

- Wave Packets and Group Velocity
- λ : Order of Magnitude
- Evidence for wave Behavior of Particle
- The "old Quantum Theory"



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I₃ Particle Waves

Recap:

I_{3,1} De Broglie Hypothesis:

Particle: Energy E
Momentum p



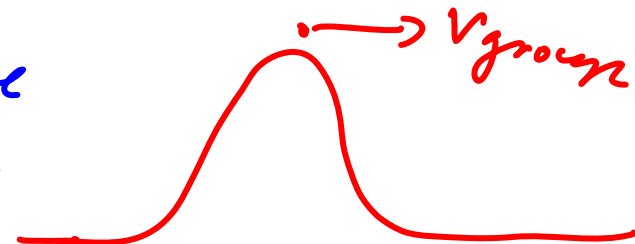
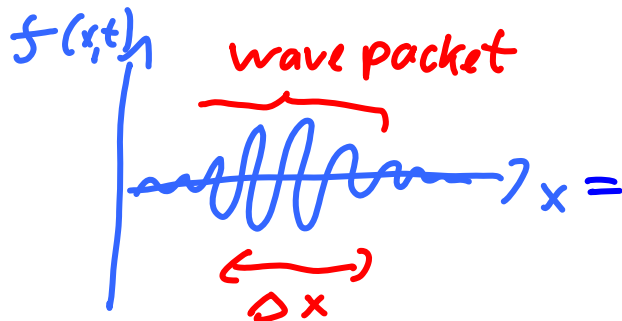
associated wave
 $\lambda = \frac{h}{p}$ $\nu = \frac{E}{h}$

I_{3,3} Superposition of Particle Waves

$$f(x,t) = \text{Re} \left\{ e^{i[k_0 x - \omega(k_0)t]} \int \phi(s) e^{is \left(x - \frac{d\omega}{dk} \Big|_{k_0} t \right)} ds \right\}$$

infinite plane wave:
crests move at
 $v_{\text{phase}} = \frac{\omega}{k} = \frac{c^2}{v}$

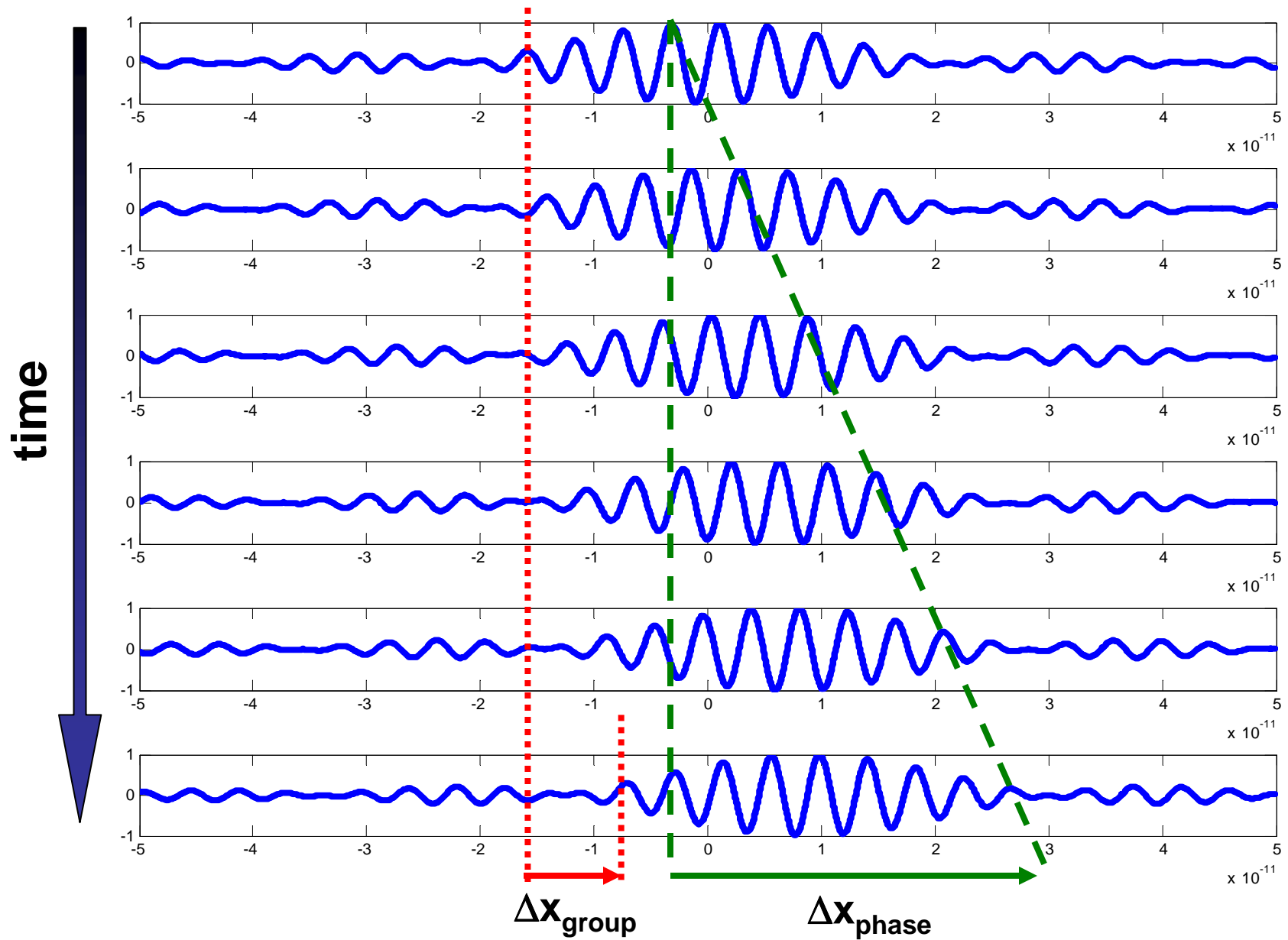
envelope function
travels at group velocity
 $v_{\text{group}} = \frac{d\omega(k)}{dk} \stackrel{!}{=} v_{\text{particle}}$



