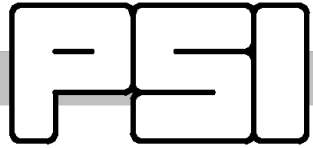
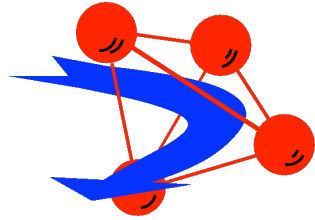


Magnetic neutron diffraction



Vladimir Pomjakushin
Laboratory for Neutron Scattering and Imaging
Paul Scherrer Institut PSI
Switzerland



The pdf-file with this talk will be
available at
<https://www.psi.ch/en/sinq/hrpt/talks>

or short link
<http://psi.ch/node/29534>

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 - 1.1. General. Intro. Experimental technics for magnetic diffraction
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2. Basic principles of magnetic neutron diffraction. (15-32)
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 - 2.2. Magnetic order parameters overview. Magnetic multipoles (22-27)
 - 2.3. Magnetic form-factors (what are neutrons sensitive to?) Expansion of Q [exp(i $\mathbf{k}\mathbf{r}$) series] (29-40)
 - 2.3.1. Dipole approximation. Examples.
 - 2.3.2. Multipole approximation, parity even, time odd. Symmetry of multipoles.
 - 2.3.3. Anapole (toroidal moment) and other parity-odd modern exotics (theory: Lovesey)
3. Description and determination of magnetic structure (41-72)
 - 3.1. Introduction to propagation vector(s) formalism star/arm (42,43,51)
 - 3.2. Magnetic structure factors. General formula 44-47
 - 3.3. Commensurate vs. incommensurate case's examples.
 - 3.4. Introduction to irreps (48-50)
 - 3.5. Magnetic Shubnikov groups (52-53)
4. Classification of the magnetic structures that are used in the literature, such as Shubnikov (or Magnetic) space groups, 3D+n superspace groups and irreducible representation (irrep) notations. Relation between two approaches. A bit of history. (54-59)
5. How can one construct all possible symmetry adapted magnetic structures for a given crystal structure and a propagation vector (a point on the Brillouine zone) by the combined use of irrep and the magnetic symmetry? A real case study of:
 - 5.1. multiferroic TmMnO₃: 2D irrep $\mathbf{k}=[1/2,0,0]$. Ferro-electric phase polar magnetic group Pbm_n21 (61-65)
 - 5.2. Topologically nontrivial skyrmionic incommensurate magnetic structure. Superspace. (66-72)

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Introduction to magnetic diffraction

neutron properties

mass $m = 1.660 \cdot 10^{-24} \text{ g} = 939 \text{ MeV}$

spin: $S = 1/2$

magnetic moment $\mu_n = \gamma \mu_N = -1.91 \text{ nuclear magnetons}$

The state of neutron is describe by its wave vector $\mathbf{k}$
plane wave $\psi \sim \exp(i\mathbf{k}\mathbf{r})$

and its spin component $S_z = \pm 1/2$

Instead of $\mathbf{k}$ we often find:

Energy $E = \frac{\hbar^2 k^2}{2m}$

momentum $\mathbf{p} = \hbar \mathbf{k}$

velocity $\mathbf{v} = \frac{\hbar \mathbf{k}}{m}$

wavelength $\lambda = \frac{2\pi}{k}$

neutron g-factor $g_n = -3.8$

$$\mu_n = g_n S [\mu_N]$$

$$\gamma = g_n / 2 = -1.91$$

nuclear magneton

$$\mu_N = e\hbar / 2m_p c$$

Bohr magneton

$$\mu_B = e\hbar / 2m_e c$$

$$m_e = 0.5 \text{ meV}$$

proton $g_p = 5.6$, electron $g_e = -2.0$

1994 Nobel Prize in Physics

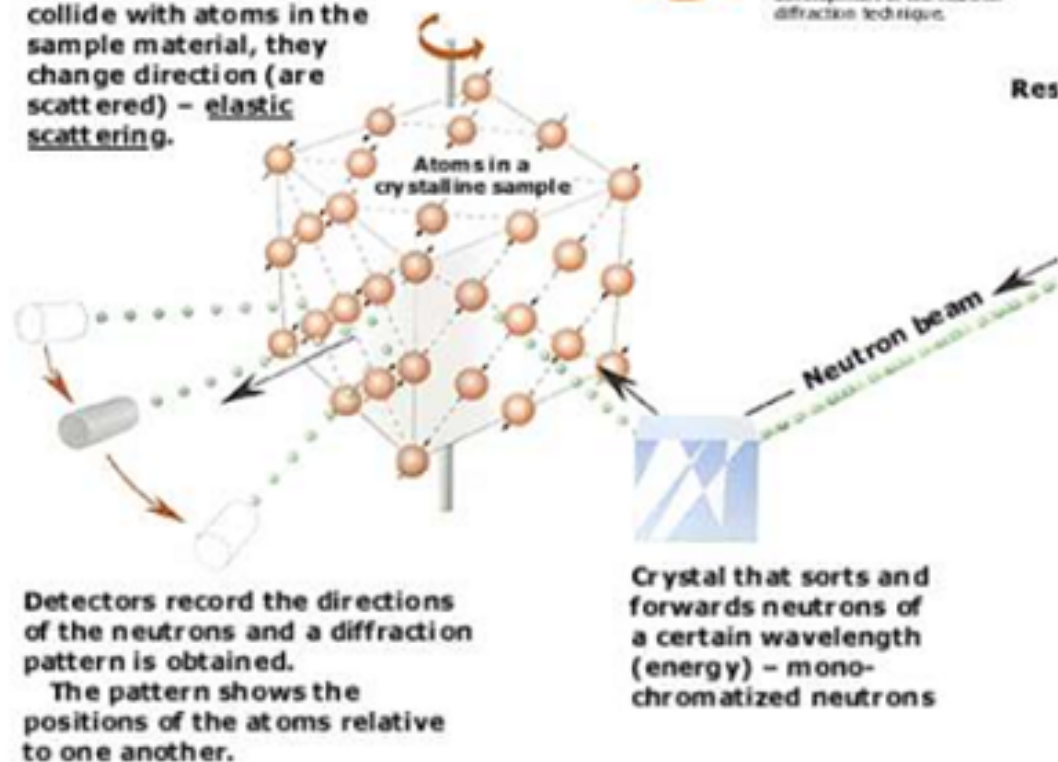
Clifford G. Shull
1915 – 2001, USA



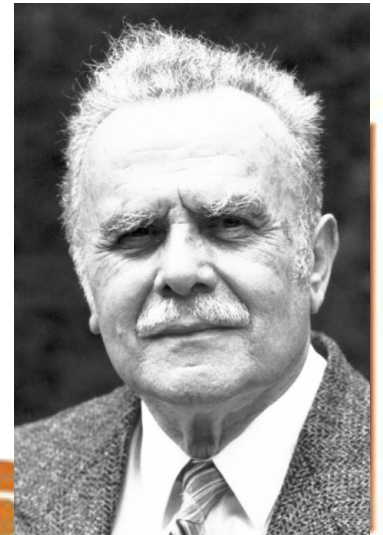
Clifford G. Shull, MIT, Cambridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.

Neutrons show where atoms are

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



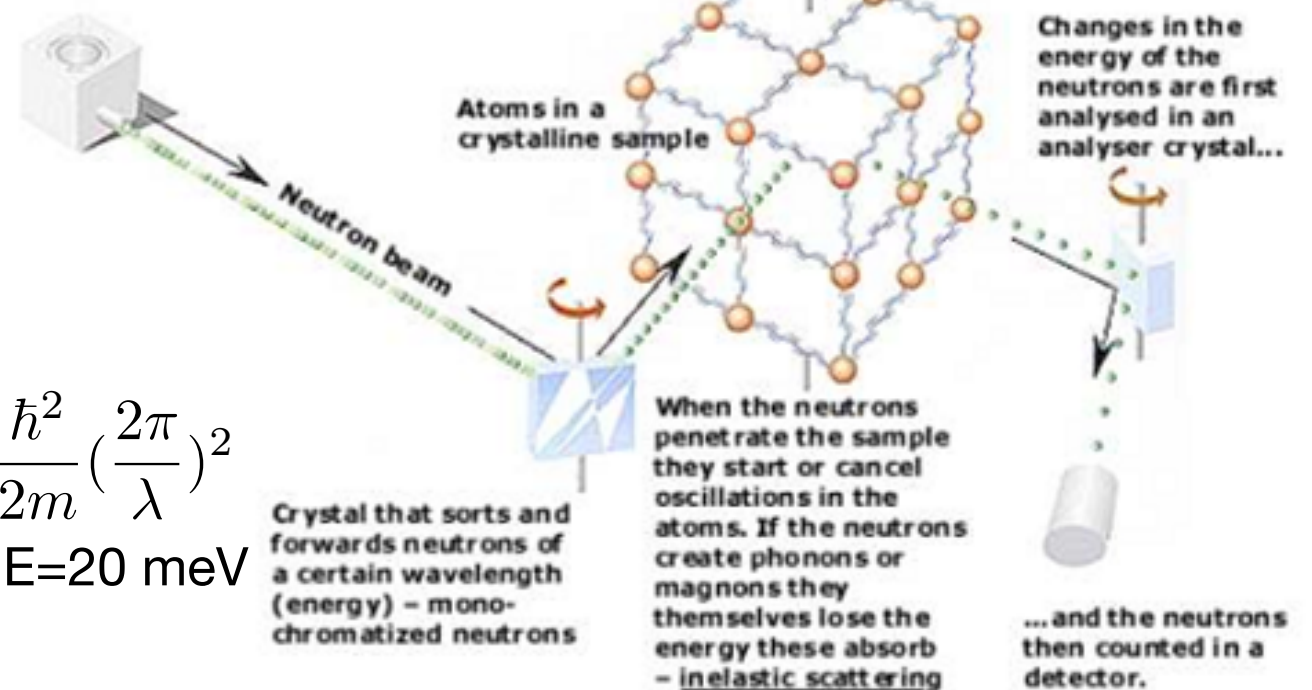
Bertram N. Brockhouse
1918 – 2003, Canada



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

Neutrons show what atoms do

3-axis spectrometer with rotatable crystals and rotatable sample



$$E = \frac{\hbar^2}{2m} \left(\frac{2\pi}{\lambda} \right)^2$$

$\lambda = 2\text{\AA}$, $E = 20\text{ meV}$

Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances

C. G. SHULL, W. A. STRAUSSER, AND E. O. WOLLAN
Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received March 2, 1951)

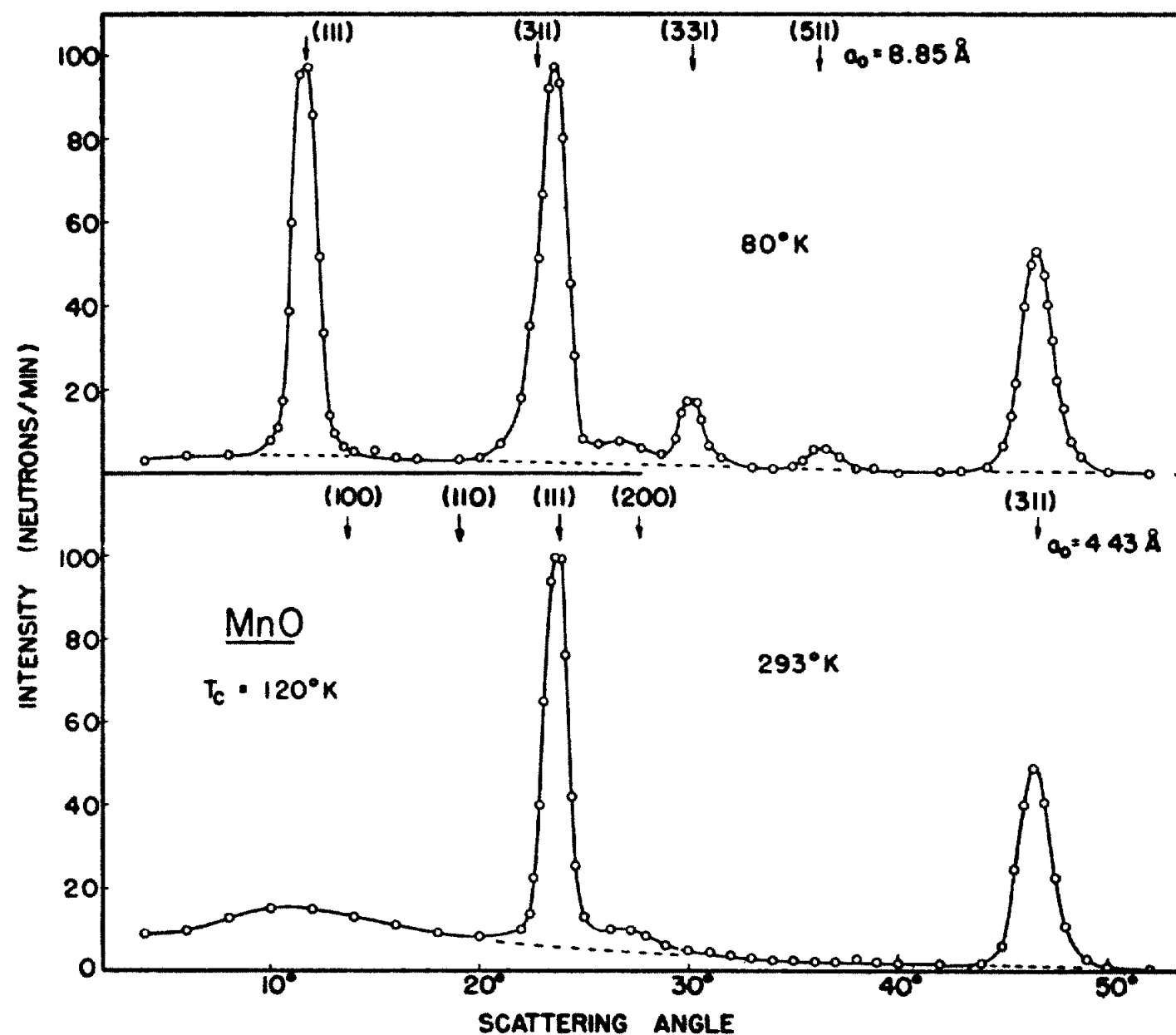


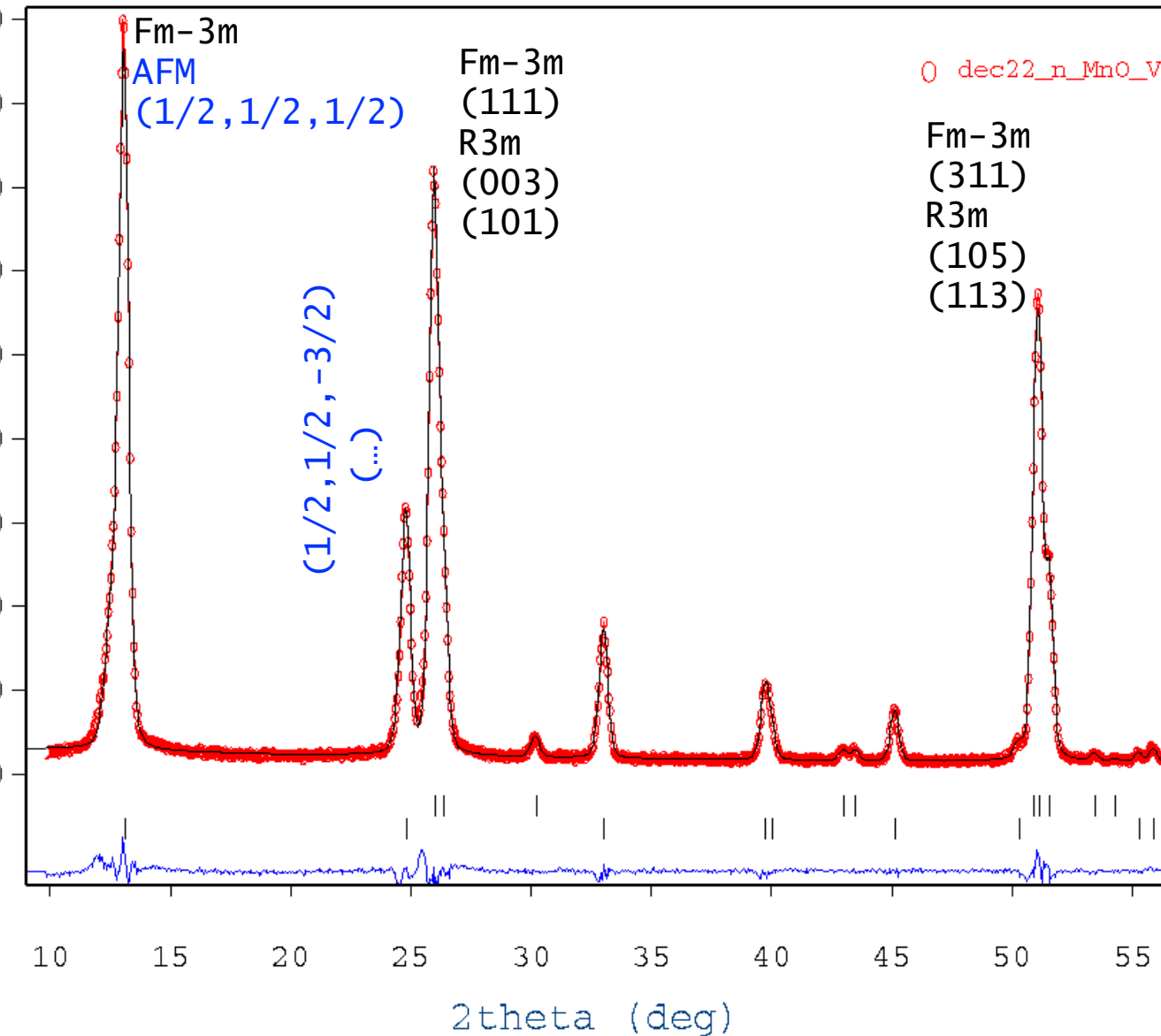
FIG. 4. Neutron diffraction patterns for MnO taken at liquid nitrogen and room temperatures. The patterns have been corrected for the various forms of extraneous, diffuse scattering mentioned in the text. Four extra antiferromagnetic reflections are to be noticed in the low temperature pattern.

