PHOT 222: Quantum Photonics
LECTURE 03

Michaël Barbier, Spring semester (2024-2025)

OVERVIEW OF THE COURSE

week	topic	Serway	Young
Week 1	Relativity	Ch. 39	Ch. 37
Week 2	**Waves and Particles**	**Ch. 40**	**Ch. 38-39**
Week 3	**Wave packets and Uncertainty**	**Ch. 40**	**Ch. 38-39**
Week 4	The Schrödinger equation and Probability		
Week 5	**Midterm exam 1**		
Week 6	Quantum particles in a potential		
Week 7	Harmonic oscillator		
Week 8	Tunneling through a potential barrier		
Week 9	The hydrogen atom, absorption/emission spectra		
Week 10	**Midterm exam 2**		
Week 11	Many-electron atoms		
Week 12	Pauli-exclusion principle		
Week 13	Atomic bonds and molecules		
Week 14	Crystalline materials and energy band structure		

Particle-wave duality

ELECTROMAGNETIC WAVES AS PARTICLES

- Electromagnetic waves can act as particles: **photons**
  - Energy $hf = \frac{hc}{\lambda}$
  - Momentum $\frac{hf}{c} = \frac{h}{\lambda}$
  - Described as particles: Photoelectric effect, Compton effect, etc.

- BUT what about diffraction of light ? This is **wave-like** behavior
  - What is the wavelength or frequency of a particle?
  - How large is a photon?

- Light is both particle and wave at the same time ?

PARTICLES WITH WAVE-LIKE BEHAVIOR

1923: Louis de Broglie: All matter is both wave and particle

- Every particle has an associated wave
  - **de Broglie wavelength** $\lambda = \frac{h}{p} = \frac{h}{mu}$ or if relativistic $\lambda = \frac{h}{\gamma mu}$
  - Associated **frequency** $f = \frac{E}{h}$ where E is the **total energy**

- Principle of complementarity:

  The wave and particle models of light and matter complement each other

ELECTRONS WITH WAVE-LIKE BEHAVIOR

- Consider an electron that has velocity $u = 1.0 \times 10^7$ m/s and mass $m_e = 9.11 \times 10^{-31}$ kg:
  - What is the associated de Broglie wavelength?

$$\lambda = \frac{h}{m_e u} = \frac{6.624 \times 10^{-34}\ \mathrm{J \cdot s}}{9.11 \times 10^{-31}\ \mathrm{kg}\ \ 1.0\ \times 10^{7} \mathrm{m/s}} \approx 7.27 \times 10^{-11}\ \mathrm{m}$$

Since 1 J = 1 kg·m^2·s^{-2} the unit of the wavelength is meter

The resulting wavelength is on the order of an Angstrom

ELECTRON DIFFRACTION: DAVISSON-GERMER EXPERIMENT

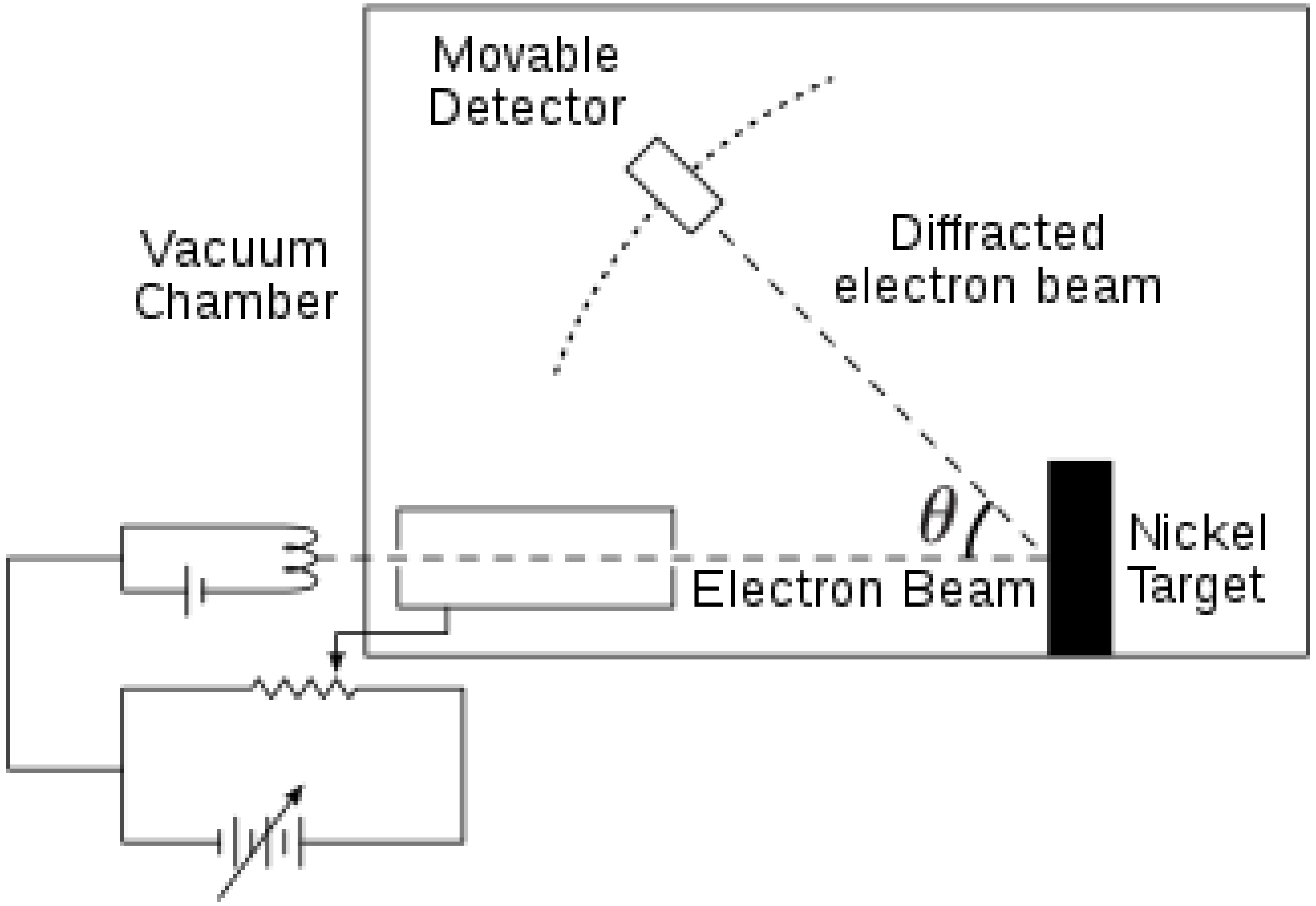
- 1927 Clinton Davisson and Lester Germer, and Thomson performed independent electron diffraction experiments

- Single crystal of Nickel:

  periodic structure

- Diffraction peaks found

- **Similar to x-ray diffraction**



X-RAY DIFFRACTION: SHORT HISTORY

- In 1895 Rontgen discovers x-rays

2. ***Ueber eine neue Art von Strahlen;***
von W. C. Röntgen.

(Zweite Mittheilung.)

Aus den Sitzungsber. der Würzburger Physik.-Medic. Gesellschaft. Jahrg. 1895.

Da meine Arbeit auf mehrere Wochen unterbrochen werden muss, gestatte ich mir im Folgenden einige neue Ergebnisse schon jetzt mitzutheilen.

