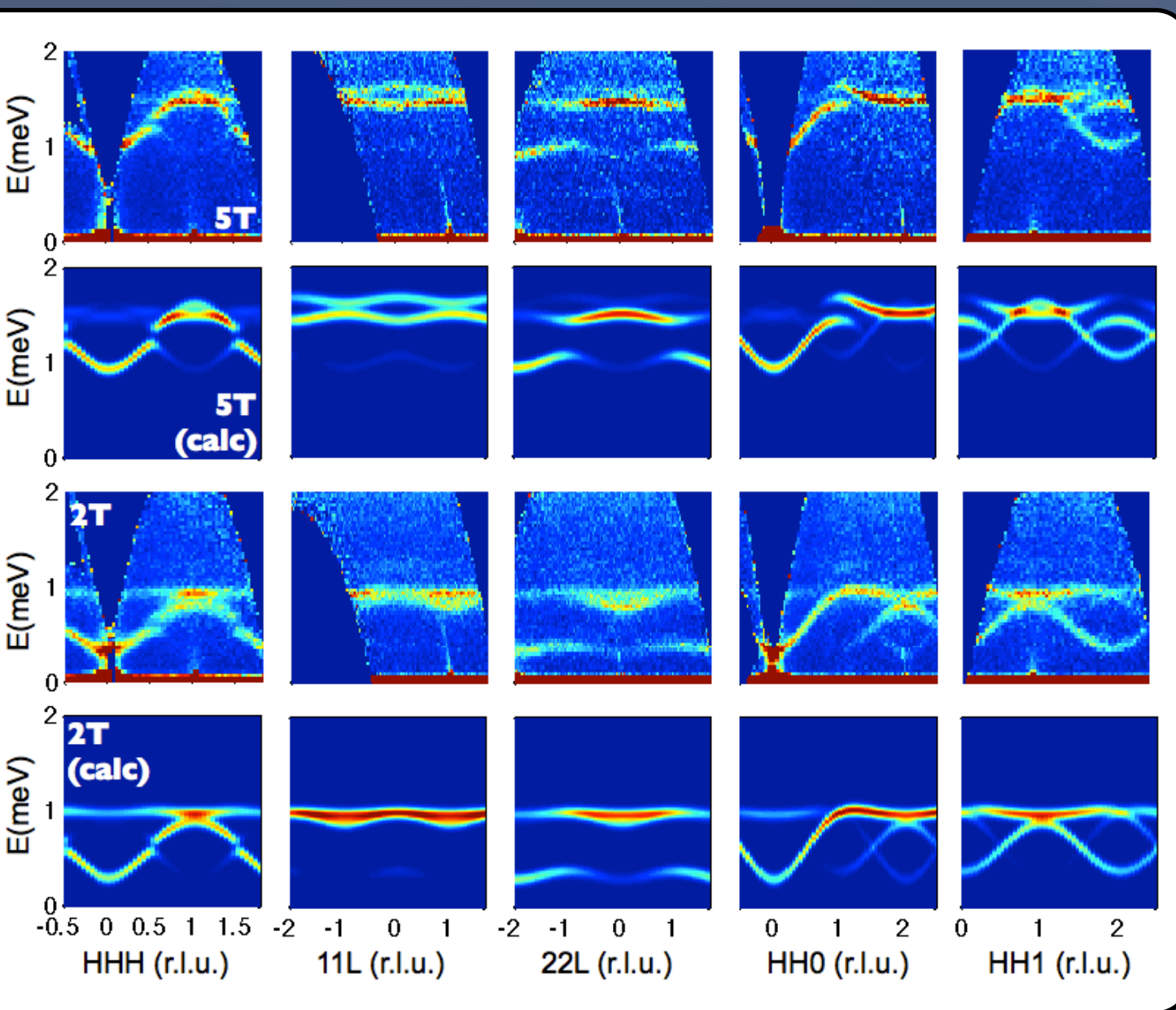


A Survey in Neutron Scattering:



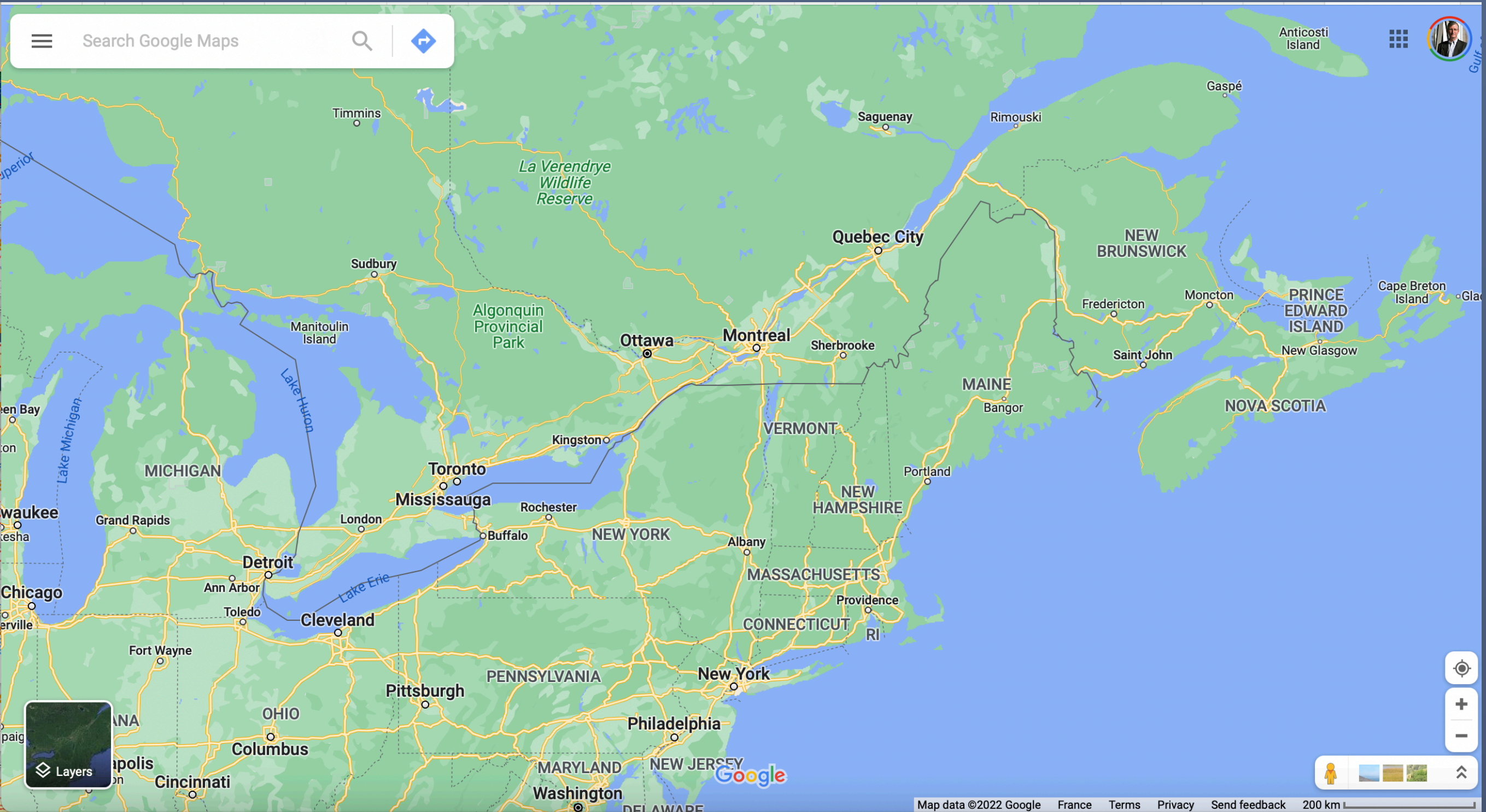
**The neutron scattering
cross section**

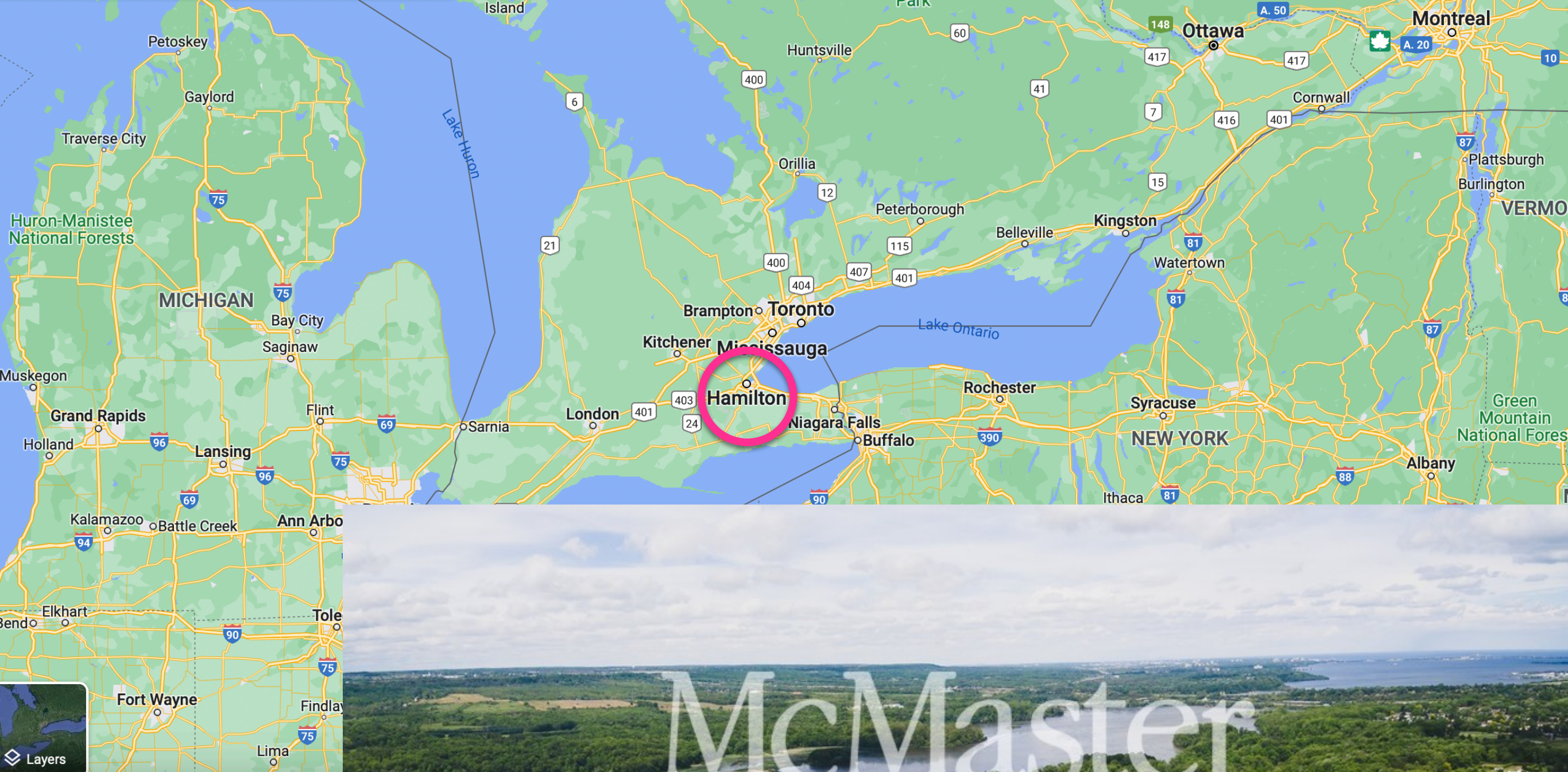
**The triple axis
spectrometer**

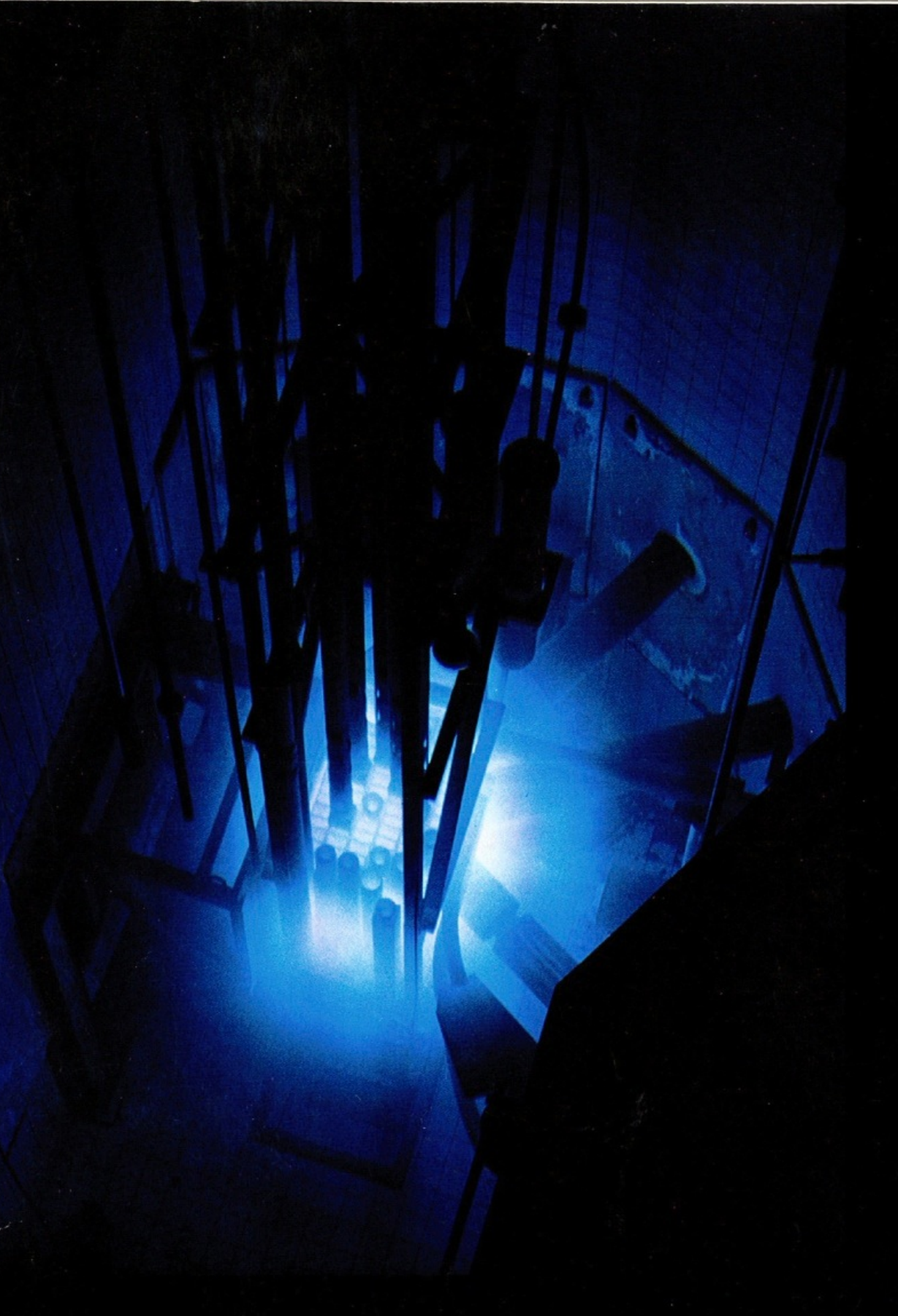
time-of-flight spectroscopy

phonons

magnetism







PHYSICS

McMASTER UNIVERSITY HAMILTON ONTARIO

Neutrons:

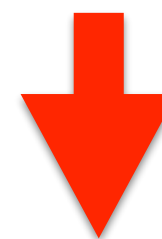
no charge

spin = 1/2

massive:

$mc^2 \sim 1 \text{ GeV}$

$^{235}\text{U} + n$

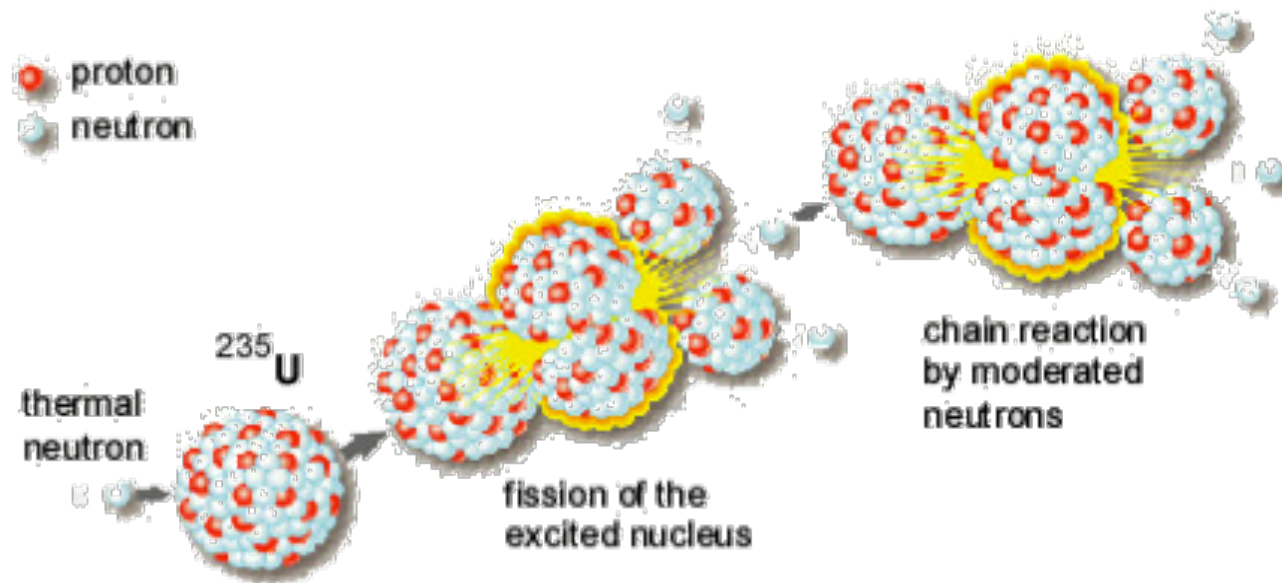


daughter nuclei

+

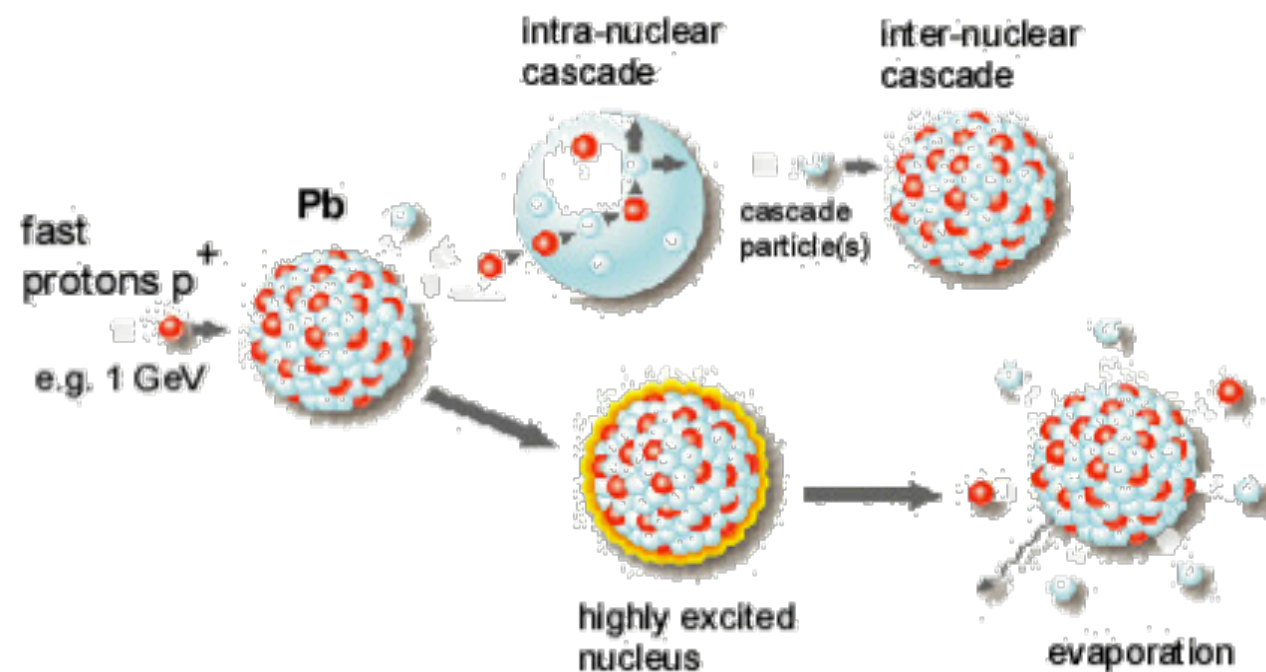
$2-3 n + \gamma\text{'s}$

How do we produce neutrons



Fission

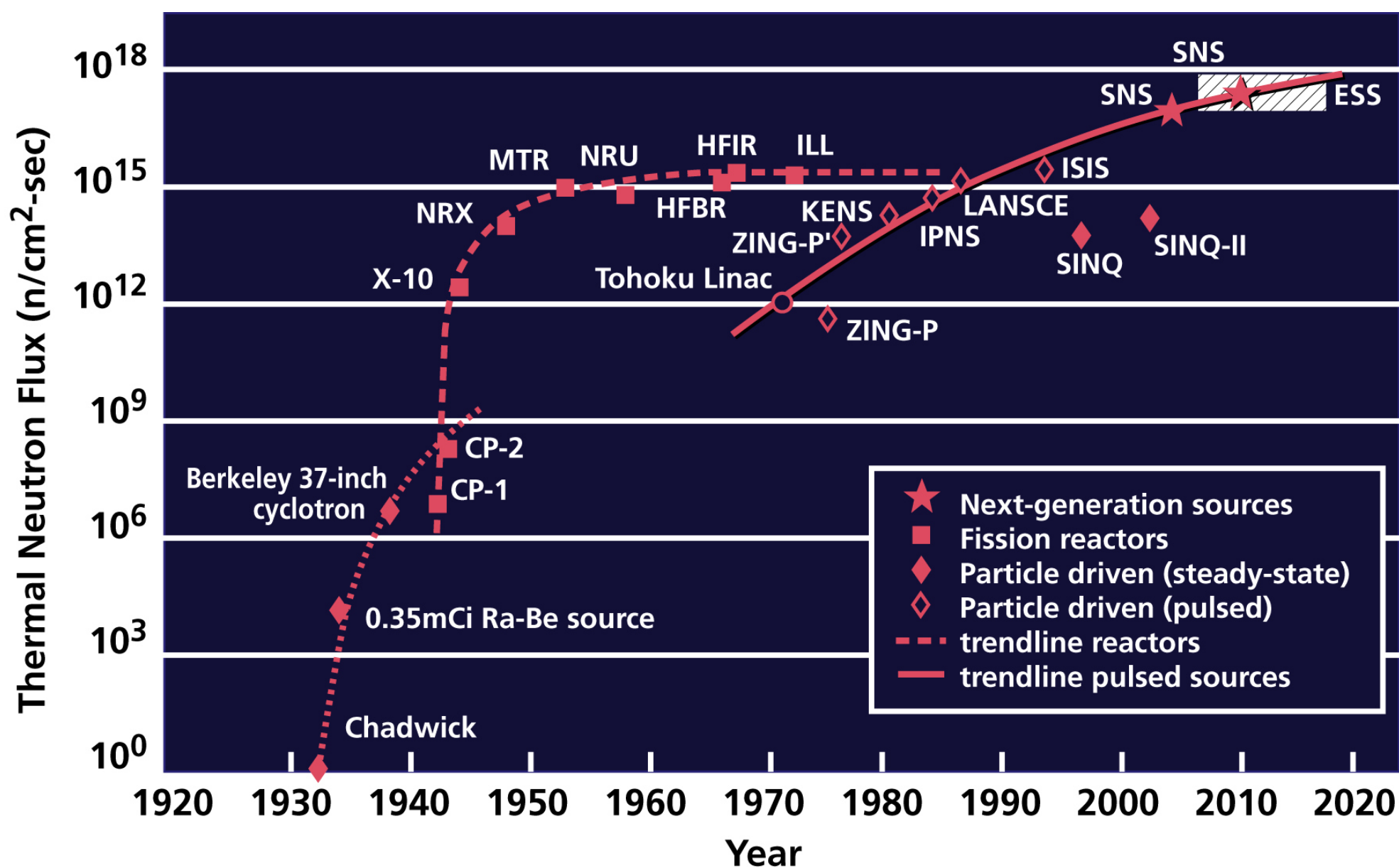
- chain reaction
- continuous flow
- 1 neutron/fission



Spallation

- no chain reaction
- pulsed operation
- 30 neutrons/proton

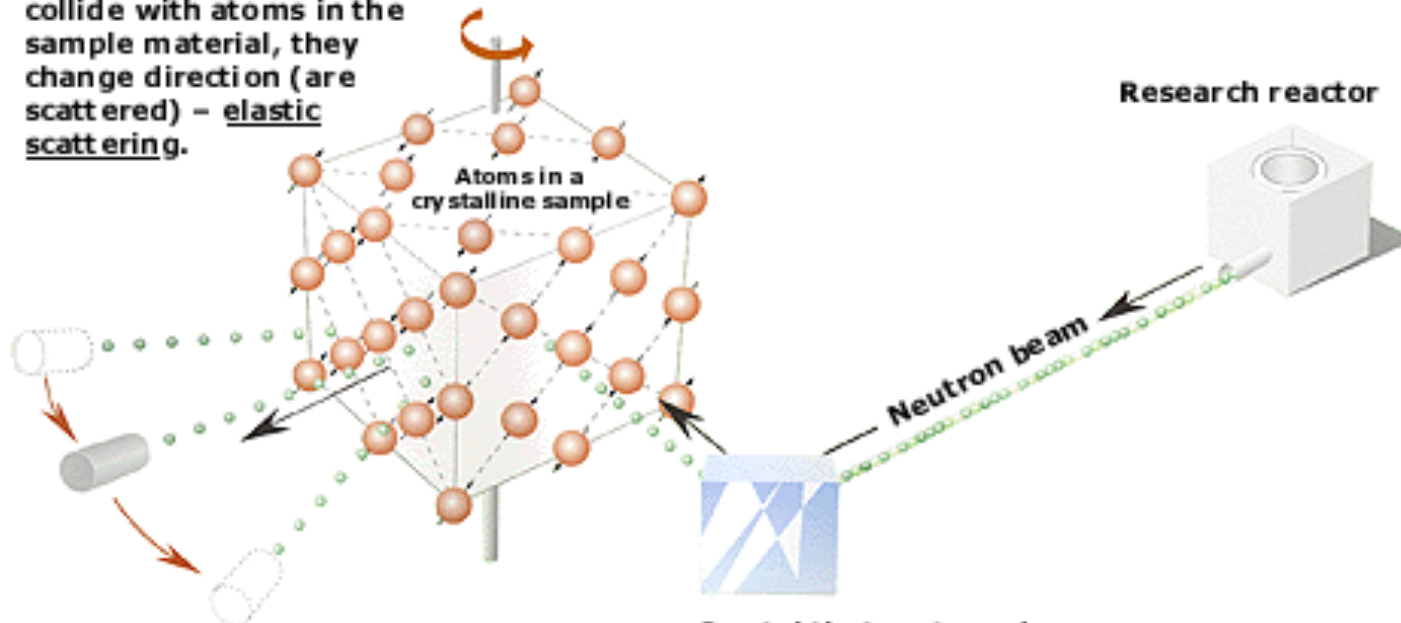
Development of Neutron Science Facilities



(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)

Brockhouse and Shull Share 1994 Nobel Prize in Physics for the invention of neutron scattering techniques

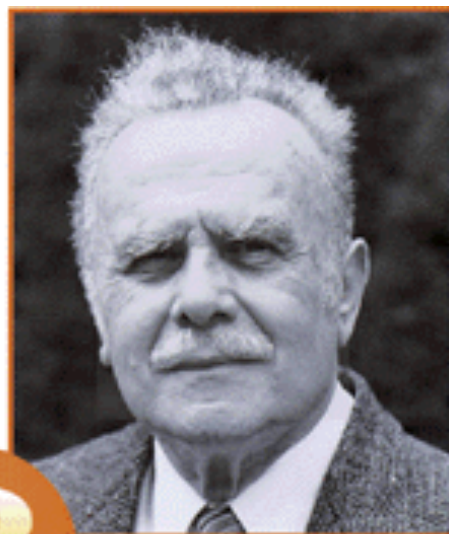
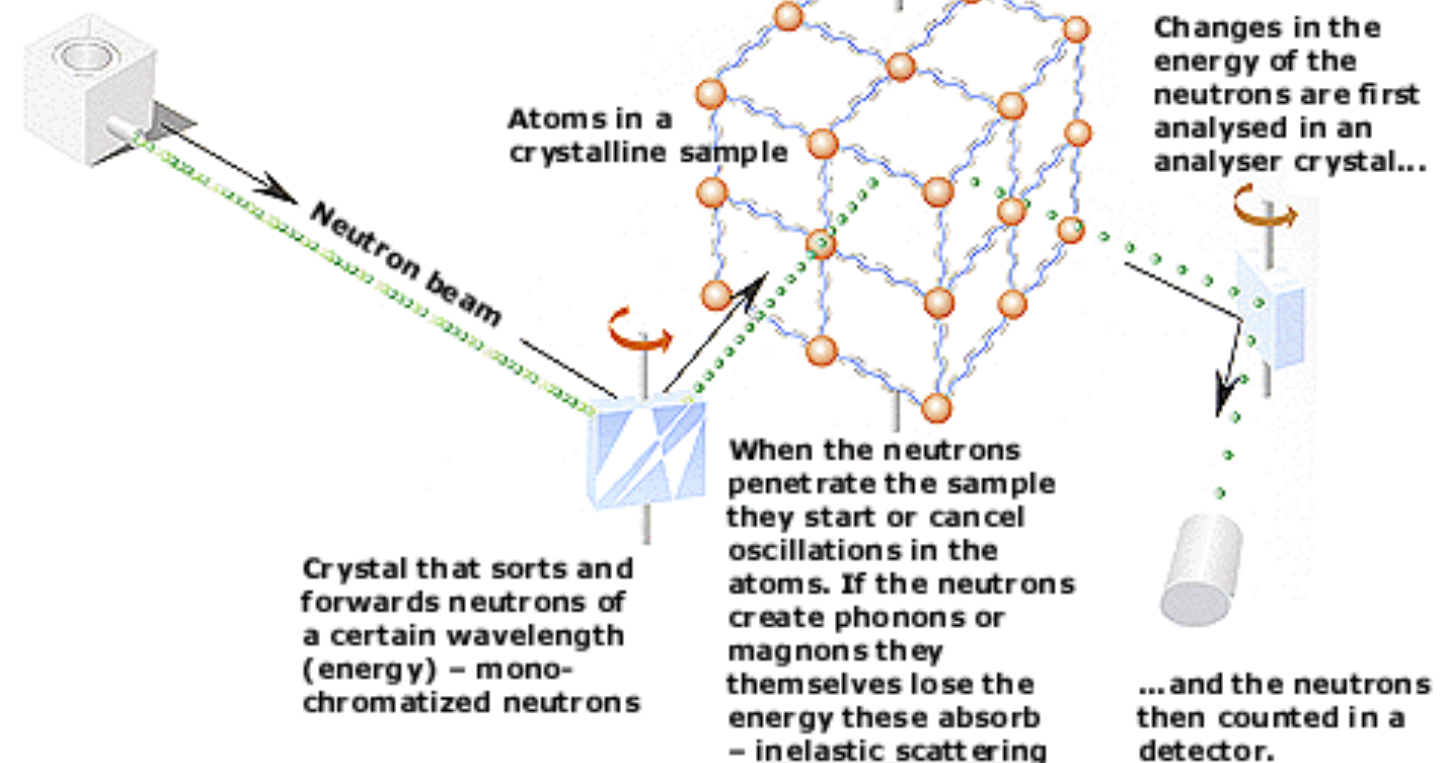
When the neutrons collide with atoms in the sample material, they change direction (are scattered) – elastic scattering.



