2 \Rightarrow F(x) = -kx$ , which we recognise as Hooke's law.
- Thus, the equation of motion of a 1D CM particle under the influence of a parabolic potential is:  $F = m\ddot{x} = -\frac{\partial V}{\partial x} = -kx$
- If we know the initial conditions, e.g.  $x(t = 0)$ ,  $v_x(t = 0)$ , then we can find  $x(t)$ .
- The derivative of the potential makes the above equation non linear.

# How do we do physics? CM particle

- The equation of motion is a 2nd-order ODE:

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

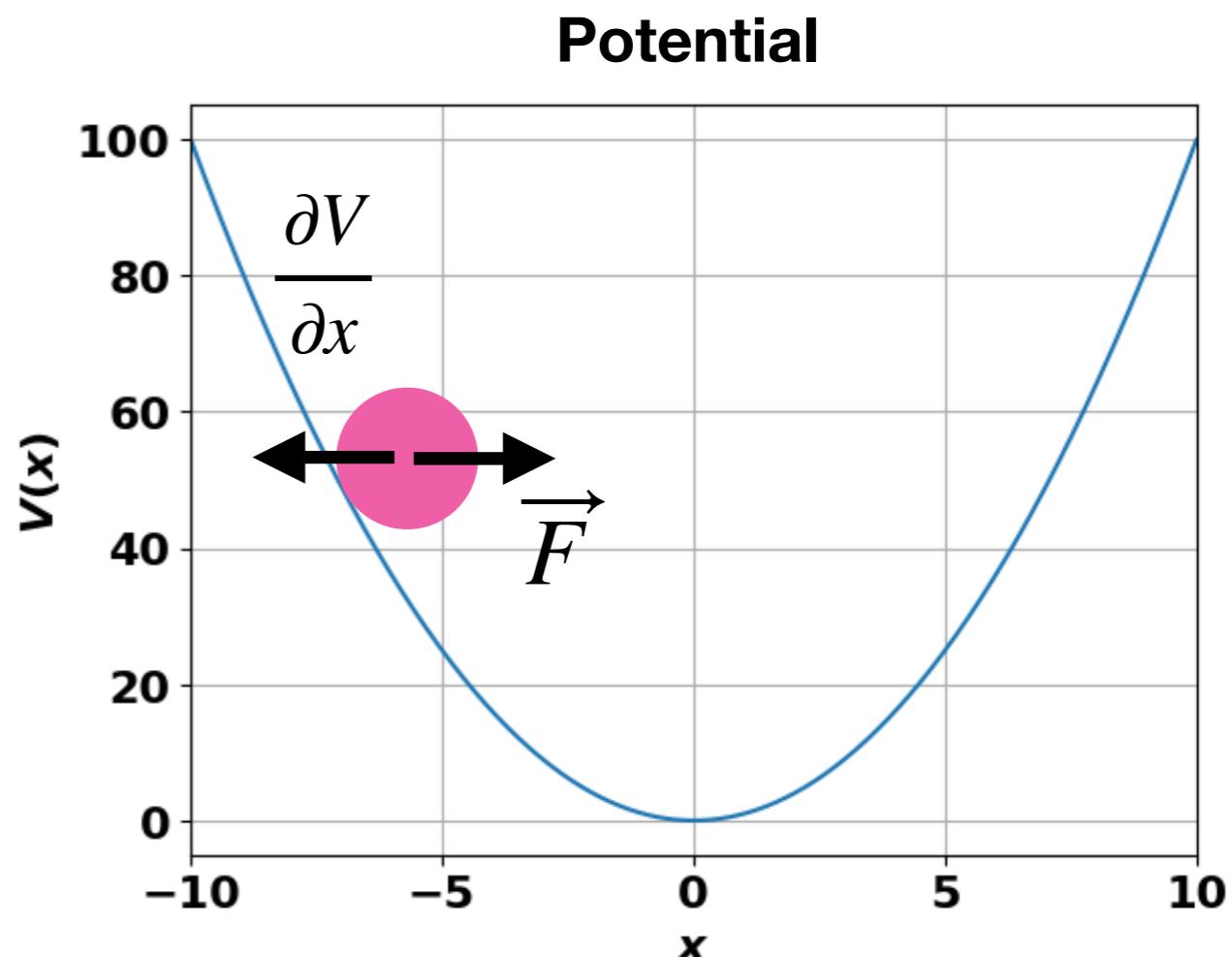
$$m\ddot{x} + kx = 0$$

- The solution to this ODE is harmonic motion:

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

where the angular frequency is:

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



# How do we do quantum mechanics?

- To study the 1D motion in quantum mechanics, we need 2 ingredients:
  1. A **dynamical variable**, which for QM is the so-called “wave function” and describes the dynamics of the QM system/particle.

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

- 2. An **equation of motion**, which is Schrödinger’s equation:

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

where  $\hat{H} = \hat{T} + \hat{V} \equiv$  Hamiltonian operator. The equation can be written as:

$$\left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \Psi = 0 \Rightarrow L \cdot \Psi = 0$$

where we can see that is is a linear equation.

# How do we do quantum mechanics?

- The Schrödinger's equation is a parabolic PDE:  $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$

where:

$$i \equiv \sqrt{-1}$$

$\hbar \equiv$  Reduced Planck constant

$\Psi \in \mathbb{C}$  (its solution is complex).

