Lesson 2: Wave-particle duality

Clara E. Alonso Alonso

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In 1887 Hertz observed

1. radiating **metals** with visible and U.V. radiation ($\nu \approx\ 10^{14} - 10^{17}$ Hz) $\rightarrow$ emission of electrons
2. there is emission if $\nu > \nu_{threshold}$ or ν_{cutoff} ($\nu_{threshold}$ depends on the radiated metal)
3. with $\nu > \nu_{threshold}$ the e^- current is proportional to the intensity of the e.m. radiation
4. the maximum kinetic energy of the emitted electrons (photoelectrons)
   - doesn't depend on the e.m. radiation intensity
   - varies linearly with ν

Clasically

- it is understood that there is e^- emission (1)
- it is not understood that there is $\nu_{threshold}$ (2)
- the energy of the incident wave (doesn't depends on ν) $\propto$ source intensity (4)
- the delay time between the radiation arrival and the electron emission (larger when the intensity is smaller) $\rightarrow$ is not observed experimentally (even whith $I\ \ll$)

Einstein $\rightarrow$ radiation $\rightarrow$ **energy quantum** $h\nu$ $\rightarrow$ absorbed by an individual e^-
- time for absorbing a quantum is smaller or similar to $10^{-9}\ s$

$$h\nu = (E_c)_{max} \; + \; W$$

W **work function** (for e^- near the surface), depends on the metal

the e^- must surmont a potential energy step at the surface of the metal, they are confined
It explains

- $\exists \quad \nu_{threshold} = \frac{W}{h}$
- $(E_c)_{max}$ linear with ν
- proporcionality between e^- current and source intensity I

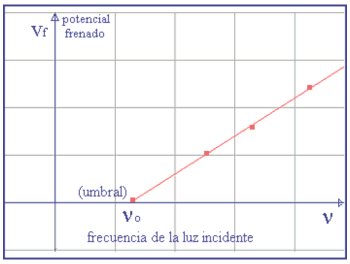
$I \gg \quad \rightarrow \quad >$ number of **photons** $\quad \rightarrow \quad >$ number of **photoelectrons**

"particle" behaviour of light

- information on metals $W \; = \; h\nu_{threshold}$
  $(W \approx eV)$
  V_f stopping potential (the polarity of the voltage source is reversed)

$$(E_c)_{max} \; = \; e\,V_f \; = \; h\nu - W$$

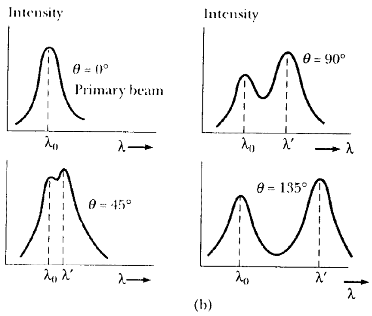
$$V_f = \frac{h}{e}\nu - \frac{W}{e}$$



Scattering of radiation of $\lambda \simeq$ Å(X rays) by metal foils

Clasically $\rightarrow$ $I(\theta) \propto 1 + \cos^2\theta$ independient of λ_{inc}

Compton observs at scattering angle θ λ_{inc} and $\lambda_{inc} + \Delta\lambda(\theta)$



Compton incident radiation $\rightarrow$ photons of energy $h\nu$
Compton effect: **elastic** scattering of e^- by photons

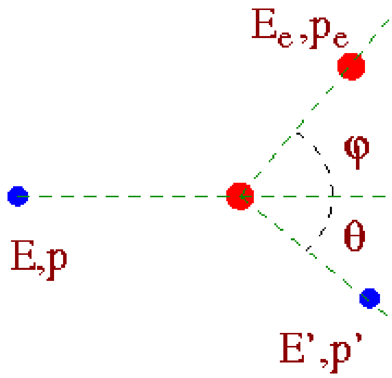
photon momentum?

