101 things you have to know about the neutron and some that you do not.

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References

- "Thermal neutron Scattering", G.L. Squires, Dover, 1996
- "Neutron Optics", V.F. Sears, Oxford, 1989
- "Neutron Data Booklet", Eds. A-J Dianoux and G.H Lander 2003. It's on Google.
- "Polarization analysis of thermal neutron scattering", R.M. Moon, T. Riste and W.C. Koehler, Phys. Rev 181, 920, 1969

Basic properties of the neutron

- Mass=1.675 10^{-27}kg
- Charge=0
- Spin=1/2
- Magnetic dipole moment μ_n=-1.913μ_N
- Bohr magneton μ_B=9.274 10^{-24} joules/tesla
- Nuclear magneton, μ_N=5.051 10^{-27} joules/tesla
- Elementary charge e=1.602 10^{-19}coulomb
- Mass of an electron m_e=9.109 10^{-31}kg
- Mass of proton m_p=1.673 10^{-27}kg
- Planck's constant h =6.626 10^{-34} joule.sec

Birth and death of the neutron

- Irène Curie and Frederic Joliot(1932). Bombarded Be with ${}_2He^4$ particles and found that the “radiation “ produced expelled protons when passed through paraffin which γ-rays never did. It was a new kind of radiation.

- Chadwick (1932) showed that this radiation consisted of a “heavy” uncharged particle

$${}_4Be^9 + {}_2He^4 = {}_6C^{12} + {}_0n^1$$

The neutron eventually decays by β-decay in 885.9 0.9sec. According to ${}_0n^1 = {}_1H^1 + {}_{-1}e$ +neutrino but we “use ‘em up” long before that.

Effect of the discovery of the neutron

- This immediately led to the understanding of the stability of the elements of the periodic table. The nucleus (small $\sim 10^{-13}$cm) is made up of *p* and *n*. There is a coulomb repulsion between *p* (e^2/r^2) and short range forces between *p* and *n* and n and n which hold the nucleus together. Eventually, around U the coulomb forces exceeds the short-ranged forces and nuclei are no longer stable.
- The neutron is made up of charged quarks (2d+1u). (2 -1/3)+1 2/3=0 whereas the proton is 1d+2u with charge 1
- The moving charges are responsible for the magnetic moment

Creation and slowing down a neutron

- The initial energy is of order Mev either in a fission reactor or spallation source and after about 100 collisions in a $_1H^1$ or $_1H^2$ moderator the energy is of order meV so not relativistic
- The Mev and keV neutron is dangerous (can knock your atoms off their sites) but an meV neutron is not so dangerous,. A “gentle probe” a mere whiff of radiation.
- It is a small, light particle so wave-particle duality should apply, i.e we think of the thermal neutron as a wave not a bullet

Units of energy

- The energy of the neutron is kinetic and so equals $\frac{1}{2}m_n v^2$. The velocity of a thermal neutron is typically 2200ms^{-1} so the energy is therefore 4.0533 10^{-21} joules or 25.301meV
- If we write the energy as $E_{kinetic}=hv$ where h is Planck's constant and v is the frequency we get v=6.1172THz which is the favoured Chalk River unit
- If we write the energy as a temperature $E_{kinetic}$=kT we get T=293.63K (the temperature of a cup of tea!)
- Finally if we write E=hc*wave-number we get the corresponding wave-number to be 204.05cm
- To summarise 1 Thz= 4.136meV= 48.000K=33.356cm^{-1}

Units of momentum and wavelength

- $m_n \mathbf{v} = \hbar \mathbf{k}$ where **k** is the wavevector.
- $k=2\pi/\lambda$ where λ is the wavelength so for our neutron of velocity $2200 \mathrm{ms}^{-1}$

  we have $\lambda=0.17982\mathrm{nm}$ or 1.7982Å.