$\hat{H} = \hat{T} + \hat{V} \equiv$  Hamiltonian operator

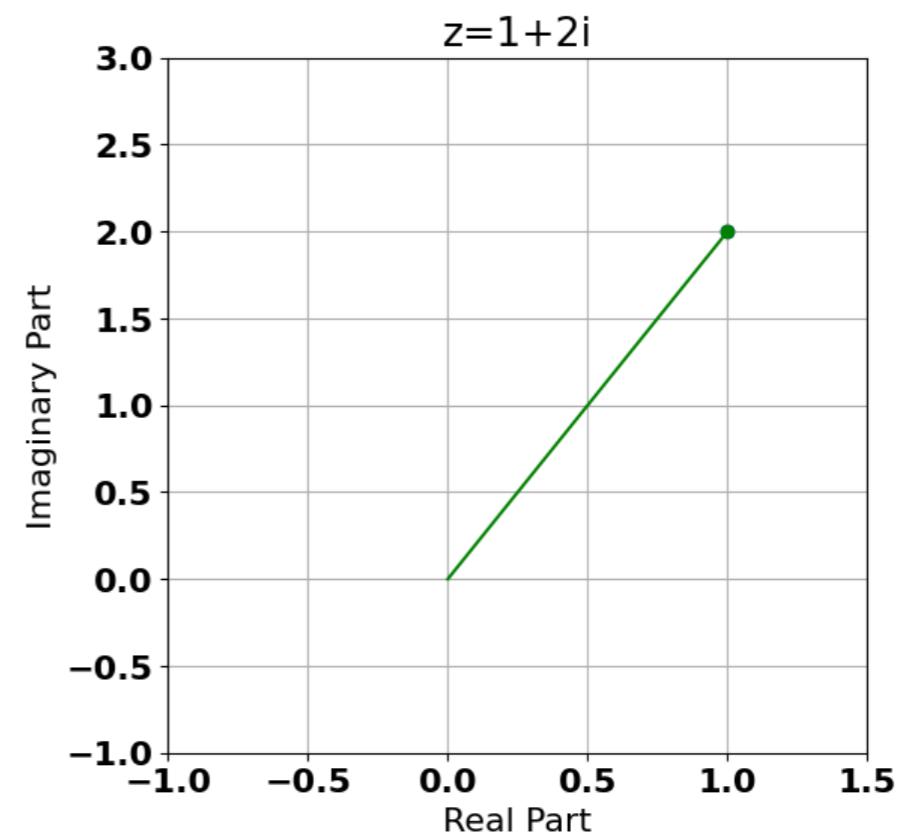
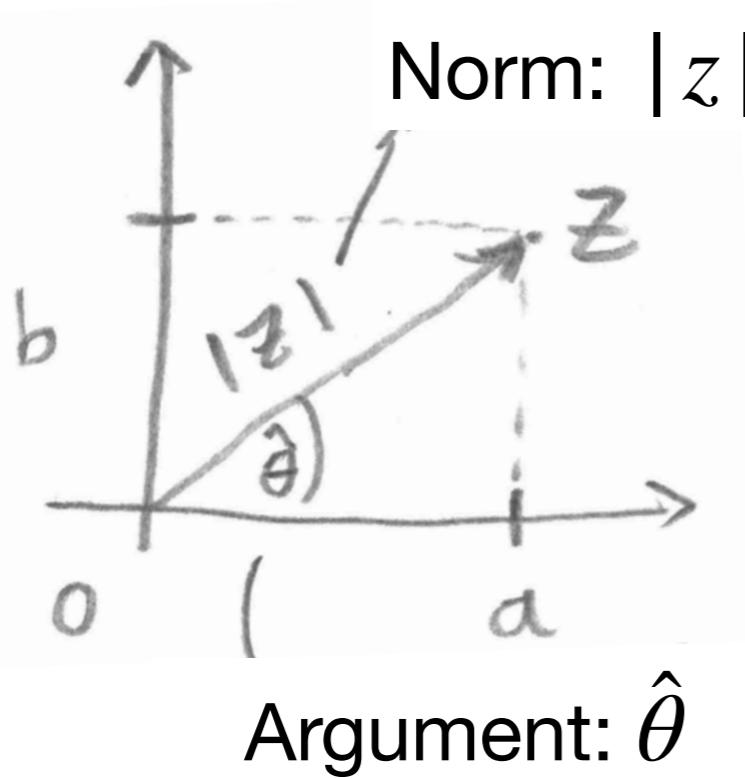
$\hat{T} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \equiv$  Kinetic energy operator

$\hat{V} \equiv$  Potential energy operator

- QM is linear, so in some sense it is simpler than CM.
- This means we can scale solutions, and add/combine solutions to create superpositions, which become new solutions.

# The necessity of complex numbers

- Why do we need complex numbers? Because  $\Psi$  is a complex number.
- The number  $i \equiv \sqrt{-1}$  is defined as the solution to the equation:  $x^2 + 1 = 0$
- A general complex number is:  $z = a + ib$ , where  $a, b \in \mathbb{R}$ . We say that the real part of  $z$  is  $\text{Re}(z)$  and imaginary part of  $z$  is  $\text{Im}(z)$ .
- Complex numbers can be represented on the so-called “complex plane”:



# Properties of complex numbers

- The complex conjugate of a complex number is:  $z^* = a - ib$
- Other notations for complex conjugates are:  $z^* = \bar{z} = \hat{z}$
- We can calculate the norm squared as follows:  $|z|^2 = z^* z \in \mathbb{R}$
- The norm of a complex number is:  $|z| = \sqrt{a^2 + b^2} \in \mathbb{R}$