HRPT/SINQ nowadays

$\lambda=1.15\text{\AA}$, MnO @ 2K.

Rhombohedral distortions are explicitly seen

R-3m and $k=003/2$



reaction by Paramagnetic and Antiferromagnetic

$\lambda=1.057\text{\AA}$

C. G. SHULL, W. A. STRAUER, AND E. O. WOLLAN
Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received March 2, 1951)

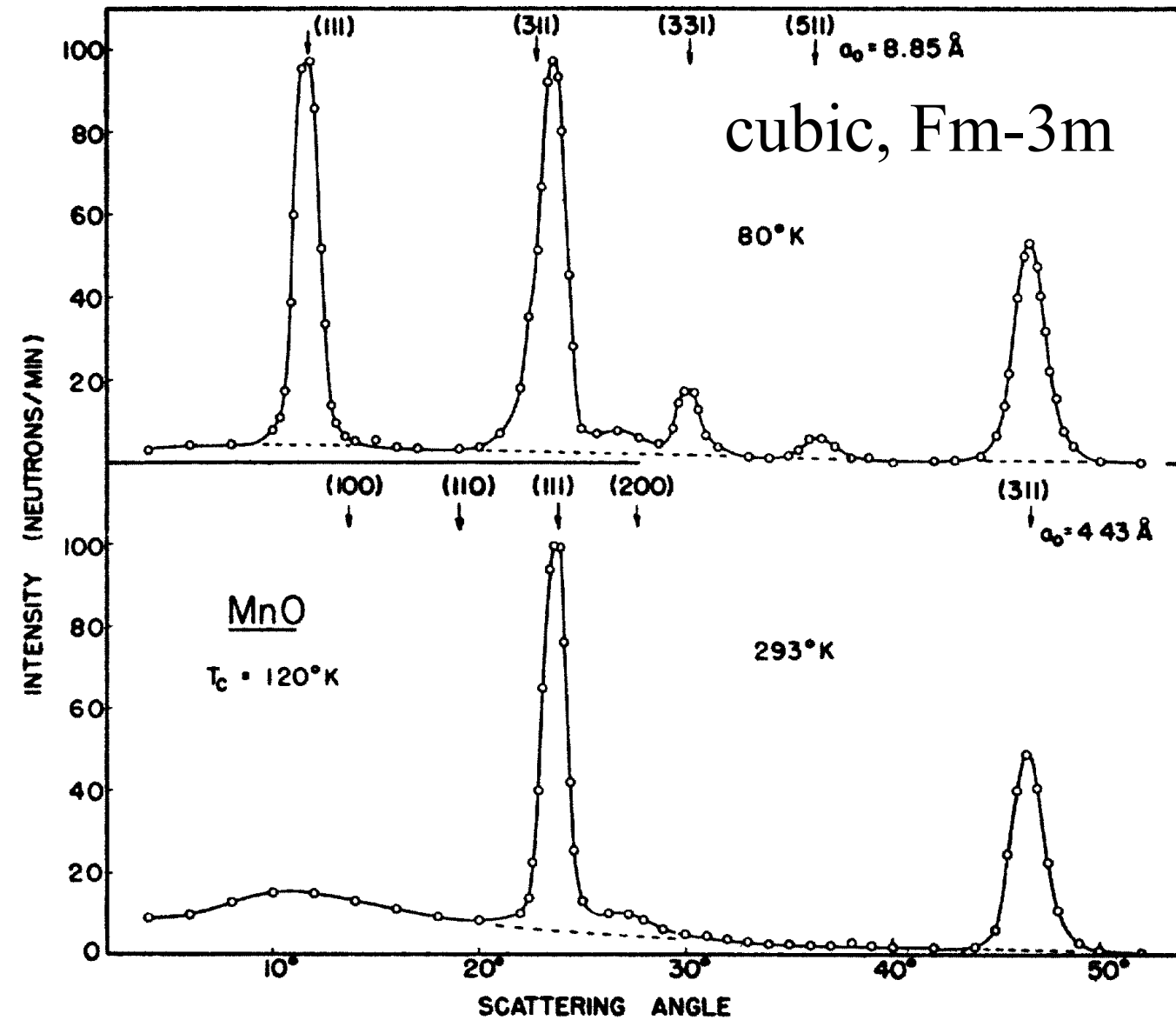


FIG. 4. Neutron diffraction patterns for MnO taken at liquid nitrogen and room temperatures. The patterns have been corrected for the various forms of extraneous, diffuse scattering mentioned in the text. Four extra antiferromagnetic reflections are to be noticed in the low temperature pattern.

Types of (magnetic) neutron diffraction techniques

Types of (magnetic) neutron diffraction techniques

- spin-polarised:
 - nuclear/magnetic interference for non-spin flip. Purely magnetic for spin-flip channel.
 - Full 3D analysis of neutron polarization - spherical neutron polarimetry.

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- $\lambda = \text{const}$: $I(2\theta)$, Time Of Flight TOF: $I(t)$, Laue

Diffraction instruments at swiss continuous spallation source SINQ. $\lambda = \text{const}$

- HRPT - High Resolution Powder Diffractometer for Thermal Neutrons, $\lambda = 0.94 - 2.96 \text{ \AA}$, High Q-range $\leq 11 \text{ \AA}^{-1}$
- DMC – High Intensity Powder Diffractometer for Cold Neutrons, $\lambda = 2.35 - 5.4 \text{ \AA}$, High flux and good resolution at low and moderate Q $\leq 4 \text{ \AA}^{-1}$
- TriCS/Zebra - Single crystal diffractometer, $\lambda = 1.18, 2.3 \text{ \AA}$, Thermal Neutrons
- TASP (triple axes) with MuPAD for polarised ND, Cold Neutrons, $\lambda = 1.8 - 6.0 \text{ \AA}$

Literature on (magnetic) neutron scattering

Neutron scattering (general)

S.W. Lovesey, “*Theory of Neutron Scattering from Condensed Matter*”, Oxford Univ. Press, 1987. Volume 2 for magnetic scattering. **Definitive formal treatment**

G.L. Squires, “*Intro. to the Theory of Thermal Neutron Scattering*”, C.U.P., 1978, Republished by Dover, 1996. **Simpler version of Lovesey.**

All you need to know about magnetic neutron diffraction. Symmetry, representation analysis

Yu.A. Izyumov, V. E. Naish and R. P. Ozerov, “*Neutron diffraction of magnetic materials*”, New York [etc.]: Consultants Bureau, 1991. **Obsolete with respect to magnetic space groups and magnetic (super)symmetry.**

Literature on magnetic neutron scattering

Modern way of magnetic symmetry and representation analysis

“Magnetic superspace groups and symmetry constraints in incommensurate magnetic phases”, J M Perez-Mato, J L Ribeiro, V Petricek and M I Aroyo, J. Phys.: Condens. Matter **24** (2012) 163201

“MAGNDATA: towards a database of magnetic structures.”

Gallego, Perez-Mato, Elcoro, Tasci, Hanson, Momma, Aroyo & Madariaga
JOURNAL OF APPLIED CRYSTALLOGRAPHY (2016) Volume: 49 Pages: 1750-1776,
1941-1956

“Tabulation of irreducible representations of the crystallographic space groups and their superspace extensions”

Harold T. Stokes, Branton J. Campbell and Ryan Cordes
Acta Cryst. (2013). A69, 388–395

Web/computer resources to perform group theory symmetry analysis, in particular magnetic structures.

General tools for representation analysis, Shubnikov groups, 3D+n, and much more...

Web sites with a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

- Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell

ISODISTORT: ISOTROPY Software Suite, <http://iso.byu.edu>

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA,

M. I. Aroyo, J. M. Perez-Mato, D. Orobengoa, E. Tasci, G. de la Flor, A. Kirov

- Bilbao Crystallographic Server

<http://www.cryst.ehu.es/>

Computer programs to construct symmetry adapted magnetic structures and fit the experimental data.

Workhorses: Computer programs for representation analysis to be used together with the diffraction data analysis programs to determine magnetic structure from neutron diffraction (ND) experiment.

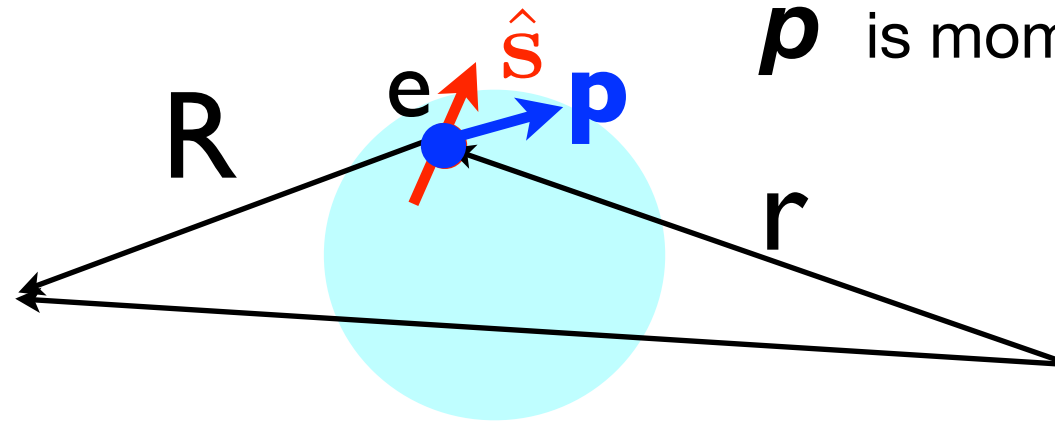
- Juan Rodríguez Carvajal (ILL) et al, <http://www.ill.fr/sites/fullprof/>
Fullprof suite
- Vaclav Petricek, Michal Dusek (Prague) Jana2006 <http://jana.fzu.cz/>

Basic principles of magnetic neutron diffraction

Magnetic neutron scattering on an atom

$$\mu_e = -2\mu_B \hat{S}$$

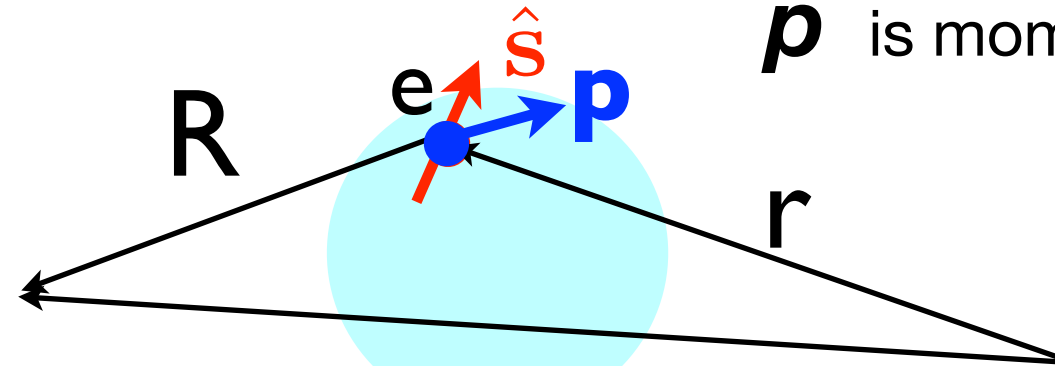
$\mathbf{p}$ is momentum



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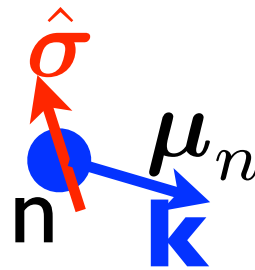


Magnetic field from an electron

$$\mathbf{H}(\mathbf{R}) = \text{rot} \left[\frac{\mu_e \times \mathbf{R}}{|\mathbf{R}|^3} \right] - \frac{2\mu_B}{\hbar} \left[\frac{\mathbf{p}_e \times \mathbf{R}}{|\mathbf{R}|^3} \right]$$

spin S orbit L

Magnetic neutron scattering on an atom

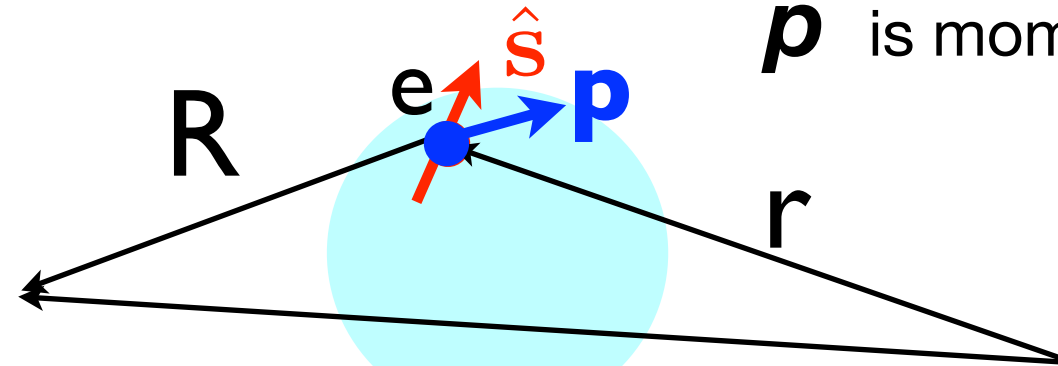


A blue dot labeled 'n' represents a neutron. A red arrow labeled $\hat{\sigma}$ points upwards and to the left, representing the spin. A blue arrow labeled $\mathbf{k}$ points to the right, representing the wave vector. A blue arrow labeled μ_n points to the right, representing the magnetic moment.