  The numerical relationship between wavelength and velocity is

  $$\lambda[\text{Å}]=3956.03/v[\mathrm{msec}^{-1}]$$

  and the relationship between energy in Thz and wavelength in Å is

  $$E=19.7801/\lambda^2$$

Wave-particle duality of the neutron as shown by diffraction through slits

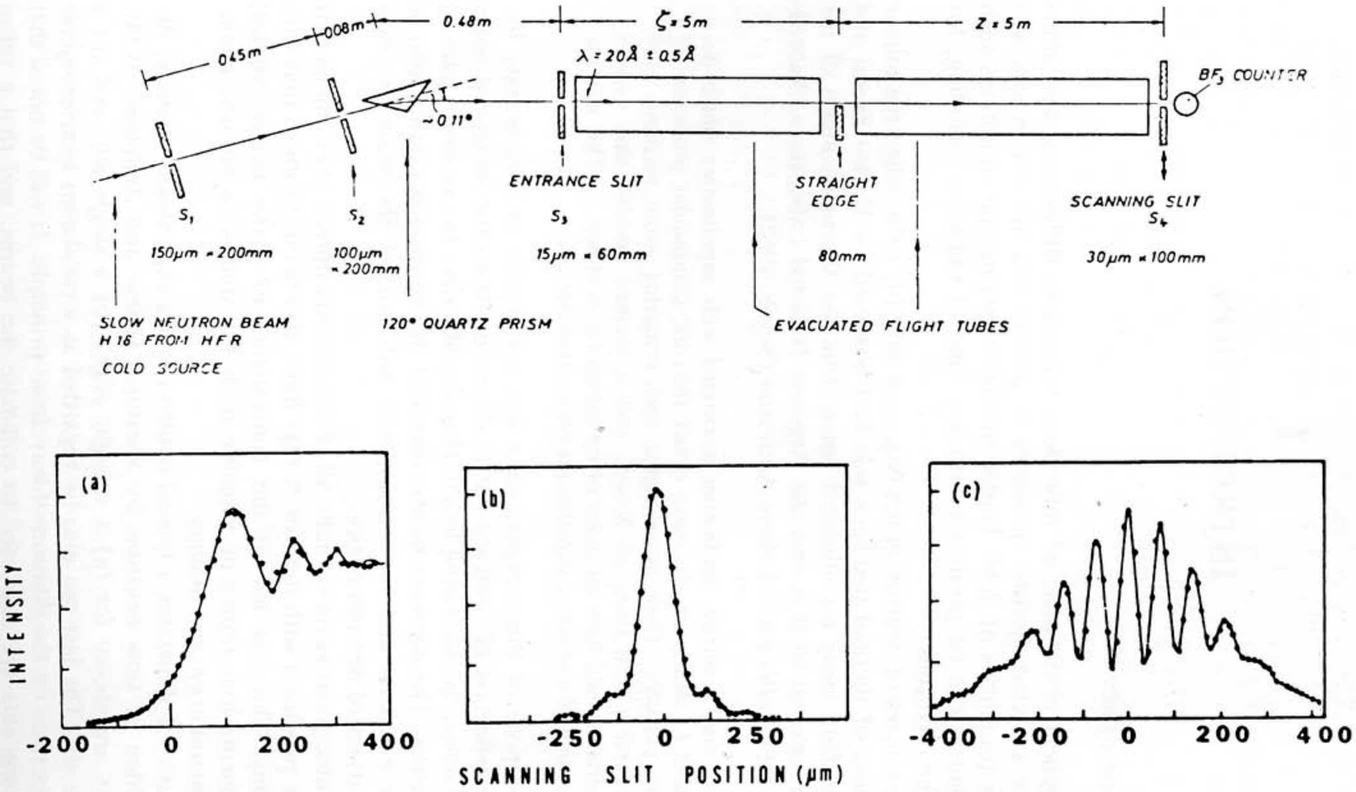


Fig. 1.1 Neutron diffraction by (a) a straight edge, (b) a single slit, and (c) a double slit (from Klein and Zeilinger, 1984).

$e^{ik^{incident} z}$

Cross section definition and form of the wave functions

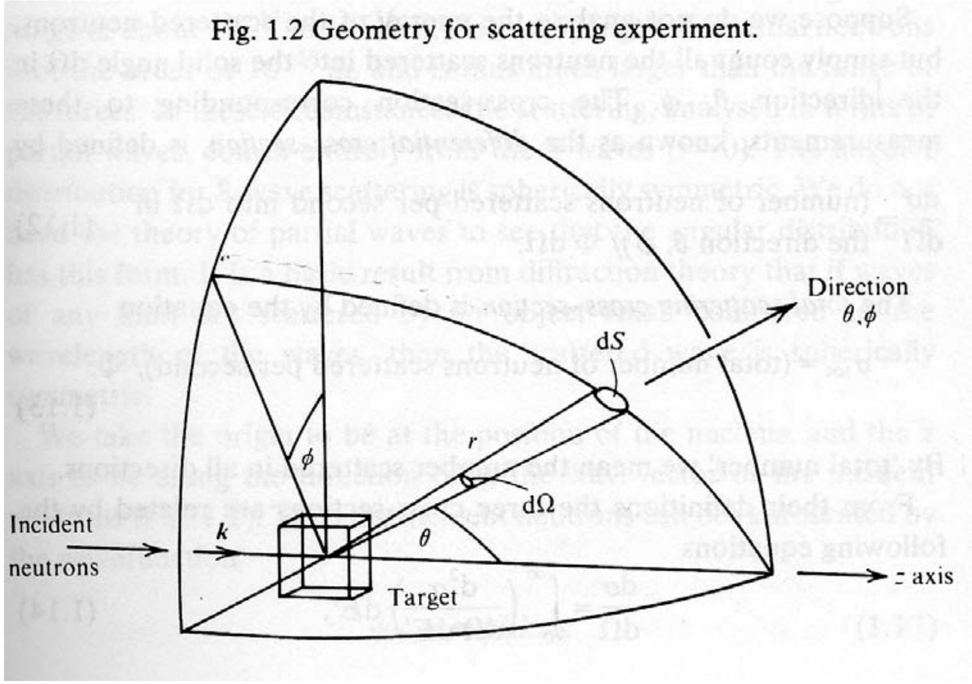


Fig. 1.2 Geometry for scattering experiment.

$$\Psi^{incident} = e^{ik^{incident} z}$$

Plane wave

$$\Psi^{scattered} = -b \frac{e^{i\underline{k}' \cdot \underline{r}}}{r}$$

Spherical wave because…

The intensity is equal to Ψ *Ψ in the usual way. b is the scattering length describing the strength of the interaction and it can be either positive or negative.

