Introduction to neutron scattering

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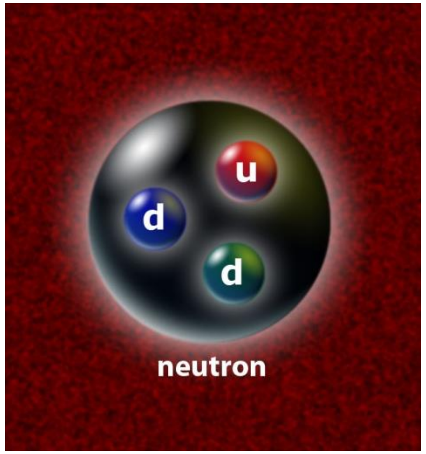
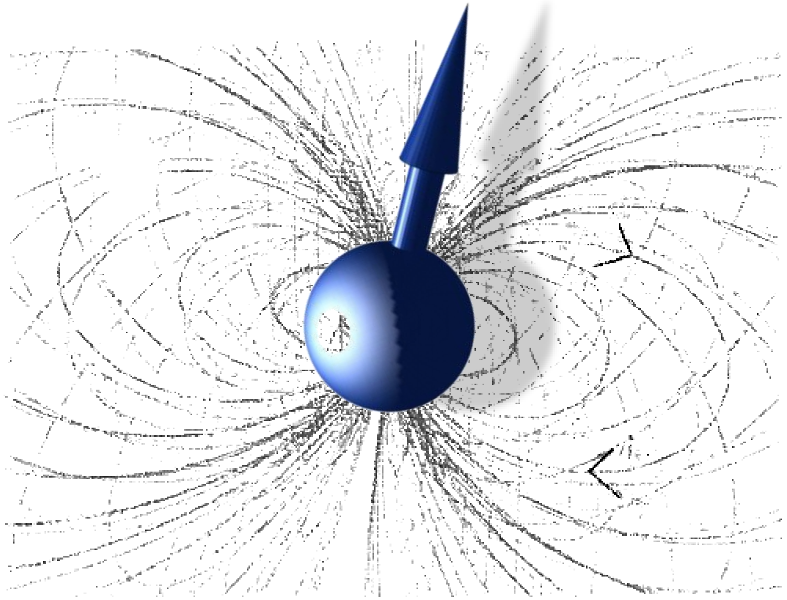
Useful reading material

- **Squires**, *Introduction to the Theory of Thermal Neutron Scattering*
  advanced text, comprehensive
- **Shirane, Shapiro and Tranquada**, *Neutron scattering with a triple-axis spectrometer*
  nicely written book which deals with more practical side of TAS
- **Lovesey**, *Theory of Neutron Scattering from Condensed Matter*
  advanced text, if you wish to go in depth
- **Furrer, Mesot and Strässle**, *Neutron Scattering in Condensed Matter Physics*
  basic introduction to theory and experiment
- **Sivia**, *Elementary Scattering Theory for X-ray and Neutron Users*
  basics of scattering theory from a slightly different perspective

Physical properties





Energy	Classification
0 - 5 meV	Cold
5 -100 meV	Thermal
100 meV - 1 eV	Epithermal
1 eV -100 eV	Resonant
100 eV - 100 keV	Intermediate
100 keV - 10 MeV	Fast
10 MeV - 10 GeV	Ultra-fast
>10 GeV	Relativistic

	Charge	Spin	Mass (MeV/c^2)	$\gamma/2\pi$ (kHz/G)
Electron	±e	1/2	0.511	2800
Muon	±e	1/2	105.7	13.6
Proton	+e	1/2	938.3	4.26
Neutron	**0**	**1/2**	**939.6**	**– 2920**

- Neutrons are subatomic particles that have a net zero charge
- Possess a magnetic moment and so are sensitive to magnetic fields

- Introduc

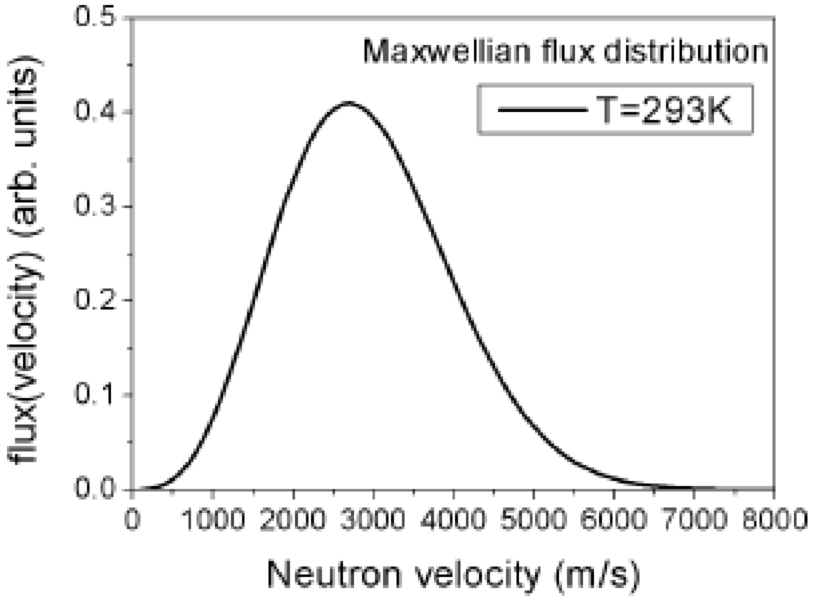
Physical properties

$$k = \frac{2\pi}{\lambda}, \quad p = \hbar k, \quad E = \frac{mv^2}{2} = \frac{\hbar^2 k^2}{2m}$$

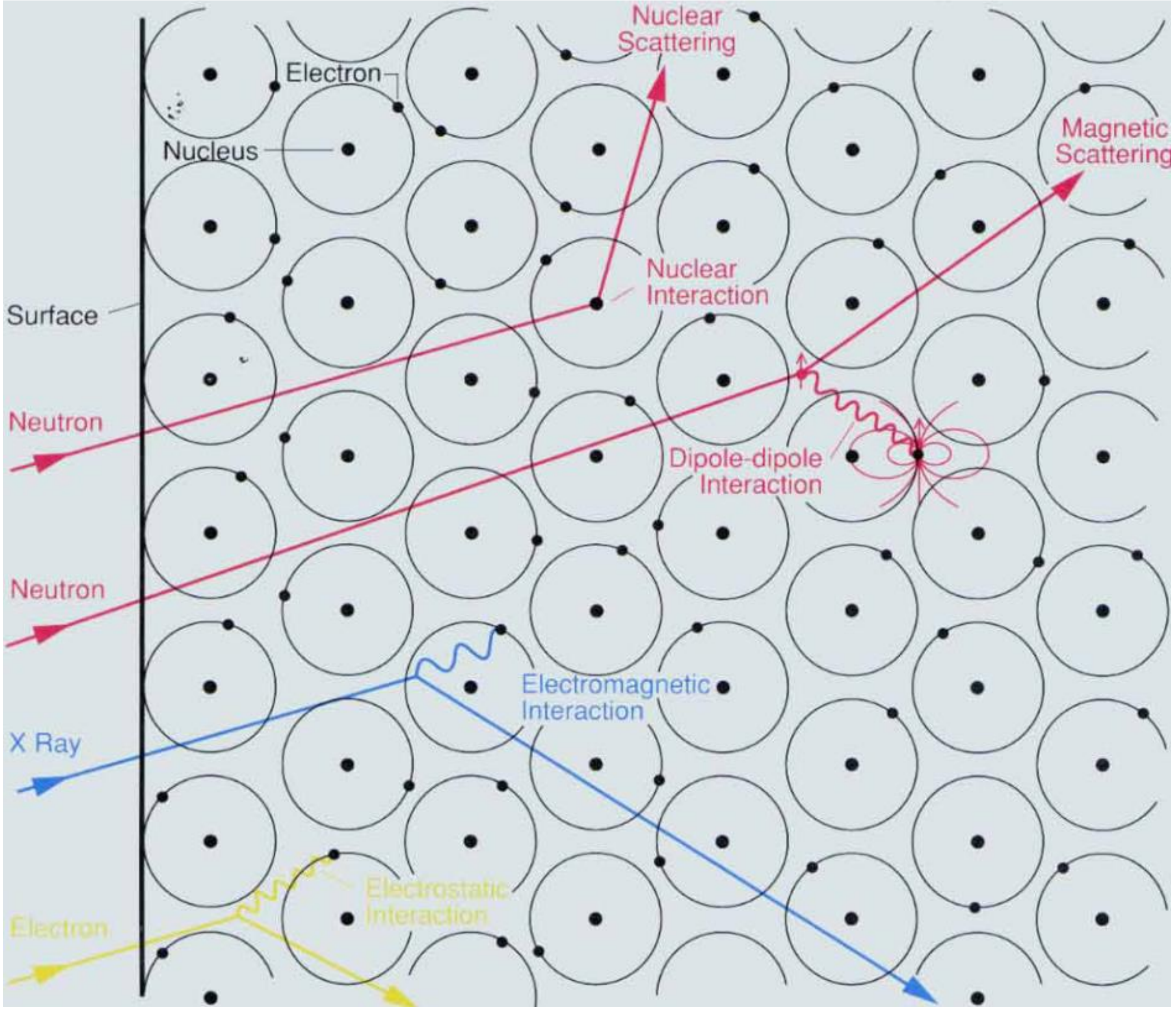
$$E[\text{meV}] = 0.08617\, T[\text{K}] = 5.227(v[\text{km/s}])^2 = 81.81 \frac{1}{(\lambda[\text{Å}])^2} = 2.072(k[\text{Å}^{-1}])^2$$

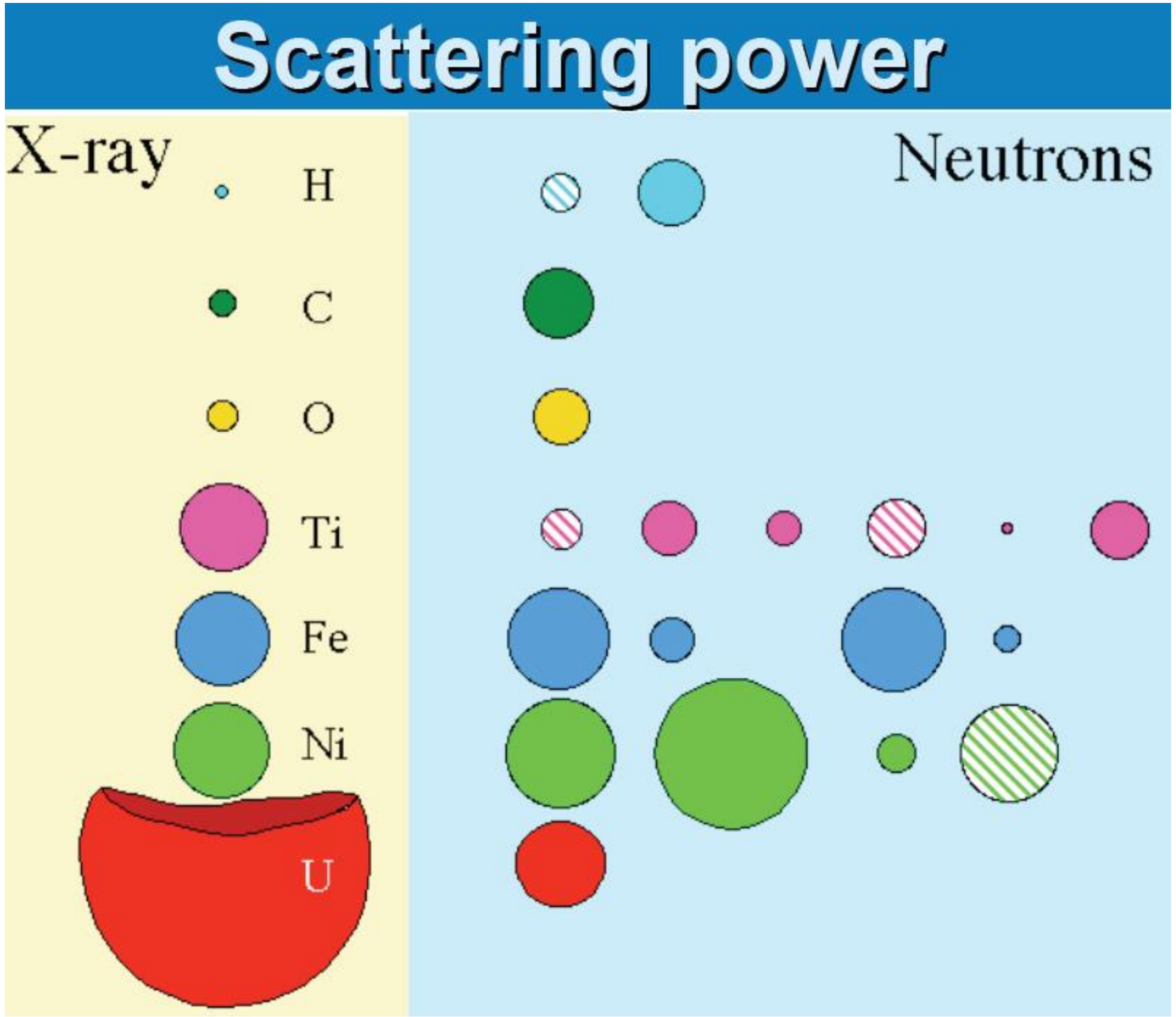
$T = 293$ K
$v = 2.20$ km/s
$E = 25.3$ meV
$\lambda = 1.798$ Å
$k = 3.49$ Å^{-1}

comparable to energy and length scales of static and dynamic correlations in condensed matter



Comparison of different scattering techniques

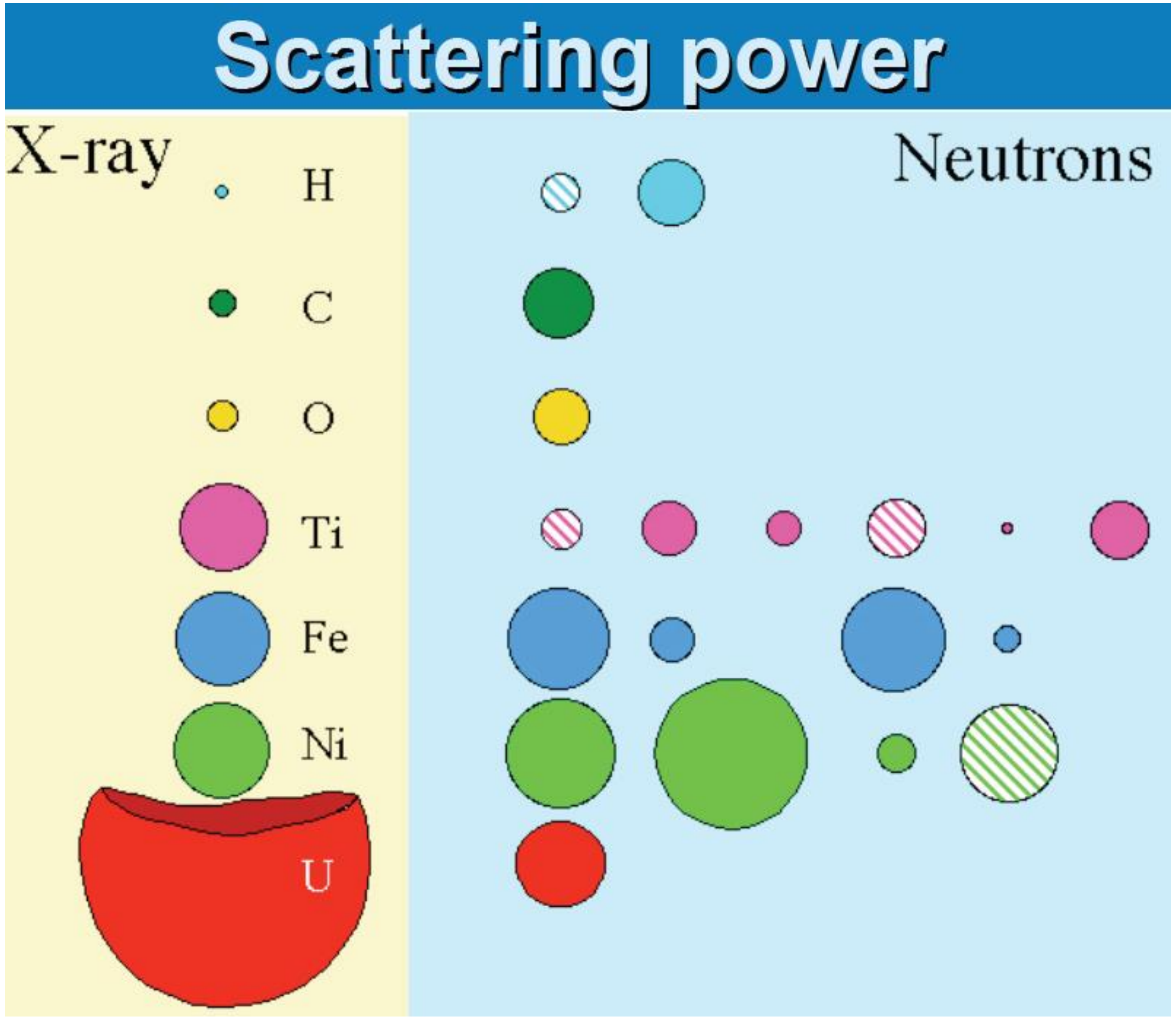




• Introduc

Neutrons vs X-rays

- X-ray sources are orders of magnitude brighter, high flux neutron source
- X-ray scattering intensity proportional to number of electrons - sees heavy elements
- Intensity of (nuclear) neutron scattering proportional to square of scattering length (strong force)
- Neutron scattering intensity randomly varies for elements - can see all elements
- X-rays scatter from electrons, neutrons scatter from nucleus
- Neutrons have large penetration depths - see through materials



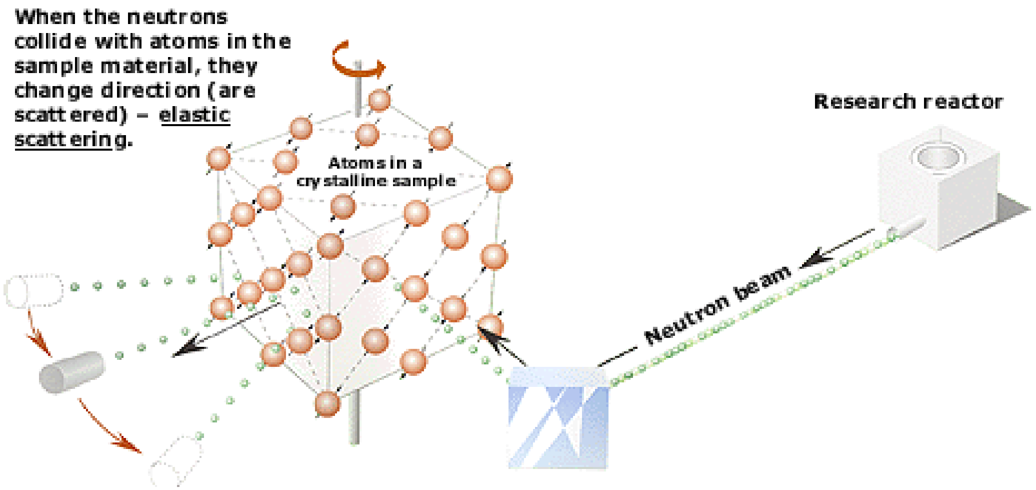
Applications in different fields of science

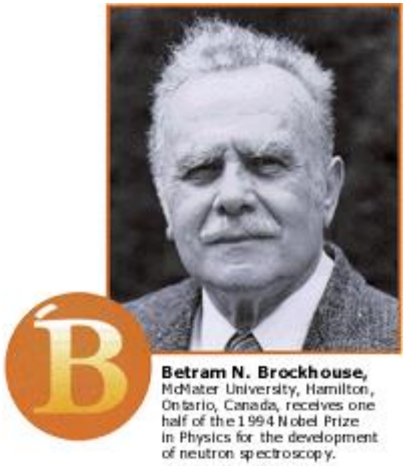
- Condensed matter physics
  (magnetism, superconductivity, glasses, liquids)
- Materials research
  (stress/strain, hydrogen in materials)
- Soft condensed matter
  (polymers, composites)
- Structural chemistry
  (catalysis, reactions, parametric studies, molecular spectroscopy)
- Geology
  (minerals at high P,T, hydrogen in rocks)
- Life sciences
  (membranes, protein structure, -dynamics, and -complexes)
- Particle physics
  (basic properties of the neutron, basic quantum mechanics)

1994 Nobel Prize in Physics

Shull

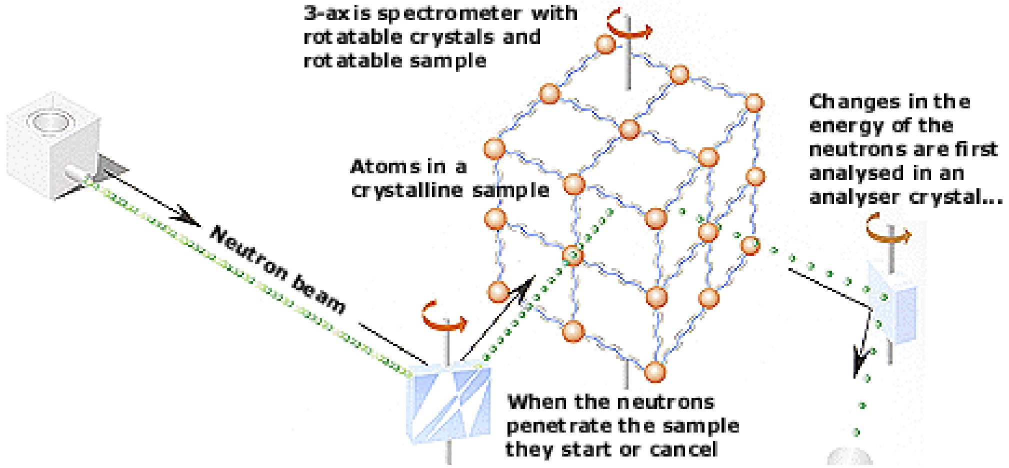
Neutrons show where atoms are





Brockhouse

Neutrons show what atoms do



Neutrons interacts with the cores of the atoms, and…

- Introduc

1994 Nobel Prize in Physics

neutrons have a (small) MAGNETIC moment.

They can be used to study:

- microscopic magnetic structure
  with atomic spatial resolution

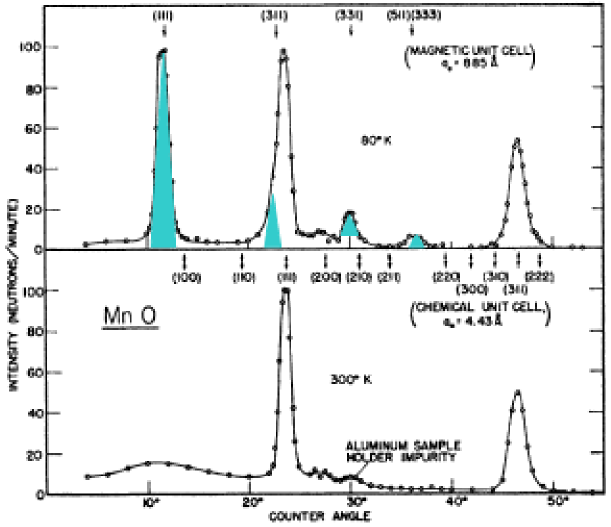
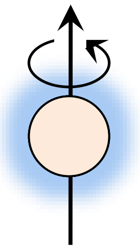
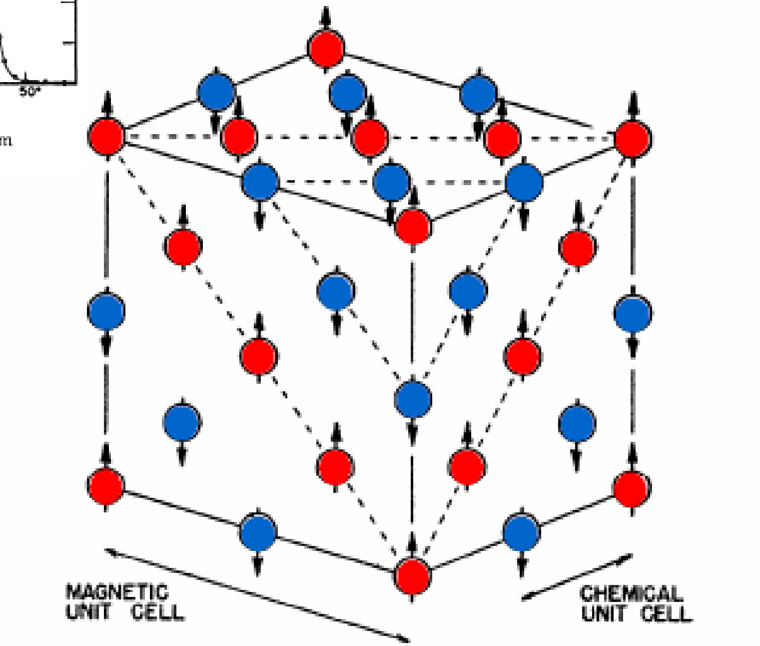


Fig. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.