Clifford G. Shull, MIT, Cambridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.



3-axis spectrometer with rotatable crystals and rotatable sample



Betram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.

The Neutron as a Wave

Energy, wave vector, wavelength, velocity :

$$k = \frac{m_n v}{\hbar} = \frac{2\pi}{\lambda}$$

$$E = k_B T = 0.08617 \text{ meV} \cdot K^{-1} \times T$$

$$E = \frac{\hbar^2 k^2}{2m_n} = \frac{\hbar^2}{2m_n} \left(\frac{2\pi}{\lambda} \right)^2 = \frac{81.81 \text{ meV} \cdot \text{\AA}^2}{\lambda^2}$$

Neutrons with λ typical of interatomic spacings ($\sim 2 \text{ \AA}$) have energies typical of elementary excitations in solids ($\sim 20 \text{ meV}$)

The Neutron as a Wave

Energy, wave vector, wavelength, velocity :

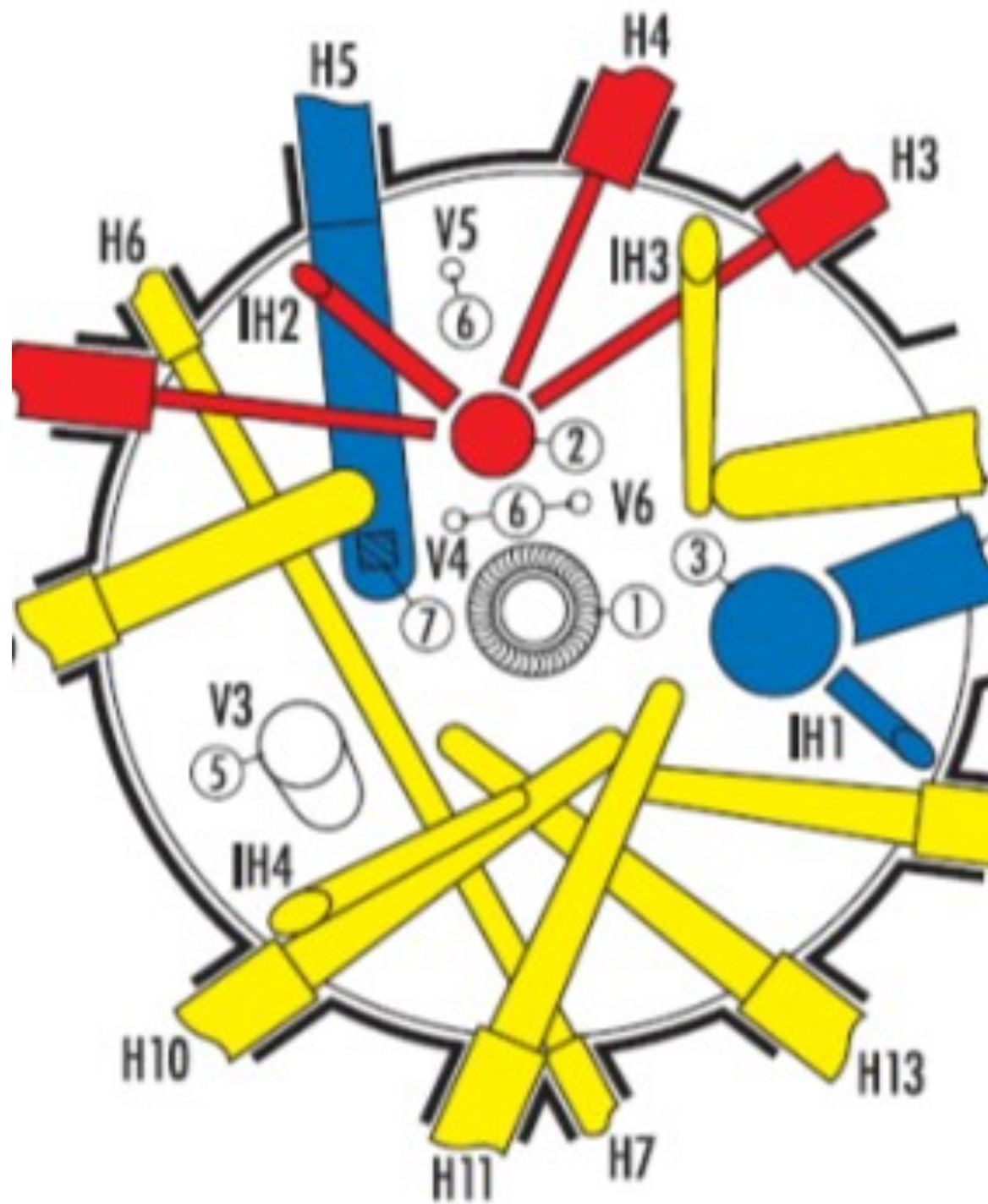
$$k = \frac{m_n v}{\hbar} = \frac{2\pi}{\lambda}$$

$$E = k_B T = 0.08617 \text{ meV} \cdot \text{K}^{-1} \times T$$

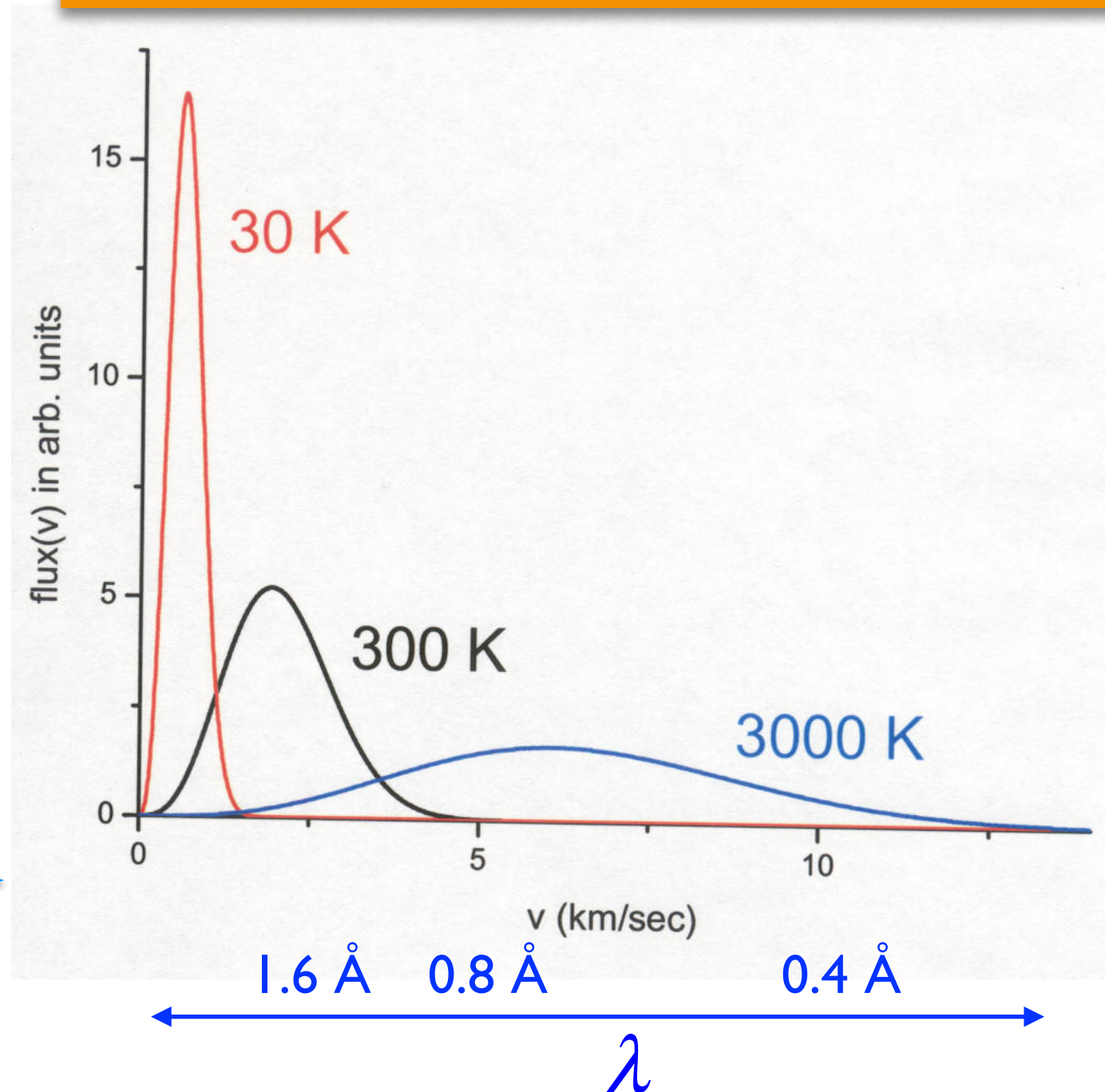
$$E = \frac{\hbar^2 k^2}{2m_n} = \frac{\hbar^2}{2m_n} \left(\frac{2\pi}{\lambda} \right)^2 = \frac{81.81 \text{ meV} \cdot \text{\AA}^2}{\lambda^2}$$

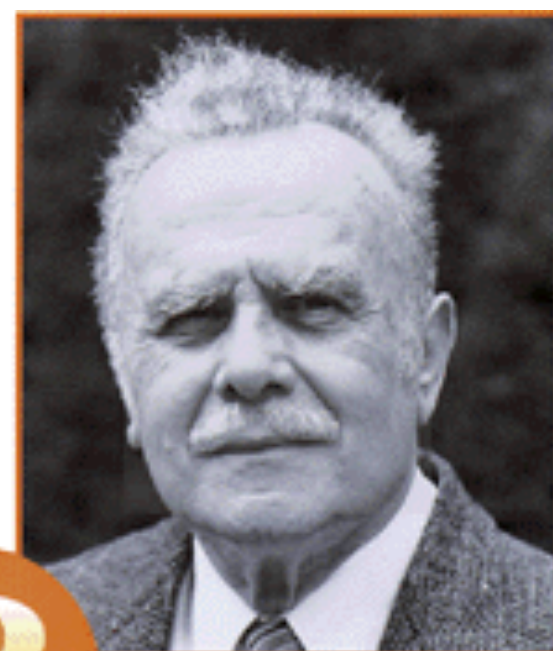
	Energy (meV)	Temperature (K)	Wavelength (Å)
Cold	0.1 – 10	1 – 120	4 – 30
Thermal	5 – 100	60 – 1000	1 – 4
Hot	100 – 500	1000 – 6000	0.4 – 1

The High Flux Reactor at the ILL and its moderators and beam ports

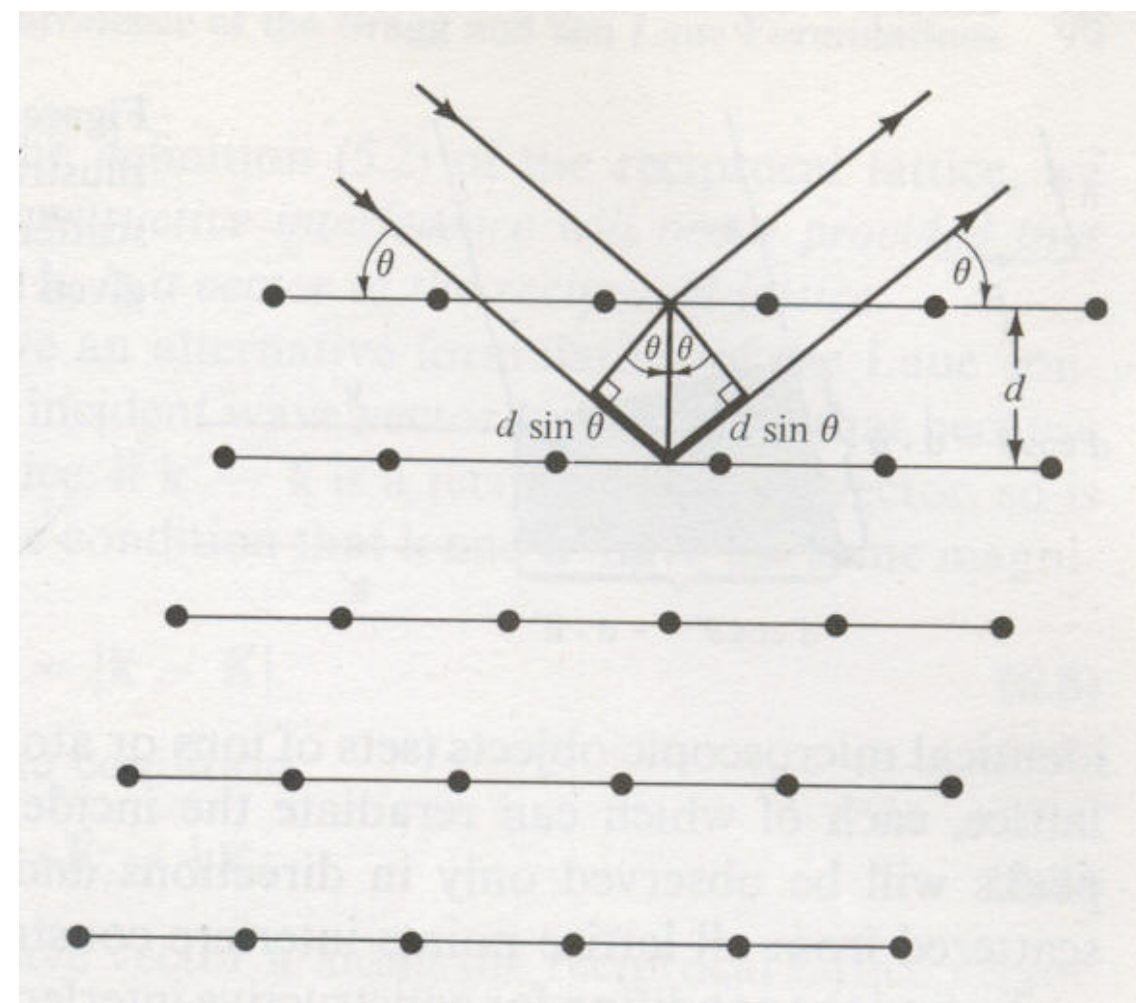
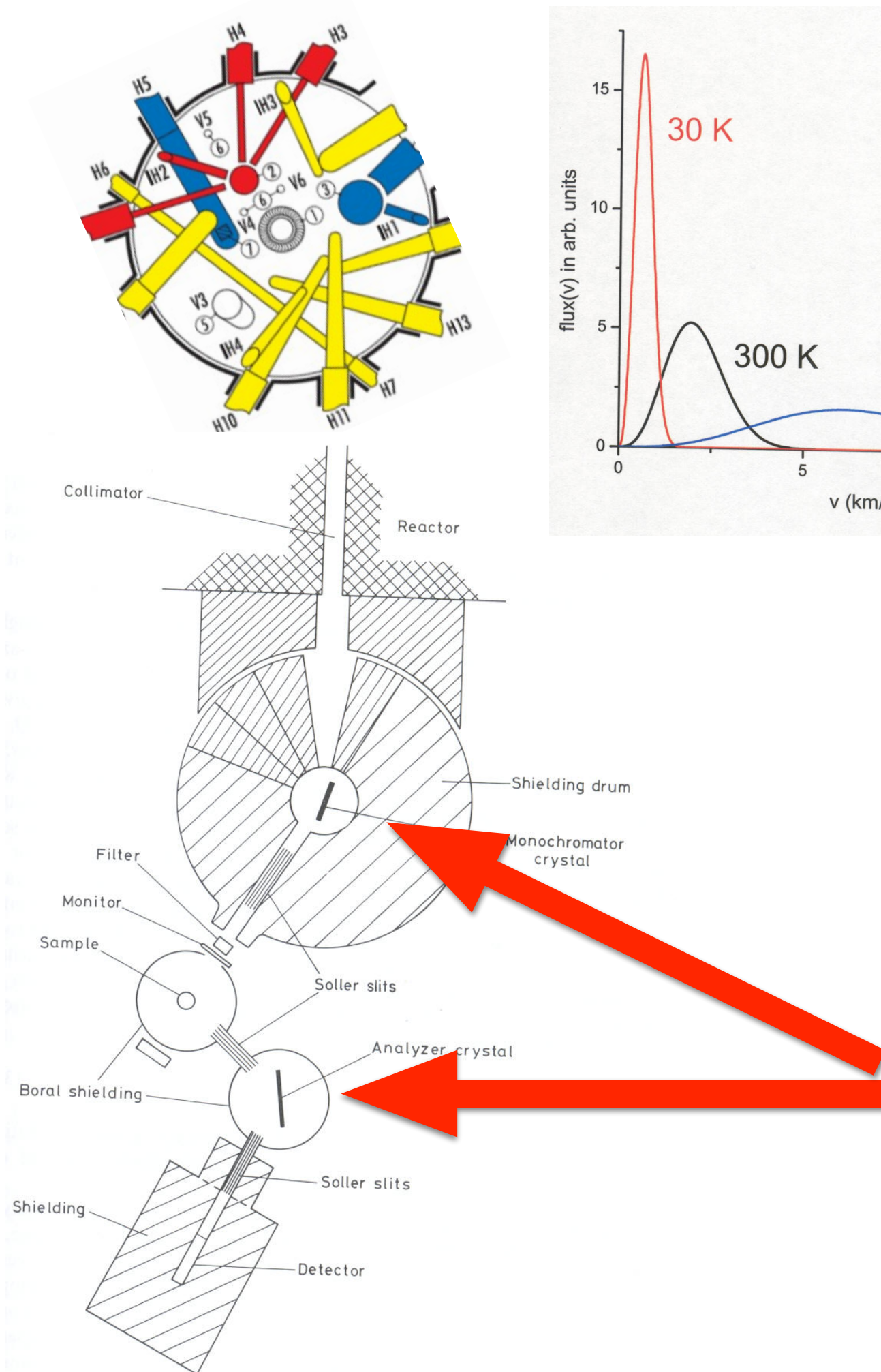
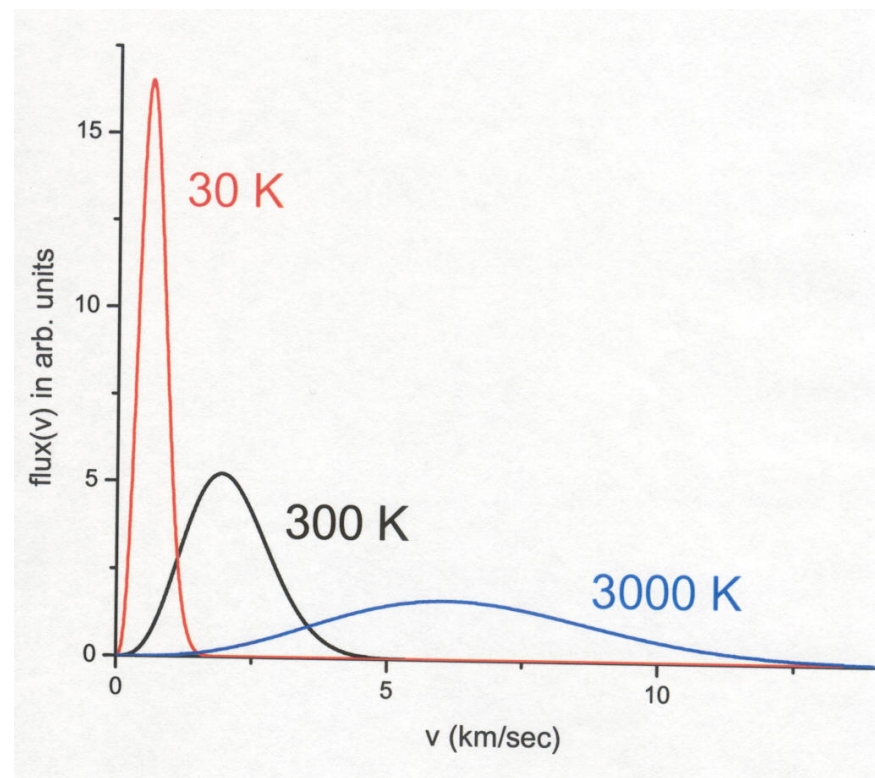


← 2.5 m →





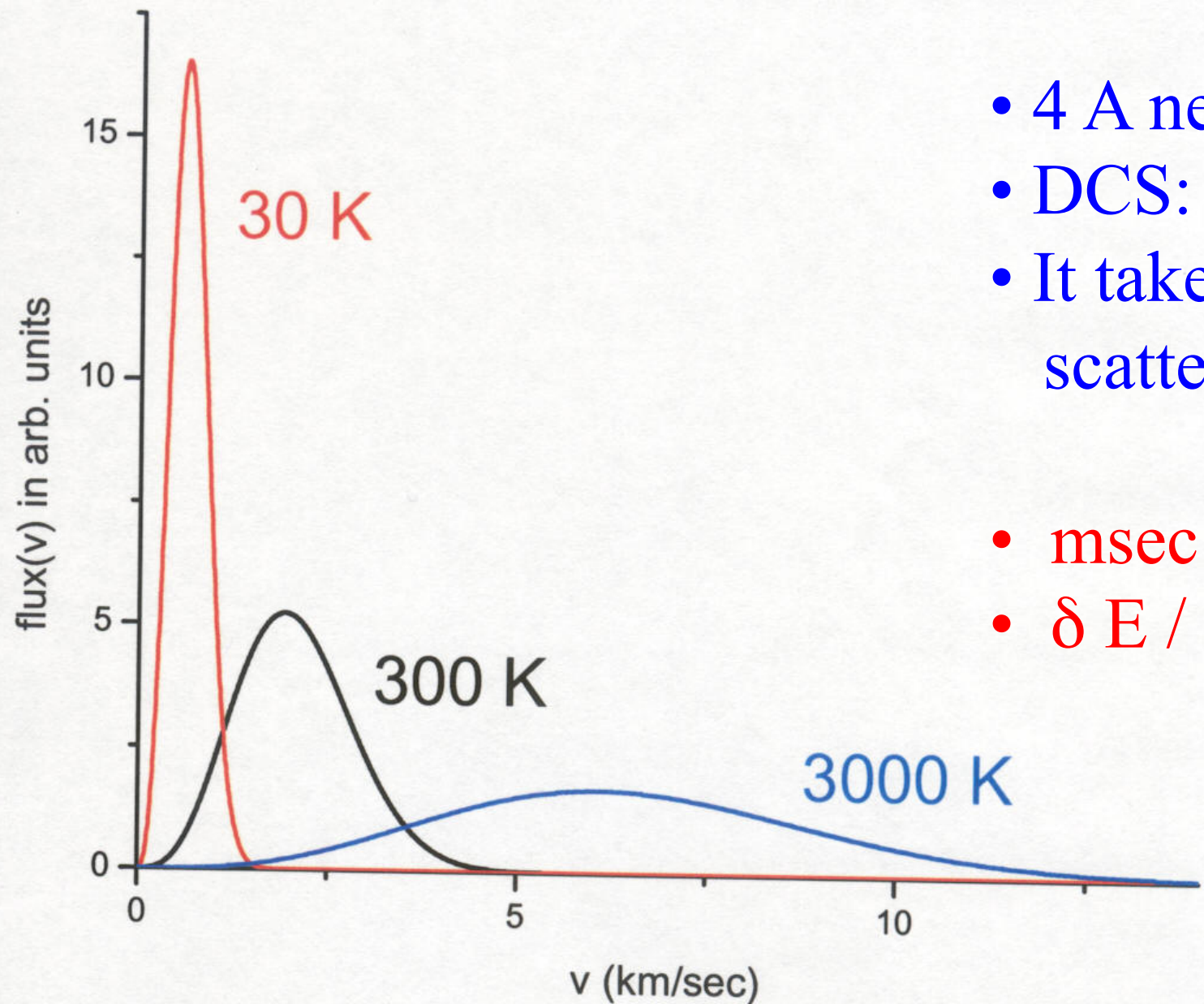
Betram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.