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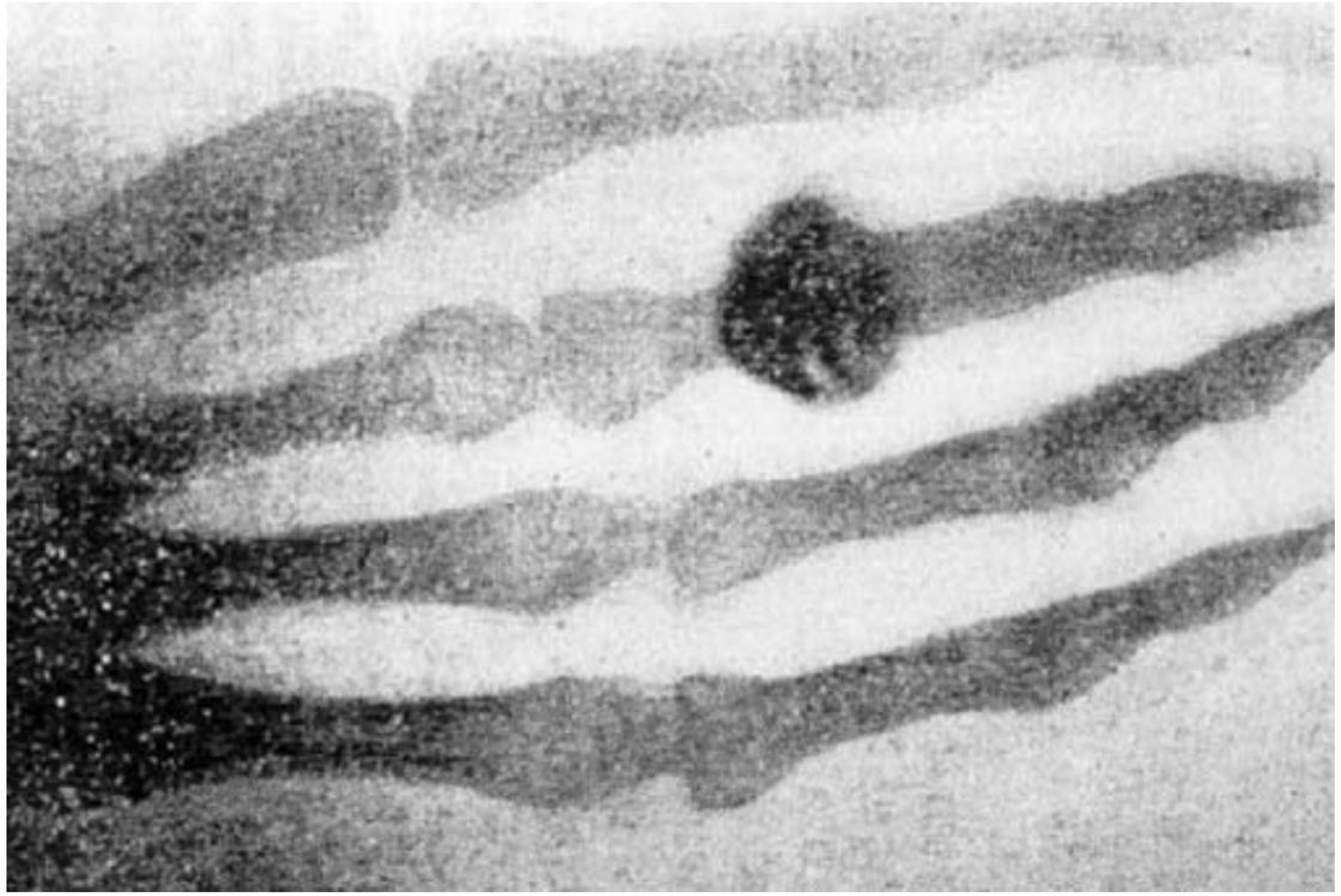
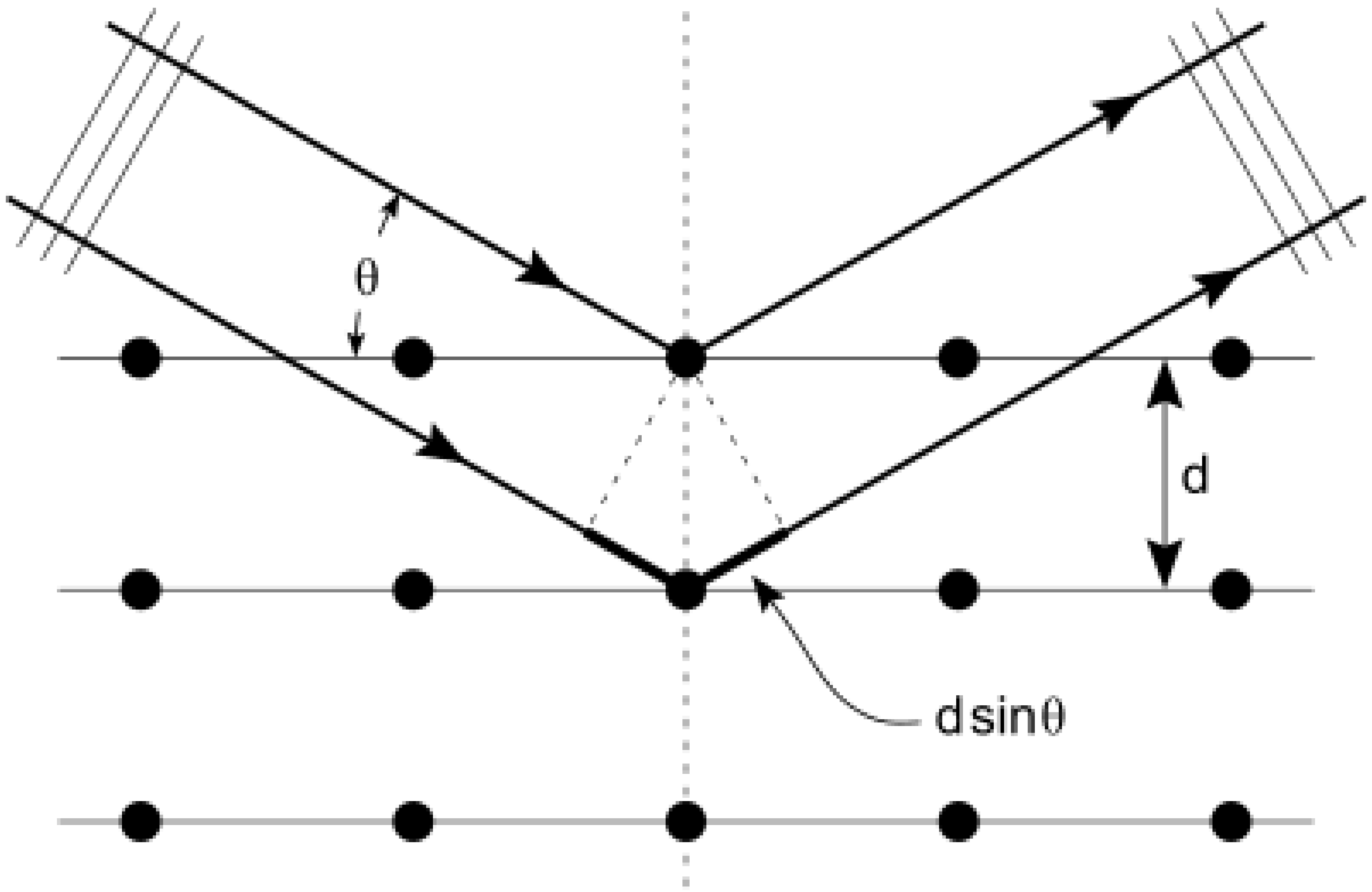


FIGURE 2 One of the first pictures using X-rays: the hand and ring of Röntgen's wife

X-RAY DIFFRACTION: SHORT HISTORY

- In 1895 Rontgen discovers x-rays
- In 1912 Von Laue found that x-rays diffract at crystals
- In 1913 Bragg formulates his Bragg equation:

$$n\lambda = 2d\sin(\theta)$$



Relates diffraction angle $\boldsymbol{\theta}$ to crystal plane distance $\boldsymbol{d}$ and $\boldsymbol{\lambda}$

X-RAY DIFFRACTION: SHORT HISTORY

- XRD experiments
- Bragg equation:

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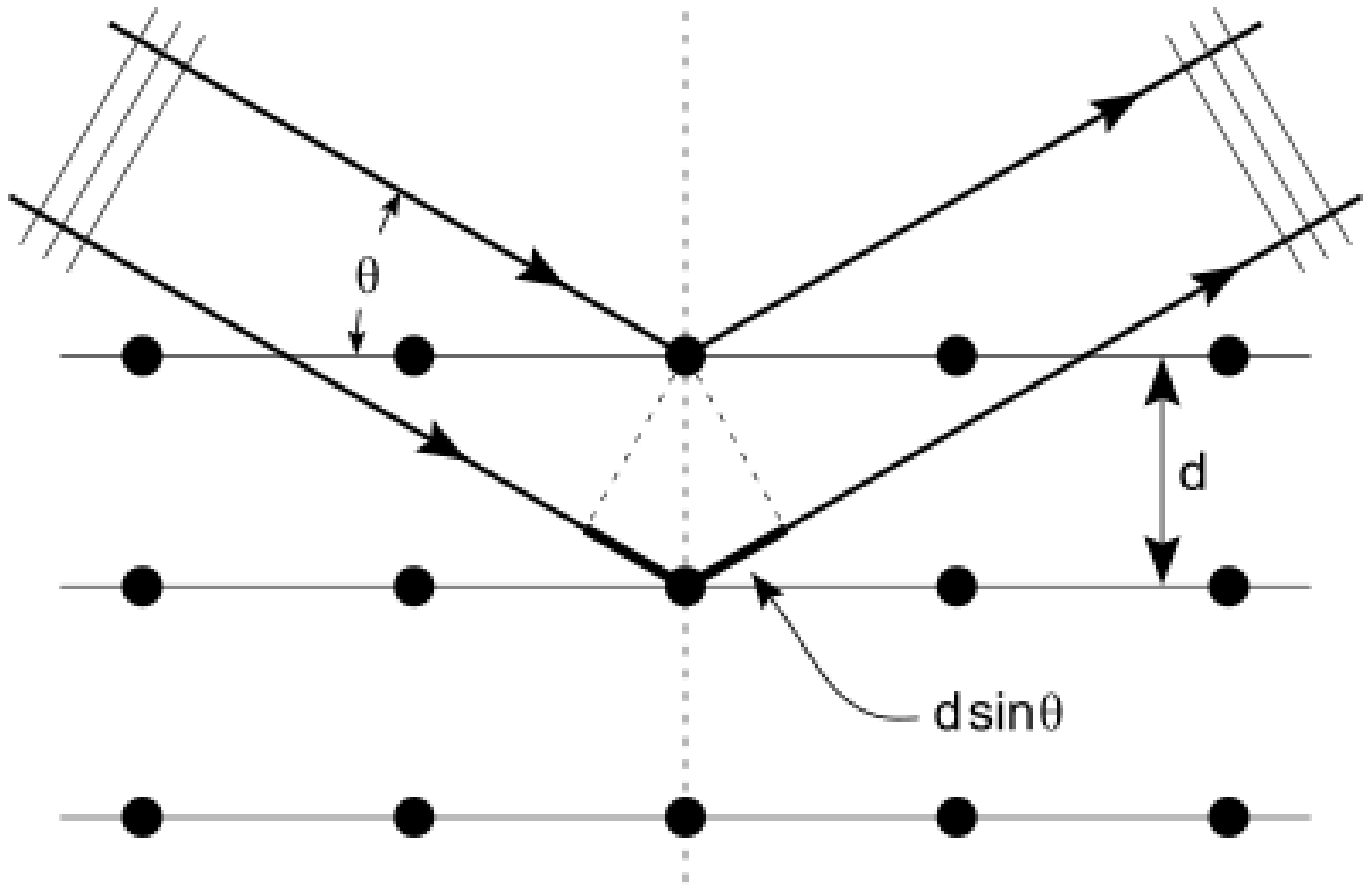
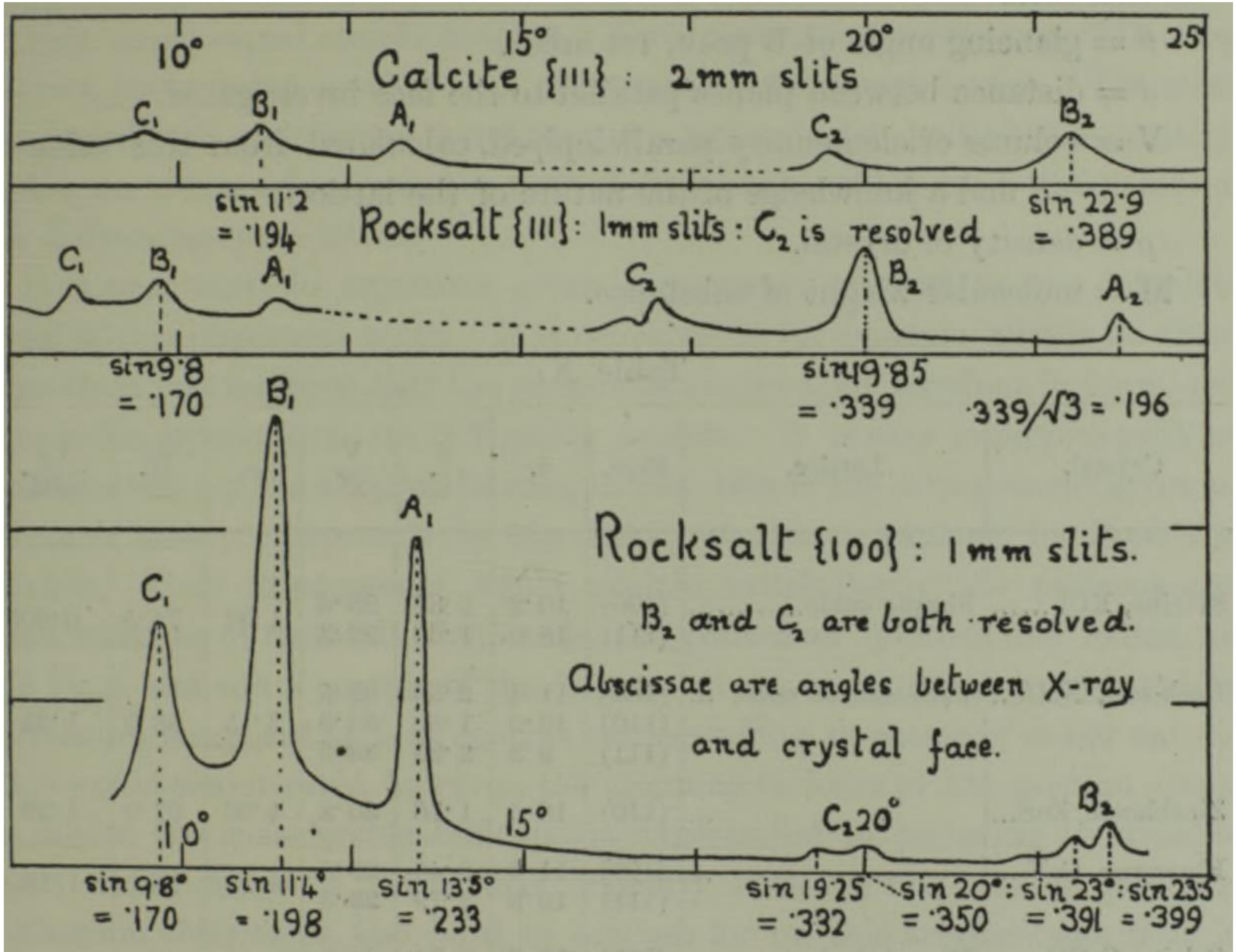




