

CHAPTER 5

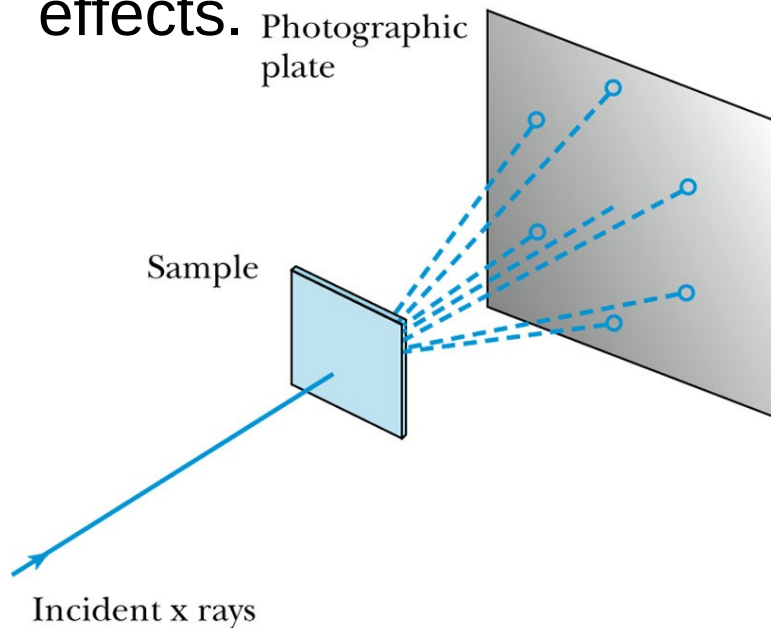
Wave Properties of Matter and Quantum Mechanics I

- 5.1 X-Ray Scattering
- 5.2 De Broglie Waves
- 5.3 Electron Scattering
- 5.4 Wave Motion
- 5.5 Waves or Particles?
- 5.6 Uncertainty Principle
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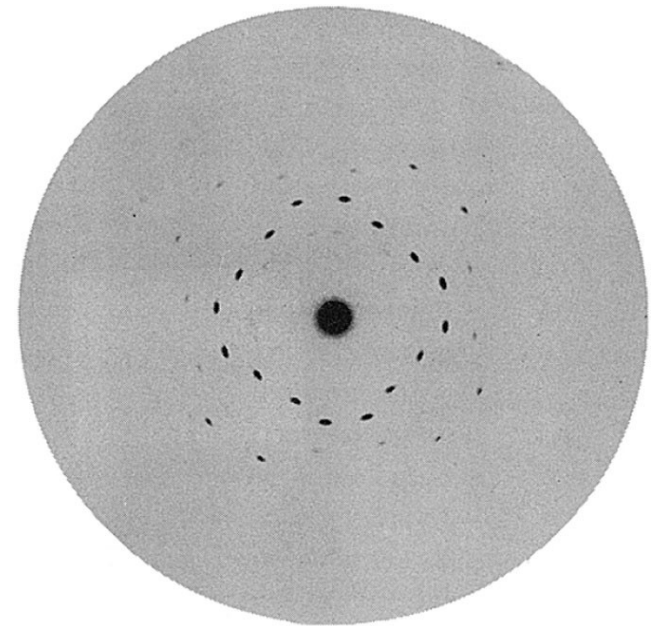
I thus arrived at the overall concept which guided my studies: for both matter and radiations, light in particular, it is necessary to introduce the corpuscle concept and the wave concept at the same time.

5.1: X-Ray Scattering

- Max von Laue suggested that if x rays were a form of electromagnetic radiation, interference effects should be observed.
- Crystals act as three-dimensional gratings, scattering the waves and producing observable interference effects.