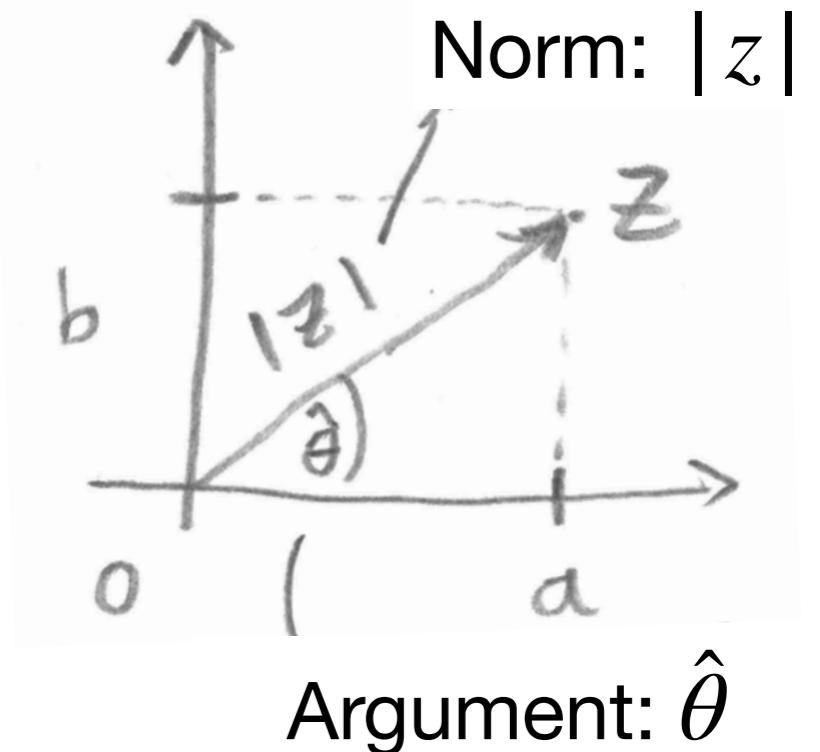
Some properties of complex numbers include:

- **Summation:**  $(a + ib) + (c + id) = (a + c) + i(b + d)$
- **Multiplication:**  $(a + ib)(c + id) = (ac - bd) + i(bc + ad)$

# The necessity of complex numbers

- We can also write complex numbers in polar coordinates, using the norm and argument:

$$\begin{aligned} a &= |z| \cos \hat{\theta} \\ b &= |z| \sin \hat{\theta} \end{aligned} \Rightarrow a = |z|(\cos \hat{\theta} + i \sin \hat{\theta}) = z e^{i\theta}$$



- **Euler formulae:**

$$e^{i\theta} = \cos \hat{\theta} + i \sin \hat{\theta},$$

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

- The wave function,  $\Psi$ , has to be a complex number to satisfy Schrödinger equation.
- In QM, we will be doing complex algebra calculations.

# The necessity of complex numbers

- What about measurement?

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

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

$|\Psi|^2 \sim$  probabilities. (Max Born)

$$|\Psi|^2 = \text{norm} \in \mathbb{R}$$

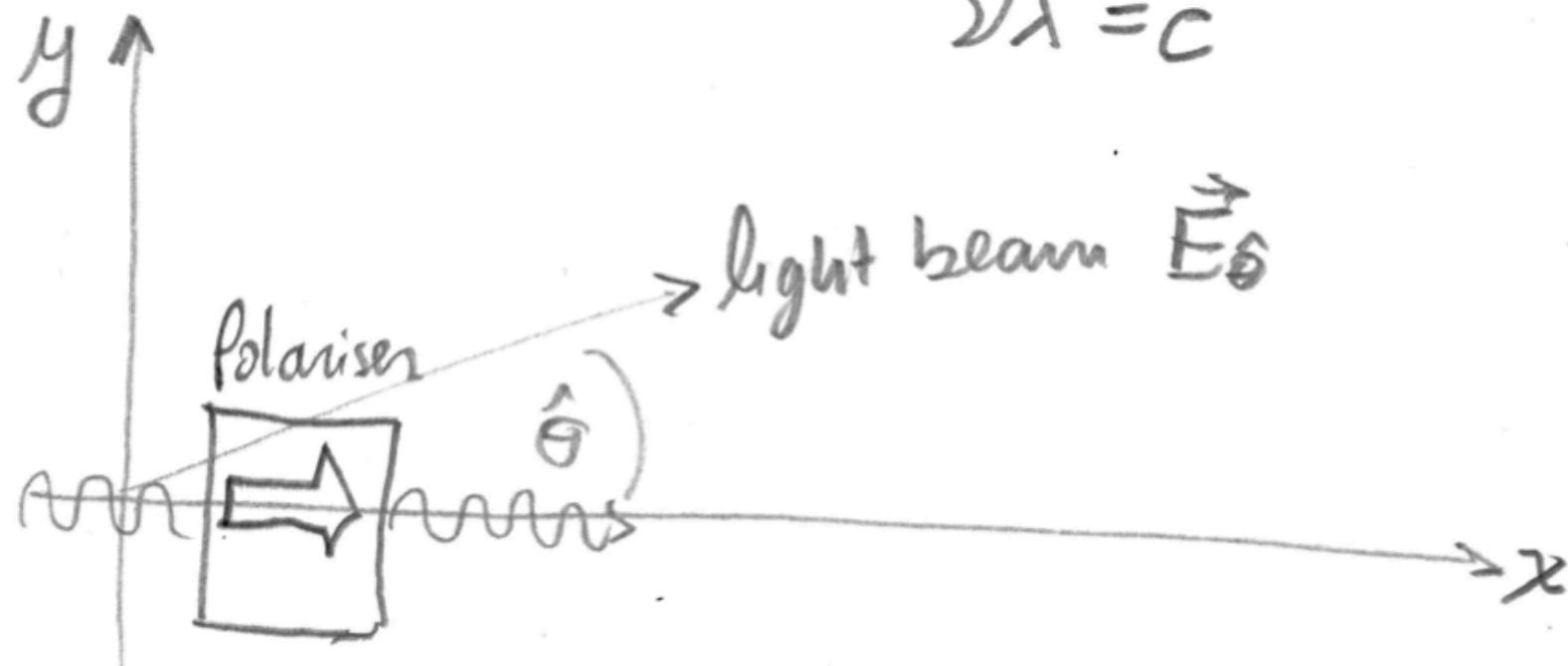
- Max Born proposes that  $\Psi$  is related to probabilities.