- magnetic fluctuations with
  1 GHz to 100 THz (10 femto-second) frequencies

- Neutrons have SPIN. They can probe quantum effects

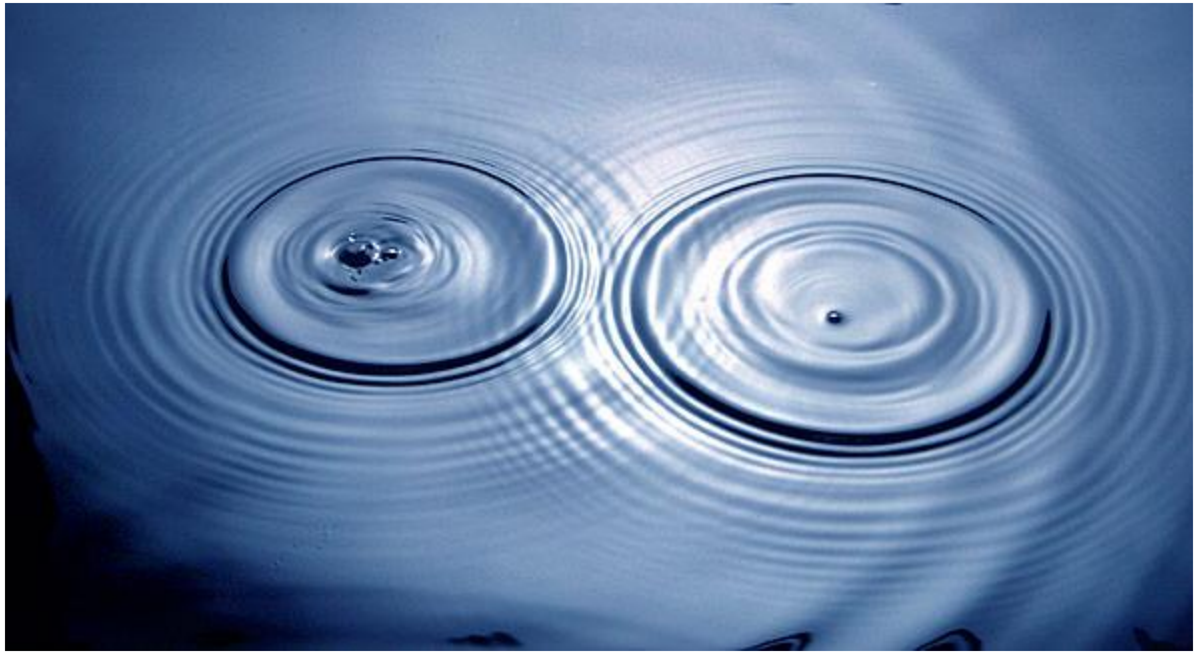


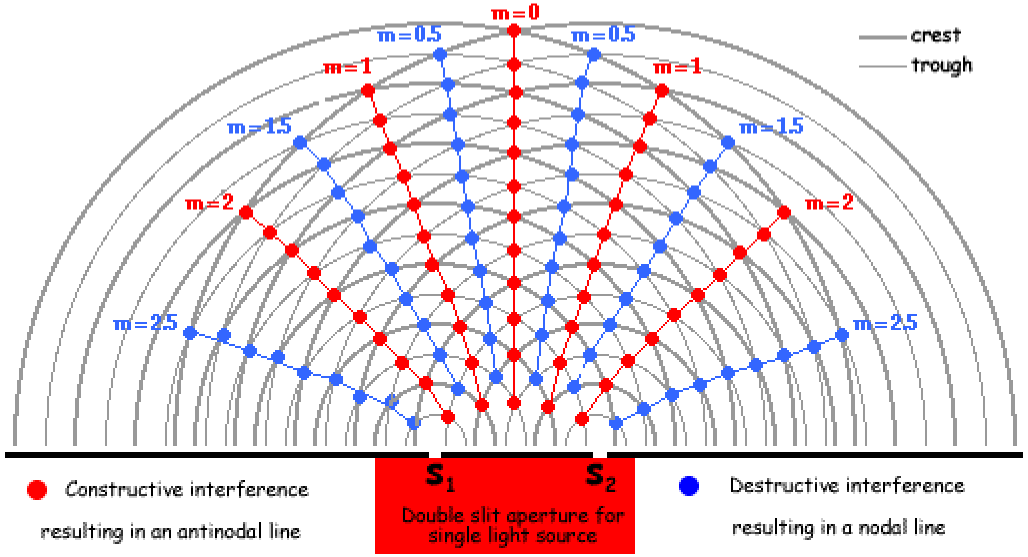


⇒ Neutron research in solid state and materials science:
currently >1000 experiments / year and similar number of publications in Europe alone

Theory of neutron scattering

Interference of waves

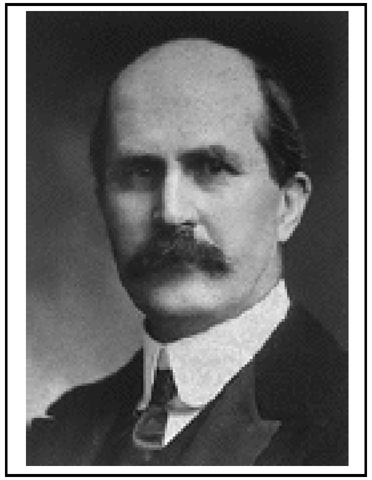




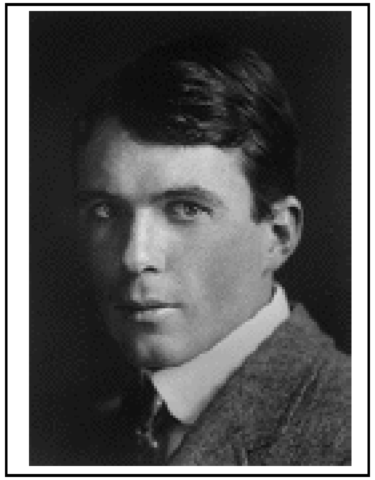
- Theory

Bragg's law

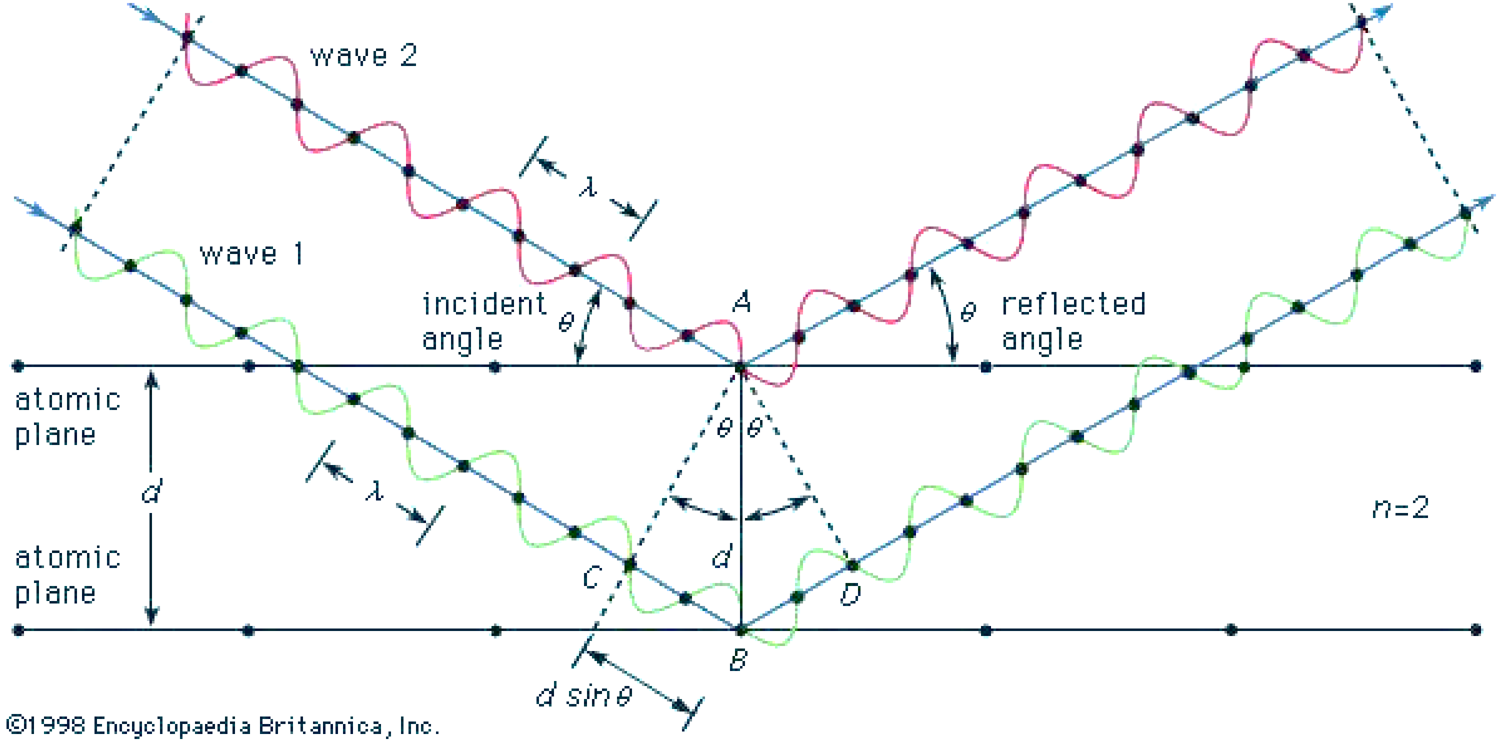
Nobel Prize 1915



W.H. Bragg
(1862–1942)



W.L. Bragg
(1890–1971)

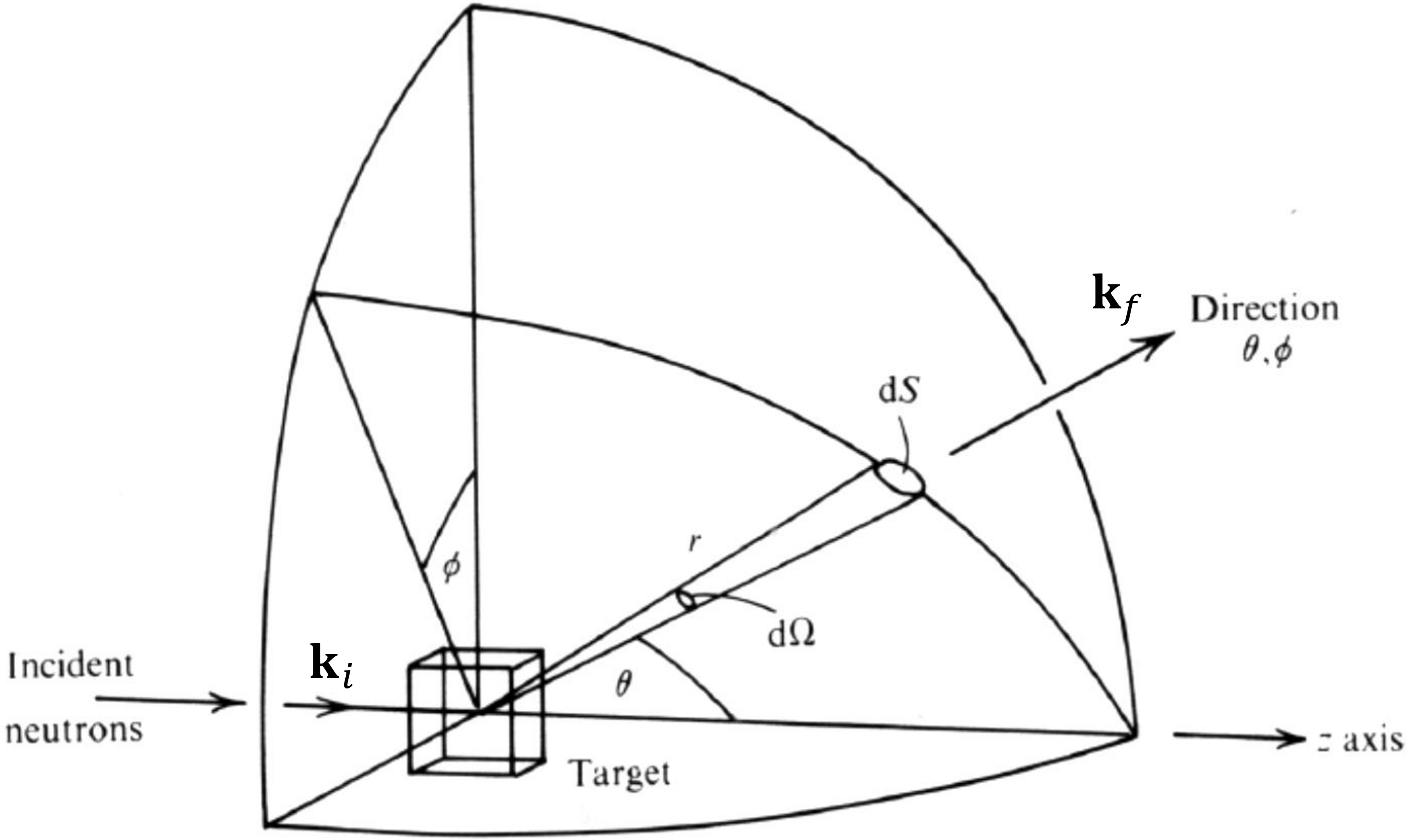


"for their services in the analysis of crystal structure by means of X-rays"

$$\lambda = 2d_{hkl} \sin \theta_{hkl}$$

- Theory

Total and differential cross-sections



- Theory

Scattering cross-section

- Flux $$\Psi = \frac{\text{number of neutrons impinging on a surface per second}}{\text{surface area perpendicular to the neutron beam direction}}$$

- Cross-section $$\sigma = \frac{1}{\Psi}\,\text{number of neutrons scattered per second}$$

- Differential cross-section

$$\frac{d\sigma}{d\Omega} = \frac{1}{\Psi}\frac{\text{number of neutrons scattered per second into solid angle } d\Omega}{d\Omega}$$

- Partial differential cross-section

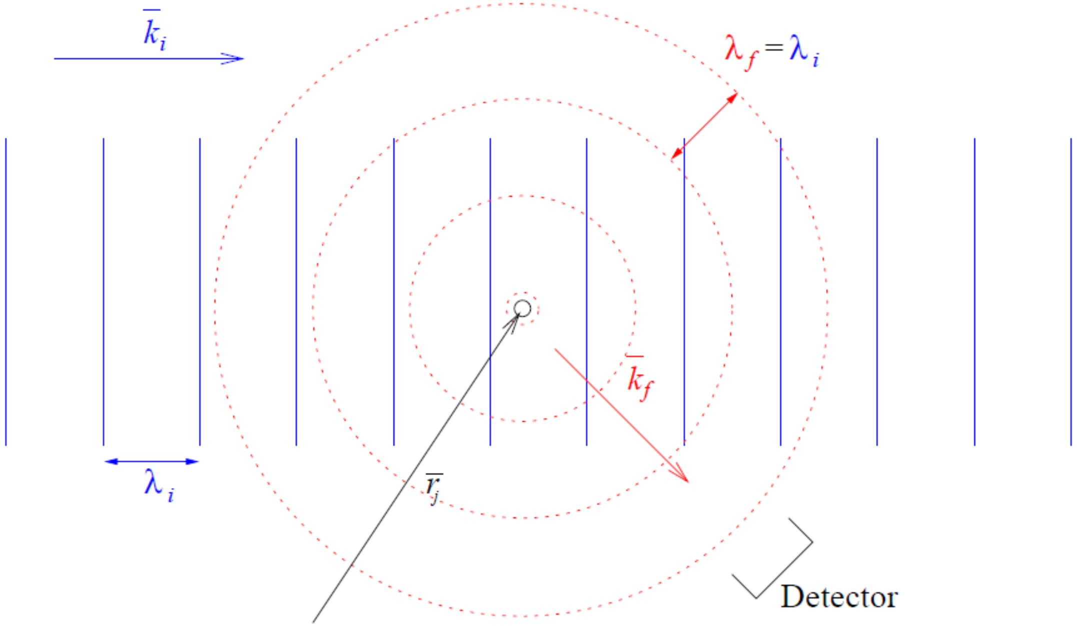
$$\frac{d^2\sigma}{d\Omega dE_\mathrm{f}} = \frac{1}{\Psi}\frac{\text{no. of neutrons scattered per sec. in } d\Omega \text{ with energies } [E_\mathrm{f}; E_\mathrm{f} + dE_\mathrm{f}]}{d\Omega dE_\mathrm{f}}$$

- Integral relations $$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega. \qquad \frac{d\sigma}{d\Omega} = \int \frac{d^2\sigma}{d\Omega dE_\mathrm{f}} dE_\mathrm{f}$$

- Theory

Neutron scattering process – scattering from a single nucleus

- We go from initial state to final state
- Initial state:
  - Of neutron: plane wave
  - Of sample
- Final state
  - Of neutron
  - Of sample



- Elastic scattering: state of sample does not change
- Final state from single particle is a spherical wave

$$\psi_{\mathrm{f}}(\mathbf{r}) = \psi_{\mathrm{i}}(\mathbf{r}_j)\frac{-b_j}{|\mathbf{r}-\mathbf{r}_j|}\exp(ik_{\mathrm{f}}|\mathbf{r}-\mathbf{r}_j|)$$

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- Theory

Neutron scattering process – scattering from a single nucleus

- Initial neutron state (*Y* is normalisation)

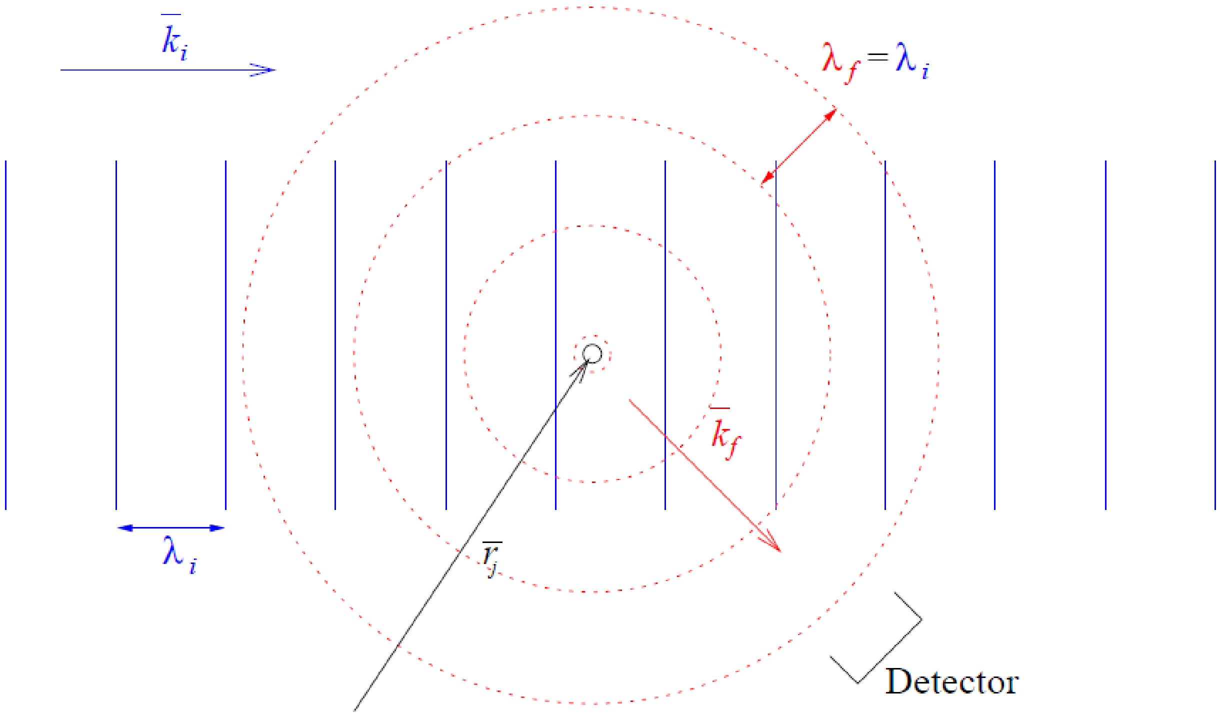
$$\psi_\mathrm{i}(\mathbf{r}) = \frac{1}{\sqrt{Y}} \exp(i\mathbf{k}_\mathrm{i} \cdot \mathbf{r})$$

neutron flux $$\Psi_\mathrm{i} = |\psi_\mathrm{i}|^2 v = \frac{1}{Y}\frac{\hbar k_\mathrm{i}}{m_\mathrm{n}}$$

Density * velocity $$v = \frac{\hbar k_\mathrm{f}}{m_\mathrm{n}}$$

- Final neutron state – spherical wave:

$$\psi_\mathrm{f}(\mathbf{r}) = \psi_\mathrm{i}(\mathbf{r}_j)\frac{-b_j}{|\mathbf{r} - \mathbf{r}_j|} \exp(ik_\mathrm{f}|\mathbf{r} - \mathbf{r}_j|)$$



Long distance approximation: $|\psi_\mathrm{f}|^2 \approx b_j^2/(Yr^2)$ $\qquad d\Omega = dA/r^2$

– Number of neutrons in dΩ per second: $\Psi_{fd\Omega} = \frac{1}{Y}\frac{b^2\hbar k_\mathrm{f}}{m_\mathrm{n}} d\Omega$

$$\frac{d\sigma}{d\Omega} = \Psi_{fd\Omega}/\Psi_i \, d\Omega = b_j^2 \, k_f/k_i = b_j^2$$

- Theory

Neutron scattering from two atoms

- Sum of two outgoing neutron waves

$$\psi_{\mathrm{f}}(\mathbf{r}) = -b\left[\frac{\psi_{\mathrm{i}}(\mathbf{r}_j)}{|\mathbf{r}-\mathbf{r}_j|}\exp(ik|\mathbf{r}-\mathbf{r}_j|) + \frac{\psi_{\mathrm{i}}(\mathbf{r}_{j'})}{|\mathbf{r}-\mathbf{r}_{j'}|}\exp(ik|\mathbf{r}-\mathbf{r}_{j'}|)\right]$$

- Approximations $\Rightarrow$

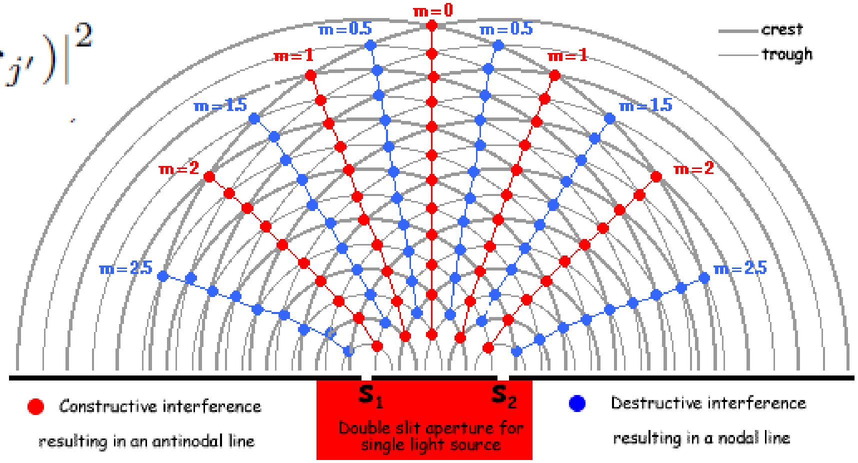
$$\psi_{\mathrm{f}}(\mathbf{r}) = -\frac{1}{\sqrt{Y}}\frac{b}{r}\exp(i\mathbf{k}_{\mathrm{f}}\cdot\mathbf{r})\left[\exp(i(\mathbf{k}_{\mathrm{i}}-\mathbf{k}_{\mathrm{f}})\cdot\mathbf{r}_j) + \exp(i(\mathbf{k}_{\mathrm{i}}-\mathbf{k}_{\mathrm{f}})\cdot\mathbf{r}_{j'})\right]$$

$$\text{no. of neutrons per sec. in } d\Omega = \frac{1}{Y}\frac{b^2\hbar k_{\mathrm{f}}}{m_{\mathrm{n}}}d\Omega\,\left|\exp(i\mathbf{q}\cdot\mathbf{r}_j) + \exp(i\mathbf{q}\cdot\mathbf{r}_{j'})\right|^2$$

- Definition: scattering vector: $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$

- Differential cross-section

$$\frac{d\sigma}{d\Omega} = b^2|\exp(i\mathbf{q}\cdot\mathbf{r}_j) + \exp(i\mathbf{q}\cdot\mathbf{r}_{j'})|^2 = 2b^2\left(1+\cos[\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_{j'})]\right)$$



- Theory

Coherent and incoherent elastic nuclear scattering

- The scattering length *b* depends on the nuclear isotope, spin relative to the neutron and nuclear eigenstate

$$\frac{d\sigma}{d\Omega} = \left|\sum_n b_n \exp i\mathbf{Q}\cdot\mathbf{r}_n\right|^2$$

$$= \sum_n \sum_m b_n b_m \exp i\mathbf{Q}\cdot(\mathbf{r}_n - \mathbf{r}_m)$$

$$\frac{d\sigma}{d\Omega} = \sum_{n\neq m} \langle b_n\rangle\langle b_m\rangle \exp i\mathbf{Q}\cdot(\mathbf{r}_n - \mathbf{r}_m) + \sum_{n=m} \langle b_n^2\rangle$$

$$= \sum_n \sum_m \langle b_n\rangle\langle b_m\rangle \exp i\mathbf{Q}\cdot(\mathbf{r}_n - \mathbf{r}_m) + \sum_{n=m} \langle b_n^2\rangle - \langle b_n\rangle^2$$

Coherent scattering — Incoherent scattering

Coherent scattering

- Correlations between the same and different nuclei – interference, structure and also collective dynamics

Incoherent scattering

- No information on structure – gives flat background

Neutron scattering: an unlikely event

σ = probability that a neutron scatters at an atom

- Theory

Neutron scattering: an unlikely event

Surface of France:

$1000 \times 1000\ \mathrm{km}^2$
$= 10^6\ \mathrm{km}^2 = 10^{12}\ \mathrm{m}^2$
$= 10^{18}\ \mathrm{mm}^2 = 10^{24}\ \mu\mathrm{m}^2$

So 1 barn = chance of hitting a $100 \times 100\ \mu\mathrm{m}^2$ spot **in France** !