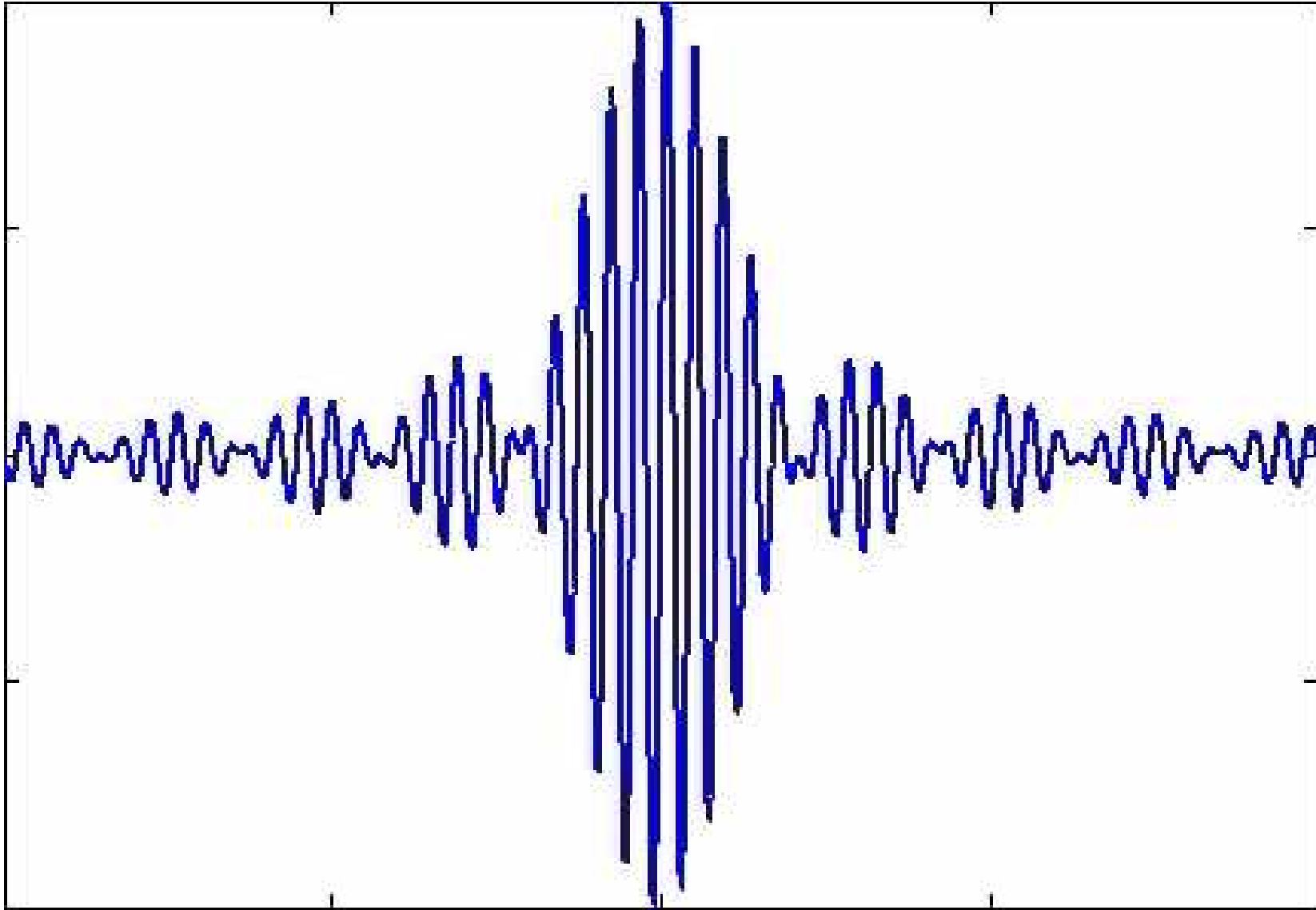
Conclusion:

- wave packet associated with "localized" particle:
 - =) position of envelope function (max. wave amplitude) matters
 - =) group velocity matters, not phase velocity
 - =) localized wave packet \Leftrightarrow momentum of particle is not well defined (uncertainty)
(small $\Delta x \rightarrow$ large Δp_x)
 - =) see free particle in Schrödinger's QM

Example: $v_{\text{group}} = v_{\text{particle}} = c/2$ $v_{\text{phase}} = c^2/v = 2c$



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The envelope function of the wave packet associated with a localized particle should be related to...

- A. The size of the particle (smaller size -> shorter envelope function)**
- B. The range of space in which the particle might be found if its position would be measured**
- C. Something else**

I_{3,4} Group and Phase Velocity for de Broglie's Particle Waves:

phase velocity: $v_{ph} = \frac{\omega}{k} = \lambda \nu = \frac{c^2}{v}$ $v \leftarrow$ speed of particle

group velocity: $v_{group} = \frac{d\omega(k)}{dk} \Rightarrow$ need $\omega(k)$

$$\begin{aligned} \omega &= 2\pi\nu = 2\pi \frac{E}{h} = \frac{2\pi}{h} \sqrt{p^2 c^2 + m_0^2 c^4} = \frac{2\pi}{h} \sqrt{\frac{h^2}{\lambda^2} c^2 + m_0^2 c^4} \\ k &= 2\pi/\lambda \quad \uparrow \quad p = h/\lambda \\ &= \frac{2\pi}{h} \sqrt{\frac{h^2}{4\pi^2} k^2 c^2 + m_0^2 c^4} = \omega(k) \end{aligned}$$

$$\Rightarrow \frac{d\omega}{dk} = \frac{2\pi}{h} \frac{1}{2} \frac{1}{\sqrt{\frac{h^2}{4\pi^2} k^2 c^2 + m_0^2 c^4}} \frac{h^2}{4\pi^2} c^2 2k = \frac{1}{E} \frac{h}{2\pi} c^2 k$$

$$= \frac{1}{E} \frac{h}{2\pi} c^2 \frac{2\pi}{\lambda} = \frac{c^2}{E} p = \frac{c^2 \gamma m_0 v}{\gamma m_0 c^2} = \underline{v} = \text{particle speed } v = \text{group velocity } \Rightarrow$$

\Rightarrow group velocity = speed of envelope function of particle wave packet = particle speed
good!

I_{3,5} $\lambda = h/p$: Order of Magnitude Estimate

Or: Why wasn't this noticed before?

thermal neutrons (300K) $\Rightarrow \lambda = 1.5 \text{ \AA}$
electrons at 100 eV $\Rightarrow \lambda = 1.2 \text{ \AA}$ } \approx atom size
neutrons at 10 MeV $\Rightarrow \lambda = 9 \cdot 10^{-15} \text{ m}$ } size of nucleus
 $m = 1g$ at 1 m/s $\Rightarrow \lambda = 7 \cdot 10^{-31} \text{ m}$
compare to visible light $\Rightarrow \lambda = 400 - 700 \text{ nm}$
 $= 4 \text{ to } 7 \cdot 10^{-7} \text{ m}$

