Particles and Waves

Outline :

- Classical Ideas and Wave Properties.
- Electromagnetic Waves.
- The Photoelectric Effect and the Particle Nature of Light.
- The Double Slit Experiment.
- Wave-Particle Duality.
- Measurement Limits and the Uncertainty Principle.
- Summary and Exercises.

Classical Ideas

Waves :

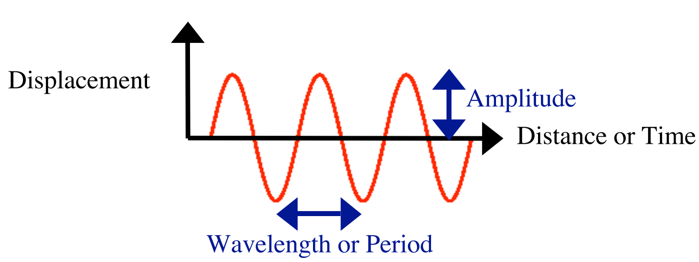
- Collective motion in some medium (electromagnetic waves ?)
- Transverse or longitudinal.
- Travelling or standing.
- Wavelength (λ), frequency (f) and speed (v) related by :

$$v = \lambda \times f$$

- Amplitude (A) : maximum displacement.
- Intensity (I) : power delivered by the wave (per unit area).

$$I \propto A^2$$

(like the energy of a simple harmonic oscillator)



Classical Ideas

Particles :

m ● ⟶ $\underline{v}$

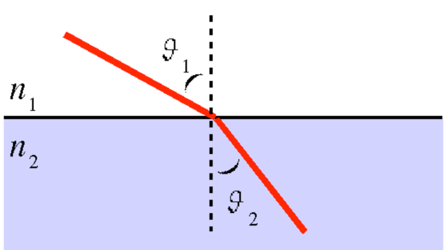
- Point-like : well defined location.
- Well defined mass, velocity, momentum and energy. At non-relativistic speeds (much smaller than the speed of light) :

$$p = m \times \underline{v} \qquad E = \frac{1}{2} m v^2 \qquad \left[\Rightarrow \; E = \frac{p^2}{2m} \right]$$

Momentum (p)   Kinetic Energy (E)

Wave Properties

(I) Refraction

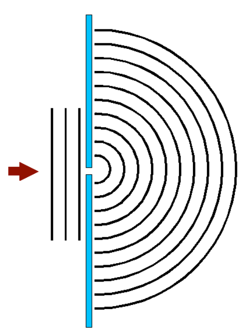


Change of velocity of wave at boundaries between different media.

Refractive index : $n_1 = \dfrac{c}{v_1}$, $n_2 = \dfrac{c}{v_2}$

Snell's Law : $n_1 \sin\theta_1 = n_2 \sin\theta_2$

(II) Diffraction



Behaviour of waves through gaps or around obstacles/boundaries.

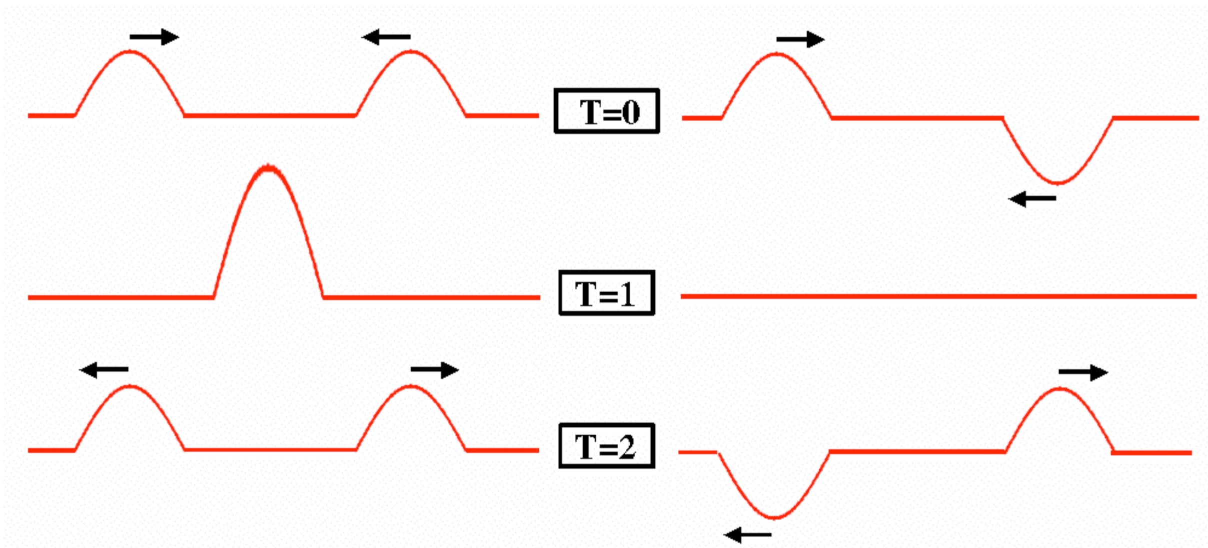
- Quantitative formulation : Huygen's principle.
- Effect is most striking when :

$$\lambda \geq a \qquad (a = \text{gap size})$$

Wave Properties

(III) Superposition

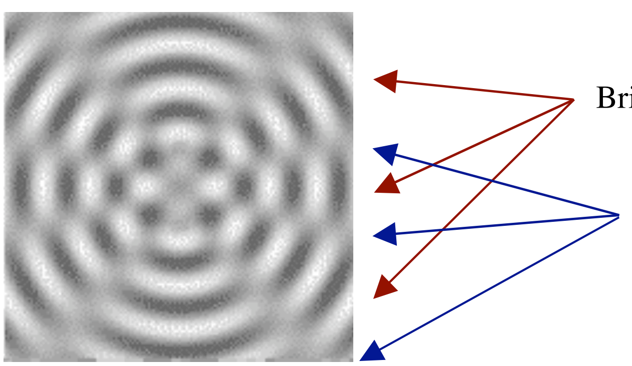
Constructive Interference | Destructive Interference



Displacements (or amplitudes) add, not intensities

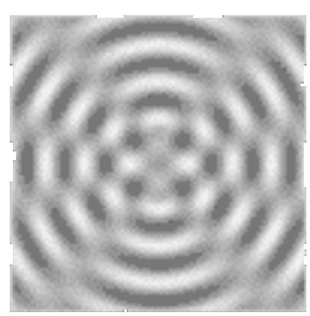
Wave Properties

- Superposition of waves from different sources gives rise to interference patterns :



Bright fringe (constructive interference).