Relativistic

$$E = \sqrt{(m_0c^2)^2 + p^2c^2}$$

$$v = \frac{dE}{dp} = \frac{pc^2}{E} = \frac{pc^2}{\sqrt{(m_0c^2)^2 + p^2c^2}}$$

for the photon $v = c \rightarrow m_0 = 0 \rightarrow p = \frac{h\nu}{c}$



- Conservation of momentum

$$\vec{p} = \vec{p}\,' + \vec{p}_e$$

$$\vec{p}_e^{\;2} = (\vec{p} - \vec{p}\,')^2 = p^2 + p'^2 - 2\vec{p}\cdot\vec{p}\,' \tag{1}$$

- Conservation of energy

$$h\nu + mc^2 = h\nu' + (m^2c^4 + p_e^2c^2)^{\frac{1}{2}}$$

$$\begin{aligned} m^2c^4 + p_e^2c^2 &= (h\nu - h\nu' + mc^2)^2 \\ &= (h\nu - h\nu')^2 + 2mc^2(h\nu - h\nu') + m^2c^4 \end{aligned} \tag{2}$$

From (1) $p_e^2 = \left(\frac{h\nu}{c}\right)^2 + \left(\frac{h\nu'}{c}\right)^2 - 2\frac{h\nu}{c}\frac{h\nu'}{c}\cos\theta$

$$p = \frac{h\nu}{c} \; ; \; p' = \frac{h\nu'}{c}$$

$$p_e^2 c^2 = (h\nu - h\nu')^2 + 2(h\nu)(h\nu')(1-\cos\theta) \tag{3}$$

From (2) and (3)

$$(h\nu)(1-\cos\theta) = \frac{mc^2}{\nu'}(\nu - \nu')$$

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

$\Delta\lambda \geq 0$

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λ_{inc} observed in expt. $\rightarrow$ scattering by atom $m \rightarrow m_{at} \rightarrow \Delta\lambda \rightarrow 0$

$\lambda_c = \frac{h}{m_e c} = 0.024$ Å Compton wavelength

- Experimentally $\rightarrow$ agreement in e^- recoil
- Simultaneity between recoil e^- and outgoing photon
- Scattering interpreted as the one of billiard balls $\rightarrow$ light could be regarded as classical particles in these experiments
- But radiation also has wave properties **(interference, diffraction)**

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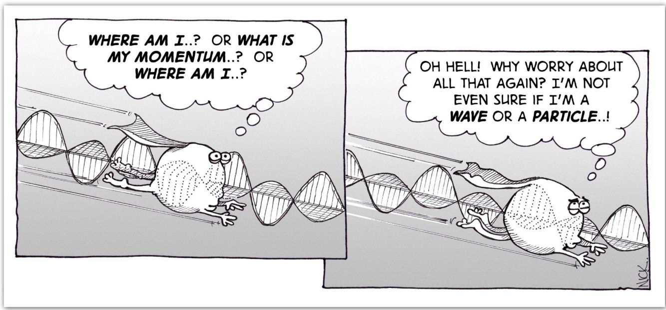


Photon self-identity issues

De Broglie hypothesis

1923 De Broglie suggests double nature **wave-particle** of matter

De Broglie relation

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

plus Einstein relation

$$E = \hbar\omega$$

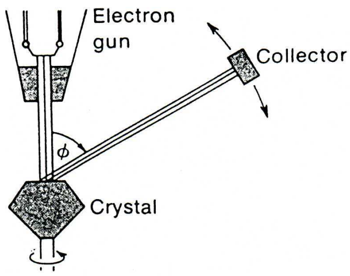
$$\hbar = \frac{h}{2\pi} \quad ; \quad \hbar c = 1970 \ eV\mathring{A}$$

He proposes to observe e^- diffraction ($E_c \sim$ tens of eV)

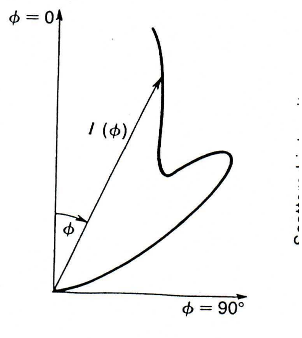
$$\Downarrow$$

Electron diffraction: Davisson and Germer experiment. Thomson experiment

DAVISSON-GERMER EXPERIMENT
e^- scattering by Ni crystal (shows preferential directions)