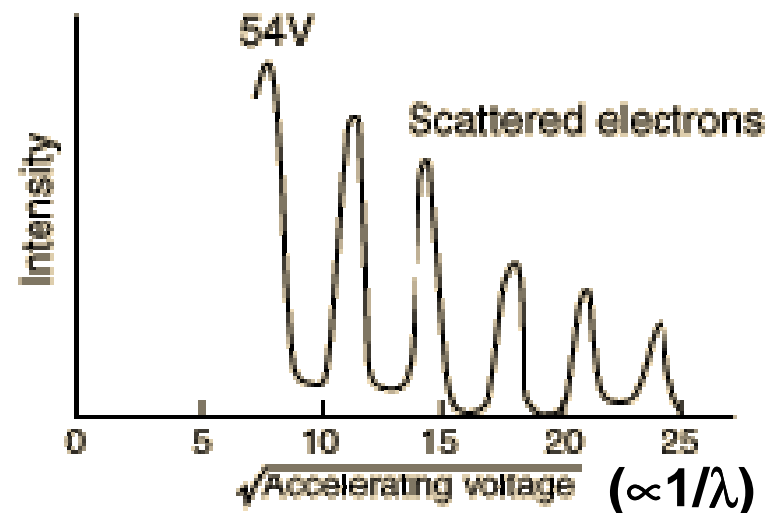
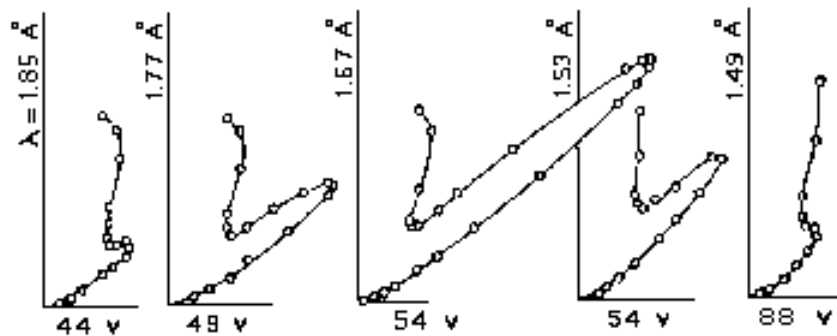
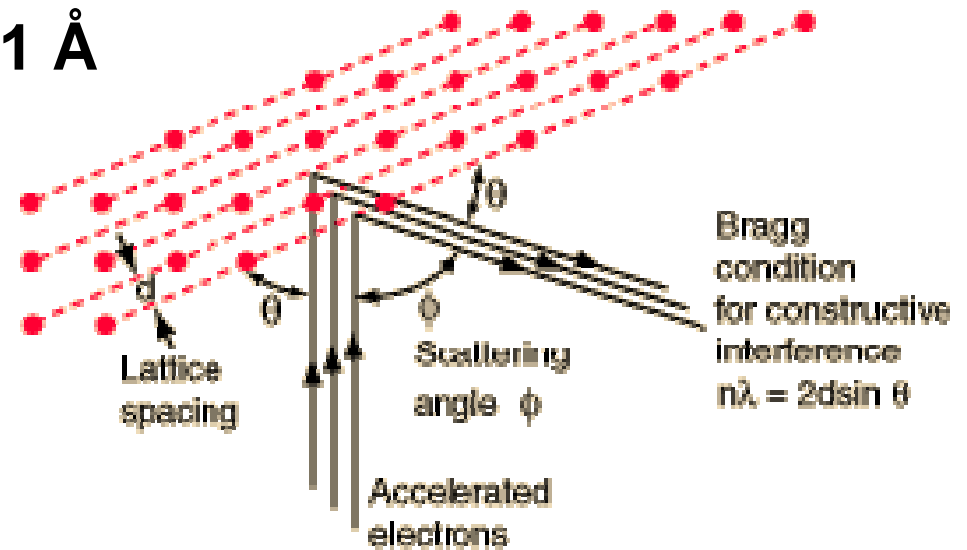
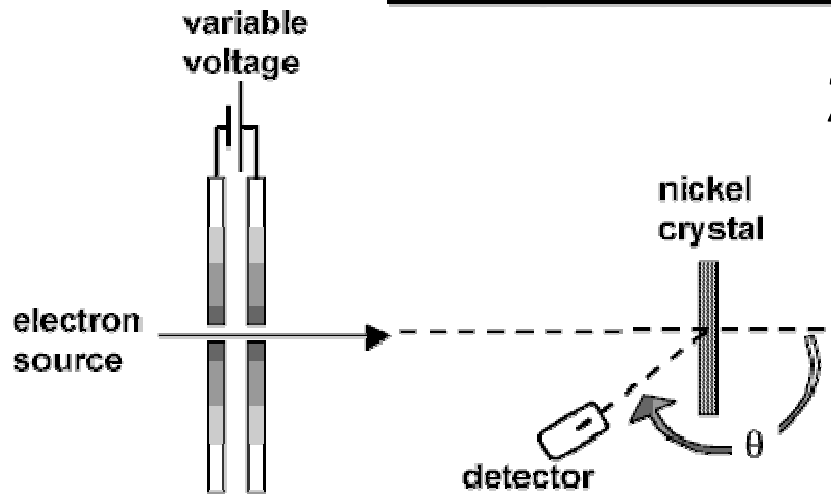
\rightarrow recall 2-slit exp.: maxima for $\sin \theta = \frac{n\lambda}{d} < 1$
need $\lambda \approx d$

\Rightarrow for particle: need "slit" spacing / diffraction grid on \AA scale (or less)
 \Rightarrow use crystals!

I_{3,6} Evidence for de Broglie's Particle Waves:

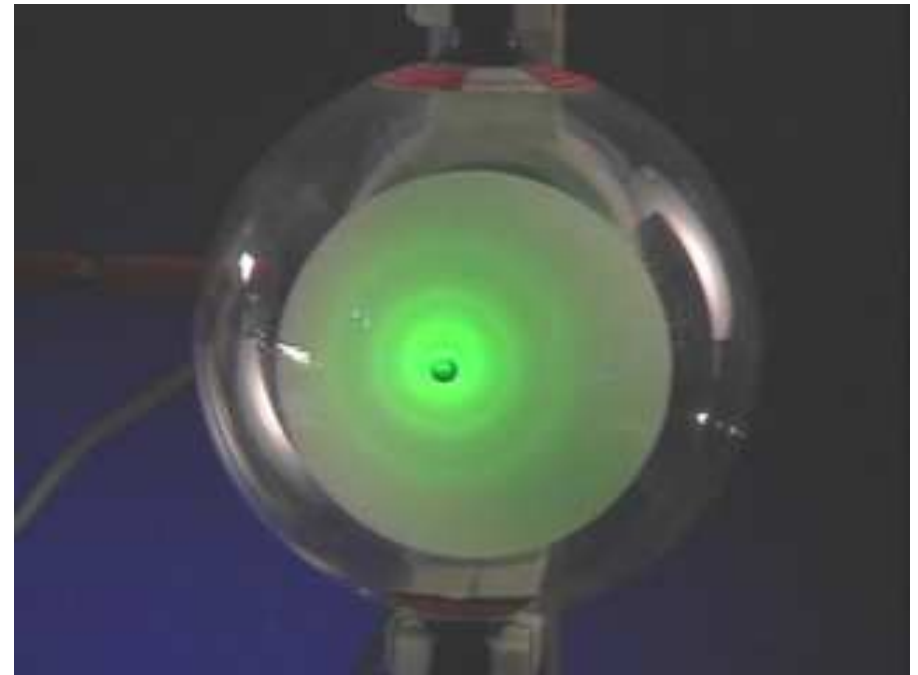
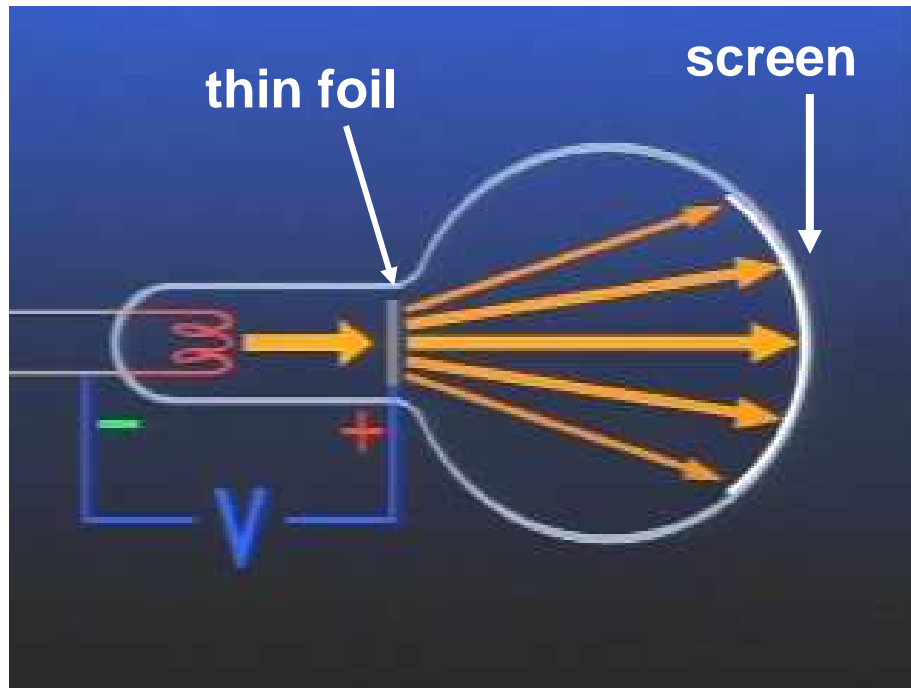
Davisson-Germer Experiment (1925): Scattering of low energy electrons by a crystal surface