Definitions of cross sections

$\frac{d^2\sigma}{d\Omega dE'}$ =number of neutrons scattered per second into a small solid angle $d\Omega$

in the direction θ, φ with final energy between E’ and E’+dE’ divided by flux

$\Phi d\Omega dE'$

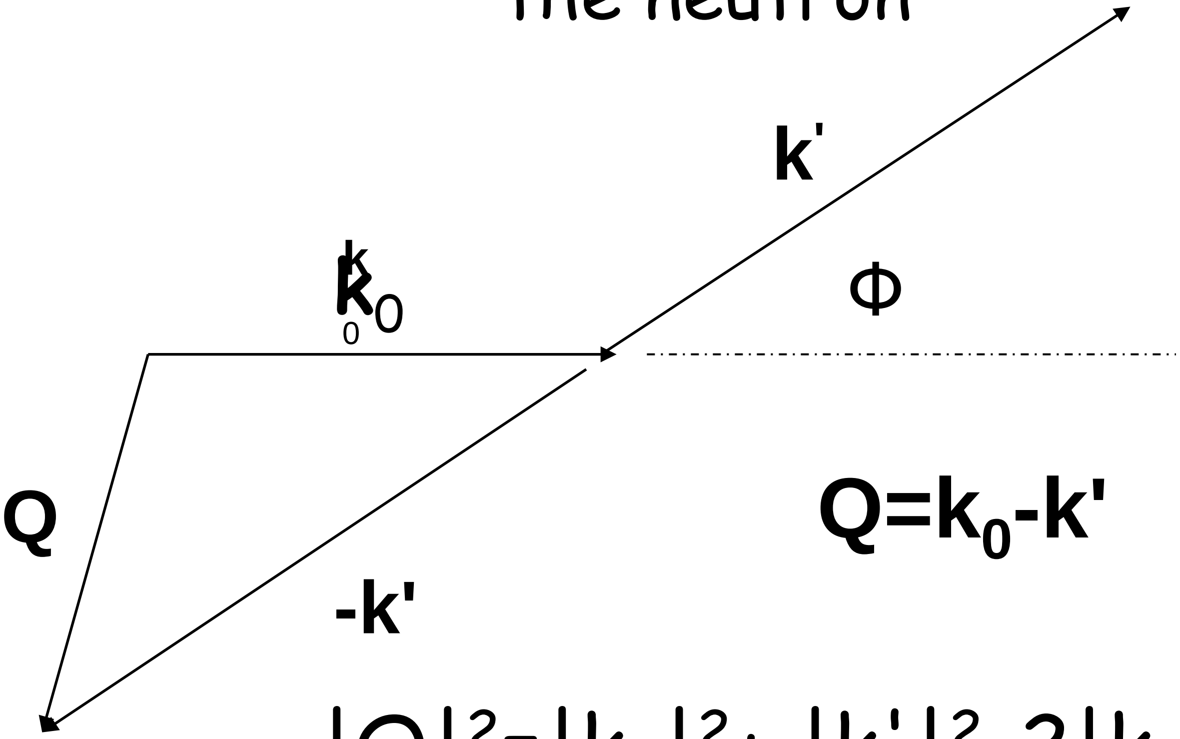
$$\frac{d\sigma}{d\Omega} = \int_o^\infty \left(\frac{d^2\sigma}{d\Omega dE'}\right) dE'$$

$\frac{d\sigma}{d\Omega}$ The number of neutrons scattered per sec into a small solid angle $d\Omega$ In the direction θ, φ divided by $\Phi d\Omega$

σ = $\int_0^\pi \frac{d\sigma}{d\Omega} 2\pi \sin\theta d\theta$

σ is the total number of neutrons scattered into 4π divided by the flux Φ

In a scattering experiment we expect to measure the energy and momentum change of the neutron