Dark fringe (destructive interference).



Displacements add :

$$d_{12}(x,y) = d_1(x,y) + d_2(x,y)$$

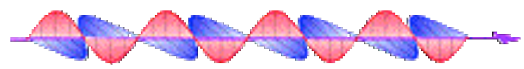
Resulting amplitude :

phase difference

$$I_{12} = I_1 + I_2 + 2\sqrt{I_1 I_2}\cos\phi$$

Electromagnetic Waves

- In a vacuum, electromagnetic waves consist of perpendicular oscillations of electric (***E***) and magnetic (***B***) fields.



- Fundamental wave equation (for example, for the electric component) :

$$\frac{d^2E}{dx^2} = \frac{1}{c^2}\frac{d^2E}{dt^2}$$

➡ c = speed of light

- The solution is :

$$E = E_0 \sin(kx - \omega t) \quad \text{or} \quad E = E_0 \cos(kx - \omega t)$$

where :

$$k = \frac{2\pi}{\lambda} \;, \quad \omega = 2\pi f \quad \text{and} \quad c = \frac{\omega}{k}$$

You can verify this by direct substitution : $E = E_0 \sin(kx - \omega t)$

$\Rightarrow \quad \frac{dE}{dx} = E_0 k \cos(kx - \omega t) \qquad \frac{d^2E}{dx^2} = -E_0 k^2 \sin(kx - \omega t)$

$\Rightarrow \quad \frac{dE}{dt} = -E_0 \omega \cos(kx - \omega t) \qquad \frac{d^2E}{dt^2} = -E_0 \omega^2 \sin(kx - \omega t)$

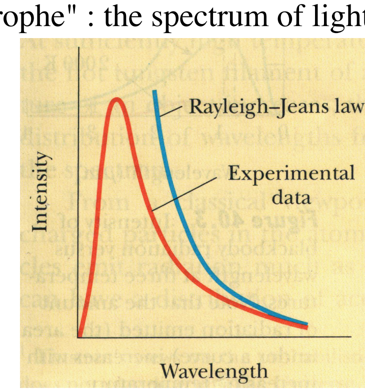
Substitute into the original equation to find $\omega^2 = k^2 \times c^2$

Problems with the Wave Theory of Light

- At the end of the 19th century, physics looked like it was wrapped up :

Electromagnetism : **Maxwell's Equations**	+	Mechanics : **Newton's Laws**

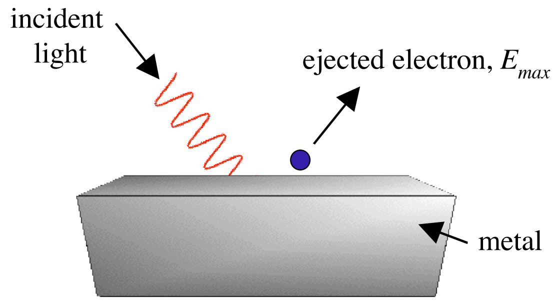
- All that was left to do was to apply these theories to explain the detailed properties and interactions of matter.
- However, difficulties emerged in the attempt to explain several phenomena :
  - ➡ "Ultraviolet catastrophe" : the spectrum of light emitted by bodies at a given temperature :

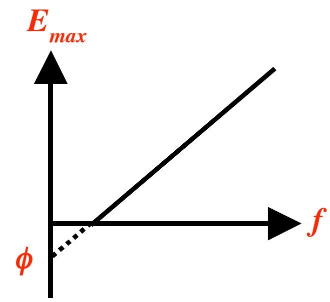


prediction of classical physics

  - ➡ "Photoelectric Effect" : the flux and energy spectrum of electrons emitted from metals due to incident electromagnetic radiation.

The Photoelectric Effect (I)





Observations :

- $E_{\text{max}} = hf - \phi$ where E_{max} is the maximum electron kinetic energy, f is the frequency of the incident light and ϕ is a constant for a given material.
- E_{max} is independent of the intensity of the incident light. Increasing the intensity only liberates more electrons but with the same energies.

➡ These observations are impossible to account for in the classical theory of the interaction between radiation and matter.

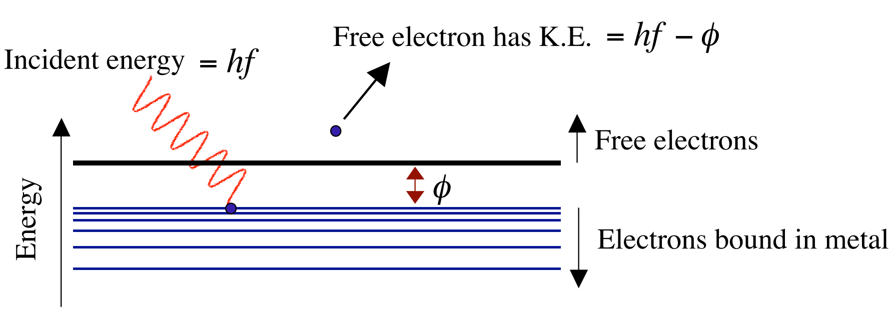
The Photoelectric Effect (II)

- These facts are easily accounted for if we imagine the energy carried by the incident electromagnetic radiation arriving in "clumps" $\rightarrow$ "**quanta**" :

$$E = hf$$ h = Planck's constant = 6.5×10^{-34} Js

or $$p = h/\lambda$$ (since $E = pc$ for objects travelling at the speed of ligl

Schematically :