$$\lambda \approx 1 \text{ \AA}$$



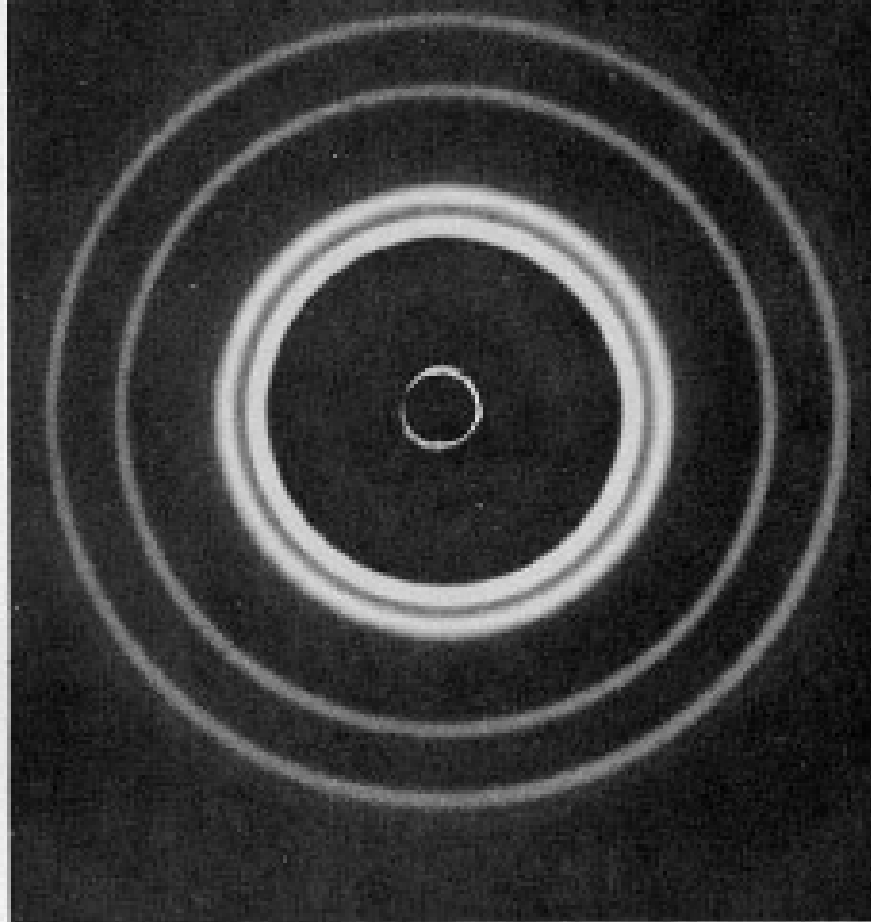
G. P. Thompson's Experiment: Diffraction of 10 – 40 keV electrons by a thin polycrystalline foil

$$\lambda \approx 0.1 \text{ \AA}$$

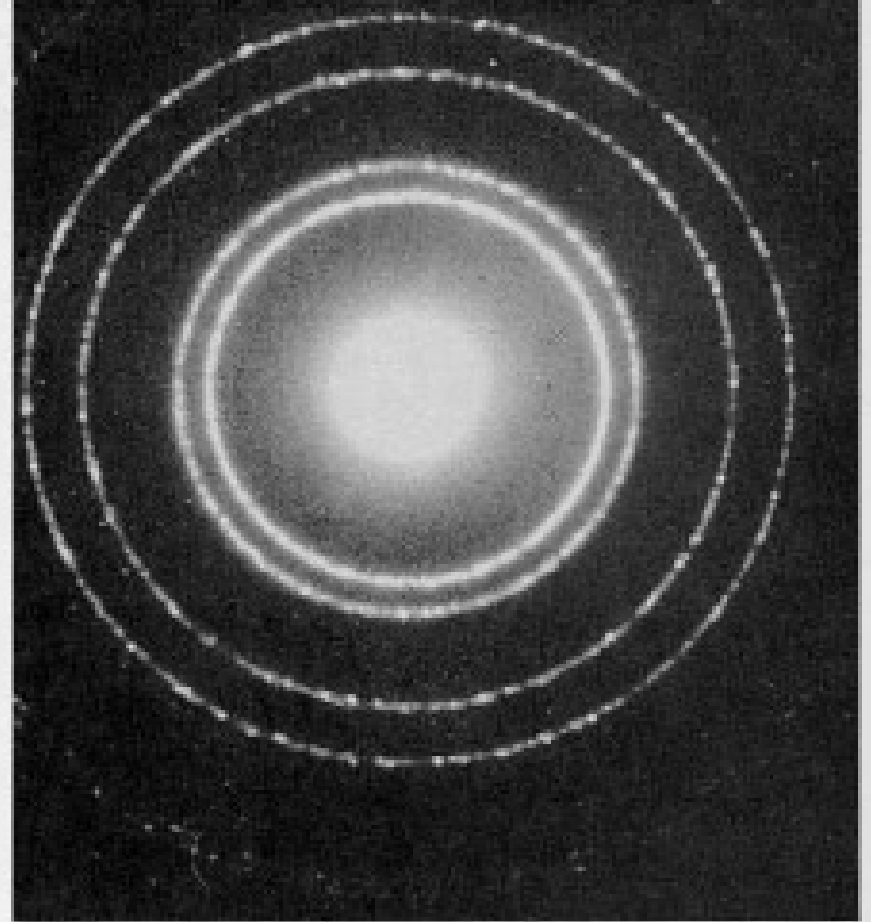


polycrystalline film \Rightarrow Bragg condition satisfied for any given reflecting plane \Rightarrow concentric circles

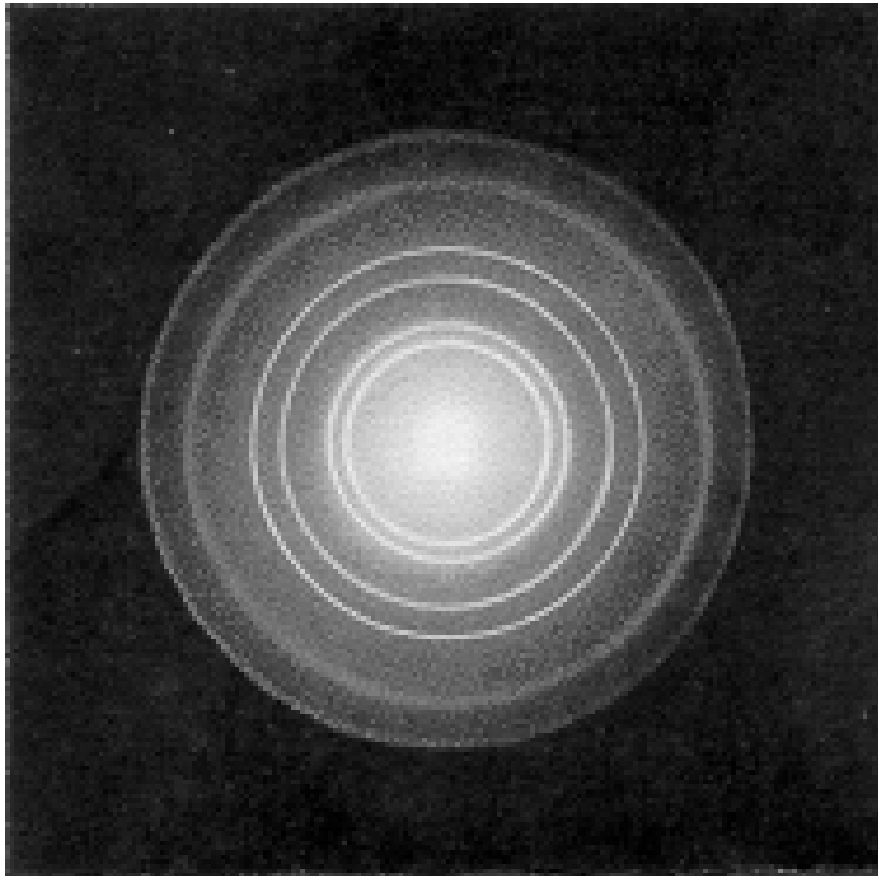
Diffraction pattern of X-ray beam passing through Al foil