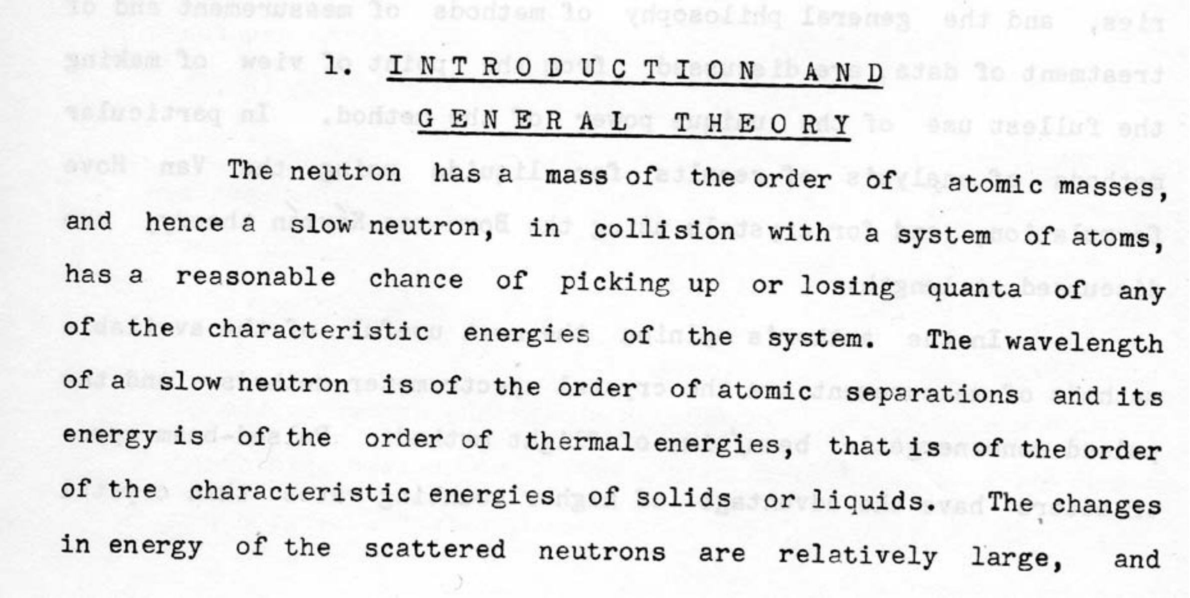
$$\mathbf{Q}=\mathbf{k_0}-\mathbf{k'}$$

$$|Q|^2=|k_0|^2+|k'|^2-2|k_0||k'|\cos\Phi$$

$$E_0-E' = h\nu = (k_0^2-k'^2)/2m_n$$

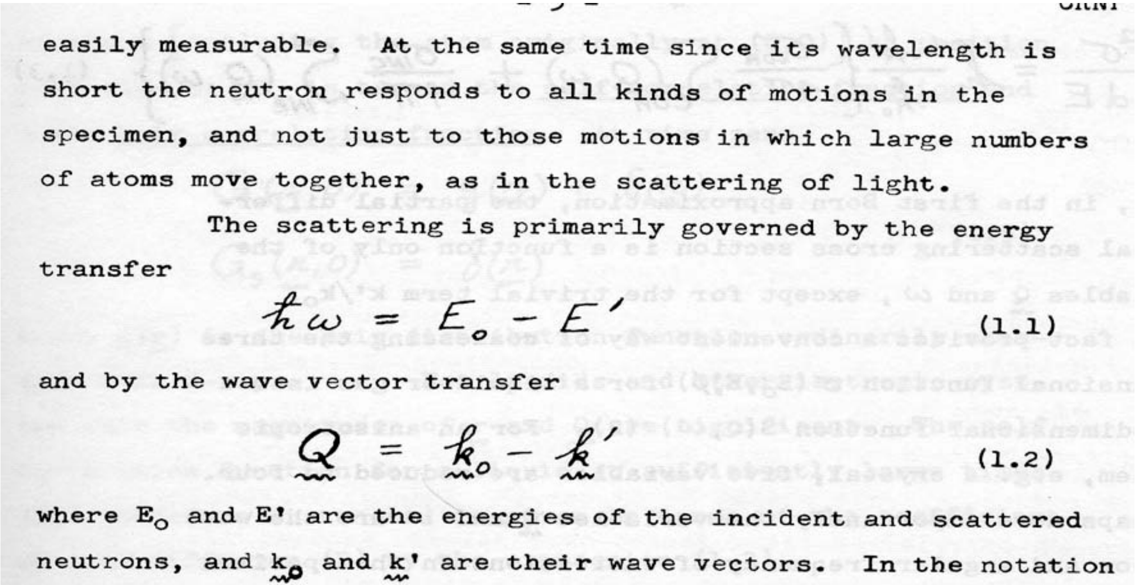
Φ is the scattering angle

This statement of Bert Brockhouse essentially embodies the whole of neutron scattering. AECL-1183, 1961



1. INTRODUCTION AND GENERAL THEORY

The neutron has a mass of the order of atomic masses, and hence a slow neutron, in collision with a system of atoms, has a reasonable chance of picking up or losing quanta of any of the characteristic energies of the system. The wavelength of a slow neutron is of the order of atomic separations and its energy is of the order of thermal energies, that is of the order of the characteristic energies of solids or liquids. The changes in energy of the scattered neutrons are relatively large, and



easily measurable. At the same time since its wavelength is short the neutron responds to all kinds of motions in the specimen, and not just to those motions in which large numbers of atoms move together, as in the scattering of light.

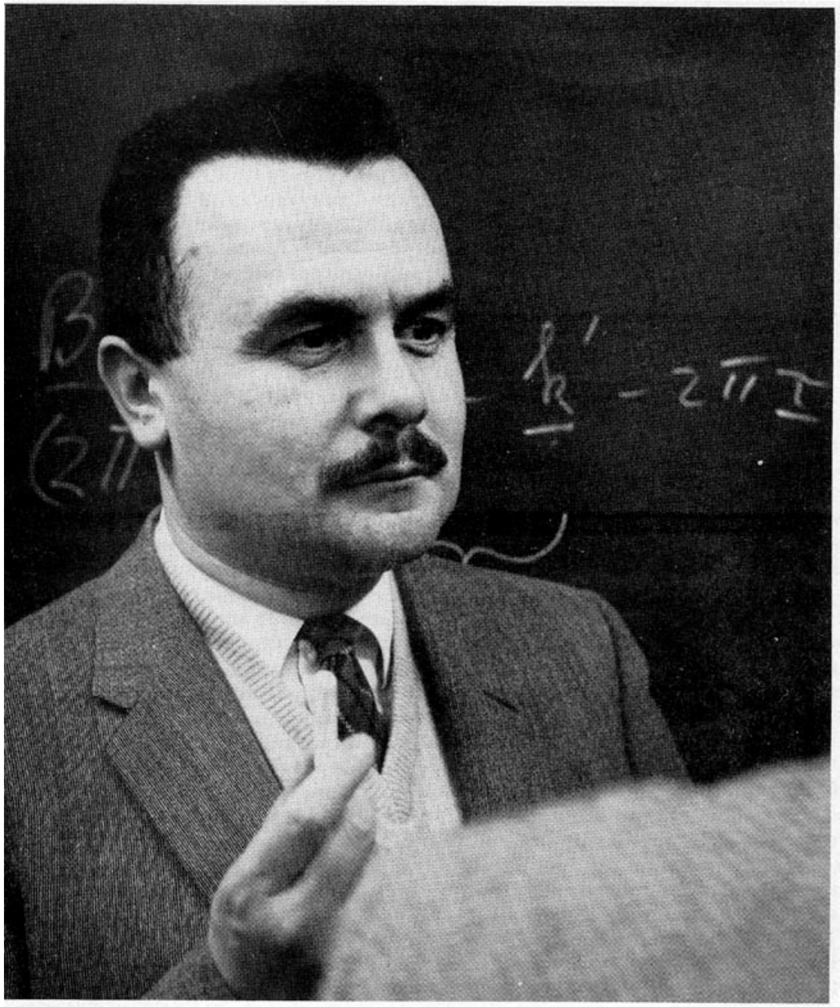
The scattering is primarily governed by the energy transfer