$$\mu_n = 2\gamma\mu_n \frac{\hat{\sigma}}{2}$$

$$\mu_e = -2\mu_B \hat{S}$$

$\mathbf{p}$ is momentum



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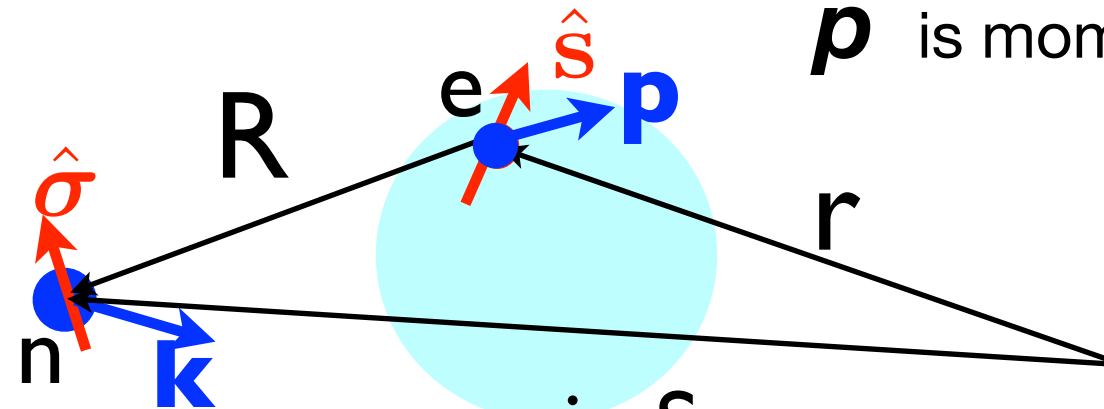
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spin S orbit L

neutron-electron dipole interaction

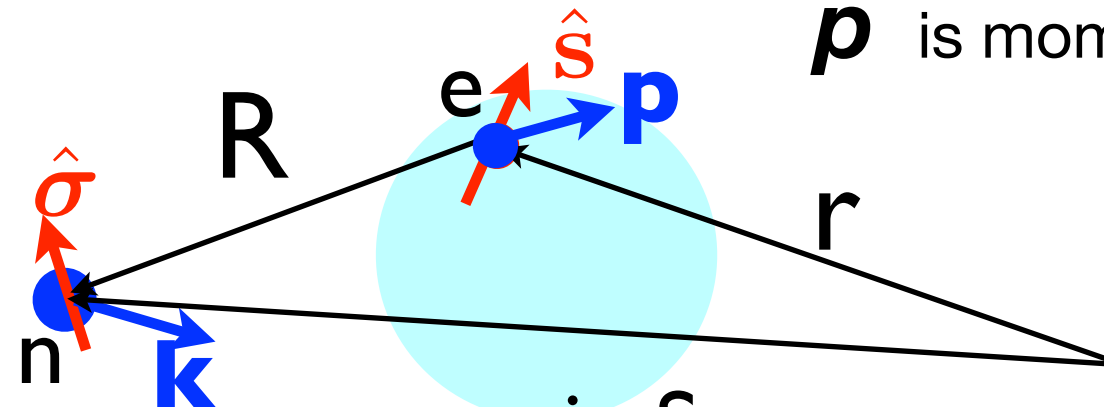
$$V(\mathbf{R}) = -\gamma\mu_n \hat{\sigma} \mathbf{H}(\mathbf{R})$$

Magnetic neutron scattering on an atom

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$$\mu_e = -2\mu_B \hat{S}$$

$\mathbf{p}$ is momentum



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spin S orbit L

neutron-electron dipole interaction

$$V(\mathbf{R}) = -\gamma\mu_n \hat{\sigma} \mathbf{H}(\mathbf{R})$$

averaging over neutron coordinates

$$\langle \mathbf{k}' | V(\mathbf{R}) | \mathbf{k} \rangle = \gamma r_e \hat{\sigma} \frac{1}{q^2} [\mathbf{q} \times [\hat{S} e^{i\mathbf{q}\mathbf{r}} \times \mathbf{q}]]$$

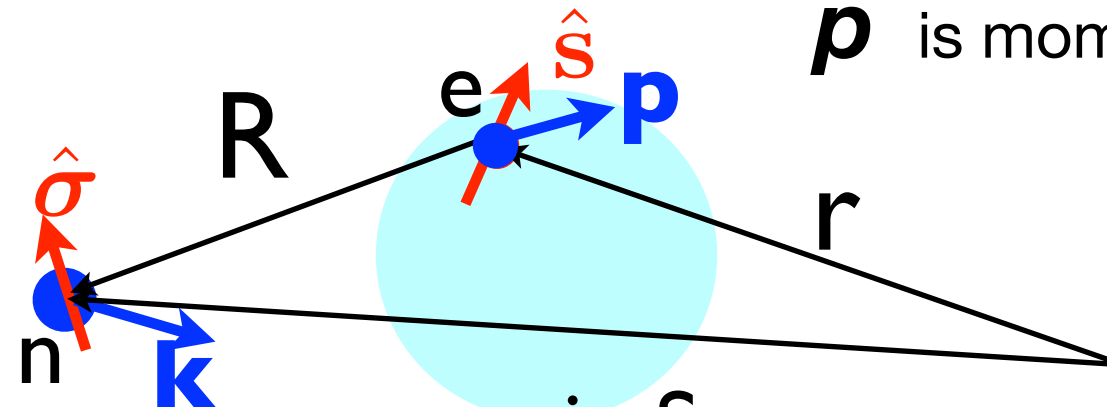
$\mathbf{q} = \mathbf{k}' - \mathbf{k}$

Magnetic neutron scattering on an atom

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$\mathbf{q} = \mathbf{k}' - \mathbf{k}$

magnetic interaction operator $\hat{\mathbf{Q}}_{\perp}$

Magnetic neutron scattering on an atom

$$\text{“magnetic scattering amplitude”} = \gamma r_e \langle \hat{\mathbf{Q}}_{\perp} \rangle ,$$

Magnetic neutron scattering on an atom

1. The size

“magnetic scattering amplitude” $= \gamma r_e \langle \hat{\mathbf{Q}}_{\perp} \rangle$,

neutron magnetic moment in $\mu_n - 1.91$ $\rightarrow$ γ

classical electron radius $\frac{e^2}{mc^2}$ $\rightarrow$ r_e

Magnetic neutron scattering on an atom

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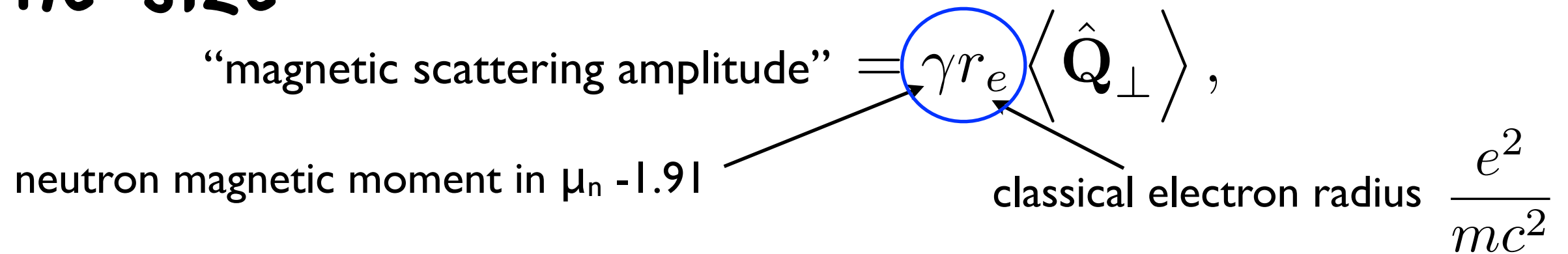
$\gamma r_e = -0.54 \cdot 10^{-12} \text{ cm} = -5.4 \text{ fm} (\times S)$
fm=fermi= 10^{-13} cm

Magnetic neutron scattering on an atom

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fm=fermi= 10^{-13} cm

x-ray scattering length: $Z r_e$

Magnetic neutron scattering on an atom

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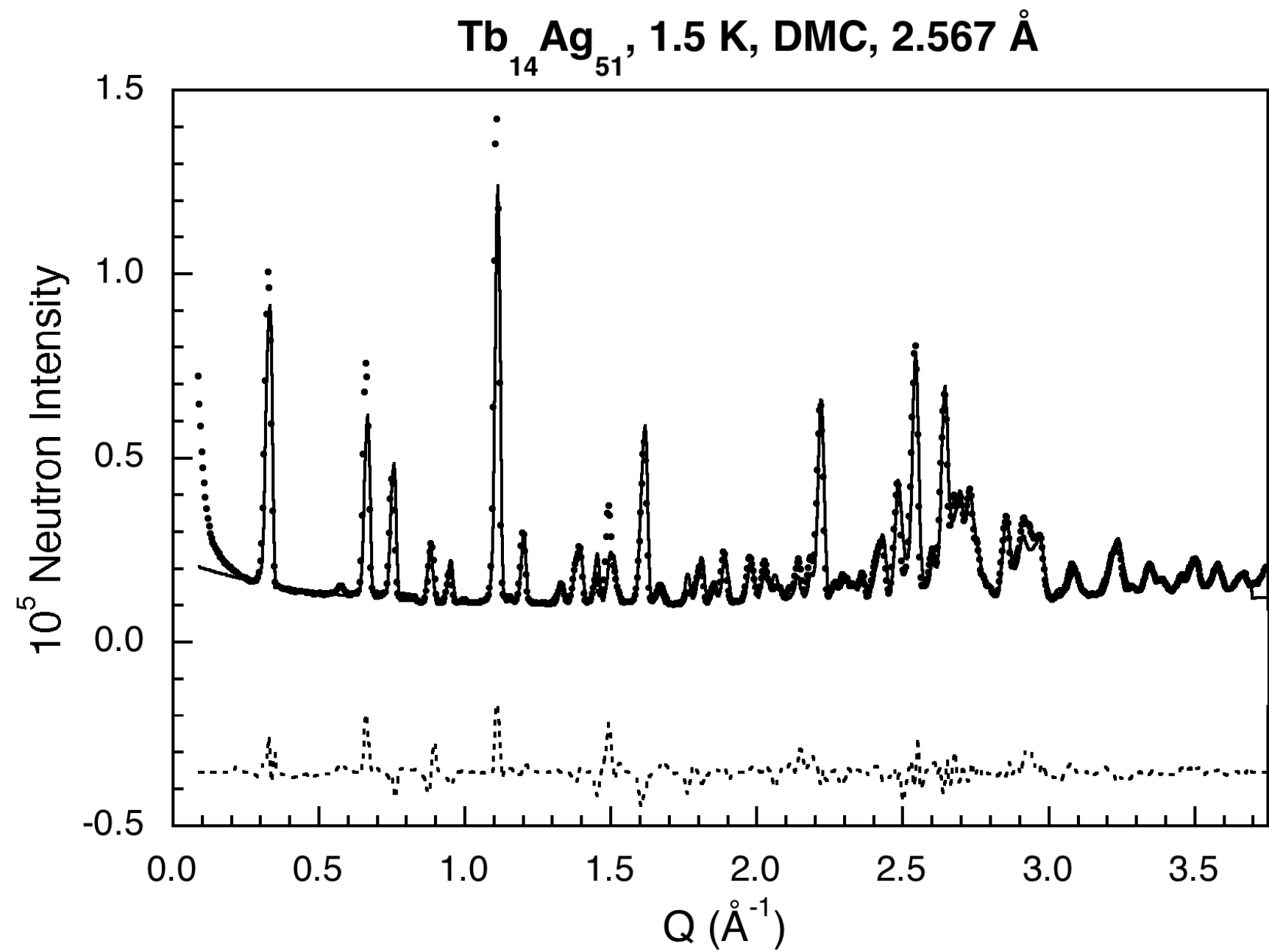
Comparison of neutron scattering lengths (fm)

magnetic

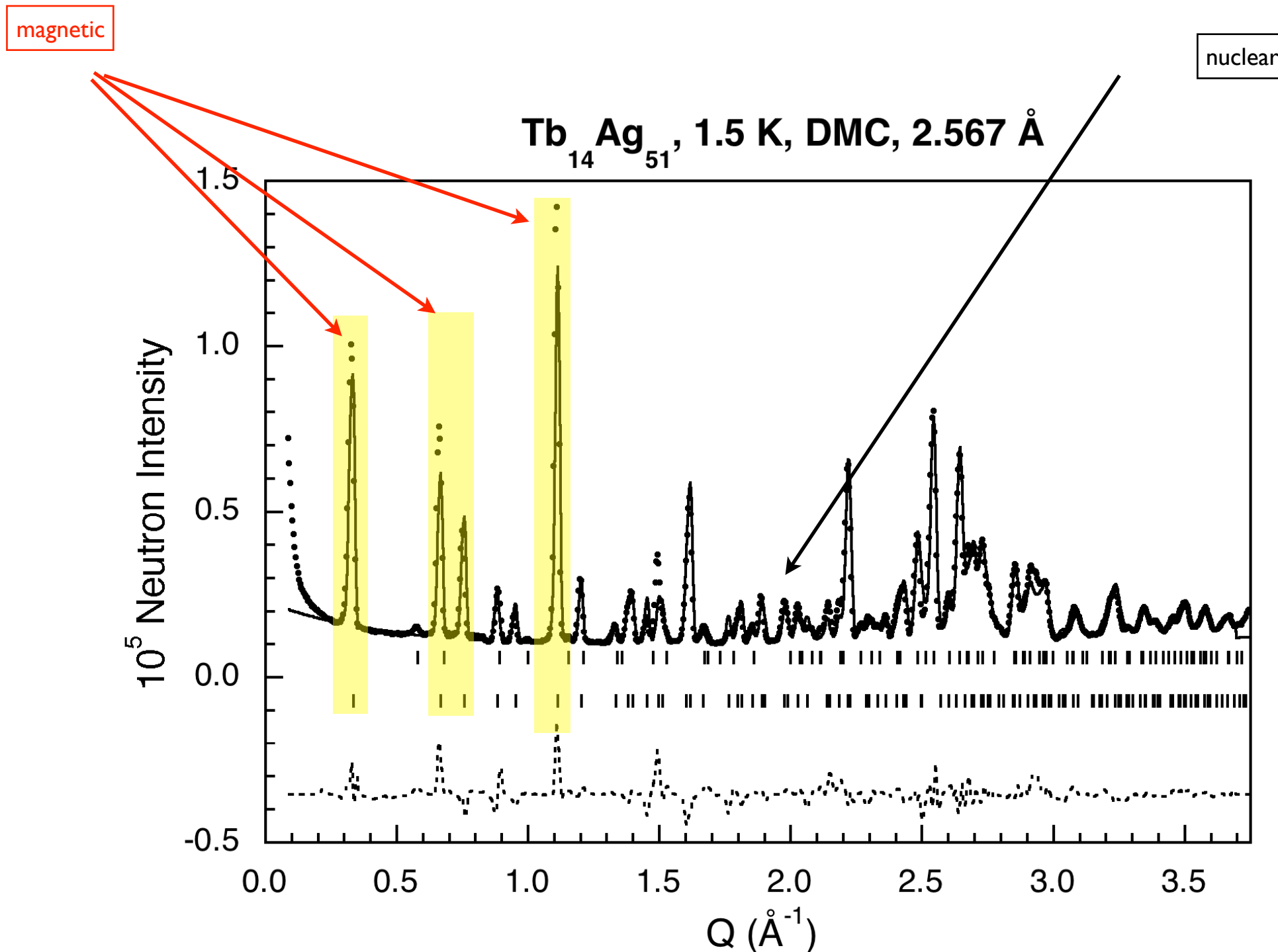
Mn³⁺ (S=2): -10.8, Cu²⁺ (S=1/2): -2.65

nuclear

Mn : -3.7, Cu: 7.7



magnetic scattering intensity can be larger than the nuclear one



Magnetic neutron scattering on an atom

$$\text{“magnetic scattering amplitude”} = \gamma r_e \langle \hat{\mathbf{Q}}_{\perp} \rangle ,$$

Magnetic neutron scattering on an atom

2. q-dependence

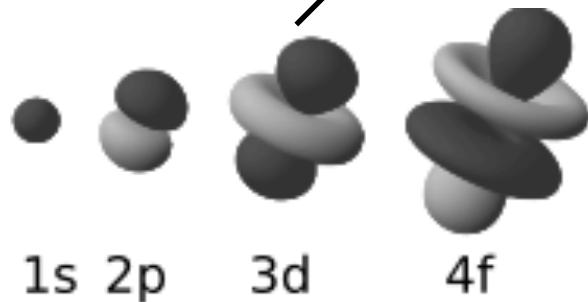
$$\text{"magnetic scattering amplitude"} = \gamma r_e \langle \hat{\mathbf{Q}}_{\perp} \rangle, \\ \frac{1}{q^2} [\mathbf{q} \times \hat{\mathbf{Q}} \times \mathbf{q}]$$

Magnetic neutron scattering on an atom

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$$\text{"magnetic scattering amplitude"} = \gamma r_e \langle \hat{\mathbf{Q}}_{\perp} \rangle, \\ \frac{1}{q^2} [\mathbf{q} \times \hat{\mathbf{Q}} \times \mathbf{q}]$$

$$\langle \hat{\mathbf{Q}} \rangle = \langle \psi | \hat{\mathbf{s}} e^{i\mathbf{q}\mathbf{r}} | \psi \rangle \simeq \mathbf{S} \int d\mathbf{r} \rho_s(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}}$$