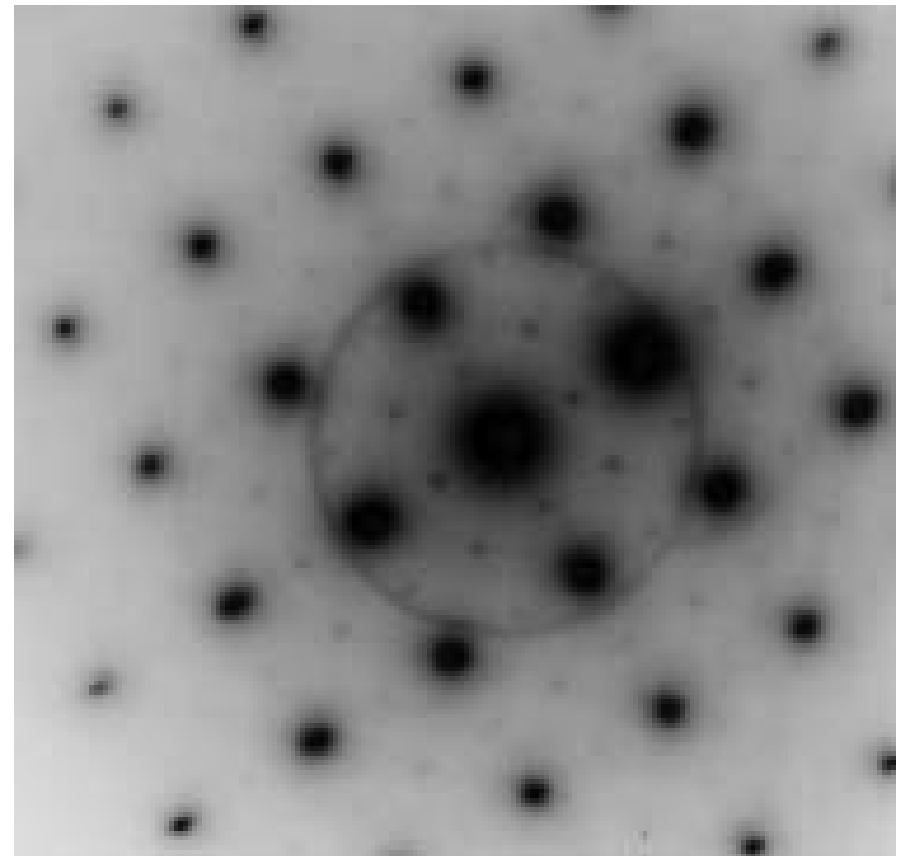
Diffraction pattern of electron beam passing through Al foil



Electron diffraction by polycrystalline aluminum

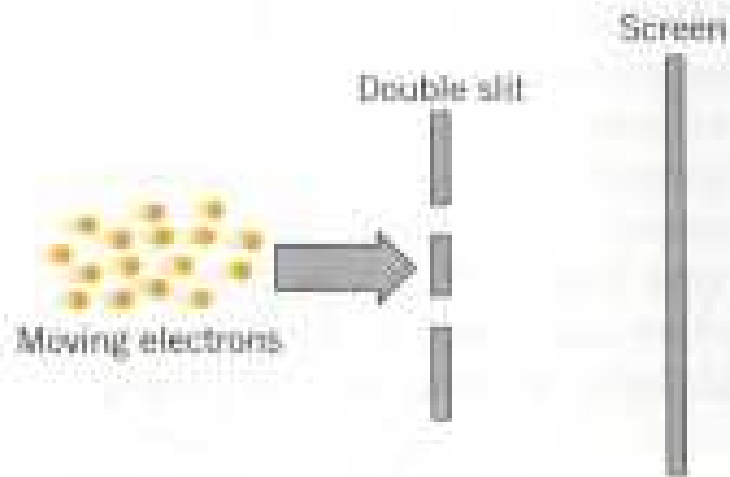


Laue pattern of electron diffraction by a single crystal



(Courtesy of Prof. Y. Soejima, Dept. of Physics, Kyushu Univ.)

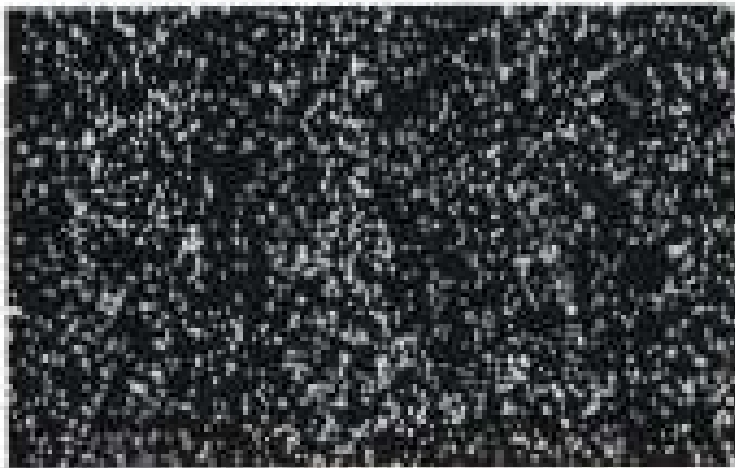
2-slit Interference of Electrons



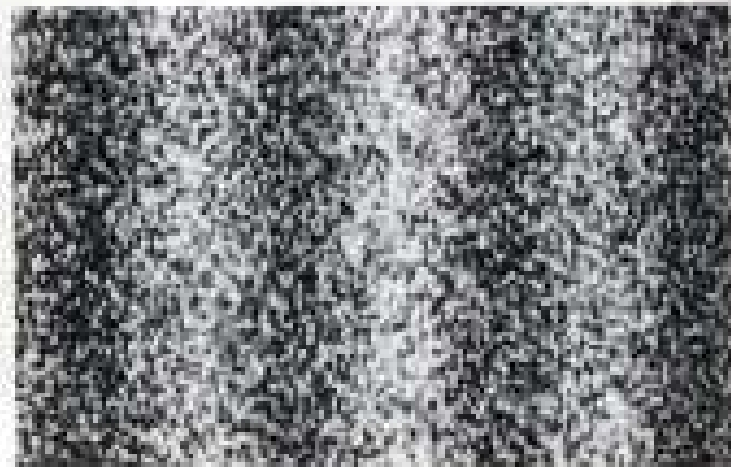
(a)