$$\hbar\omega = E_o - E' \qquad (1.1)$$

and by the wave vector transfer

$$\underset{\sim}{Q} = \underset{\sim}{k}_o - \underset{\sim}{k}' \qquad (1.2)$$

where E_o and E' are the energies of the incident and scattered neutrons, and $\underset{\sim}{k}_o$ and $\underset{\sim}{k}'$ are their wave vectors. In the notation



Bertram N. Brockhouse

Phonon dispersion relations
Kohn anomalies
Spin waves in magnetite
Spin waves in metals (CoFe)
Crystal fields
Excitations in Liquid Lead
Scattering in water
Scattering in He
Texture of U
Triple axis spectrometer
1950-62

Absorption cross sections

- This refers to the capture of a neutron by the nucleus, creating an unstable isotope which then usually, but not always, decays by the emitting other particles or γ-rays.
- Examples include Cd (2520 bn.), B^{10} (3835bn, alpha +Li), Li^6 (70.5bn.), Gd (49700bn.) and U^{235} (681bn, fission)

Experiments are difficult with these elements but they are very useful for shielding, i.e. stopping unwanted neutrons, and for counting them. Sometimes isotopes that are non-absorbing can be separated at great cost to do experiments on these materials.

There is usually a 1/velocity variation to the absorption cross section; the low energy tail of a resonance

Cross section for scattering from a single nucleus

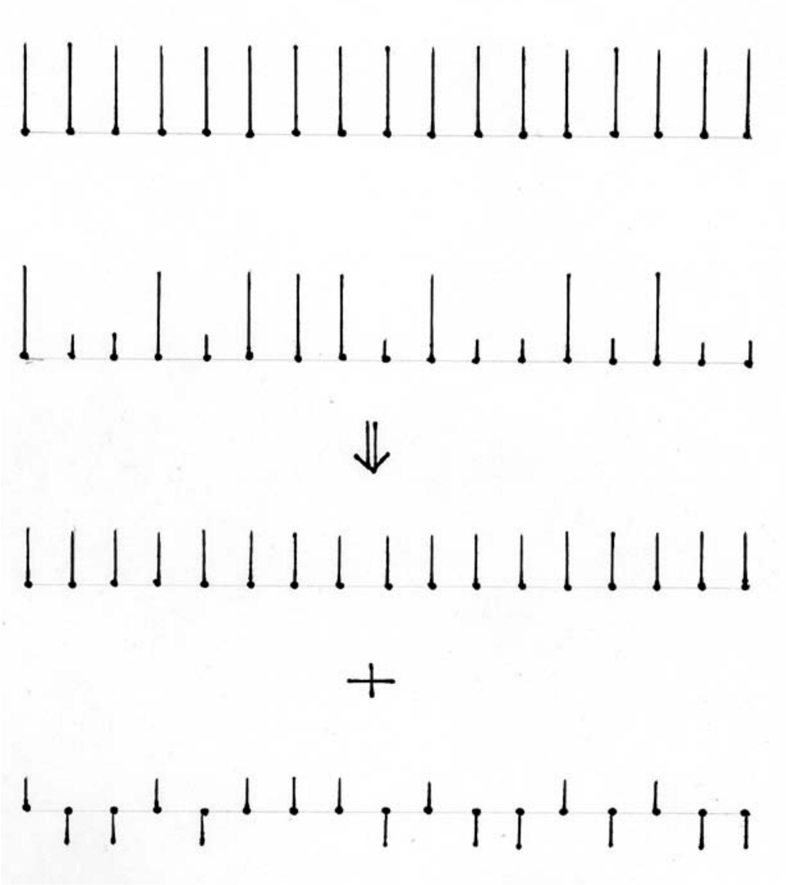
- We do not know the functional form of the neutron-nucleus interaction but we do know that it is short-ranged and can be represented by a delta function, δ(r). (Fermi pseudopotential). The quantity b can either be positive or negative and is a measured quantity with magnitude ~10^{-12} cm.
- If we work out the total cross section from a single fixed nucleus with scattering length b we have

$$\sigma=4\pi b^2$$

Since the nucleus is fixed we have no energy transfer but we do have momentum transfer since the neutron changes direction in the scattering event.