(a)

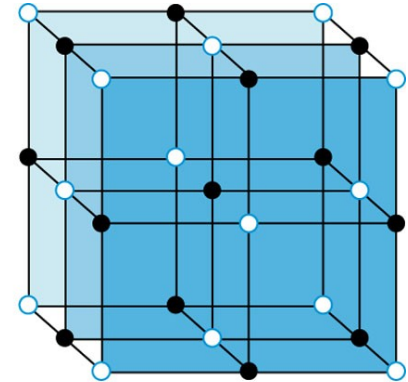
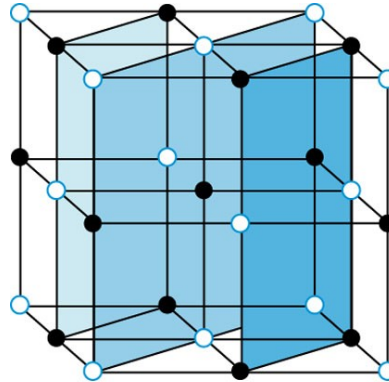


(b)

Bragg's Law

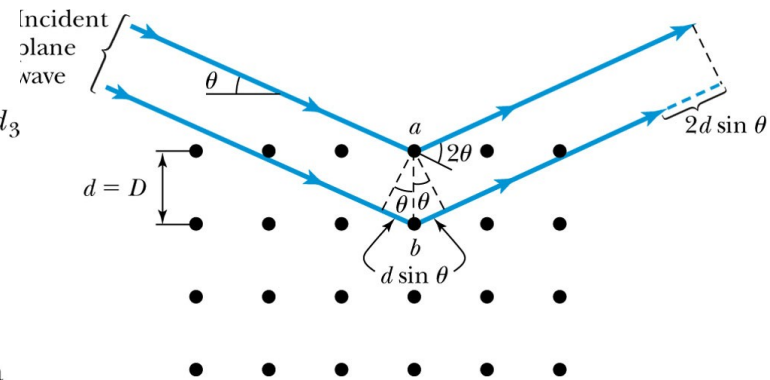
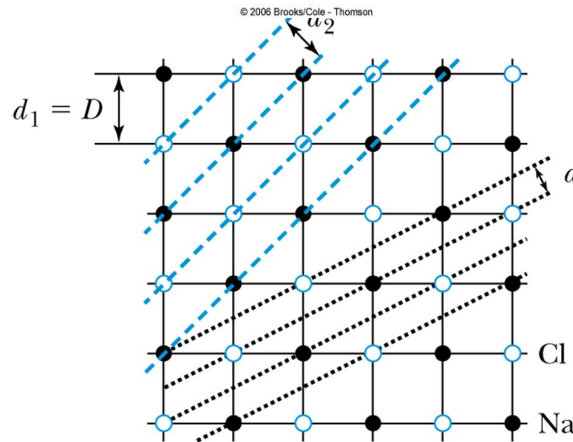
- William Lawrence Bragg interpreted the x-ray scattering as the reflection of the incident x-ray beam from a unique set of planes of atoms within the crystal.
- There are two conditions for constructive interference of the scattered x rays:

- The angle of incidence must equal the angle of reflection of the outgoing wave.
- The difference in path lengths must be an integral number of wavelengths.