(b) After 100 electrons



(c) After 3000 electrons



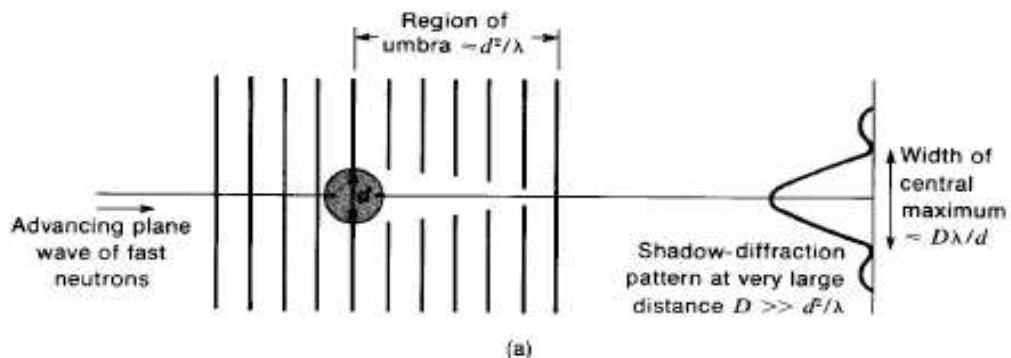
(d) After 70 000 electrons

Diffraction of Neutrons

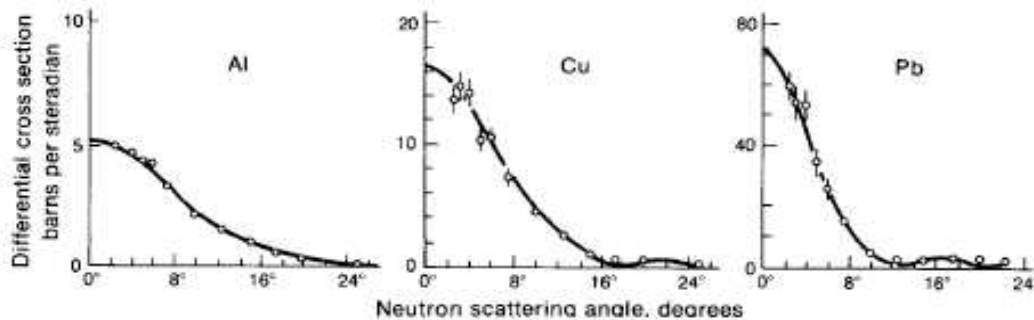
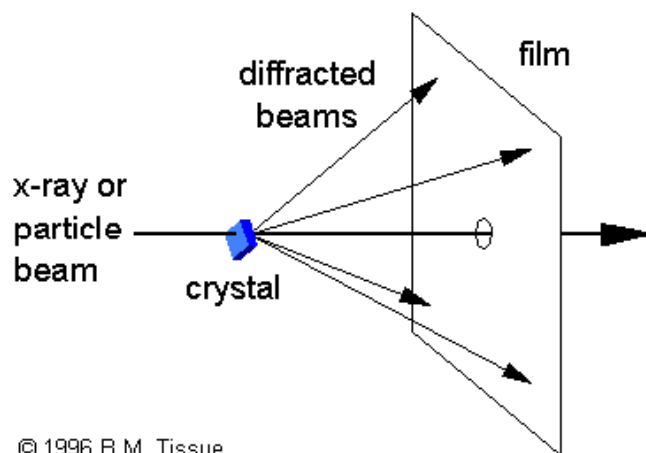
$\lambda = \text{several } \text{\AA} \text{ down to } <10^{-14} \text{ m}$



FIGURE 4.7 Diffraction of neutrons by a sodium chloride crystal.

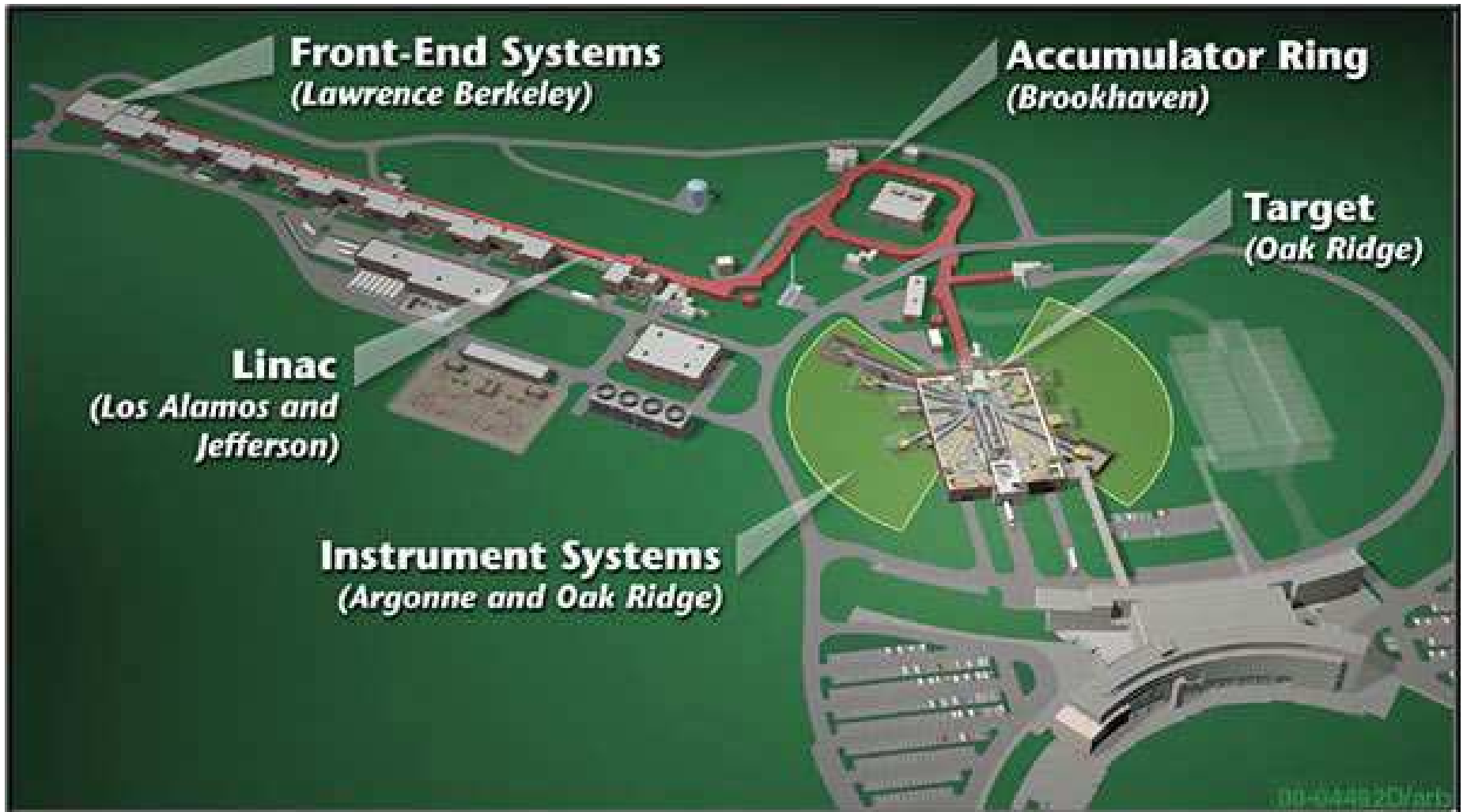


from Krane



Diffraction of fast neutrons from Al, Cu, and Pb nuclei. [from French, after A Bratenahl, Phys Rev 77, 597 (1950)]

The Spallation Neutron Source (SNS) in Oak Ridge, TN



Why Neutrons?

Neutrons are **NEUTRAL** particles. They

- are highly penetrating,
- can be used as nondestructive probes, and
- can be used to study samples in severe environments.

Neutrons have a **MAGNETIC** moment. They can be used to

- study microscopic magnetic structure,
- study magnetic fluctuations, and
- develop magnetic materials.

Neutrons have **SPIN**. They can be

- formed into polarized neutron beams,
- used to study nuclear (atomic) orientation, and
- used for coherent and incoherent scattering.

The **ENERGIES** of thermal neutrons are similar to the energies of elementary excitations in solids. Both have similar