The unit of cross section is barns (10^{-24}cm^2)

Scattering from a periodic array of nuclei:coherent and incoherent scattering



Case of single isotope

Element consisting of two isotopes

Construction of <*b*>

Construction of the variance of <b> namely $\surd(\langle b^2\rangle - \langle b\rangle^2)$

We work out the intensity from the product of the wavefunction with its complex conjugate

Definitions of scattering lengths and cross sections

$$b_{coh} = \overline{b} = (\langle b_{\xi} \rangle_{iso})_{spin}$$

$$b_{inc} = \sqrt{(}\langle b^2 \rangle - \langle b \rangle^2)$$

$$\sigma_{coh} = 4\pi b_{coh}^2$$

$$\sigma_{inc} = 4\pi b_{inc}^2$$

In addition to the isotopic incoherence there is a contribution to incoherent scattering if the nucleus has a nuclear spin

The values of these experimental constants for the elements and their isotopes are given in say, “The Neutron Data Booklet“

Variation of b_{coh} across the periodic table as a function of Z

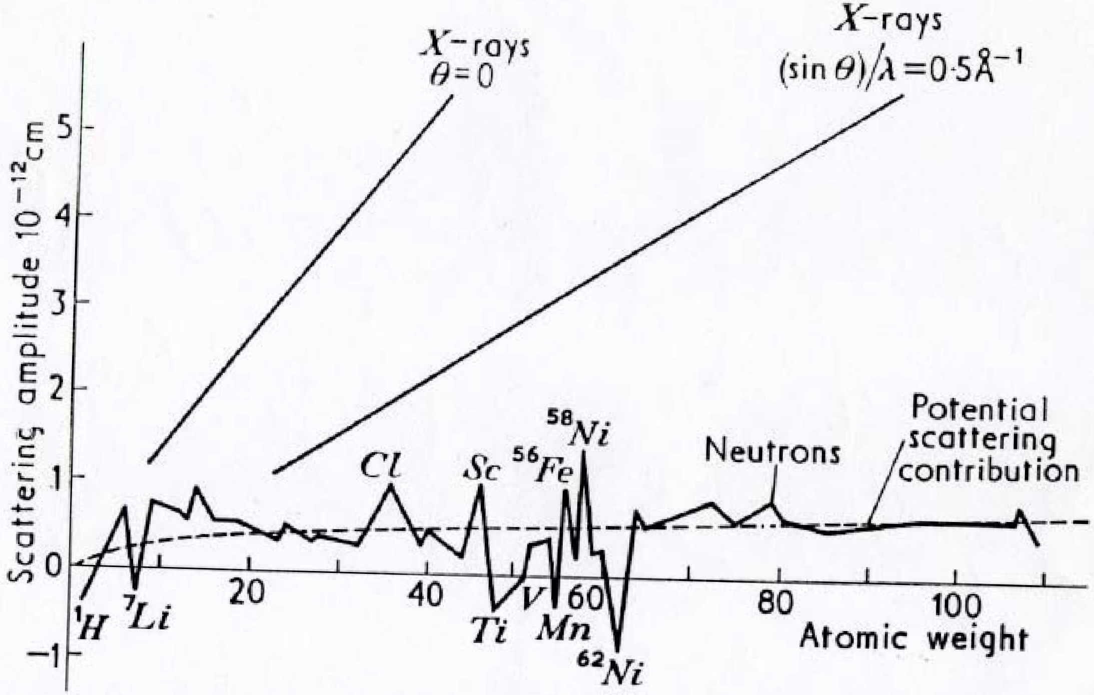


FIG. 14. Irregular variation of neutron scattering amplitude with atomic weight due to superposition of 'resonance scattering' on the slowly increasing 'potential scattering': for comparison the regular increase for X-rays is shown. (From *Research*, London, 7, 257, 1954.)

Note negative values, especially for D: very important for biology

Note small variation overall and irregular variation with Z

Light/heavy nucleus distinction

Some scattering lengths and cross sections

	H	D	Li	Al	Ti	Mn	Ni	U	U^{235}
b	-.37 $\times 10^{-12}$ cm	.67 $\times 10^{-12}$ cm	-.19 $\times 10^{-12}$ cm	.34 $\times 10^{-12}$ cm	-.34 $\times 10^{-12}$ cm	-.38 $\times 10^{-12}$ cm	1.03 $\times 10^{-12}$ cm	0.84 $\times 10^{-12}$ cm	1.05 $\times 10^{-12}$ cm
σ_{inc}	80.3 Bn S	2.05 Bn S	.92 Bn S+I	.008 bn	2.87 Bn S+I	0.4 Bn S	5.2 Bn I	.005 bn	.2 bn S
σ_{abs}	.33 bn	.005 bn	70.5 bn	.23 bn	6.09 bn	13.3 bn	4.49 bn	7.57 bn	681 bn

Coherent scattering

- Corresponds to the interference of the scattered wavelets from all the nuclei. The scattering is seen at special points in **Q (** the Laue spots from a crystal) or discrete angles (the Debye-Scherrer cones from a powder)
- The signal from lattice vibrations is seen at special locations, namely the wavevector **q** of the vibration **(Q-τ)** corresponding to a particular energy $\hbar\nu_{phonon}$.
- The cross sections for these phenomena are all proportional to $\langle b \rangle^2$
- If we have correlations between atom positions, for example in short-range order, then these are seen through $\langle b \rangle^2$