Luckily, we have 10^{23} atoms

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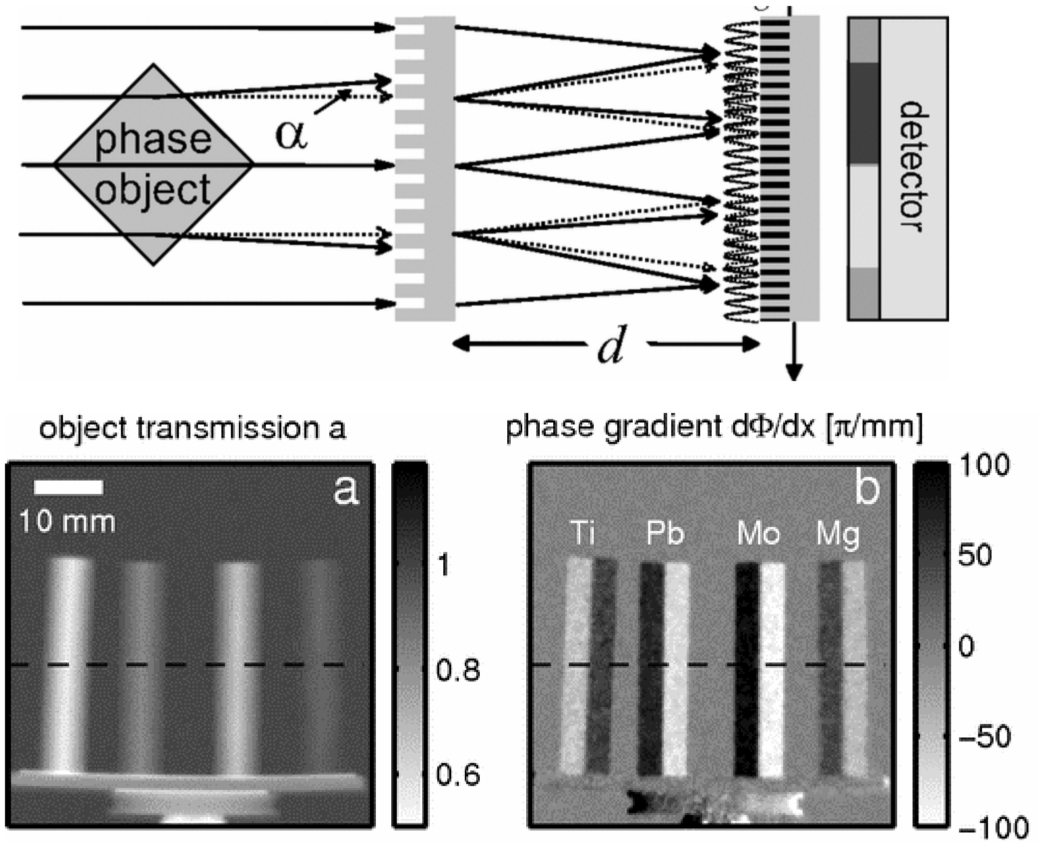
- Theory

Scattering lengths



$$n = 1 + \delta + i\beta$$

Pfeiffer et al., PRL **96** 215505 (2006)

Z	Nucleus	Scattering length b (10^{-15} m)	Incoherent scattering σ_{inc} (10^{-28} m^2)	Absorption $\sigma_{a,th}$ (10^{-28} m^2)
1	^{1}H	-3.742	80.27	0.3326
1	^{2}D	6.674	2.05	0.000519
2	^{3}He	5.74	1.532	5333
2	^{4}He	3.26	0	0
3	Li	-1.90	0.92	70.5
4	Be	7.79	0.0018	0.0076
5	B	5.30	1.70	767
6	C	6.6484	0.001	0.00350
7	N	9.36	0.50	1.90
8	O	5.805	0	0.00019
9	F	5.654	0.0008	0.0096
10	Ne	4.566	0.008	0.039
11	Na	3.63	1.62	0.530
12	Mg	5.375	0.08	0.063
13	Al	3.449	0.0082	0.231
14	Si	4.1507	0.004	0.171
15	P	5.13	0.005	0.172
16	S	2.847	0.007	0.53
17	Cl	9.5792	5.3	33.5
18	Ar	1.909	0.225	0.675
19	K	3.67	0.27	2.1
20	Ca	4.70	0.05	0.43
21	Sc	12.1	4.5	27.5
22	Ti	-3.37	2.87	6.09
23	V	-0.443	5.08	5.08
24	Cr	3.635	1.83	3.05
25	Mn	-3.750	0.40	13.3
26	Fe	9.45	0.40	2.56
27	Co	2.49	4.8	37.18
28	Ni	10.3	5.2	4.49
29	Cu	7.718	0.55	3.78
30	Zn	5.68	0.077	1.11
32	Ge	8.185	0.18	2.20
48	Cd	4.83	3.46	2520

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- Theory

Absorption cross-section

Neutrons can be absorbed in the nuclei

e.g.: $^3He + n \rightarrow {^3H} + {^1H} + 765$ keV

No scattering, so only total cross-section

Absorption cross-section: $v_{\text{th}} = 2.2$ km/s

$$\sigma_a = \sigma_{a,\,th} \frac{v_{th}}{v} = \sigma_{a,\,th} \frac{\lambda}{\lambda_{th}}$$

Attenuation:

$$\Psi(z) = \Psi(0)\exp(-\mu z)$$

$$\mu_a = \sum_i \frac{N_i \sigma_{a,i}}{V} = \sum_i n_i \sigma_{a,i}$$

$$\mu_{tot} = \mu_{scatt} + \mu_a$$

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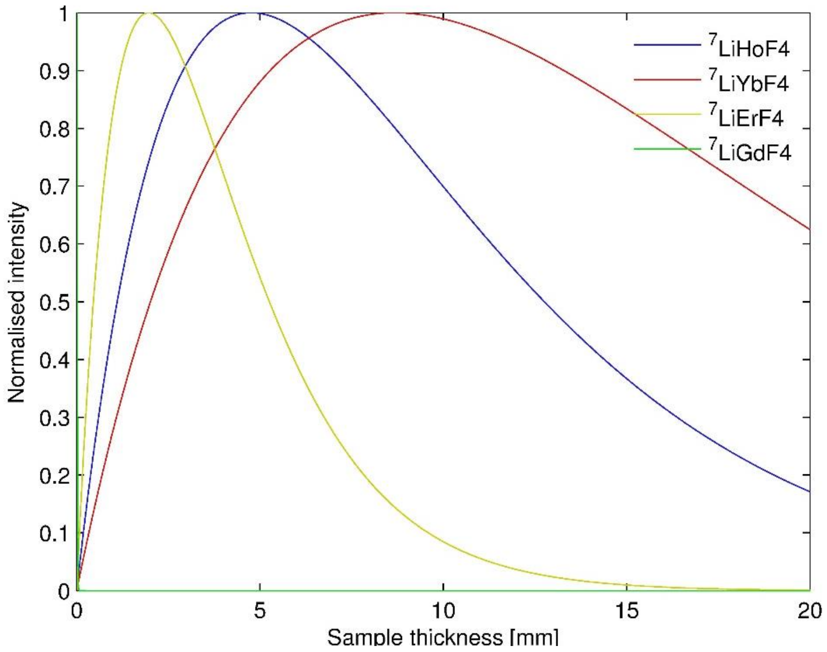
transparent (C, Al)

highly absorbing (^{3}He, Cd)

Coherent and incoherent scattering



Neutron scattering lengths and cross sections							
Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
Er	---	7.79	---	7.63	1.1	8.7	159.(4.)
162Er	0.14	8.8	0	9.7	0	9.7	19.(2.)
164Er	1.56	8.2	0	8.4	0	8.4	13.(2.)
166Er	33.4	10.6	0	14.1	0	14.1	19.6(1.5)
167Er	22.9	3.0	1.0	1.1	0.13	1.2	659.(16.)
168Er	27.1	7.4	0	6.9	0	6.9	2.74
170Er	14.9	9.6	0	11.6	0	11.6(1.2)	5.8

NIST http://www.ncnr.nist.gov/resources/n-lengths/elements/er.html

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- Theory

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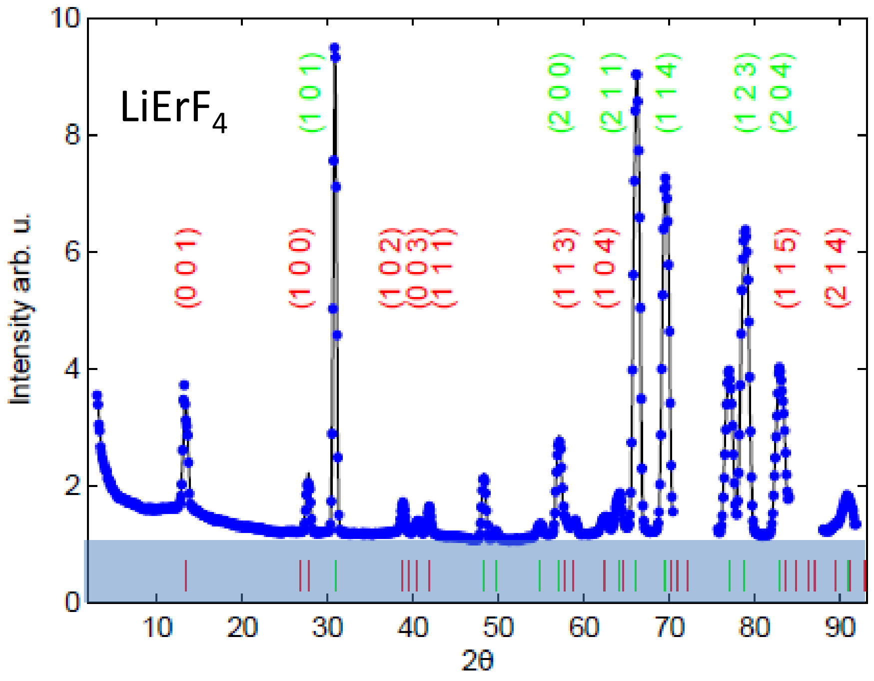
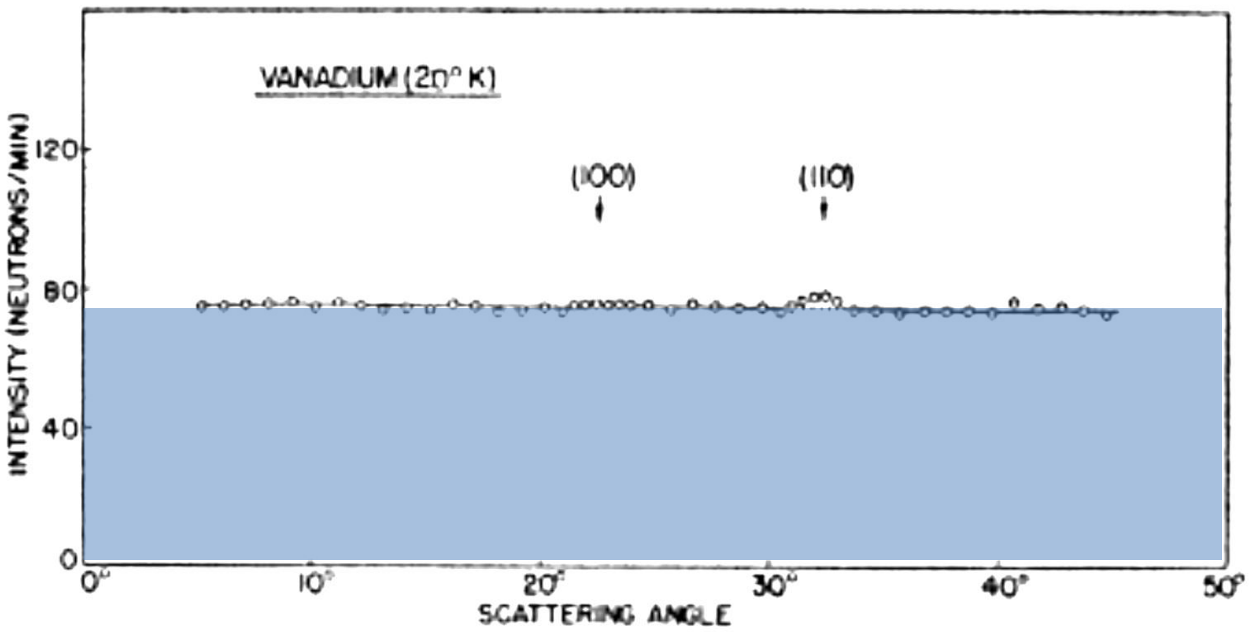
Total cross-section of a system of particles

$$\frac{d^2\sigma}{d\Omega dE_f} = \sum_j \frac{d^2\sigma_j}{d\Omega dE_f}\bigg|_{\mathrm{inc}} + \frac{d^2\sigma}{d\Omega dE_f}\bigg|_{\mathrm{coh}} + \sum_j \frac{d\sigma_j}{d\Omega}\bigg|_{\mathrm{inc}} \delta(\hbar\omega) + \frac{d\sigma}{d\Omega}\bigg|_{\mathrm{coh}} \delta(\hbar\omega)$$

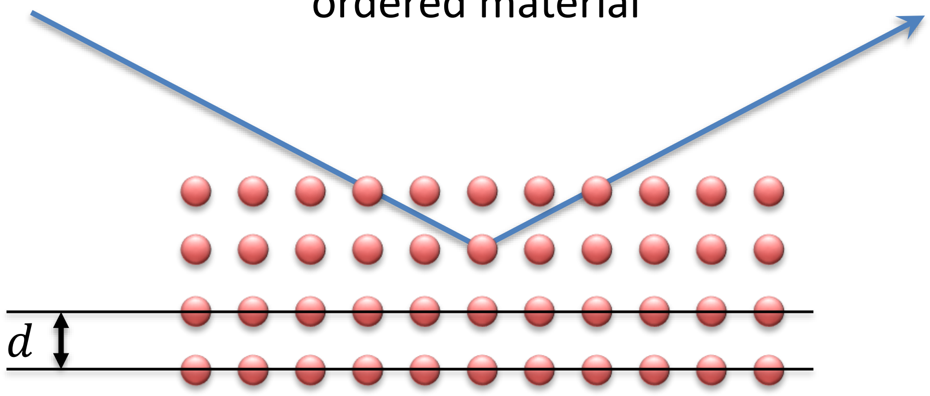




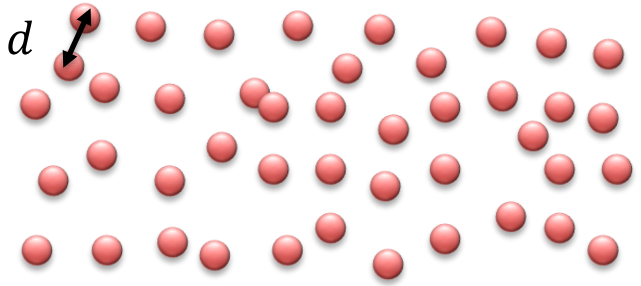
- Theory

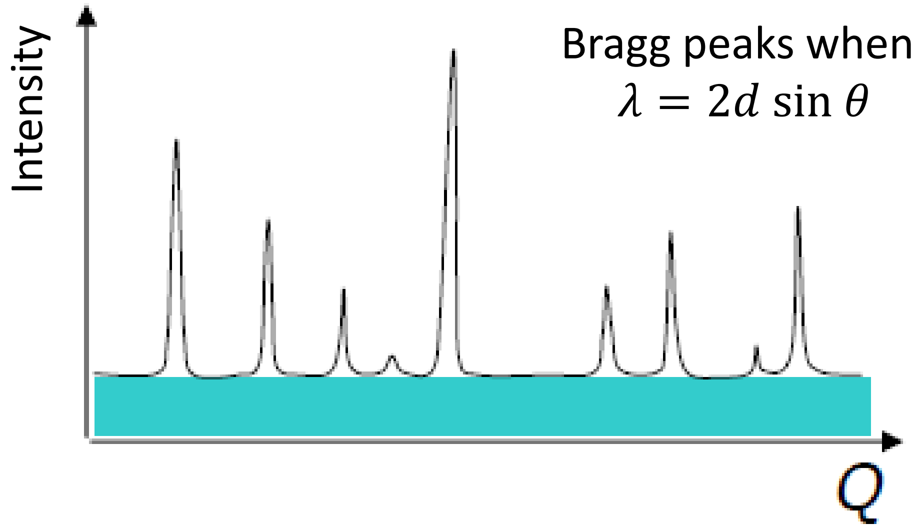
Diffraction

Diffraction from an ordered material

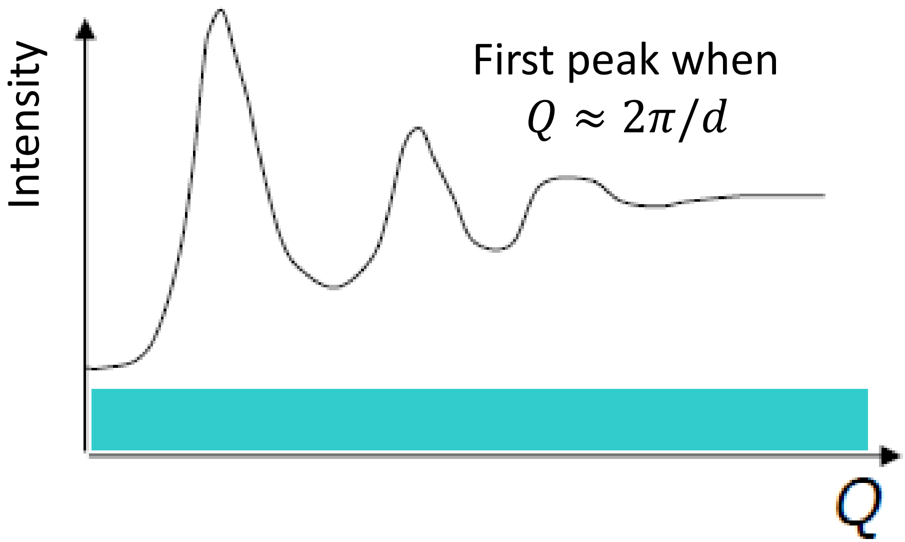


Diffraction from a disordered material





Bragg peaks when
$\lambda = 2d \sin\theta$

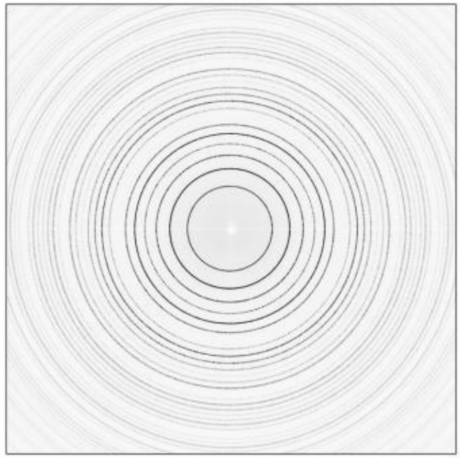


First peak when
$Q \approx 2\pi/d$

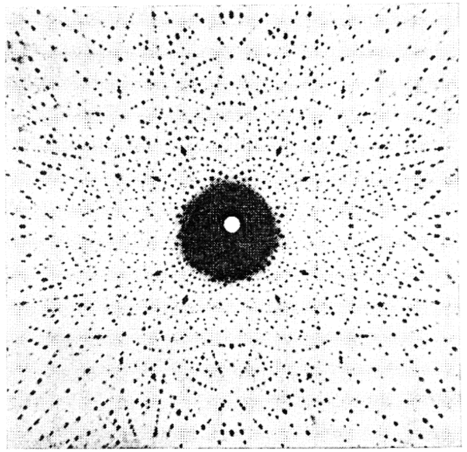
- Theory

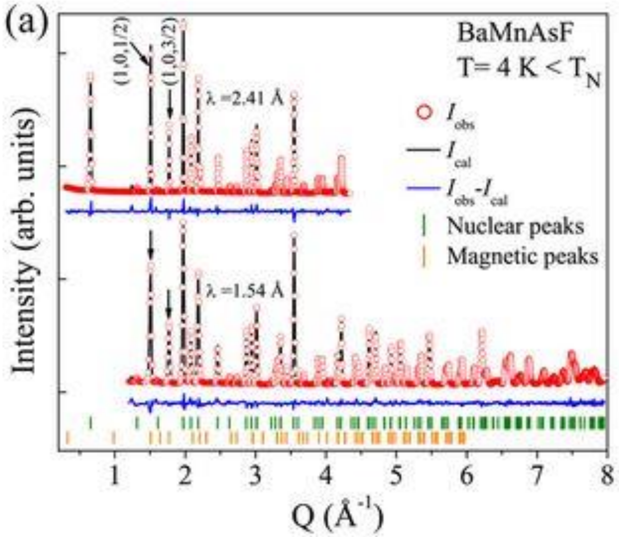
Diffraction

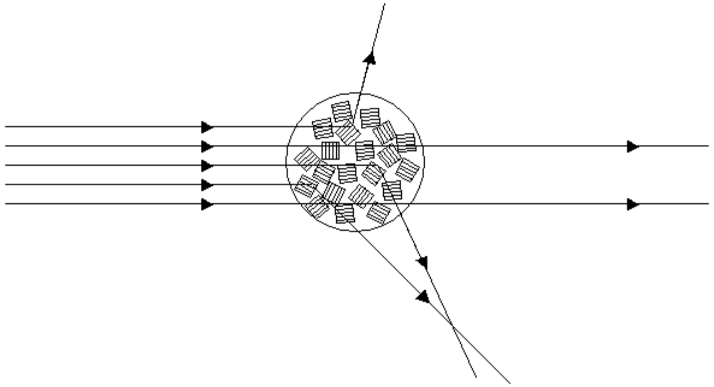
Polycrystal

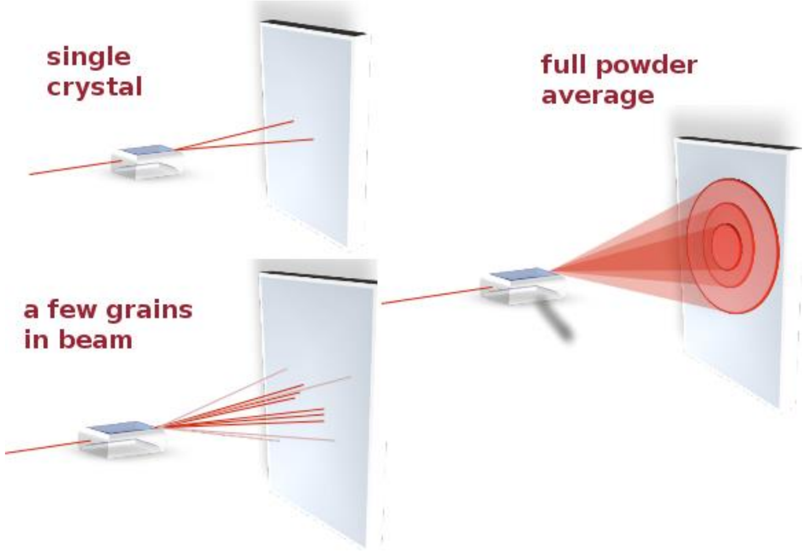


Single crystal









- Theory

Magnetic neutron scattering

Master equation for scatteting – Fermi's Golden rule

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E_f} = \sum_{\lambda_i} p_{\lambda_i} \sum_{\sigma_i,\sigma_f} p_{\sigma_i} \sum_{\lambda_f} \left.\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E_f}\right|_{\sigma_i,\lambda_i\to\sigma_f,\lambda_f}$$

Fermi's Golden Rule:

- Interaction between neutron and sample

$$\left.\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E_f}\right|_{\sigma_i,\lambda_i\to\sigma_f,\lambda_f} = \frac{k_f}{k_i}\left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\langle\sigma_f,\mathbf{k}_f,\lambda_f|\hat{V}|\sigma_i,\mathbf{k}_i,\lambda_i\rangle\right|^2 \delta(E_i - E_f + \hbar\omega)$$

Scattering potential

Final state of sample

Initial state of sample

Final spin and wave state of neutron

Initial spin and wave state of neutron

Magnetic scattering potential

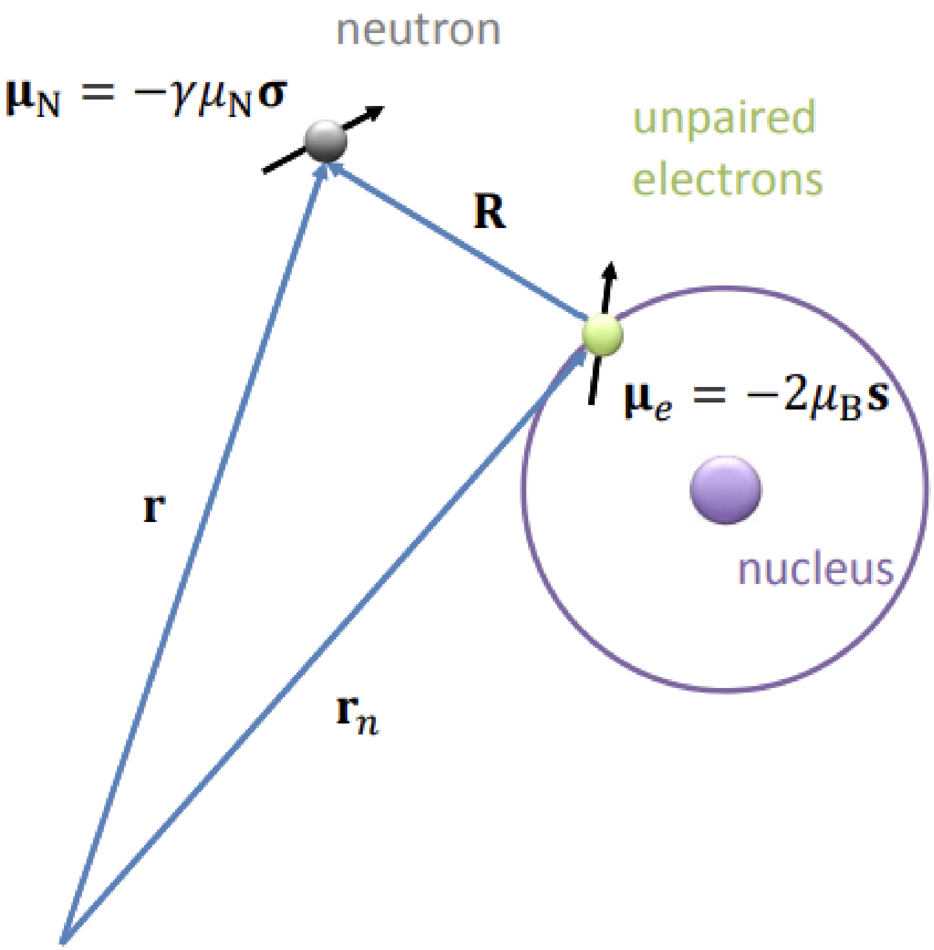
- Magnetic interaction potential:

$$V_{\mathrm{M}}(\mathbf{R}) = -\boldsymbol{\mu}_{\mathrm{N}} \cdot \mathbf{B}(\mathbf{R})$$

$\boldsymbol{\mu}_{\mathrm{N}}$ neutron magnetic moment

$\mathbf{B}(\mathbf{R})$ magnetic field from distribution of electron spin and orbital currents

$$-\boldsymbol{\mu}_{\mathrm{N}} \cdot \mathbf{B} = \frac{\mu_0}{4\pi}\gamma\mu_{\mathrm{N}} 2\mu_B \boldsymbol{\sigma} \cdot \frac{1}{R^2}\left[\nabla \times \mathbf{s} \times \widehat{\mathbf{R}} - \frac{1}{\hbar}\mathbf{p} \times \widehat{\mathbf{R}}\right]$$



Spatial and temporal Fourier transform

$$\left(\frac{d^2\sigma}{d\Omega\, dE_f}\right)_{\lambda_i\to\lambda_f} = \frac{k_f}{k_i}\left(\frac{m_n}{2\pi\hbar^2}\right)^2 \underline{|\langle \mathbf{k}_f\lambda_f\, |V|\, \mathbf{k}_i\lambda_i\rangle|^2}\, \delta(E_{\lambda_i} - E_{\lambda_f} + \hbar\omega)$$

Neutrons treated as plane waves:

$$|\mathbf{ks}_n > = V^{-1/2}\exp(i\mathbf{k}\cdot\mathbf{r}_n)\,|\mathbf{s}_n >$$

Energy conservation ⇒ integral rep.:

$$\delta(\hbar\omega + E_i - E_f) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{i(\hbar\omega + E_i - E_f)t/\hbar}dt$$