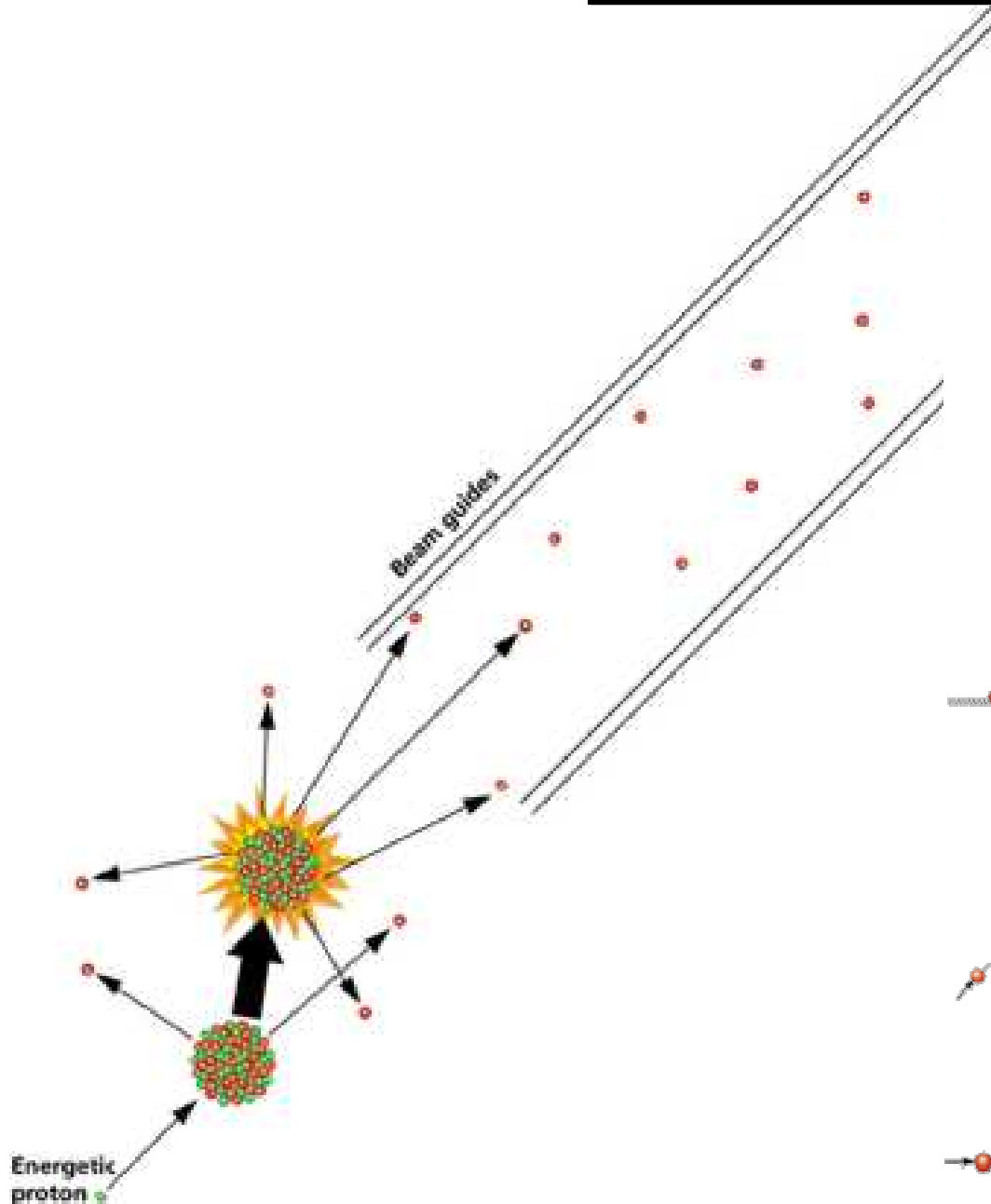
- molecular vibrations,
- lattice modes, and
- dynamics of atomic motion.

The **WAVELENGTHS** of neutrons are similar to atomic spacings. They can determine

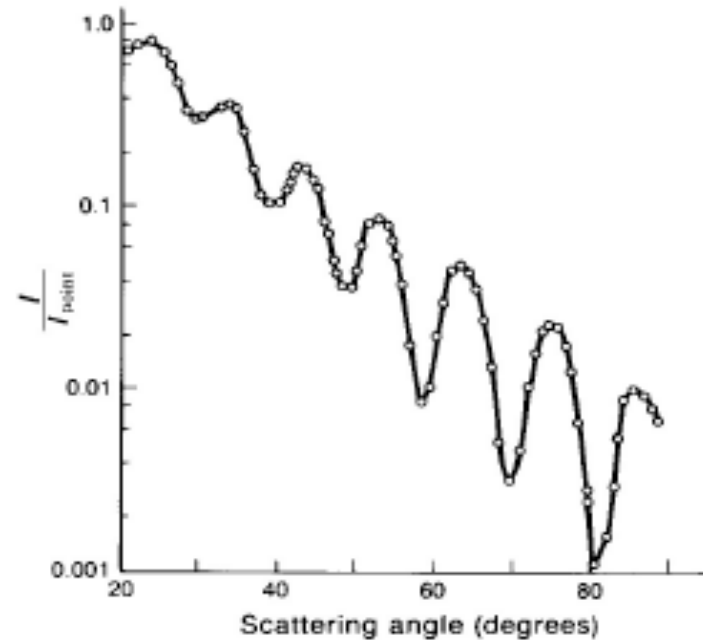
- structural sensitivity,
- structural information from 10^{-13} to 10^{-4} cm, and
- crystal structures and atomic spacings.

Neutrons "see" **NUCLEI**. They

- are sensitive to light atoms,
- can exploit isotopic substitution, and
- can use contrast variation to differentiate complex molecular structures.



Scattering of Alpha Particles



Angular distribution of 40 MeV alpha particles scattered from niobium nuclei.

[from French after G. Igo et al., Phys Rev 101, 1508 (1956)]

Crystal Diffraction of Neutral Helium (1930)

$$\lambda \approx 1 \text{ \AA}$$

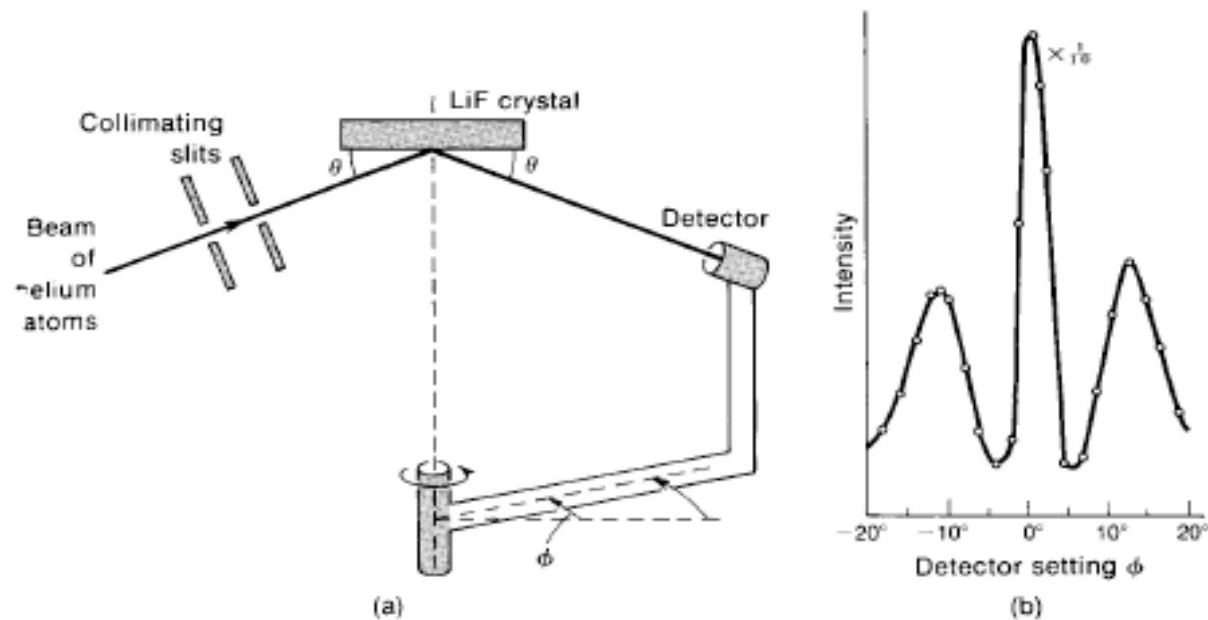
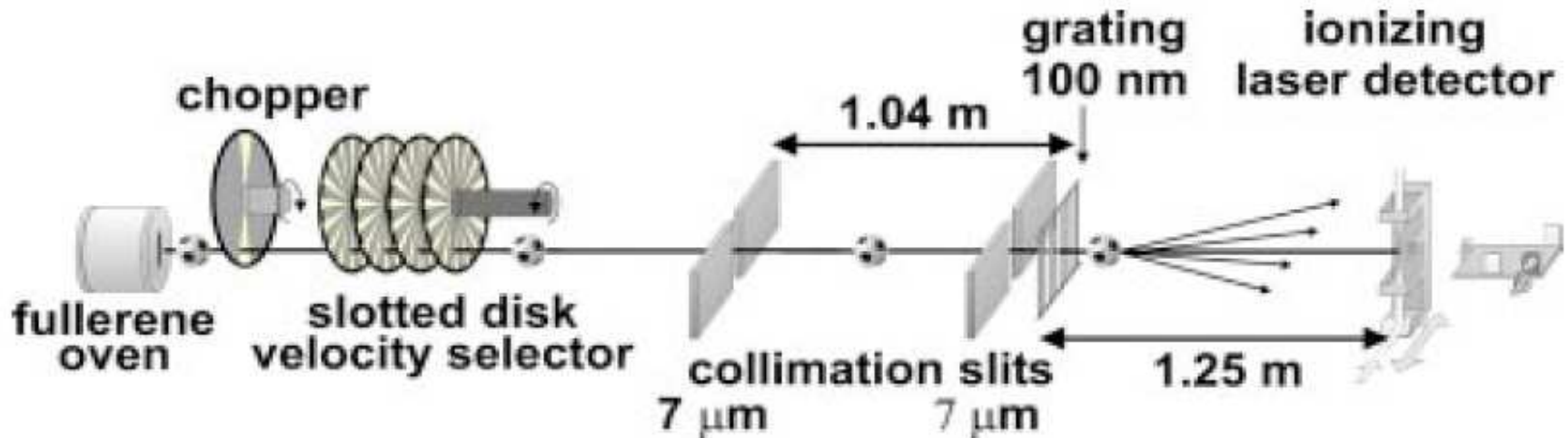