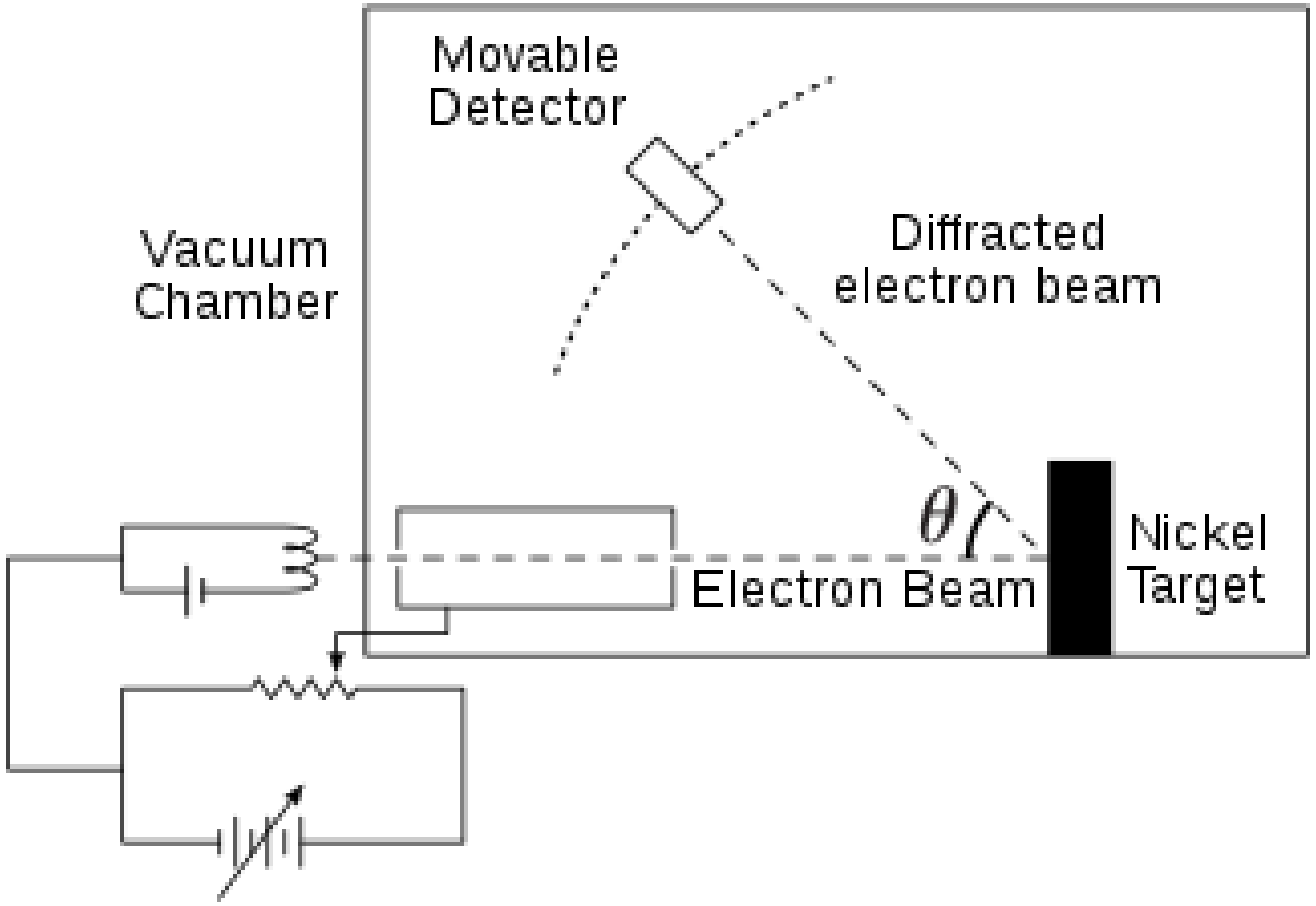
ELECTRON DIFFRACTION: DAVISSON-GERMER EXPERIMENT

- 1927 Clinton Davisson and Lester Germer, and Thomson performed independent electron diffraction experiments

- Single crystal of Nickel:
  periodic structure

- Diffraction peaks found

- Electrons of $54\ \mathrm{eV} \rightarrow\ 50°$



ELECTRON DIFFRACTION: DAVISSON-GERMER EXPERIMENT

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Letters to the Editor.

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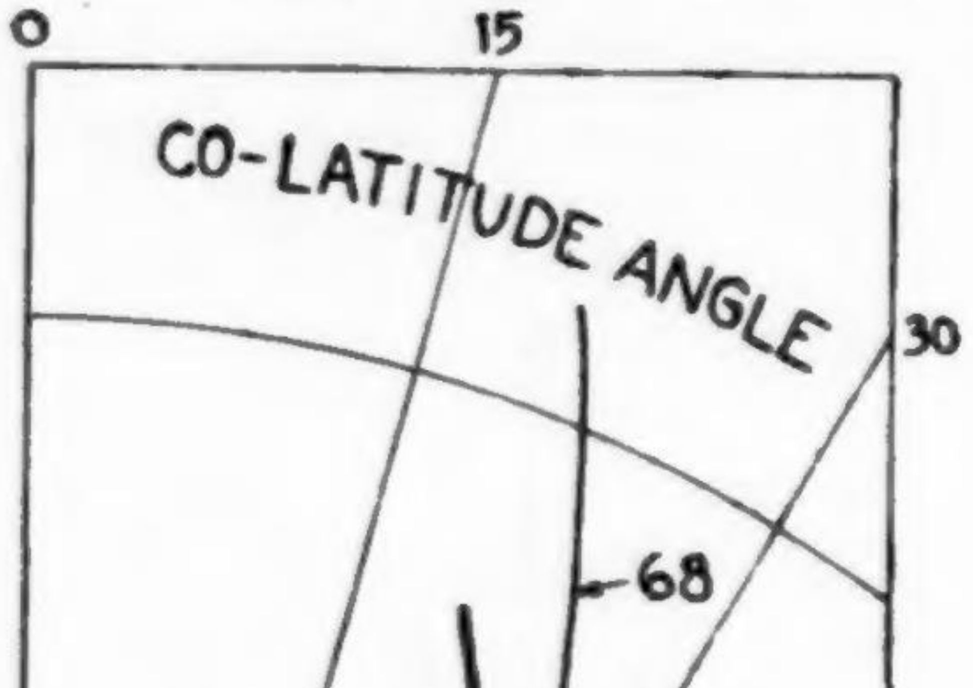
The Scattering of Electrons by a Single Crystal of Nickel.