Neutrons have *mass*

so higher energy means faster – lower energy means slower

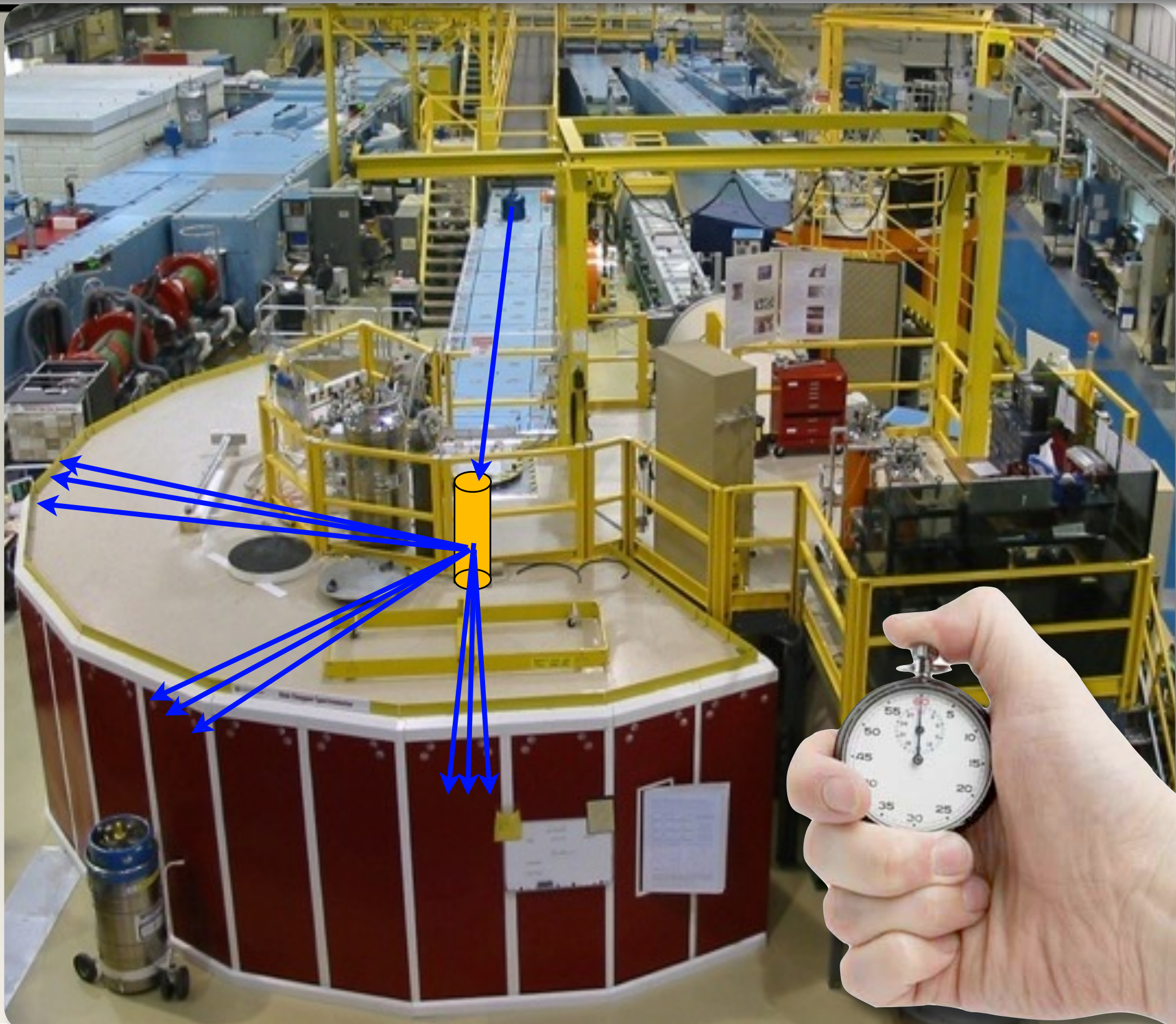
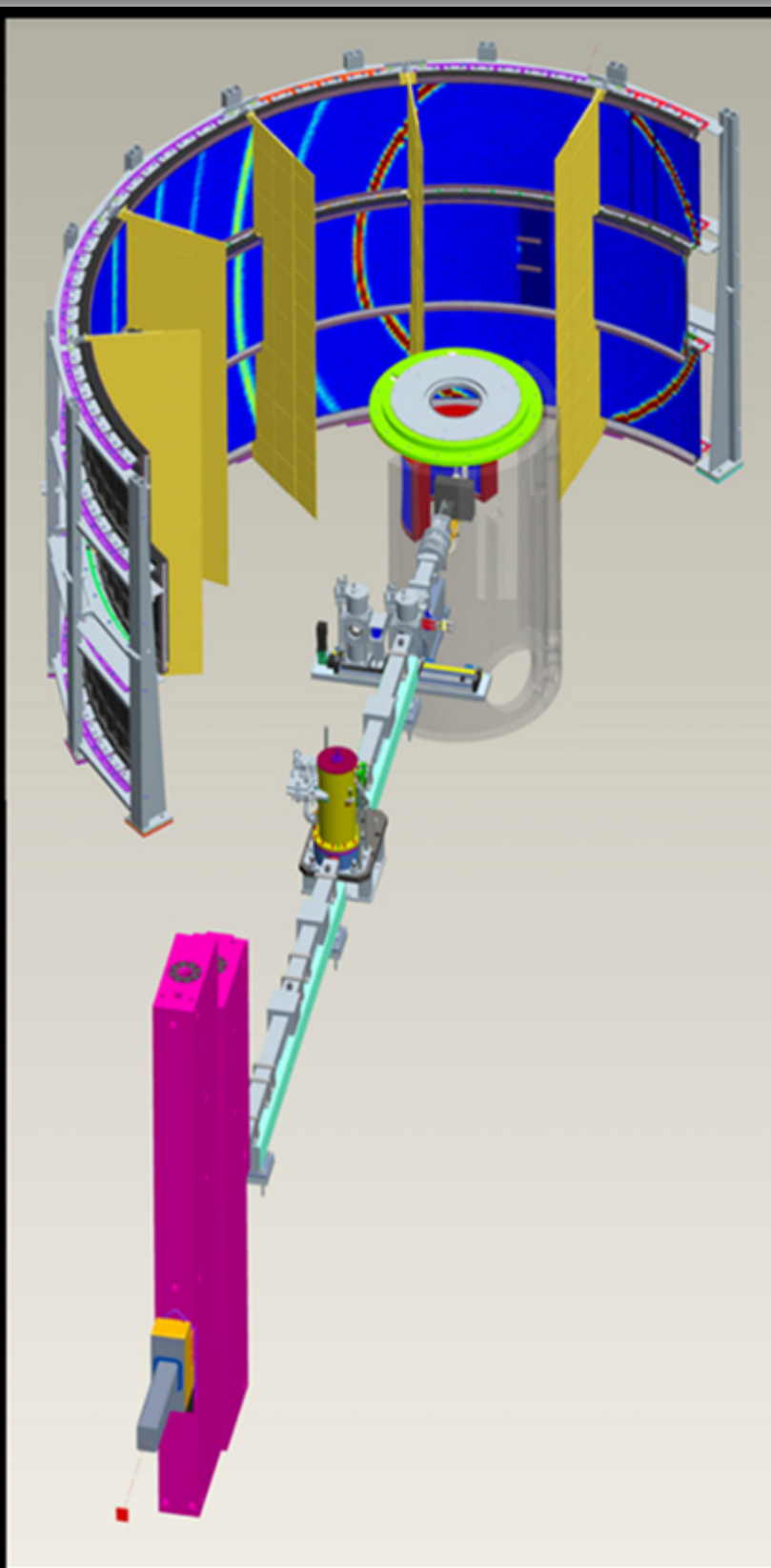
$$v \text{ (km/sec)} = 3.96 / \lambda \text{ (Å)}$$



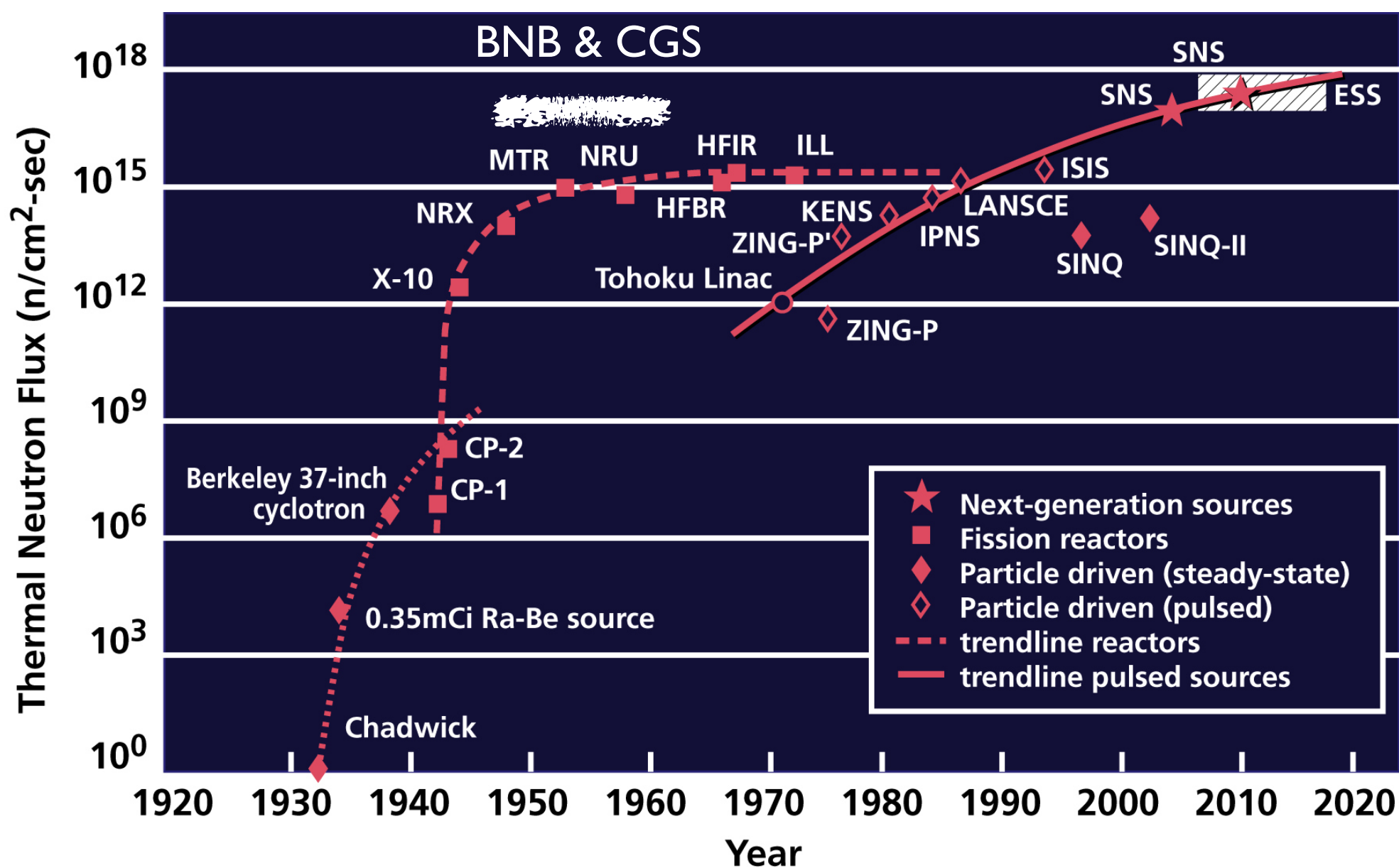
- 4 Å neutrons move at ~ 1 km/sec
- DCS: 4 m from sample to detector
- It takes 4 msec for elastically scattered 4 Å neutrons to travel 4 m
- msec timing of neutrons is easy
- $\delta E / E \sim 1\text{-}3\%$ - very good !

We can measure a neutron's energy, wavelength by measuring its *speed*

Time of Flight Neutron Scattering



Development of Neutron Science Facilities

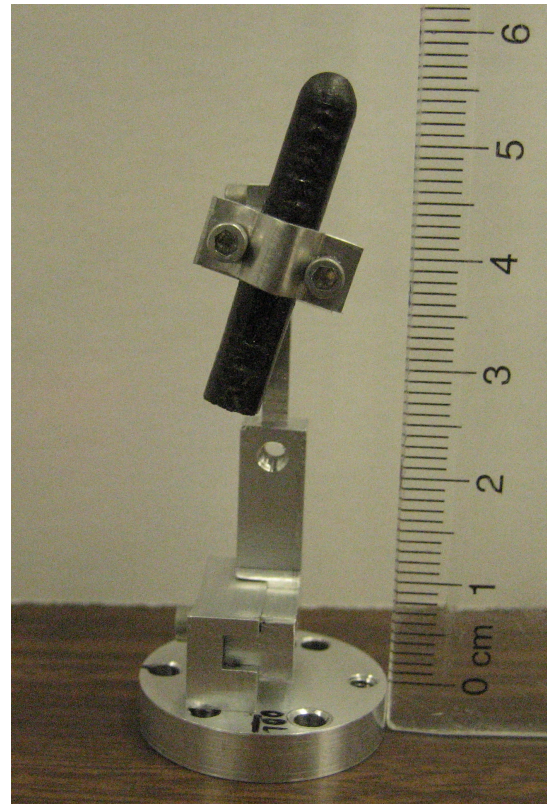


(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)

The Basic Neutron Scattering Experiment



Incident Beam



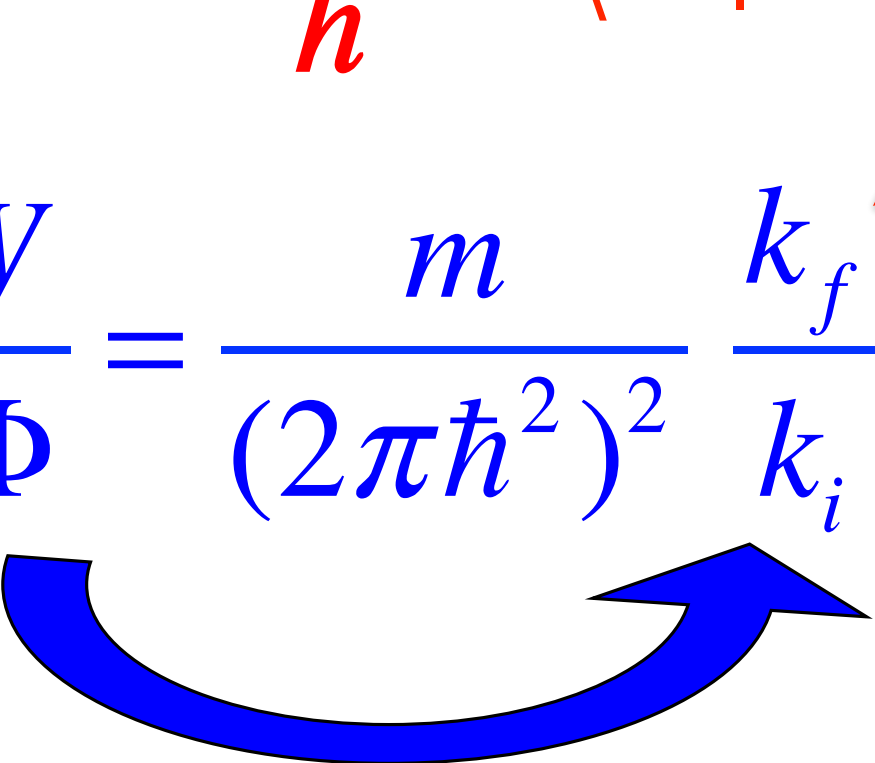
Scattered Beam

- **Monochromatic**
- **“White”**
- **“Pink”**

- **Resolve its energy**
- **Don't resolve its energy**
- **Filter its energy**

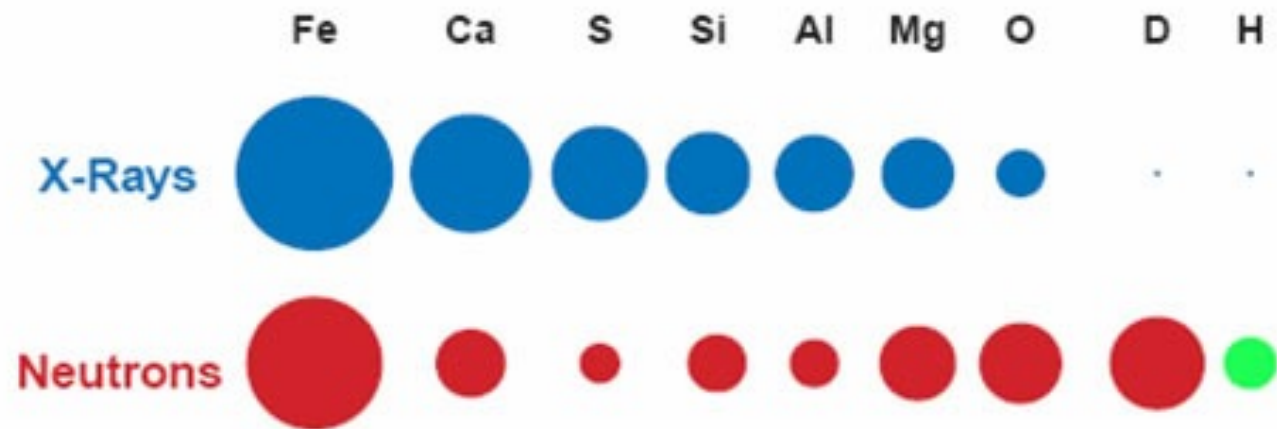
Fermi's Golden Rule within the 1st Born approximation

$$W = \frac{2\pi}{\hbar} |\langle f | V | i \rangle|^2 \rho(E_f)$$

$$\frac{\partial \sigma}{\partial \Omega} = \frac{W}{\Phi} = \frac{m}{(2\pi\hbar^2)^2} \frac{k_f}{k_i} |\langle f | V | i \rangle|^2 \partial \Omega$$


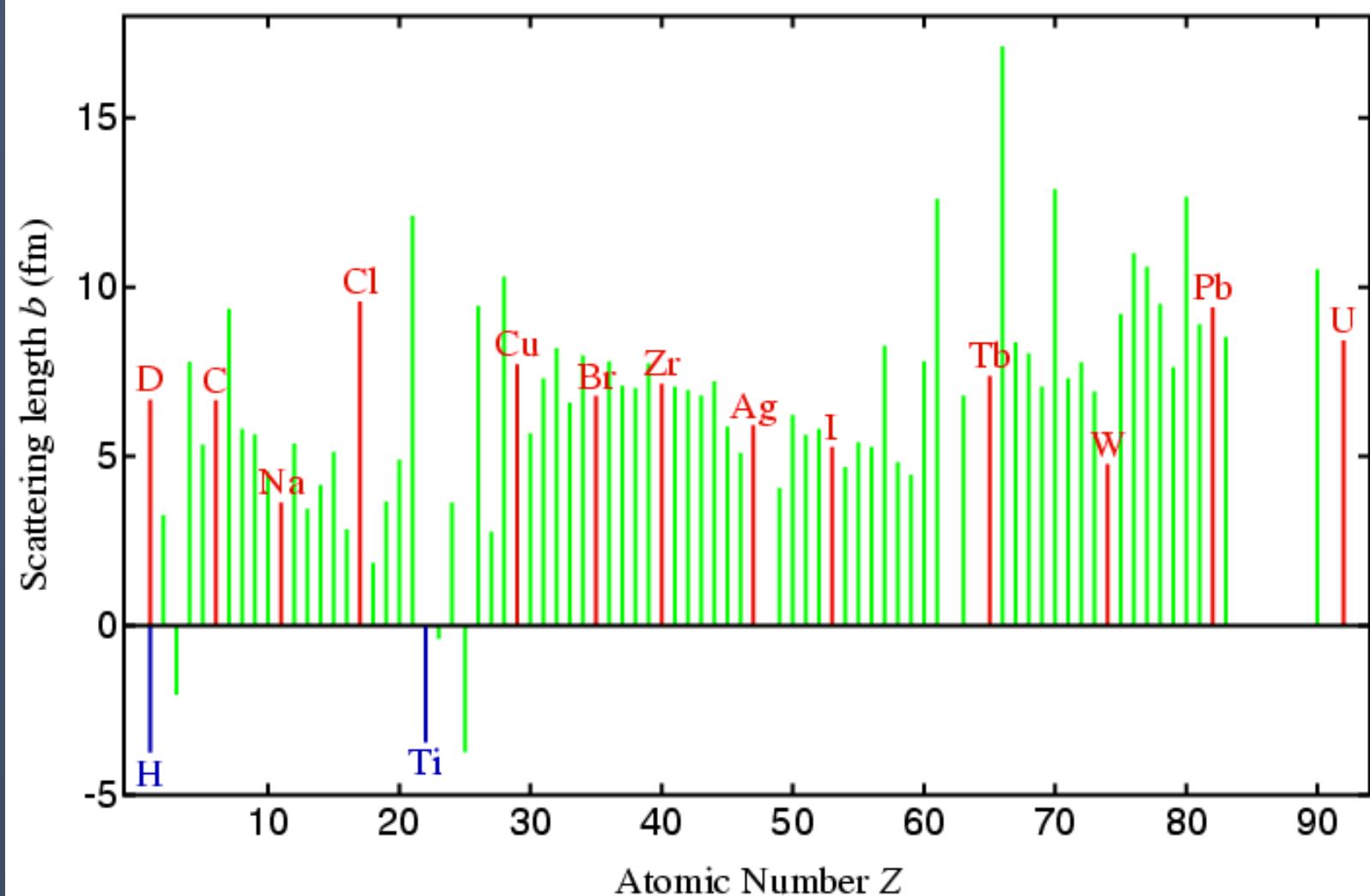
$$\frac{\partial^2 \sigma}{\partial \Omega \partial E_f} = \frac{k_f}{k_i} \frac{\sigma_{coherent}}{4\pi} N S_{coherent}(\vec{Q}, \hbar\omega)$$

Neutrons scatter off *nuclei*



**Neutrons “see”
nuclei and
magnetism**

**X-rays -
electromagnetic
radiation
“see” electrons**



Dipole moment of the neutron interacts with the magnetic field generated by the electron

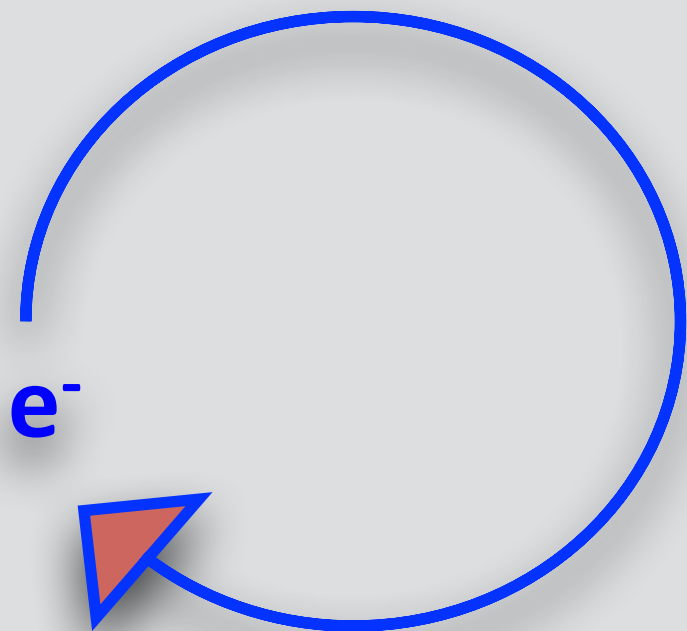
$$\mu_n = -\gamma \mu_N \sigma$$

$$\gamma = 1.913$$

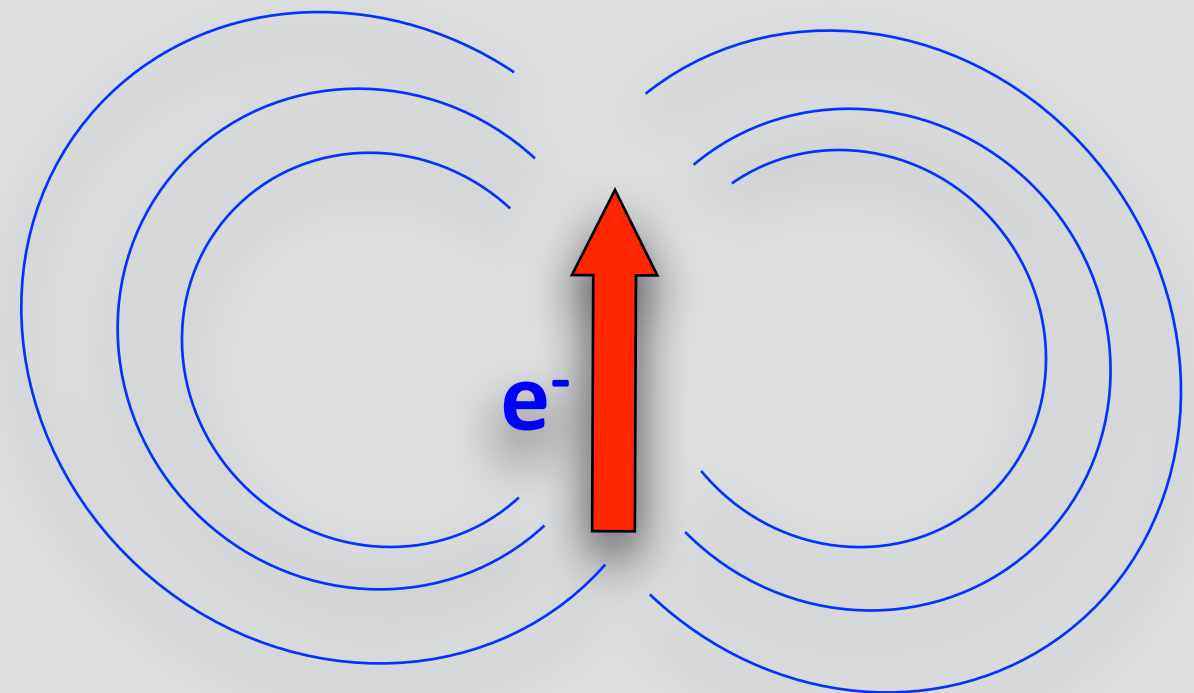
$$\text{nuclear magneton} = e \hbar / 2m_n$$

Pauli spin operator

$$V_M = -\vec{\mu}_n \cdot \vec{B}_{\text{electrons}}$$



Dipole field due to orbital currents

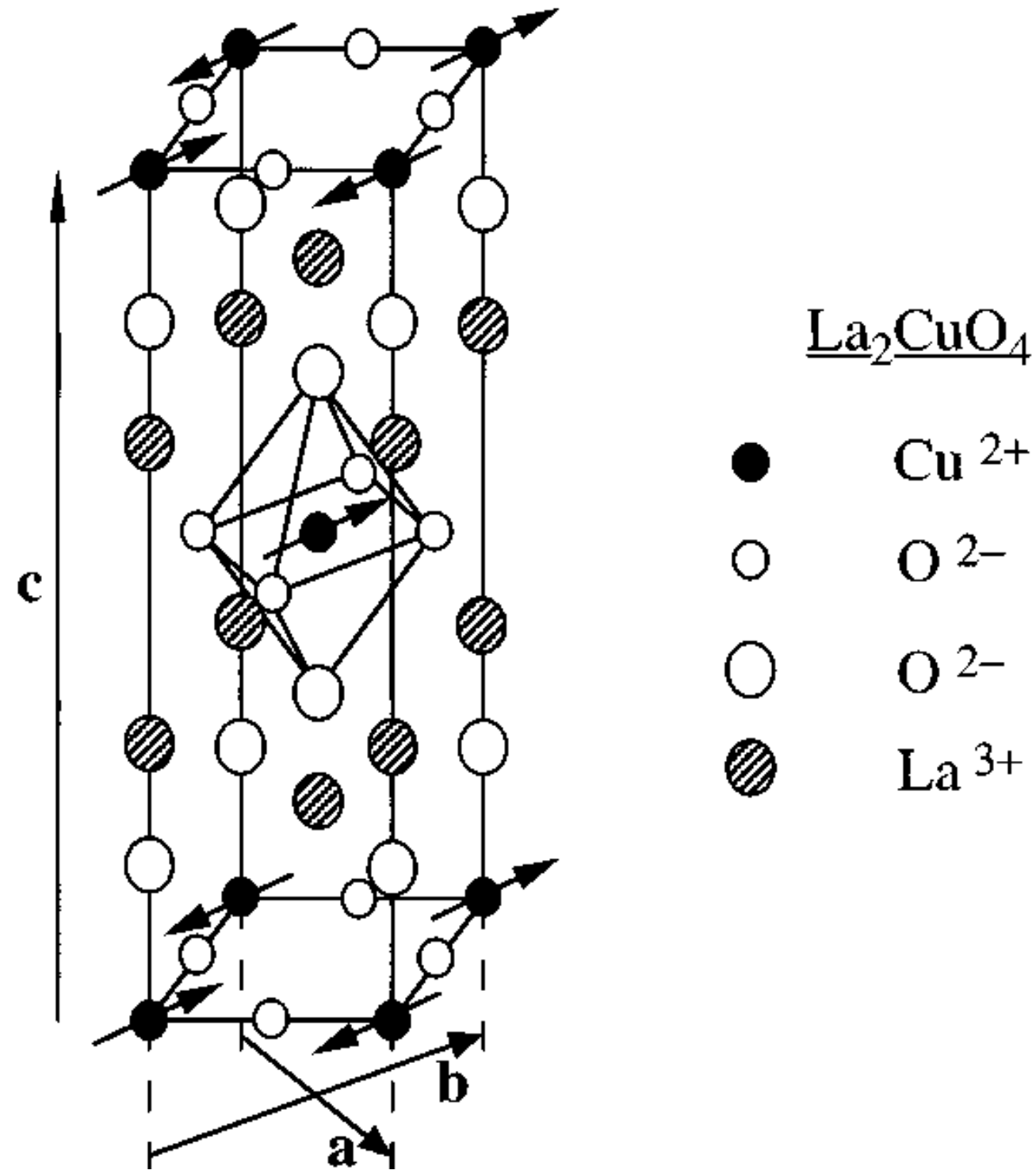


Dipole field due to Spin of the electron(s)