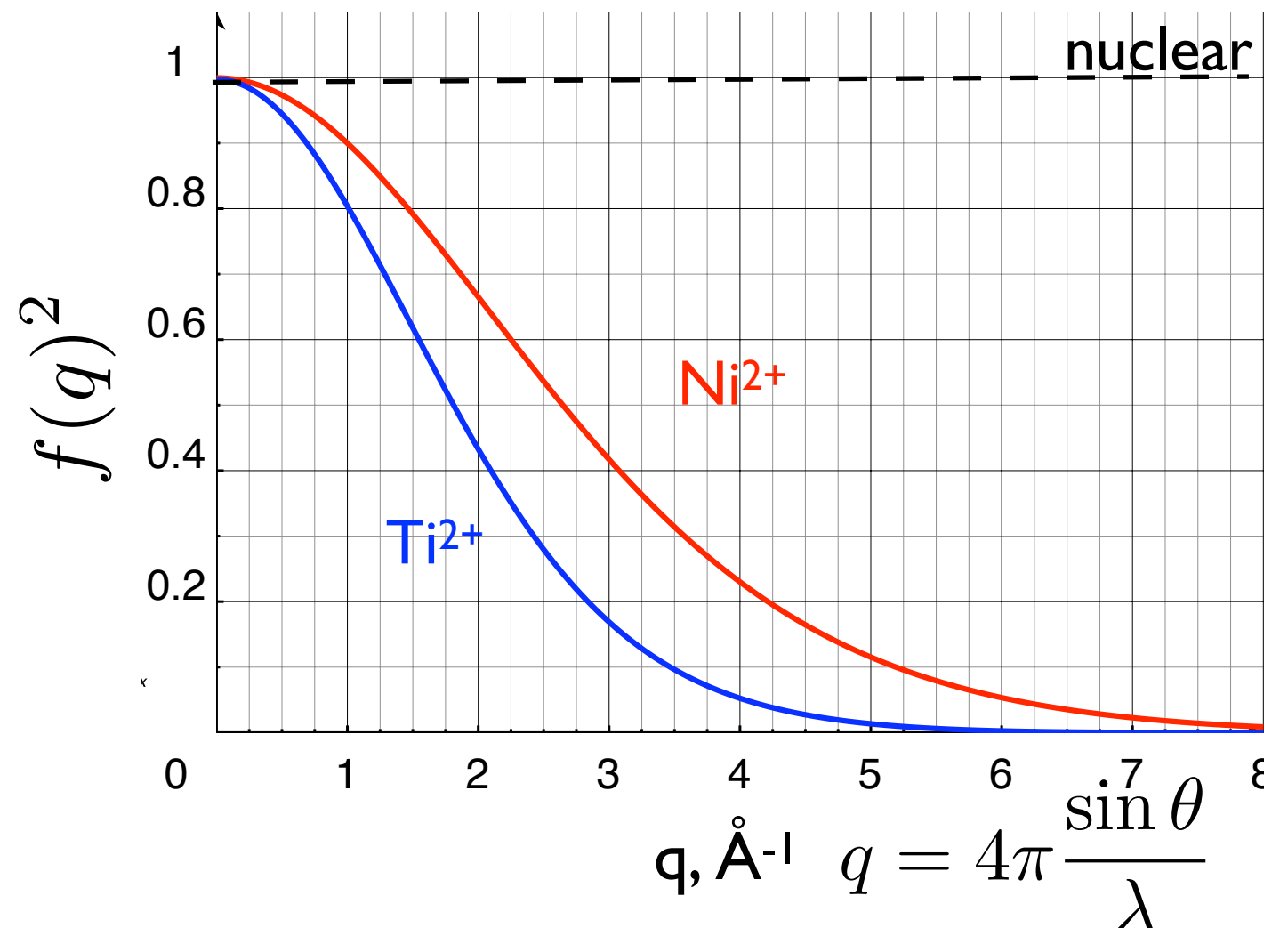
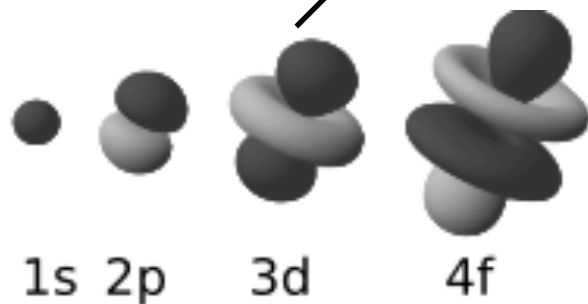
Magnetic neutron scattering on an atom

2. q-dependence

“magnetic scattering amplitude” = $\gamma r_e \langle \hat{\mathbf{Q}}_{\perp} \rangle$,

Fourier image of the spin density in atom
or magnetic form-factor

$$\langle \hat{\mathbf{Q}} \rangle = \langle \psi | \hat{\mathbf{s}} e^{i\mathbf{q}\mathbf{r}} | \psi \rangle \simeq \mathbf{S} \int d\mathbf{r} \rho_s(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}} = \mathbf{S} f(q)$$



Magnetic neutron scattering on an atom

$$\text{“magnetic scattering amplitude”} = \gamma r_e \langle \hat{\mathbf{Q}}_{\perp} \rangle$$

$$\mathbf{Q}_{\perp} = \tilde{\mathbf{q}} \times \mathbf{Q} \times \tilde{\mathbf{q}} = [\tilde{\mathbf{q}} \times \mathbf{S} \times \tilde{\mathbf{q}}] f(q)$$

$$\tilde{\mathbf{q}} = \mathbf{q}/q$$

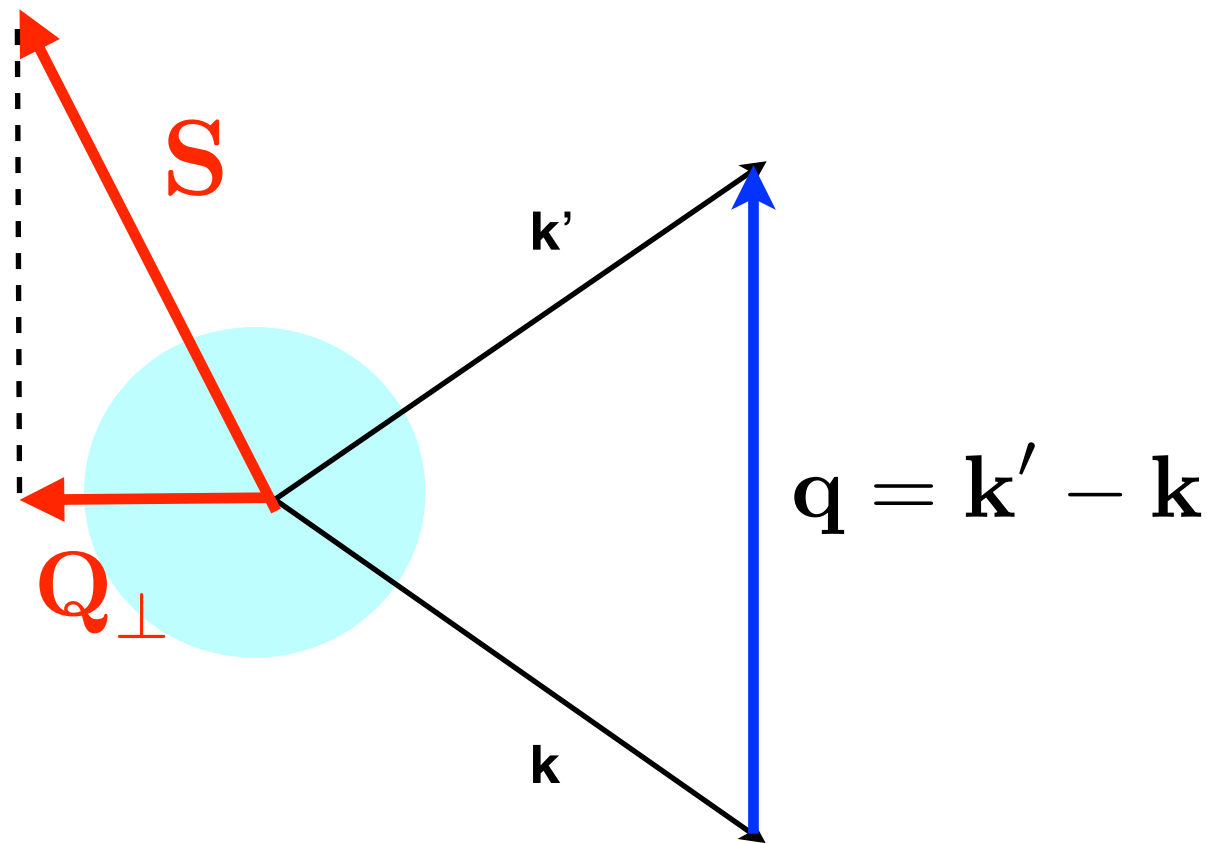
Magnetic neutron scattering on an atom

3. geometry

“magnetic scattering amplitude” = $\gamma r_e \langle \hat{\mathbf{Q}}_{\perp} \rangle$

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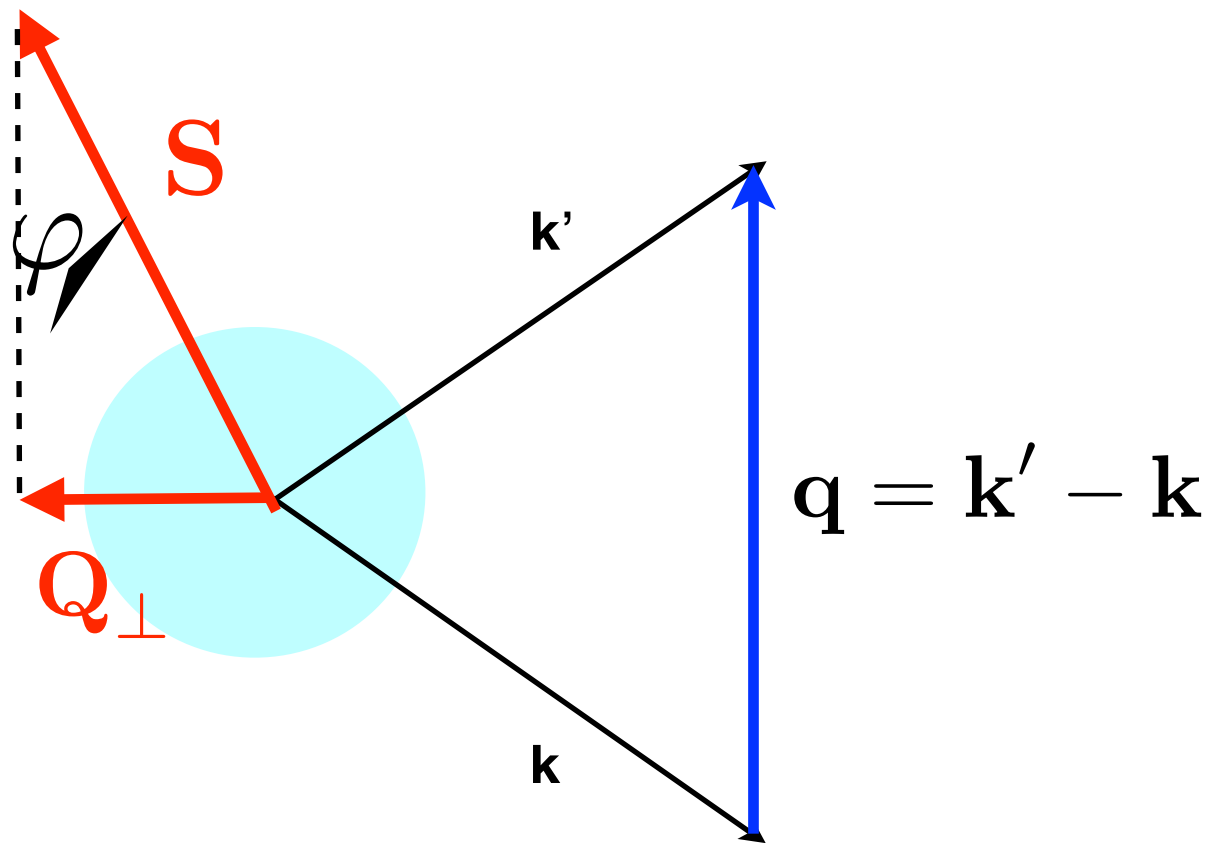
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$$|\mathbf{Q}_{\perp}| = |\mathbf{S}| \sin(\varphi)$$

Elastic scattering intensity

Neutron scattering cross-section (for unpolarised neutron beam)

$$\frac{d\sigma}{d\Omega} \propto | \langle \hat{\mathbf{Q}}_{\perp} \rangle |^2$$

Magnetic order parameters overview

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Term **FerroMagnetism (FM)**: lodestone in Greek writings by the year 800 B.C., magnetit $\text{FeO-Fe}_2\text{O}_3$ used as compass. First “theory” Rene Descartes (1596-1650)



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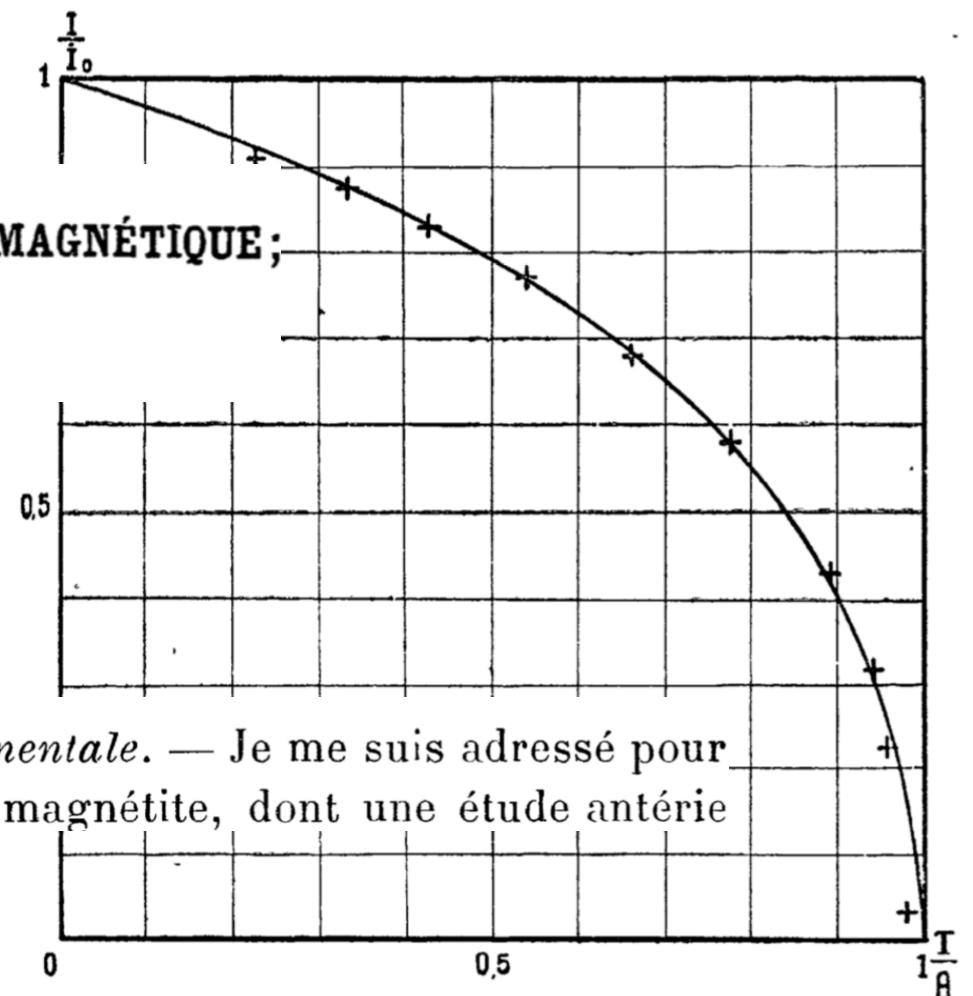


Order parameter: FM seen macroscopically

L'HYPOTHÈSE DU CHAMP MOLÉCULAIRE ET LA PROPRIÉTÉ FERROMAGNÉTIQUE;

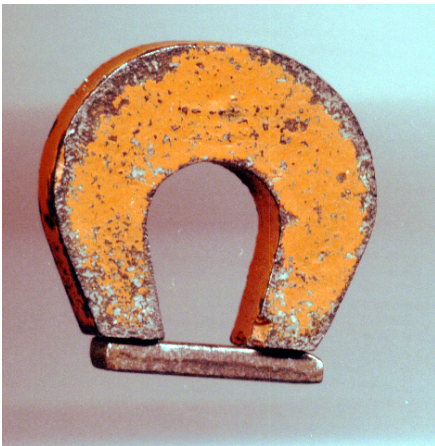
Par M. PIERRE WEISS ⁽¹⁾.