- Bragg's Law:**

$$n\lambda = 2d \sin \theta$$
 $(n = \text{integer})$

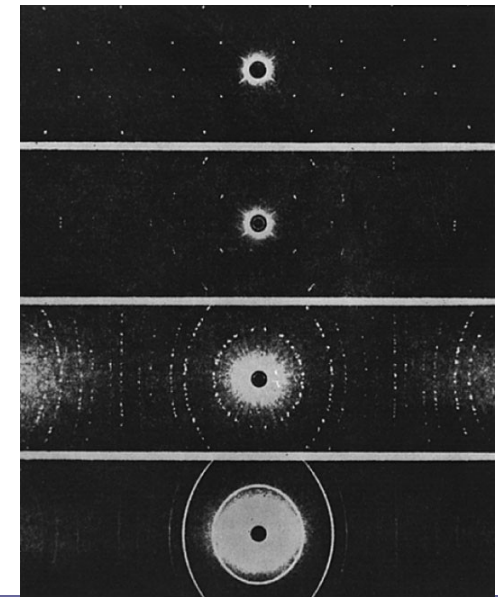
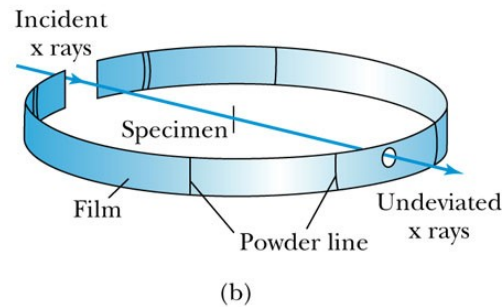
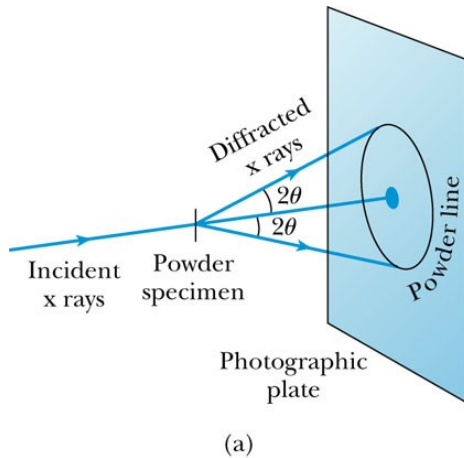
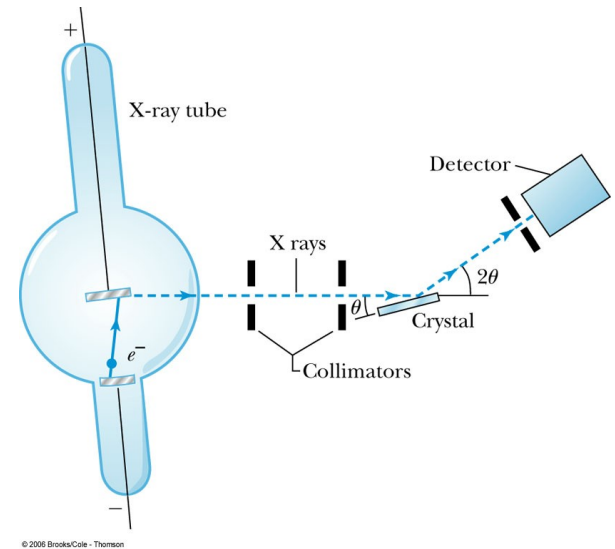


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The Bragg Spectrometer

- A Bragg spectrometer scatters x rays from several crystals. The intensity of the diffracted beam is determined as a function of scattering angle by rotating the crystal and the detector.
- When a beam of x rays passes through the powdered crystal, the dots become a series of rings.



(c)

5.2: De Broglie Waves

- Prince Louis V. de Broglie suggested that mass particles should have wave properties similar to electromagnetic radiation.
- The energy can be written as $hf = pc = p\lambda f$
- Thus the wavelength of a matter wave is called the de Broglie wavelength:

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

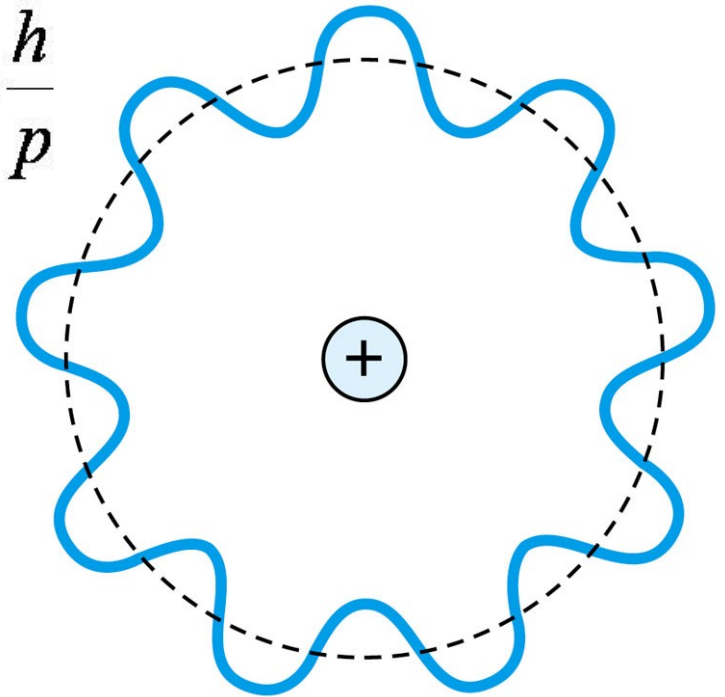
Bohr's Quantization Condition

- One of Bohr's assumptions concerning his hydrogen atom model was that the angular momentum of the electron-nucleus system in a stationary state is an integral multiple of $h/2\pi$.
- The electron is a standing wave in an orbit around the proton. This standing wave will have nodes and be an integral number of wavelengths.

$$2\pi r = n\lambda = n \frac{h}{p}$$

- The angular momentum becomes:

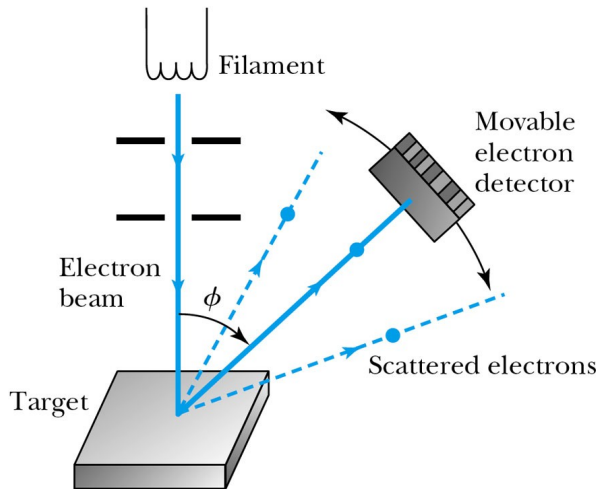
$$L = rp = \frac{nh}{2\pi} = n\hbar$$



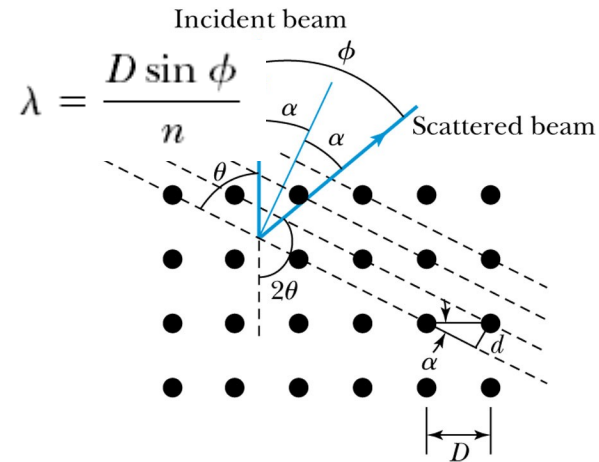
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5.3: Electron Scattering

- Davisson and Germer experimentally observed that electrons were diffracted much like x rays in nickel crystals.

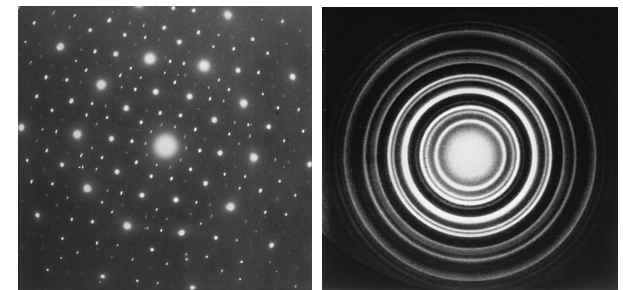


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- George P. Thomson (1892–1975), son of J. J. Thomson, reported seeing the effects of electron diffraction in transmission experiments. The first target was celluloid, and soon after that gold, aluminum, and platinum were used. The randomly oriented polycrystalline sample of SnO_2 produces rings as shown in the figure at right.



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5.4: Wave Motion

- De Broglie matter waves suggest a further description. The displacement of a wave is

$$\Psi(x, t) = A \sin \left[\frac{2\pi}{\lambda} (x - vt) \right]$$

- This is a solution to the wave equation

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2}$$

- Define the wave number k and the angular frequency ω as:

$$k \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad \omega = \frac{2\pi}{T}$$

- The wave function is now: $\Psi(x, t) = A \sin (kx - \omega t)$.