(a)



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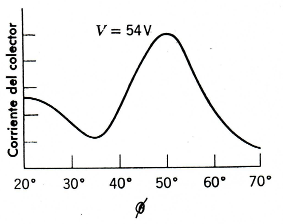
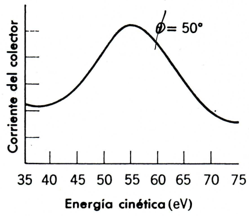
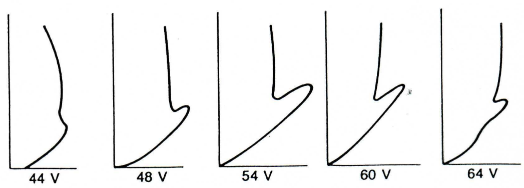


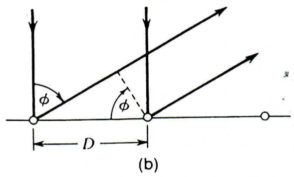


$\lambda_{DB} = \frac{h}{\sqrt{2m_e Ve}} \rightarrow \lambda_{DB}(\AA) = \left(\frac{150}{V}\right)^{\frac{1}{2}}$ (V in volts)
(no relativistic; $m_e = 0.511 \frac{MeV}{c^2}$)

- For $V = 54\ V \rightarrow \lambda_{DB} = 1.66$ Å (for other V less intense phenomenon)

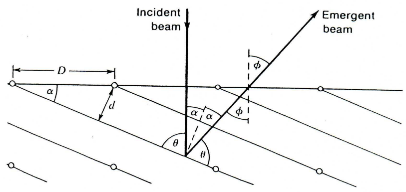
Fig. 2-6 Polar plots of scattered intensity showing dependence of diffraction pattern on accelerating voltage. (Based on data of Davisson and Germer.)





If the effect depended only on the rows of atoms in the surface $\rightarrow$ any voltage V $\rightarrow$ strong diffraction peak at $\phi = \sin^{-1}\frac{\lambda}{D}$ Electrons of E very different from $54\ eV$ $\rightarrow$ much reduced diffraction intensities

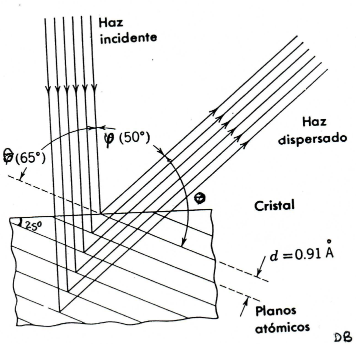
Observations explained by $\rightarrow$ **reflections from atomic planes**

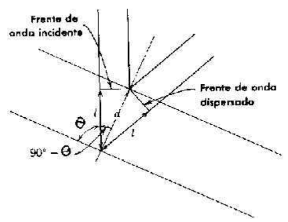


$$d = D\sin\alpha \quad \text{and} \quad D = 2.15\mathring{A}$$

$$\theta = \frac{\pi}{2} - \alpha \quad ; \quad \phi = 2\alpha \ ;$$

$$\alpha = 25^\circ \quad \rightarrow \quad \phi = 50^\circ \quad ; \quad d = 0.91\mathring{A}$$





$$l \;=\; d\sin\theta$$

path difference

$$\delta \;=\; 2l \;=\; 2d\sin\theta \;=\; 2\times 0.91\mathring{A}\times\sin 65^\circ \;=\; 1.65\mathring{A}$$

path difference $\;=\; n\lambda$ **Bragg's law** (condition of reinforcement)

$n=1\rightarrow\lambda \;=\; 2d\sin\theta \;=\; D\sin\phi \;=\; 1.65\mathring{A}$ (first order diffraction maximum)