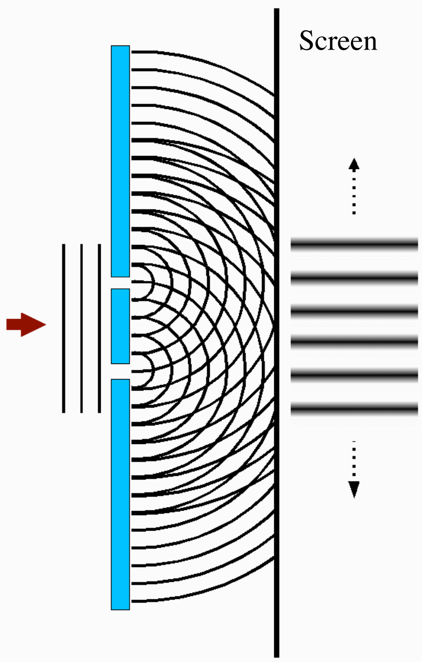
$\Rightarrow$ Concept of energy levels will become clearer later

The Double Slit Experiment (I)

Richard Feynman : "...We choose to examine a phenomenon which is impossible to explain, *absolutely* impossible, to explain in any classical way, and which has in it the heart of quantum mechanics. In reality, it contains the *only* mystery."

Feynman Lectures, Vol 3.

Coherent light source (for example, provided by a laser). Plane wave diffracts at narrow slits.

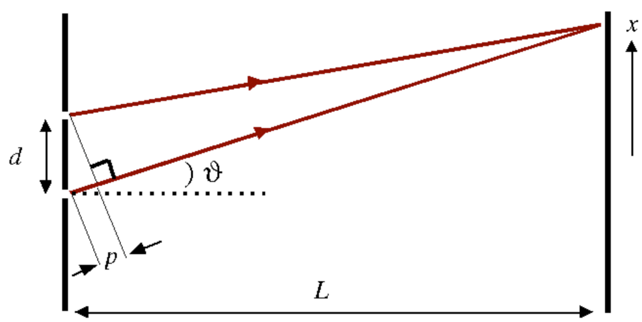


Interference fringes show that light is behaving as a wave through the apparatus.

The photo-electric effect shows that light arrives as a particle.

⇒ Paradox ?

The Double Slit Experiment (II)



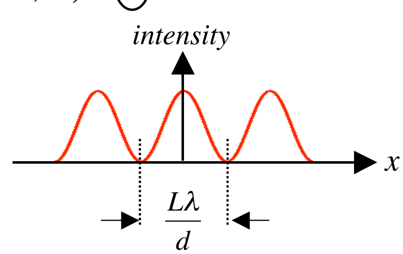
$x = L\sin\vartheta$ (1)
(for small ϑ)

- If $L >> d$ then the path difference p is given by : $p = d\sin\vartheta$
- A bright fringe corresponds to the path difference being equal to an integer number of wavelengths, in order to give rise to constructive interference :

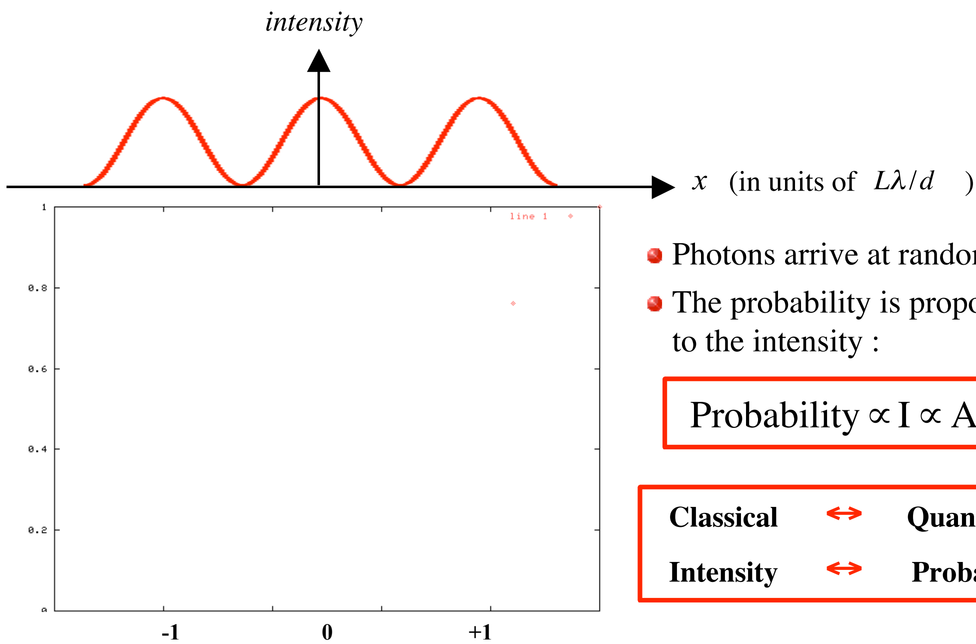
$$d\sin\vartheta = n\lambda \qquad (n = 0, \pm1, \pm2, \ldots) \quad (2)$$

- Eliminating $\sin\vartheta$ from (1) and (2):

$$x_{\mathrm{BRIGHT}} = \frac{Ln\lambda}{d}$$



The Double Slit Experiment (III)



- Photons arrive at random.
- The probability is proportional to the intensity :