# The loss of determinism

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

$\gamma$ : waves/particles :  $E = h\nu$

$$2\nu\lambda = c$$



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

$$\vec{E}_0 = E_0 \cos \hat{\theta} \hat{e}_x + E_0 \sin \hat{\theta} \hat{e}_y$$

Electric field before the polariser.

# The loss of determinism

After the polariser:

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

magnitude of E field  
↑  
fraction of E that goes thru,

Now we send  $\gamma$  one by one:

**In CM:** identical  $\gamma$  should either get absorbed or go thru.

**In QM:** identical  $\gamma$  sometimes go thru / sometimes they don't

$\Rightarrow$  We lose predictability / we lose determinism.

# The loss of determinism

- A  $\gamma$  either gets thru or not.
- We can only predict probabilities.  
wavefunction / states / vectors
- $\Psi$  of a  $\gamma$  polarised in the  $X$  direction; Dirac's notation,

$|\gamma; x\rangle$

vector  
wavefunction  
represents a possible state

$|\gamma; y\rangle$       polarised along Y.

# The loss of determinism

Photon state before the polariser:

$$|\gamma; \theta\rangle = |\gamma; x\rangle \cos\hat{\theta} + |\gamma; y\rangle \sin\hat{\theta}$$

superposition

Photon state after the polariser:

$$|\gamma; x\rangle \quad \text{when it goes thru, the whole } \gamma \text{ goes thru.}$$

Einstein's view:

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

# The statistical interpretation

- What is the wave function?

Ⓐ light

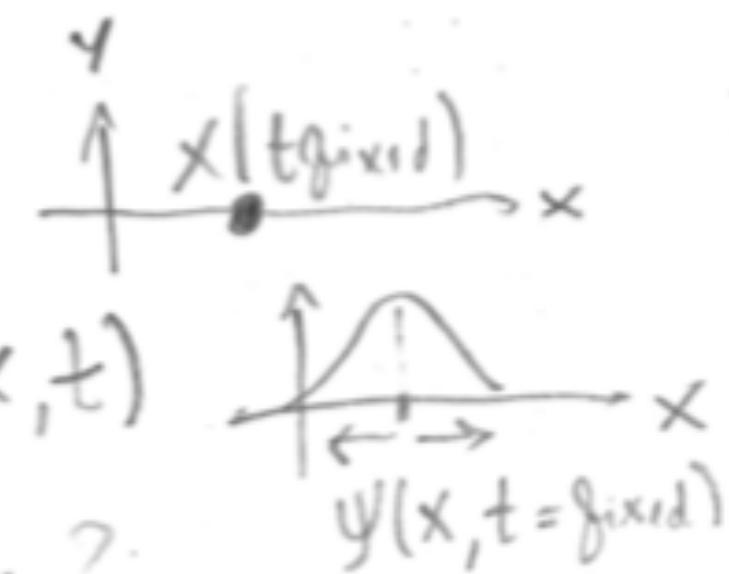
Ⓑ matter

- Particle  $\rightarrow$  located at a point  $x(t)$

- wave function  $\rightarrow$  spread out in space  $\Psi(x, t)$

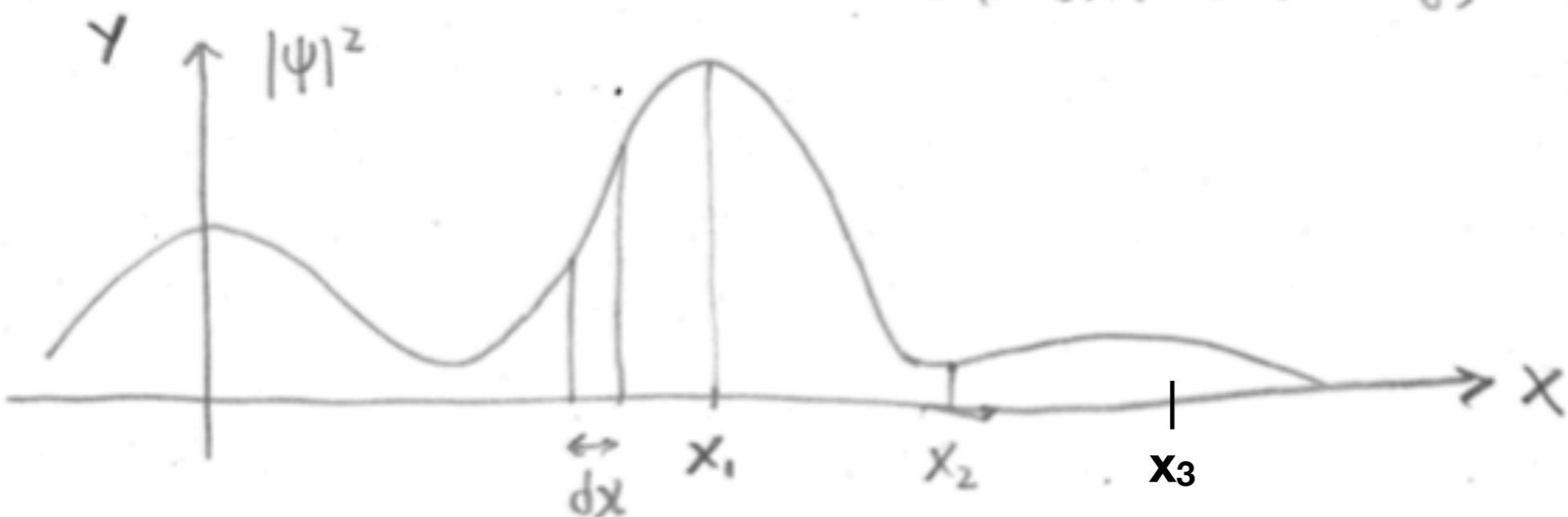
- How can  $\Psi$  describe the state of a particle?