In a series of experiments now in progress, we are directing a narrow beam of electrons normally against a target cut from a single crystal of nickel, and are measuring the intensity of scattering (number of electrons per unit solid angle with speeds near that of the bombarding electrons) in various directions in front of the target. The experimental arrangement is such that the intensity of scattering can be measured

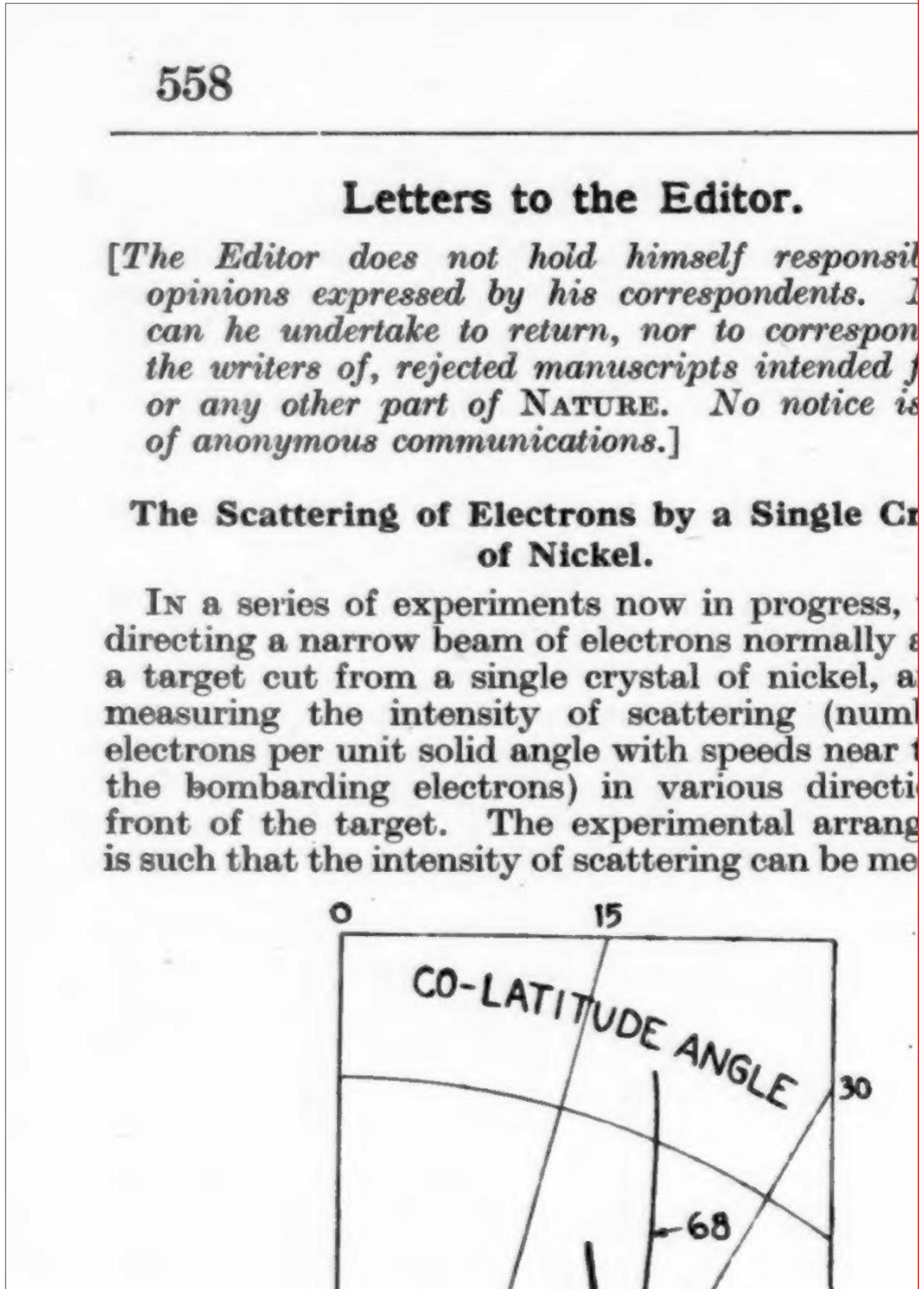


target. There are six such azimuths, and any one of these will be referred to as a {110}-azimuth. It follows from considerations of symmetry that if the intensity of scattering exhibits a dependence upon azimuth as we pass from a {100}-azimuth to the next adjacent {111}-azimuth (60°), the same dependence must be exhibited in the reverse order as we continue on through 60° to the next following {100}-azimuth. Dependence on azimuth must be an even function of period $2\pi/3$.

In general, if bombarding potential and azimuth are fixed and exploration is made in latitude, nothing very striking is observed. The intensity of scattering increases continuously and regularly from zero in the plane of the target to a highest value in co-latitude 20°, the limit of observations. If bombarding potential and co-latitude are fixed and exploration is made in azimuth, a variation in the intensity of scattering of the type to be expected is always observed, but in general this variation is slight, amounting in some cases to not more than a few per cent. of the average intensity. This is the nature of the scattering for bombarding potentials in the range from 15 volts to near 40 volts.

At 40 volts a slight hump appears near 60° in the co-latitude curve for azimuth-{111}. This hump develops rapidly with increasing voltage into a strong spur, at the same time moving slowly upward toward the incident beam. It attains a maximum intensity in co-latitude 50° for a bombarding potential of 54 volts, then decreases in intensity, and disappears

ELECTRON DIFFRACTION:



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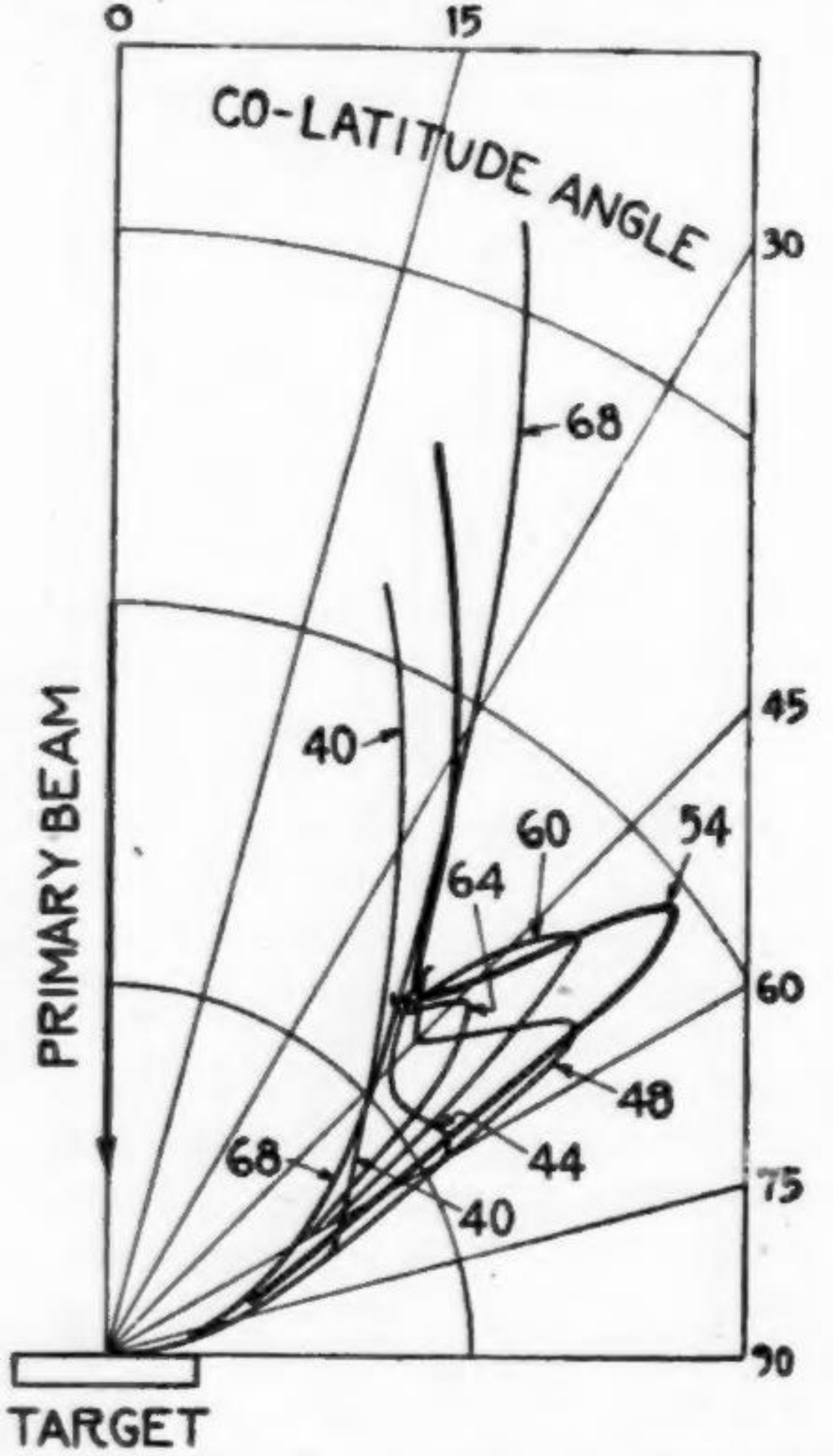
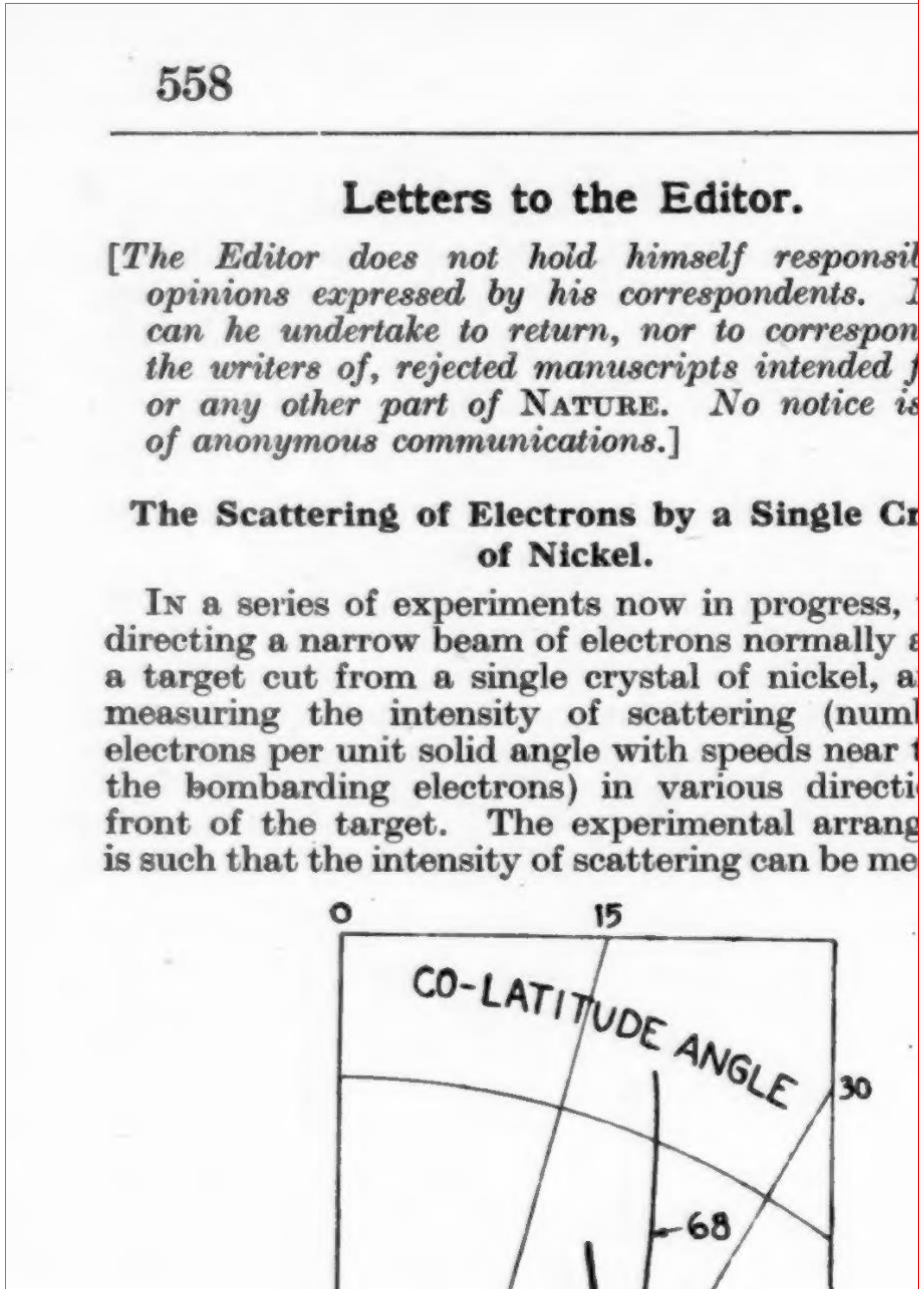