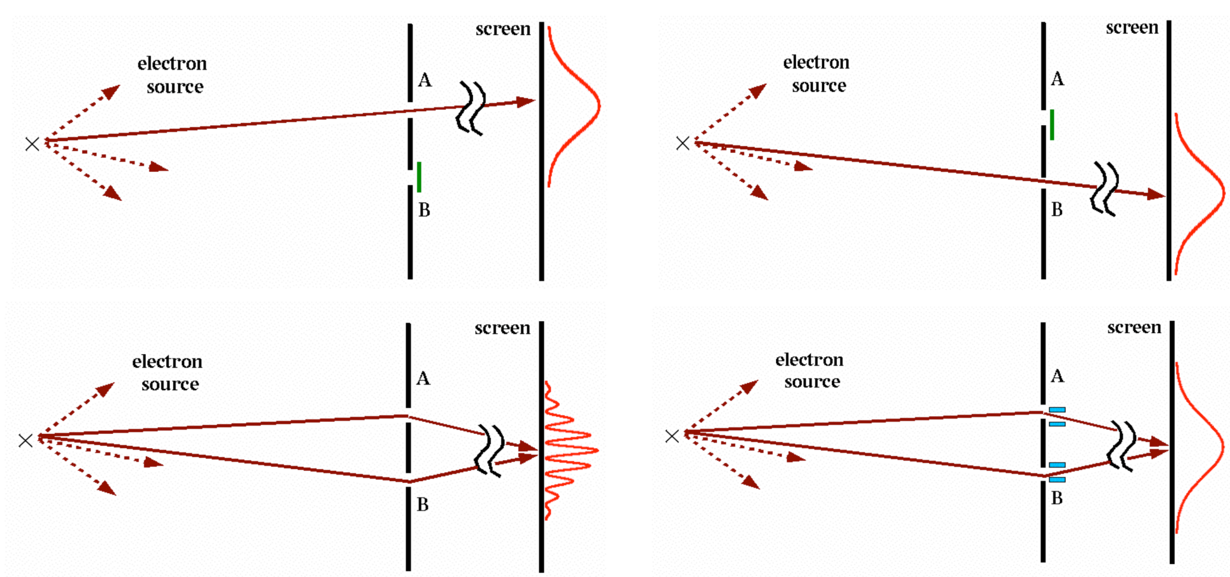
$$\text{Probability} \propto \text{I} \propto \text{A}^2$$

Classical	↔	**Quantum**
Intensity	↔	**Probability**

- As far as we know quantum mechanics is **truly** random. The probabilities are not just a statement of our ignorance about the true inner workings of quantum mechanical systems.
- The interference pattern emerges even if the average number of light quanta in the apparatus at any given time is **< 1.**

The Double Slit Experiment (IV)

- Try the experiment with something more "particle-like" : electrons.



- An interference pattern also emerges with both slits open.
- If detectors are installed to try and figure out which slit each electron passes through, the interference pattern disappears !

Wave Particle Duality (I)

- We have arrived at a picture in which light and even electrons appears to travel as waves, yet arrive as a particles.
- **De Broglie** made the amazing suggestion that ***all*** objects display both particle and wave-like properties, as characterised by the following equations :

$$p = h/\lambda$$
$$E = h \times f$$

De Broglie equations (*)

where λ and f are the De Broglie wavelength and frequency.

- For example, take an electron with an energy of 1 eV :

$$m_e = 9.1 \times 10^{-31} \quad \text{kg}$$

$$p = \sqrt{2 m_e E} = \sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}} = 0.54 \times 10^{-24} \quad \text{kg m s}^{-1}$$

$$\lambda = \frac{h}{p} = \frac{6.6 \times 10^{-34}}{0.54 \times 10^{-24}} \approx 1 \times 10^{-9} \text{ m} = 1 \text{ nm}$$

(*) We often use related quantities : $k = \dfrac{2\pi}{\lambda}$, $\omega = 2\pi f$ and $\hbar = \dfrac{h}{2\pi}$

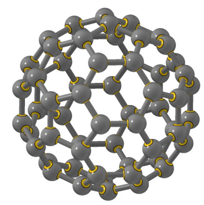
Wave Particle Duality (II)

- De Broglie's hypothesis has been widely confirmed by experiments at many different wavelength scales.

increasing mass ↓

- Light : conventional optics & X-ray diffraction
- Electrons : electron diffraction from crystals & nuclei
- Neutrons : neutron diffraction (atomic structure)
- Atoms : atom interferometry
- Simple Molecules
- Complex Molecules ← Limit of current experiments
- DNA
- Virus
- Single Cell
- ...

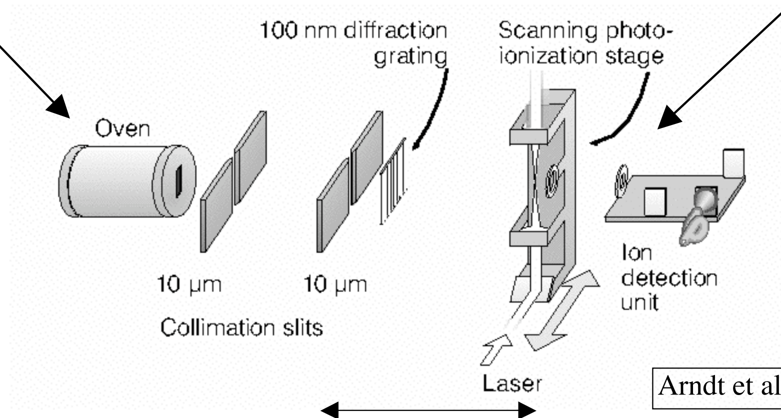
Example : C_{60} Molecules



1 nm

Source of C_{60} molecules at a temperature of between 900 and 1,000 K.

Laser scans across the interference pattern, ionising the C_{60} molecules which are then detected downstream.

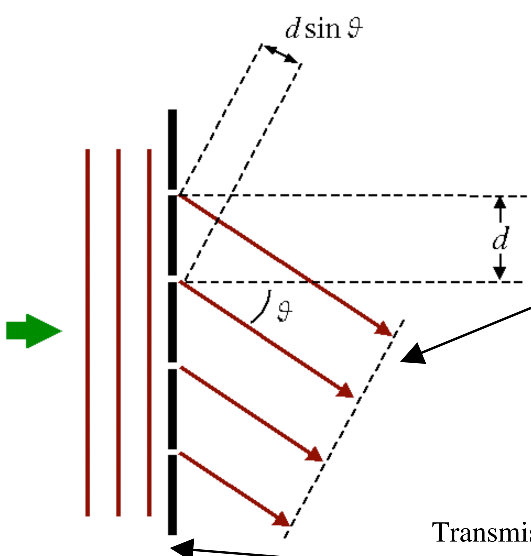


Arndt et al., Nature **401**, 1999

Diffraction Grating

- The principle is very similar to the double slit experiment. Multiple slits provide much brighter fringes, since the amplitudes from N slits multiply the intensity from a single slit :

$$I_{max} = N^2 I_0$$ where I_0 is the maximum intensity from a single slit.