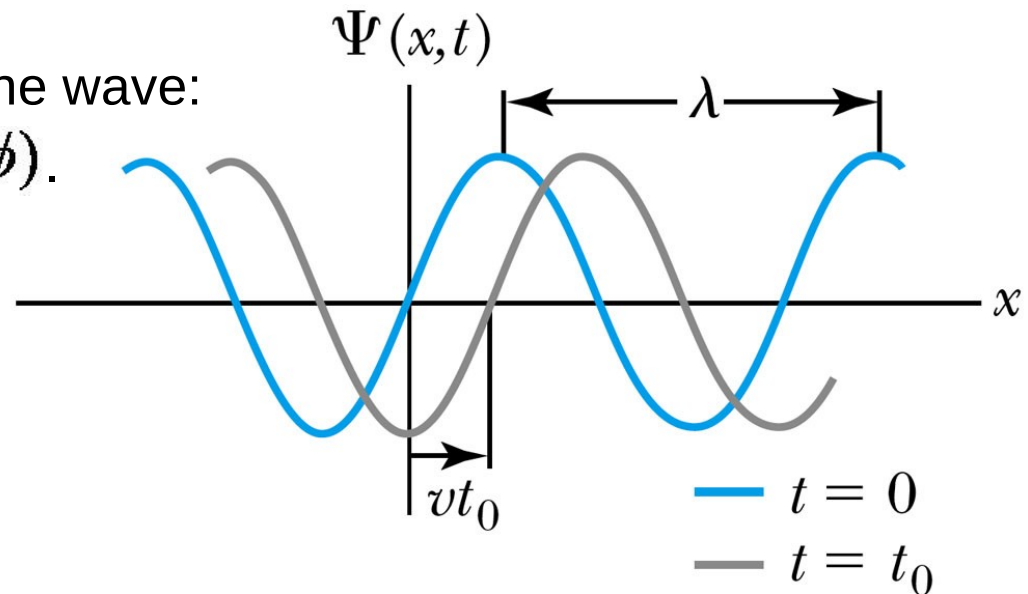
Wave Properties

- The phase velocity is the velocity of a point on the wave that has a given phase (for example, the crest) and is given by

$$v_{\text{ph}} = \frac{\lambda}{T} = \frac{\omega}{k}$$

- A phase constant Φ shifts the wave:

$$\Psi(x, t) = A \sin(kx - \omega t + \phi).$$



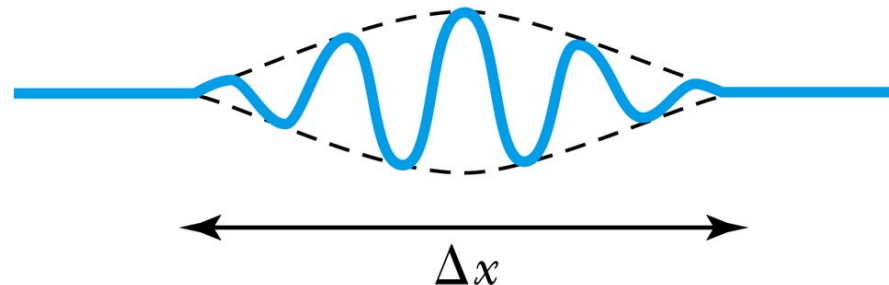
Principle of Superposition

- When two or more waves traverse the same region, they act independently of each other.
- Combining two waves yields:

$$\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t) = 2A \left(\frac{\Delta k}{2} x - \frac{\Delta \omega}{2} t \right) \cos(k_{av} x - \omega_{av} t)$$

- The combined wave oscillates within an envelope that denotes the maximum displacement of the combined waves.
- When combining many waves with different amplitudes and frequencies, a pulse, or **wave packet**, is formed which moves at a **group velocity**:

$$u_{gr} = \Delta \omega / \Delta k.$$



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Fourier Series

- The sum of many waves that form a wave packet is called a **Fourier series**:

$$\Psi(x, t) = \sum_i A_i \cos(k_i x - \omega_i t)$$

- Summing an infinite number of waves yields the Fourier integral:

$$\Psi(x, t) = \int \tilde{A}(k) \cos(kx - \omega t) dk$$

Wave Packet Envelope

- The superposition of two waves yields a wave number and angular frequency of the wave packet envelope.

$$\frac{\Delta k}{2}x - \frac{\Delta \omega}{2}t$$

- The range of wave numbers and angular frequencies that produce the wave packet have the following relations:

$$\Delta k \Delta x = 2\pi \qquad \Delta \omega \Delta t = 2\pi$$

- A **Gaussian wave packet** has similar relations:

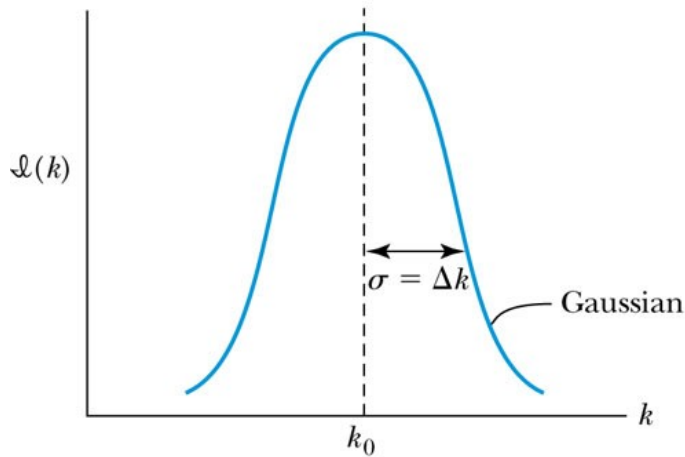
$$\Delta k \Delta x = 1/2 \qquad \Delta \omega \Delta t = \frac{1}{2}$$