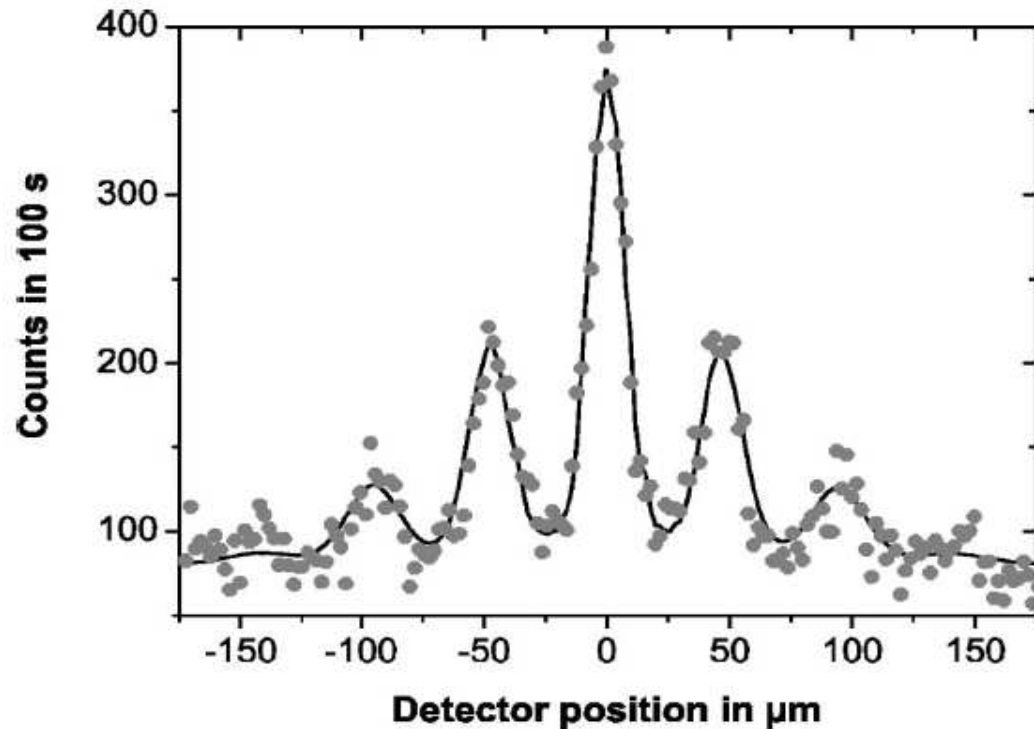
Fig. 2-16 (a) Experimental arrangement used by Stern et al. to investigate crystal diffraction of neutral helium atoms. (b) Experimental results showing central reflection peak ($\phi = 0^\circ$), plus first-order diffraction peaks ($\phi = 11^\circ$). In the experiment, $\theta = 18.5^\circ$.

from French after Estermann and Stern, Z Phys 61, 95 (1930)

Interference of Molecules



Fullerene molecule C₆₀, consisting of 60 carbon atoms

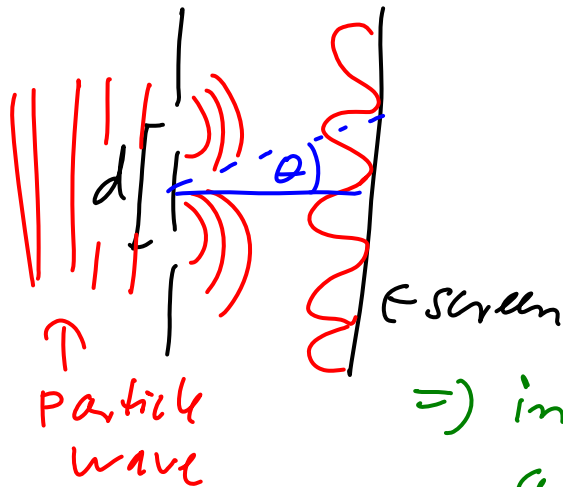


I₄ The "Old Quantum Theory"

I_{4,1} Key Ideas / Concepts / Postulates:

- 1) Photons, all particles have both particle-like and wave-like properties
- 2) Precisely-defined trajectories do not exist at the quantum level
- 3) The exact behavior of a given particle cannot be predicted → only its probable behavior
⇒ statistical interpretation
- 4) The probability that a single particle is observed in a given region is proportional to intensity of its associated wave field: $I \propto |A|^2$
⇒ $P \propto |A|^2$

=> recall 2-slit experiment



wave amplitude on screen:

- one slit open: A_0

- both slits open: interference

$$A_{\text{total}} = 2 A_0 \cos\left(\frac{\pi d}{\lambda} \sin \theta\right)$$

=> intensity on screen \propto probability for a particle to arrive at a given region along the screen \propto statistical distribution of large number of particles on the screen

$$I(\theta) \propto P(\theta) \propto |A_{\text{total}}|^2 = 4|A_0|^2 \cos^2\left(\frac{\pi d}{\lambda} \sin \theta\right)$$

\uparrow probability

=> $\sqrt{P} \propto |A|$ also called probability amplitude
(quantum amplitude)

later: wavefunctions Ψ (complex) $\Rightarrow P \propto |\Psi|^2$

2-slit experiment with particles: Assume that only one slit is open, and that the probability of a particle to arrive at a small section Δx of the screen is F . What is the **maximum** probability of finding a particle in that section Δx of the screen if both slits are open simultaneously?

A. $\sqrt{2} F$

~~B. $2 F$~~

C. $4 F$

D. $2 \sqrt{F}$

E. F^2

- one slit open: prob.
probability $F \Rightarrow$ amplitude = \sqrt{F} · complex phase factor
- both slits open:
 \Rightarrow add probability amplitudes!
 \Rightarrow max. probability amplitude = $2 \sqrt{F}$
 \Rightarrow max. probability = $(2 \sqrt{F})^2 = \underline{\underline{4 F}}$

5) If a particle is confined into a small volume, its energy is quantized \Rightarrow "energy levels"
"energy states"

6) de Broglie - Einstein postulates:

$$\lambda = h/p \quad (p = \hbar k) \quad k = \text{wave number}$$

$$v = E/h \quad (E = \hbar \omega) \quad \omega = \text{angular frequ.}$$

7) Superposition principle