A bright fringe is formed when this wavefront is comprised of rays that are exactly in phase :

$$d\sin\vartheta = n\lambda$$

where $n = 0, \pm1, \pm2, \ldots$

"First order" maximum

"Second order" maximum

Transmission grating. Reflection gratings are also possible.

Example : C_{60} Molecules

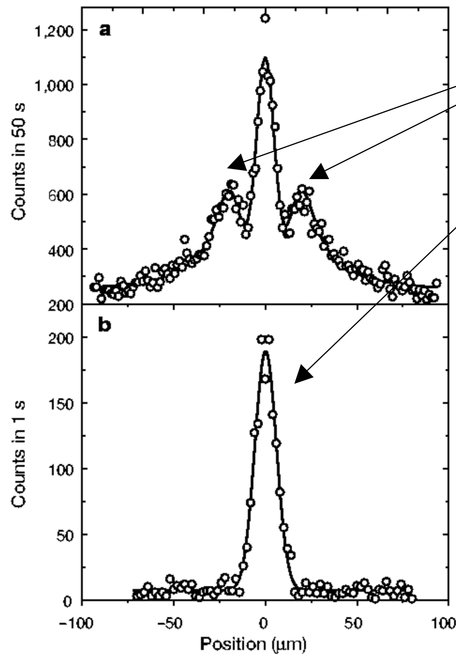


Figure 2 Interference pattern produced by C_{60} molecules. **a**, Experimental recording (open circles) and fit using Kirchhoff diffraction theory (continuous line). The expected zeroth and first-order maxima can be clearly seen. Details of the theory are discussed in the text. **b**, The molecular beam profile without the grating in the path of the molecules.

First order maxima clearly visible

Width of the beam *without* diffraction.

<u>Estimating the wavelength from the data :</u>

Position of first order peak ≈ 25 µm.

$$\sin\vartheta \approx \frac{25\times10^{-6}}{1.25} \approx 2\times10^{-5}$$

$$\lambda = d\sin\vartheta \quad (n=1)$$

$$\Rightarrow \lambda = \underbrace{100\times10^{-9}}_{\text{100 nm slit spacing}} \times 2\times10^{-5} = 2\ \text{pm}$$

100 nm slit spacing

Example : C_{60} Molecules

<u>Estimating the De Broglie wavelength :</u>

$$M = 60\times12\times u = 720\times931.5 \quad \text{MeV/c}^2$$

$$v = 220\ \text{m/s} = 7.33\times10^{-7}\ \text{c}$$

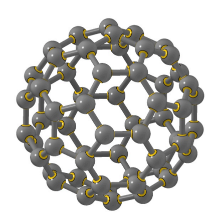
$$p = M\times v = 670{,}680\ \ \text{MeV/c}^2\times7.33\times10^{-7}\ \text{c}$$

$$= 0.4918\ \ \text{MeV/c}$$

$$\Rightarrow \lambda = \frac{h}{p} = 2\pi\frac{\hbar c}{pc} = 2\pi\frac{197\ \text{MeV fm}}{0.4918\ \ \text{MeV}}$$

$$= 2.5\times10^{-12}\ \text{m} = 2.5\ \text{pm}$$

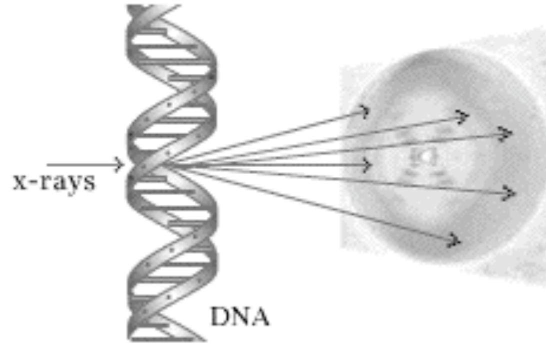
$$\lambda_{\text{De Broglie}} \ll d_{C_{60}}$$

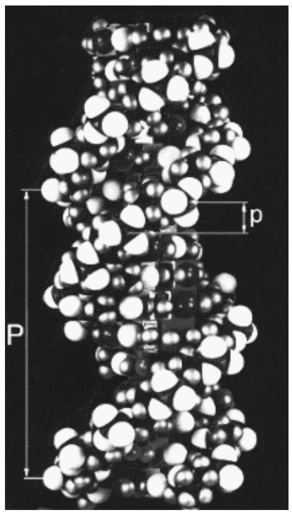


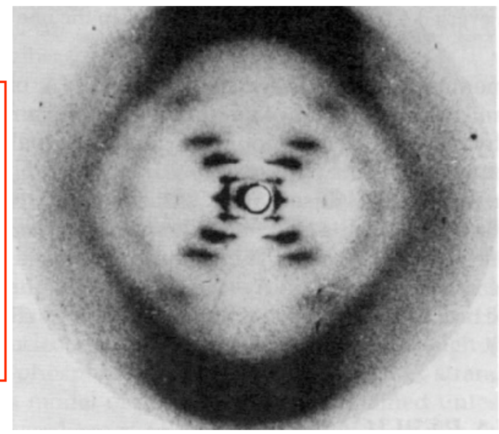
➨Agreement with the data shows that the C_{60} molecules are behaving quantum mechanically as single bodies.