FIG. 1.—Intensity of electron scattering vs. co-latitude angle for various bombarding voltages—azimuth-{111}-330°.

ELECTRON DIFFRACTION:



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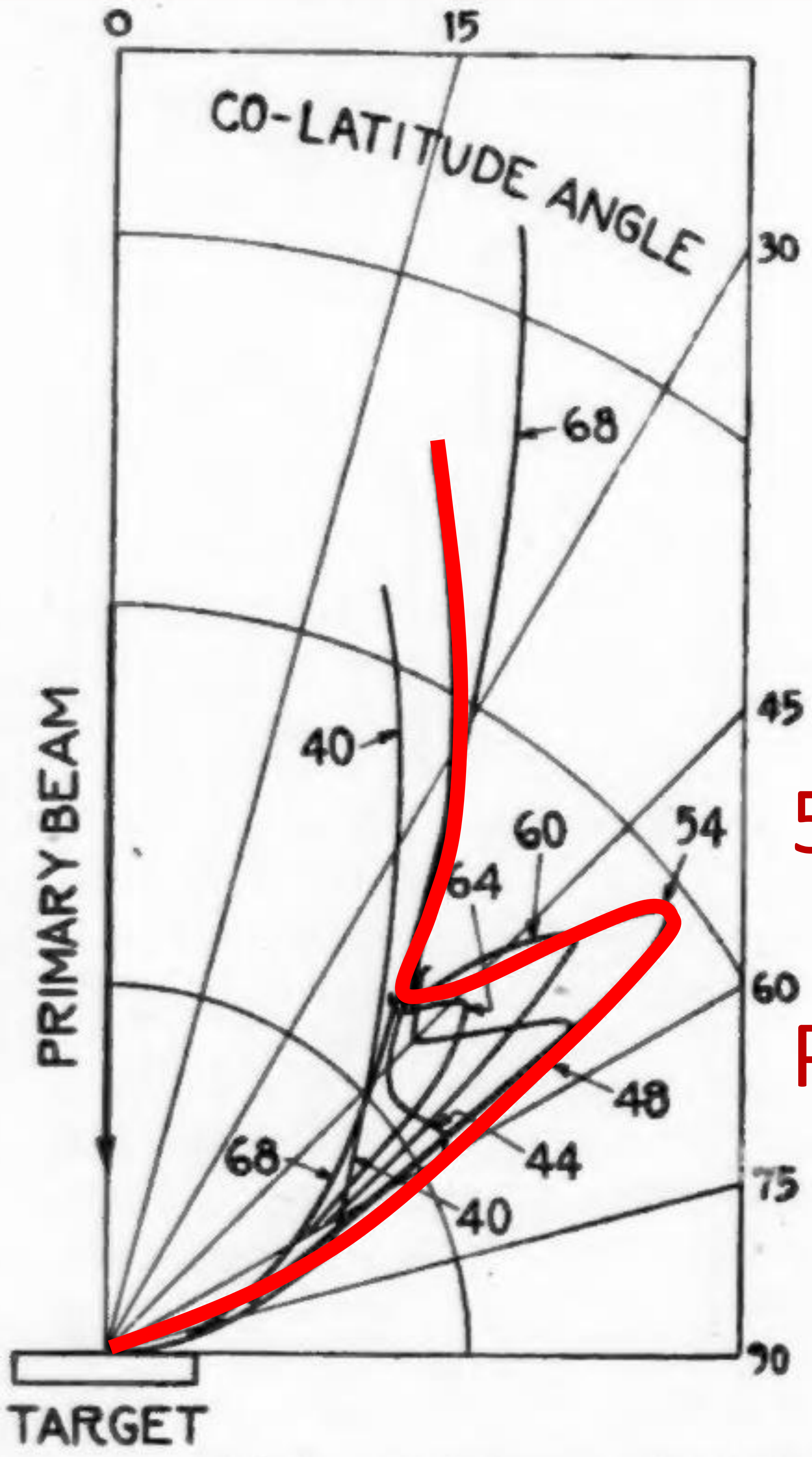


54 eV

Peak at 50º

FIG. 1.—Intensity of electron scattering vs. co-latitude angle for various bombarding voltages—azimuth-{111}-330°.

ELECTRON DIFFRACTION: DAVISSON-GERMER EXPERIMENT

- 1927 Clinton Davisson and Lester Germer, and Thomson performed independent electron diffraction experiments

$$54\ \text{eV}, \qquad 50° \ \rightarrow \ \theta = \frac{130°}{2} = 65°$$

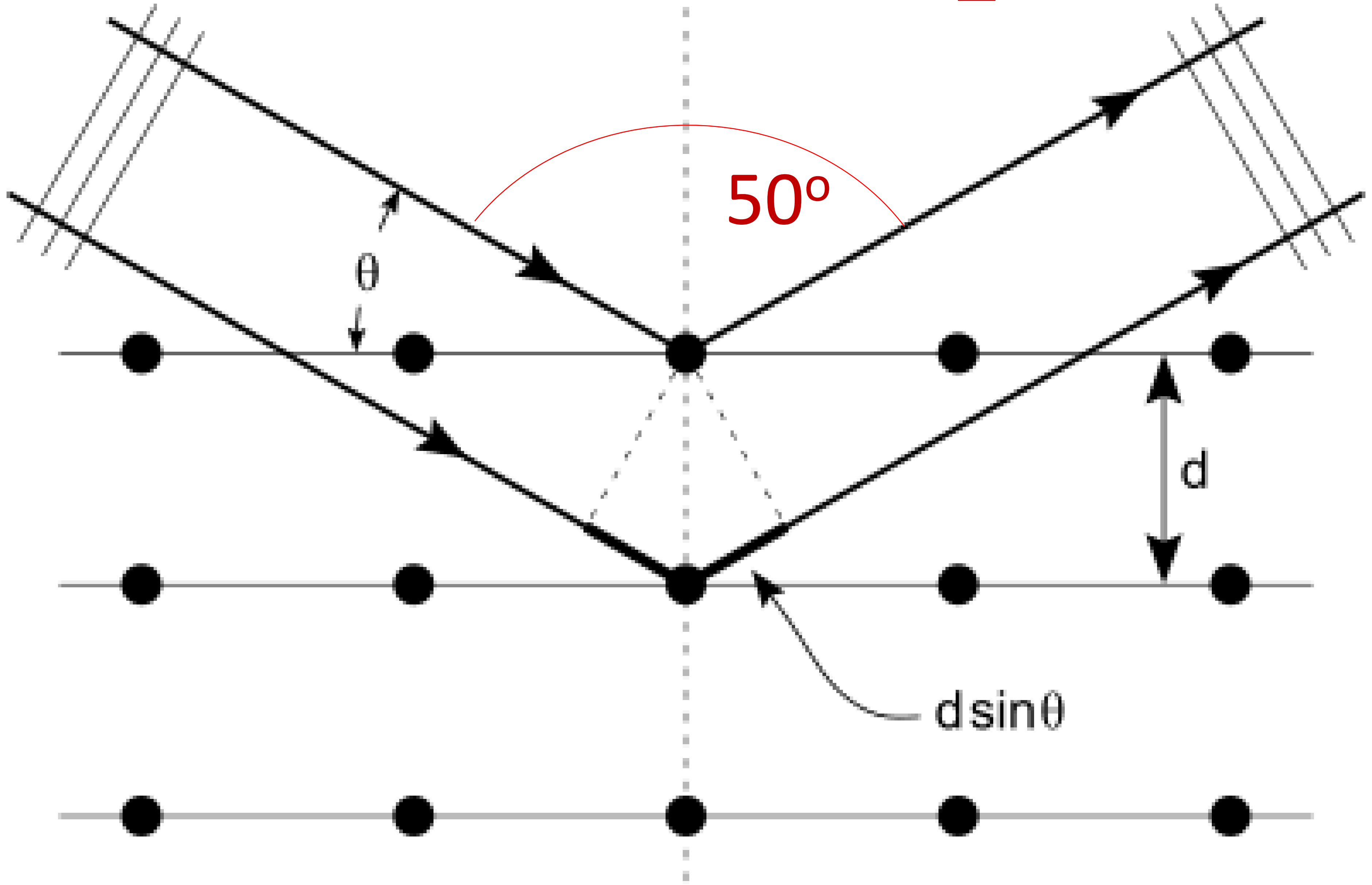
- Single crystal of Nickel:

  periodic structure

- Bragg equation:

  $$n\lambda = 2d\sin(\theta)$$

- x-ray diffraction: $\mathrm{d} = 0.091\ \mathrm{nm}$



ELECTRON DIFFRACTION: DAVISSON-GERMER EXPERIMENT

- x-ray diffraction tells us that:

$$\lambda = 2d\sin(\theta) = 2\,(0.091\,\text{nm}) \times \sin(65°) = 0.165\,\text{nm}$$