- The localization of the wave packet over a small region to describe a particle requires a large range of wave numbers. Conversely, a small range of wave numbers cannot produce a wave packet localized within a small distance.

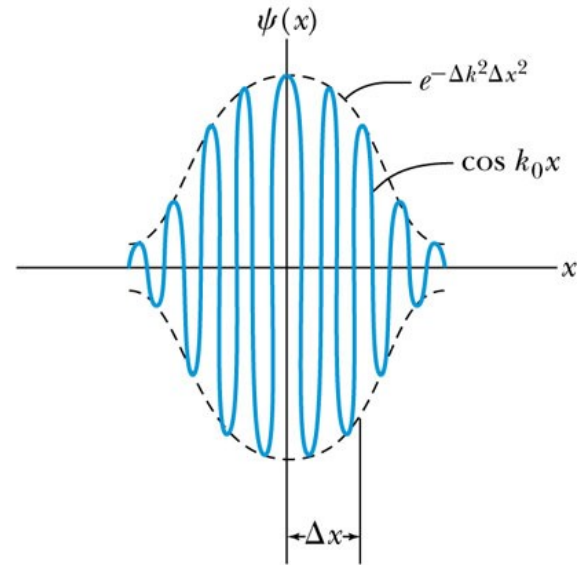
Gaussian Function

- A Gaussian wave packet describes the envelope of a pulse wave.

$$\Psi(x, 0) = \Psi(x) = Ae^{-\Delta k^2 x^2} \cos(k_0 x)$$



(a)



(b)

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- The group velocity is $u_{\text{gr}} = \frac{d\omega}{dk}$.

Dispersion

- Considering the group velocity of a de Broglie wave packet yields:

$$u_{\text{gr}} = \frac{dE}{dp} = \frac{pc^2}{E}$$

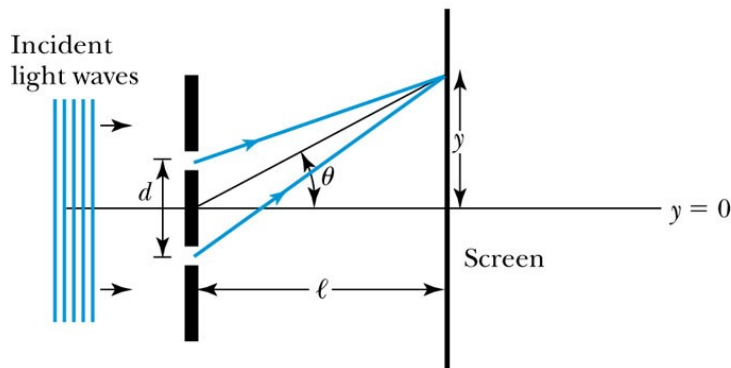
- The relationship between the phase velocity and the group velocity is

$$u_{\text{gr}} = \frac{d\omega}{dk} = \frac{d}{dk}(v_{\text{ph}}k) = v_{\text{ph}} + k \frac{dv_{\text{ph}}}{dk}$$

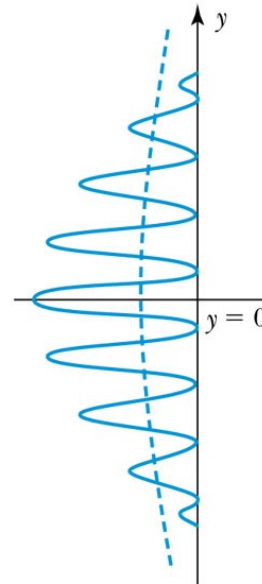
- Hence the group velocity may be greater or less than the phase velocity. A medium is called nondispersive when the phase velocity is the same for all frequencies and equal to the group velocity.

5.5: Waves or Particles?