Fourier transform in

- space/momentum
- time/energy

Magnetic neutron scattering cross-section

$$|\langle \mathbf{k}_f \lambda_f \; | V | \; \mathbf{k}_i \lambda_i \rangle|^2$$

$$V_{\text{mag}}(\mathbf{r}) = -\frac{\mu_0}{4\pi} 2\gamma \mu_N \mu_B \, \boldsymbol{\sigma}_n \cdot \left(\nabla \times \left(\frac{\mathbf{s} \times \hat{\mathbf{R}}}{|\mathbf{R}|^2} \right) + \frac{1}{\hbar} \frac{\mathbf{p} \times \hat{\mathbf{R}}}{|\mathbf{R}|^2} \right)$$

$$\left(\frac{d^2\sigma}{d\Omega dE_f} \right)_{\text{mag}} = \frac{(\gamma r_0)^2}{2\pi\hbar} \frac{k_f}{k_i} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) |g F_R(Q)|^2 \sum_{RR'} \int dt e^{iQ(R-R')-i\omega t} \langle S_R^\alpha(0) S_{R'}^\beta(t) \rangle$$

cross-section

pre factor

dipole factor

magnetic form factor

Fourier transform

spin-spin correlation function

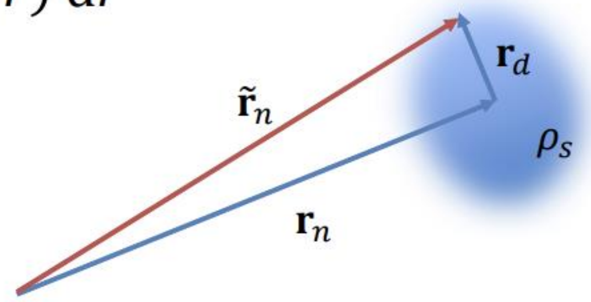
Magnetic form factor

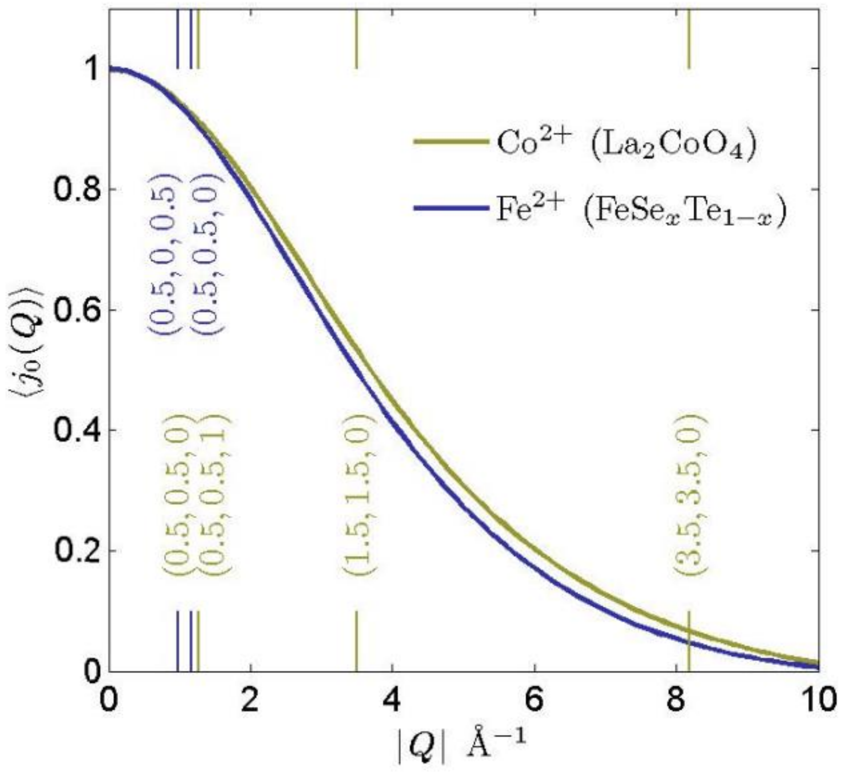
- A magnetic moment is spread out in space due to spatial distribution of unpaired electrons around a magnetic ion

- Dipole approximation:

$$M_n(\mathbf{Q}) \approx -\mu_\mathrm{B}[(\langle j_0(\mathbf{Q})\rangle + \langle j_2(\mathbf{Q})\rangle)\mathbf{L}_n + 2\langle j_0(\mathbf{Q})\rangle \mathbf{S}_n]$$

$$\langle j_m(\mathbf{Q})\rangle = \int_0^\infty r^2 \rho_s(r) j_m(Qr)\,\mathrm{d}r$$





Dipole factor – neutrons see only component perp to Q

$$|\mathbf{M}_\perp| = |\mathbf{M}|\sin\alpha$$

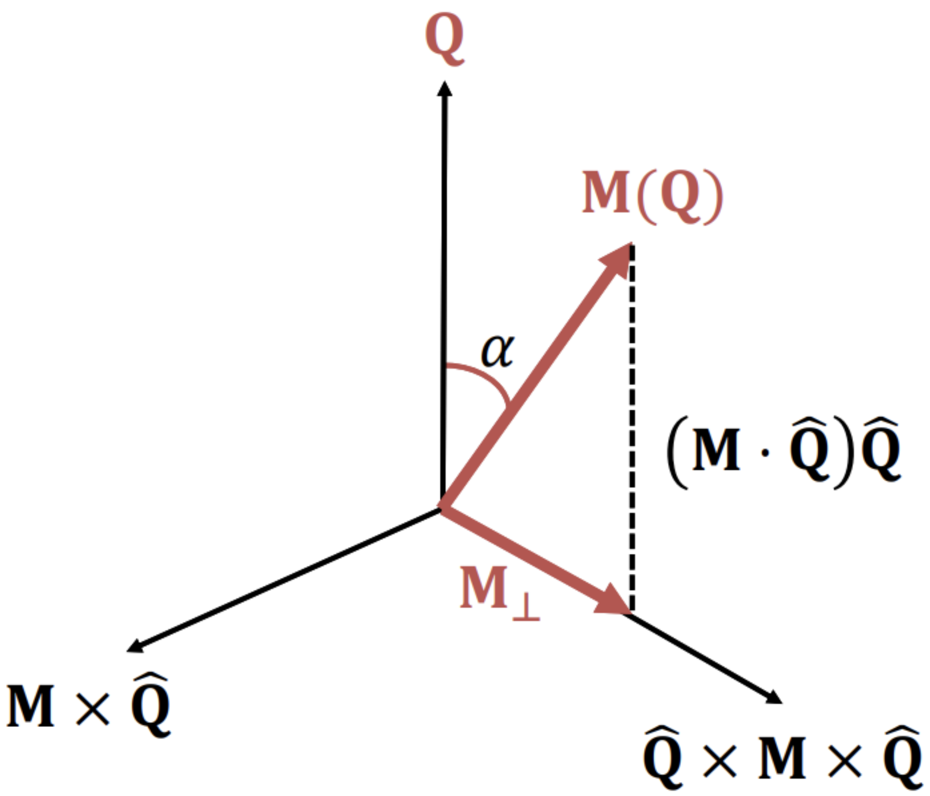
Geometrically:

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

$$\mathbf{M}_\perp^* \cdot \mathbf{M}_\perp = \sum_{\alpha\beta}(\delta_{\alpha\beta} - \hat{Q}_\alpha\hat{Q}_\beta)M_\alpha^* M_\beta$$

Summation over $\{x, y, z\}$

Kronecker delta



Dynamic, Static and Instantaneous structure factor

- **Dynamic structure factor: inelastic**

$$S(\mathbf{Q},\omega) \propto \int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t} \langle \hat{S}_m(t)\hat{S}_n(0)\rangle$$

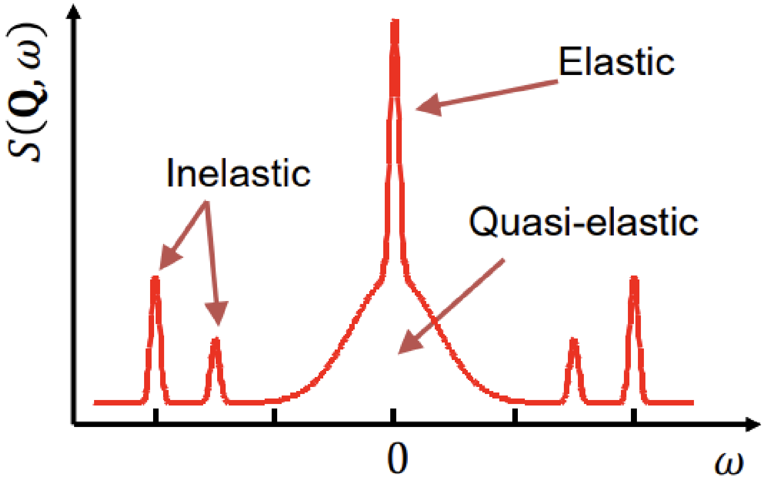
  - Periodic, $\sin(\omega_0 t) \Rightarrow$ peak at $\delta(\omega_0 - \omega)$
  - Decay, $\exp(-t/\tau) \Rightarrow$ Lorentzian $1/(1+\omega^2\tau^2)$

- **Static structure factor: elastic**

  as $t \to \infty$, $\langle \hat{S}_m(t)\hat{S}_n(0)\rangle$ becomes independent of time

$$S(\mathbf{Q},\omega=0) \propto \langle \hat{S}_n\rangle\langle \hat{S}_m\rangle$$

  - Bragg peaks at $\omega = 0$



- **Instantaneous structure factor – integrate over energy**

$$S(\mathbf{Q}) = \int d\omega\, S(\mathbf{Q},\omega) \propto \int_{-\infty}^{\infty} \mathrm{d}t\, \delta(t)\langle \hat{S}_m(t)\hat{S}_n(0)\rangle = \langle \hat{S}_m(t)\hat{S}_n(t)\rangle$$

  - Finite time/length scale of correlations

Magnetic diffraction

Elastic magnetic cross section

$$\left.\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right|_{\mathrm{M}} \propto |\mathbf{F}_{\perp\mathrm{M}}(\mathbf{Q})|^2 \delta(\mathbf{G} - \mathbf{Q} \pm \mathbf{k})$$

$$\mathbf{F}_{\perp\mathrm{M}}(\mathbf{Q}) = \hat{\mathbf{Q}} \times \mathbf{F}_{\mathrm{M}}(\mathbf{Q}) \times \hat{\mathbf{Q}}$$

$$\mathbf{F}_{\mathrm{M}}(\mathbf{Q}) = \sum_n f_n(Q) \boldsymbol{\mu}_n e^{-W_n} e^{i\mathbf{Q}\cdot\mathbf{r}_n}$$

Differences from nuclear Bragg scattering

- Magnetic intensity proportional to the square of the magnetic moment
  can track the temperature dependence of the magnetic moment
- **Q**-dependence – decreasing intensity at larger **Q**
  magnetic peaks strongest at small **Q**
- Measure component of magnetisation perpendicular to **Q**
  can use external magnetic field to change spin orientations
- Polarisation analysis
  provide additional information about the spin structure and domains

EPFL

Defining a magnetic structure

The general magnetic moment distribution $\mathbf{m}_n$ at position $\mathbf{r}_n$ for a single-$\mathbf{k}$ structure

$$\mathbf{m}_n = \mathbf{S}_n^{\mathbf{k}} \exp(i\mathbf{k}.\mathbf{l}) + \mathbf{S}_n^{-\mathbf{k}} \exp(-i\mathbf{k}.\mathbf{l})$$

$\mathbf{S}_n^{-\mathbf{k}} = (\mathbf{S}_n^{\mathbf{k}})^*$ to ensure $\mathbf{m}_n$ is real

$\mathbf{S}_n^{\mathbf{k}}$	*basis vector*	complex-valued basis vector which describes the direction in which a moment is pointing
$\mathbf{k}$	*propagation vector*	describes how moments on equivalent atoms are related in nuclear cells
$\mathbf{l}$	*translation vector*	real space translation vector between unit cells

Defining a magnetic structure

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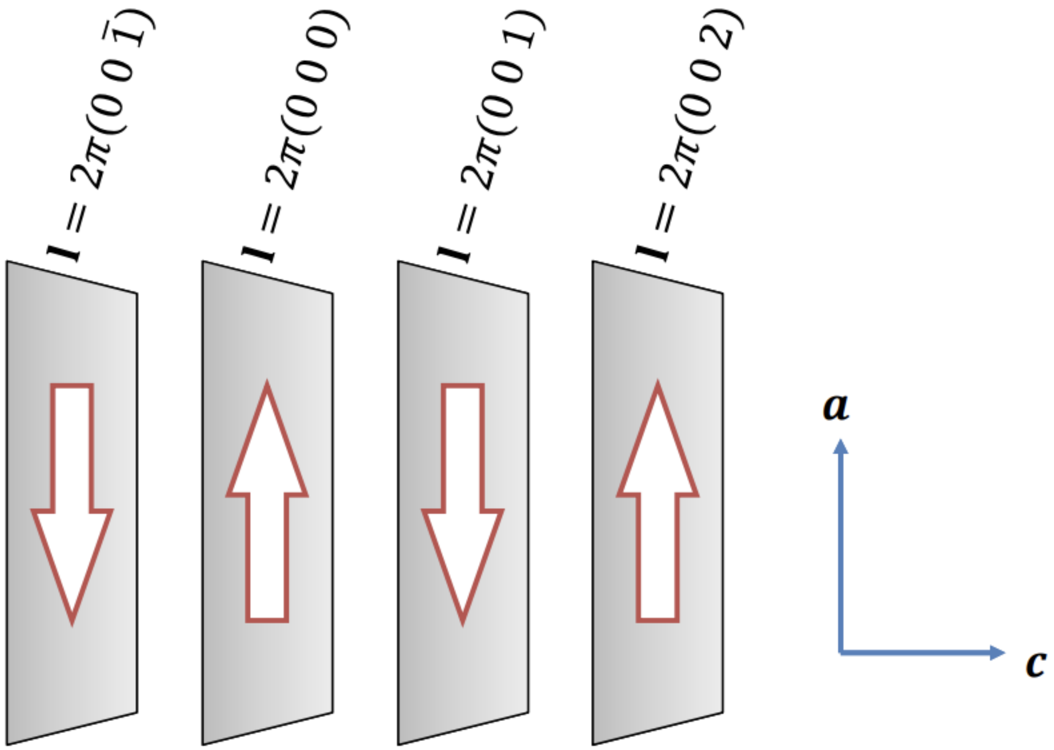
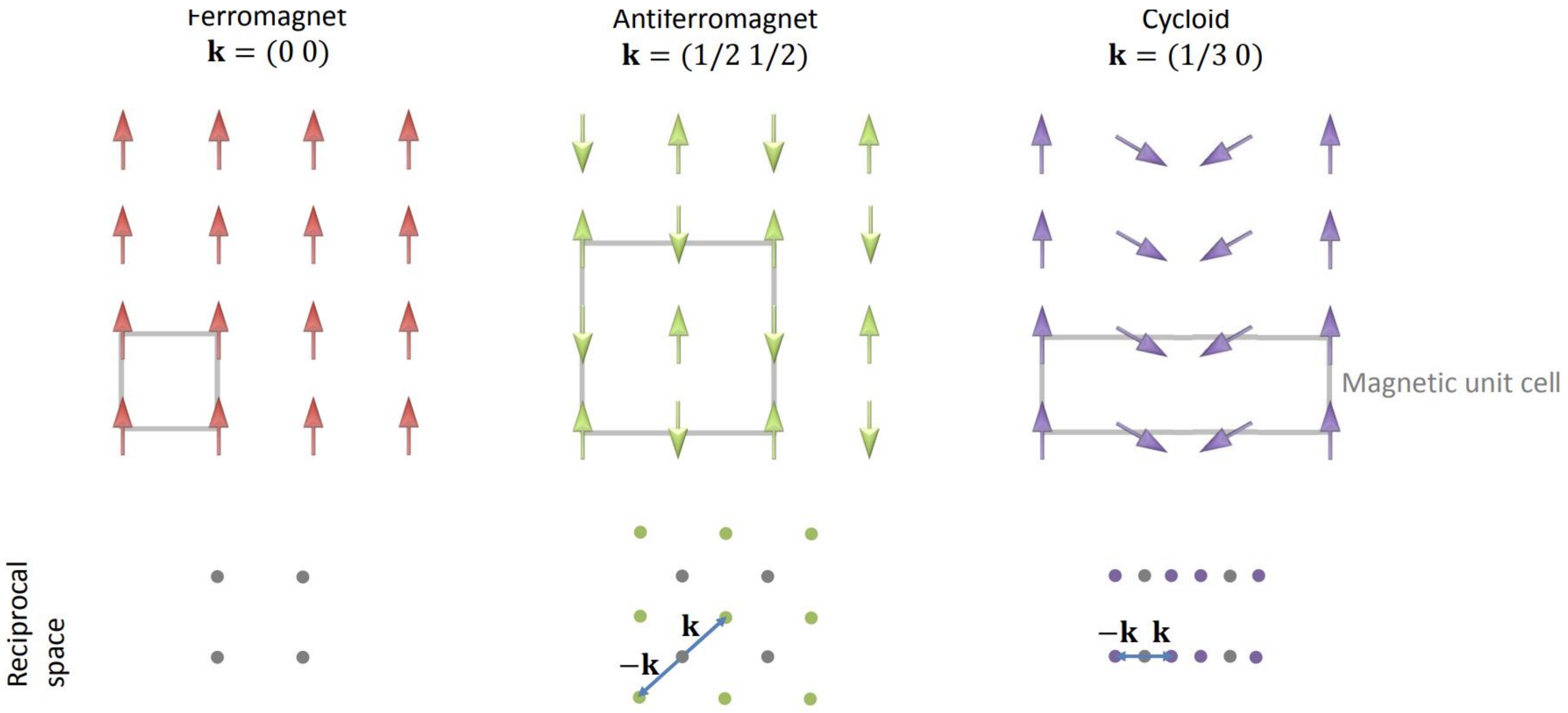


Example

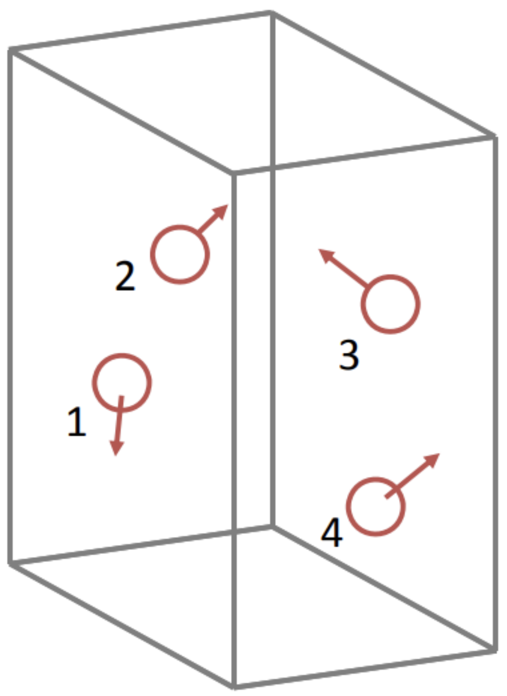
- $\mathbf{k} = \left(0\ 0\ \frac{1}{2}\right)$
- $\mathbf{S}_n^{\mathbf{k}} = (1\ 0\ 0)$

Therefore, if we know $\mathbf{k}$ and $\mathbf{S}_n^{\mathbf{k}}$ we can calculate the magnetic moment orientation in any cell of the nuclear lattice

Magnetic structures and their propagation vectors



Representation analysis



If we have n atoms in the unit cell, we would in general have for each ion, $\mathbf{S}_n^k$ which for is a vector along $\{x, y, z\}$ and can be complex, along with ϕ_n we would need to determine $2 \times 3 \times j + (j - 1)$ parameters (one phase can be fixed)!

For 4 atoms in the cell, this would correspond to 27 parameters.

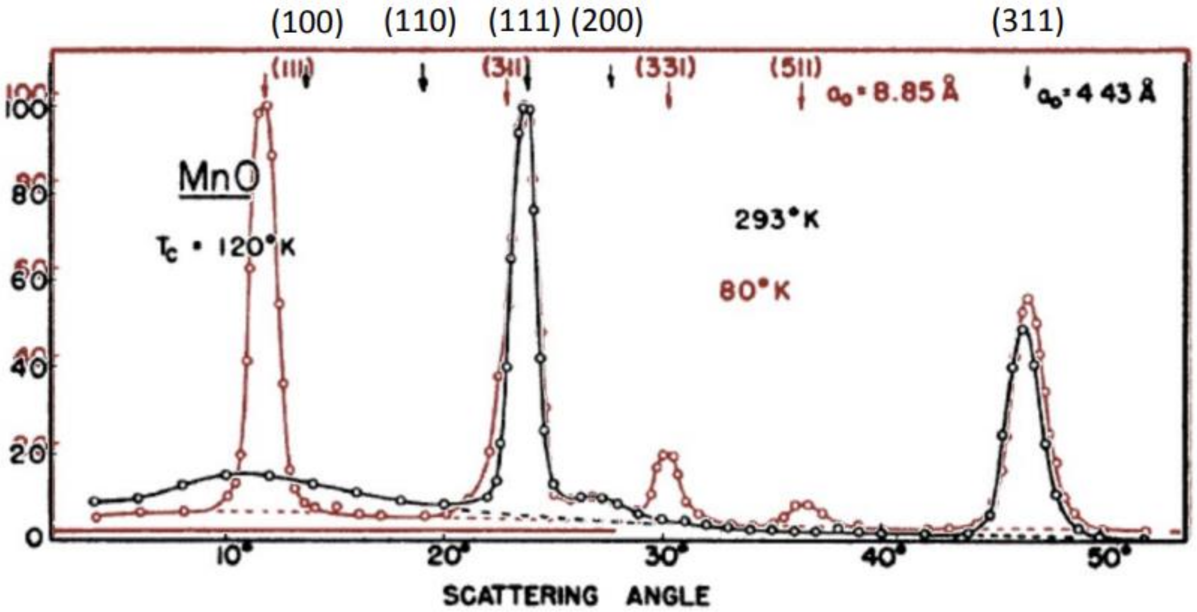
Fortunately we can apply use the symmetry of the crystal structure to greatly reduce the number of free parameters that need to be fitted provided,

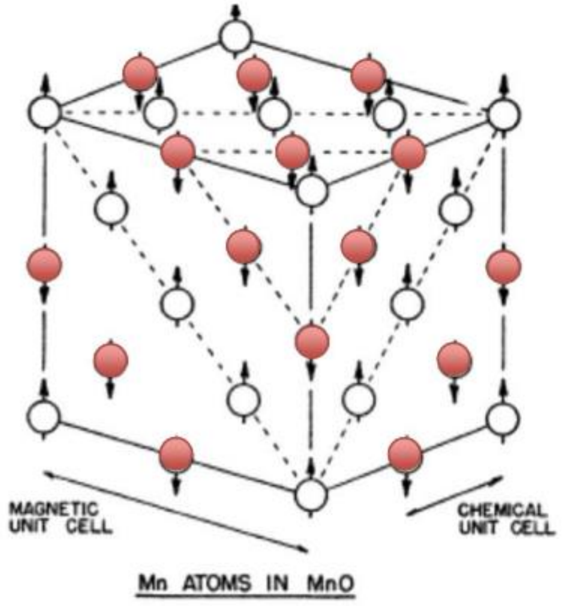
a) $\mathbf{k}$ propagation vector and
b) crystal symmetry are known

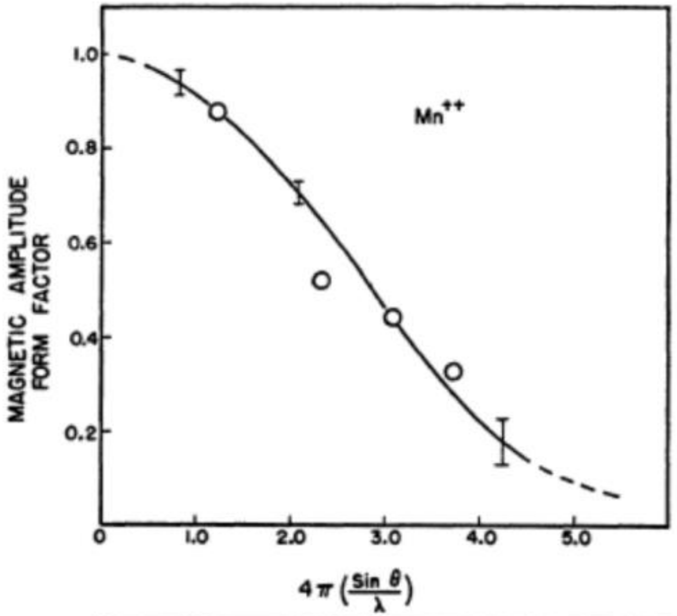
Some software packages are available to help:

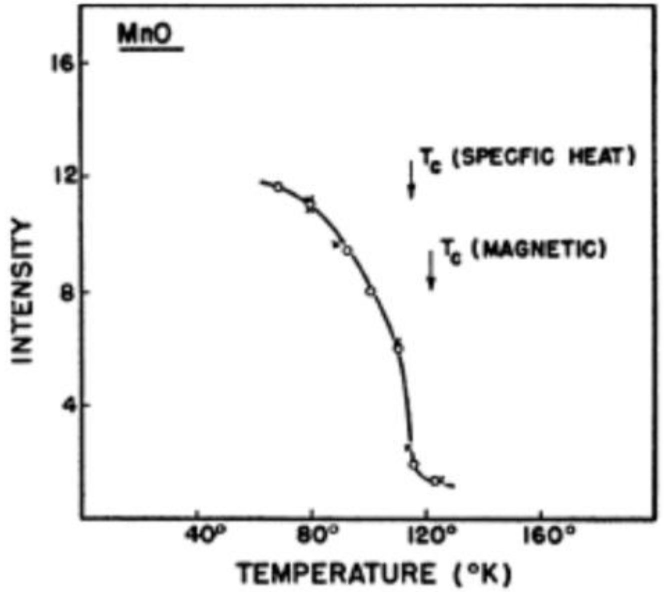
- SARAh
- BasIreps
- Isotropy

First magnetic diffraction







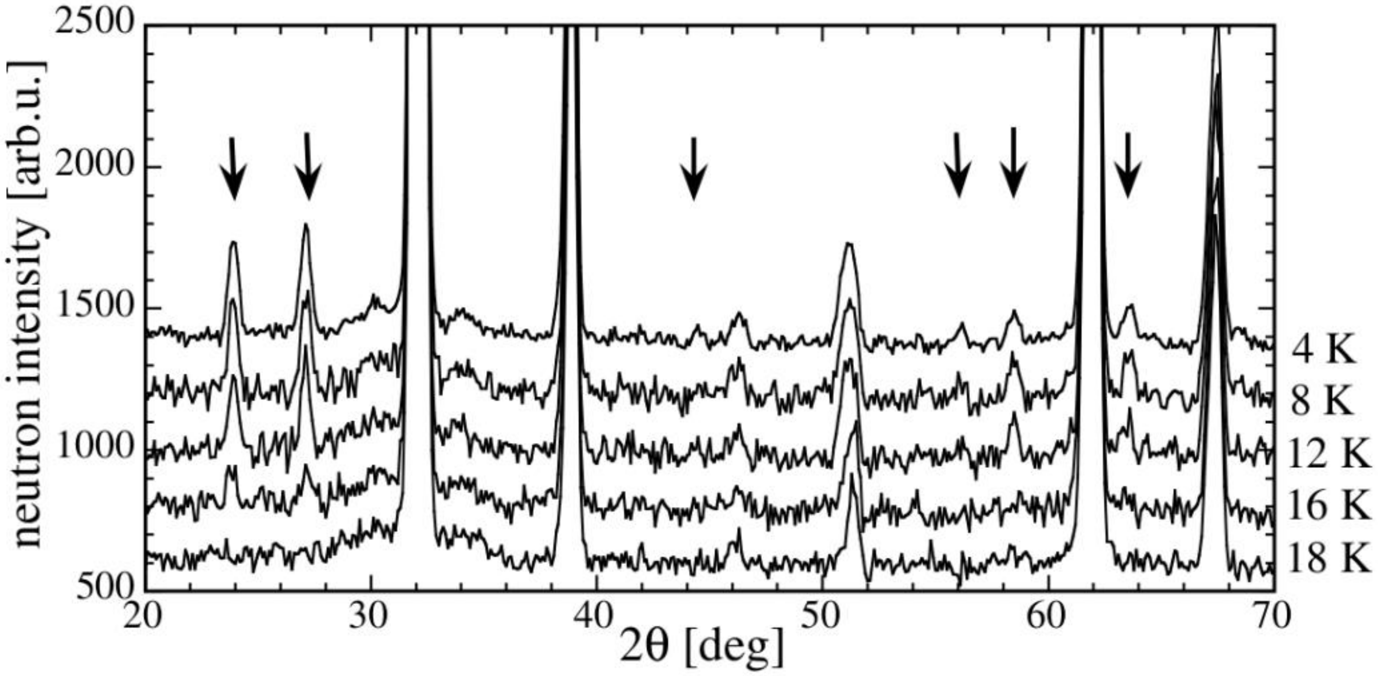


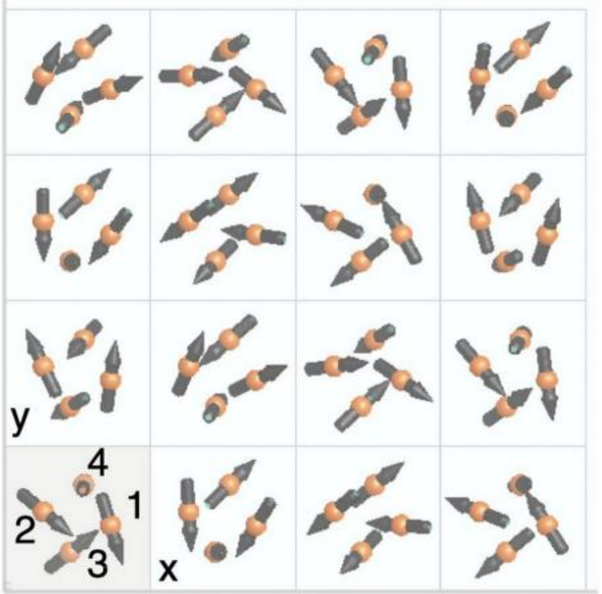
Pioneering work by Shull and Brockhouse showed by neutron scattering that MnO orders magnetically below 120 K with AFM planes stacked along (111) direction.