Application : X-ray Diffraction

- X-ray wavelengths (0.1 - 1.0 nm) are appropriate for the investigation of molecular structures.
- e.g. DNA :



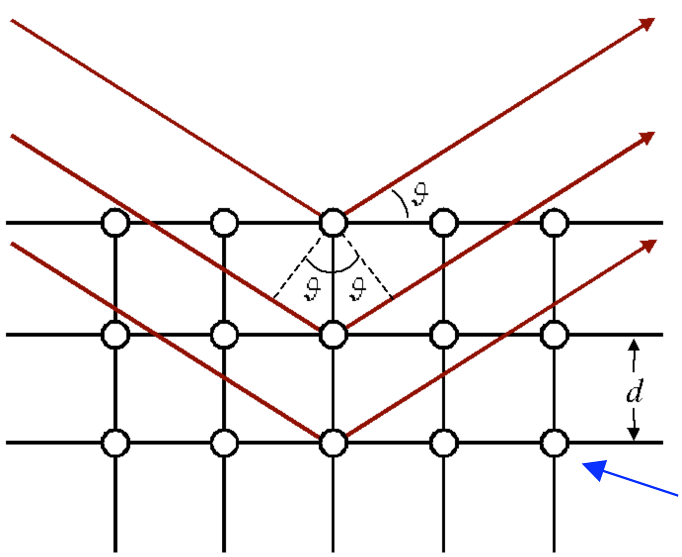




Rosalind Franklin, 1953

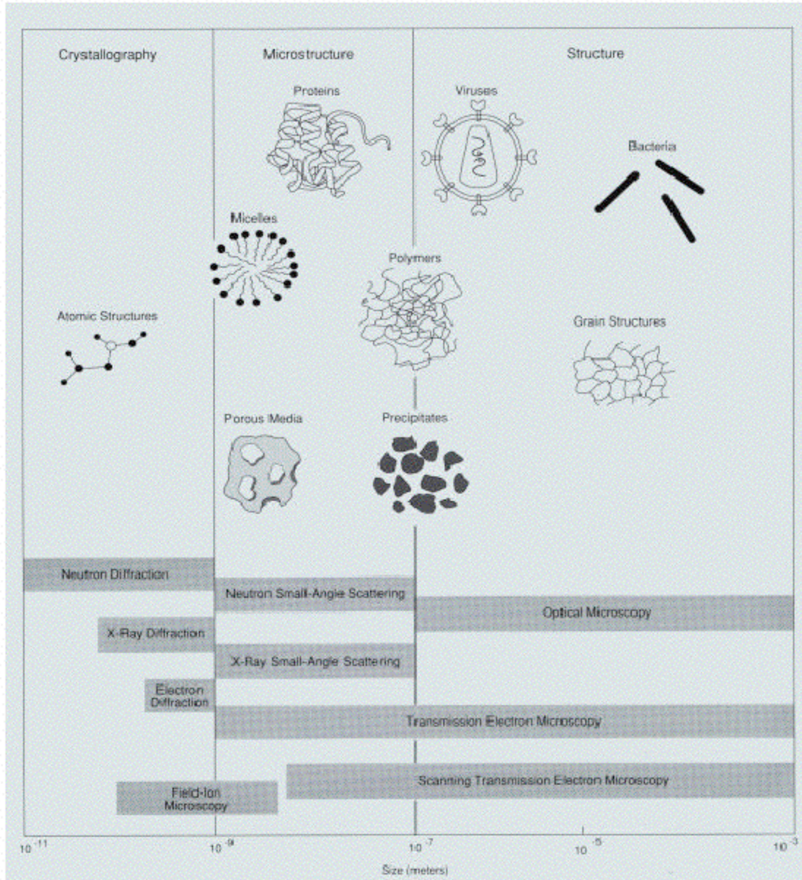
Application : Neutron Diffraction

- De Broglie wavelength comparable to typical inter-atomic distances.
- Neutrons have little electromagnetic interaction with materials.
- Each nucleus can be thought of as a scattering centre (similar to each slit in a transmission grating).
- e.g. determination of crystal structures :



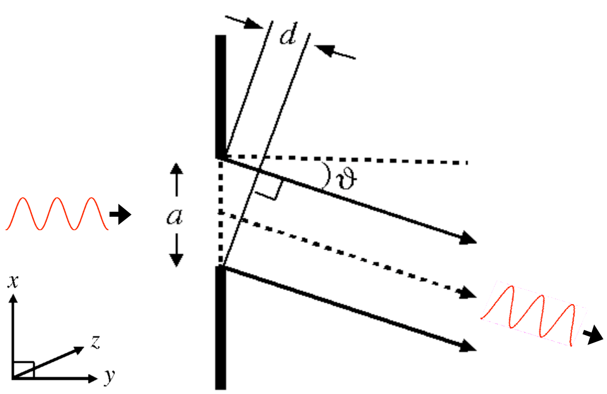
Bright fringe when incident and outgoing angles satisfy :

$$n\lambda = 2d\sin\vartheta$$



Measurement Limits : Example I

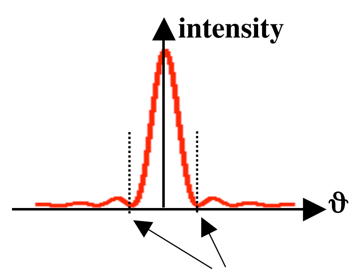
- Goal : try to measure the position and momentum of photons of light .
- One way to measure the location of a photon is to require that it pass through a single slit :



Uncertainty in x-location of photon :

$\Delta x \approx a$

But we know that as a is decreased, diffraction effects will increase :



$$\sin\vartheta = \frac{d}{a} = \frac{\lambda}{a}$$

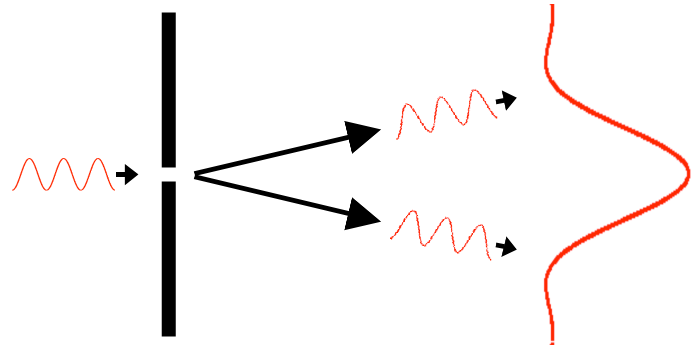
From the position of the first minimum :

$$\Delta p_x \approx p\sin\vartheta \approx \frac{p\lambda}{a}$$

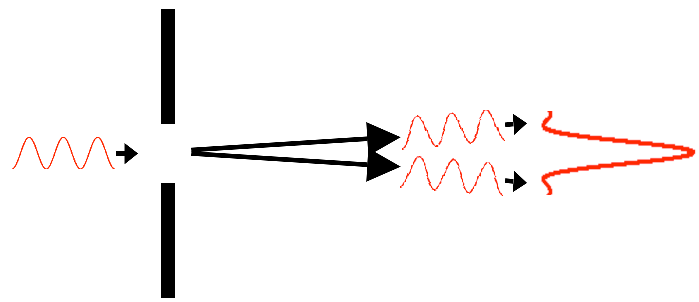
$$\Rightarrow \quad \Delta p_x \Delta x \approx p\lambda$$