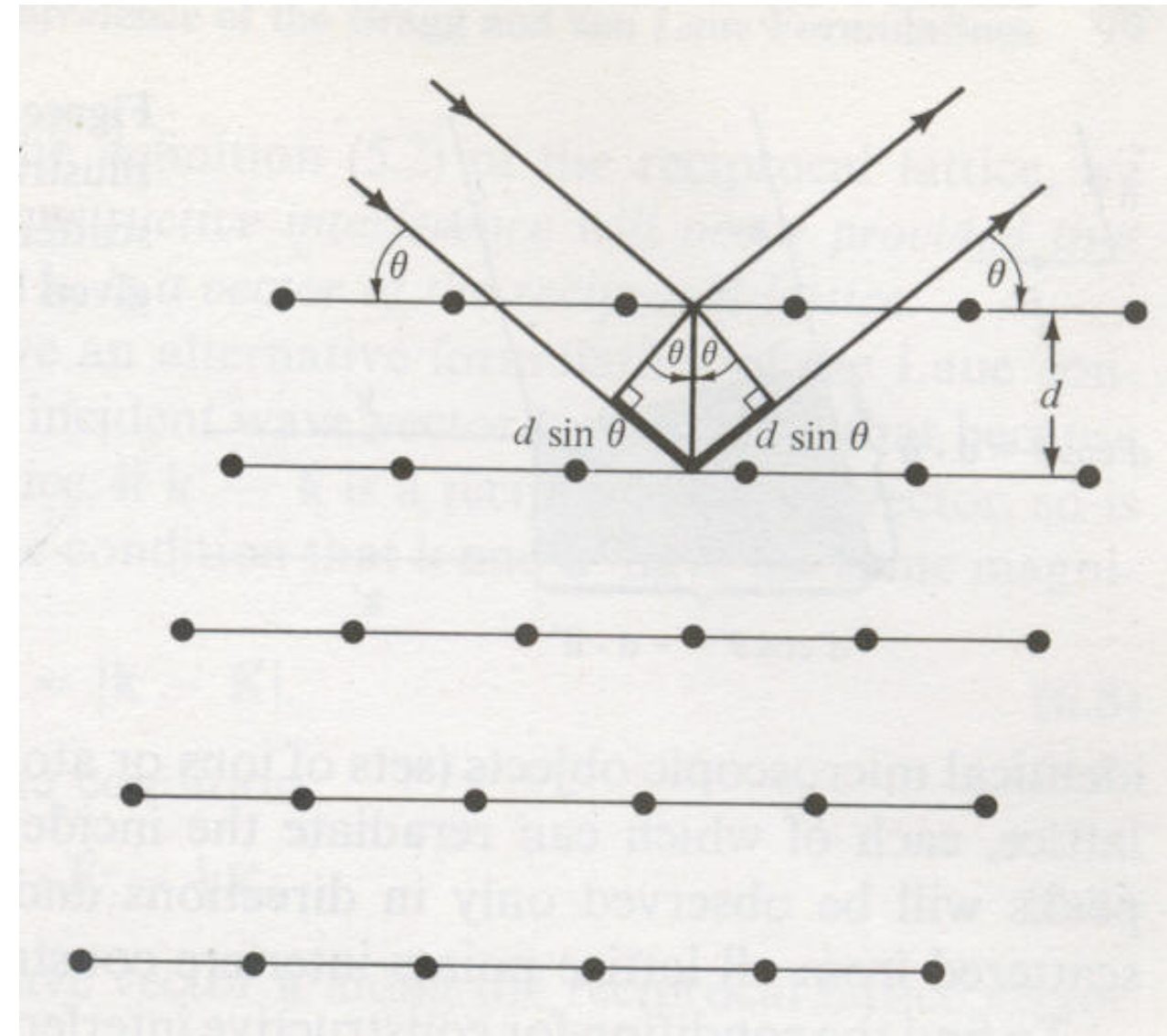
“Killer Applications” for Neutron Scattering

- **Magnetism**
- **Hydrogenous materials**
- **4D $\vec{Q}, \hbar\omega$ studies**
- **Studies at depth**

What are we typically trying to understand?



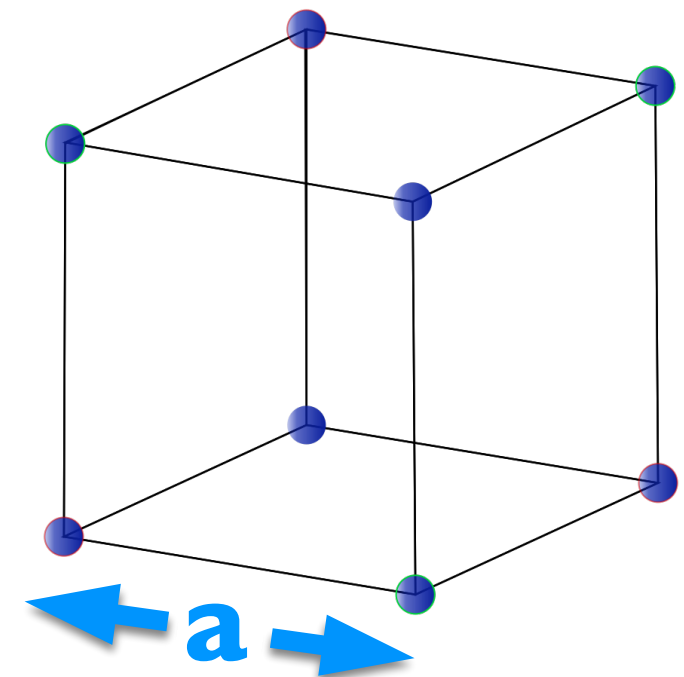
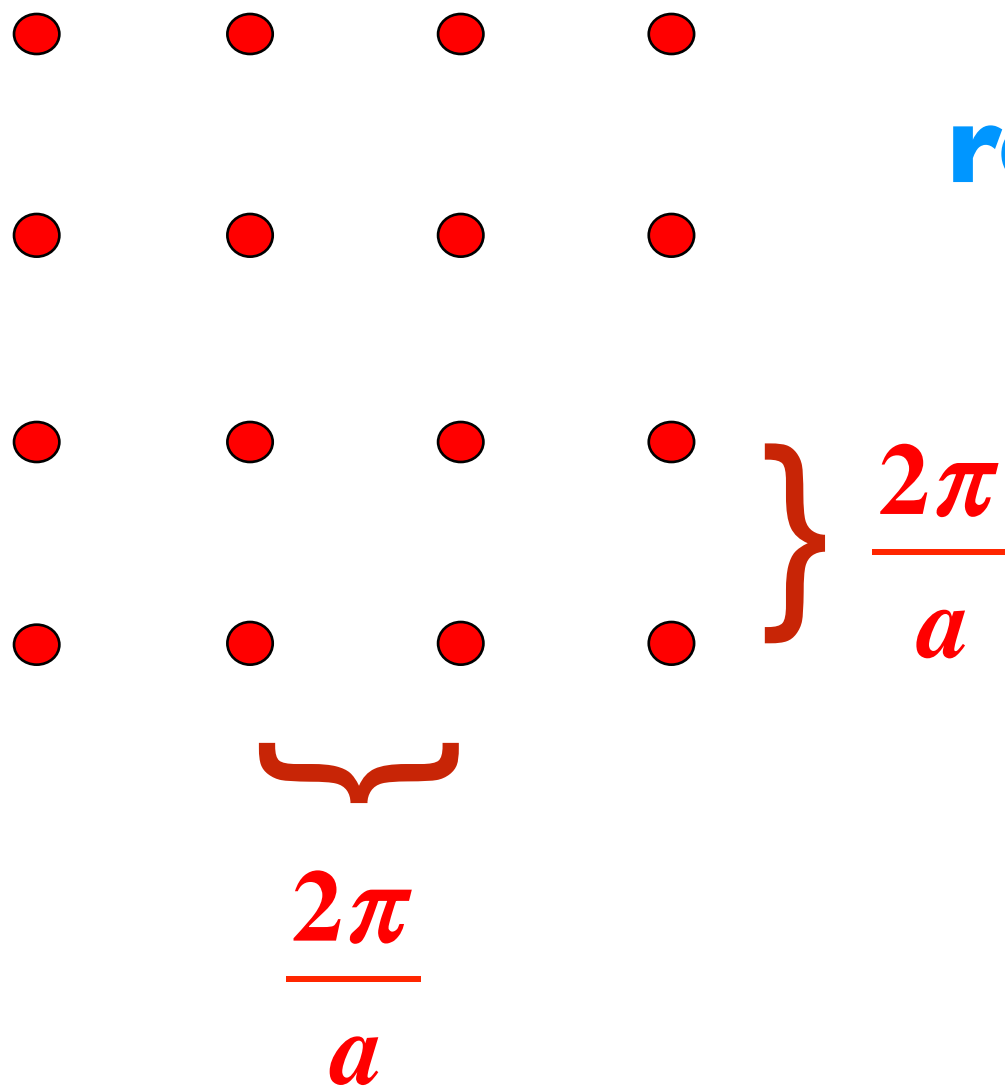
Bragg's law: $n\lambda = 2d \sin(\theta)$



- **What is the atomic and magnetic structure of new materials?**
- **What are the dynamic properties of the atoms and the magnetic moments?**
- **How are structure and dynamics related to physical properties?**

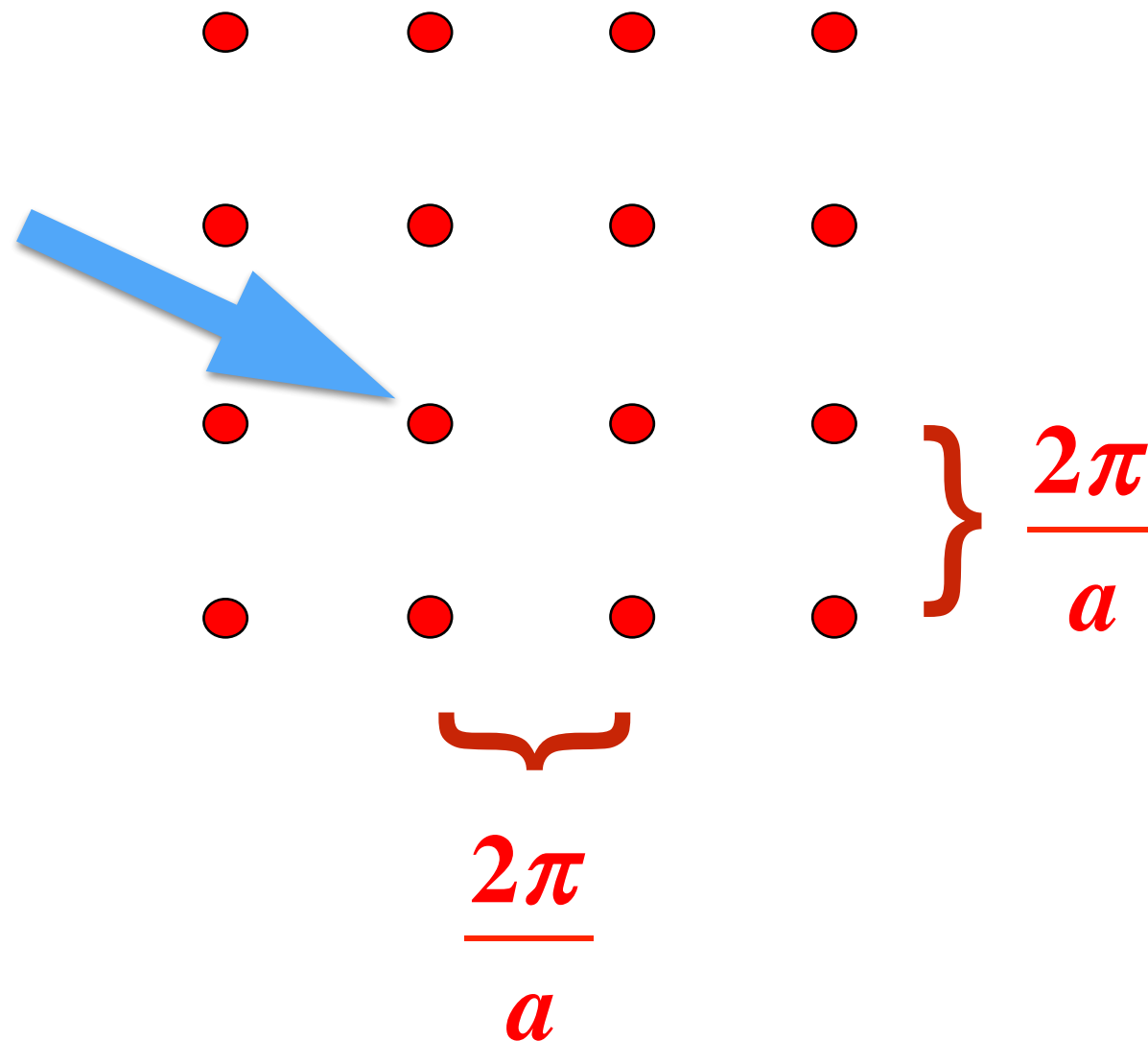
Diffraction in Momentum (Q) space

**In momentum space,
our sample is
represented
by its
reciprocal lattice**



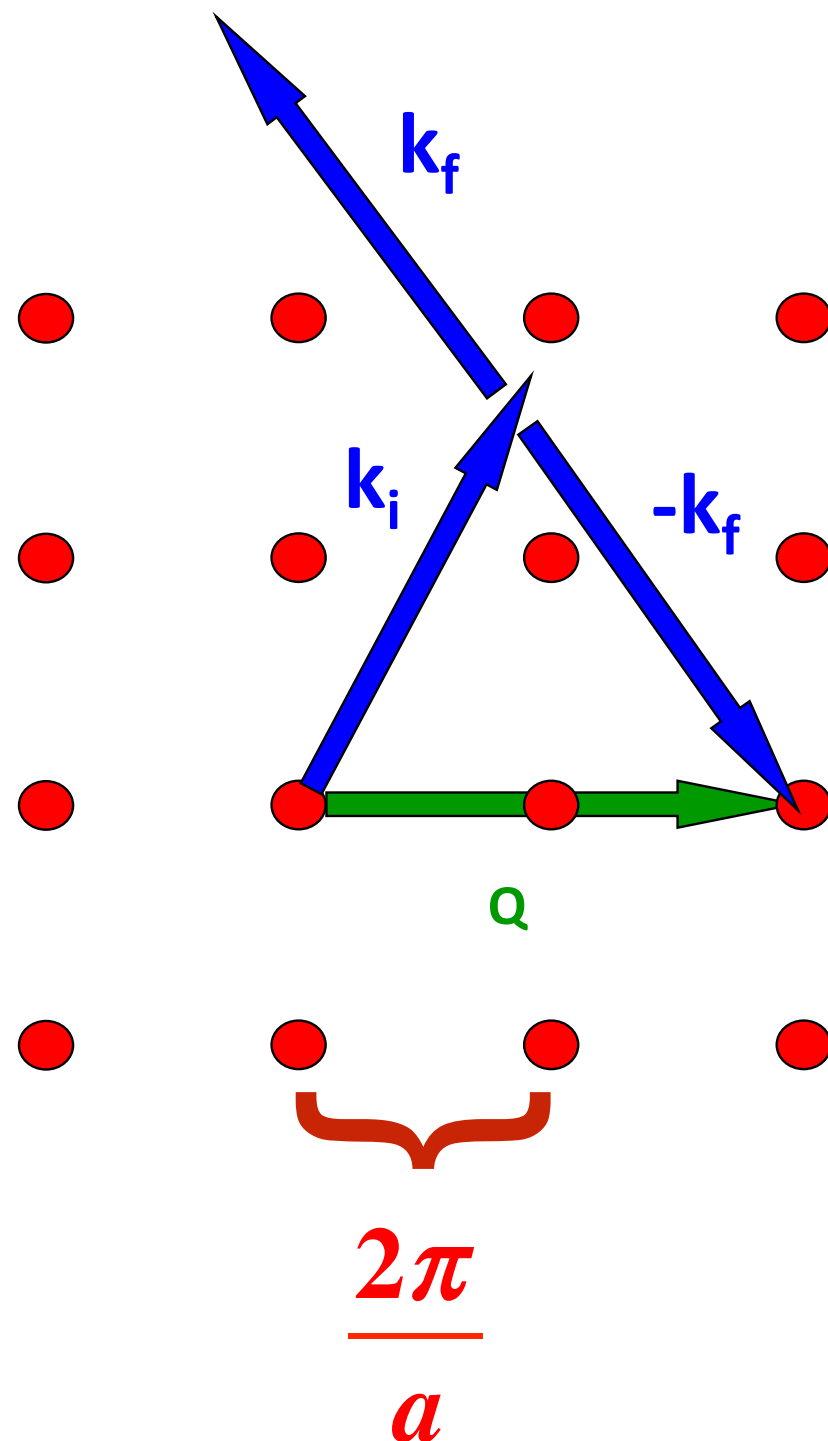
Diffraction in Momentum (Q) space

**Origin of
reciprocal
space**



**Remains
fixed for
all sample
orientations**

Diffraction in Momentum (Q) space



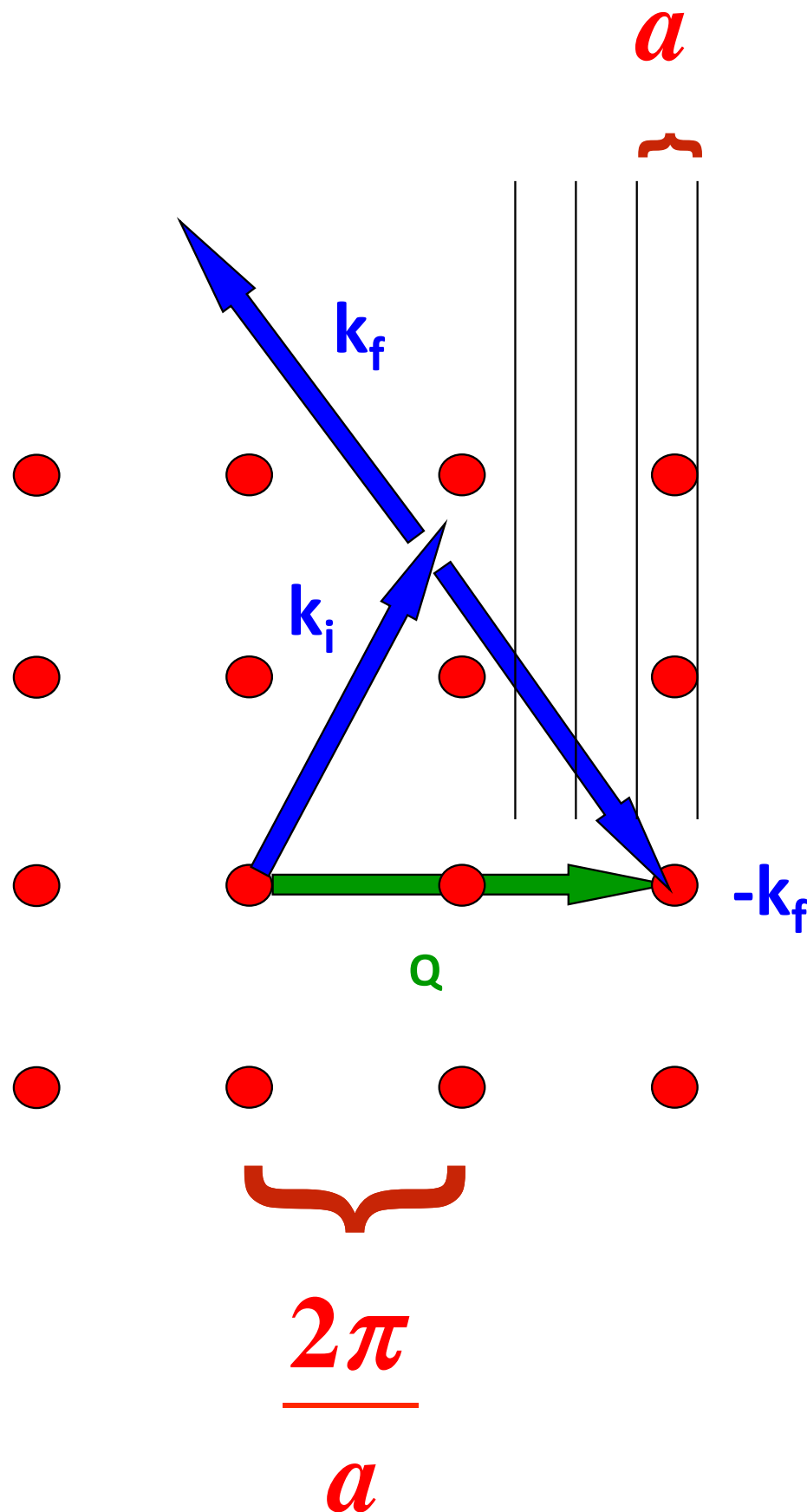
Bragg diffraction

**constructive
interference when**

$$\vec{Q} = \vec{k}_i - \vec{k}_f = \vec{\tau}$$

**= a reciprocal lattice
vector**

Diffraction in Momentum (Q) space



Bragg diffraction

**constructive
interference when**

$$\vec{Q} = \vec{k}_i - \vec{k}_f = \vec{\tau}$$

**= a reciprocal lattice
vector**

Phonon Polarizations



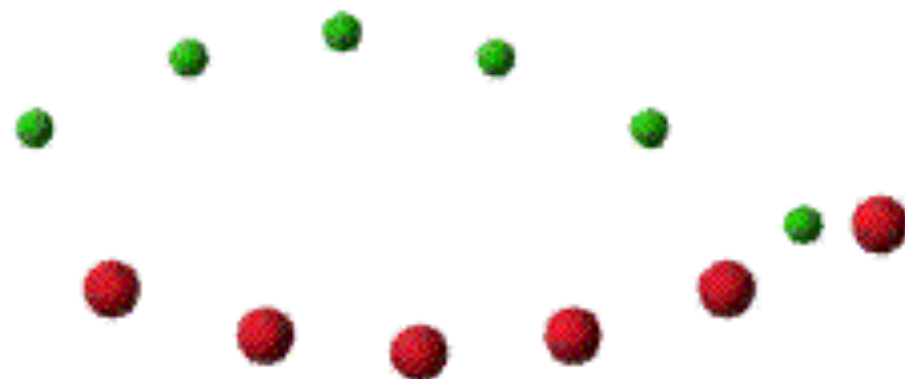
Longitudinal Acoustic



Transverse Acoustic

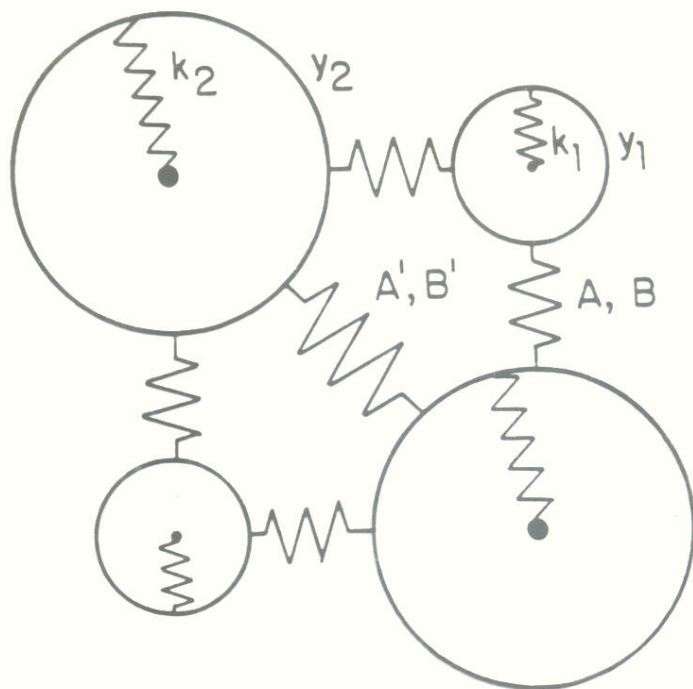
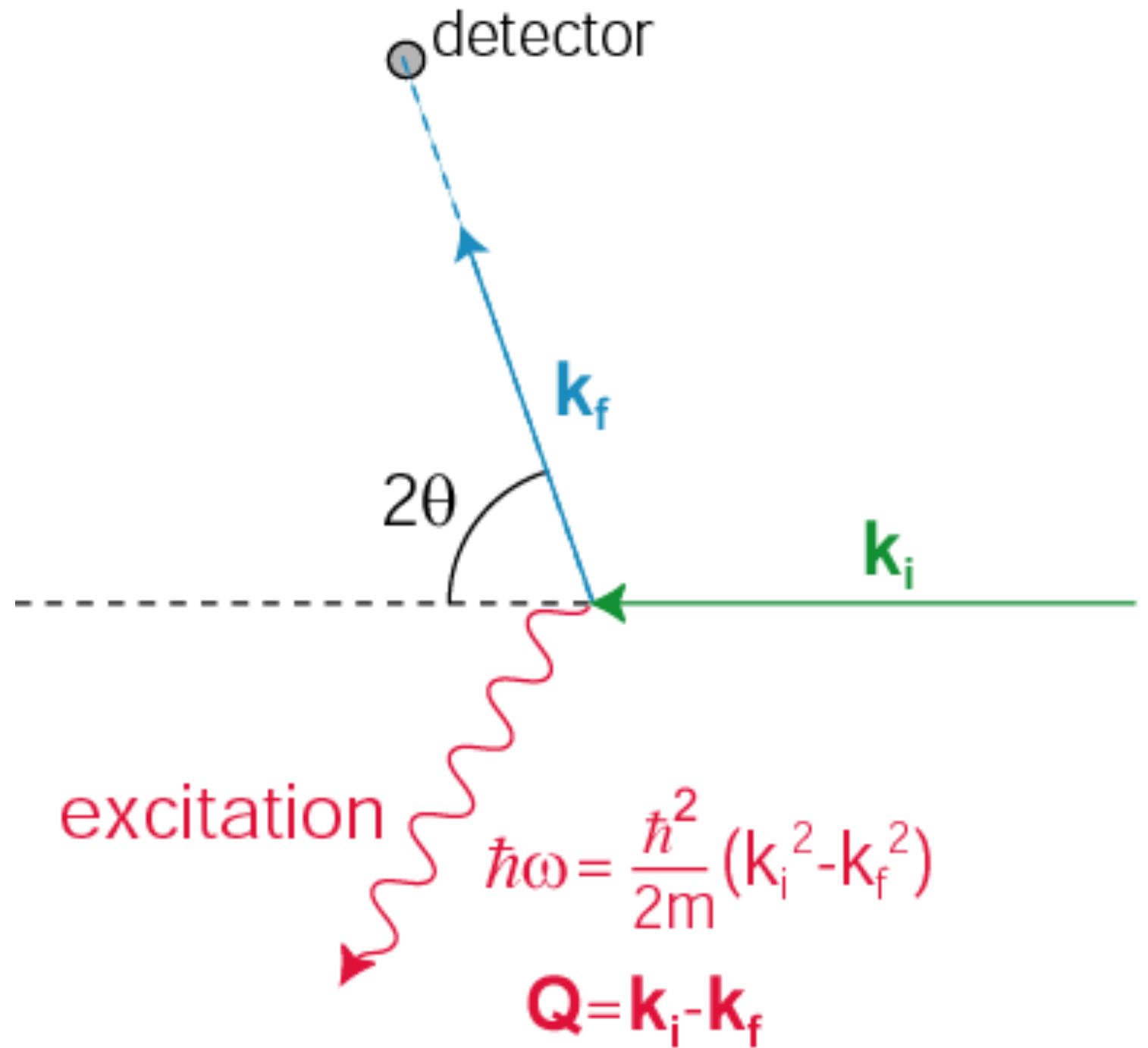
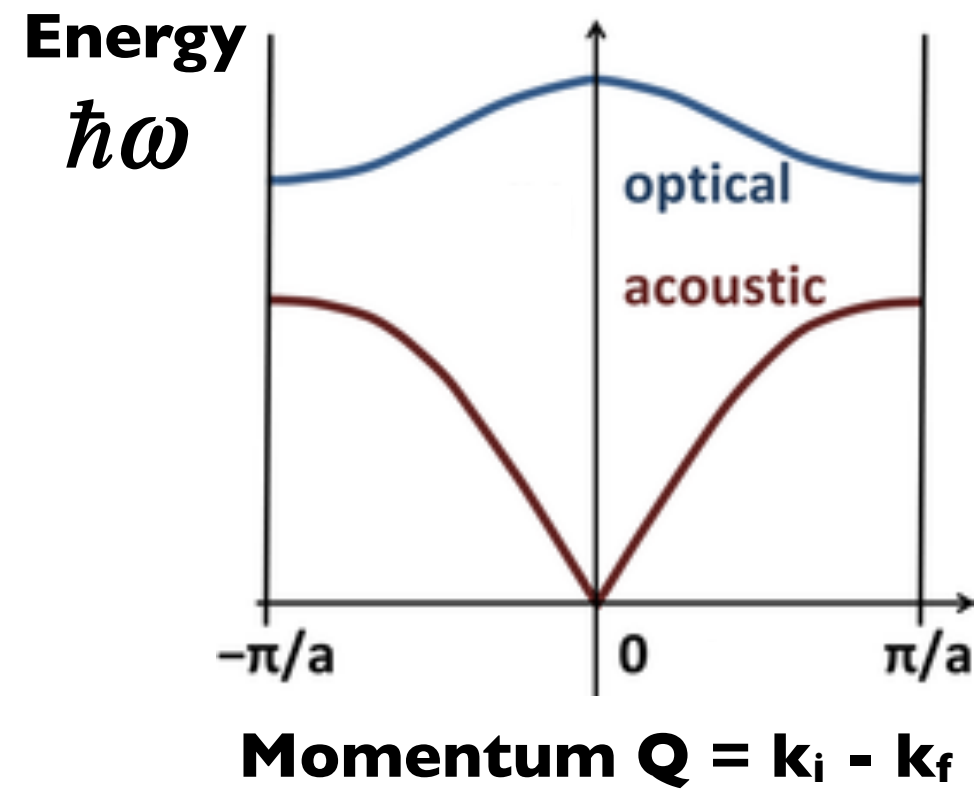