- De Broglie:

$$\lambda = \frac{h}{\gamma m_e u}$$

$$\approx \frac{h}{m_e u} = \frac{h}{\sqrt{2 m_e K}} = \frac{6.63\times10^{-34}\ \text{J}\cdot\text{s}}{\sqrt{2\ (9.1\times10^{-31})\ (54\ eV)\left(1.6\times10^{-19}\frac{\text{J}}{\text{eV}}\right)}} = 0.166\,\text{nm}$$

ELECTRON DIFFRACTION: DAVISSON-GERMER EXPERIMENT

- x-ray diffraction tells us that:

$$\lambda = 2d\sin(\theta) = 2\,(0.091\text{ nm}) \times \sin(65°) = 0.165\text{ nm}$$

- De Broglie: $E = K + m_e c^2 = \gamma m_e c^2$

$$\lambda = \frac{h}{\gamma m_e u} \quad \text{where } K\ (54\text{ eV}) \ll m_e c^2 (0.5\text{ MeV}) \Rightarrow \gamma \approx 1$$

$$\approx \frac{h}{m_e u} = \frac{h}{\sqrt{2 m_e K}} = \frac{6.63\times10^{-34}\text{ J}\cdot\text{s}}{\sqrt{2\ (9.1\times10^{-31})\,(54\ eV)\left(1.6\times10^{-19}\frac{\text{J}}{\text{eV}}\right)}} = 0.166\text{ nm}$$

ELECTRON MICROSCOPY

- In 1873 **Abbe diffraction limit** in light microscopy :

$$\text{Resolution } \Delta = \frac{\lambda}{2\, n \,\sin\theta} = \frac{\lambda}{2\text{NA}} \approx \frac{\lambda}{2.8}$$

- Visible light is in the interval: 380 - 700 nm

$$\text{Resolution } \Delta > 135 \text{ nm}$$

- Electrons can have very small de Broglie wavelengths
- Previously: a low energy of 54 eV resulted in $\lambda = 0.166 \text{ nm}$
- Formula for TEM: $\Delta \approx \frac{0.753}{\theta \sqrt{V}}$ with V the acceleration voltage

ELECTRON MICROSCOPY

- Electrons can have very small de Broglie wavelengths

- 2002 model at EMAT, University of Antwerp: resolution = 0.135 nm

ELECTRON MICROSCOPY

- Electrons can have very small de Broglie wavelengths
- 2002 model at EMAT, University of Antwerp: resolution = 0.135 nm
- 2010 model at EMAT, University of Antwerp: resolution = 0.070 nm

SUMMARY PARTICLE-WAVE DUALITY

- Electrons show wave-like behavior when accelerated
- De Broglie: particles-wave duality
  - Associated wave with a particle
  - Wavelength $\lambda = \frac{h}{\gamma m_e u} \approx \frac{h}{m_e u}$
  - Proof by electron diffraction experiments
- Electron microscopy: wave-like behavior electrons

Probability, Wave packets, and uncertainty

WAVES DESCRIBING PROBABILITY OF A PARTICLE

- What are the de Broglie waves associated with the particles ?
- When we measure accurately, we can measure single photons

In 1926 Max Born: Probability interpretation:

Wave is determined by the wave function $\Psi(x, y, z, t)$

Probability to find a particle at position (x, y, z) at time t is proportional to $|\Psi(x, y, z, t)|^2$

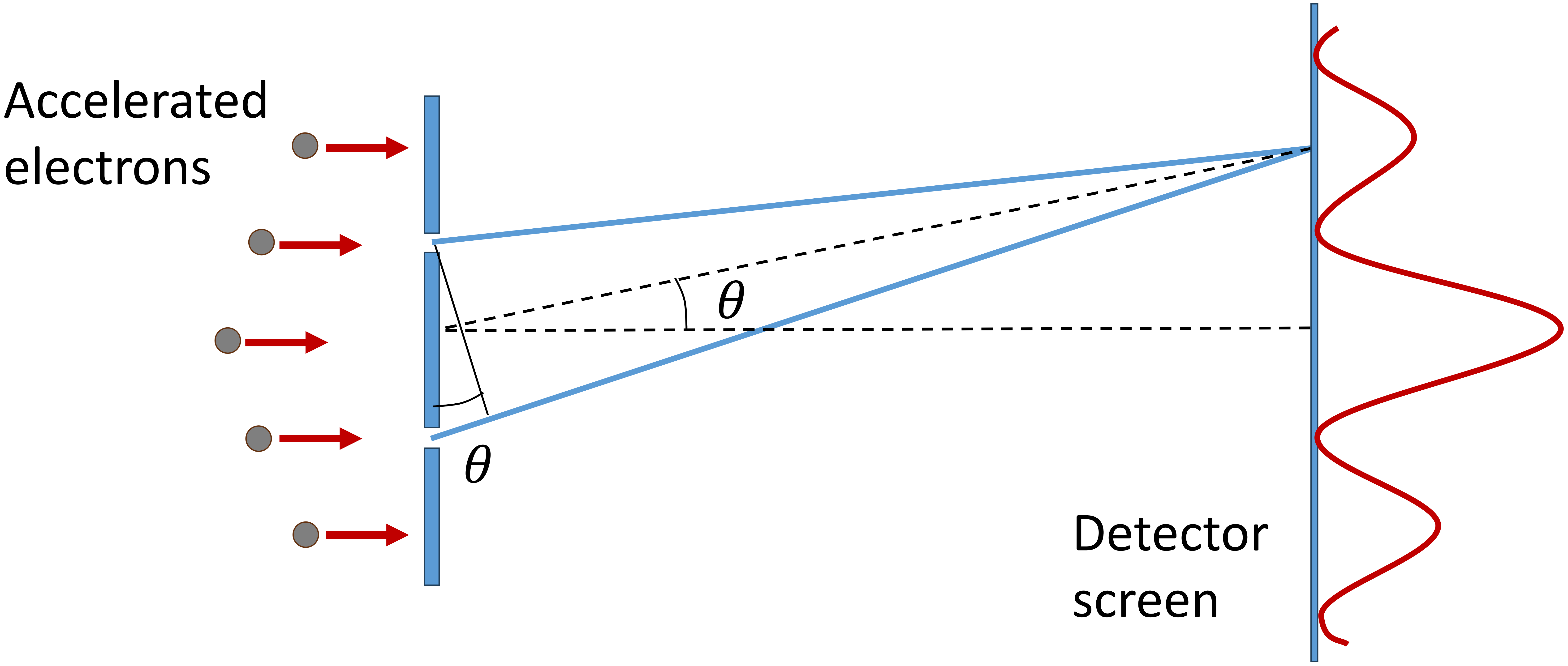
WAVES DESCRIBING PROBABILITY OF A PARTICLE

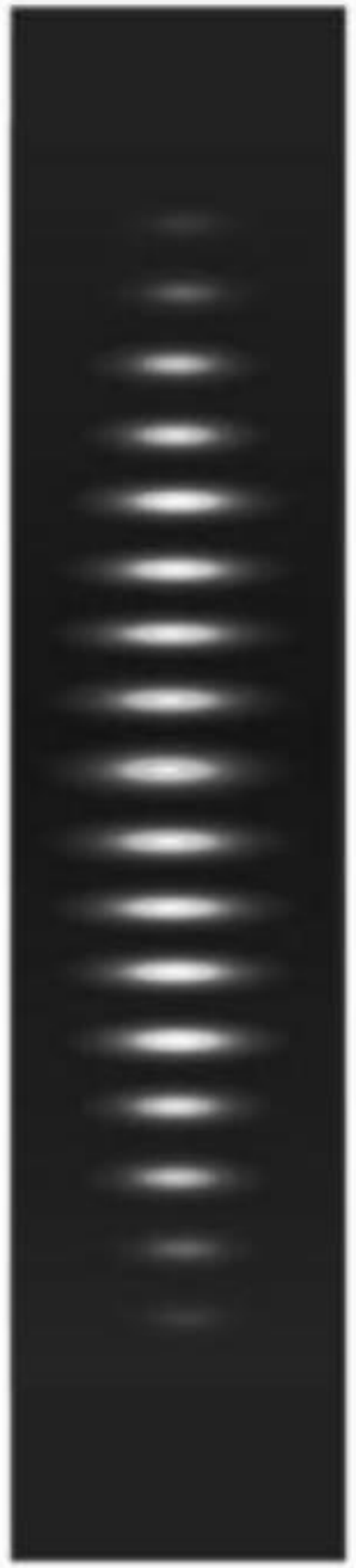
Wave is determined by the wave function $\Psi(x, y, z, t)$

Probability to find a particle at position (x, y, z) at time t is proportional to $|\Psi(x, y, z, t)|^2$