Incoherent scattering

- The scattering from the nuclei , which may be perfectly periodically arranged, are all out of phase with each other. There is no adding up in phase from different sites. There is still scattering but it is just from every site separately. Every nucleus for itself! The scattering is seen at all scattering angles, all **Q**. It does not tell us about structure!
- It does tell us about what is happening at the same site as a function of time. Every site experiences the effect of every phonon so it gives is the sum of all modes, or the density of vibrational states by inelastic scattering
- Basically a pest because it competes with other scattering cross sections which are more useful

Neutron-magnetic moment interaction

$$\underline{B}_S + \underline{B}_L = \frac{\mu_0}{4\pi}\left(curl\,\frac{\mu_e \wedge \underline{R}}{R^2} - \frac{2\mu_B}{\hbar}\frac{\underline{p} \wedge \underline{R}}{R^2} \right)$$

The spin and orbital moment on the atom generate a magnetic field which the magnetic moment on the neutron feels

Note that there is a vector character to the interaction which will mean that we can get at the x,y,z component of the spin and orbital moment

Note that there are different interactions in different directions because of the anisotropy of the field

Since the magnetism is distributed in real space on a scale of Å there is a form factor and the scattering decreases with **Q**

For magnetic scattering we replace the scattering potential specified by <b> by

$-\gamma r_0 \underline{\sigma} \cdot \underline{M}_\perp$ and multiply by the complex conjugate

where $\underline{M}_\perp = \sum_i e^{i\underline{Q}\cdot\underline{r}_i} (\hat{Q} \wedge (\underline{S}_i \wedge \hat{Q} + \frac{i}{\hbar|Q|}(\underline{p}_i \wedge \hat{Q}))$

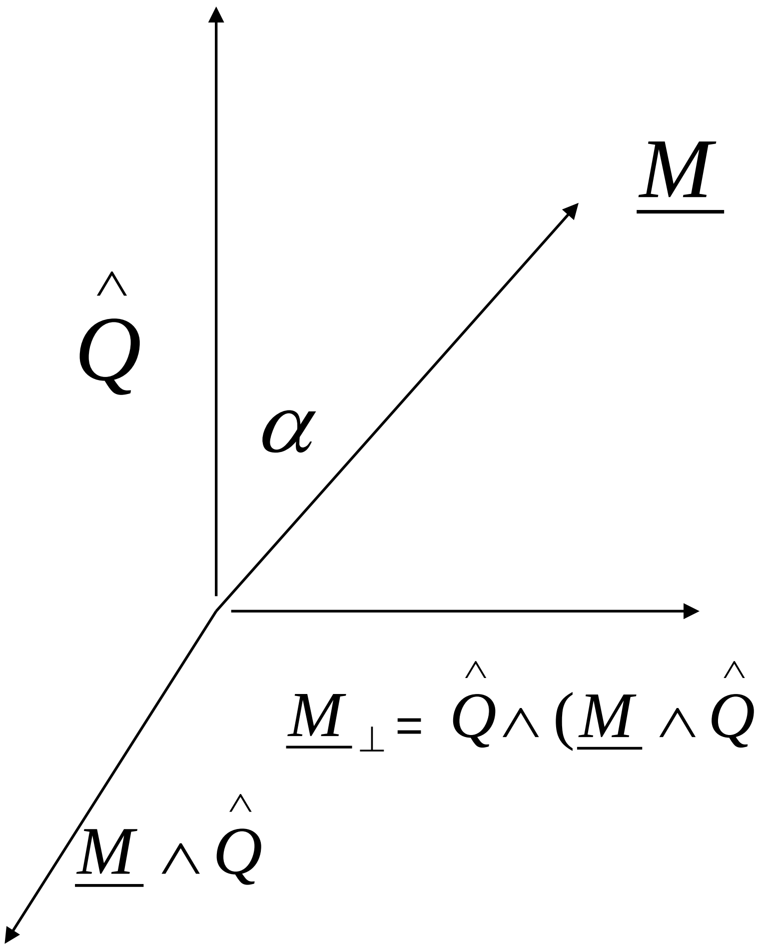
γ is the neutron gyromagnetic ratio, 1.913, and r_0 is the classical electron radius and **σ** is the Pauli spin operator

$\underline{M}_\perp$ is a spin and orbital angular momentum operator.

We can write $\underline{M}_\perp = \hat{Q} \wedge (\underline{M} \wedge \hat{Q})$

The relationship to the magnetic moment is

$\underline{M} = \frac{-1}{2\mu_B} \mathrm{M}^{moment}$ and $\underline{\mathrm{M}}^{moment}(\underline{Q}) = \int e^{i\underline{Q}\cdot\underline{r}} \underline{\mathrm{M}}^{moment}(\underline{r}) d\underline{r}$



$$\underline{M}_\perp = \hat{Q}\wedge(\underline{M}\wedge\hat{Q})$$

$$\underline{M}_\perp = |M|\sin\alpha(\hat{Q}\wedge(\hat{M}\wedge\hat{Q})$$

$$\underline{M}_\perp = \underline{M} - (\underline{M}\cdot\hat{Q})\hat{Q}$$

Physical significance of $\underline{M}_\perp$

Making use of the direction dependence of the scattering

$$\underline{M}_{\perp}^{z} = \left|M^{z}\right| \sin\alpha(\hat{Q} \wedge (\hat{M}_{z} \wedge \hat{Q})$$

Consider the z component of $\underline{M}_{\perp}$ which represents the magnetic moment. If it is perpendicular to **Q** sinα=1 and the scattering is switched on. If it is parallel to **Q** sinα=0 and the scattering is switched off.