Transverse Acoustic

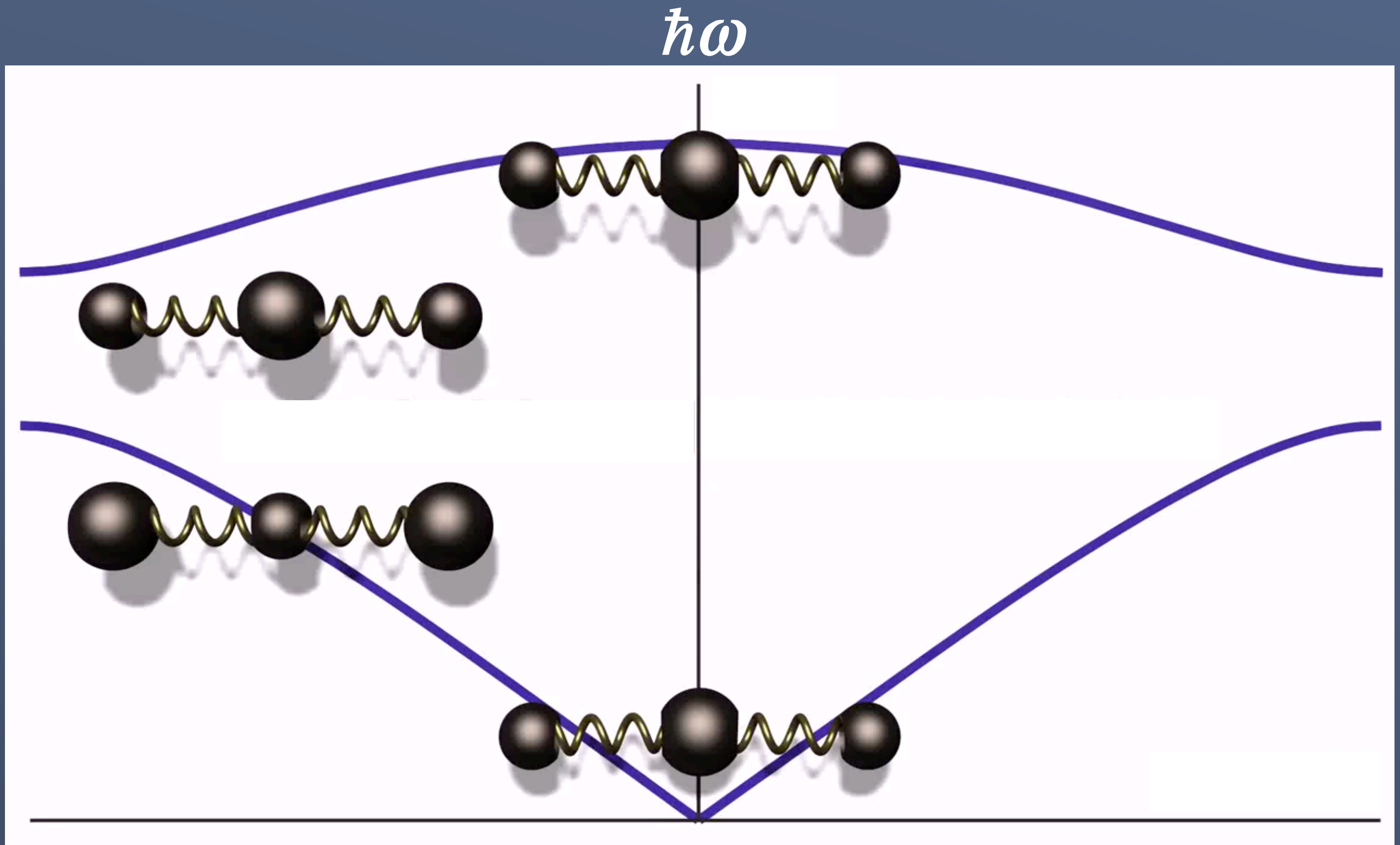


Transverse Optic

Elementary Excitations

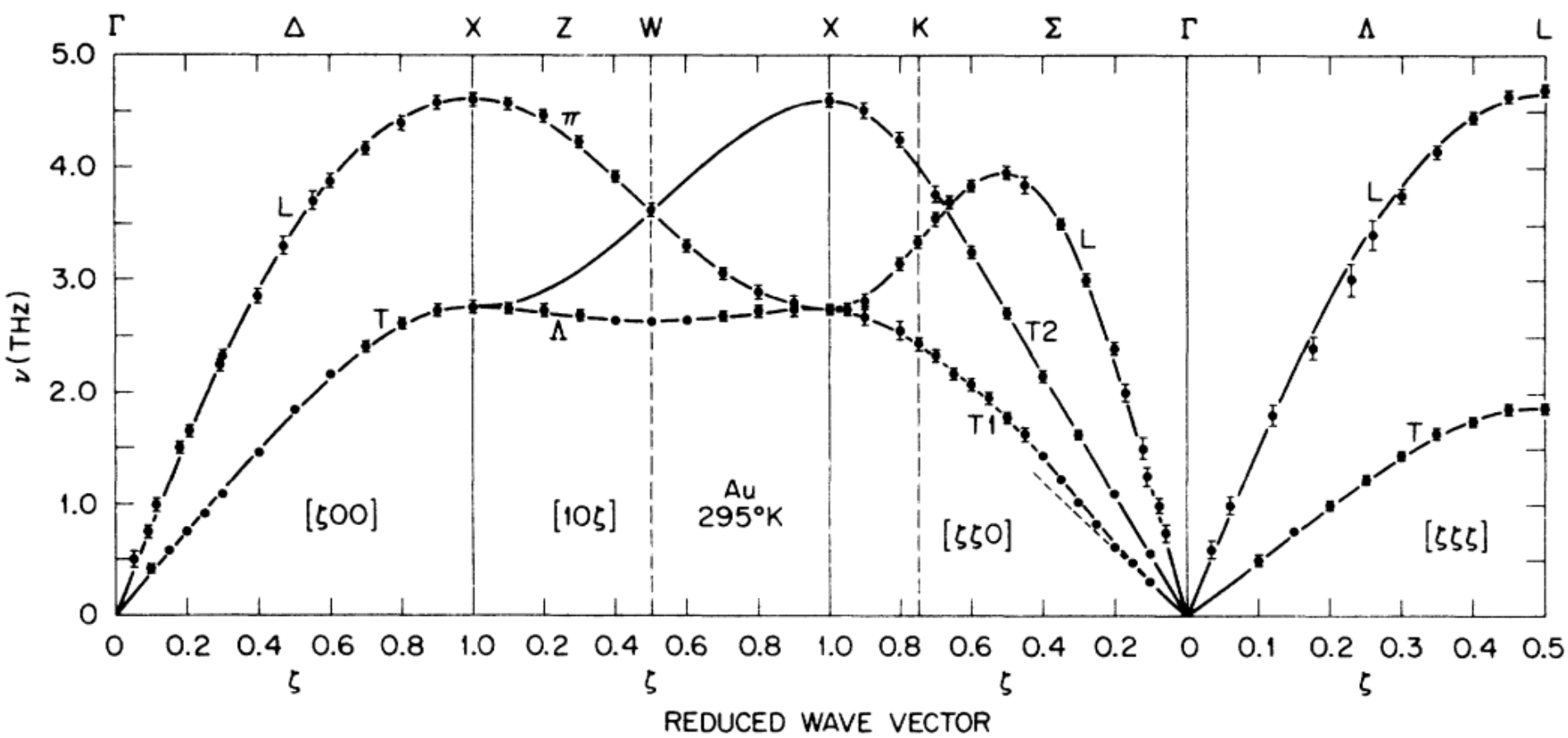


Phonon eigenvectors and eigenvalues

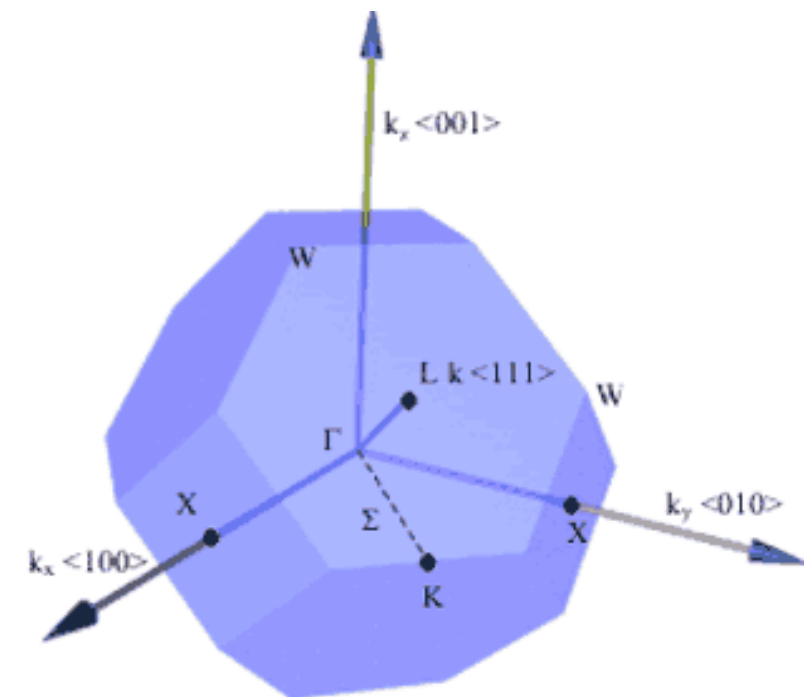
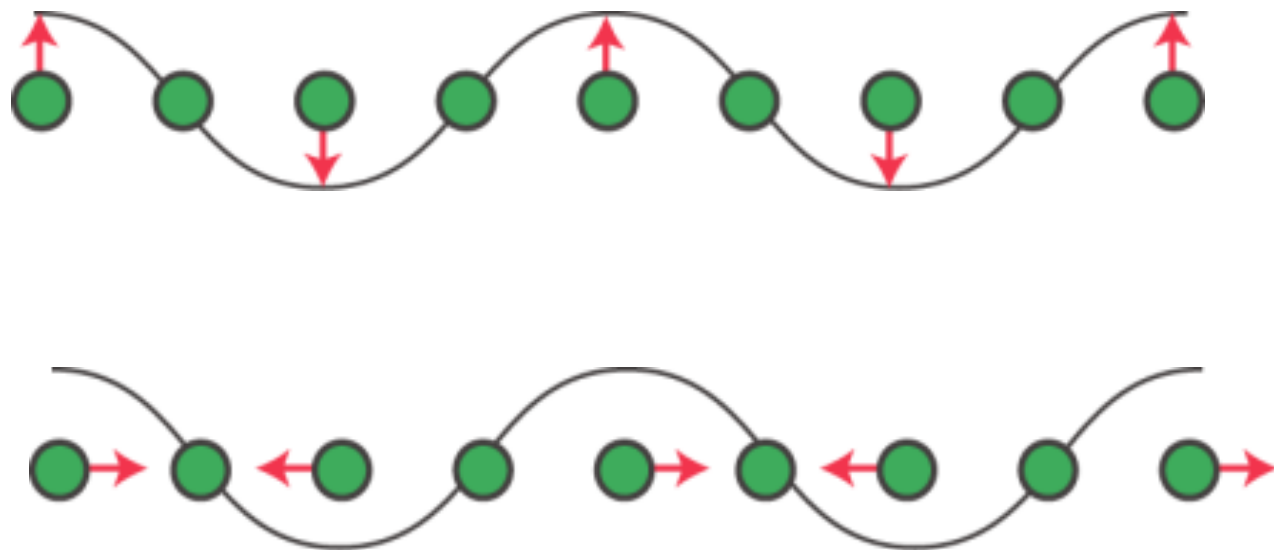
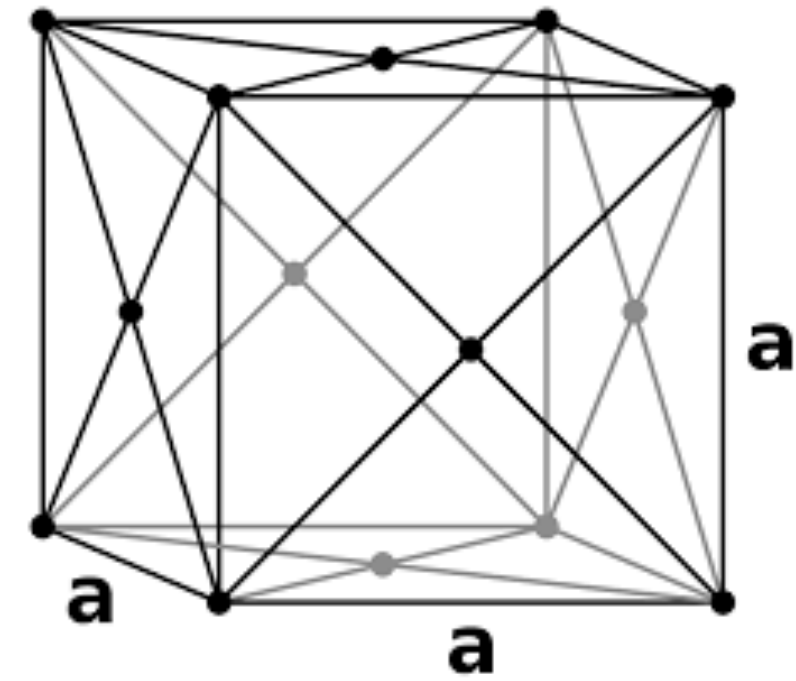


Momentum $Q = k_i - k_f$

Phonons in 3D

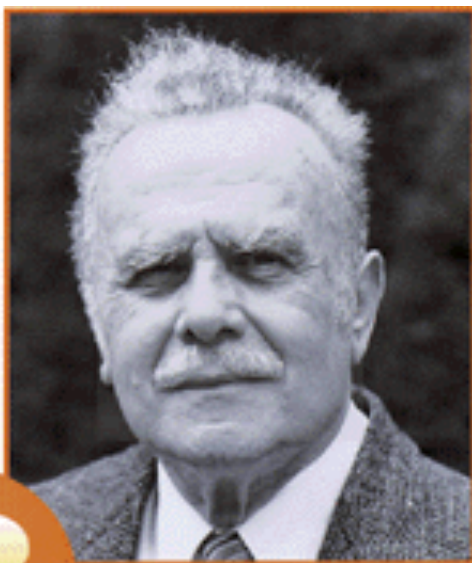


Lynn, et al., *Phys. Rev. B* **8**, 3493 (1973).

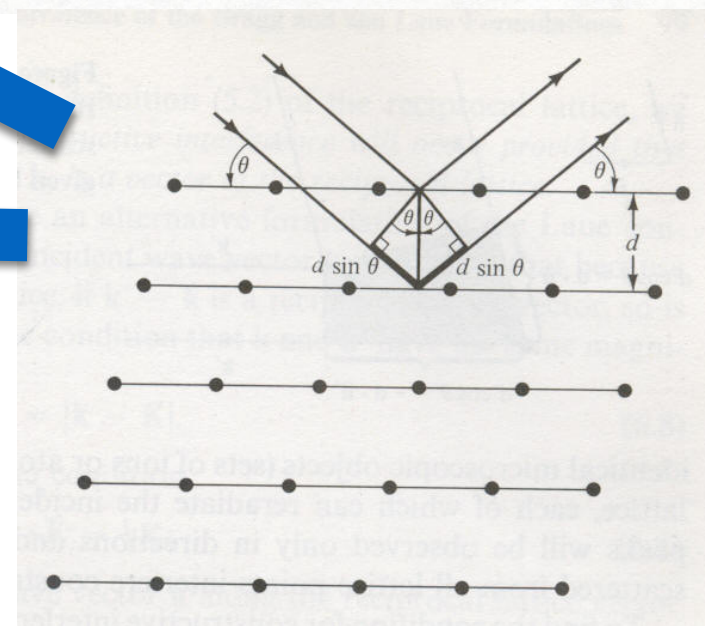
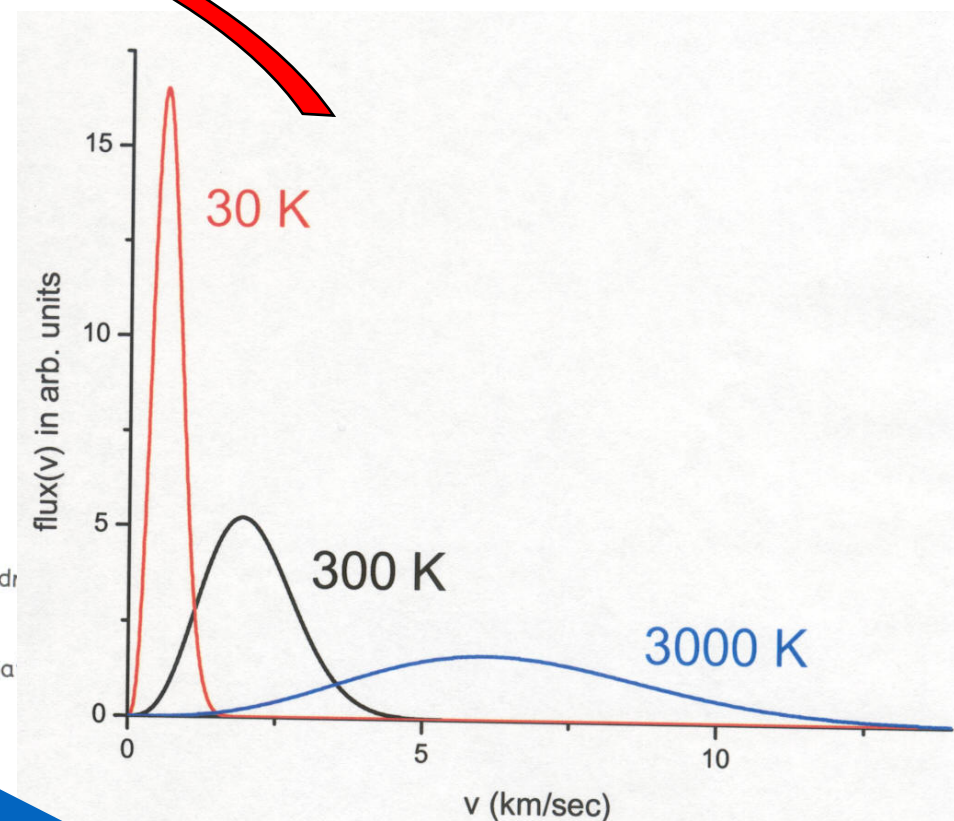
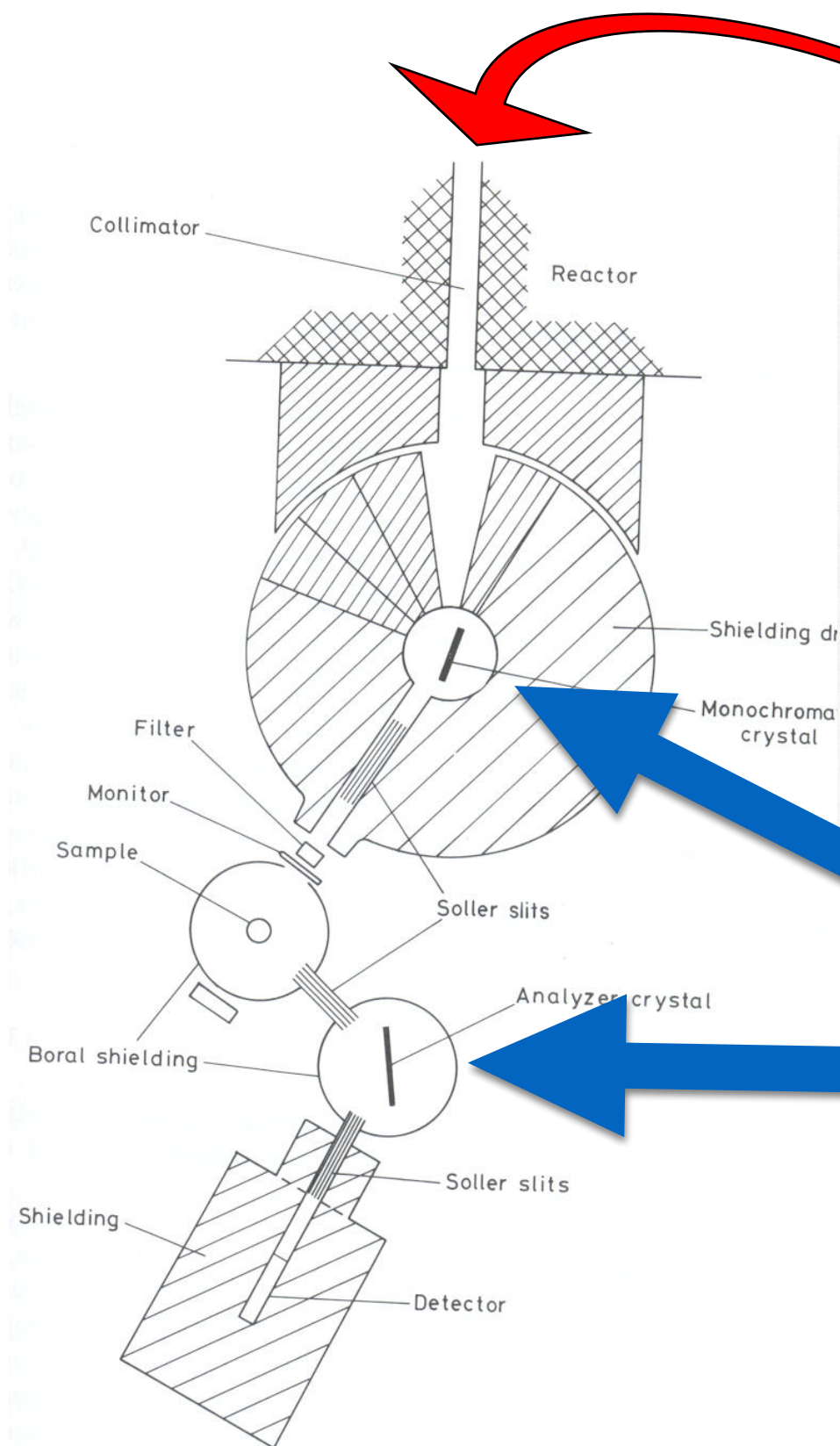


FCC Brillouin zone

Brockhouse's Triple Axis Spectrometer

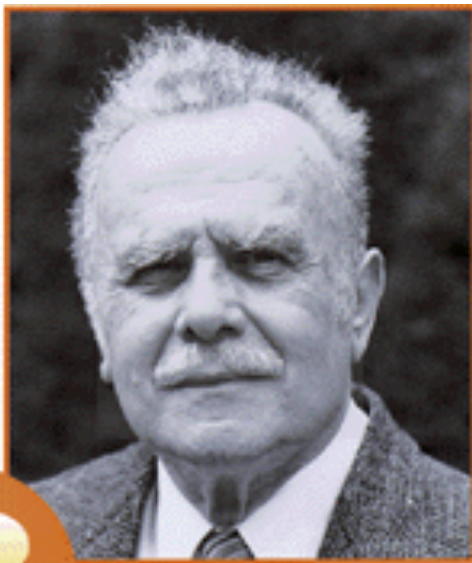


Betram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.