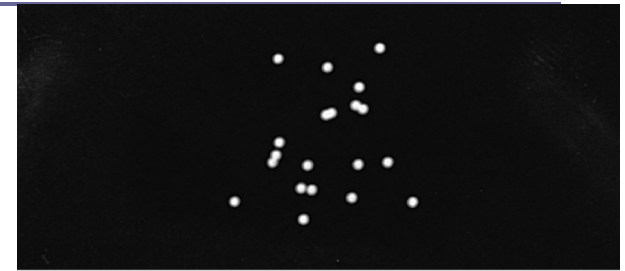
- Young's double-slit diffraction experiment demonstrates the wave property of light.
- However, dimming the light results in single flashes on the screen representative of particles.



(a)



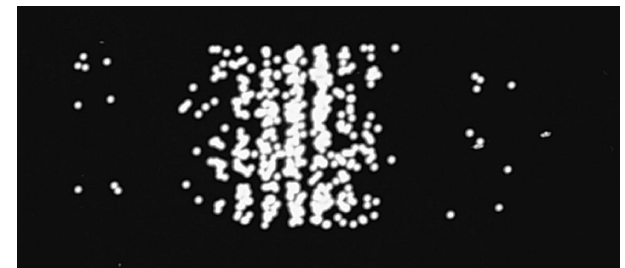
(b)



(a) 20 counts



(b) 100 counts



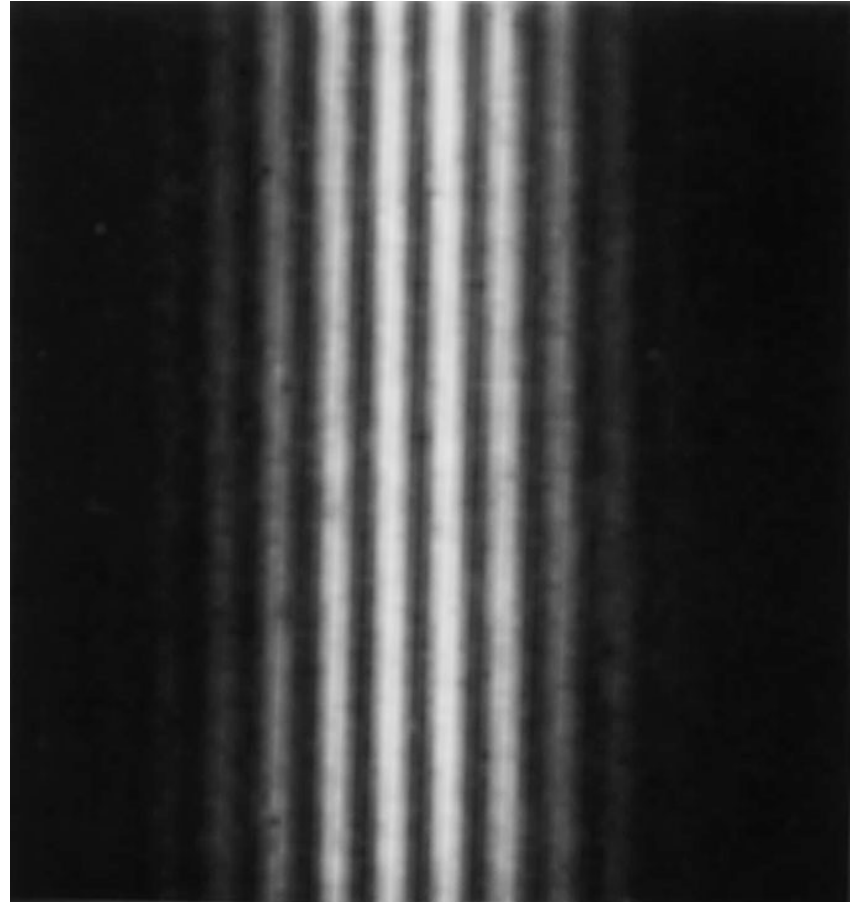
(c) 500 counts



(d) ~4000 counts

Electron Double-Slit Experiment

- C. Jönsson of Tübingen, Germany, succeeded in 1961 in showing double-slit interference effects for electrons by constructing very narrow slits and using relatively large distances between the slits and the observation screen.
- This experiment demonstrated that precisely the same behavior occurs for both light (waves) and electrons (particles).



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Which slit?