Submitted on 1 Jan 1907



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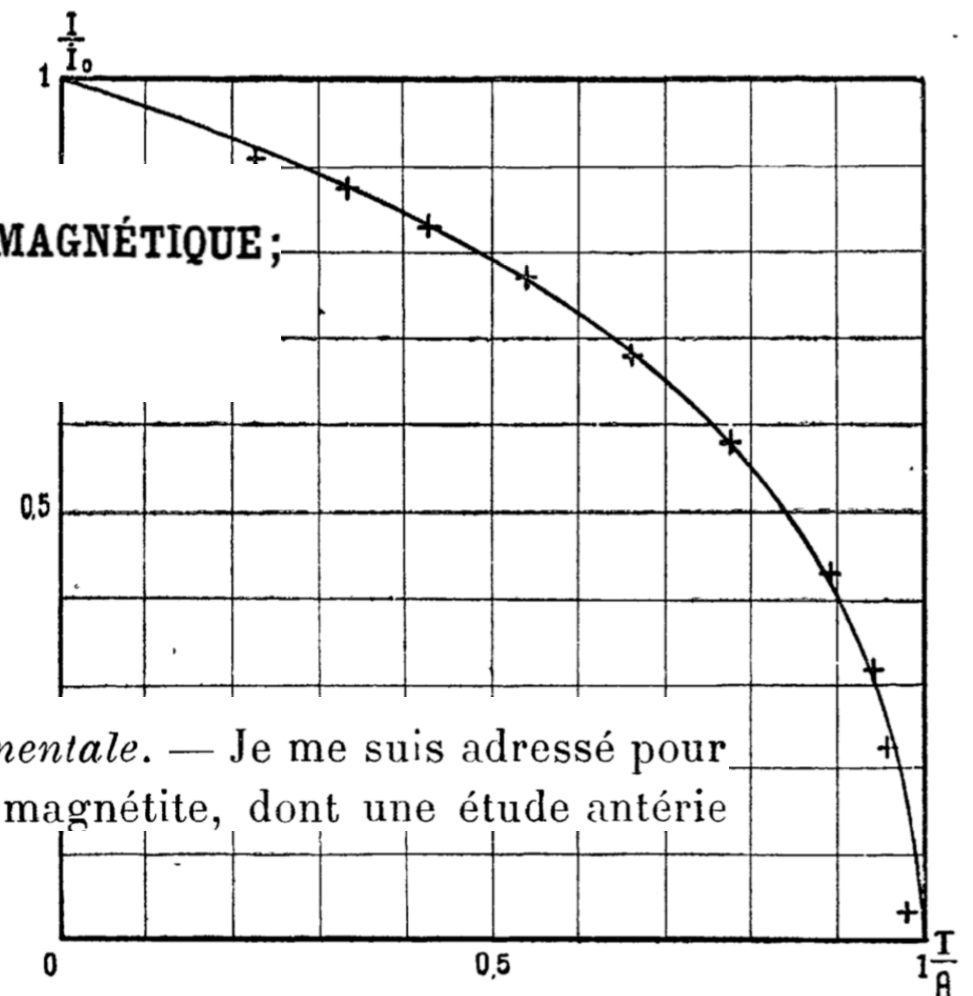
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FM is not possible in classical physics! Bohr–van Leeuwen theorem was discovered by Niels Bohr in 1911 in his doctoral dissertation

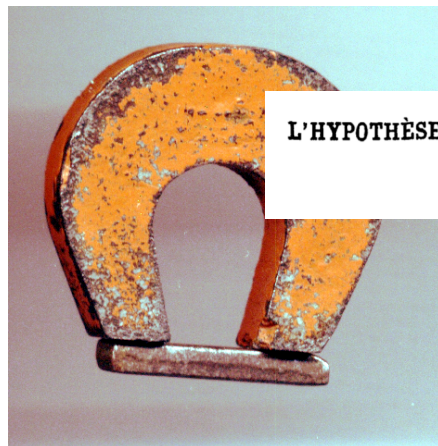
QM 1925-27



Magnetic order parameters overview

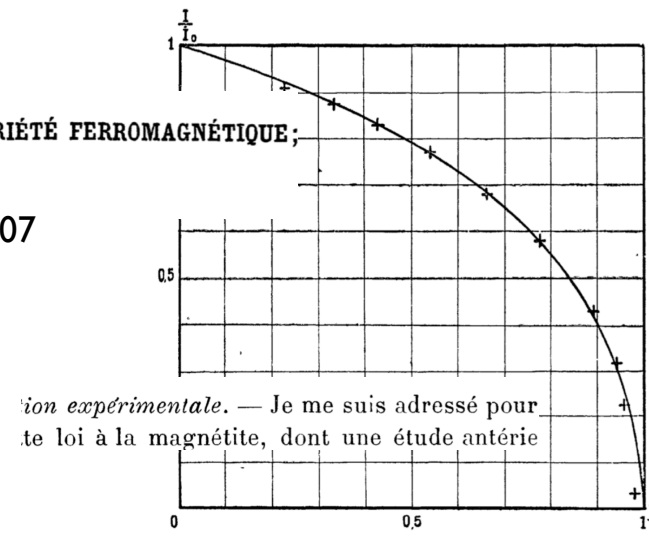
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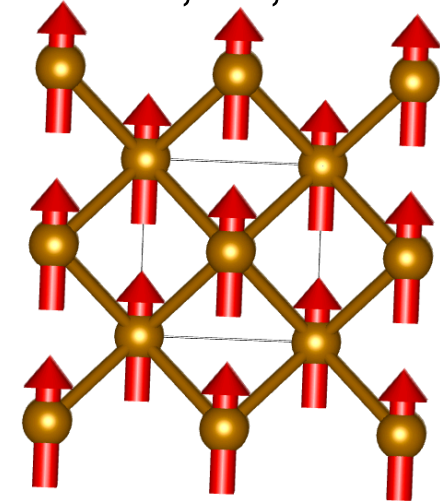


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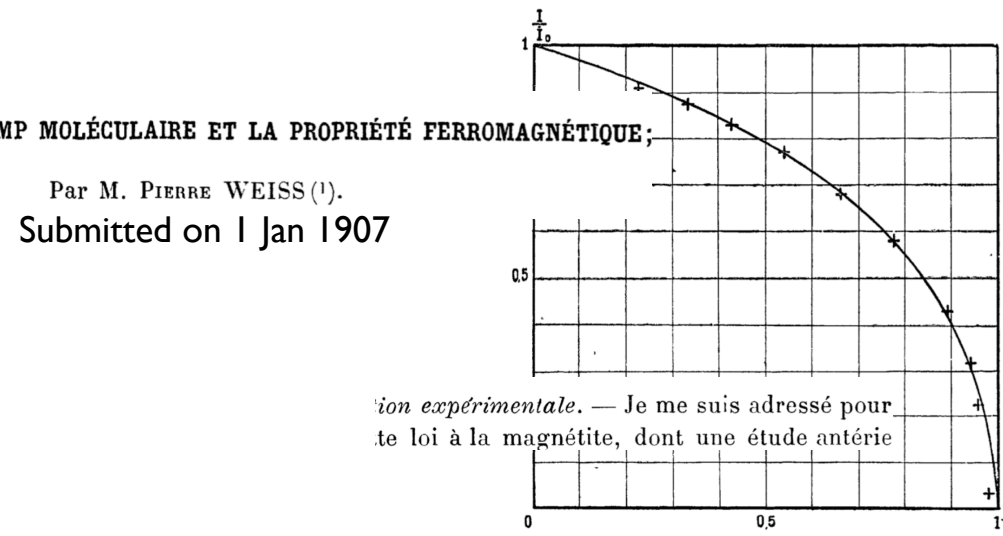
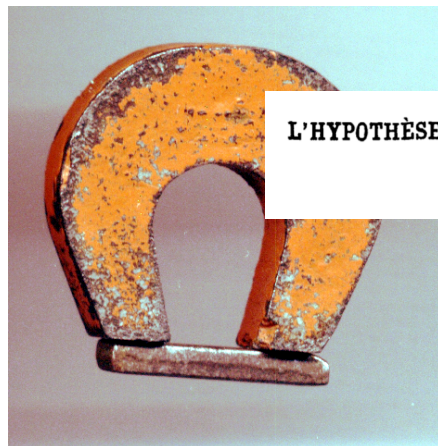
bcc iron, Fe, $I4/m\bar{m}'m'$



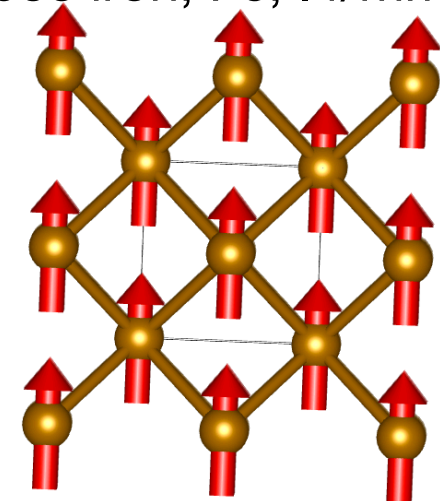
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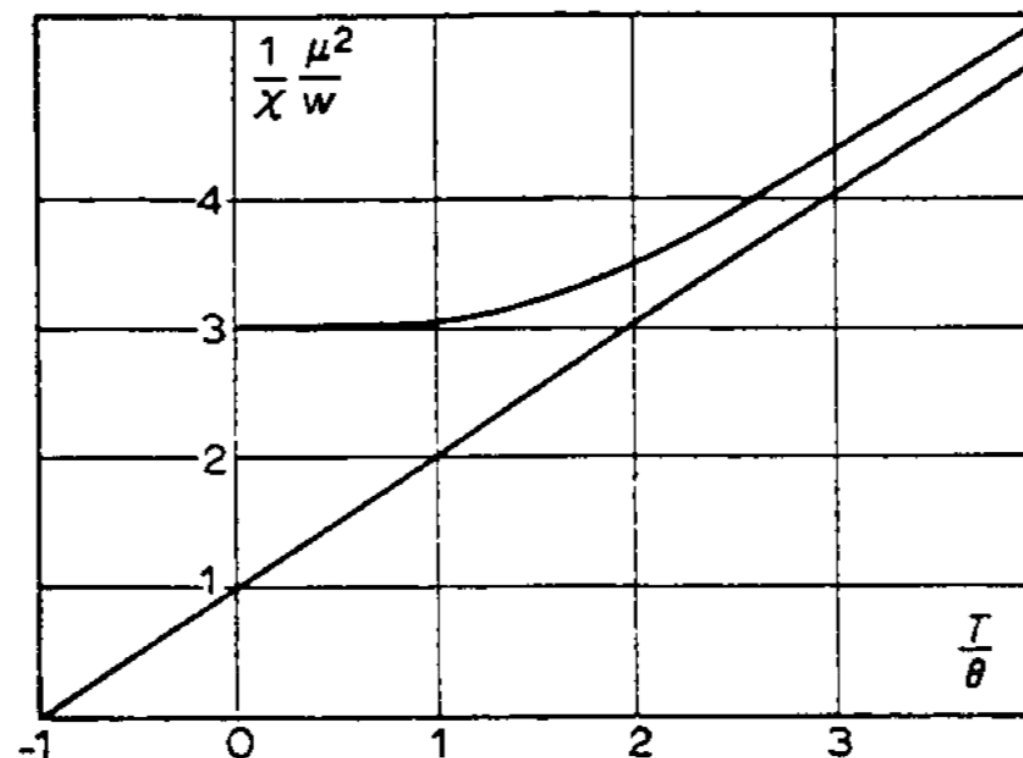
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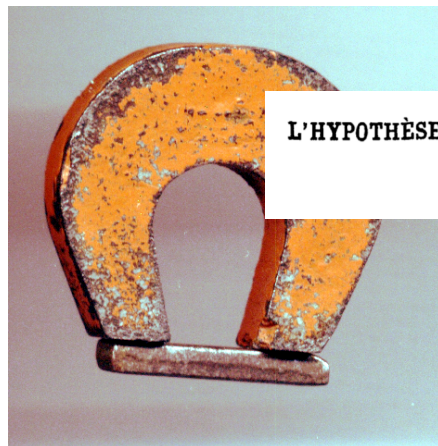
AntiFerroMagnetism (AFM): In 1932, Néel put forward the idea of antiferromagnetism to explain the temperature independent paramagnetic susceptibility of such metals as Cr and Mn



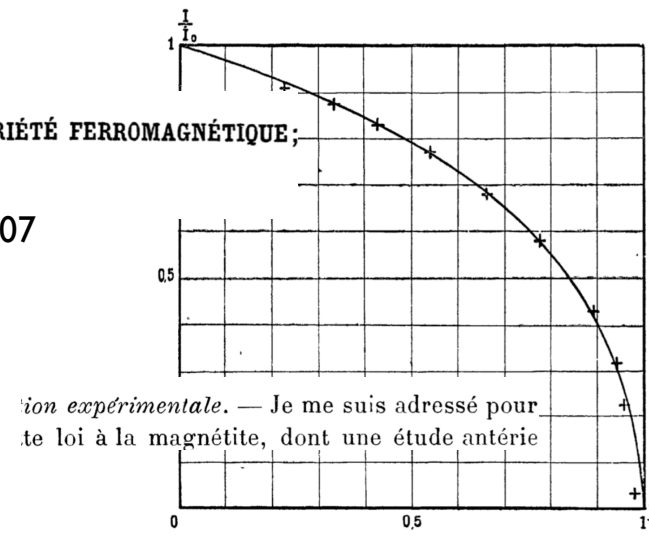
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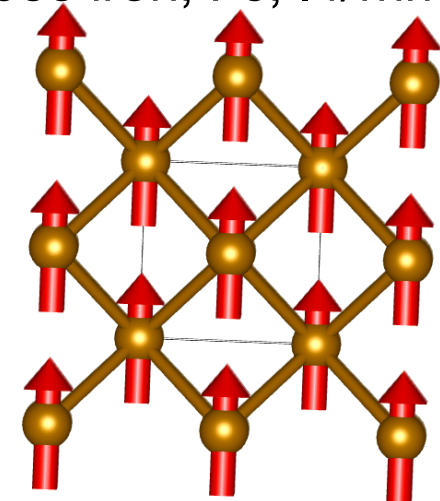
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Par M. PIERRE WEISS (1).
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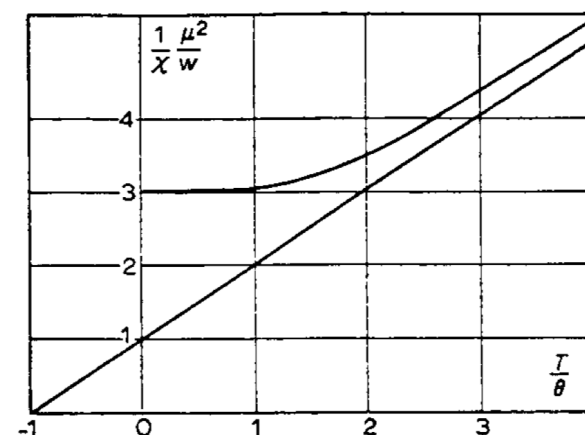
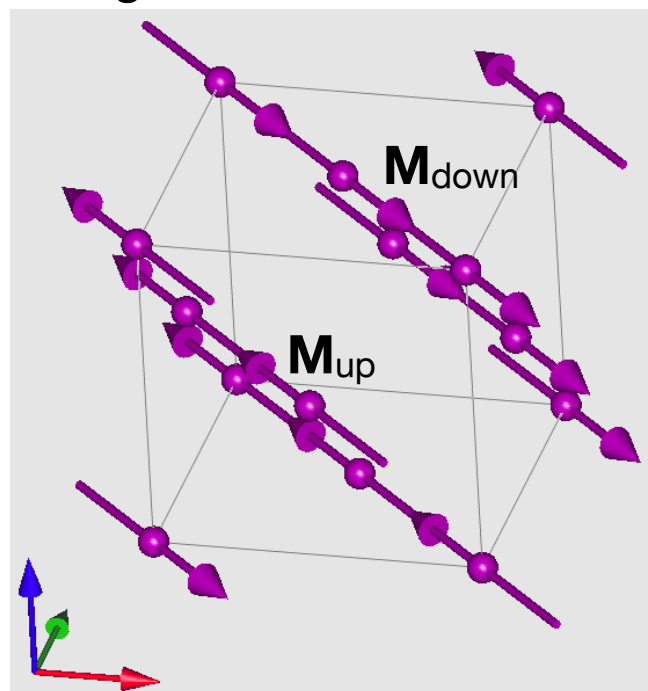
bcc iron, Fe, I4/mmm'