$\hookrightarrow$  Born's statistical interpretation of  $\Psi$



# 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  $\Psi$  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  $x_3$

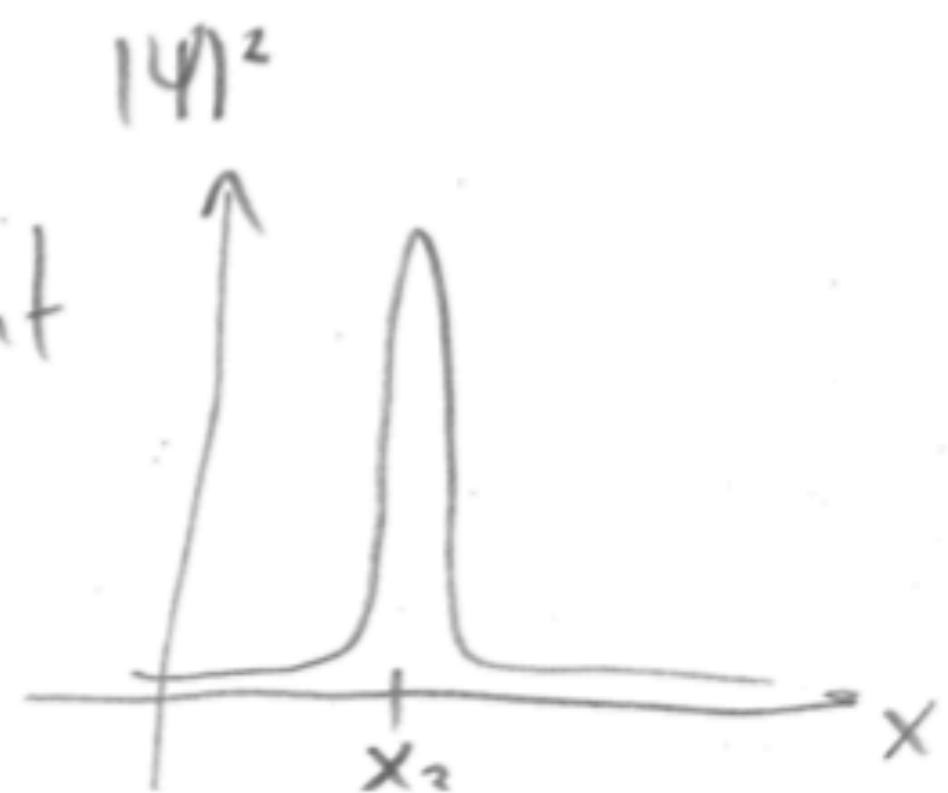
# Views on determinism

\* 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 variable, 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 weighing of  $\Psi$ .  
Second measurement?
- Must return the same value
- Measurement alters the  $\Psi$
- The  $\Psi$  collapses upon measurement



# Processes in Quantum Mechanics

In QM; there are two physical processes:

- ① Ordinary :  $\Psi$  evolves according to S. eq.
- ② Measurement :  $\Psi$  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  $\Psi$  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  $\alpha_x = \alpha_y = \alpha$

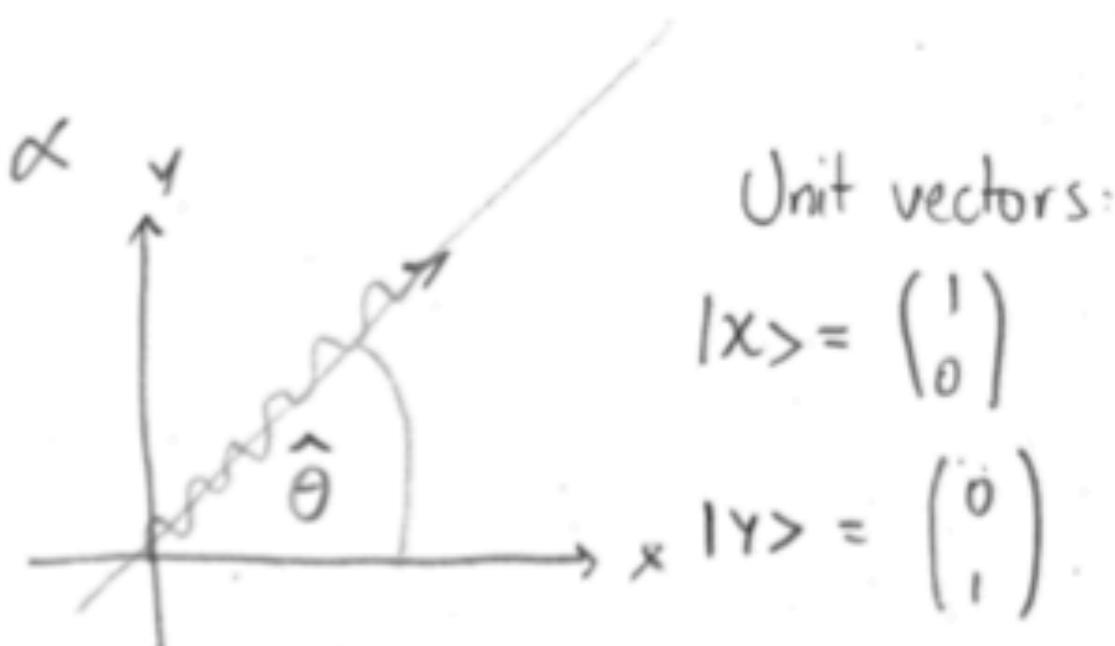
$$\Rightarrow |\Psi\rangle = \begin{pmatrix} \cos \hat{\theta} \\ \sin \hat{\theta} \end{pmatrix} e^{i\alpha}$$

$$\Rightarrow |\Psi\rangle = \underbrace{\cos \hat{\theta} e^{i\alpha}}_{\alpha} |x\rangle + \underbrace{\sin \hat{\theta} e^{i\alpha}}_{\beta} |y\rangle$$

$$\Rightarrow |\Psi\rangle = \Psi_x |x\rangle + \Psi_y |y\rangle \quad \text{Superposition} \quad (1)$$