De Broglie : $p = \dfrac{h}{\lambda}$ $\Rightarrow$ $\boxed{\Delta p_x \Delta x \approx h}$

Measurement Limits : Example I



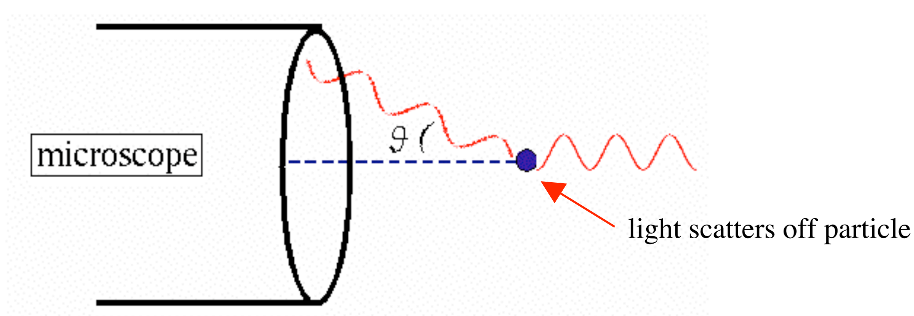
- Well defined position.
- Poorly defined momentum.



- Well defined momentum.
- Poorly defined position.

Measurement Limits : Example II

- Measure the position of a particle using a single photon of light.



Bigger lens means smaller resolution (optics) ⇒ $\Delta x \approx \dfrac{\lambda}{\sin\vartheta}$

Photon enters lens at unknown angle about the microscope axis. Imparts recoil momentum on particle ⇒ $\Delta p_x \approx p\sin\vartheta$

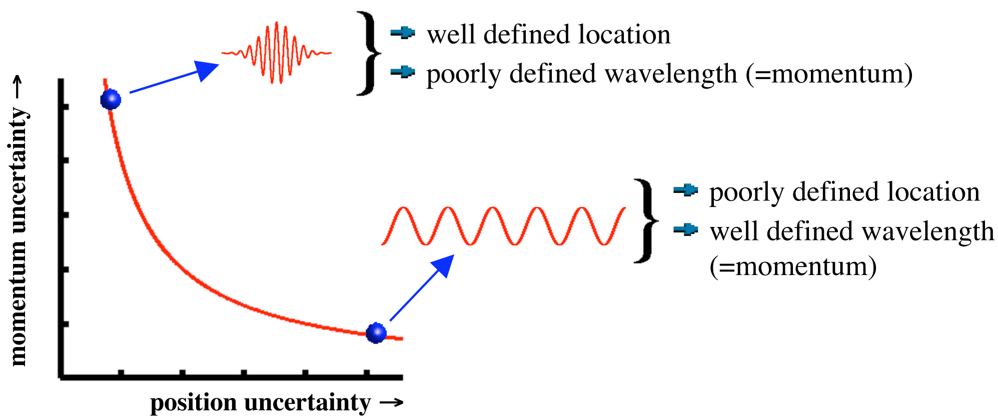
All other experiments yield the same bound. Cannot measure both position and momentum simultaneously to arbitrary precision.

$$\Delta x \Delta p_x \approx \lambda \times p \approx h$$

Uncertainty Principle (I)

- It turns out that we can never do better than dictated by the uncertainty principle :

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$



Uncertainty Principle (II)

- Formally, the theory of quantum mechanics predicts many uncertainty relations between different pairs of observables.
- Another common uncertainty relation is between measurements of energy and time :

$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$

- The uncertainty relations are rigorous results in quantum theory if Δa and Δb are defined as the root-mean-square deviations of the observables ***a*** and ***b***.

Summary (I)

- All objects display both wave and particle properties
  - ➨ Principle of complementarity.
- The De Broglie equation gives the relationship between momentum and wavelength :

$$p = h / \lambda$$

- Diffraction effects are most noticeable when the De Broglie wavelength is similar to the size of the gap or obstacle → probing the structure of matter.
- Quantum mechanics is intrinsically probabilistic. Classical waves are replaced by "probability waves", usually denoted by ψ . Classical intensities, obtained by squaring the amplitudes, become quantum mechanical probabilities :

$$\text{Probability} \propto |\psi|^2$$

ψ is generally complex

Summary (II)

- Probability waves add like classical waves :

$$\text{Probability} \propto |\psi_1 + \psi_2|^2$$

- Bright fringes due to constructive interference correspond to path differences for coherent sources equal to a whole number of wavelengths. This is the basis for most of our experiments and calculations.
- Quantum mechanical description of interference patterns : bright fringes correspond to regions of high probability for the arrival of quanta (e.g. photons). Dark fringes correspond to regions of low probability. With very large numbers of quanta, the classical interference pattern is built up ("correspondence principle").
- Simultaneous quantum mechanical measurements are limited in their precision by the uncertainty principle :

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$

Next Lecture

- Examine some of the properties of quantum mechanical probability waves.
- Look at the Schrödinger equation, governing the behaviour of these probability waves :
  - Particle in a box.
  - Quantisation of energy.
  - More complicated example : the hydrogen atom.
- Quantum mechanical view of fields and forces and interactions between elementary particles :
  - Range of forces.
  - Feynman diagrams.