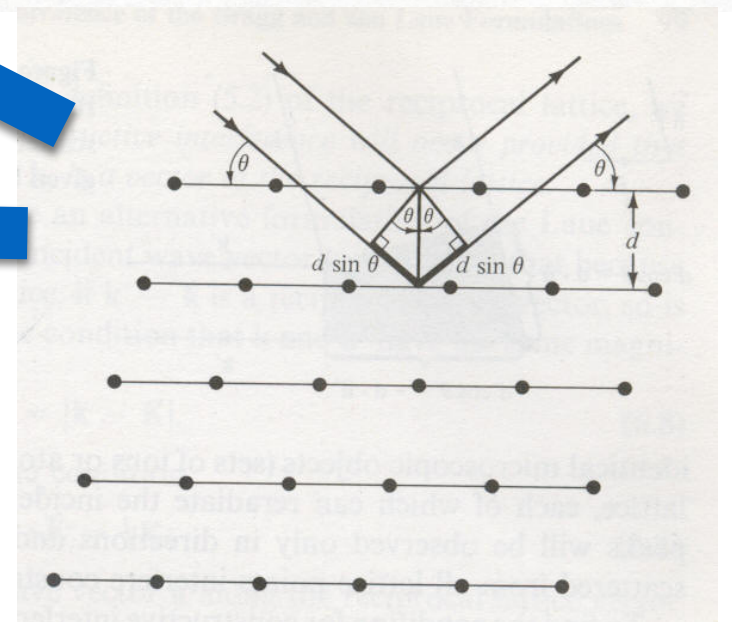
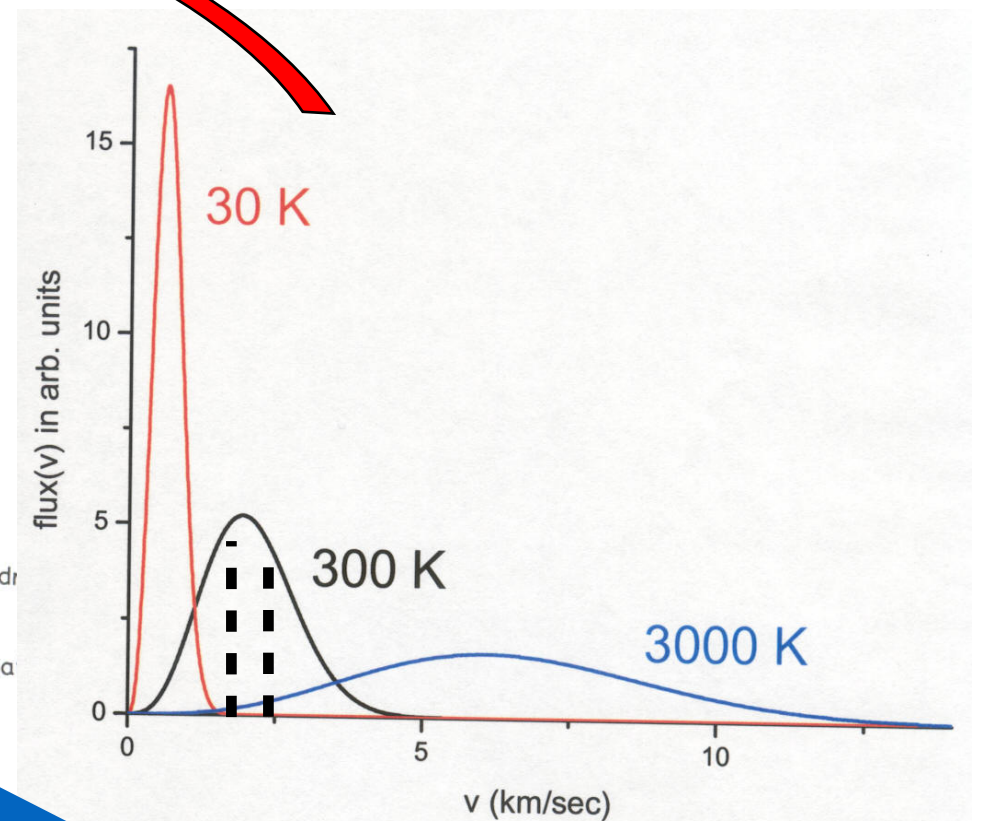
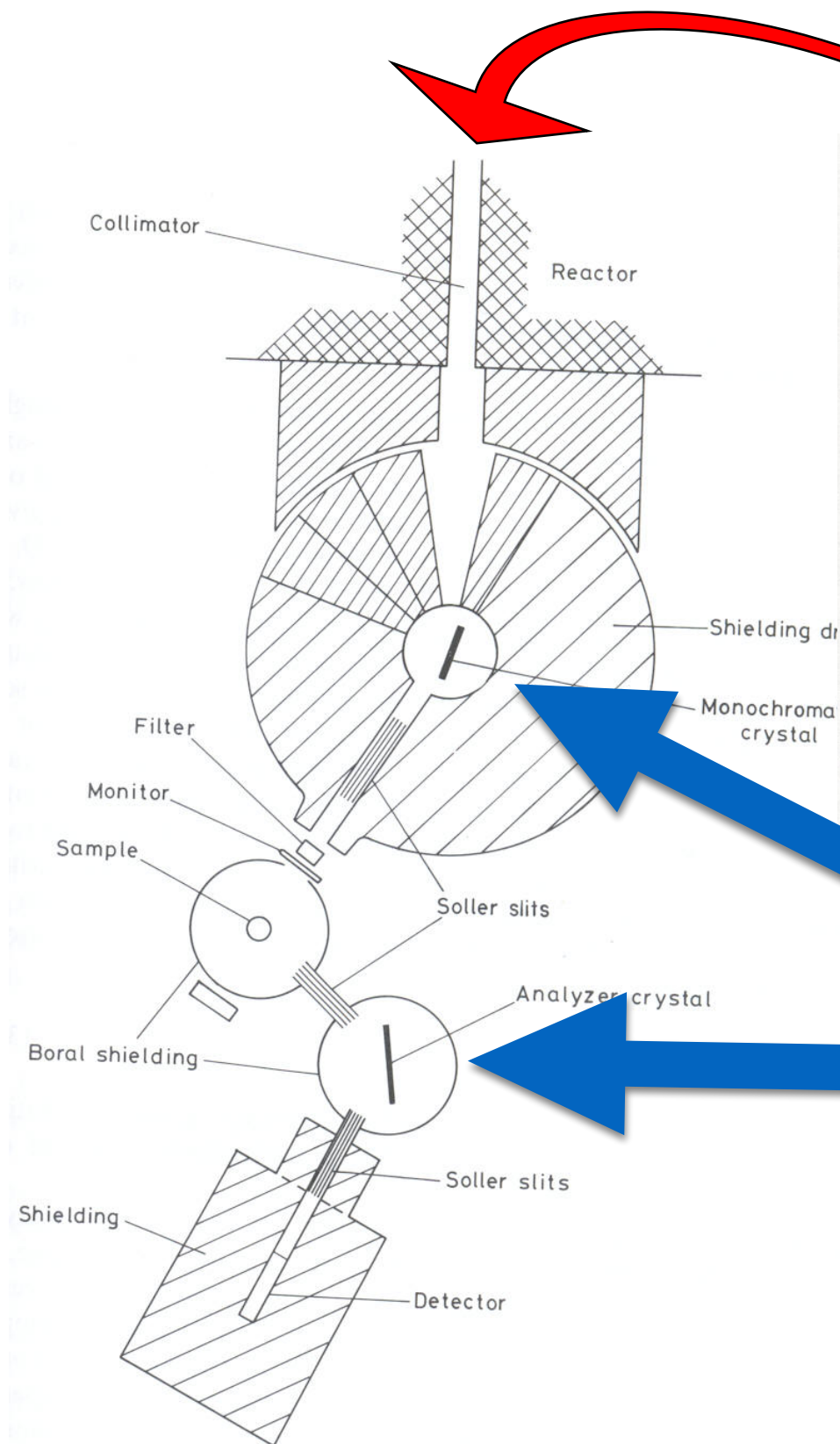


$$n\lambda = 2d \sin \theta$$

Brockhouse's Triple Axis Spectrometer

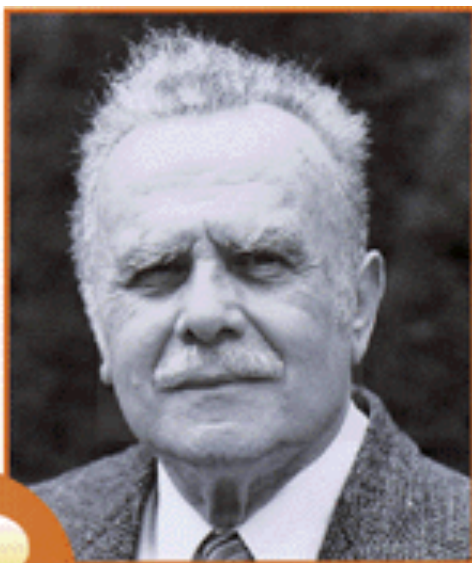


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$$n\lambda = 2d \sin \theta$$

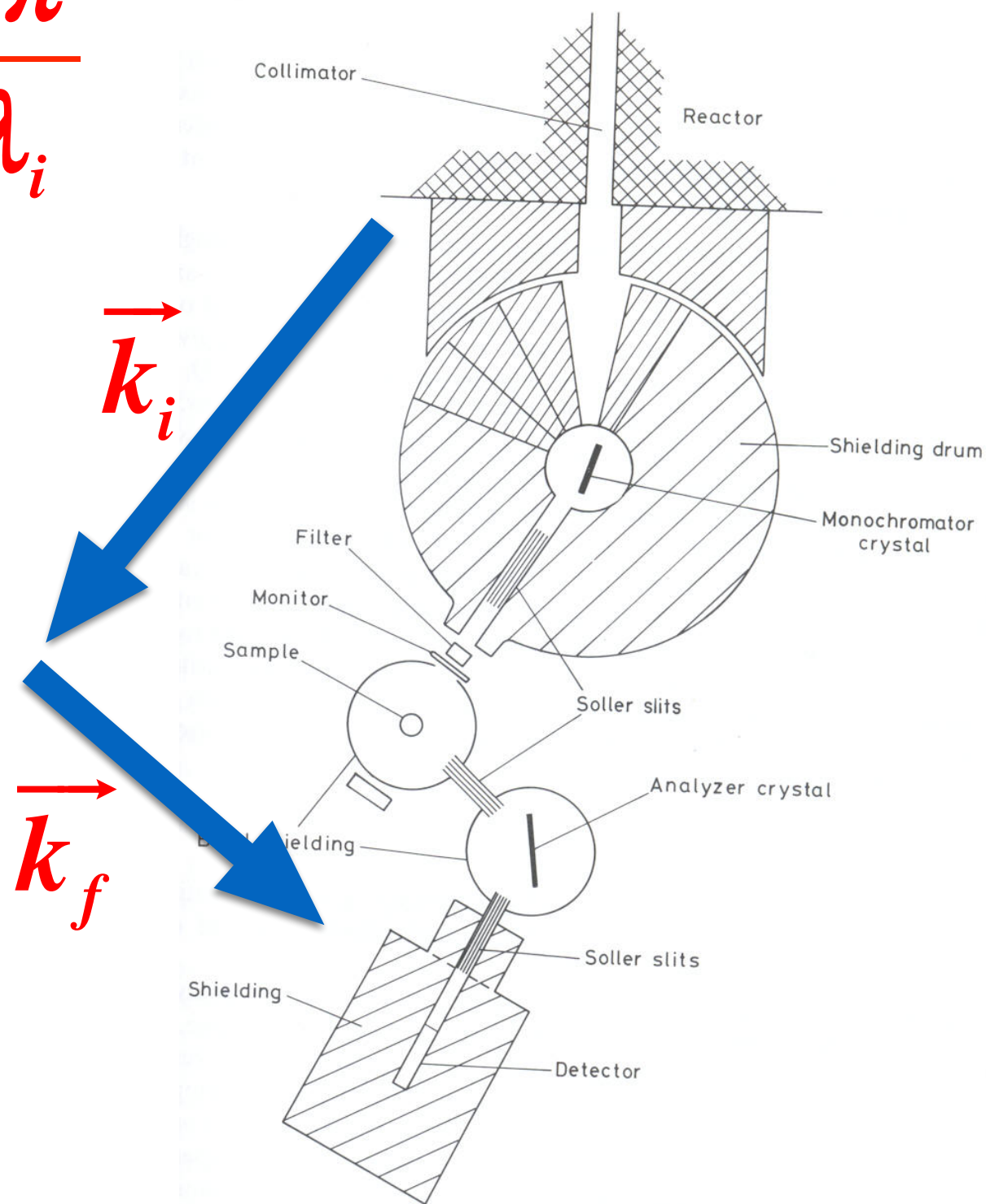
Brockhouse's Triple Axis Spectrometer



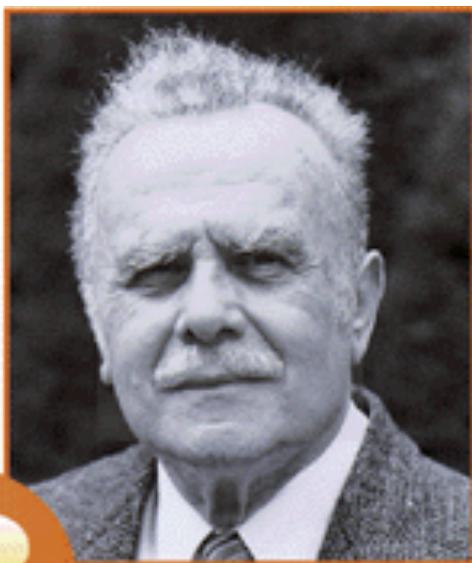
Betram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.

$$|\vec{k}_i| = \frac{2\pi}{\lambda_i}$$

$$|\vec{k}_f| = \frac{2\pi}{\lambda_f}$$



Brockhouse's Triple Axis Spectrometer



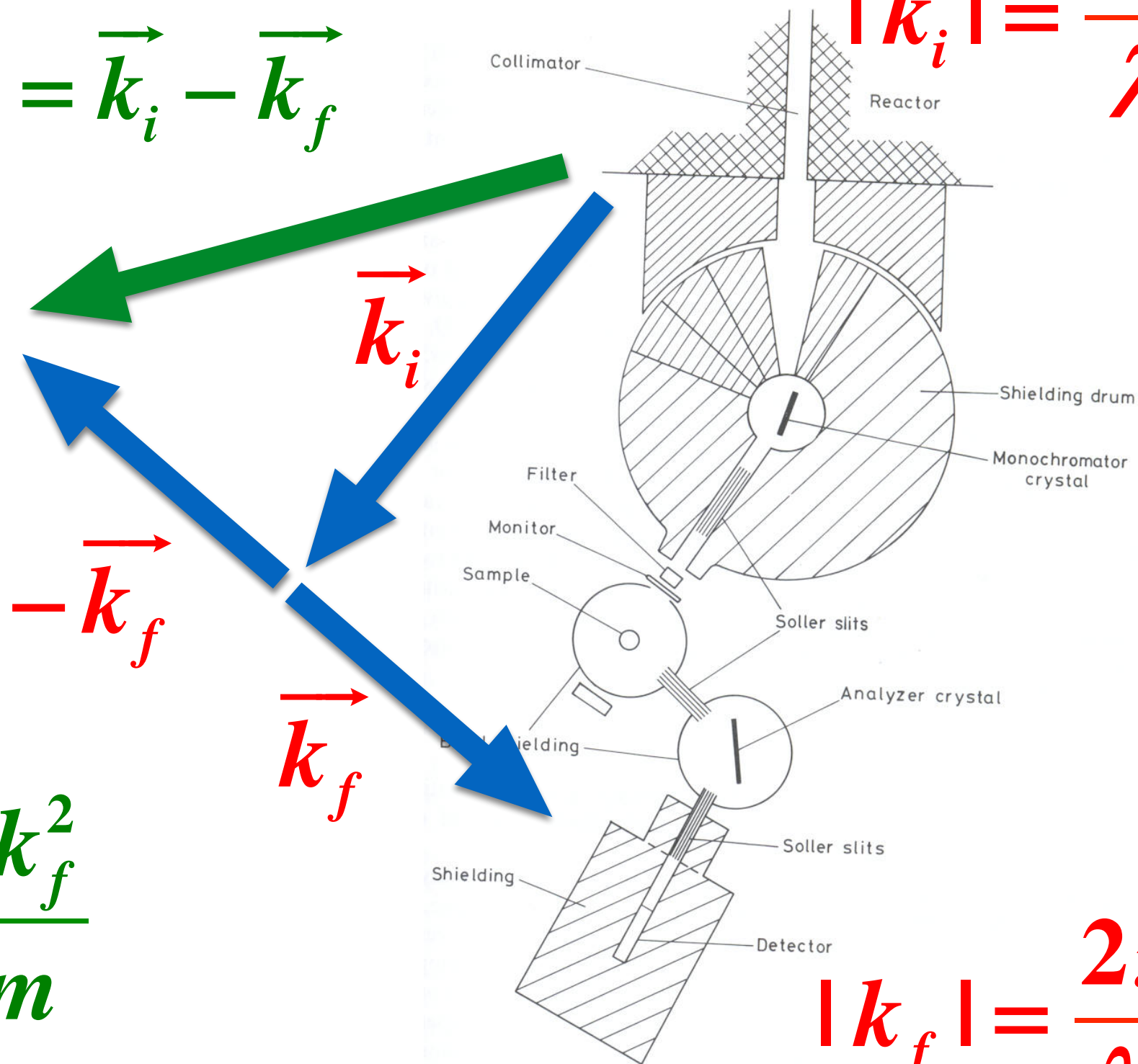
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$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

$$|\vec{k}_i| = \frac{2\pi}{\lambda_i}$$

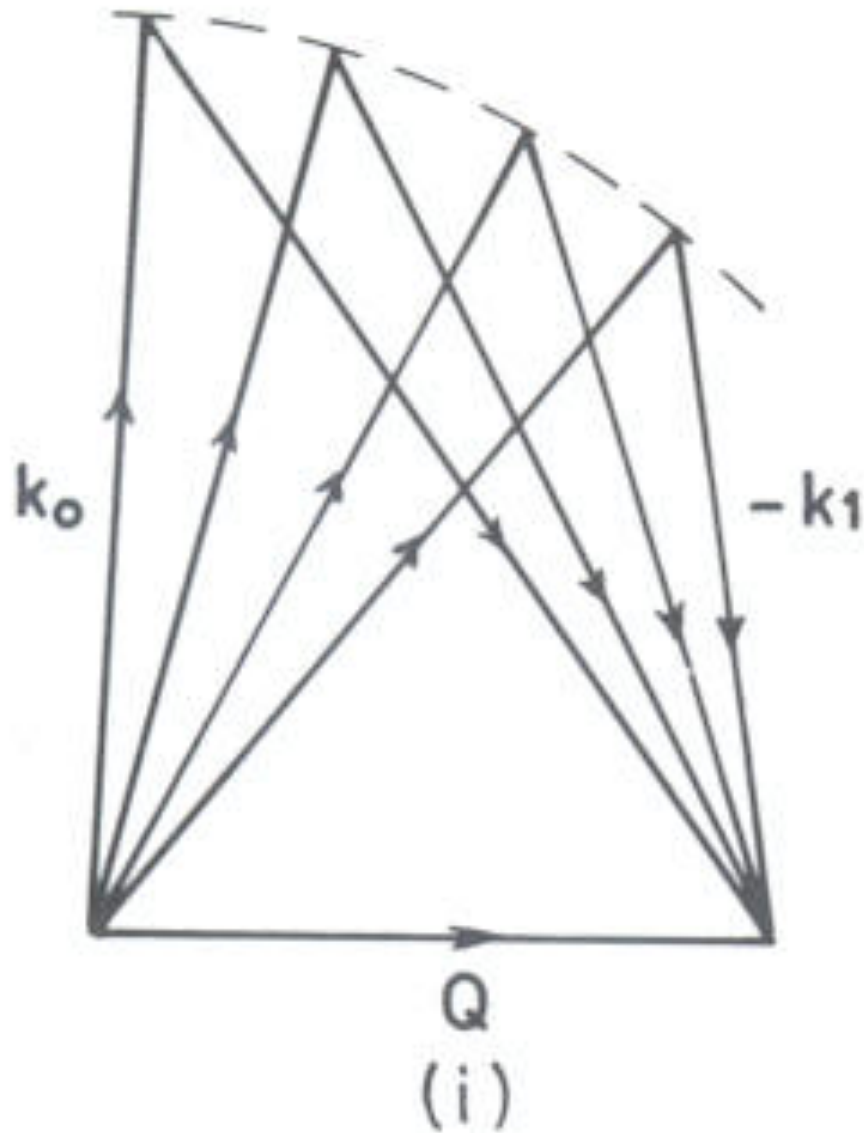
$$\hbar\omega = \frac{\hbar^2 k_i^2}{2m} - \frac{\hbar^2 k_f^2}{2m}$$

$$|\vec{k}_f| = \frac{2\pi}{\lambda_f}$$

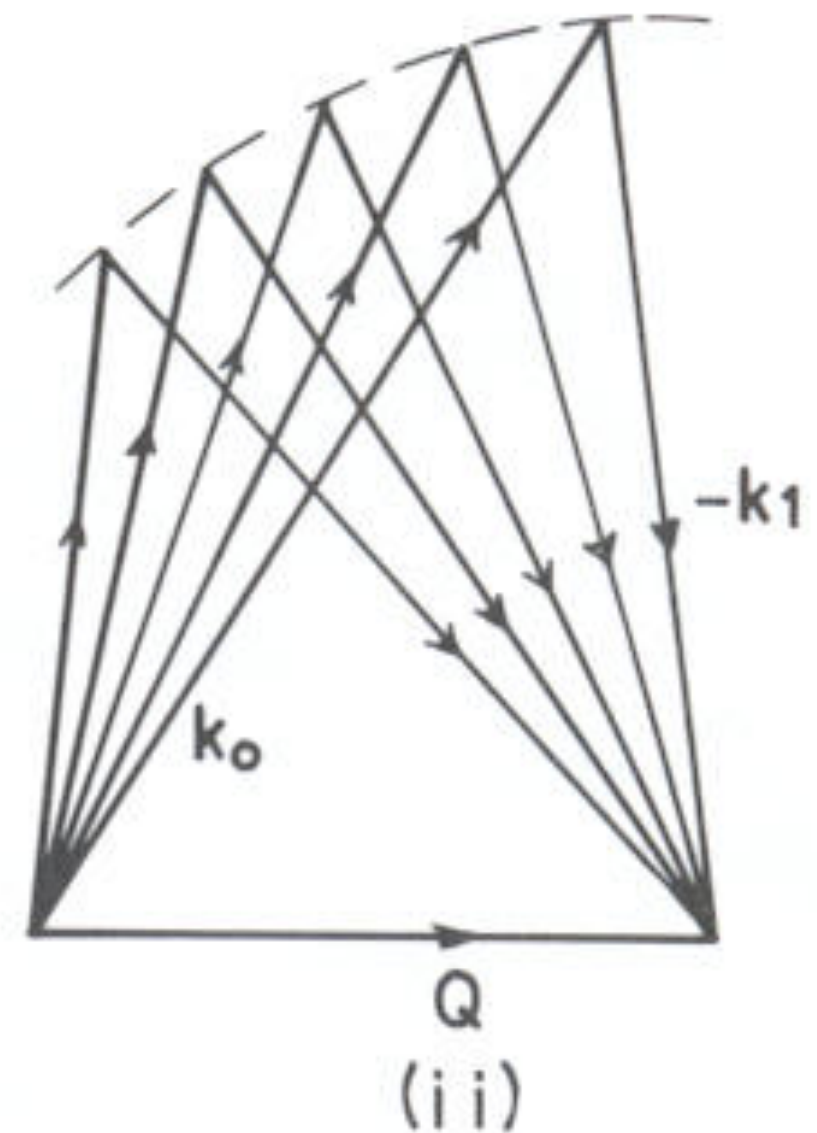


Two different ways of performing constant-Q scans

$$Q = k_i - k_f$$



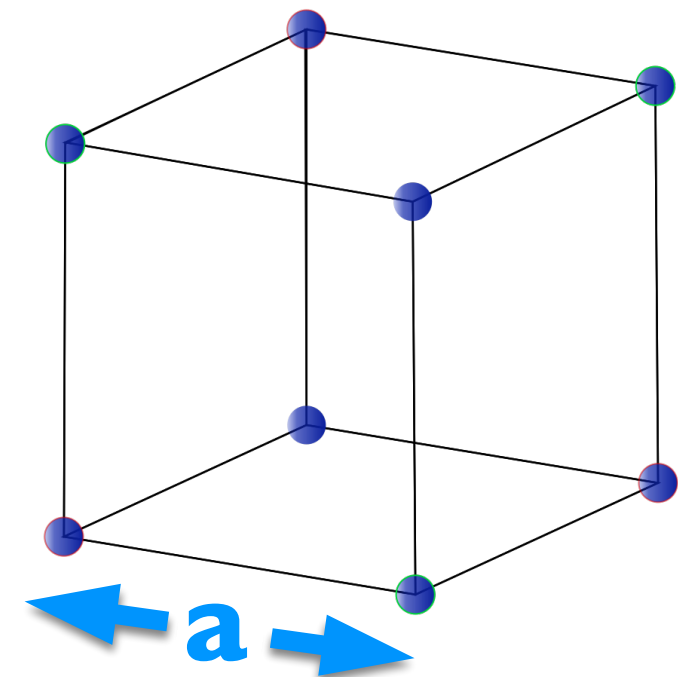
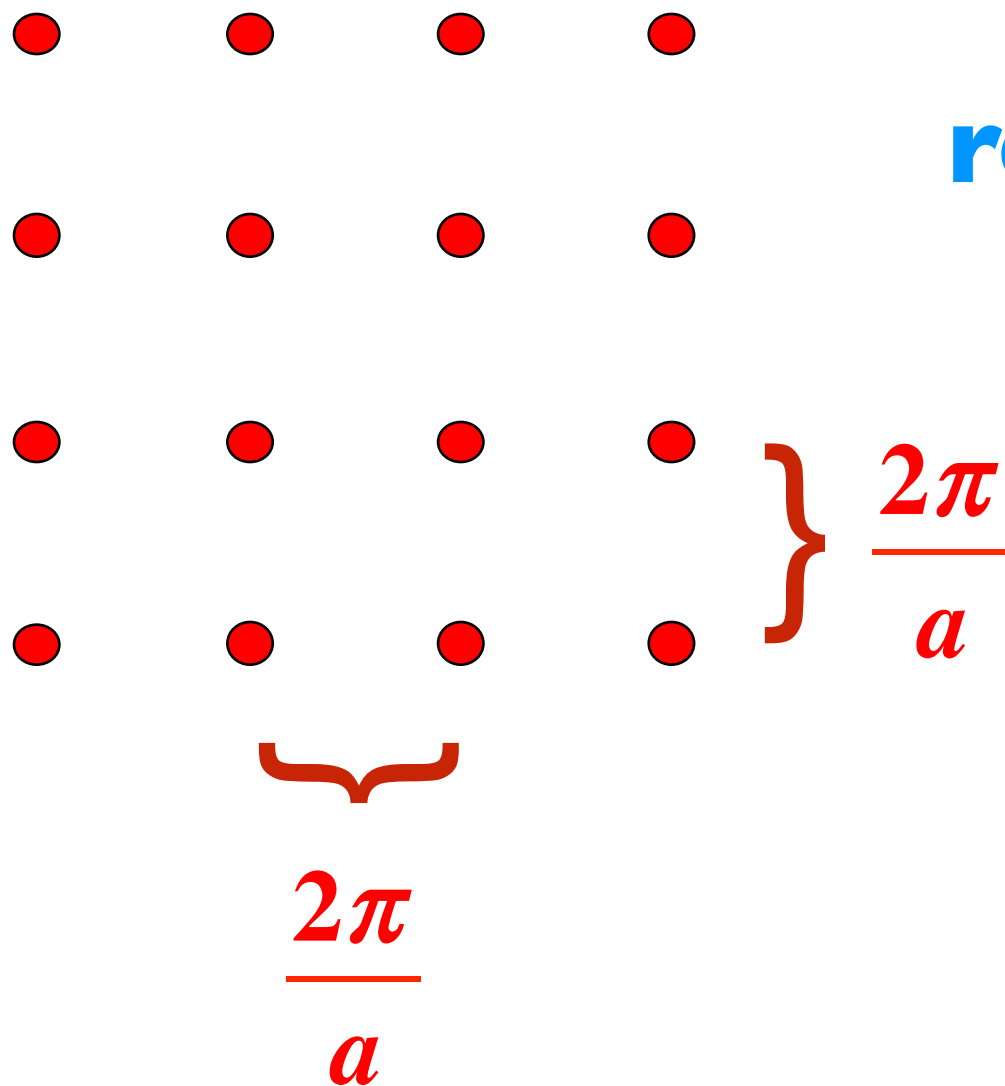
$$Q = \text{Constant } k_i$$



$$Q = \text{Constant } k_f$$

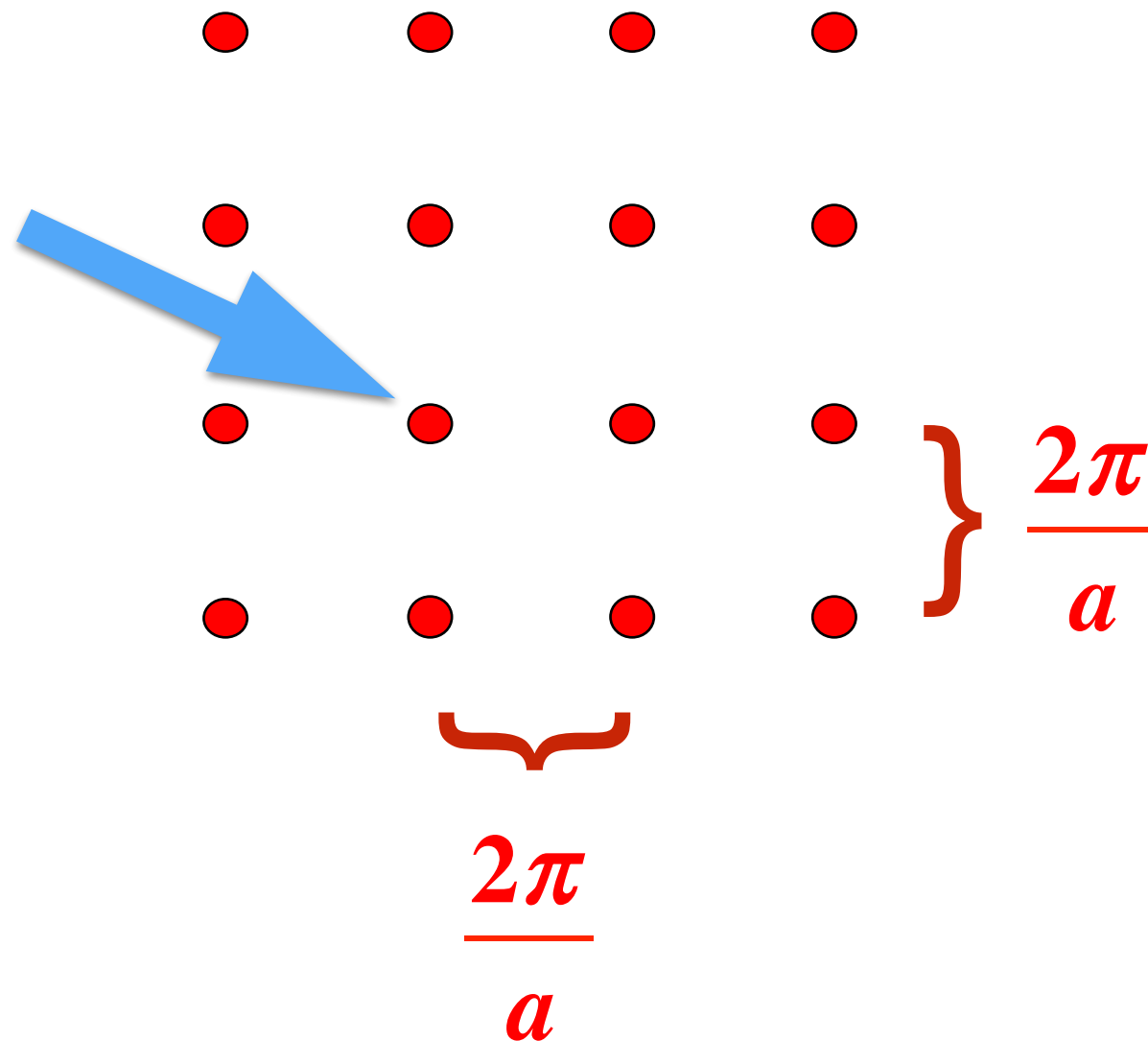
Mapping Momentum (Q) and Energy ($\hbar\omega$) space