Example of very complicated magnetic structure

$Cu_2Te_2O_5X_2$ (X = Br, Cl)

$\mathbf{Q}_{Br}$ = (0.158, 0.354, 0.5), T_N = 11 K
$\mathbf{Q}_{Cl}$ = (0.150, 0.422, 0.5), T_N = 18 K





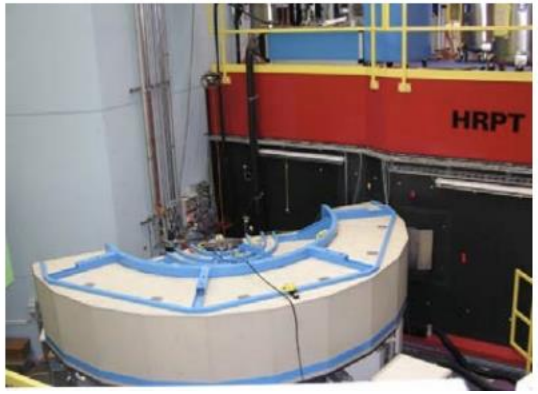
O. Zaharko *et al.*, *Phys. Rev. Lett.* **93**, 217206 (2004)

Magnetic structure determination

Powder neutron diffraction

+ Search for propagation vector
+ Cover all of reciprocal space
+ Can obtain absolute units and no corrections for extinction or absorption

- Find many peaks which may not be easy to index
- Not sensitive to small moments $\approx 0.1\mu_B$
- Sometimes difficult to refine complex magnetic structures such as cycloids and helices
- Cannot study effects of applied magnetic fields, pressure, etc along specific directions



HRPT, PSI

Single-crystal neutron diffraction

+ Often can separate nuclear and magnetic reflections in **Q**
+ Can perform experiments in field, pressure, etc.
+ Can focus on particular **Q** to have greater sensitivity to small moments

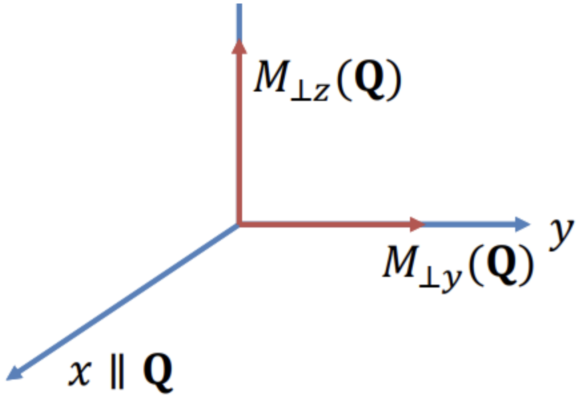
- Need to worry about corrections
- Only look at certain **Q** positions, may miss something
- Require a large, good quality single-crystal which are harder to synthesise

TRICS, PSI

Polarized neutron scattering

Scattering of neutrons from *nucleus* and *electron cloud*:

$$\frac{d^2\sigma}{d\Omega dE_f} \propto \left|\langle \sigma_f, \mathbf{k}_f, \lambda_f | b + B\boldsymbol{I}.\boldsymbol{\sigma} - \boldsymbol{M}_\perp.\boldsymbol{\sigma} | \sigma_i, \mathbf{k}_i, \lambda_i \rangle\right|^2 \delta(E_i - E_f + \hbar\omega)$$



Consider a neutron beam polarised along z:

Initial spin \ Final spin state	$\vert\uparrow\rangle$	$\vert\downarrow\rangle$
$\vert\uparrow\rangle$	**NSF** $\sigma(z,z) = b - M_{\perp z} + BI_z$	**SF** $\sigma(-z,z) = -iM_{\perp y} + B(I_x + iI_y)$
$\vert\downarrow\rangle$	**SF** $\sigma(z,-z) = iM_{\perp y} + B(I_x - iI_y)$	**NSF** $\sigma(-z,-z) = b + M_{\perp z} - BI_z$

- Coherent nuclear scattering is non spin-flip (NSF)
- Magnetization parallel to neutron spin is non-spin-flip (NSF)
- Magnetization perpendicular to neutron spin is spin-flip (SF)
- Can separate incoherent, coherent nuclear and magnetic scattering
- Can determine directions of magnetic moments from one or few Bragg peaks
- Nuclear-magnetic interference can determine magnetization densities

EPFL

Magnetic Inelastic Neutron Scattering

Magnetic neutron scattering cross-section

$$|\langle \mathbf{k}_f \lambda_f \;|V|\; \mathbf{k}_i \lambda_i \rangle|^2$$

$$V_{\text{mag}}(\mathbf{r}) = -\frac{\mu_0}{4\pi} 2\gamma \mu_N \mu_B \, \boldsymbol{\sigma}_n \cdot \left(\nabla \times \left(\frac{\mathbf{s} \times \hat{\mathbf{R}}}{|\mathbf{R}|^2} \right) + \frac{1}{\hbar} \frac{\mathbf{p} \times \hat{\mathbf{R}}}{|\mathbf{R}|^2} \right)$$

$$\left(\frac{d^2\sigma}{d\Omega dE_f} \right)_{\text{mag}} = \frac{(\gamma r_0)^2}{2\pi\hbar} \frac{k_f}{k_i} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) |gF_R(Q)|^2 \sum_{RR'} \int dt e^{iQ(R-R') - i\omega t} \langle S_R^\alpha(0) S_{R'}^\beta(t) \rangle$$

cross-section

pre factor

dipole factor

magnetic form factor

Fourier transform

spin-spin correlation function

Dynamic structure factor

Spin-spin correlation function

$$S^{\alpha\beta}(Q,\omega) = \frac{1}{2\pi}\sum_{RR'}\int dt e^{iQ(R-R')-i\omega t}\langle S_R^\alpha(0)S_{R'}^\beta(t)\rangle$$

Dynamic structure factor

Theory !

$$\left(\frac{d^2\sigma}{d\Omega\, dE_f}\right)_{\text{mag}} = \frac{1}{\hbar}\frac{k_f}{k_i}p^2\exp(-2W)\sum_{\alpha\beta}(\delta_{\alpha\beta}-\hat{\mathbf{Q}}_\alpha\hat{\mathbf{Q}}_\beta)S^{\alpha\beta}(\mathbf{Q},\omega)$$

Fluctuation dissipation theorem $\Rightarrow$ gen. susceptibility

$$S(\mathbf{Q},\omega) = [n(\omega)+1]\,\chi''(\mathbf{Q},\omega) = \frac{\chi''(\mathbf{Q},\omega)}{1-\exp(-\hbar\omega/k_BT)}$$

intrinsic dynamics $\Leftrightarrow$ response to perturbation

Generalized susceptibility

- Magnetic susceptibility χ relates how magnetisation $\mathbf{M}$ changes with applied field $\mathbf{H}$

$$\mathbf{M} = \chi \mathbf{H}$$

- If the applied field varies in space and time, we would measure the generalised susceptibility $\chi(\mathbf{Q}, \omega)$

$$\mathbf{M}(\mathbf{Q}, \omega) = \chi(\mathbf{Q}, \omega)\mathbf{H}(\mathbf{Q}, \omega)$$

  this applies when the system responds linearly to the applied field

- In general $\mathbf{M}$ is not in phase with $\mathbf{H}$ and χ is complex

$$\chi(\mathbf{Q}, \omega) = \chi'(\mathbf{Q}, \omega) - i\chi''(\mathbf{Q}, \omega)$$

- Neutrons are a probe which provides a magnetic perturbation which varies in *space* and *time*

$$\tilde{S}^{\alpha\beta}(\mathbf{Q}, \omega) = \frac{1}{\pi}\frac{1}{1 - e^{-\hbar\omega/k_B T}}\chi''(\mathbf{Q}, \omega) = \frac{1}{\pi}(1 + n)\chi''(\mathbf{Q}, \omega)$$

Inelastic magnetic scattering: Lets take the scenic route…

Selected examples

- Spin-flip, singlet-triplet, dispersive triplets
- 1D spin chain
  – spinons vs spin waves
- 2D HAF zone boundary anomaly
  – as instability of spin waves ?
  – the smoking gun of RVB ?

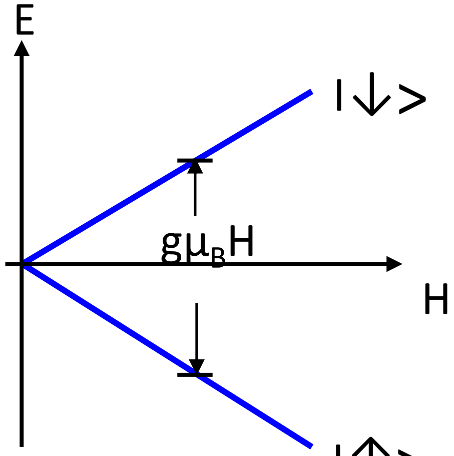
Between long range ordered states

… and spin liquids

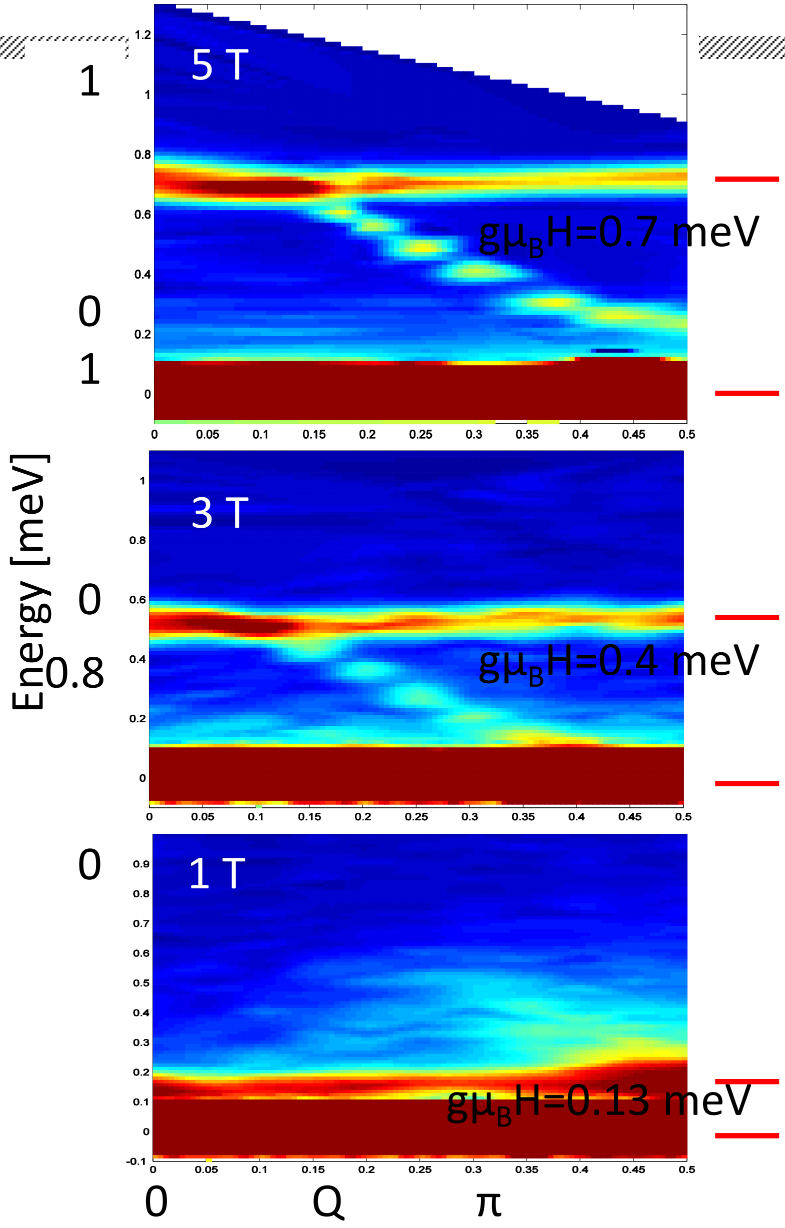
paramagnetic spins S=1/2

- Two states |↑⟩, |↓⟩, can be magnetized
- Zeemann-split energy of the levels
- A gap for transitions

$CuSO_4 \cdot 5D_2O$



Spin-flip excitation



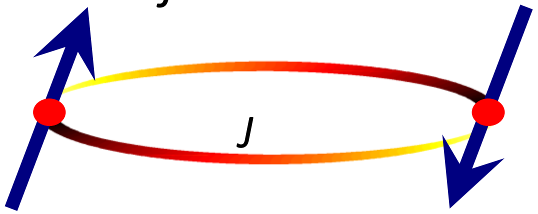
- Local excitation

  ⇒ no Q-dependence

EPFL

Take two – the spin pair

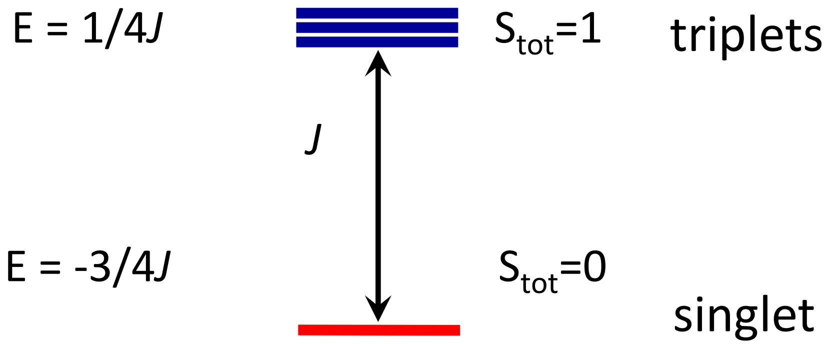
$$\mathcal{H} = J \sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$



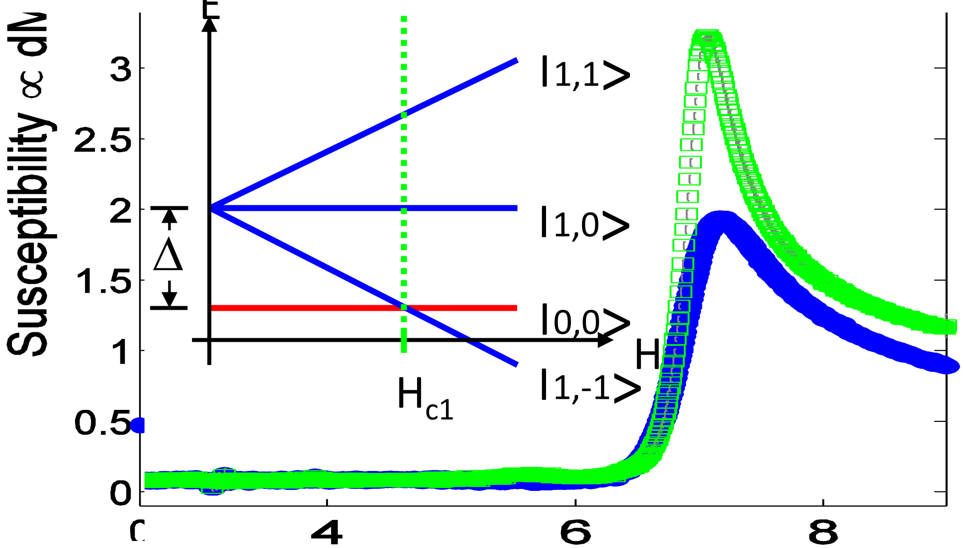
No magnetization or susceptibility up to critical field

Antiferromagnetic: $J > 0$

$|\uparrow\uparrow\rangle,\ |\downarrow\downarrow\rangle,\ |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$

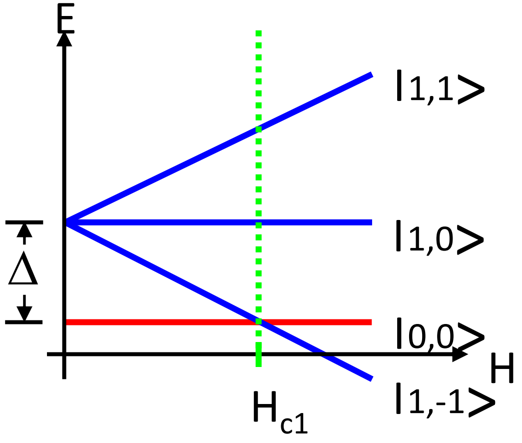


$|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$



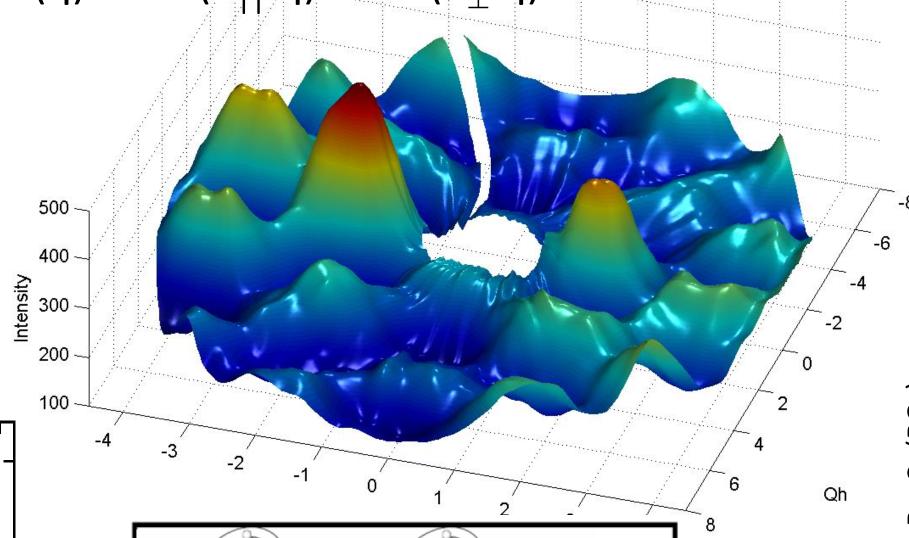
Singlet ground state: $\langle S^z_1 \rangle = \langle S^z_2 \rangle = 0$

Take two – the spin pair

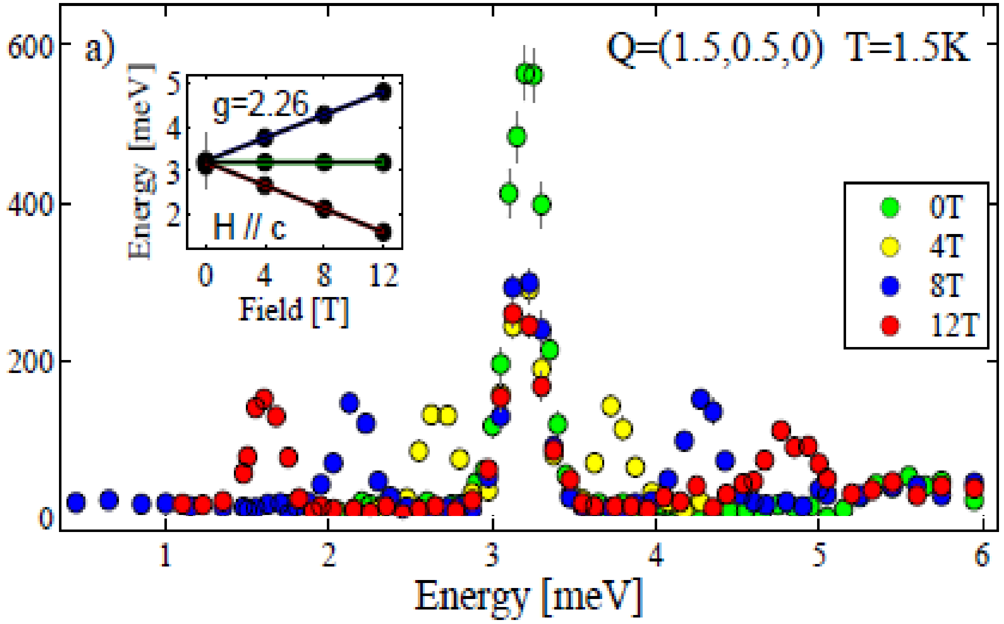


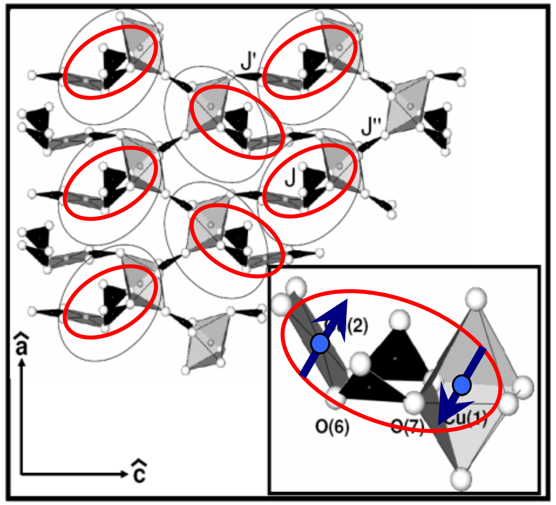
Structure factor along pairs:

$S(q) \sim \cos(d_{||} \cdot q) + \cos(d_{\perp} \cdot q)$



$Ba_2Cu(BO_3)_2$
Rüegg, HMR, Demmel *et al.*





$SrCu_2(BO_3)_2$
Zayed, Rüegg, HMR *et al.*

The Heisenberg model

- Seem innocently simple for a spin pair

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

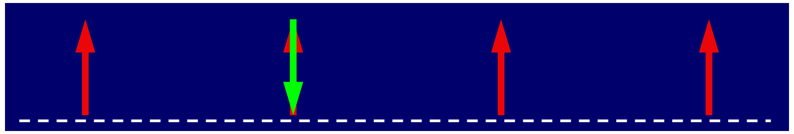
- for extended systems, do we understand it well enough ?