AntiFerroMagnetism (AFM): In 1932, Néel put forward the idea of antiferromagnetism to explain the temperature independent paramagnetic susceptibility of such metals as Cr and Mn

bcc MnO, MnS, Fm-3m,
magnetic C₂/c

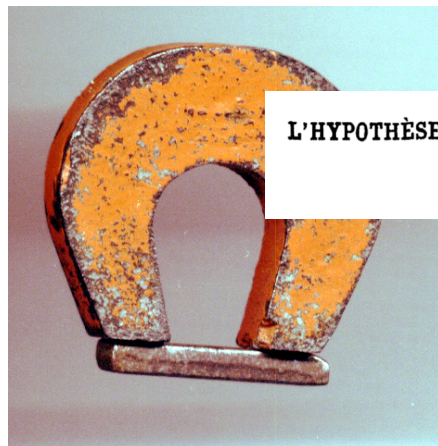
Order parameter: sub-lattice
magnetisations $\mathbf{M}_{\text{up}}$ $\mathbf{M}_{\text{down}}$ are not
directly seen macroscopically



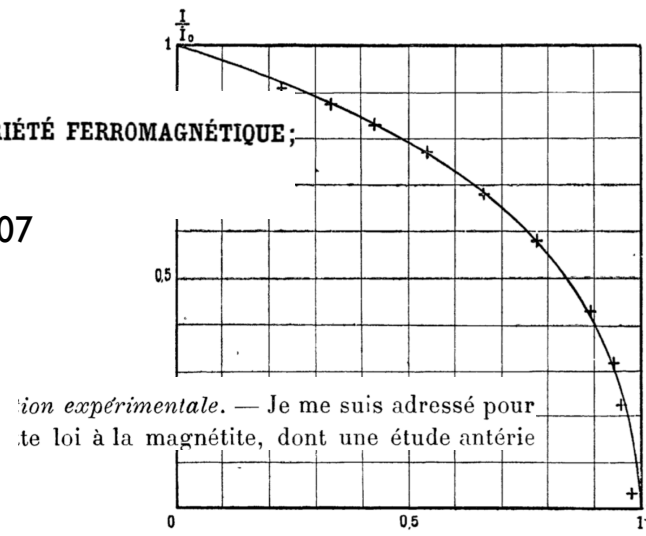
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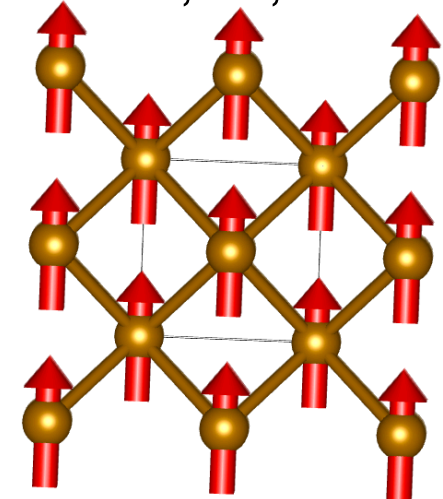
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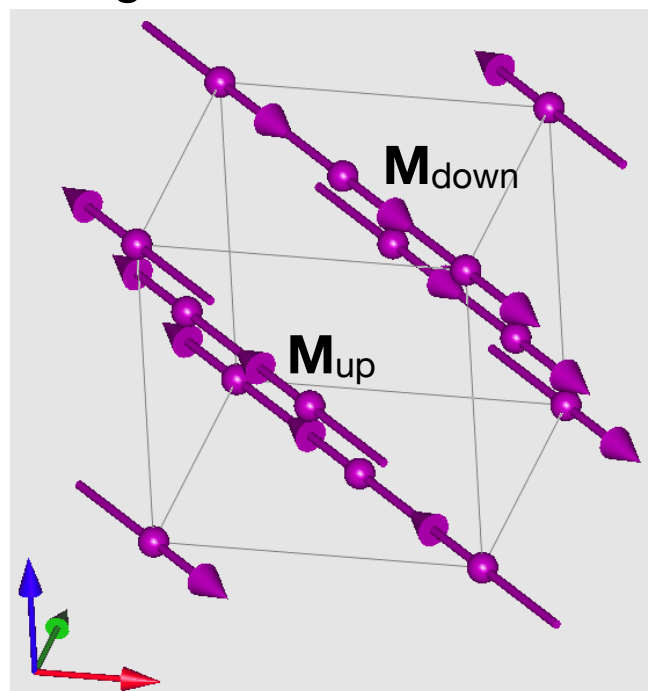


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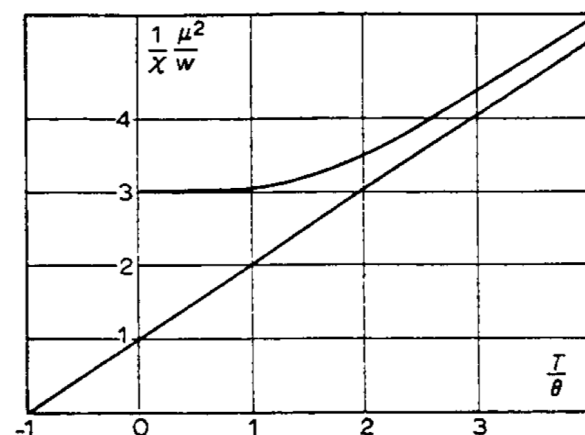


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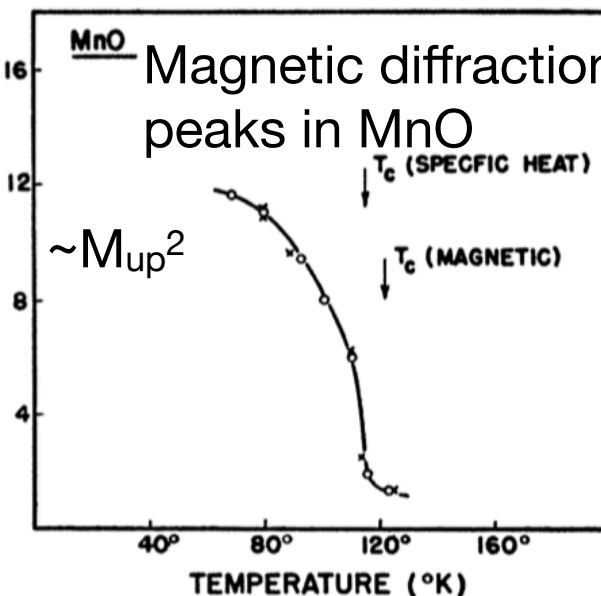
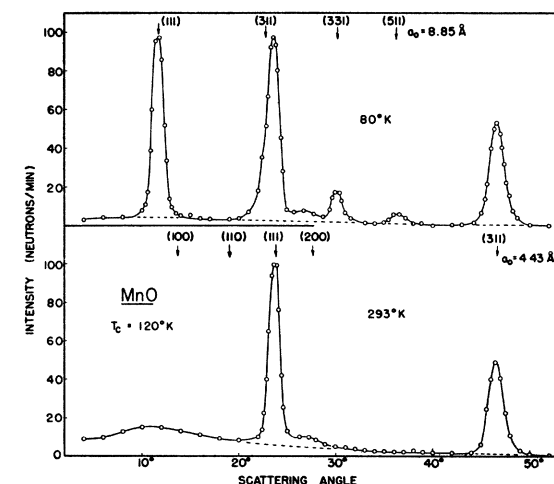
bcc MnO, MnS, $Fm\bar{3}m$,
magnetic C_2/c



Order parameter: sub-lattice magnetisations $\mathbf{M}_{up}$ $\mathbf{M}_{down}$ are not directly seen macroscopically

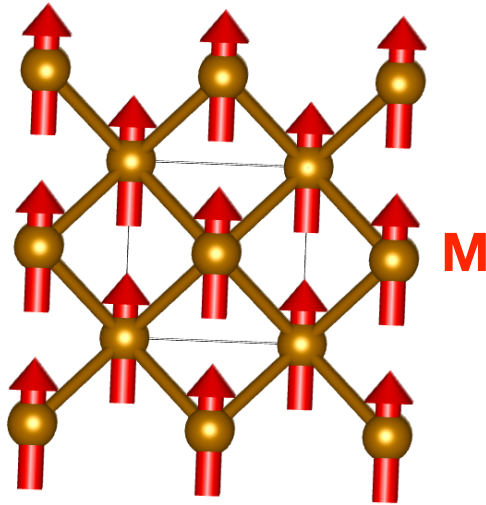


Neutron diffraction: one of the direct techniques
Shull, et al 1951

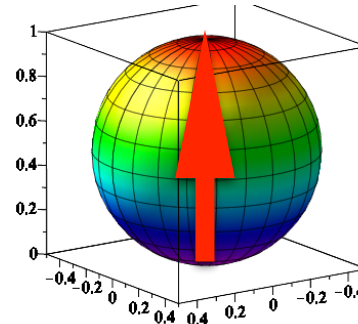


Magnetic order parameters overview

FerroMagnetism (FM), AntiFerroMagnetism (AFM), Ferrimagnetism, ...



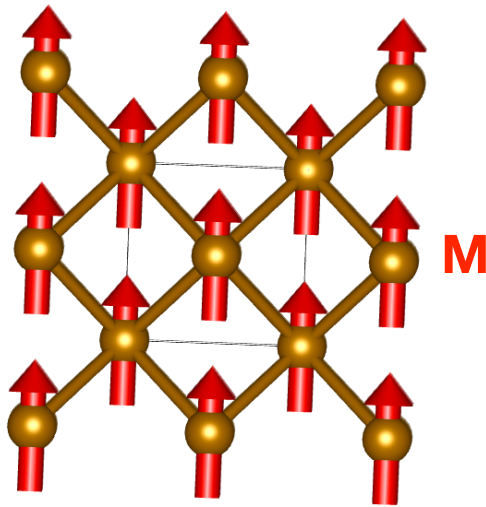
Order parameter is a magnetic moment of the atom: an axial vector **M: dipole, or tensor of rank 1: M_i , $i=1..3$**



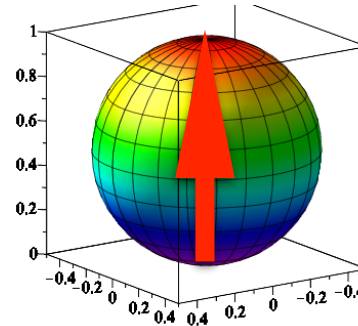
spherically symmetric
distribution of moment
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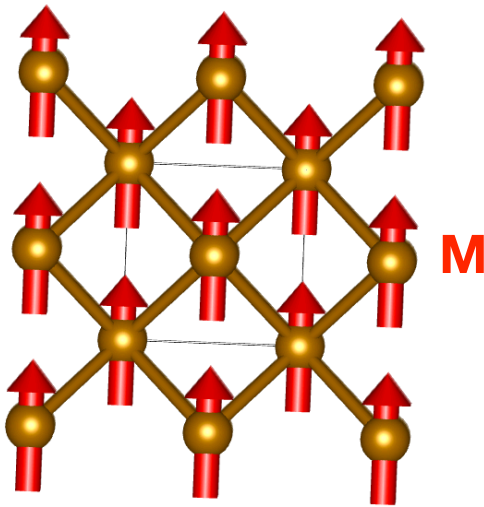


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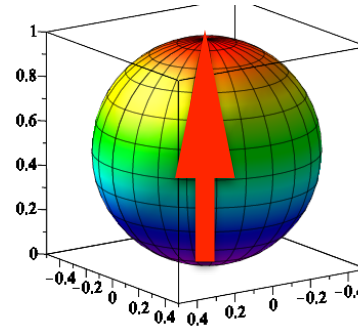
If M is small or zero: Can we have another magnetic order parameter?

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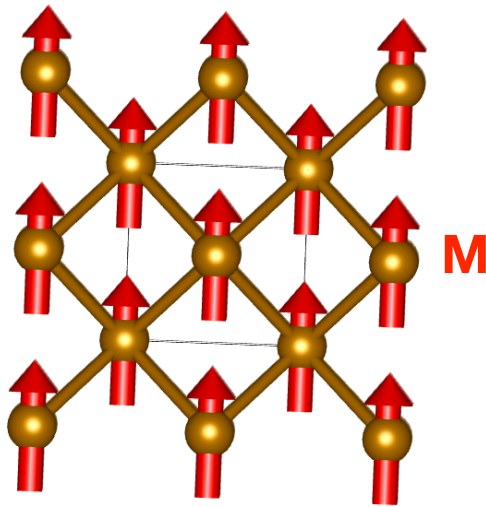
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Yes we can! We can have ordering of **multipoles, or tensors of rank >1 : $M_{ijk}...$**

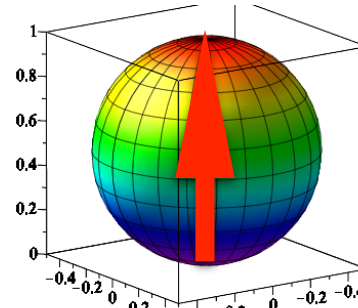
Deviations from spherically symmetric
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quadrupole, octupole, ...

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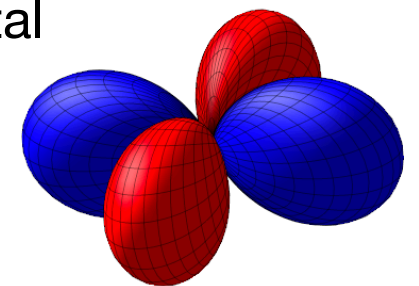
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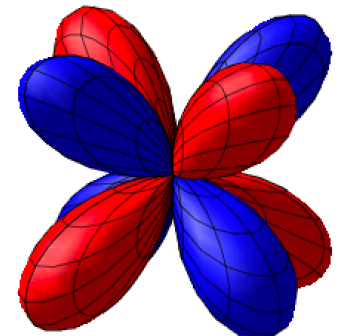
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Deviations from spherically symmetric distribution of moment density: quadrupole, octupole, ...

d-orbital
 Y_{22}



f-orbital
 Y_{32}



magnetic multipole moments: 3D-tensors of rank R

Dipole, tensor of rank $R=1$: $2^1=2$ charges



$$M_i = \sum_n S_{ni} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$i, j, k \dots = 1, 2, 3 (x, y, z)$
 n runs over all dipoles

nomenclature is Greek 2^R -numbers

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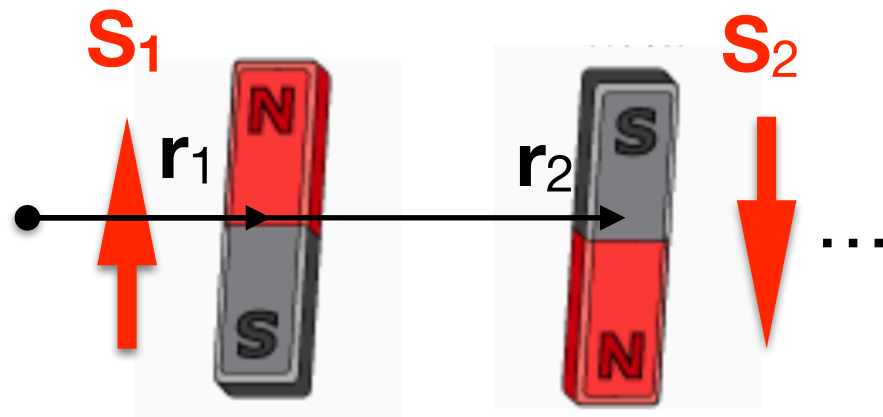