Expressions necessary to obtain the last relation of previous page

$$d = D\sin\alpha = D\cos\theta$$

$$2d\sin\theta = 2D\cos\theta\sin\theta = D\sin 2\theta = D\sin\phi$$

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Thomson experiment (1927-28)

- e^- wave properties are observed
- Differs from Davisson-Germer experiment:
  - Energy of e^- $\rightarrow 10 - 40KeV \rightarrow \lambda_{DB} \approx 0.1\AA$ (D.G.$\rightarrow 30 - 600eV \rightarrow \lambda_{DB} \approx 1$ $\AA$) $\rightarrow e^-$ much more penetrating, pass through thin films (≈ 1000 $\AA$ thickness) $\rightarrow$ TRANSMISSION
  - Many hundred of atomic planes contribute to the diffracted wave
  - Polycrystal (aggregate of very small crystals oriented at random)
  - Independently confirms the De Broglie relation
    Diffraction pattern are concentric circles

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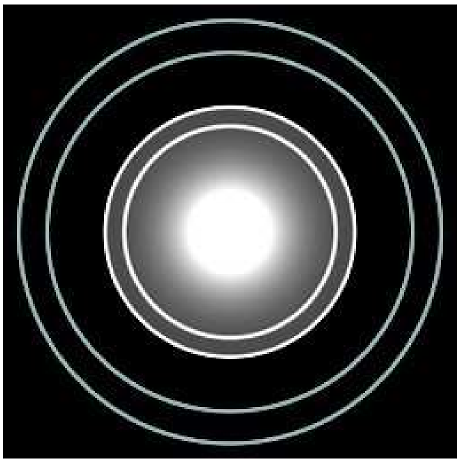

Electron diffraction by gold crystals

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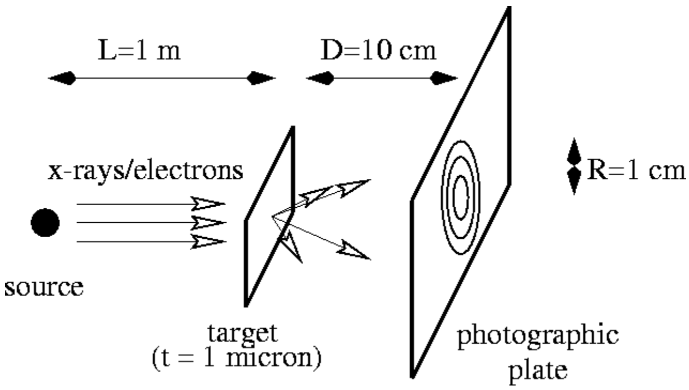
- Diffracted beams are collected on photographic plates located far from the diffracting film
- Results similar to those of X-rays (clasically is radiation)
- This experiment verifies the applicability of the De Broglie relation to higher energies



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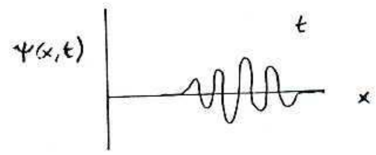
De Broglie assigns λ to particles
Which is the responsible wave?
Ej. Representation of $\Psi(x,t)$ versus x at an instant t



We expect something like this plot for particles moving in the $x-$axis

- Modulate amplitude
- Different from zero in finite region of x-axis

Plane wave $\rightarrow e^{i(\vec{k}\cdot\vec{r}-\omega t)}$ **is not localized** in espace (it has plane wavefronts, $\vec{k}$ vector of module $\frac{2\pi}{\lambda}$ and direction the one of the wave propagation
The need arises for wavepackets (superposition of plane waves with different amplitudes)

$$\Psi(\vec{r},t) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int d^3\vec{p}\; A(\vec{p}) e^{\frac{i(\vec{r}\cdot\vec{p}-E(\vec{p})t)}{\hbar}}$$

$$A(\vec{p}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int d^3\vec{r}\; \Psi(\vec{r},0)\; e^{-\frac{i\vec{r}\cdot\vec{p}}{\hbar}}$$

where $\vec{p} = \hbar\vec{k}$ (De Broglie) and $E = \hbar\omega = \frac{p^2}{2m}$