For magnetic scattering with unpolarized neutrons there is no cross term between nuclear and magnetic scattering but we can change the magnitude of the scattering by aligning the moment with a magnetic field in a ferromagnet

A famous example: Detection of antiferromagnetism in MnO

New peaks arise because the periodicity of the antiferromagnetic cell is larger than that of the lattice. In a cubic system with a powder sample the orientation of the moments cannot be determined, because of domain effects. In MnO we now know the spins lie almost along the <111> axes

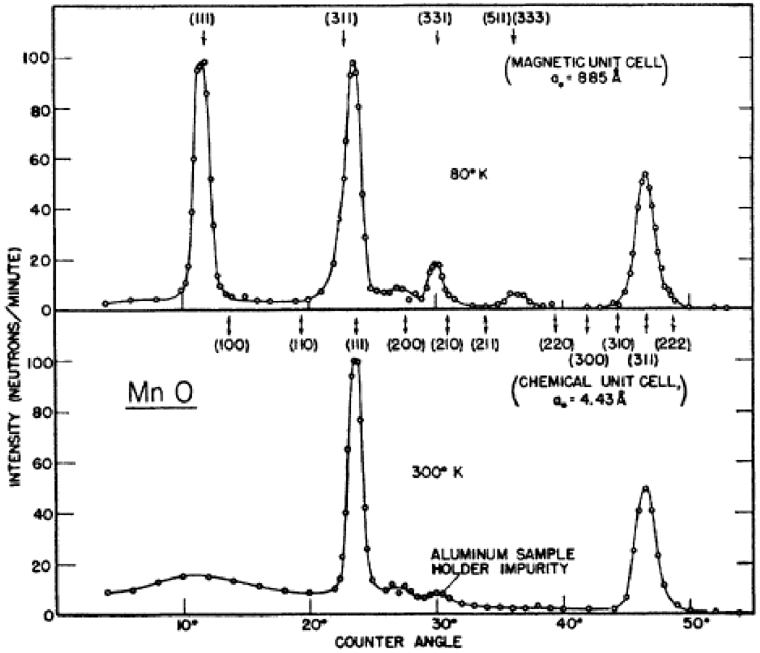
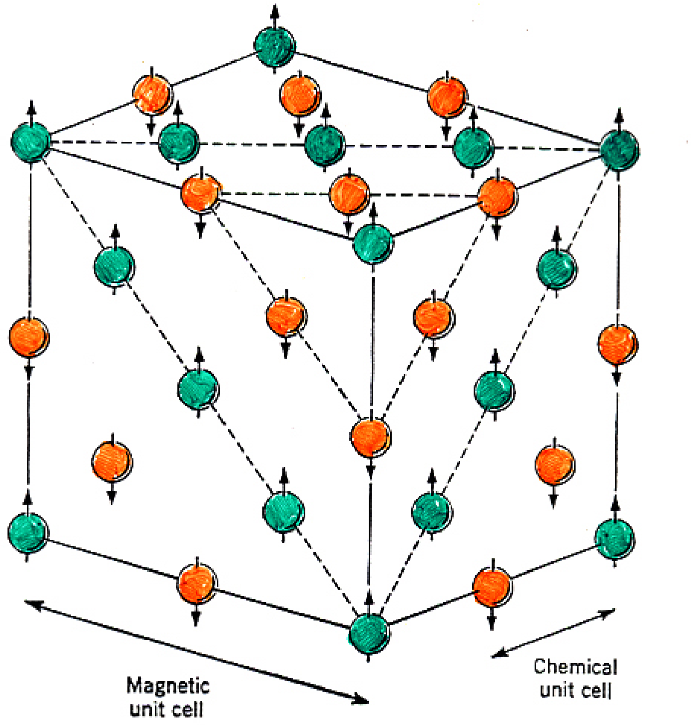


FIG. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.



C. G. Shull and J. S. Smart, Phys. Rev <u>76</u>, 1256 (1949)

Advantages of neutrons (1)

- Variation of b_{coh} allows sensitivity to light elements in the presence of heavy ones
- Large difference between b for H and D: biology, contrast matching in soft matter
- Presence of large σ_{inc} for H. Follow diffusion processes for H, follow water kinetics in batteries
- Neutrons have low energies allowing inelastic processes to be measured easily
- 1.8Å neutron 25.2meV and 1.8Å x-ray 6.89 keV . Note however that one can now attain meV resolution with a keV synchrotron x-ray beam!!! So one can now do triple axis spectroscopy with x-rays

Advantages of neutrons (2)

- Neutrons have a magnetic moment and hence interact strongly with unpaired spins in magnetic materials
- They generally have high penetration. Can use big samples, and make windows of furnaces and cryostats easily and there are many engineering applications
- Weak interaction with matter (say compared with electrons) so the cross sections have a quantitative interpretation

Disadvantages of neutrons

- Not enough of them. Experiments are intensity limited. Even with new sources we now have fluxes that are comparable to x-ray tubes in the 1940's whereas synchrotrons have extended x-ray fluxes by a whopping 10^{10}
- Powder diffraction minimum 100mg
- Single crystal diffraction few mg
- Single crystal inelastic scattering 100-1000mg
- Do not use neutrons if you can solve the problem with x-rays
- As an experimentalist use both neutrons and synchrotron x-rays

Finale

- I hope you have as much fun doing lots of different kinds of experiments with neutrons as I did
- Best of luck with your careers