... n-dipoles

$$M_i = \sum_n S_{ni} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

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Quadrupole, tensor of rank $R=2$: $2^R=2^2=4$ charges



$$M_{ij} = \sum_n S_{ni} r_{nj} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

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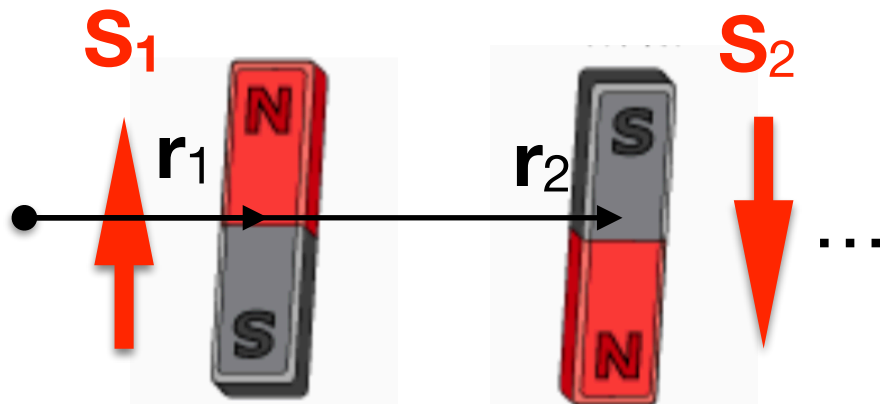


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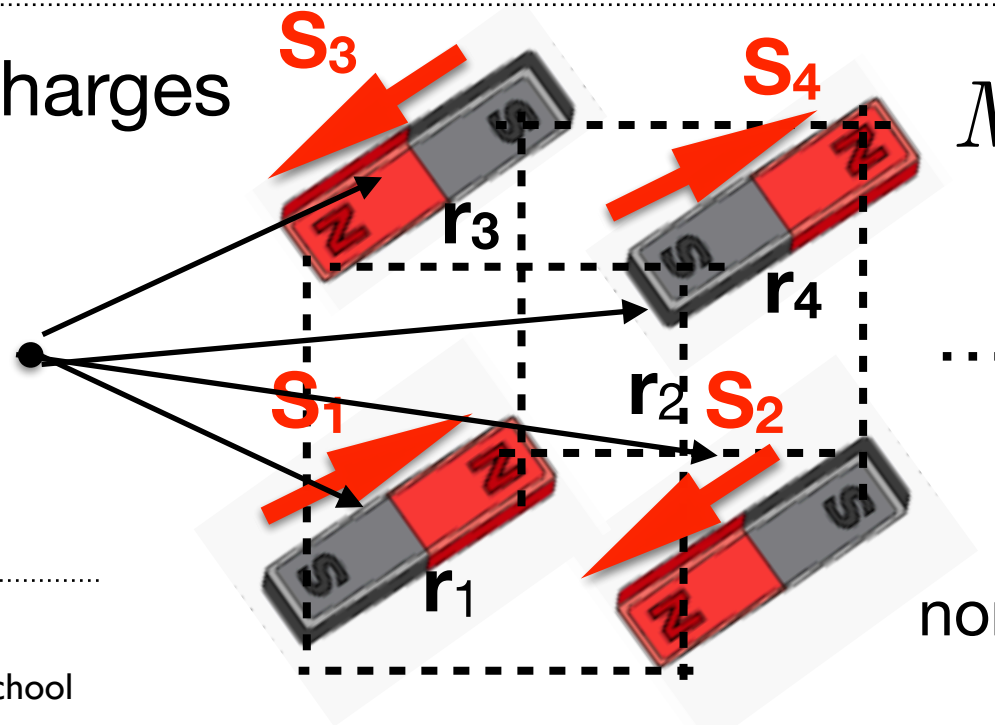
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Octupole, $R=3$: $2^3=8$ charges



$$M_{ijk} = \sum_n S_{ni} r_{nj} r_{nk}$$

Hexadecapole $R=4$...

nomenclature is Greek 2^R -numbers

Magnetic order parameters overview

Magnetic-octupoles ordering

PHYSICAL REVIEW B 72, 144401 2005

NpO₂

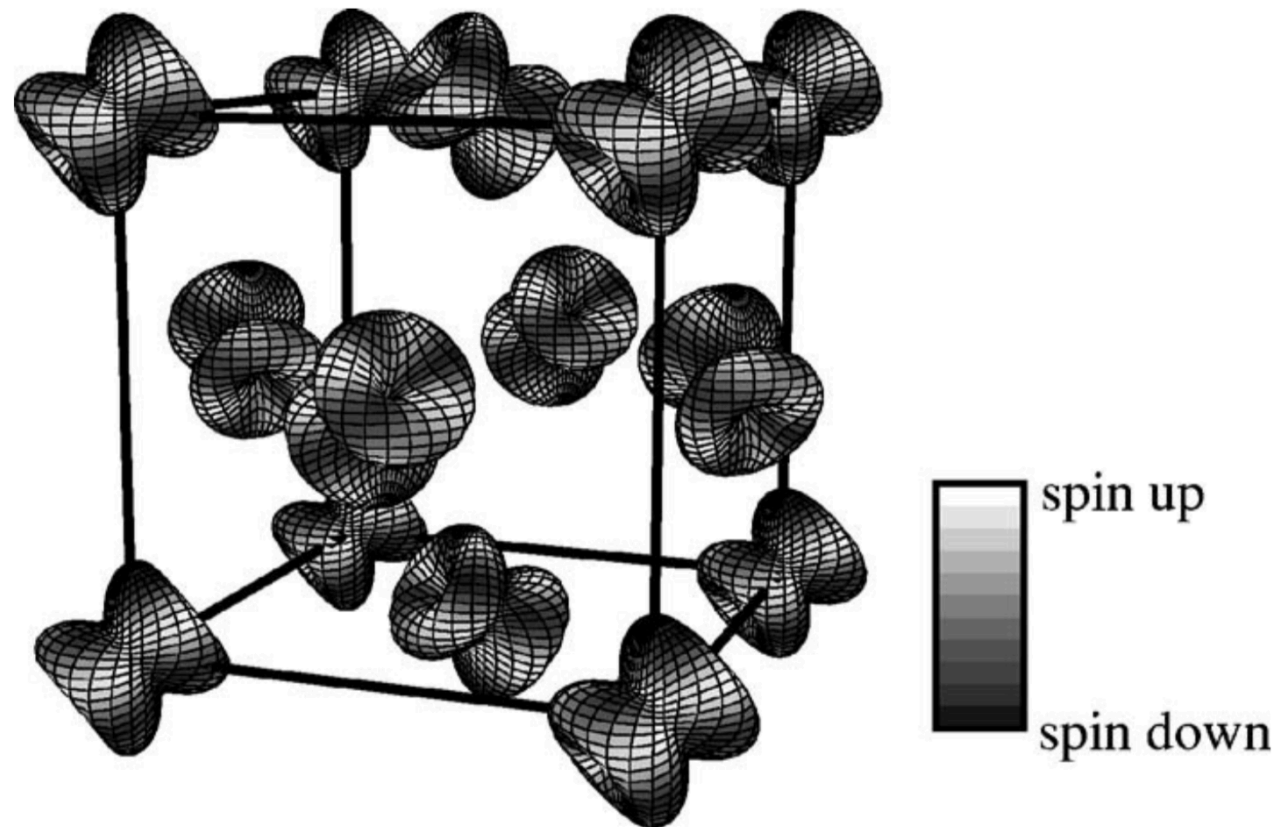


FIG. 7. The triple- $\mathbf{q}$ Γ_{5u} octupole state. The surface is defined by $S = [\sum_{\sigma} |\psi(\theta, \phi, \sigma)|^2]^{1/2}$ in the polar coordinates, when the $5f$ wave function is represented by $\Psi(r, \theta, \phi, \sigma) = R(r)\psi(\theta, \phi, \sigma)$, where σ denotes real spin. White shift of the surface indicates the increase of

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Magnetic-octupoles ordering

PHYSICAL REVIEW B 72, 144401 2005

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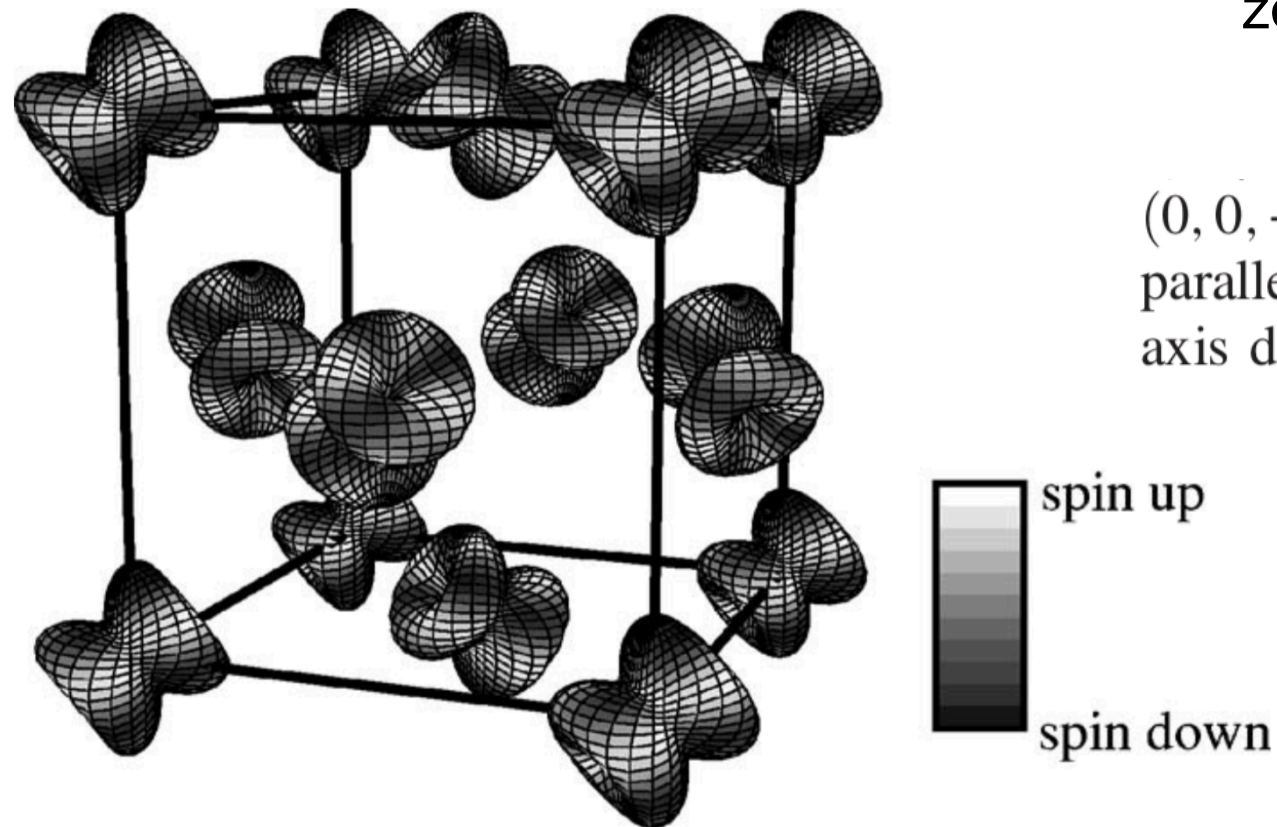
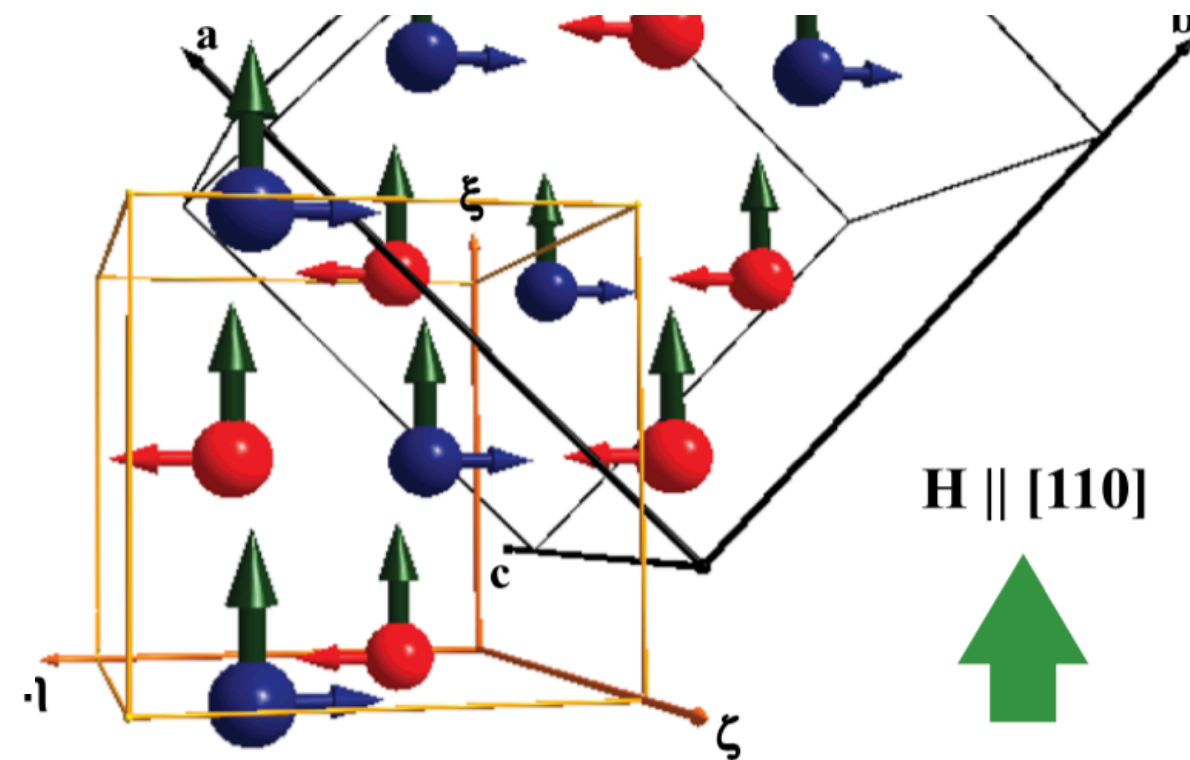


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New exotics!

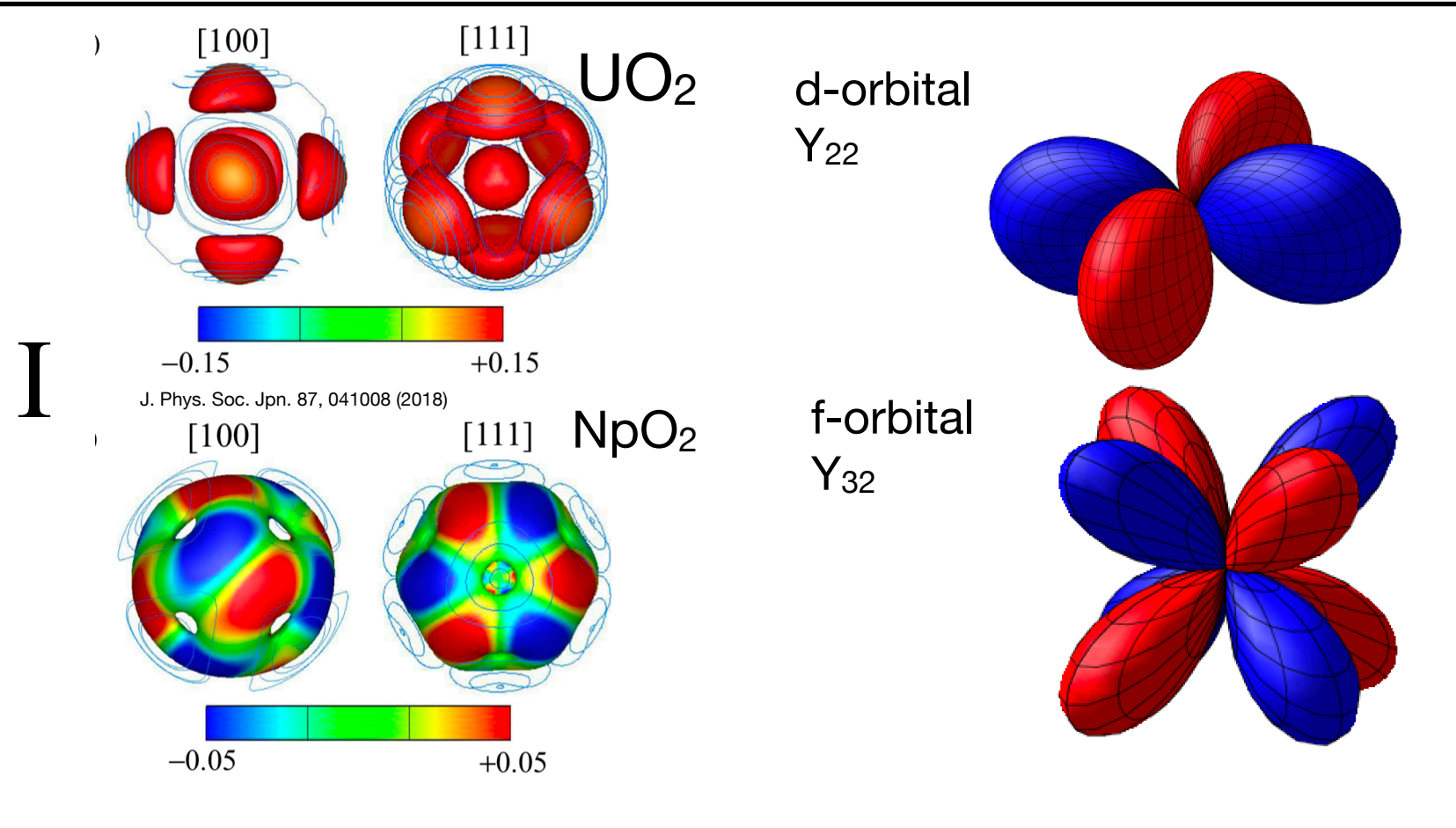
Dirac magnetoelectric dipole (anapole) in zero-magnetization ferromagnet Sm_{0.97}Gd_{0.02}Al₂
S W Lovesey et al PRL 122, 047203 (2019)

(0, 0, -1) outlined in yellow. Green arrows are axial dipoles parallel to the ξ axis, while blue and red arrows that lie along the η axis denote anapoles related by point inversion.