EPFL

Ferromagnets are easy, exact solution:

$H=-\sum_{rr'}J_{rr'}S_r\cdot S_{r'} = -J\sum_{<r,r'=r+d>} S^z_r S^z_{r'} + ½(S^+_r S^-_{r'} + S^-_r S^+_{r'})$

⇑ nearest neighbour ⇑



Ordered ground state, all spin up: $H|g\rangle = E_g|g\rangle$, $E_g=-zNS^2J$

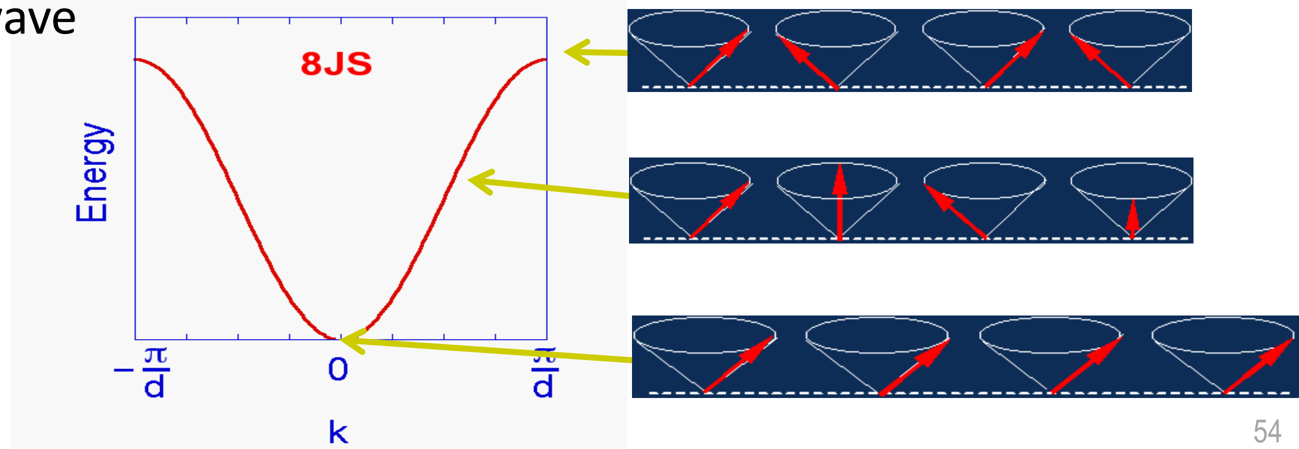
Single spin flip not eigenstate: $|r\rangle = (2S)^{-½} S^-_r|g\rangle$, $S^-_{r'}S^+_r|r\rangle = 2S|r'\rangle$

$H|r\rangle=(-zNS^2J+2zSJ)|r\rangle - 2SJ\sum_d |r+d\rangle$ flipped spin moves to neighbors

Periodic linear combination: $|k\rangle = N^{-½}\Sigma_r e^{ikr}|r\rangle$ plane wave

Is eigenstate: $H|k\rangle = E_g+E_k|k\rangle$, $E_k=SJ\Sigma_d 1-e^{ikd}$ dispersion = 2SJ (1-cos(kd)) in 1D

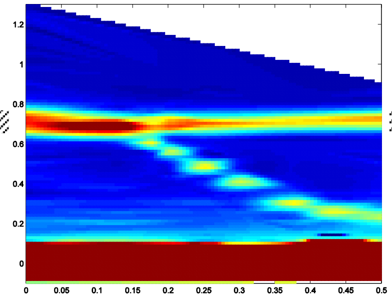
Time evolution: $|k(t)\rangle = e^{iHt}|k\rangle = e^{iE_k t}|k\rangle$ sliding wave

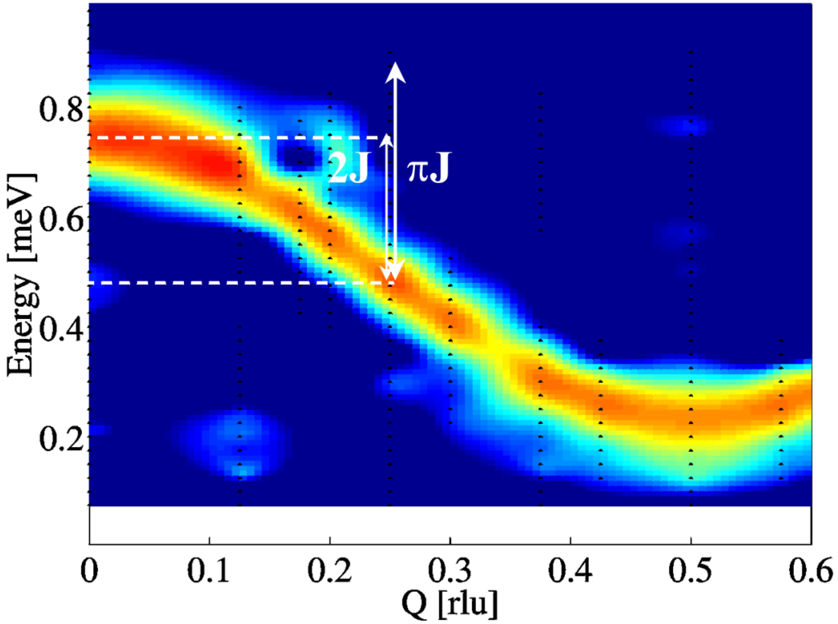


Dispersion:
relation between time- and space-modulation period

Same result in classical
calculation ⇒ precession:

Spin waves in a “ferromagnet”





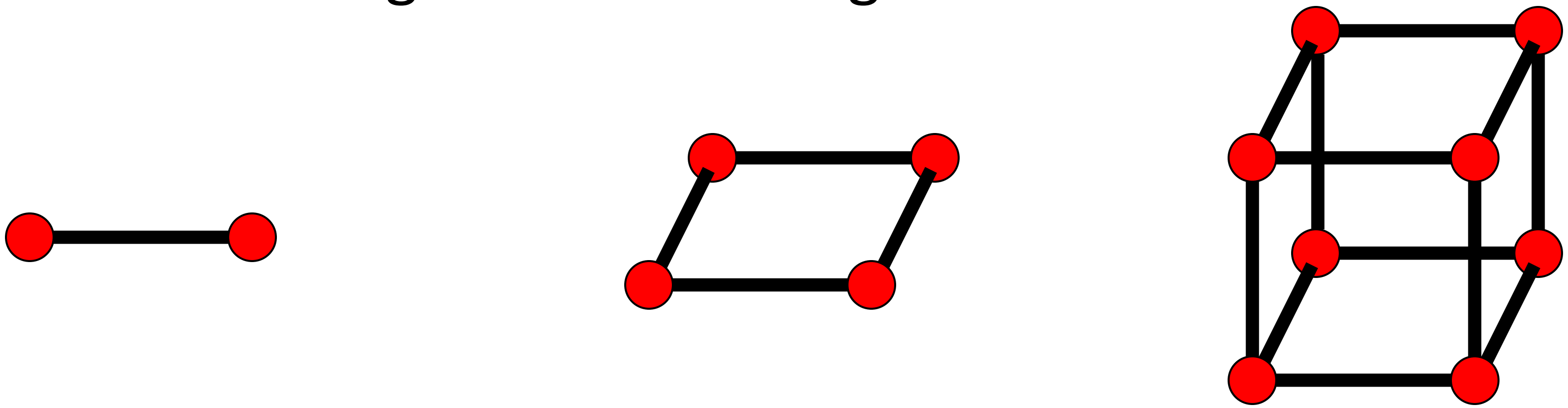
$CuSO_4 \cdot 5D_2O$
=
$Cu_2(SO_4)_2 \cdot 10D_2O$
=
1 Cu S=1/2 uncoupled
1 Cu S=1/2 chain

dispersion = 2SJ (1-cos(kd))

Actually it is an antiferromagnet polarized by 5T field

Quantum antiferromagnets are tricky

Fluctuations stronger for fewer neighbours



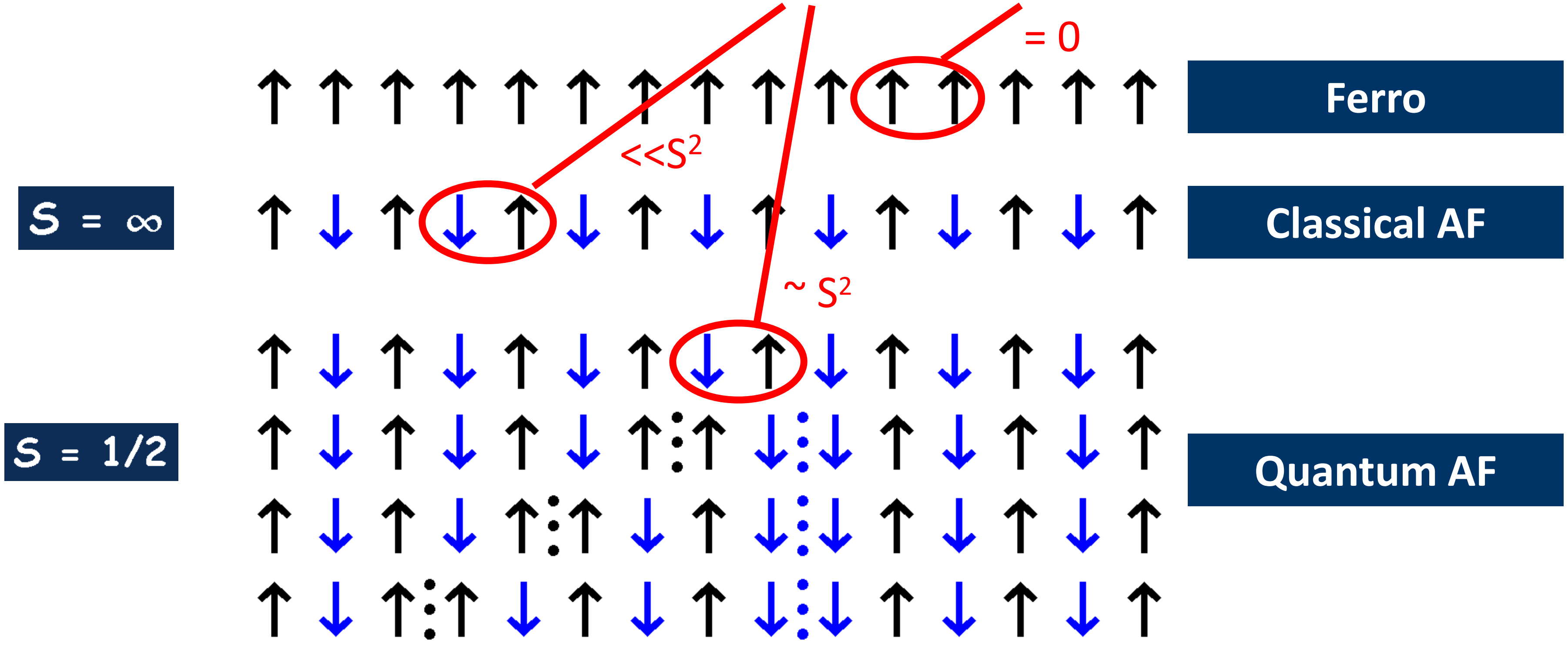
1D: Ground state ‘quantum disordered’ spin liquid of S=1/2 spinons. Bethe ansatz ‘solves’ the model

2D: Ground state ordered at T=0 <S> = 60% of 1/2 (although not rigorously proven).

3D: Ground state long range ordered, weak quantum-effects

antiferromagnetic spin chain

$$\mathcal{H} = J \sum S^z_n S^z_{n+1} + \frac{1}{2}\left(S^+_n S^-_{n+1} + S^-_n S^+_{n+1}\right)$$



Ground state (Bethe 1931) – a soup of domain walls

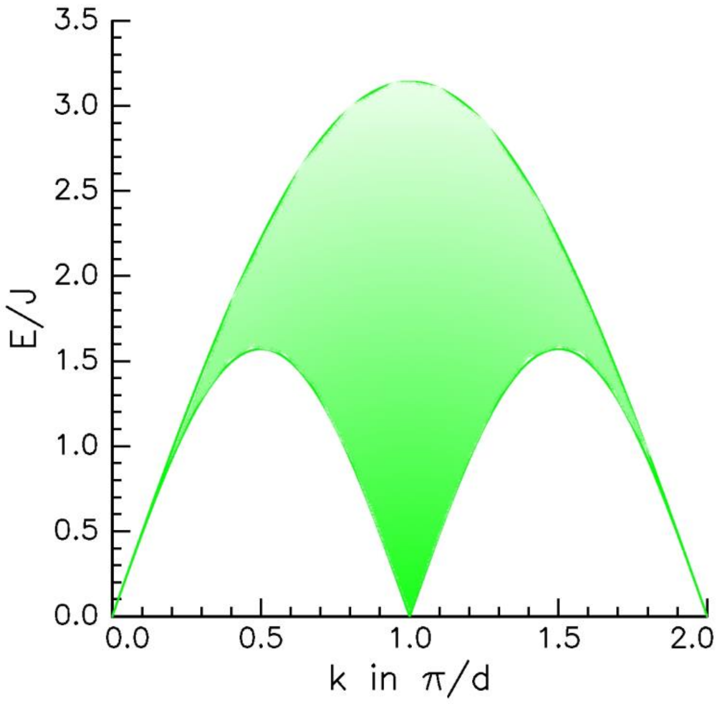
Spinon excitations

Elementary excitations:
- "Spinons": spin S = ½ domain walls with respect to local AF 'order'
- Need 2 spinons to form S=1 excitation we can see with neutrons

↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓ ↑
↑ ↓ ↑ ↓ ↑ ↓ ↑ ⁝ ↑ ↓ ⁝ ↓ ↑ ↓ ↑ ↓ ↑
↑ ↓ ↑ ↓ ↑ ⁝ ↑ ↓ ↑ ↓ ⁝ ↓ ↑
↑ ↓ ↑ ⁝ ↑ ↓ ↑ ↓ ↑ ↓ ⁝ ↓ ↑

Energy: $E(q) = E(k_1) + E(k_2)$
Momentum: $q = k_1 + k_2$
Spin: $S = \frac{1}{2} \pm \frac{1}{2}$

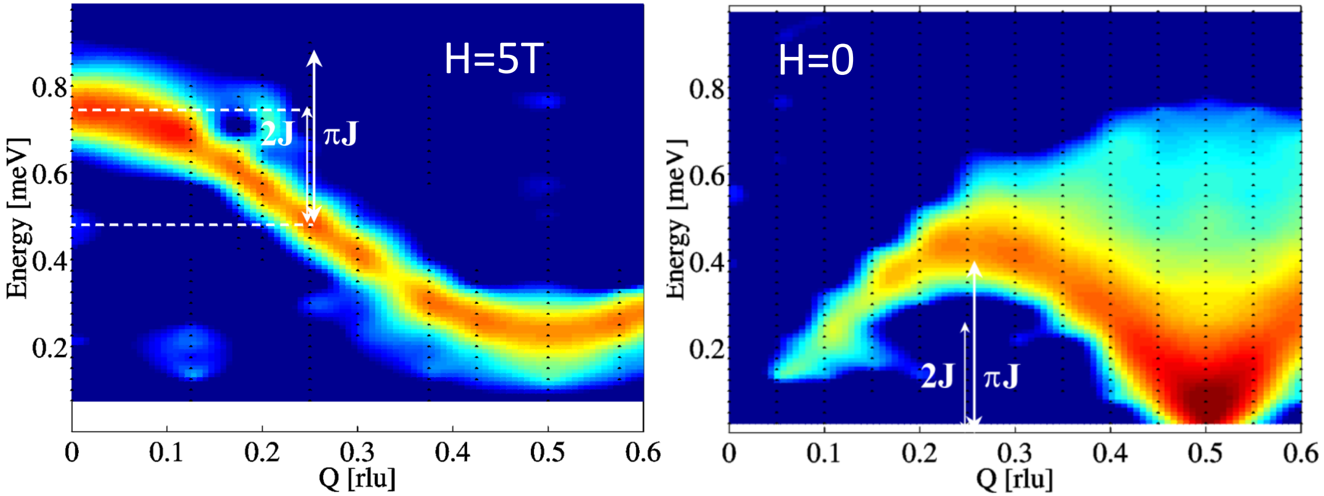
Continuum of scattering ⇒



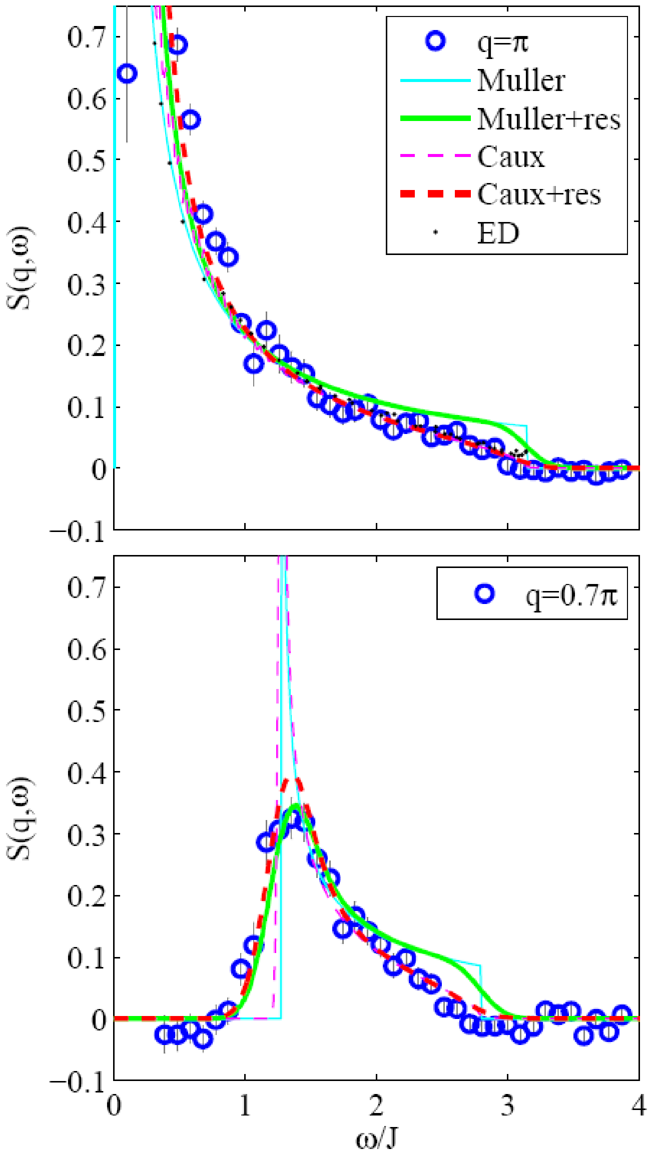
The *antiferromagnetic* spin chain

FM: ordered ground state (in 5T mag. field)
- semiclassical spin-wave excitations

AFM: quantum disordered ground state
- Staggered and singlet correlations
- Spinon excitations

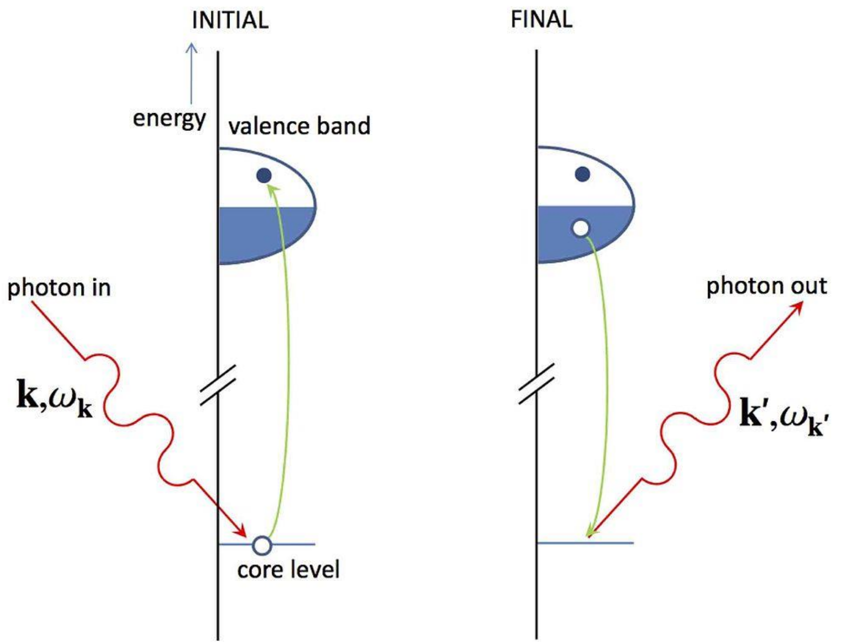


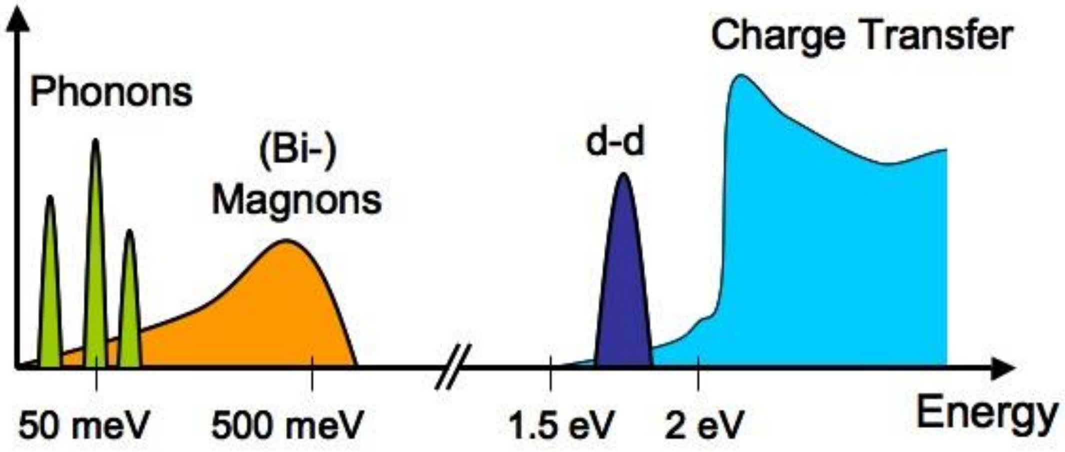
– Algebraic Bethe ansatz for inelastic lineshape
– Beyond Müller-conjecture ⇒

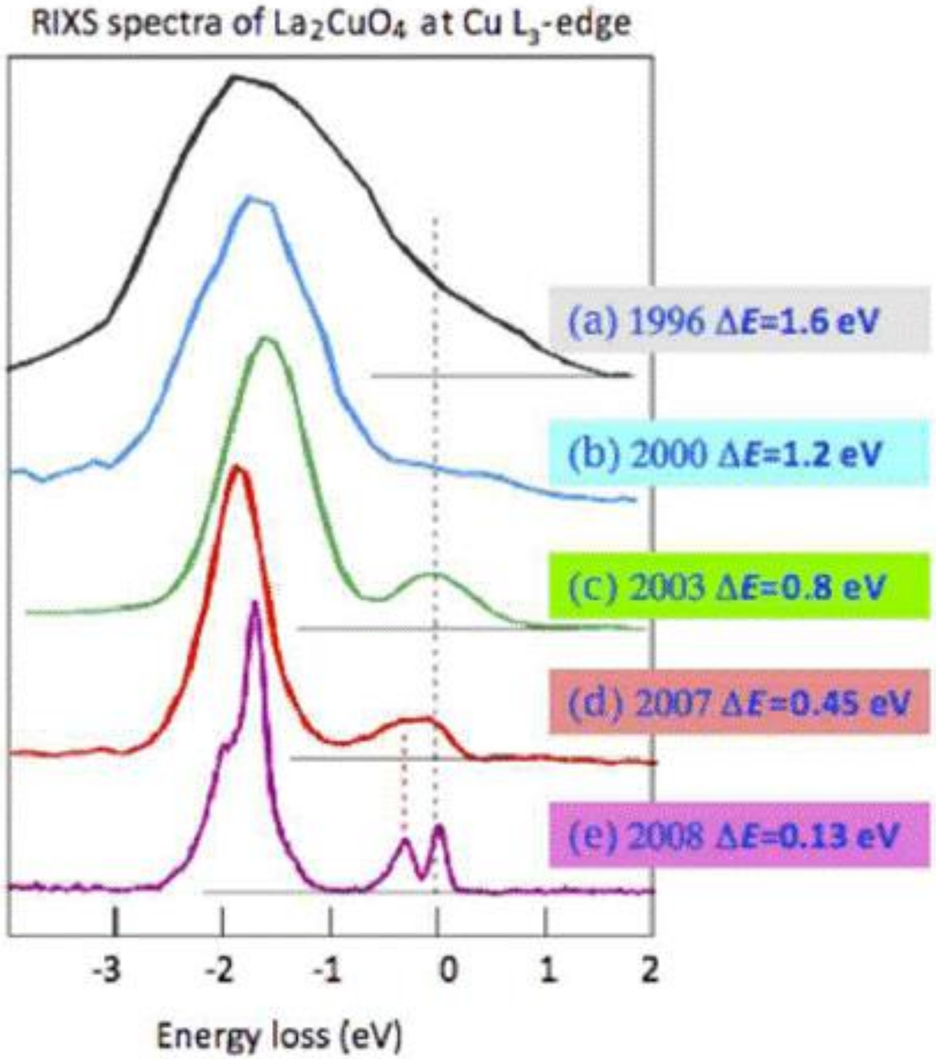


Mourigal *et al.* Nat Phys **9**, 435 (2013)

Resonant Inelastic X-ray scattering







New measure of magnetic excitations

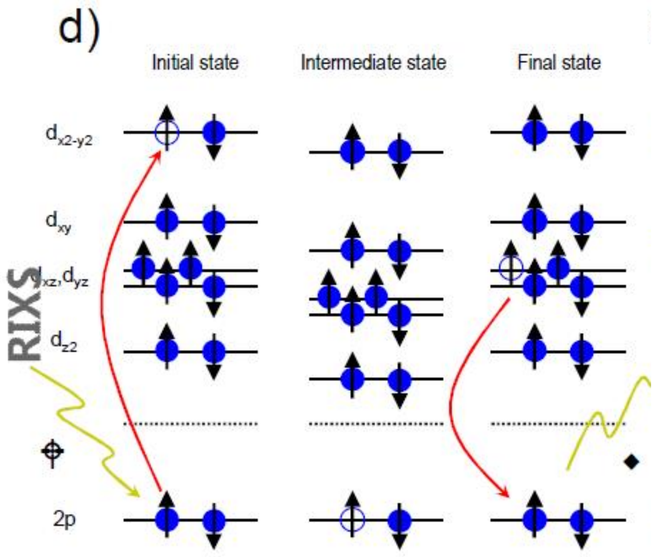
EPFL

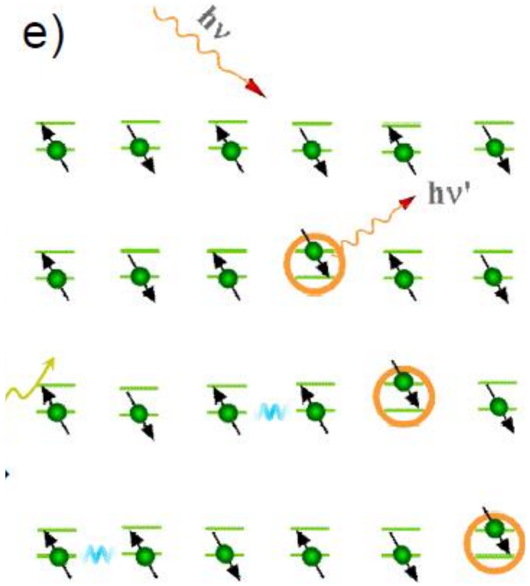
RIXS and new correlation functions

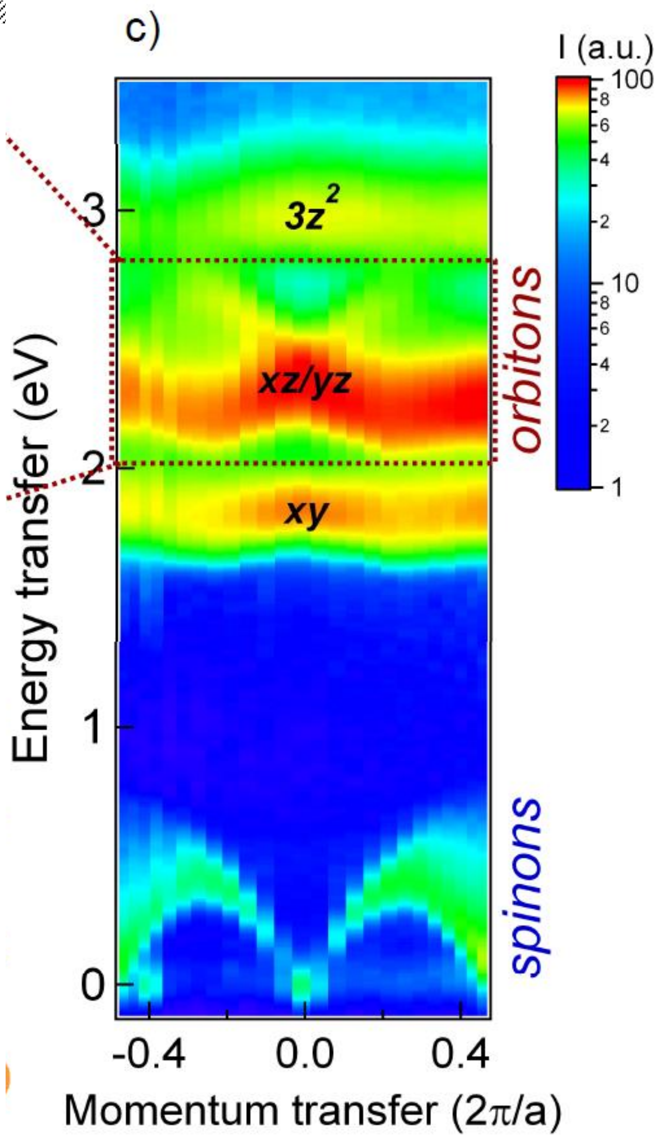
Sr_2CuO_3 Much higher energy scale

Resonant Inelastic X-ray scattering

- Sees both magnetic and orbital excitations
- Dispersive 'orbitons'
- Spinon-orbiton separation



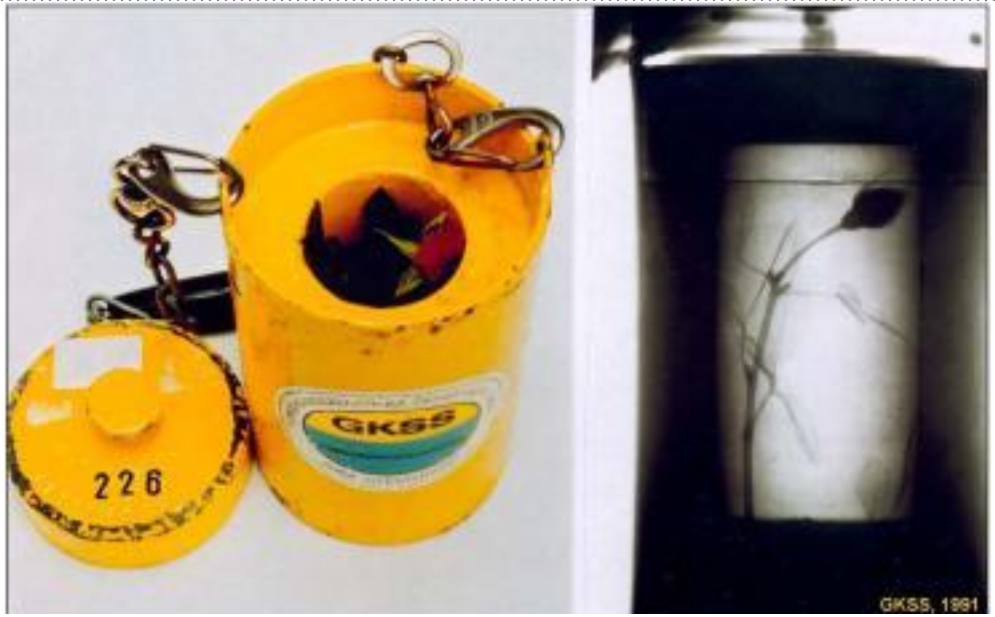




J. Schlappa *et al.*, Nature **485**, 82 (2012)

Other applications of neutron scattering technique

Neutron radiography



Rose inside a lead container (source: FRMII)

... Superman would do better with neutron vision...