- To determine which slit the electron went through: We set up a light shining on the double slit and use a powerful microscope to look at the region. After the electron passes through one of the slits, light bounces off the electron; we observe the reflected light, so we know which slit the electron came through.
- Use a subscript “ph” to denote variables for light (photon). Therefore the momentum of the photon is

$$p_{\text{ph}} = \frac{h}{\lambda_{\text{ph}}} > \frac{h}{d}$$

- The momentum of the electrons will be on the order of $p_{\text{el}} = \frac{h}{\lambda_{\text{el}}} \sim \frac{h}{d}$.
- The difficulty is that the momentum of the photons used to determine which slit the electron went through is sufficiently great to strongly modify the momentum of the electron itself, thus changing the direction of the electron! The attempt to identify which slit the electron is passing through will in itself change the interference pattern.

Wave particle duality solution

- The solution to the wave particle duality of an event is given by the following principle.
- **Bohr's principle of complementarity:** It is not possible to describe physical observables simultaneously in terms of both particles and waves.
- **Physical observables** are those quantities such as position, velocity, momentum, and energy that can be experimentally measured. In any given instance we must use either the particle description or the wave description.

5.6: Uncertainty Principle

- It is impossible to measure simultaneously, with no uncertainty, the precise values of k and x for the same particle. The wave number k may be rewritten as

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = p \frac{2\pi}{h} = \frac{p}{\hbar}$$

- For the case of a Gaussian wave packet we have

$$\Delta k \Delta x = \frac{\Delta p}{\hbar} \Delta x = \frac{1}{2}$$

Thus for a single particle we have Heisenberg's **uncertainty principle**:

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

Energy Uncertainty

- If we are uncertain as to the exact position of a particle, for example an electron somewhere inside an atom, the particle can't have zero kinetic energy.

$$K_{\min} = \frac{p_{\min}^2}{2m} \geq \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2}{2m\ell^2}$$

- The energy uncertainty of a Gaussian wave packet is

$$\Delta E = h \Delta f = h \frac{\Delta \omega}{2\pi} = \hbar \Delta \omega$$

combined with the angular frequency relation

$$\Delta \omega \Delta t = \frac{\Delta E}{\hbar} \Delta t = \frac{1}{2}$$

- Energy-Time Uncertainty Principle: $\Delta E \Delta t \geq \frac{\hbar}{2}$.

5.7: Probability, Wave Functions, and the Copenhagen Interpretation

- The wave function determines the likelihood (or probability) of finding a particle at a particular position in space at a given time.

$$P(y) dy = |\Psi(y,t)|^2 dy$$

- The total probability of finding the electron is 1. Forcing this condition on the wave function is called normalization.

$$\int_{-\infty}^{\infty} P(y) dy = \int_{-\infty}^{\infty} |\Psi(y,t)|^2 dy = 1$$

The Copenhagen Interpretation

- Bohr's interpretation of the wave function consisted of 3 principles:
 - 1) The uncertainty principle of Heisenberg
 - 2) The complementarity principle of Bohr
 - 3) The statistical interpretation of Born, based on probabilities determined by the wave function

- Together these three concepts form a logical interpretation of the physical meaning of quantum theory. According to the Copenhagen interpretation, physics depends on the outcomes of measurement.

5.8: Particle in a Box

- A particle of mass m is trapped in a one-dimensional box of width L .
- The particle is treated as a wave.
- The box puts boundary conditions on the wave. The wave function must be zero at the walls of the box and on the outside.
- In order for the probability to vanish at the walls, we must have an integral number of half wavelengths in the box.

$$\frac{n\lambda}{2} = \ell \quad \text{or} \quad \lambda_n = \frac{2\ell}{n} \quad (n = 1, 2, 3, \dots)$$

- The energy of the particle is $E = \text{K.E.} = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$.
- The possible wavelengths are quantized which yields the energy:

$$E_n = \frac{h^2}{2m} \left(\frac{n}{2\ell} \right)^2 = n^2 \frac{h^2}{8m\ell^2} \quad (n = 1, 2, 3, \dots)$$

- The possible energies of the particle are quantized.

Probability of the Particle

- The probability of observing the particle between x and $x + dx$ in each state is

$$P_n dx \propto |\Psi_n(x)|^2 dx$$

- Note that $E_0 = 0$ is not a possible energy level.
- The concept of energy levels, as first discussed in the Bohr model, has surfaced in a natural way by using waves.