**In momentum space,
our sample is
represented
by its
reciprocal lattice**



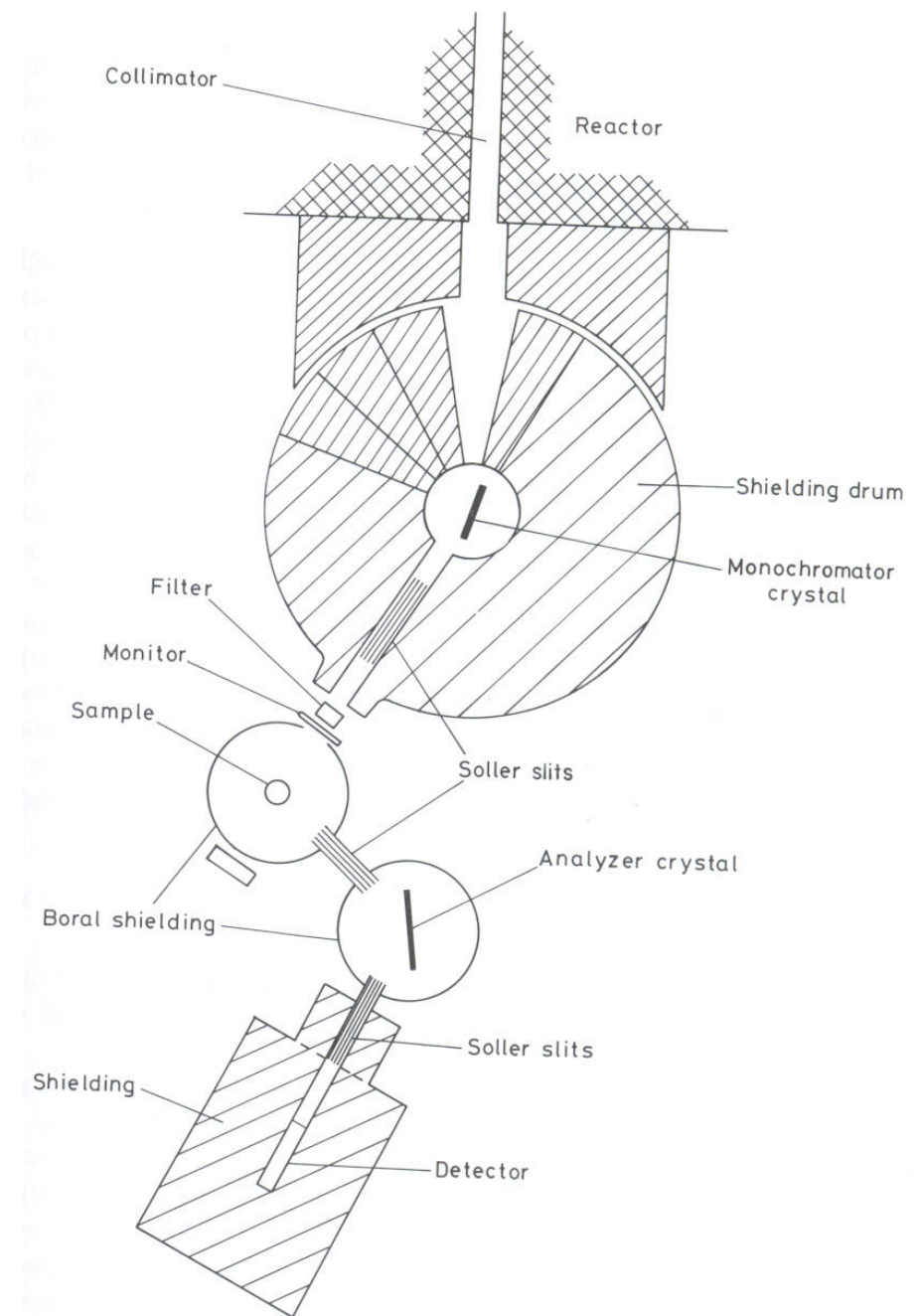
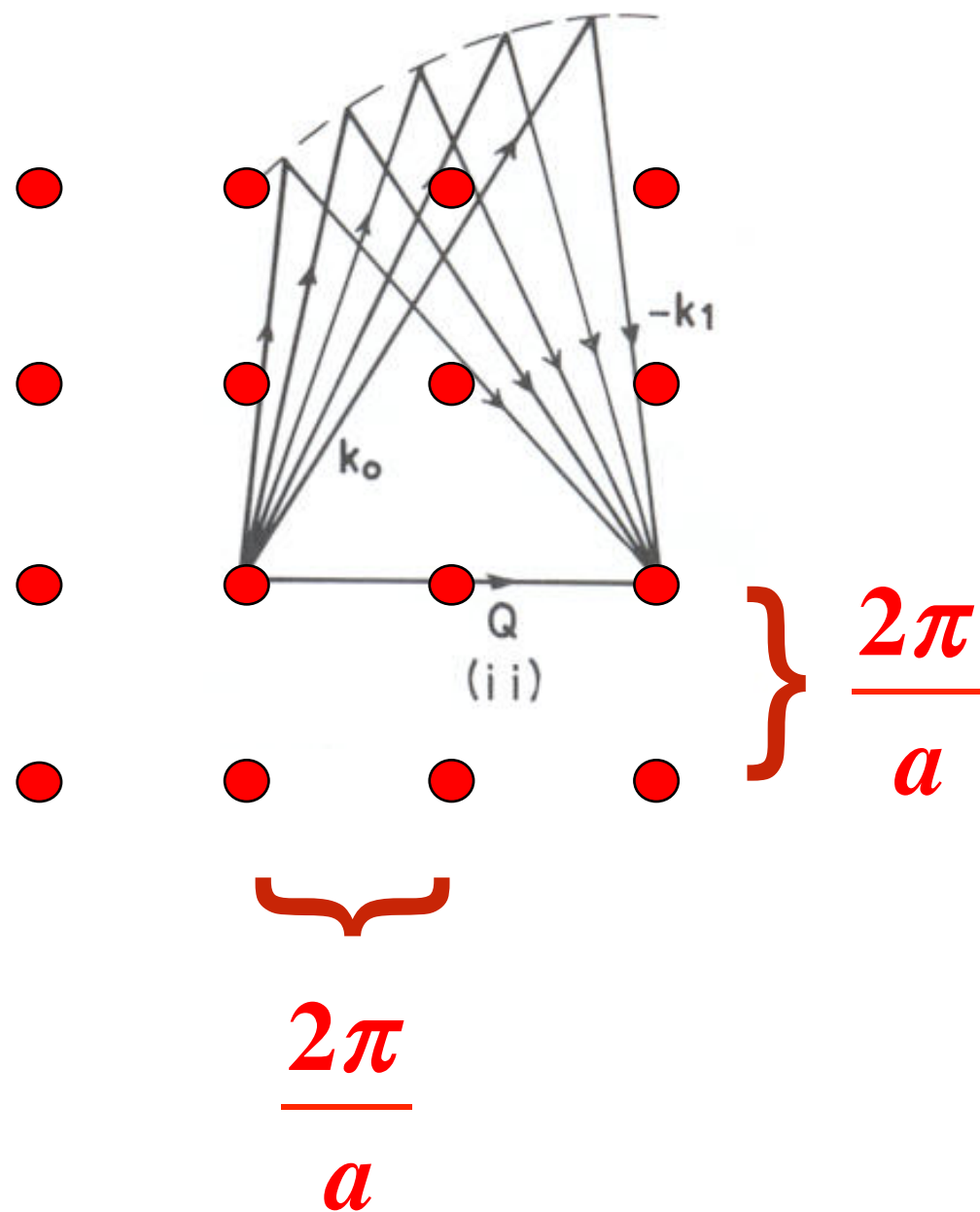
Mapping Momentum (Q) and Energy ($\hbar\omega$) space

**Origin of
reciprocal
space**

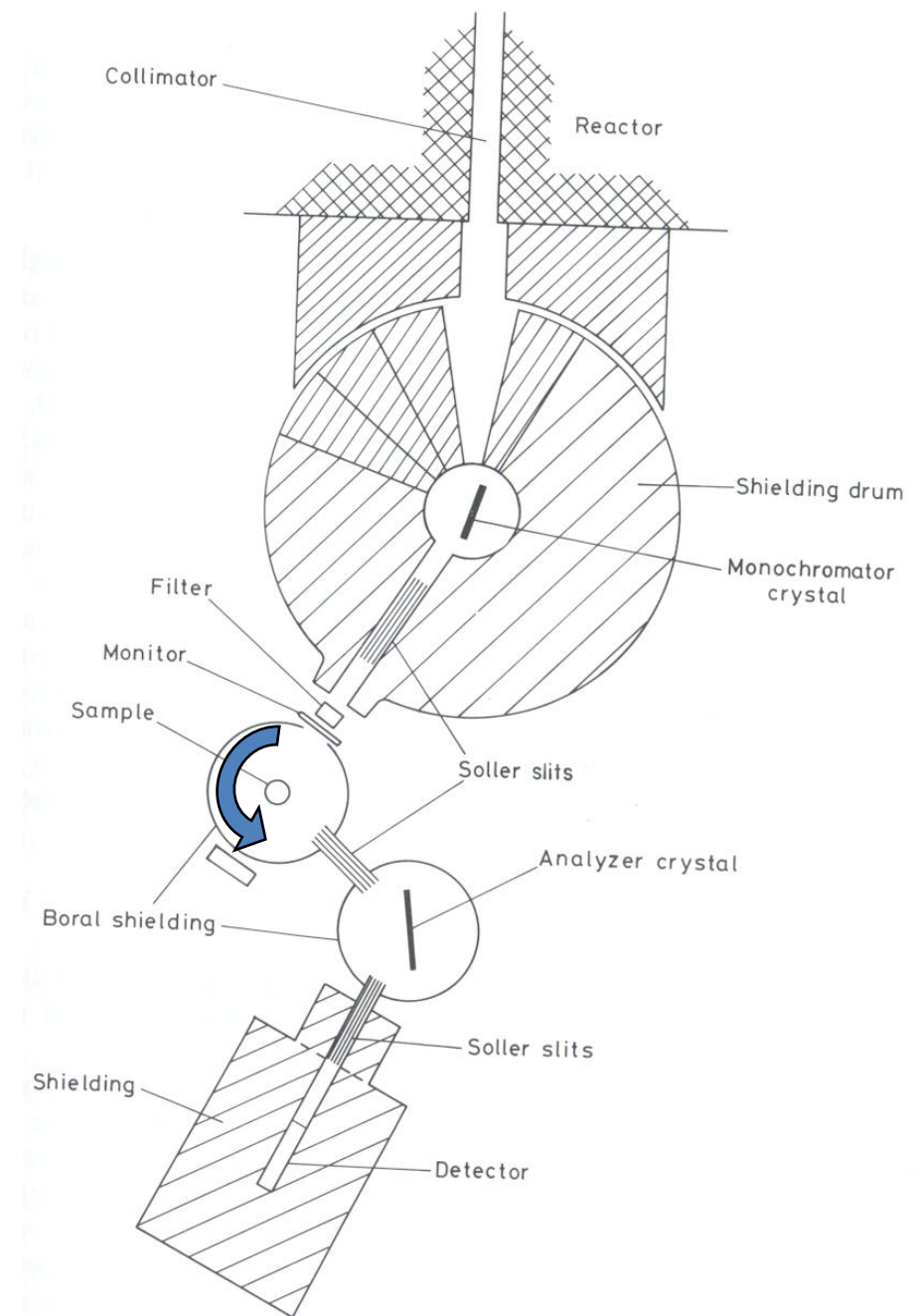
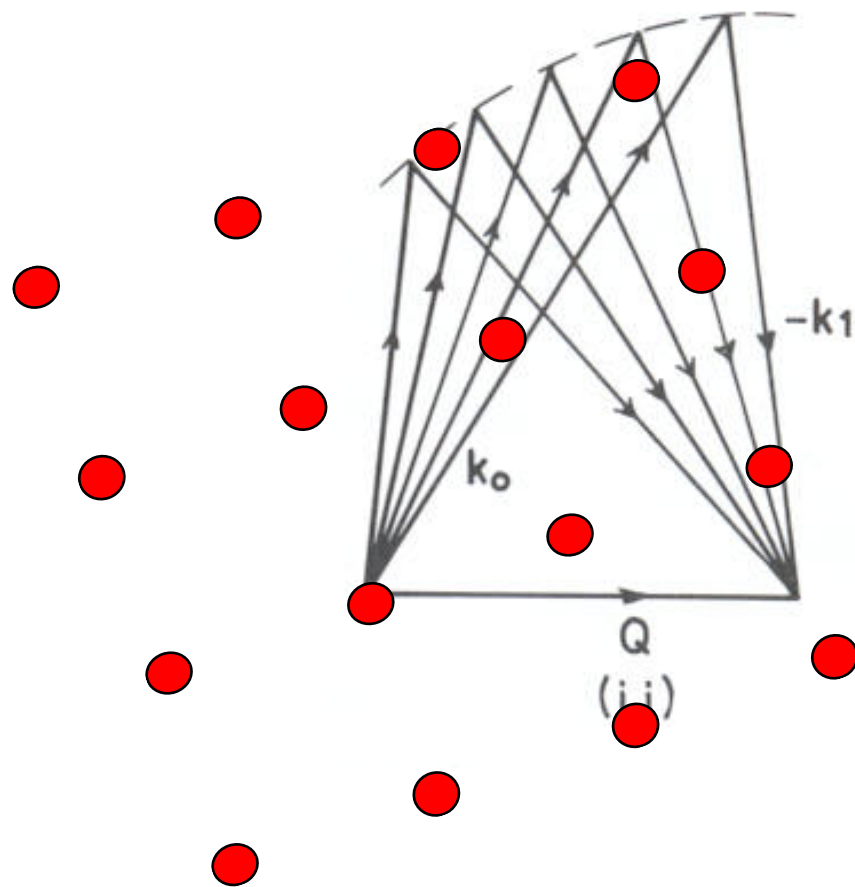


**Remains
fixed for
all sample
orientations**

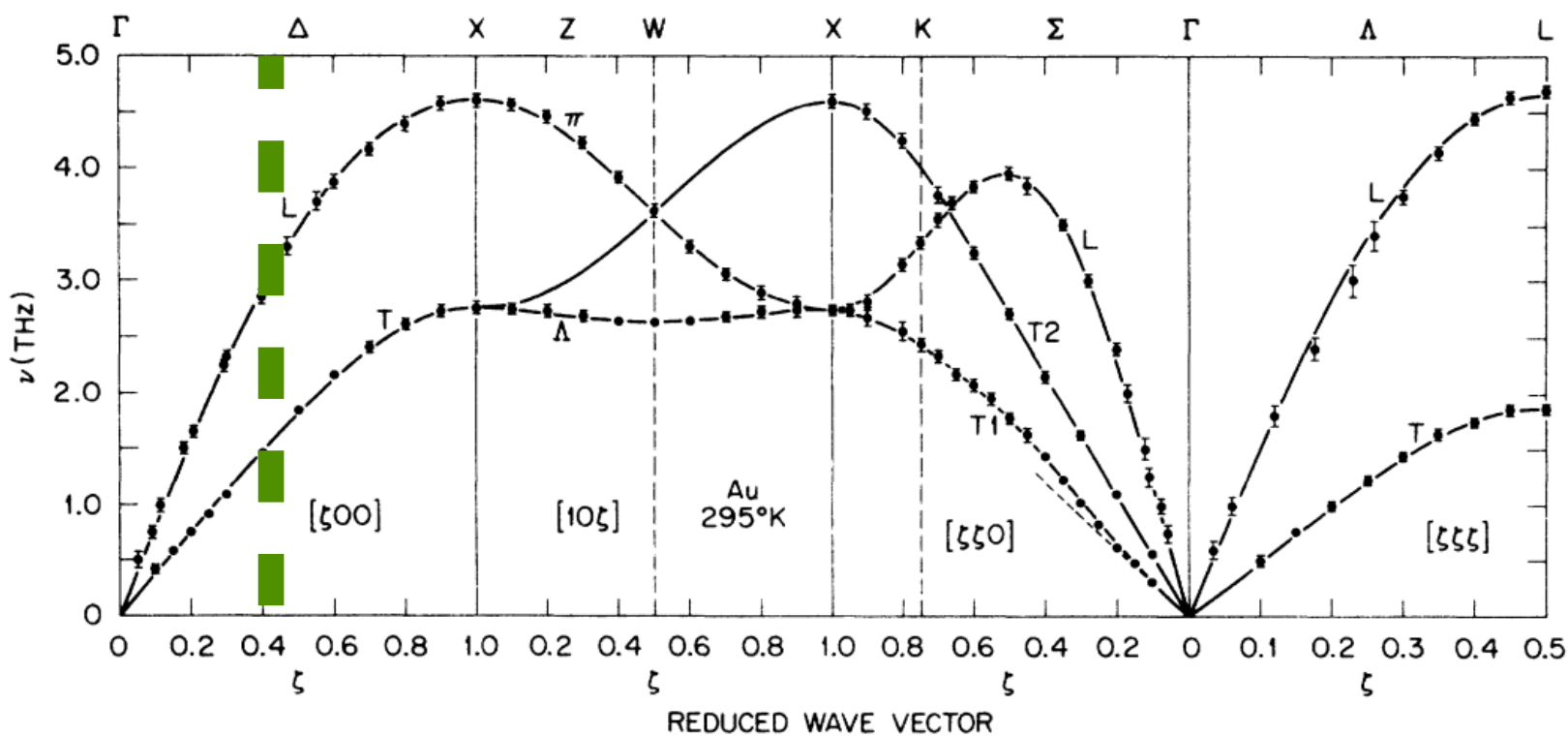
Putting the Q-map of the scattering with the reciprocal lattice of the crystal



Putting the Q-map of the scattering with the reciprocal lattice of the crystal

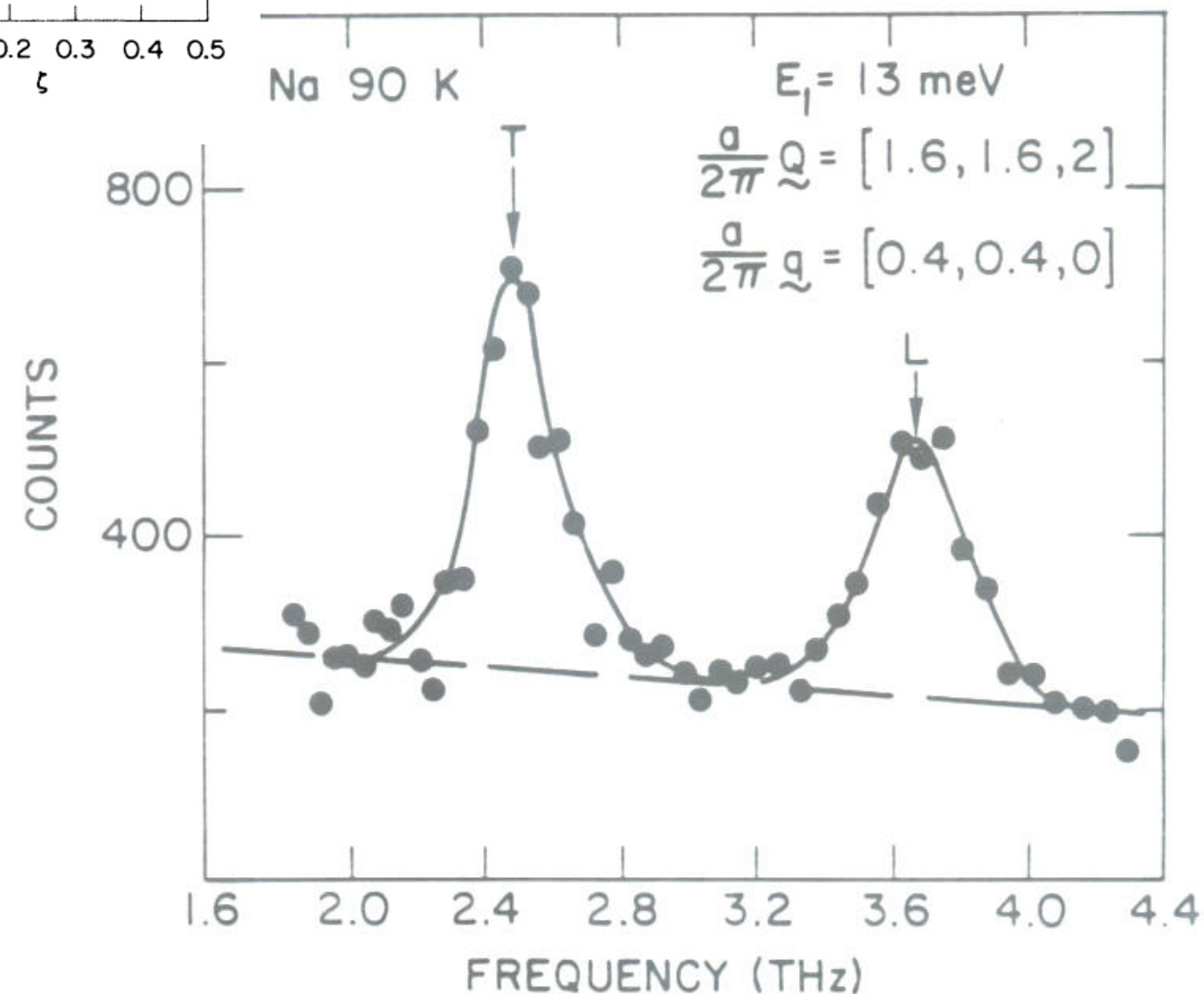


Constant-Q triple axis data

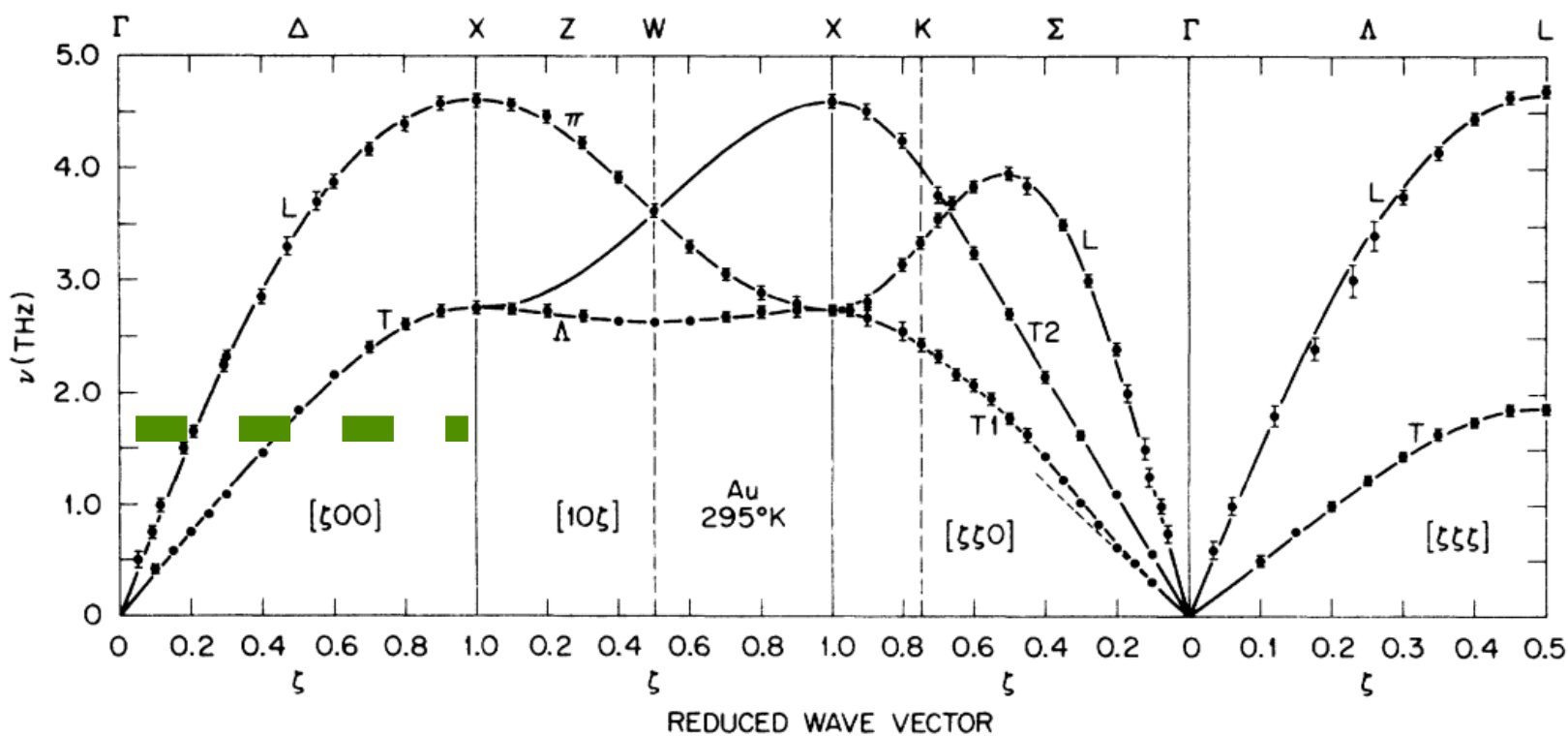


Lynn, et al., *Phys. Rev. B* 8, 3493 (1973).