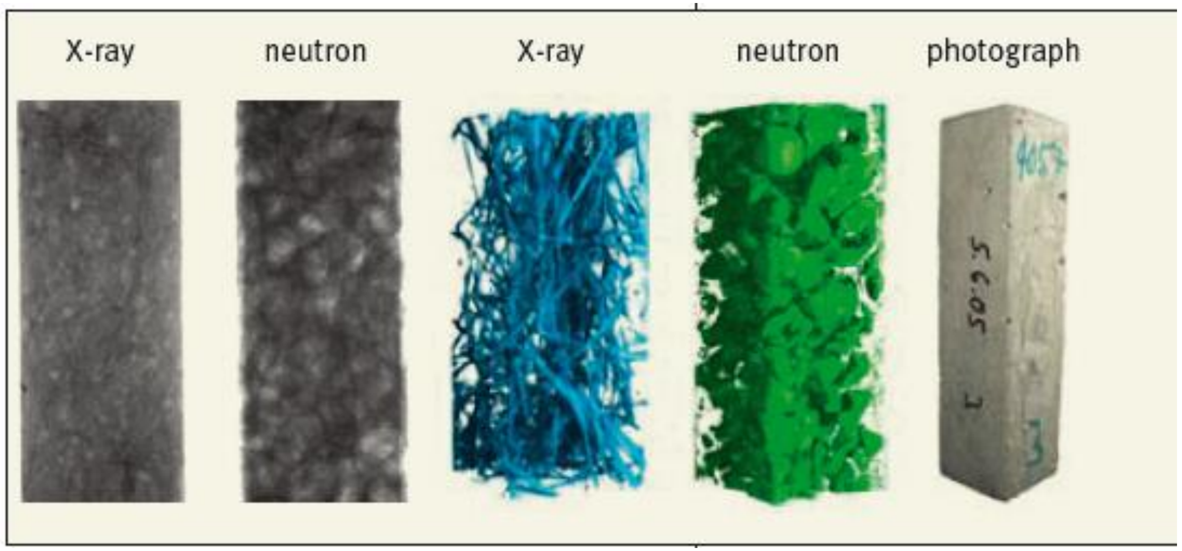


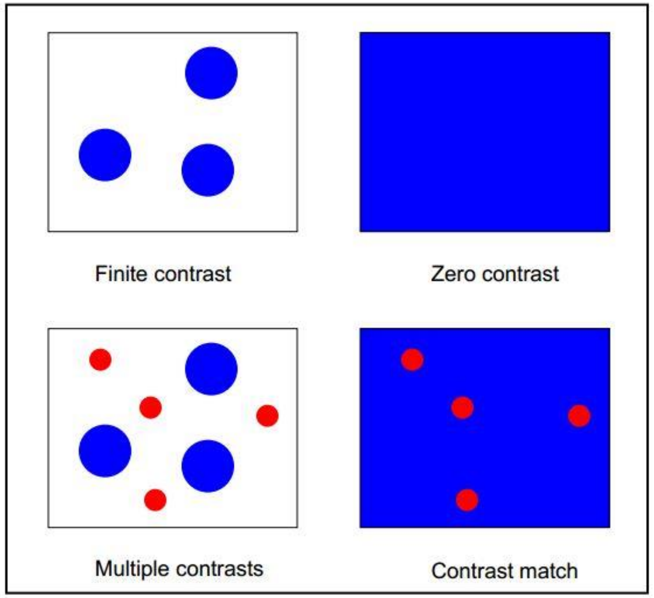
Figure 7: Transmission radiographs (left) and tomographic views (middle) made from a concrete sample embedded with steel fibres with X-ray and neutrons.

X-rays and neutrons yield complementary information

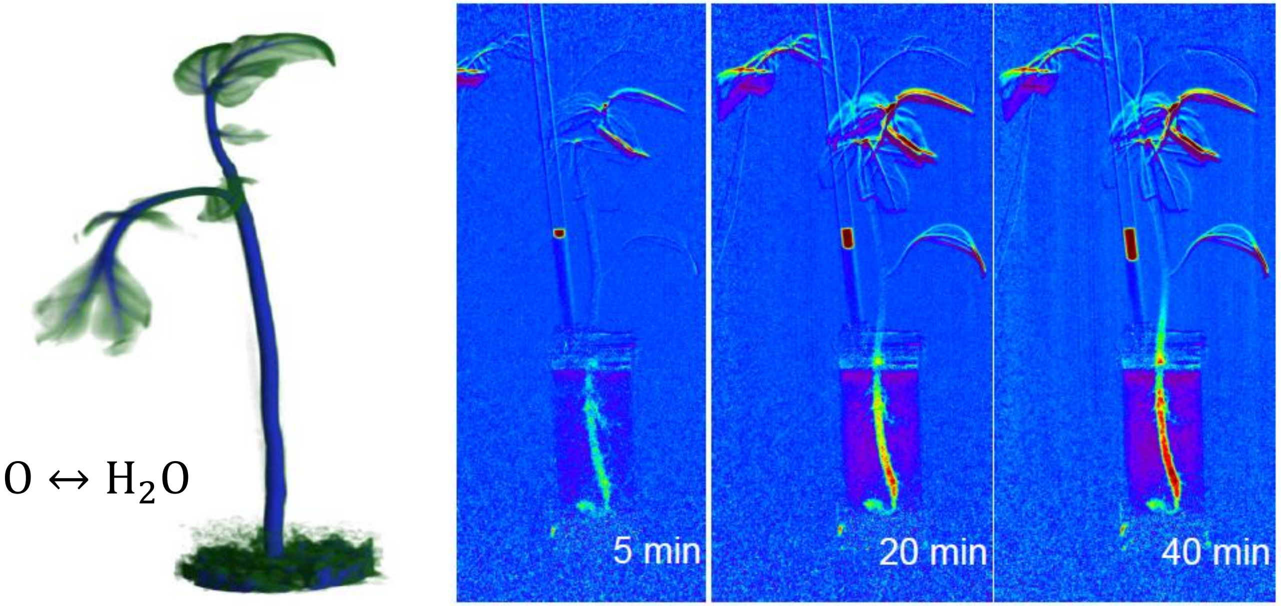
- Applicat
- Radiogra

Phase contrast

- H hydrogen negative, D deutrium positive – phase contrast
- Alter H and D ratio to see different individual parts of materials
- Examine different parts of biological samples
- Examine material on surfaces of water (cleaning products)

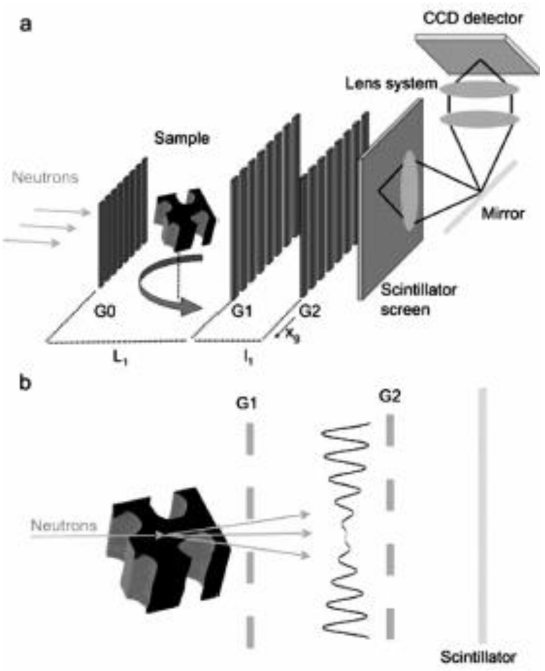


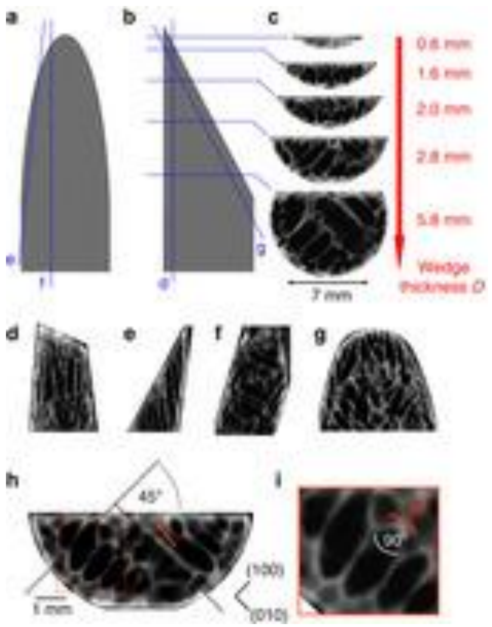
$D_2O \leftrightarrow H_2O$

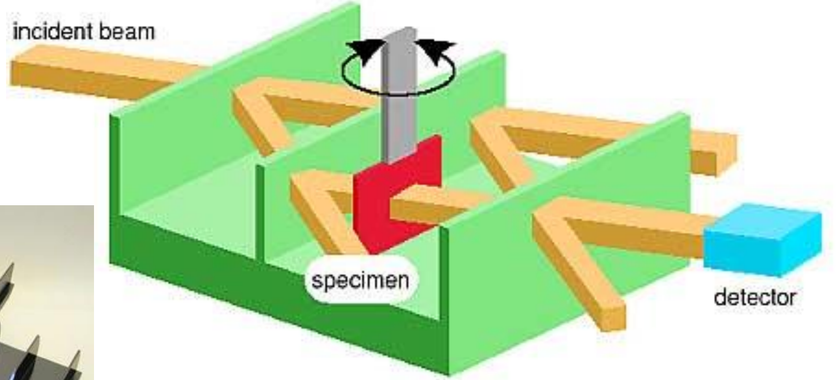


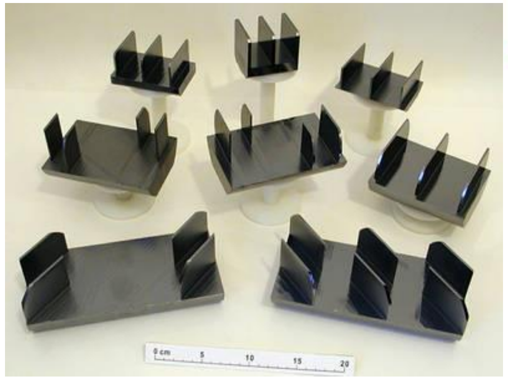
- Applicat

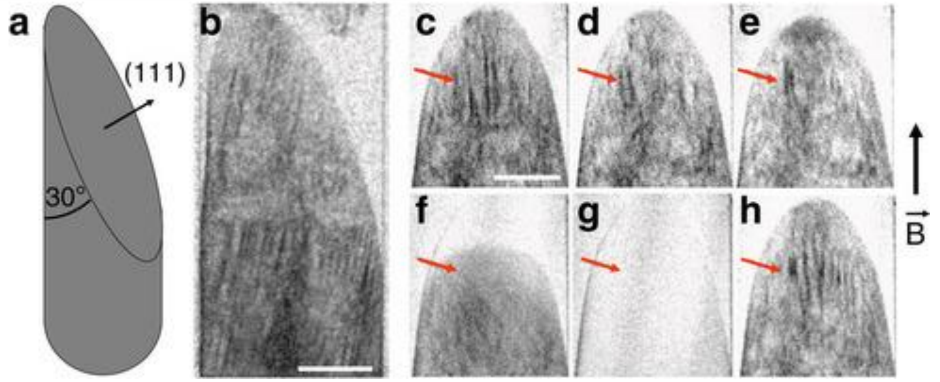
Neutron tomography











Strobl, PRL **101**, 123902 (2008)
Manke, Nature **1**, 125 (2010)

- Neutrons undergo magnetic refraction when transversing non-uniform magnetic fields
- Phase-sensitive detection using Talbot-Lau neutron imaging
- Allows for a 3D imaging of magnetic domains in FeSi

- Applicat

Biological applications

Particle form factor:

(spheres)

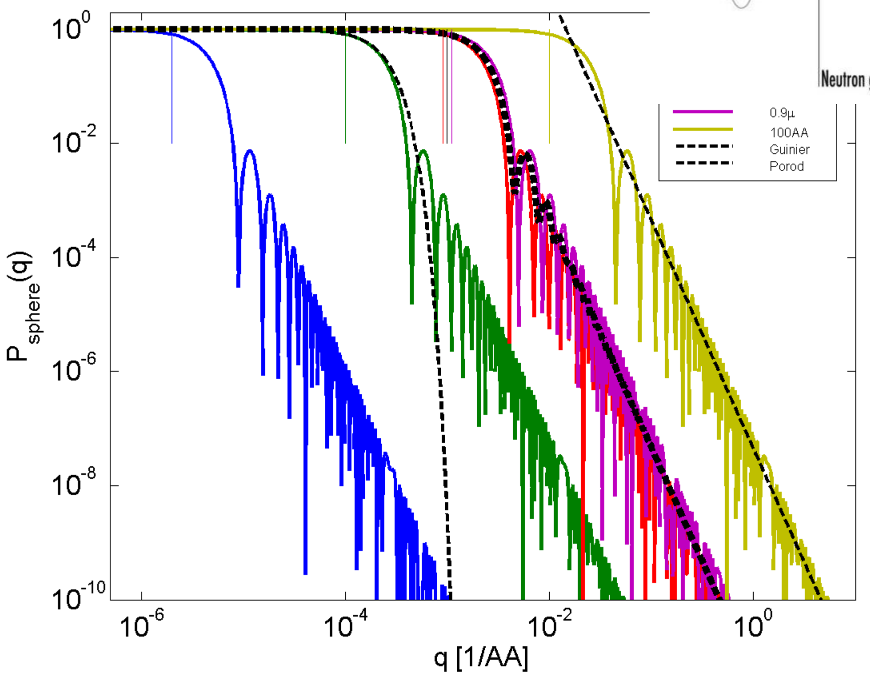
$$\left(3\frac{\sin(qR)-qR\cos(qR)}{(qR)^3}\right)^2$$

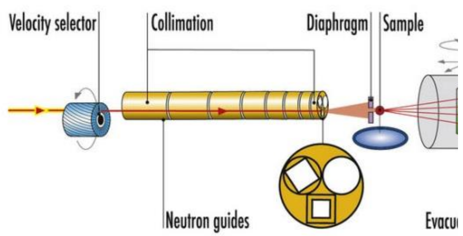
Small q: Guinier

$$\approx \exp\left(-\tfrac{1}{3}(qR)^2\right)$$

Large q: Porod

$$\approx \frac{9}{2}(qR)^{-4}$$





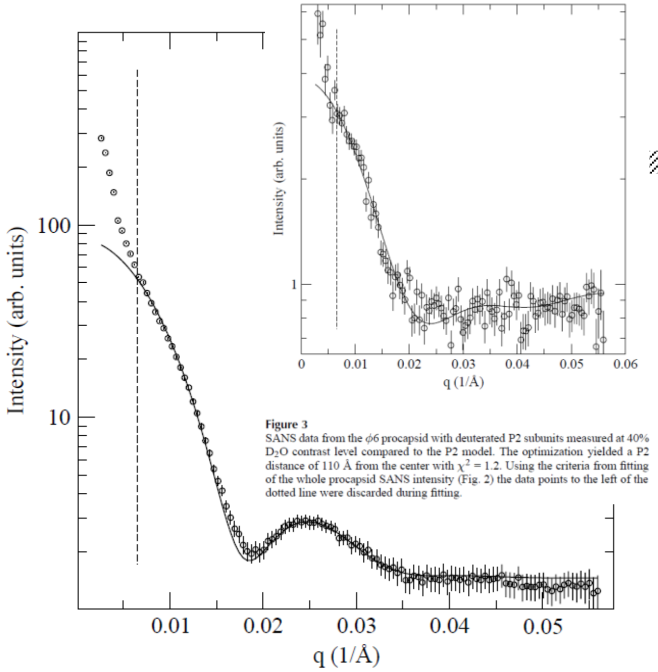
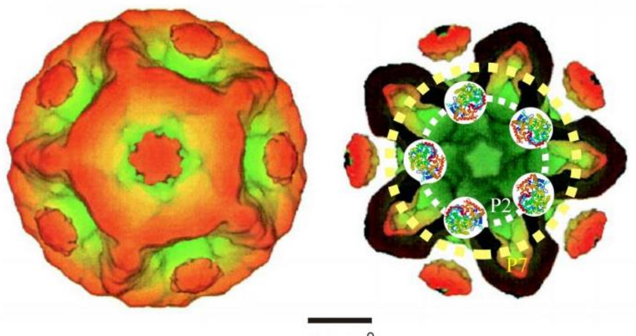


Figure 3
SANS data from the $\phi6$ procapsid with deuterated P2 subunits measured at 40% D_2O contrast level compared to the P2 model. The optimization yielded a P2 distance of 110 Å from the center with $\chi^2 = 1.2$. Using the criteria from fitting of the whole procapsid SANS intensity (Fig. 2) the data points to the left of the dotted line were discarded during fitting.

A comparison of SANS intensity measured from the $\phi6$ procapsid at 100% D_2O contrast and a smeared spherical shell model with $R_{out} = 230$ Å and $R_{in} = 100$ Å, $\chi^2 = 1.6$. Data points to the left of the dotted line were discarded during fitting.

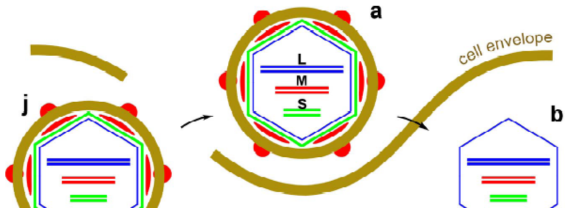


Locating the minor components of double-stranded RNA bacteriophage $\phi6$ by neutron scattering

Teemu Ikonen,[a] Denis Kainov,[b] Peter Timmins,[c] Ritva Serimaa[a] and Roman Tuma[b]*

[a]Department of Physical Sciences, P.O. Box 64, FIN-00014, University of Helsinki, Finland, [b]Institute of Biotechnology, P.O. Box 56, FIN-00014, University of Helsinki, Finland, [c]Large Scale Structures Group, Institut Laue-Langevin, 212-ILL20, 6, rue Jules Horowitz, BP 156 - 38042 Grenoble Cedex 0, France.
E-mail: roman.tuma@helsinki.fi

The polymerase core of double-stranded (ds) RNA virus provides the molecular machinery for RNA packaging and replication. Procapsid of bacteriophage $\phi6$ constitutes the best studied model of such dsRNA-

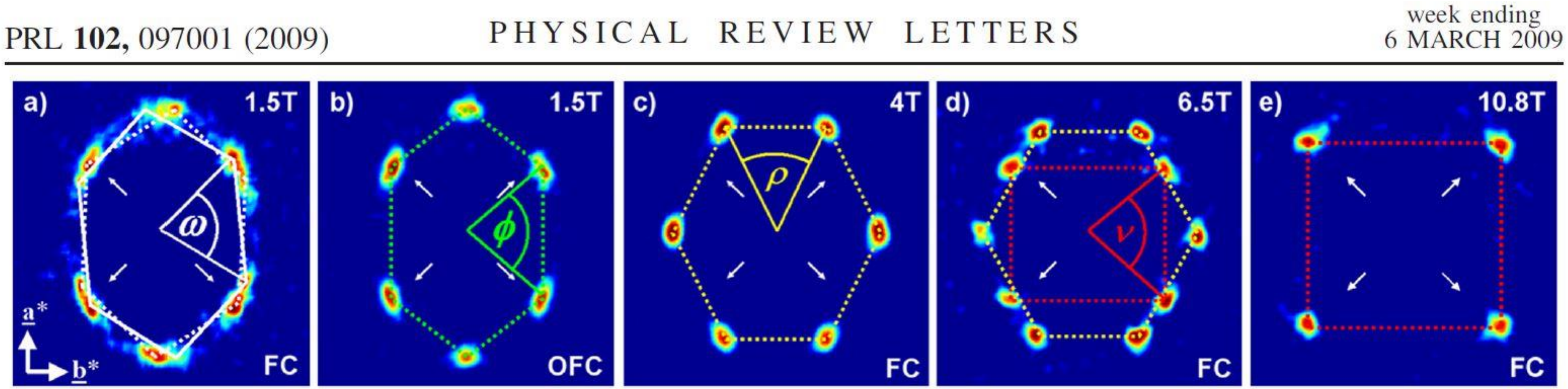


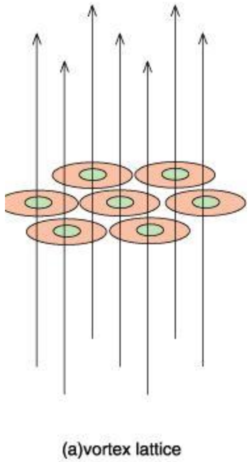
SANS and soft-condensed matter growing field of NS

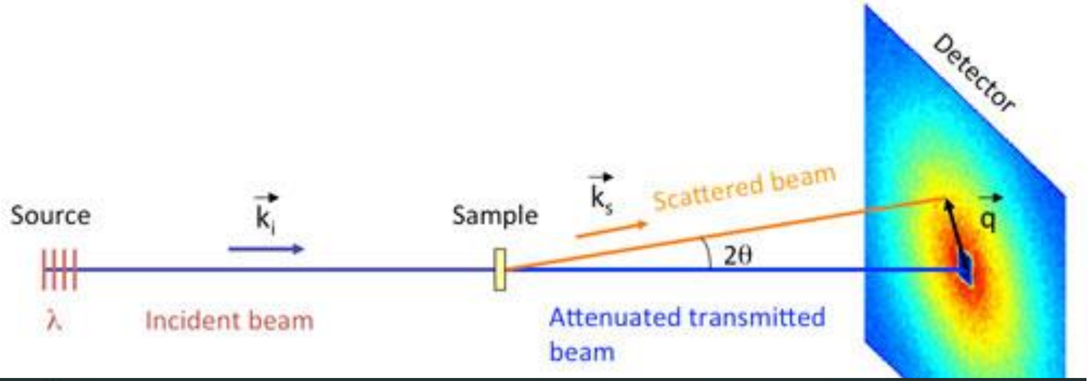
Contrast variation H_2O/D_2O

- Applicat

Flux vortices





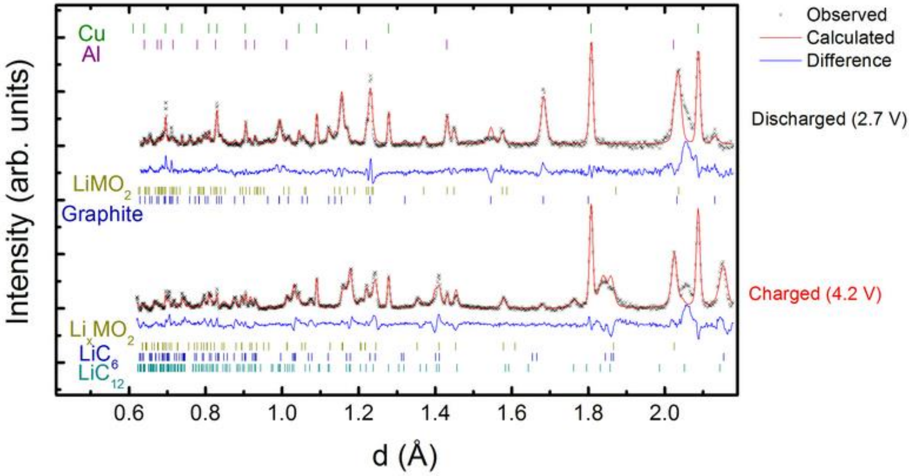


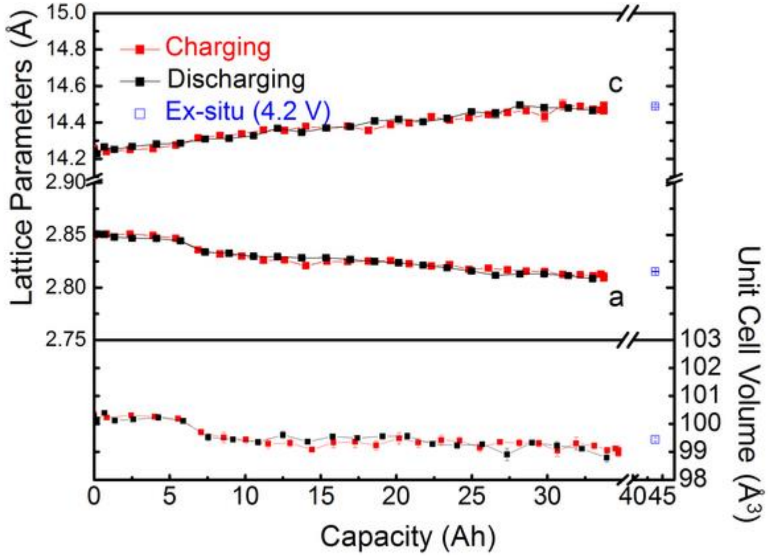
- Measured SANS on single crystal
- Symmetry of reflections implies hexagonal vortex lattice at low fields, wavevector **Q** of observed reflections implies spacing of vortices
- Scattering at small angles, small **Q**, large structure
- At higher fields get (nearly) square lattice