(superimposed plane waves have different λ and ν)

Group velocity $v_g = \frac{d\omega(k)}{dk}|_{\bar{k}} = 2\pi \frac{d\nu}{dk}|_{\bar{k}}$ ($\neq v_\Phi = \frac{\omega}{k}$ monochromatic waves, phase velocity)

$$\omega = \frac{\hbar k^2}{2m} \quad \rightarrow \quad v_g = \frac{\hbar \bar{k}}{m} = \frac{\bar{p}}{m} = \bar{v}$$

$$v_p = \frac{dE}{dp} = \frac{\hbar k_p}{m} \qquad \text{(particle)}$$

we want $v_g = v_p$

it is achieved if the wave packet is chosen with $\bar{k} = \frac{m v_p}{\hbar}$

Wave packets and Schrödinger equation. Superposition principle

Achievements with the wavepacket

- location in space
- $v_g = v$ of the particle

we seek the wave equation whose solution is the wavepacket

Conditions

- Linear equation (so that the **superposition principle** applies) $\rightarrow$ it contains the first power of $\Psi, \frac{\partial\psi}{\partial x_i}, \frac{\partial^2\psi}{\partial x_i^2}, \frac{\partial\psi}{\partial t}, \frac{\partial^2\psi}{\partial t^2} \cdots$

Linear $\rightarrow$ If Ψ_1 and Ψ_2 they are solutions of the equation $\Psi = c_1\Psi_1 + c_2\Psi_2$ it is also solution $c_1,\ c_2 \in \mathcal{C}$

Wavepacket = linear combination of plane waves

$$\Downarrow$$

the plane wave must be solution of the wave equation sought
We postulate the Schrödinger equation

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

$$\bigtriangledown^2 \;=\; \triangle \;=\; \sum_i \frac{\partial^2}{\partial x_i^2} \qquad \text{(laplacian operator)}$$

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The Schrödinger equation is valid for nonrelativistic particle of mass m subjected to potential V

Free particle $V = 0 \quad \rightarrow \quad \Psi = e^{i(\vec{k}\cdot\vec{r} - \omega t)}$ is solution of Schrödinger eq. with

$$\omega = \frac{E}{\hbar} \quad ; \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

Matter waves are superimposed linearly as the classical → there should result interference phenomena

(eg, Davisson-Germer, double slit)

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If Ψ_1 and Ψ_2 describe physical situations

$$\Downarrow$$

also $\Psi = c_1\Psi_1 + c_2\Psi_2 \quad ; \quad c_1,\ c_2 \in \mathcal{C}$

Waves are added, not intensities

$$I \propto |\Psi|^2$$

$$\Psi_1 \to I_1 \propto |\Psi_1|^2 \quad ; \quad \Psi_2 \to I_2 \propto |\Psi_2|^2$$

$$\Psi_1,\ \Psi_2 \to I_t \propto |\Psi_1 + \Psi_2|^2$$

interference

$$I_t \neq I_1 + I_2$$

The superposition principle explains interference and diffraction $\to$ we adopt it for quantum mechanics

- If we have a plane wave associated with a free particle moving in one dimension in the direction of increasing x

$$\Psi_1(x,t) = A\ e^{i(kx-\omega t)}$$

- idem moving in one dimension in the direction of decreasing x

$$\Psi_2(x,t) = A\ e^{i(-kx-\omega t)}$$

If in $t = 0$

$$\Psi(x,0) = \Psi_1(x,0) + \Psi_2(x,0) = 2A\cos kx = A\left(e^{ikx} + e^{-ikx}\right)$$

by the principle of superposition of waves they evolve independently in time

$$\Psi(x,t) = A\left(e^{i(kx-\omega t)} + e^{-i(kx+\omega t)}\right)$$

Ψ is complex in general. Intensities $\propto |\Psi|^2$ are real

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