DOUBLE SLIT EXPERIMENTS WITH SINGLE ELECTRONS

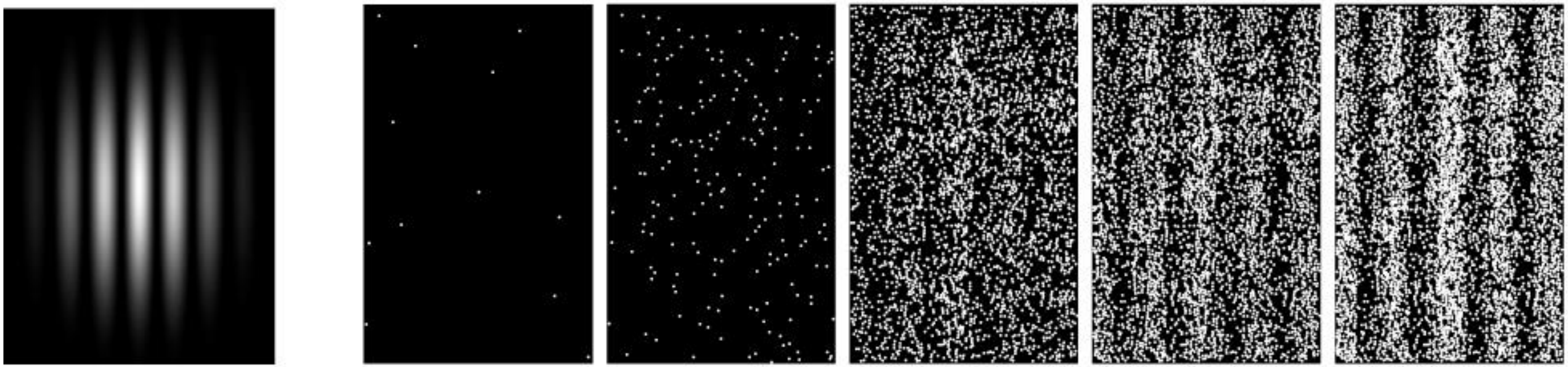
- Electrons accelerated ➡ corresponding de Broglie wavelength
- When reducing number of electrons: “single electrons”





DOUBLE SLIT EXPERIMENTS WITH SINGLE ELECTRONS

- Electrons arrive one by one
- probability to find an electron at coordinates $(x, y, t) = |\Psi(x, y, t)|^2$
- Higher photon densities ⇨ diffraction pattern: $|\Psi(x, y, t)|^2$
- “Similar” to the intensity of electric waves: $\mathrm{I} \propto E^2$



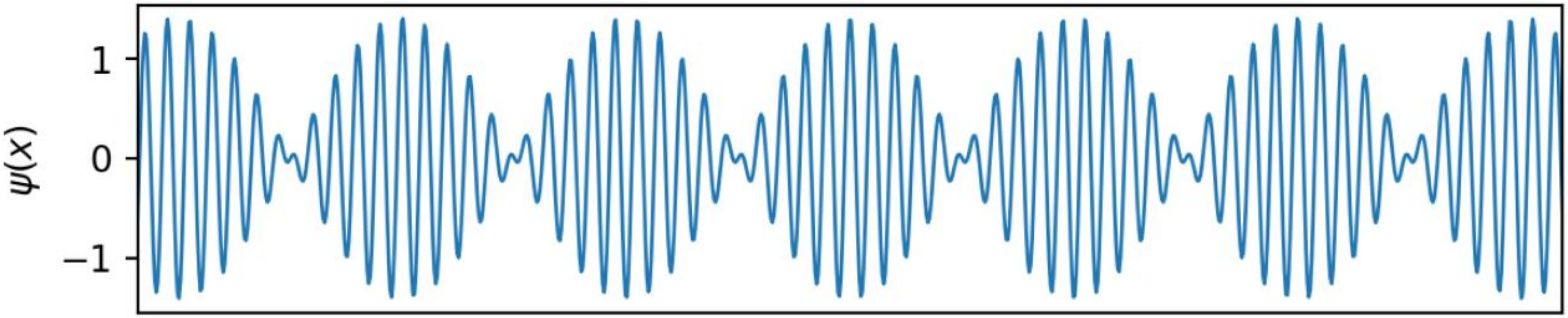
WAVE PACKETS

- A single wave can be written:

$$y = \cos(kx - \omega t) \text{ with } k = \frac{2\pi}{\lambda},\ \omega = 2\pi f$$

- Superposition of 2 cosine waves:

$$y_1 + y_2 = \cos(k_1 x - \omega_1 t) + \cos(\mathrm{k_2 x} - \omega_2 t)$$



WAVE PACKETS

- Goniometric identity:

$$\cos(a) + \cos(\mathrm{b}) = 2\cos\left(\frac{\mathrm{a}-\mathrm{b}}{2}\right)\cos\left(\frac{\mathrm{a}+\mathrm{b}}{2}\right)$$

- Superposition of 2 cosine waves:

$$\begin{aligned} y_1 + y_2 &= \cos(k_1 x - \omega_1 t) + \cos(\mathrm{k}_2\mathrm{x} - \omega_2 t) \\ &= 2\cos(\Delta k\, x - \Delta\omega\, t) \times \cos\left((k_1+k_2)x - (\omega_1+\omega_2)t\right) \end{aligned}$$

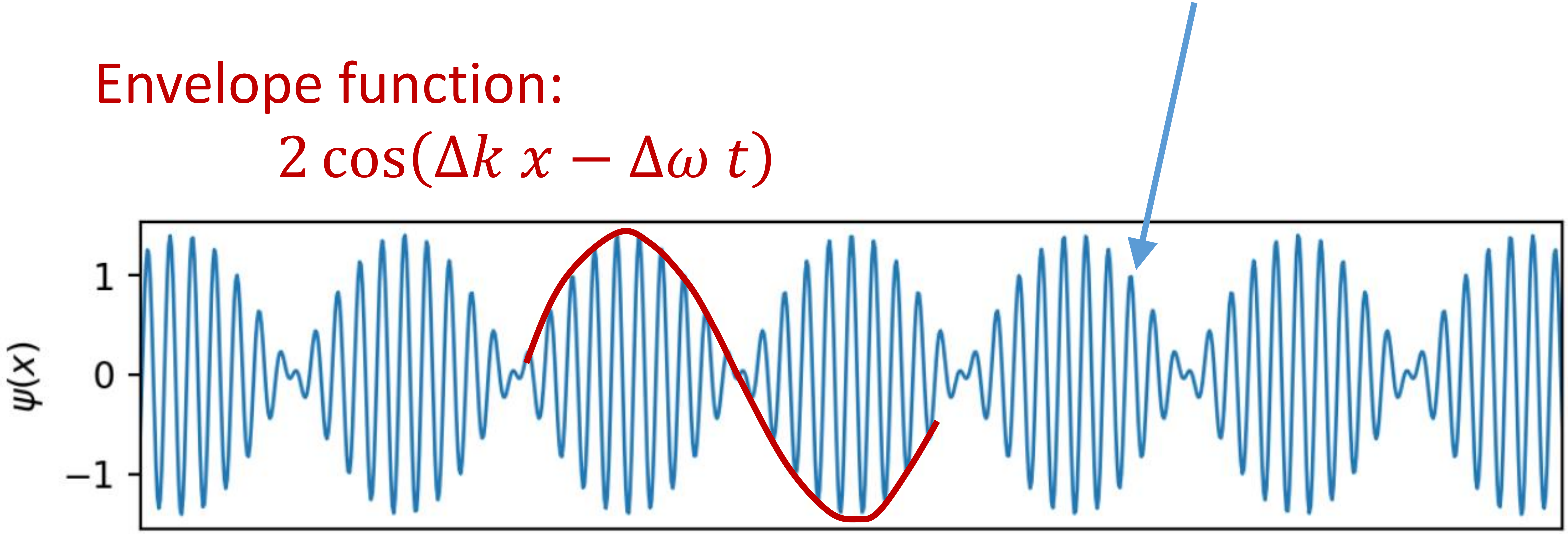
WAVE PACKETS

- Superposition of 2 cosine waves:

$$\Psi(x,t) = 2\cos(\Delta k\, x - \Delta\omega\, t) \times \cos\big((k_1+k_2)x - (\omega_1+\omega_2)t\big)$$

Envelope function:

$$2\cos(\Delta k\, x - \Delta\omega\, t)$$



WAVE PACKETS

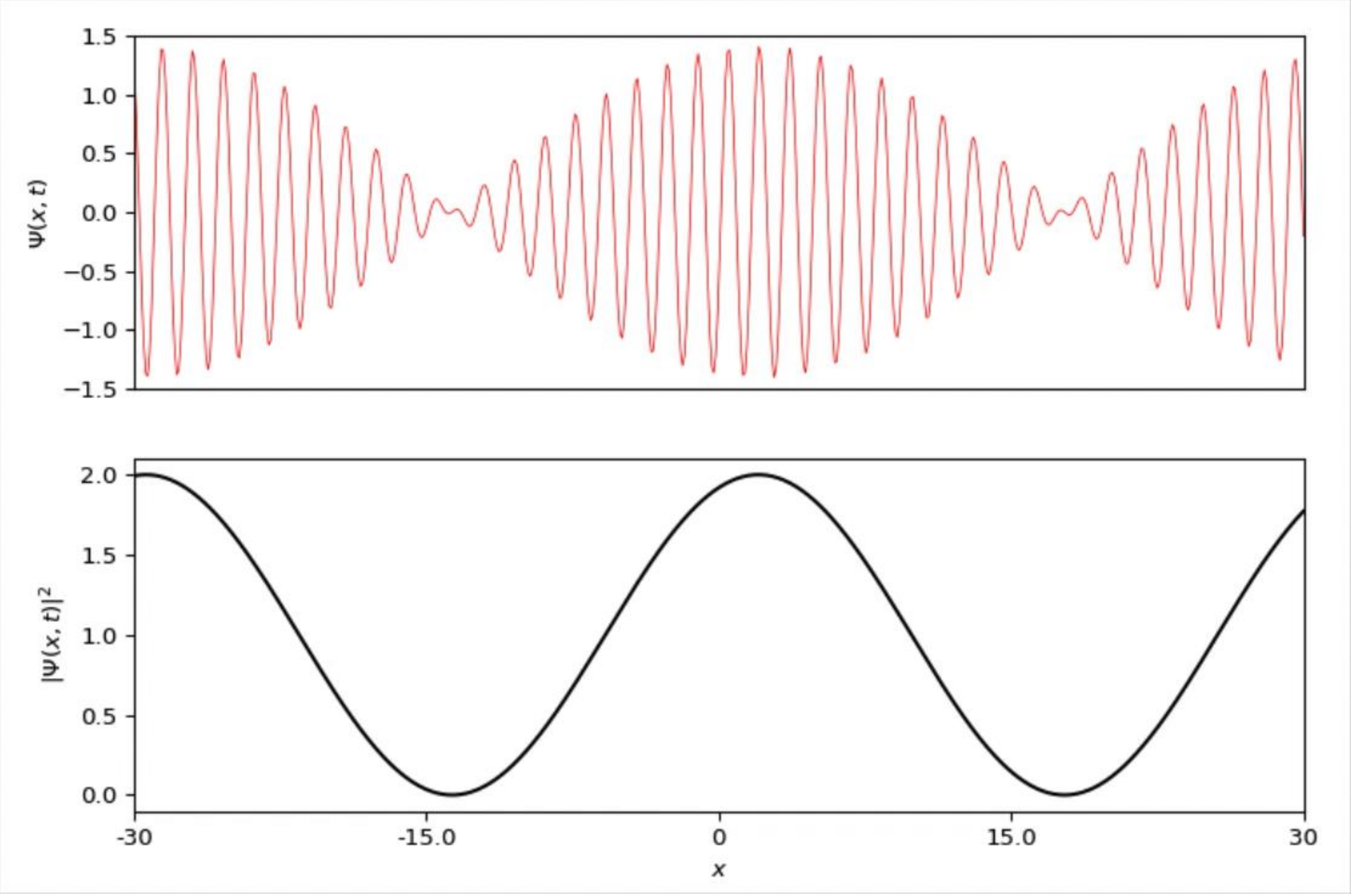
- Superposition

- Phase velocity:

$$v_{\text{phase}} = \frac{\omega}{k}$$

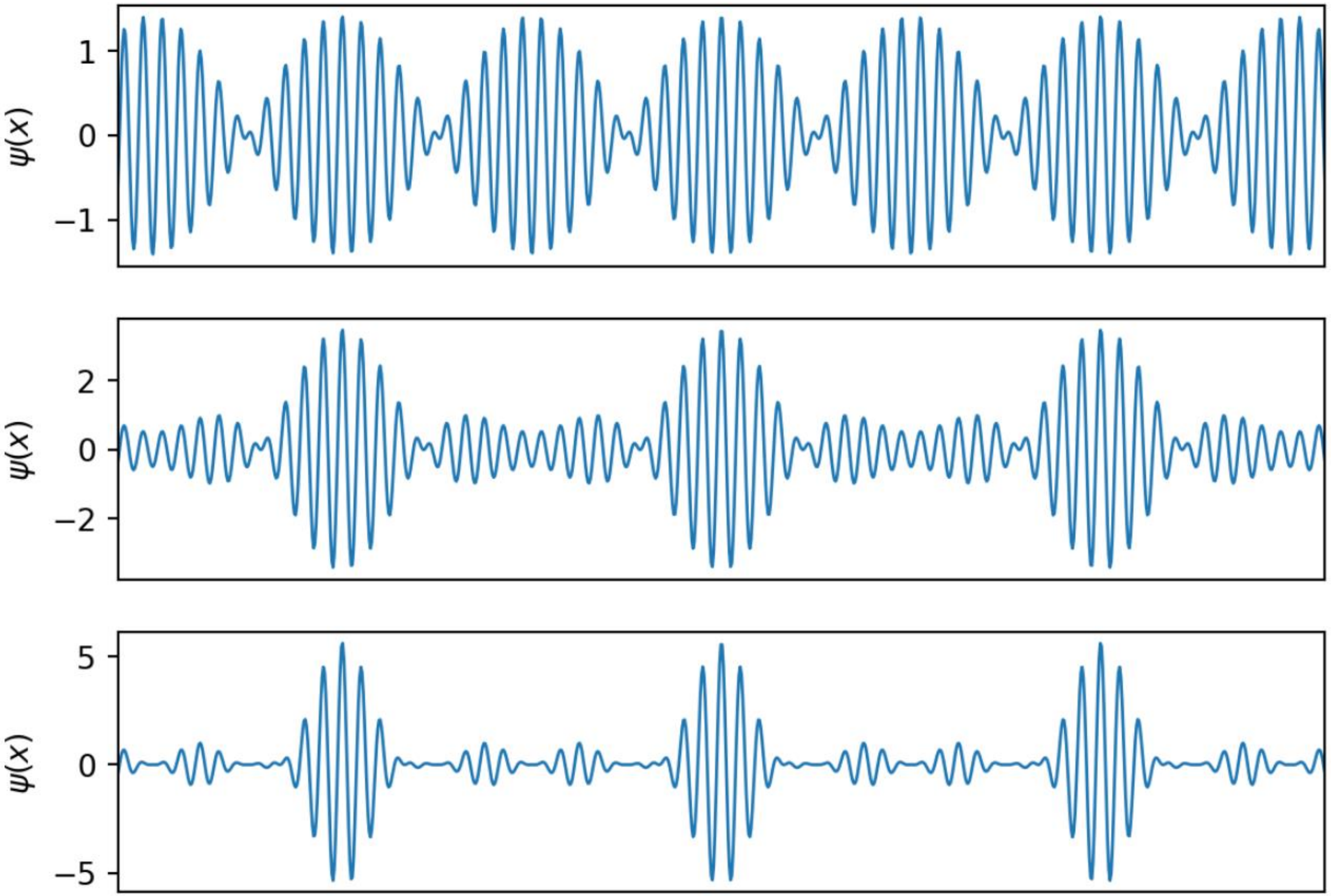
- Group velocity:

$$v_{\text{group}} = \frac{\Delta\omega}{\Delta k}$$



WAVE PACKETS

- Superposition of waves
- Many waves can form a wave packet
- Localized wave



GROUP VELOCITY OF WAVE PACKETS

- Superposition of many waves

$$v_{\text{group}} = \frac{\Delta\omega}{\Delta k} \rightarrow \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{d(\hbar\omega)}{d(\hbar k)} \qquad \text{where } \hbar = \frac{h}{2\pi}.$$

- Numerator: $\hbar\omega = \frac{h}{2\pi} 2\pi f = hf = E$
- Denominator: $\hbar k = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \frac{h}{\lambda} = p$

$$\Rightarrow \quad v_{\text{group}} = \frac{dE}{dp} = \frac{d\left(\frac{p^2}{2m}\right)}{dp} = \frac{p}{m} = u$$

- So group velocity equals the particle associated with the wave

UNCERTAINTY RELATION

- In 1927 Heisenberg introduces his uncertainty principle:

If position and momentum of a particle are measured simulaneously with uncertainties Δx and Δp_x then:

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

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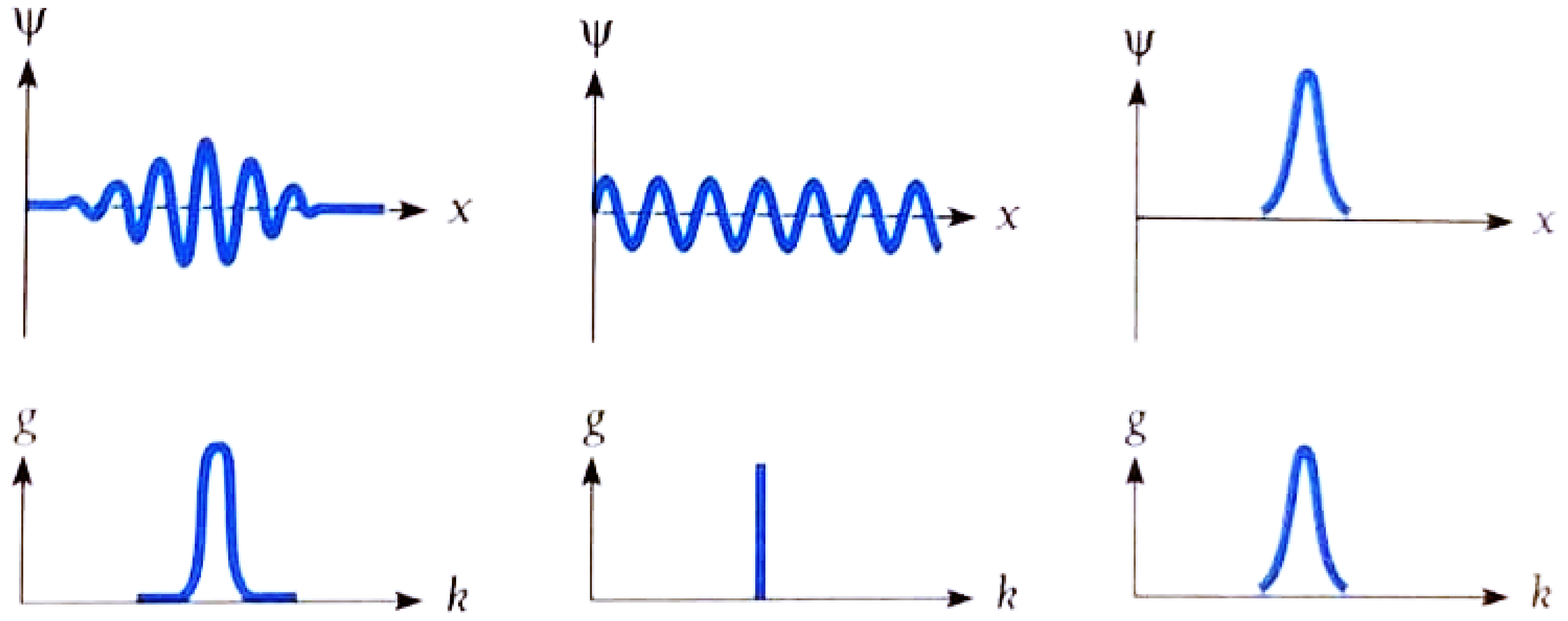

SUMMARY PROBABILITY & WAVE FUNCTIONS

- Wave function $\Psi(x, y, z, t)$ interacts in a wave-like manner
- Probability to find a particle determined by the probability density function $|\Psi(\mathrm{x}, \mathrm{y}, \mathrm{z}, \mathrm{t})|^2$
- Wave packets describe “localized” particles
- Uncertainty relation: impossible to know both velocity and location