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

$$|\Psi, \hat{\theta}\rangle = \cos \hat{\theta} |\Psi, x\rangle + \sin \hat{\theta} |\Psi, y\rangle \quad \begin{matrix} \text{Before} \\ \text{After} \end{matrix}$$
$$|\Psi, x\rangle$$



Unit vectors:

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

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

# Quantum Superposition

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

In Q.M.:  $|\Psi_1\rangle$  and  $|\Psi_2\rangle$  are two states  $\xrightarrow[\text{same property}]{\text{measurement}} |\Psi_1\rangle \rightarrow a$  always!

Superposition:

$$|\Psi\rangle = \alpha|\Psi_1\rangle + \beta|\Psi_2\rangle, \alpha, \beta \in \mathbb{C} \rightarrow \} \text{ either } a \text{ or } b$$

What happens if you measure the same property?

- No certain answer
- No intermediate answer
- $\alpha, \beta$  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:

$$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle, \alpha, \beta \in \mathbb{C} \rightarrow \left\{ \begin{array}{l} \text{either } a \text{ or } b \end{array} \right.$$

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  $\Rightarrow$  After  
measurement  $|\psi\rangle = |\psi_1\rangle$

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 phys. 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

$$|\psi\rangle = \alpha|1\rangle_x + \beta|1\rangle_y$$

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

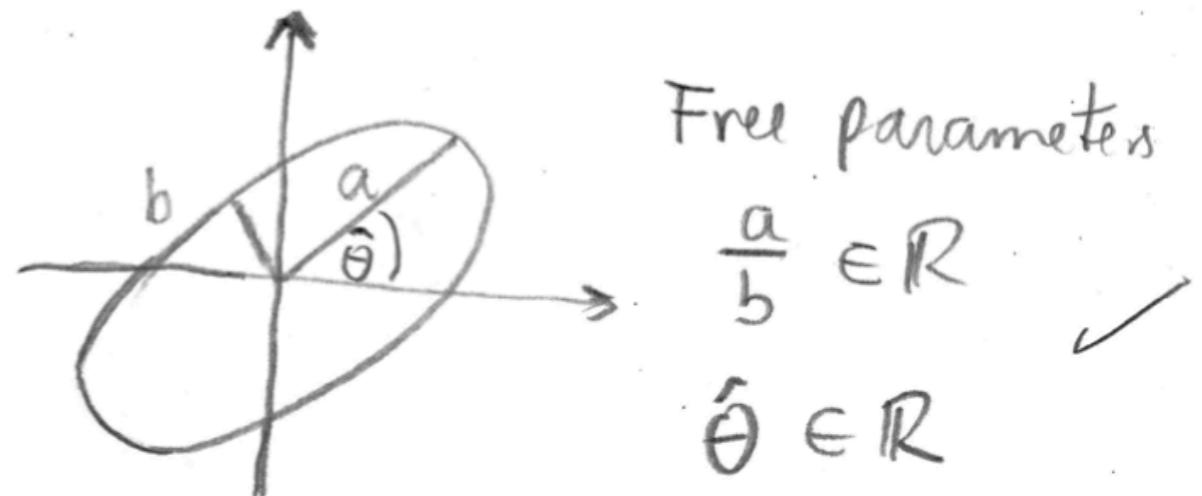
> 4 R parameters ( $a, b, c, d$ )

but thanks to physical equivalence:

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

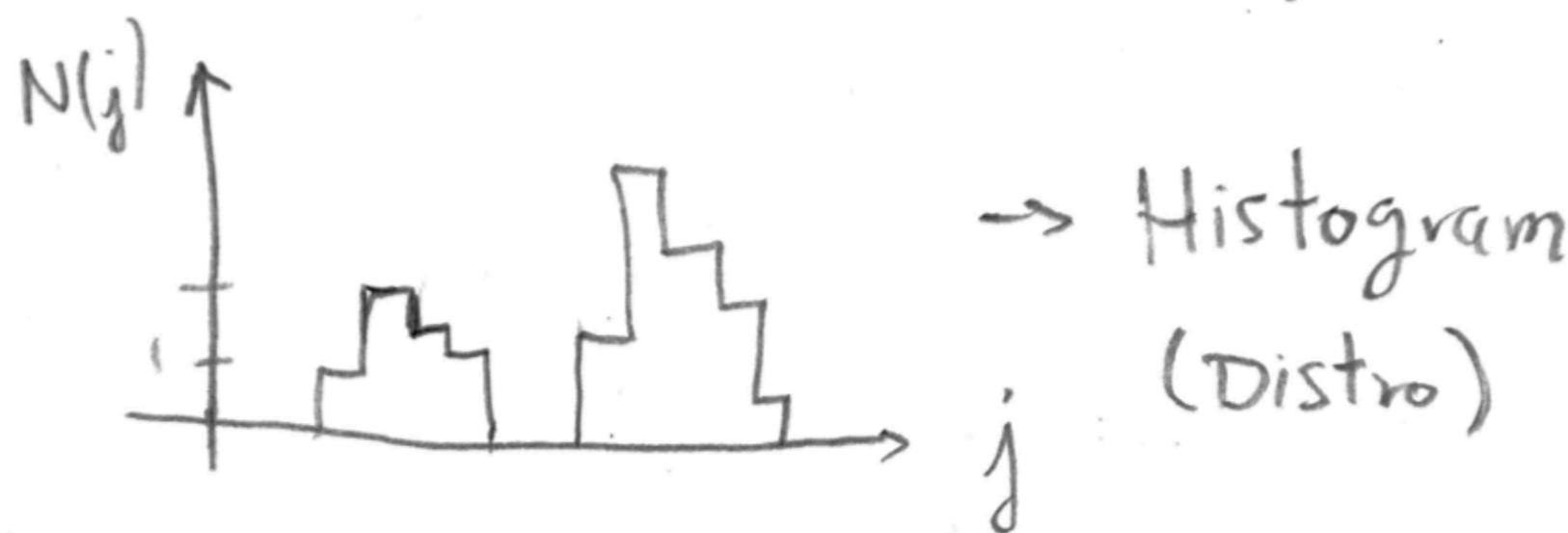
$$> \frac{\beta}{\alpha} \in \mathbb{C} \Rightarrow \frac{\beta}{\alpha} = p + q i$$