Constant **Q**, constant **E**
triple axis techniques
allow us to put **Q** and **E**
on a grid, and scan through
as we choose

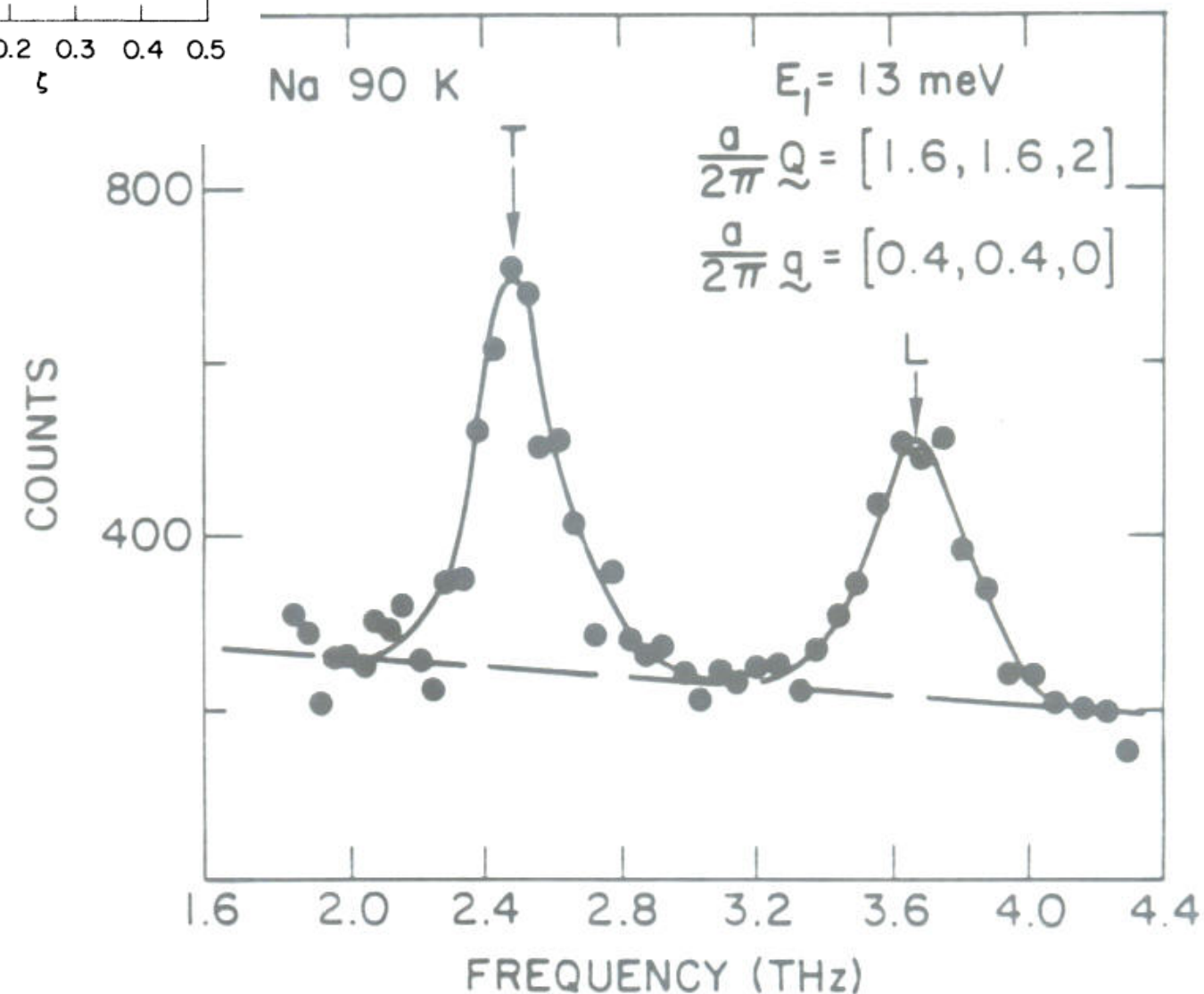


Constant-E triple axis data



Lynn, et al., *Phys. Rev. B* 8, 3493 (1973).

Constant **Q**, constant E
triple axis techniques
allow us to put **Q** and E
on a grid, and scan through
as we choose



The coherent neutron scattering cross section for phonons

$$S(\vec{Q}, \hbar\omega) = \frac{1}{2NM} e^{-Q^2 \langle u^2 \rangle} \sum_{j, \vec{q}} |\vec{Q} \cdot \vec{\varepsilon}_j(\vec{q})|^2 \frac{1}{\omega_j(\vec{q})}$$

The displacement (eigenvectors) of the atoms must be // to the momentum transfer

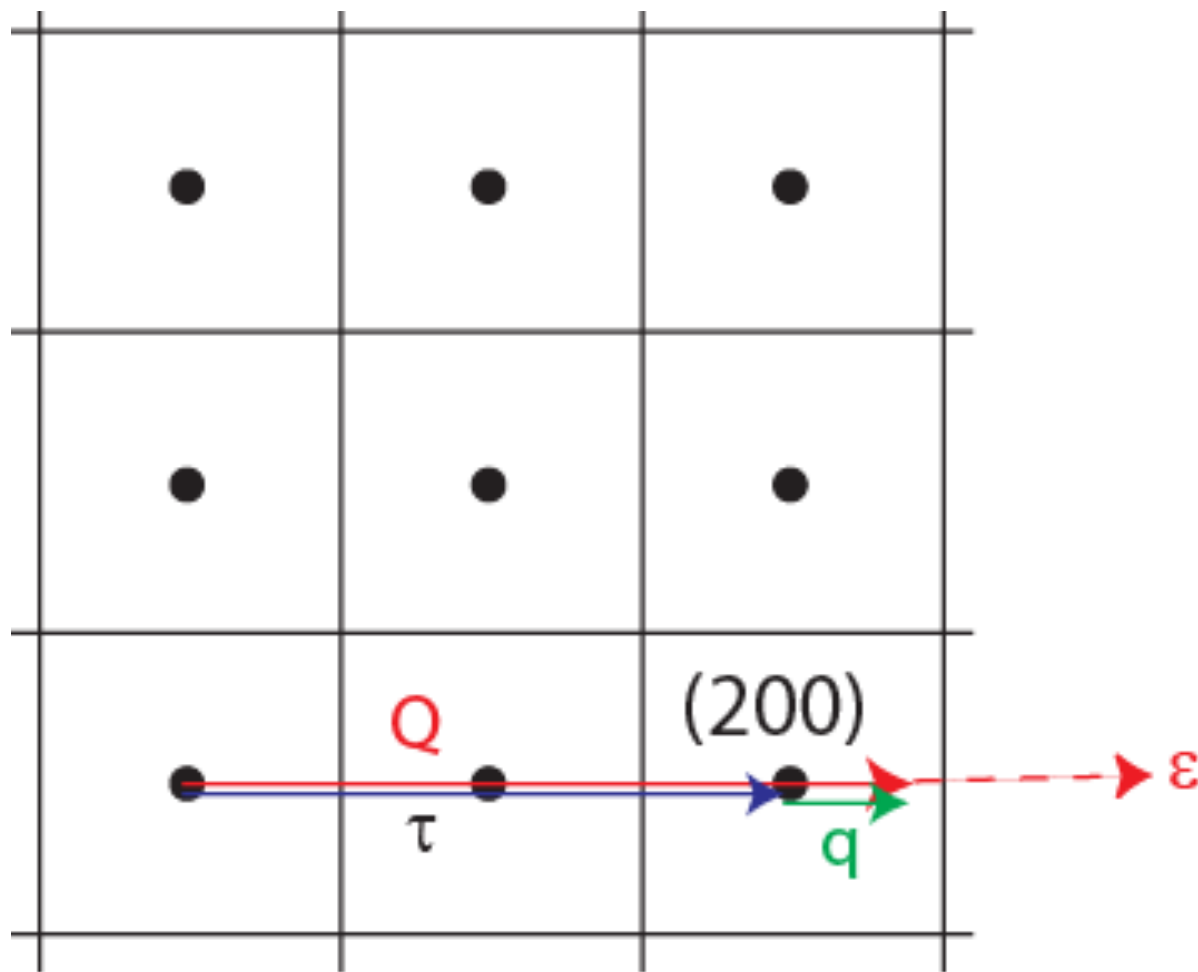
$$\times (1 + n(\hbar\omega)) \delta(\vec{Q} - \vec{q} - \vec{\tau}) \delta(\hbar\omega - \hbar\omega_j(\vec{q}))$$

The neutron can always create a phonon, but it cannot destroy a phonon unless one is already present

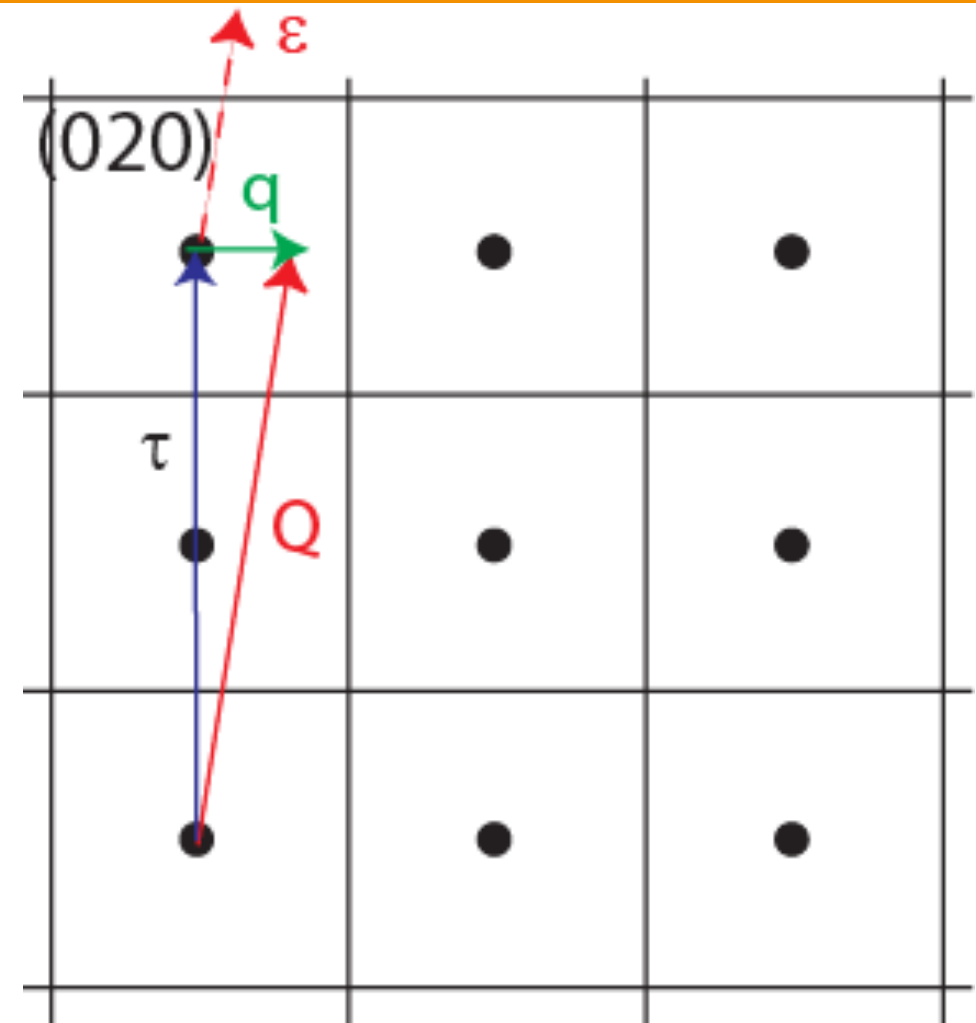
Momentum must be conserved

Energy must be conserved

The coherent neutron scattering cross section for phonons



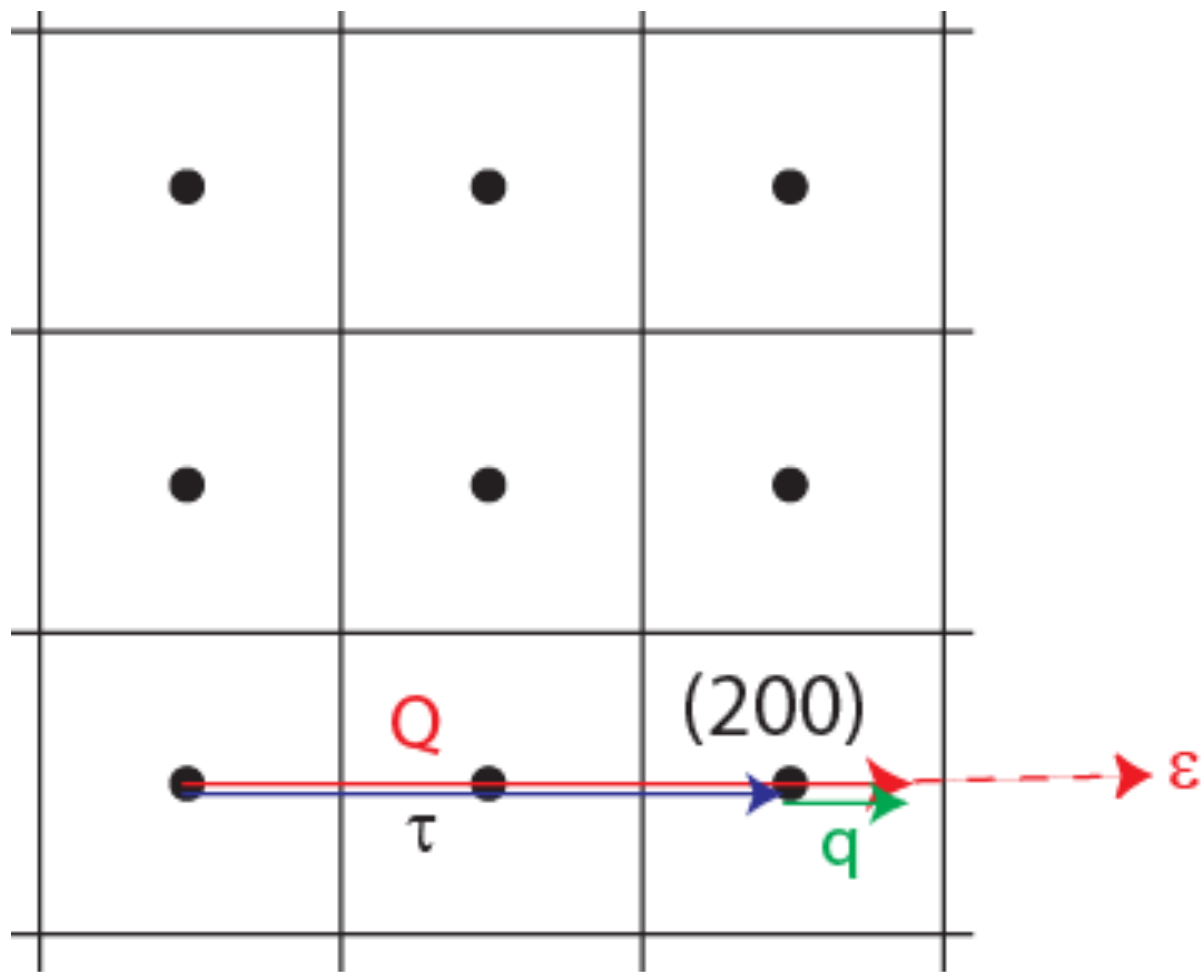
Longitudinal scan, $\mathbf{q} \parallel \boldsymbol{\varepsilon}$



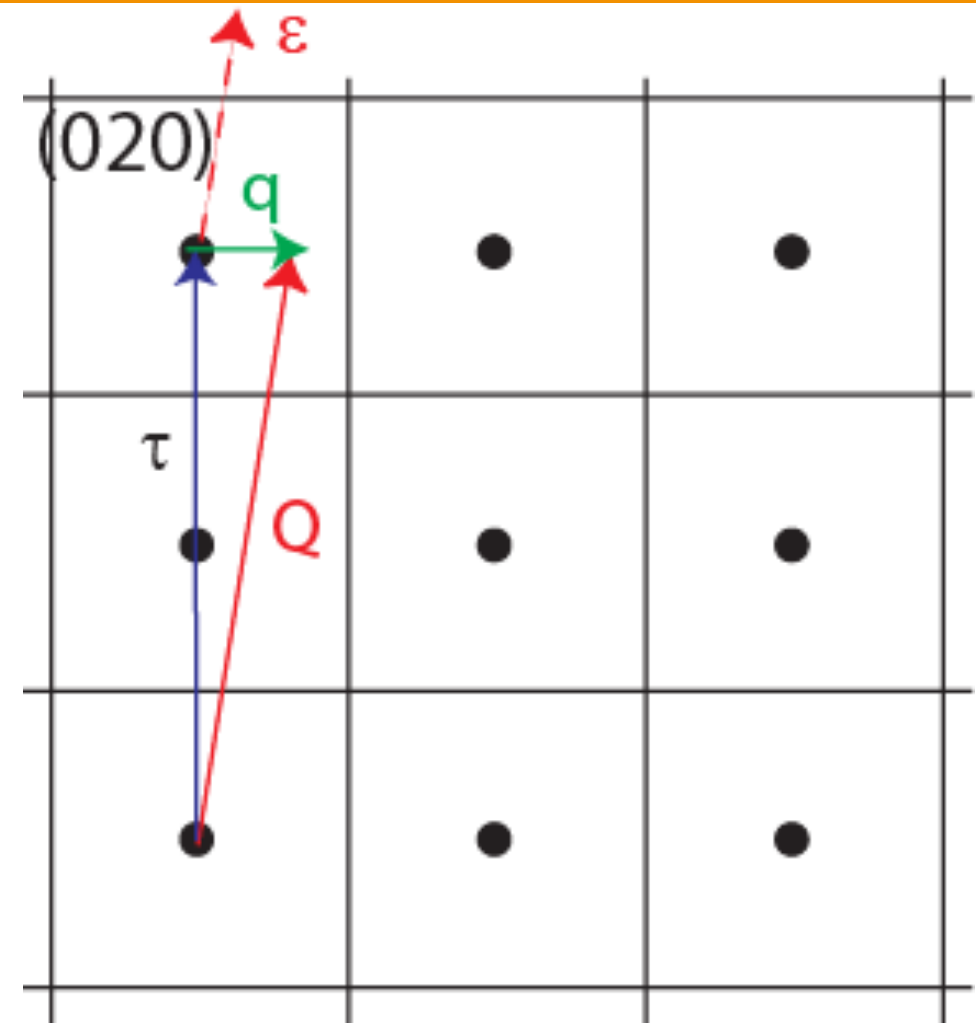
Transverse scan, $\mathbf{q} \perp \boldsymbol{\varepsilon}$

$$S(\vec{Q}, \hbar\omega) = \frac{1}{2NM} e^{-Q^2 \langle u^2 \rangle} \sum_{j, \vec{q}} |\vec{Q} \cdot \vec{\varepsilon}_j(\vec{q})|^2 \frac{1}{\omega_j(\vec{q})} \\ \times (1 + n(\hbar\omega)) \delta(\vec{Q} - \vec{q} - \vec{\tau}) \delta(\hbar\omega - \hbar\omega_j(\vec{q}))$$

The coherent neutron scattering cross section for phonons



Longitudinal scan, $\mathbf{q} \parallel \varepsilon$



Transverse scan, $\mathbf{q} \perp \varepsilon$



$$S(\vec{Q}, \hbar\omega) = \frac{1}{2NM} e^{-Q^2 \langle u^2 \rangle} \sum_{j, \vec{q}} |\vec{Q} \cdot \vec{\varepsilon}_j(\vec{q})|^2 \frac{1}{\omega_j(\vec{q})}$$

The Magnetic Cross Section

What fraction of neutrons scatter off the sample with a particular:

- **Change in momentum:**

$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

- **Change in energy:**

$$\hbar\omega = \frac{\hbar^2 k_i^2}{2m} - \frac{\hbar^2 k_f^2}{2m}$$

Fermi's Golden Rule: 1st order perturbation theory

$$\frac{\partial^2 \sigma}{\partial \Omega \partial E_f} : i, \vec{k}_i, \sigma_i \rightarrow f, \vec{k}_f, \sigma_f$$

$$= \frac{m}{(2\pi\hbar^2)^2} \frac{k_f}{k_i} \left| \left\langle f, \vec{k}_f, \sigma_f \left| V \right| i, \vec{k}_i, \sigma_i \right\rangle \right|^2 \delta(E_i - E_f - \hbar\omega)$$

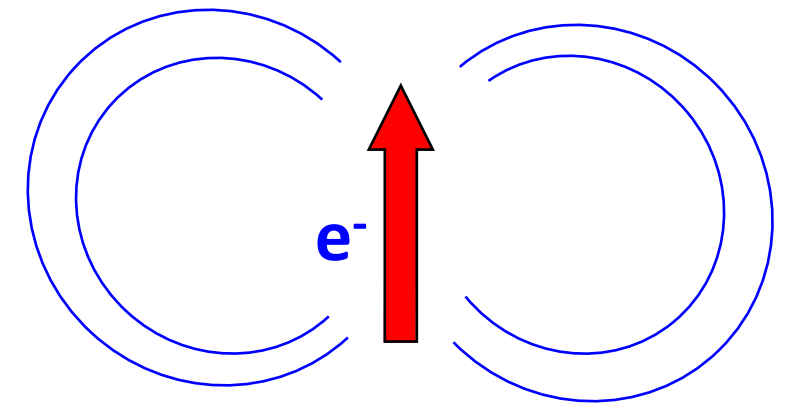
kinematic

**interaction
matrix element**

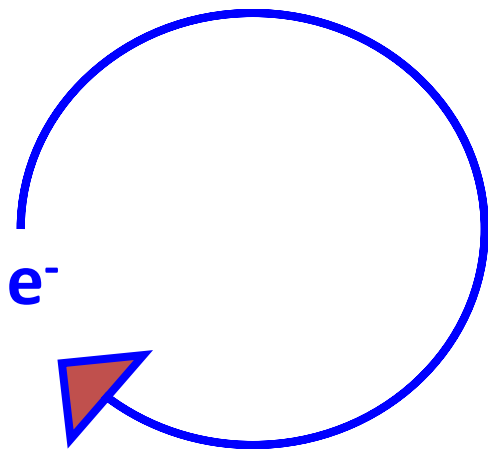
**energy conserving
delta function**

Understanding this means understanding:

$$V_M = \vec{\mu}_n \cdot \vec{B}_{electrons}$$



**magnetic field
due to $S=1/2$ of
unpaired electrons:
 B_s**



**magnetic field
due to orbital motion
of electrons: B_L**

**neutron
spin**

Bottom lines for magnetic neutron scattering

- Comparable in strength to nuclear scattering
- $(\frac{g}{2}F_d(Q))^2$ Goes like magnetic form factor squared
- $\sum_{\alpha,\beta}(\delta_{\alpha,\beta} - \hat{Q}_\alpha \hat{Q}_\beta)$ Sensitive only to components of magnetic moment $\perp \vec{Q}$
- Dipole selection rules :
Goes like $\langle f | S_{d'}^\alpha | i \rangle$ with $S_{d'}^z$ $S_{d'}^+$ $S_{d'}^-$

Magnetic Form Factors:

Magnetic electrons are extended in space around the nucleus

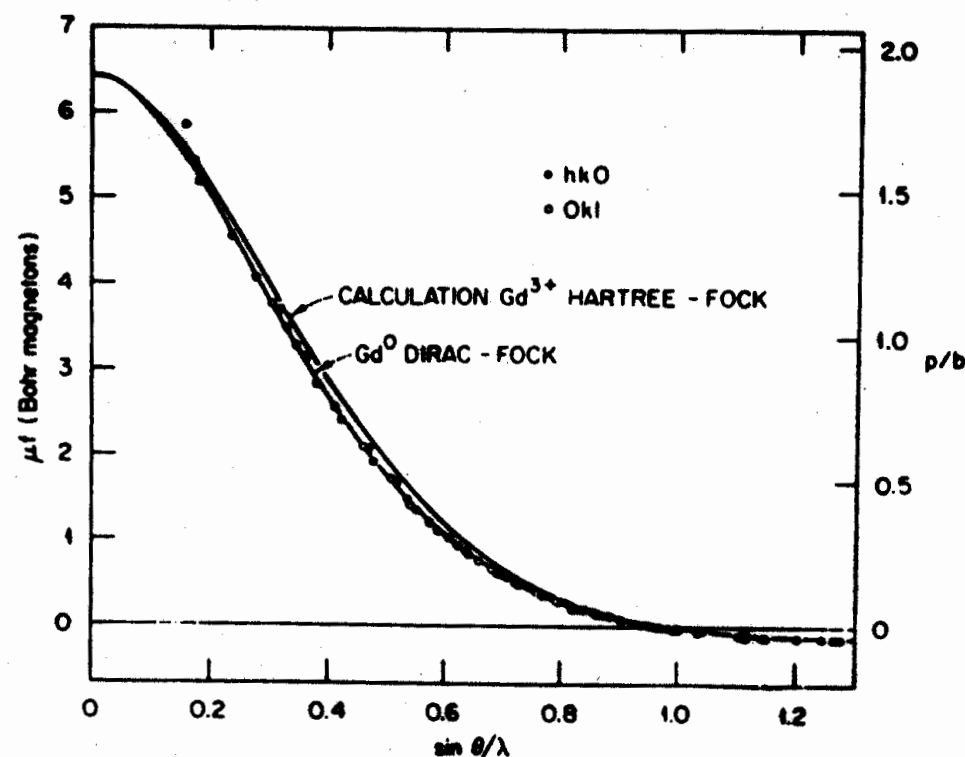
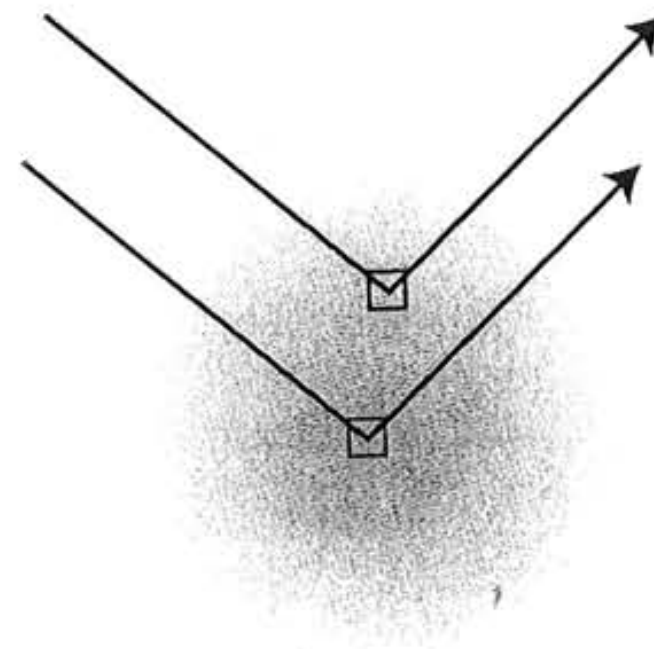


FIG. 13. Comparison of the experimental ^{160}Gd form factor at 96 K as measured by Moon *et al.*⁴⁷ with nonrelativistic Hartree-Fock and relativistic Dirac-Fock calculations by Freeman and Desclaux.³⁶



Neutrons can interfere destructively from the same magnetic electron cloud

The magnetic form factor, $F_d(Q)$, is the Fourier transform of the spatial distribution of magnetic electrons. It usually falls off with Q on scale of $\frac{\pi}{1 \text{ \AA}} \sim 3 \text{ \AA}^{-1}$