EPFL • Applicat • Flux

Chemistry and dynamics in batteries

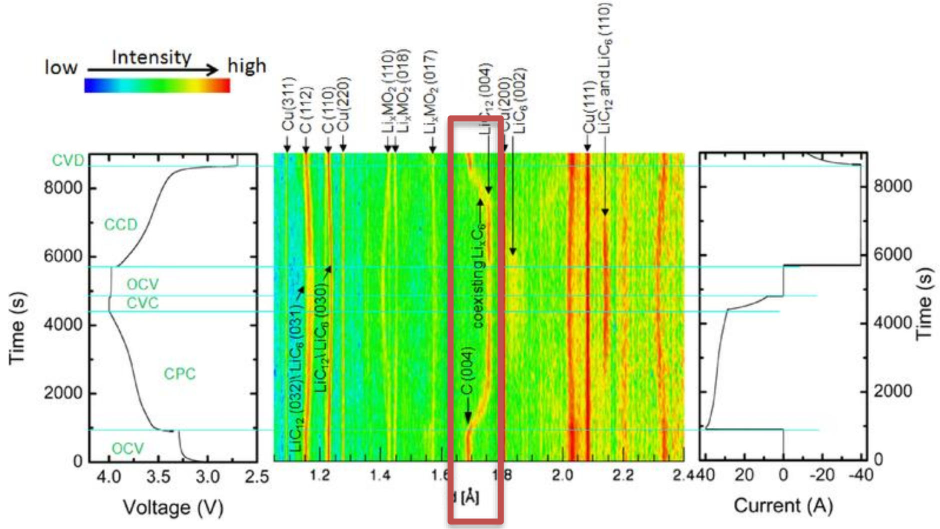
- Perform time- and spatially-resolved neutron diffraction experiments
- Clear contrast between charge and discharge cycles
- Observe changes in structure and chemistry in *in-situ* measurements in 2.5 min bins over 1.5 hours of charging



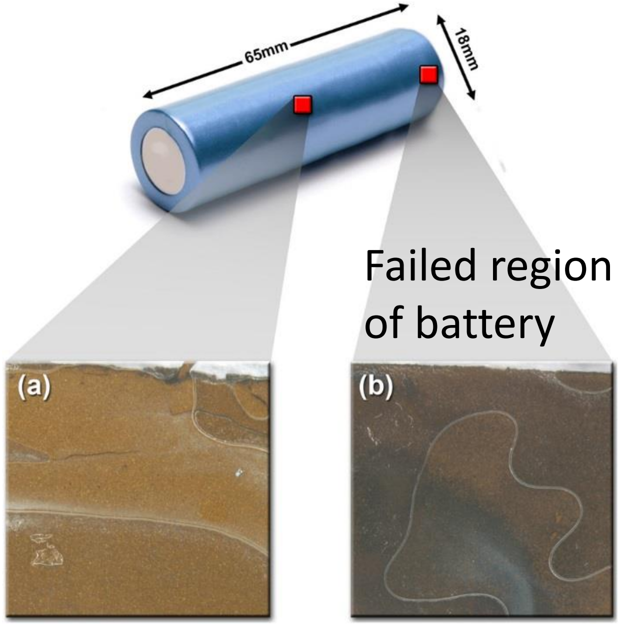


Discharging

Charging



Wang et al, Scientific Report 2, 747 (2012)



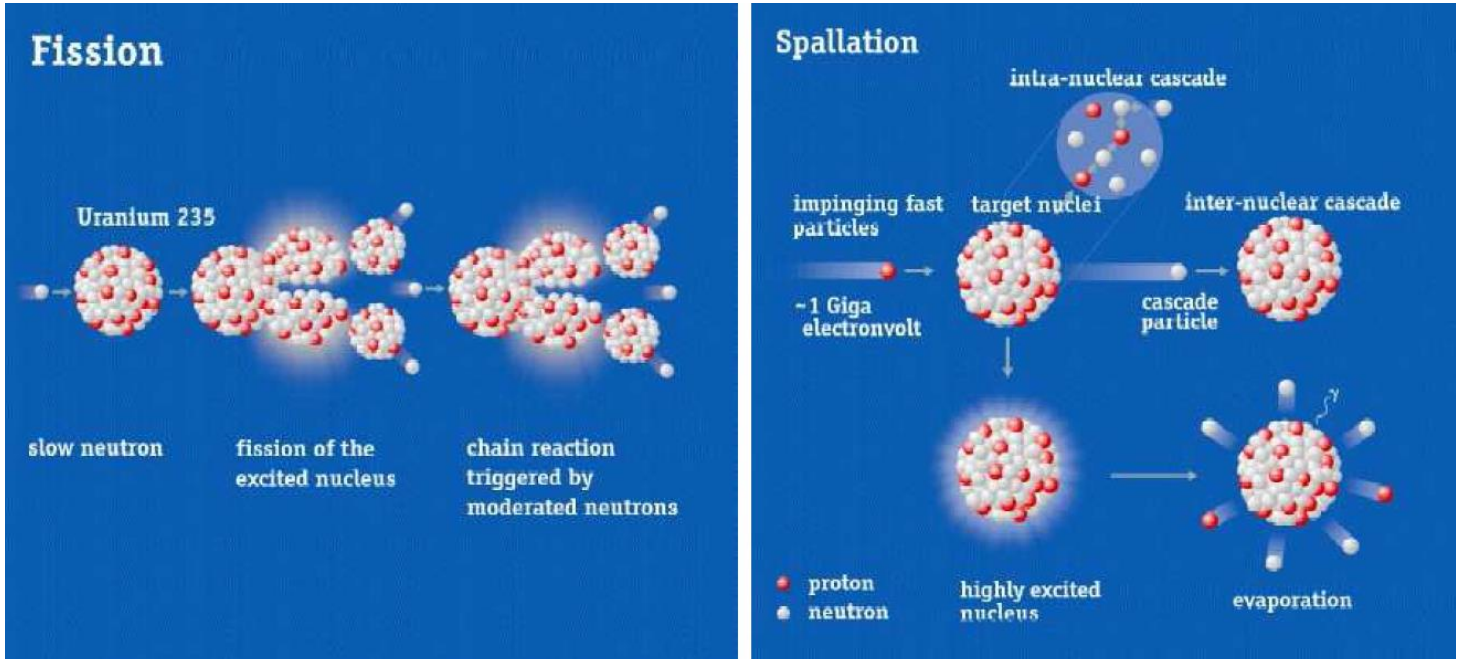
Failed region of battery

EPFL

- Applicat

Neutron facilities and instrumentation

Generating neutrons for solid state physics: fission vs spallation



Fission

- Neutron absorption causes unstable nuclei
- Nuclei decays and releases neutrons
- Nuclear reactor: a continuous neutron source

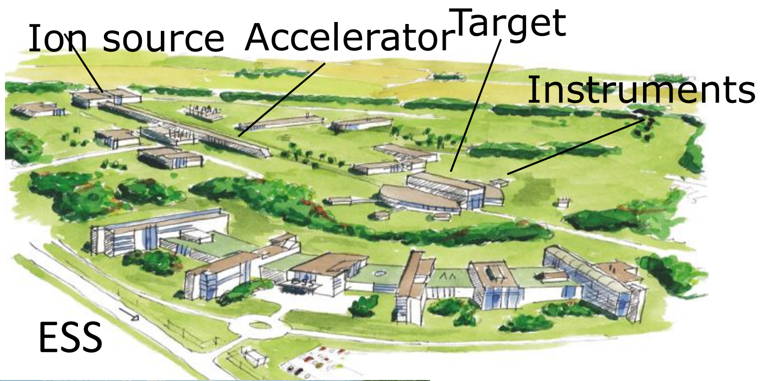
Spallation

- Accelerated proton fired into heavy element nuclei
- Excess energy makes nuclei unstable, neutrons released

• Instrum

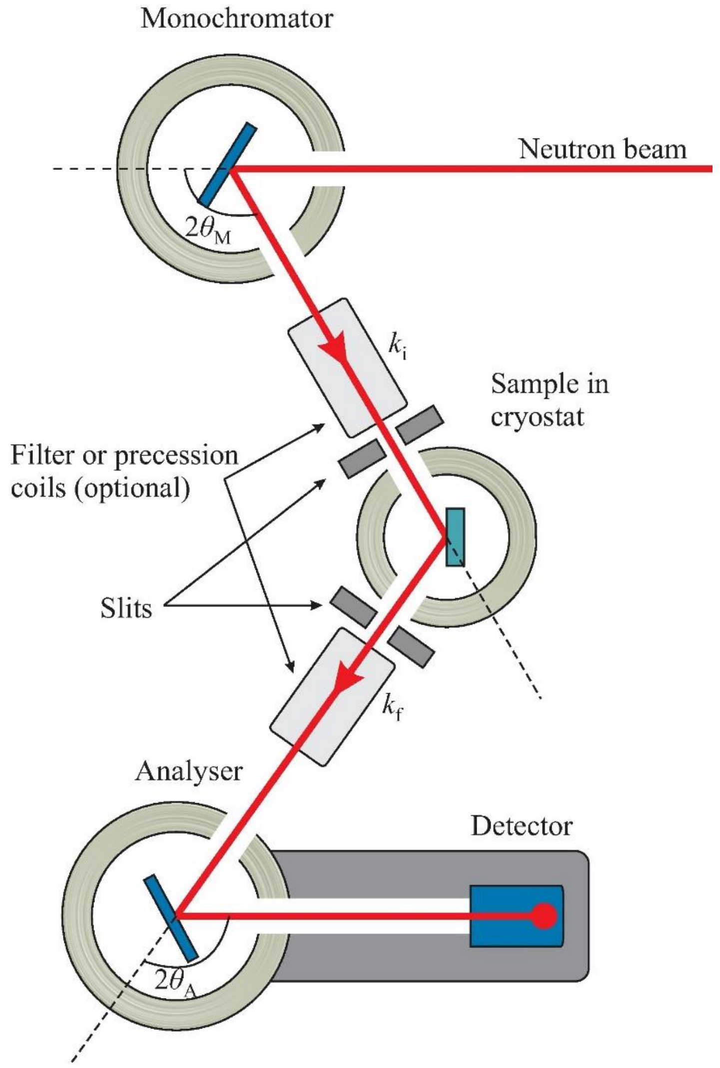
Evolution of neutron scattering

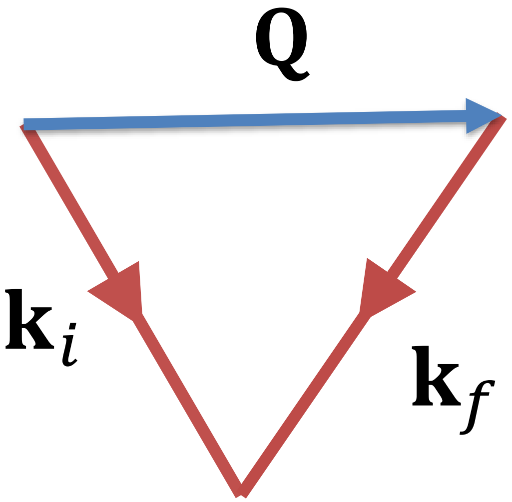
- 1st generation facilities:
  - re-use research reactors
- 2nd generation facilities:
  - Dedicated to neutron scattering:
  - ILL, France, FRMII Germany, SINQ Switzerland
    ISIS, UK etc.
- 3rd generation facilities:
  - SNS, US 1.4b$, commission 2006
  - J-Parc, Japan 150b¥, commission 2008
  - ESS, Sweden 1.8b€, start 2015, commission 2020
  - (China Spallation source, start 2011, commission 2018)
- 2nd to 3rd generation gains of 10-1000 times!
  - Faster experiments, smaller samples, better data
  - Time resolved physics
  - New fields of science



• Instrum

Triple-axis spectrometer





Advantages

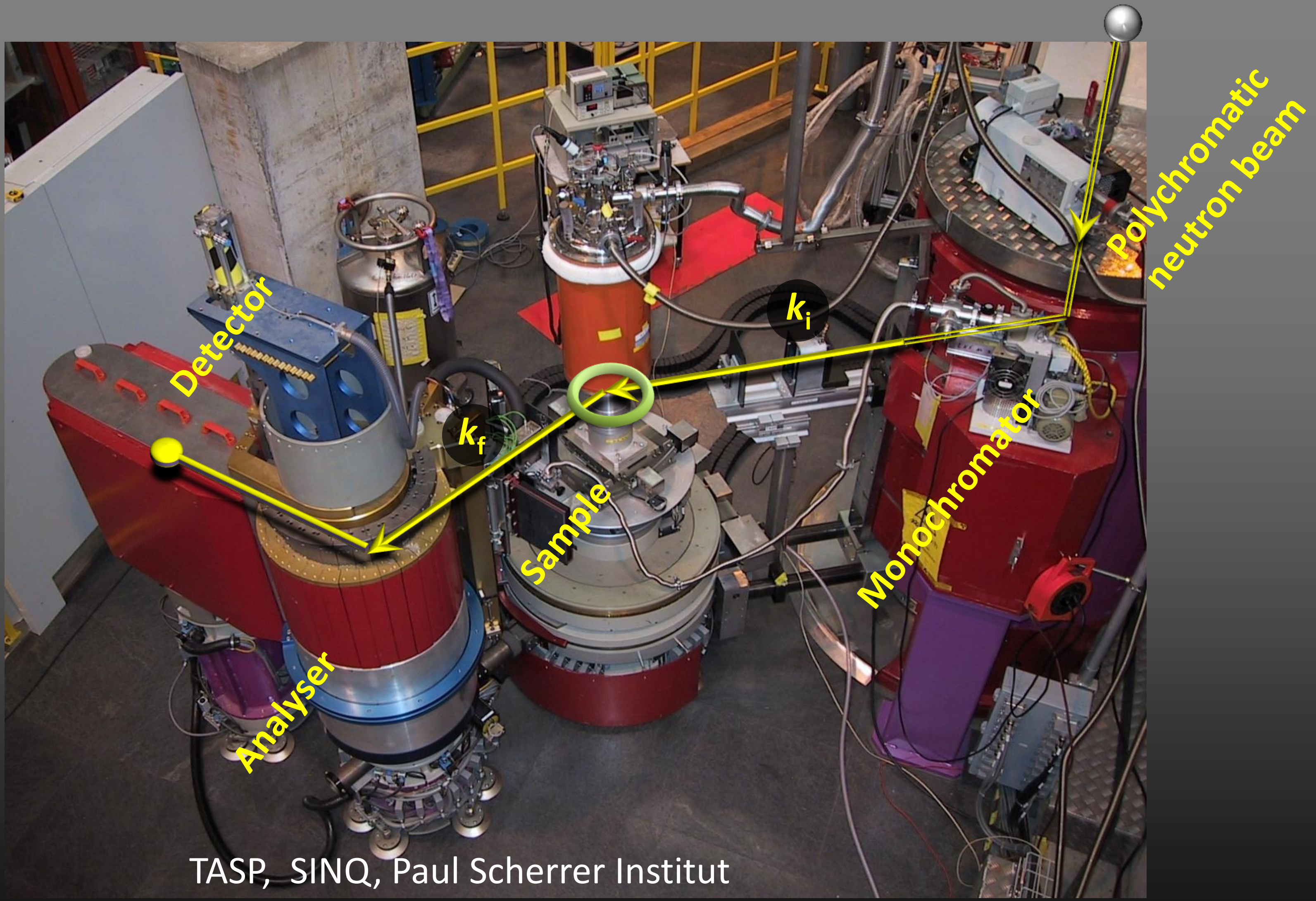
- Precise control of (**Q**, *E*)
- Can focus on a particular (**Q**, E) point
- Can use polarisation analysis
- Can obtain constant-*E* or constant-**Q** scans
- Ability to tune using focusing and collimation to trade between flux and resolution

Disadvantages

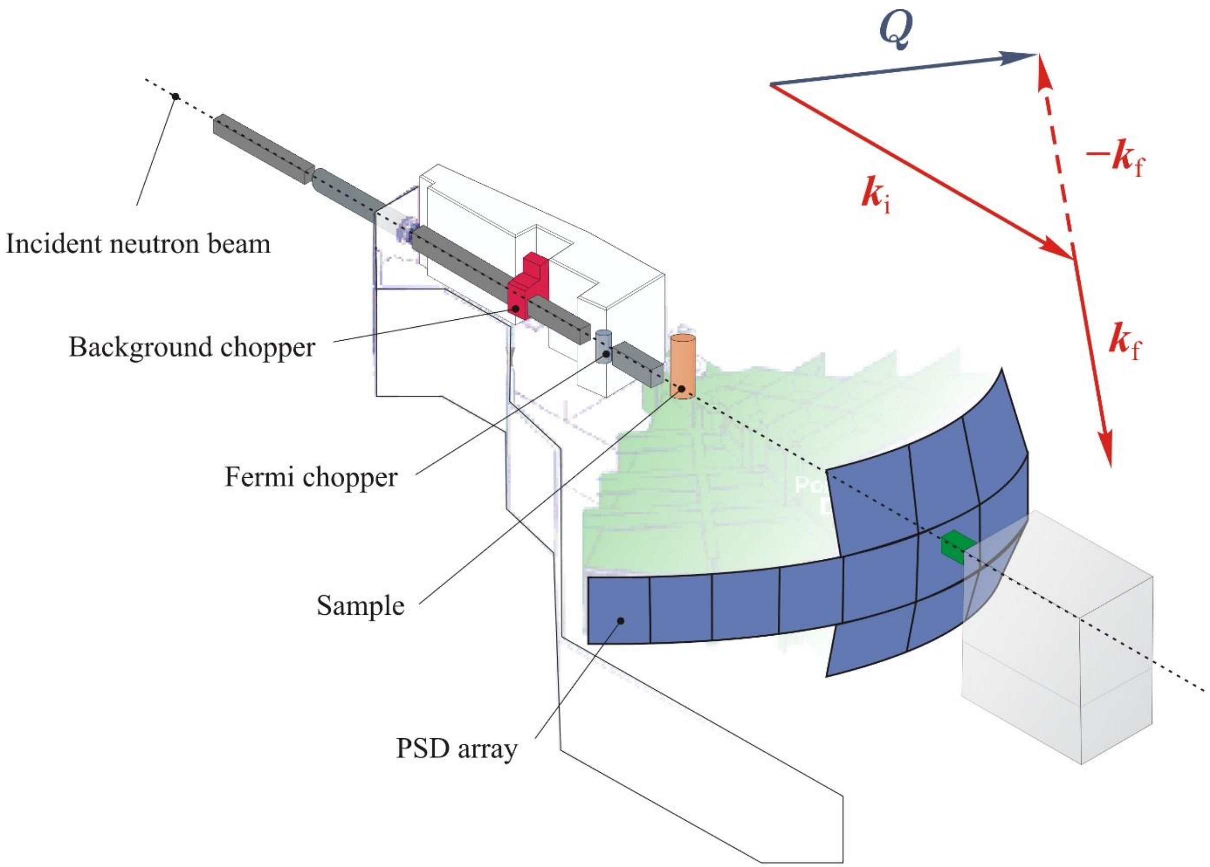
- Scan requires movement of various arms of spectrometer – lose time on moving
- Requires understanding of the instrument and how it works
- Cannot get an overview of (**Q**, *E*)-space

- Instrum

Neutron scattering measurement



Time-of-flight spectrometer



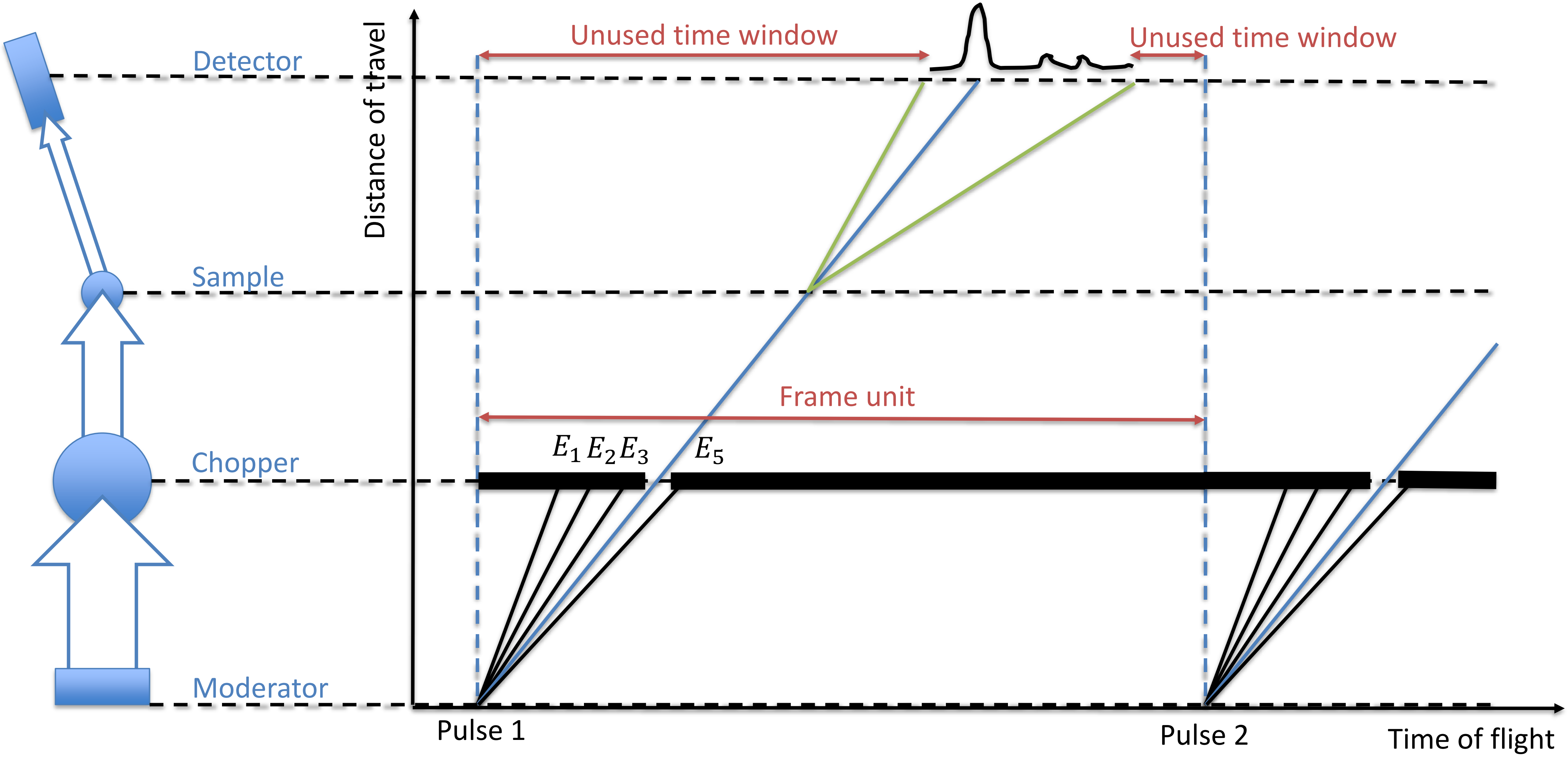
Advantages

- Capture a large volume of (**Q**, *E*)-space in one time
- Can obtain intensity in absolute units which can be compared to theory
- Relatively new technique which may improve further

Disadvantages

- Cannot perform constant-E or constant-**Q** scans
- Less flexible
- Optimum need a large number of detectors – Helium-3 expensive and in short supply
- Sample environment can block large portions of the detectors
- Requires pulsed beam

Creating a monochromatic beam: choppers



EPFL

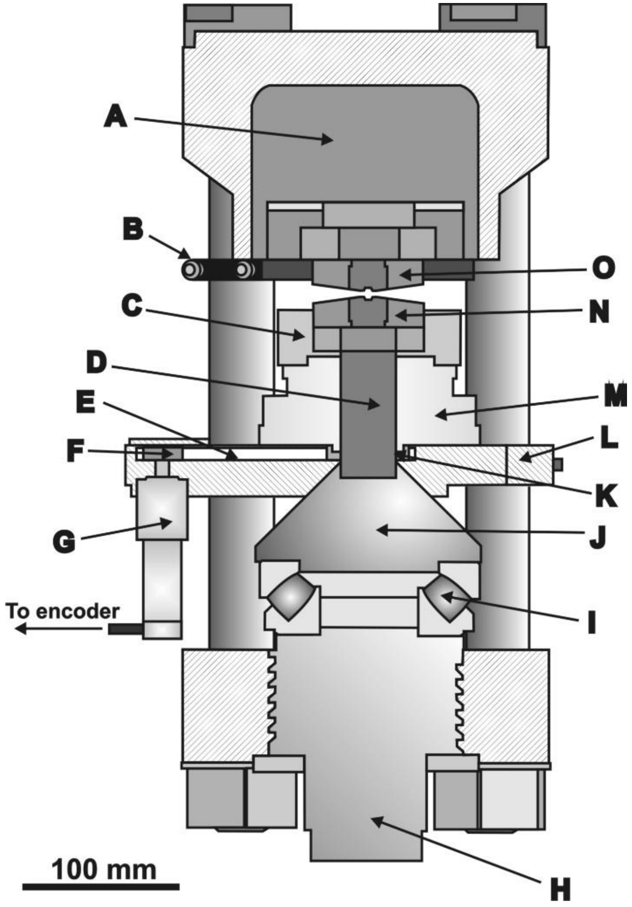
• Instrum

Sample environment

High magnetic fields

Low/high temperatures

Applied pressure



EPFL

- Instrum