> 2 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



- Total # of elements :

$$N = \sum_j^\infty N(j)$$

# Probabilities

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

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

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

$\Rightarrow$  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?

$$\langle j \rangle = \frac{\sum j N(j)}{N} = \sum_j j P(j)$$

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?

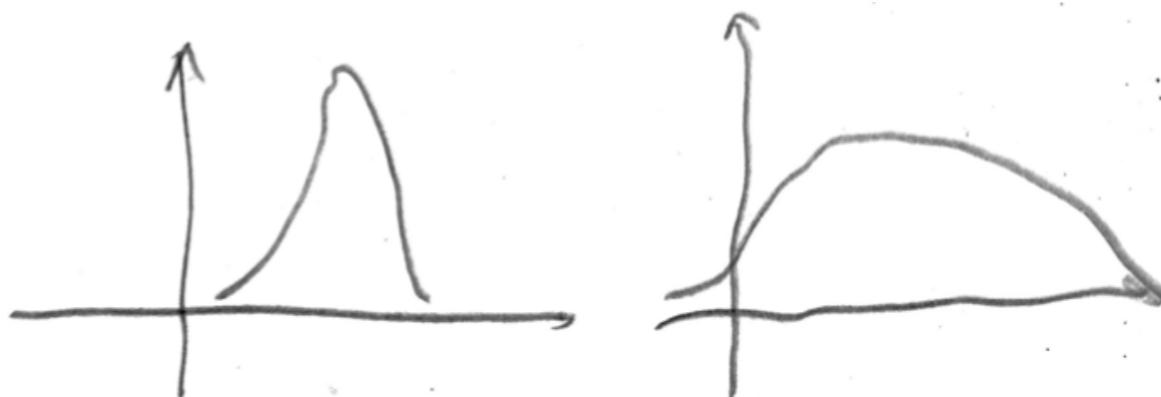
$$\langle j^2 \rangle = \frac{\sum_j j^2 N(j)}{N} = \sum_j j^2 P(j)$$

Therefore, in general:

$$\langle f(j) \rangle = \sum_j f(j) P(j)$$

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?

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

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

constant. } does not  
change when changing  
 $j$

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

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

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

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

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

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

= for distros with no spread.

## Continuous functions

③ What about continuous densities?

The  $P(j) = 0$  precisely if

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

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

$\rho(x)$  = probability density

- The prob that "x" lies between "a"  $\wedge$  "b":

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

# Continuous functions

Same rules as for discrete distros:

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

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

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

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

## Normalisation

$$\underbrace{|\Psi(x,t)|^2 dx}_{\text{P of finding a particle between } x \wedge x+dx \text{ at time t.}}$$

Probability density for finding the particle at  $x$  at  $t$ .

The particle has to be somewhere:

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

Is this compatible 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  $\otimes$  satisfied? We must pick A so that  $\otimes$  is satisfied.

↳ This process is called normalisation of  $\Psi$ .

In some cases:  $\left\{ \begin{array}{l} \int |\Psi(x,t)|^2 dx \rightarrow \infty \\ \Psi(x,t) = 0 \end{array} \right\}$  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  $\Psi$ .

**Proof:**

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

# Normalisation

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

$\xrightarrow{\text{SEq}}$

$$\left\{ \begin{array}{l} \frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi \\ \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^* \end{array} \right.$$

Remember:

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

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

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

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

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

## Normalisation

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

$\psi(x,t) \rightarrow 0$  when  $x \rightarrow \pm\infty$

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

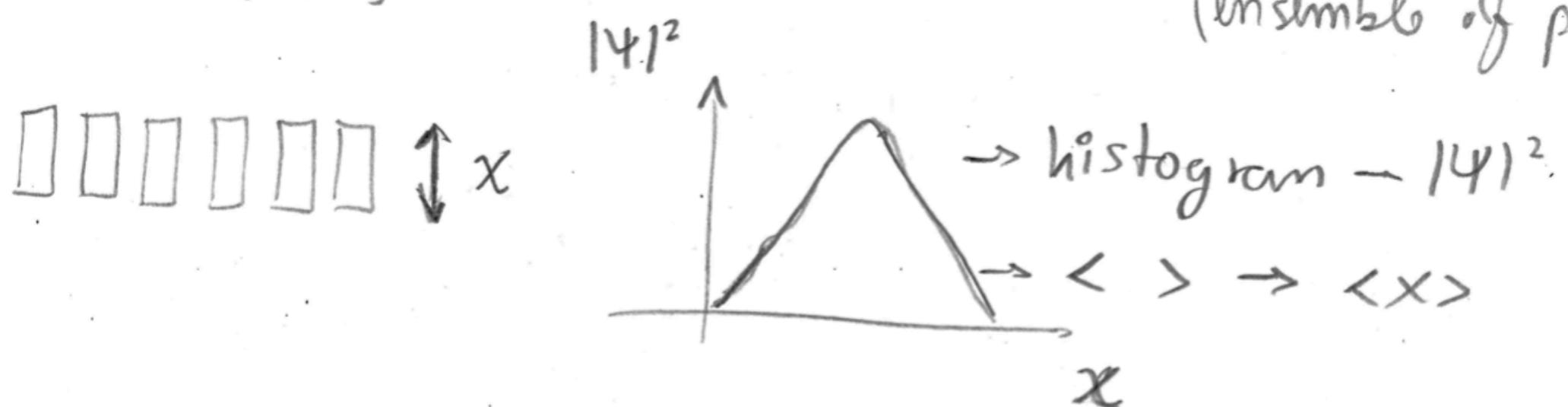
constant  $\Rightarrow$  normalisation is preserved!