Exercises

1) The size of the atomic nucleus is of order 10^{-14} m. High energy electrons used to probe the size and shape of atomic nuclei need to have a De Broglie wavelength of similar size.
   i. Use the formula $p = h/\lambda$ to estimate the momentum of the electrons.
   ii. How does the kinetic energy of the electrons compare to their rest energy ? [you might need to wait until after the relativity lecture to answer this]
2) What advantages might neutrons have over other particles as probes of the structure of matter ? What disadvantages might they have ?
3) The size of the hydrogen atom is approximately 0.53×10^{-10} m. You can use this as an estimate of the uncertainty on the position of the electron orbiting the nucleus. Then use the uncertainty relation in the form $\Delta p \approx \hbar/\Delta x$ to calculate the typical linear momentum of the electron in the hydrogen atom.

[You will find it easier to read the appendix on units and then use $\hbar c = 197.3$ eVnm . You should first calculate the quantity $\Delta p \times c$ which you will need in the next part of the question.]

Exercises

4) Classically, the energy of the electron in the hydrogen atom would be given by the combination of kinetic energy and potential energy :

$$E = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r}$$

Use the momentum calculated in (3), together with the given size of the hydrogen atom, to estimate the ionisation energy of hydrogen. How accurate is this estimate ?

[You will find it easier to re-write the first term above as $(pc)^2/2mc^2$ and also use the following :

$m(\text{electron}) = 0.511 \quad \text{MeV/c}^2$

$\frac{e^2}{4\pi\varepsilon_0} = 1.440 \quad \text{eV nm}$]

Appendix : Units

- Energy : **eV**
  - Electron Volt = energy acquired by an electron as it falls through a potential difference of 1 Volt = 1.6×10^{-19} Joules.
  - 1 keV = 1000 eV = 10^3 eV.
  - 1 MeV = 1000 keV = 10^6 eV.
  - 1 GeV = 1000 MeV = 10^9 eV.
- Velocity : **c**
  - c = speed of light = 3×10^8 m/s
- Momentum : **eV/c**
  - 1 eV/c = 5.3×10^{-28} kg m/s.
- Mass : **eV/c²**
  - 1 eV/c^2 = 1.8×10^{-36} kg.

Why are these useful ?

- Mass of the proton = 938 MeV/c^2 ≈ 1 GeV/c^2
- ***E = mc²*** : if the mass of the proton is 1 GeV/c^2, it takes an energy of 1 GeV to create a proton.
- ***E = pc*** (for photons and highly relativistic particles) : if a particle is moving close to the speed of light, its momentum in units of (GeV/c) is numerically similar to its energy in units of (GeV/c^2)

Appendix : Units

- We've already seen Planck's constant :

$$\hbar = \frac{h}{2\pi} = 1.054 \times 10^{-34} \quad \text{J s}$$

- An extremely useful combination of constants is :

$$\hbar c = 197 \;\text{MeV fm} \;=\; 197 \;\text{eV nm}$$

$1 \text{ fm} = 10^{-15}$ m

- Occasionally equations will appear that do not seem to be dimensionally consistent. They can always be made consistent by inserting combinations of $\hbar$ and c.

Appendix : Complex Numbers

- Imaginary number :

$$bi \qquad \text{where} \;\; i^2 = -1 \;\; \text{and} \;\; b \;\; \text{is real.}$$

- Complex number :

$$c = a + bi \qquad \text{where} \;\; a \;\; \text{and} \;\; b \;\; \text{are real.}$$

- Real and Imaginary parts :

$$\mathrm{Re}(c) = a, \quad \mathrm{Im}(c) = b$$

- Some properties :
  - $c = 0$ if and only if $\mathrm{Re}(c) = 0$ and $\mathrm{Im}(c) = 0$
  - $c = d$ if and only if $\mathrm{Re}(c) = \mathrm{Re}(d)$ and $\mathrm{Im}(c) = \mathrm{Im}(d)$
  - addition and subtraction :

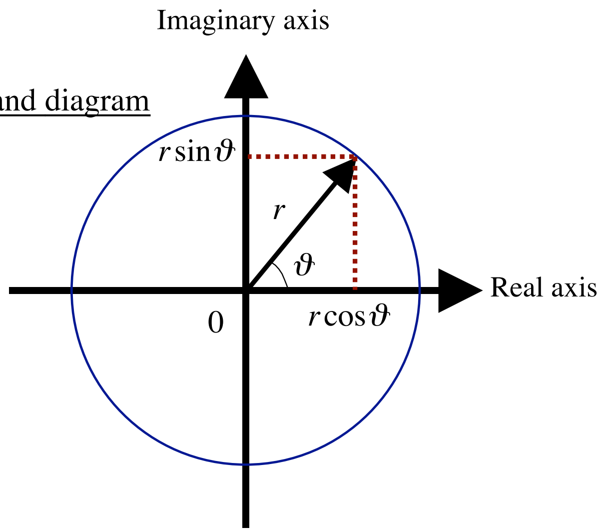
$$e = c + d \quad \text{means} \quad \begin{array}{l} \mathrm{Re}(e) = \mathrm{Re}(c) + \mathrm{Re}(d) \\ \mathrm{Im}(e) = \mathrm{Im}(c) + \mathrm{Im}(d) \end{array} \quad \text{etc.}$$

  - magnitude of a complex number :

$$|c| = \sqrt{(a^2 + b^2)} \quad \Rightarrow \text{similar to Cartesian vector}$$

Appendix : Complex Numbers

<u>Argand diagram</u>



- This provides a simple pictorial representation of certain complex number operations :

$$e = c \times d \quad \Rightarrow \quad \begin{array}{l} r_e = r_c \times r_d \\ \vartheta_e = \vartheta_c + \vartheta_d \end{array}$$

- A very useful complex number is :

$$e^{i\omega t}$$

Both real and imaginary parts describe SHM with angular frequency ω. Waves.

<u>Proof :</u> $e^{i\vartheta} = 1 + (i\vartheta) + \frac{(i\vartheta)^2}{2!} + \ldots$

$$e^{i\vartheta} = 1 - \frac{\vartheta^2}{2!} + \frac{\vartheta^4}{4!} \ldots \quad + \quad i(\vartheta - \frac{\vartheta^3}{3!} + \ldots) \quad \Rightarrow \quad \boxed{e^{i\vartheta} = \cos\vartheta + i\sin\vartheta}$$