# Expectation values

For a particle in state  $\Psi$ , 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.
- 1<sup>st</sup> measurement  $\rightarrow \Psi$  collapses  $\rightarrow$  same result.
- $\langle x \rangle$  is the  $\langle \rangle$  of measurements performed on particles all in the state  $\Psi$  (ensemble of particles)



# Expectation values

Velocity of the expectation value of x:

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

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

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

Expectation value of the velocity:

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

# Expectation values

Momentum :  $p = m\sigma$

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

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

Derivatives

Multiplication

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

operator  $x$

operator  $p$

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

$\Rightarrow$  to calculate expectation values:  $\psi^* \text{op.} \psi$

# Expectation values

What about other dynamical variables?

④ Kinetic energy:  $T = \frac{1}{2}mv^2 = \frac{\vec{p}^2}{2m}$

④ Angular momentum:  $\vec{L} = \vec{r} \times m\vec{v} = \vec{r} \times \vec{p}$

In general:

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

expectation value  
of any dyn. var.  
for a particle in  
state  $\psi$ .

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:

Expectation values obey classical laws.

$$\textcircled{1} \quad \langle p \rangle = m \frac{d\langle x \rangle}{dt}$$

$$\textcircled{2} \quad \frac{d\langle p \rangle}{dt} = \left\langle -i\hbar \frac{\partial \psi}{\partial x} \right\rangle$$

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

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

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

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

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

# 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):

$$\Rightarrow \frac{d\langle p \rangle}{dt} = -i\hbar \left\{ \left[ -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V\Psi^* \right] \frac{\partial \Psi}{\partial x} + \Psi^* \frac{\partial}{\partial x} \left[ \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V\Psi \right] \right\} dx \\ - i\hbar \left\{ \frac{i\hbar}{2m} \left[ \Psi^* \frac{\partial^3 \Psi}{\partial x^3} - \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} \right] + \frac{i}{\hbar} \left[ V\Psi^* \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial}{\partial x} (V\Psi) \right] \right\} dx$$

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

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

I<sub>2</sub>

# The Ehrenfest Theorem

$$I_2 = \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} dx = \left[ \frac{\partial \Psi^*}{\partial x} \frac{\partial \Psi}{\partial x} \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} \frac{\partial^2 \Psi}{\partial x^2} dx$$

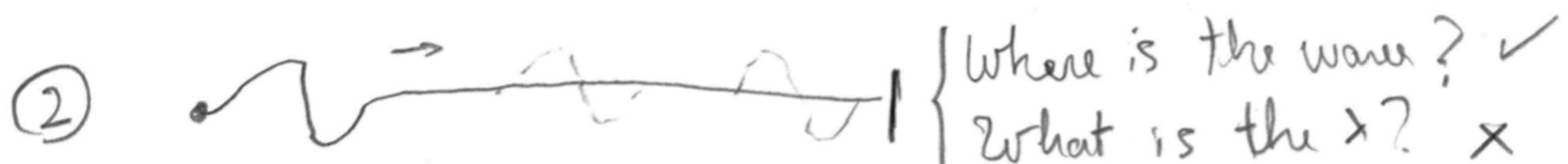
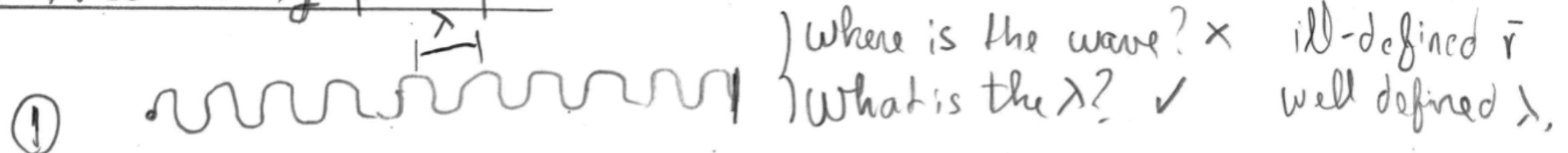
$$\begin{aligned} I_2 &= - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} \frac{\partial^2 \Psi}{\partial x^2} dx \\ &= - \left[ \Psi^* \frac{\partial^2 \Psi}{\partial x^2} \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \Psi^* \frac{\partial^3 \Psi}{\partial x^3} dx \end{aligned}$$

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

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

# The Uncertainty Principle

The uncertainty principle:



- The more precise the wave position is, the less precise its  $\lambda$ , and vice versa.
- Also, applies to waves in QM.

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

$x$  of  $y$ .

$\Rightarrow$  a spread in  $\lambda \rightarrow$  a spread in  $p$ .

# Heisenberg's Uncertainty Principle

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}}$$

$$\left. \begin{array}{l} \Delta x \equiv \text{std dev of } x \\ \Delta p \equiv \text{std dev of } p \end{array} \right\}$$

- \* Position measurements
- \* Momentum measurements
- \* Measurements on identical systems do not yield consistent results
- \* Q system where  $x$  measurements by making  $\Psi$  a localised spike,  $p$  measurements will be widely scattered.
- \* " " "  $p$  measurements by a long sine wave,  $x$  " " "
- \* No limit on how big  $\Delta x, \Delta p$  can be.