Magnetic objects neutrons sensitive to

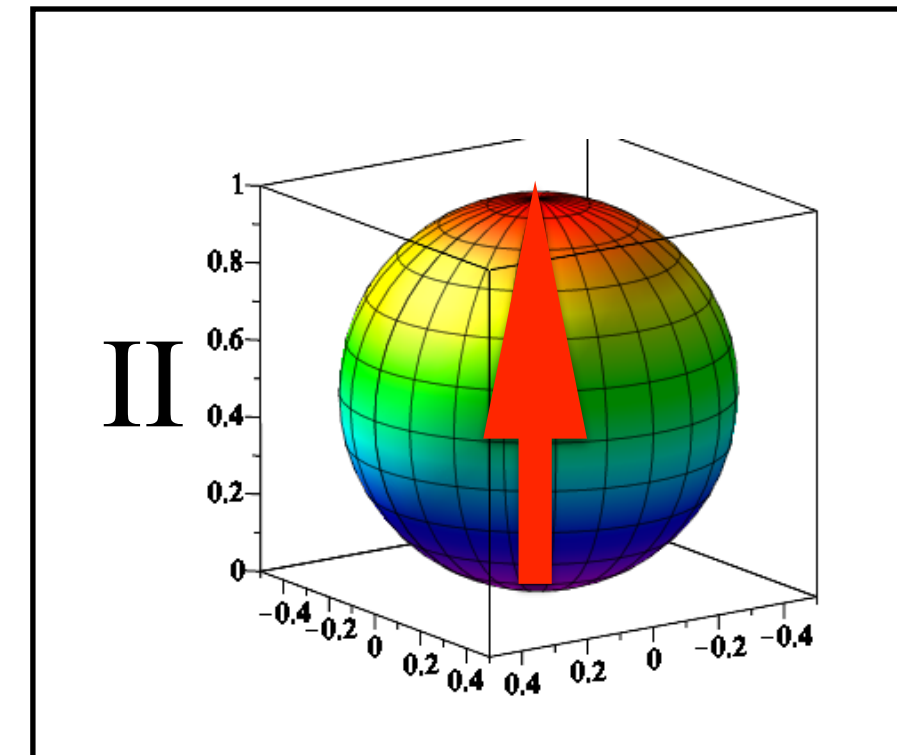
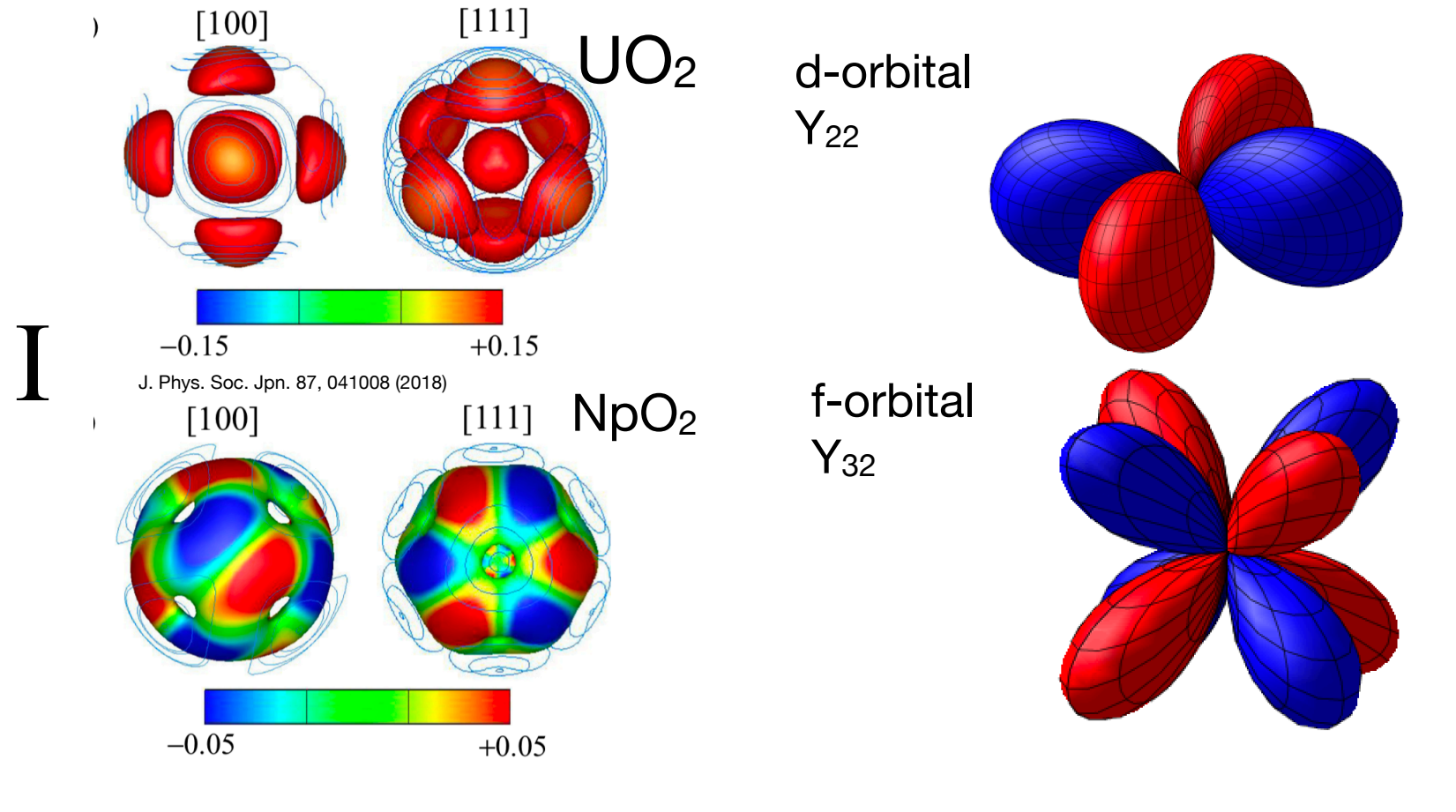
sketch of multipole expansion, octupoles



Magnetic objects neutrons sensitive to

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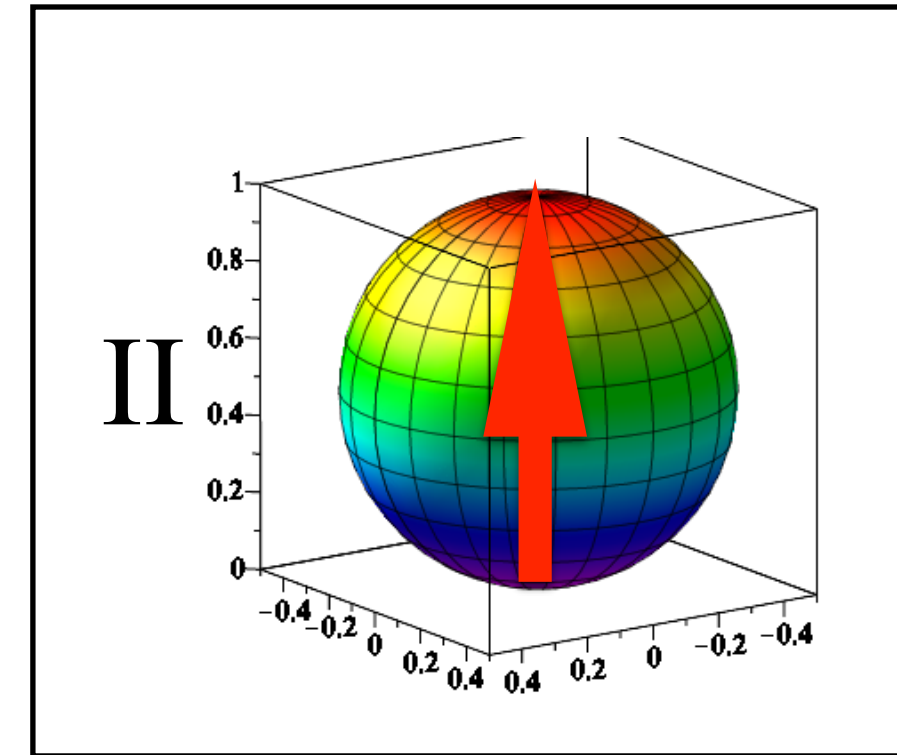
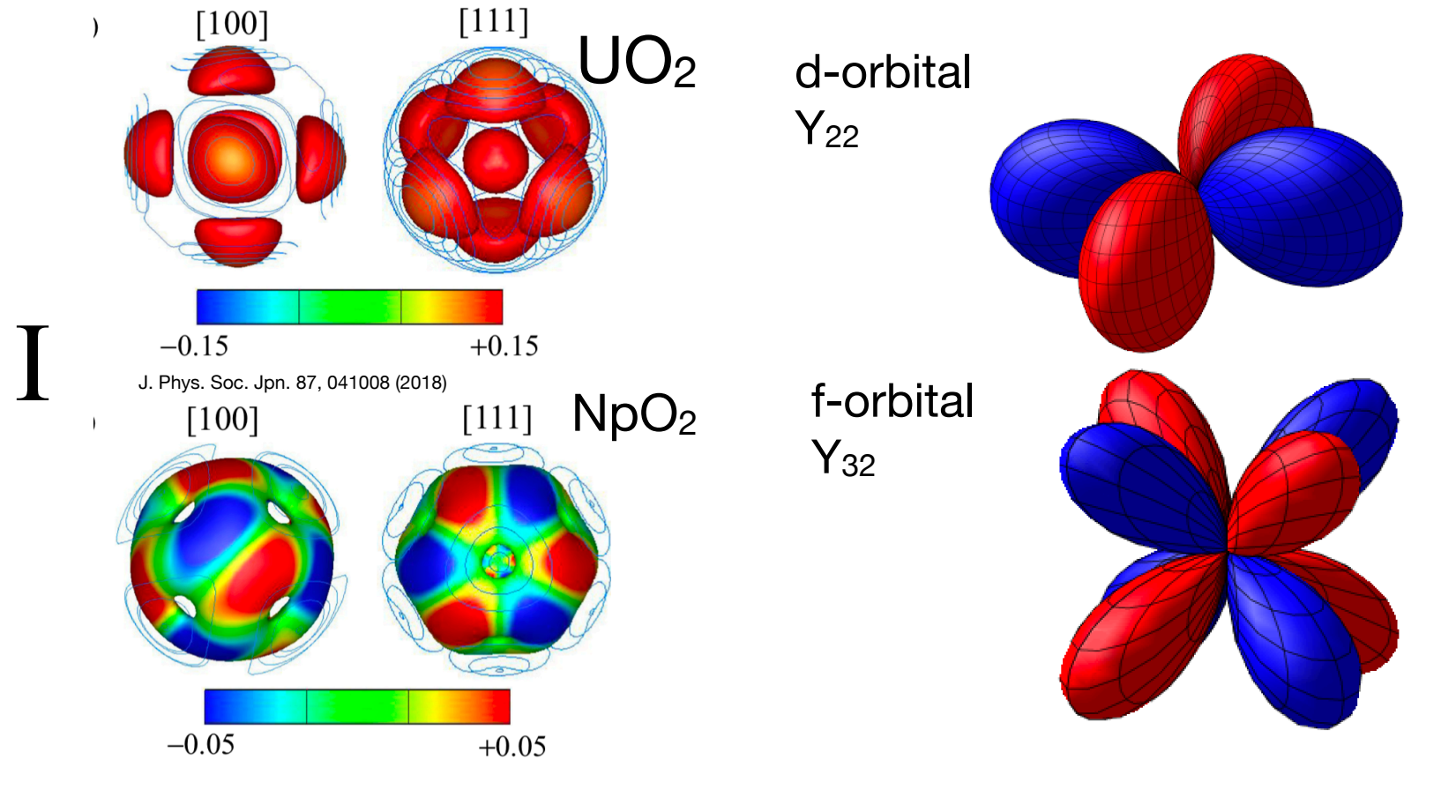
Dipole approximation



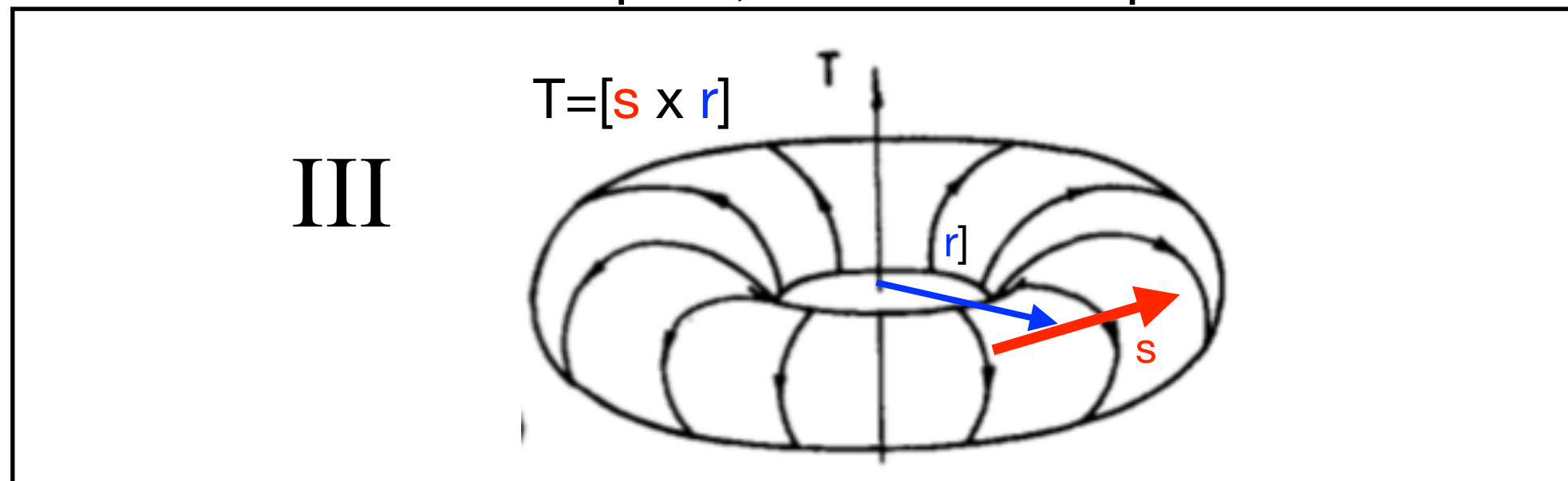
Magnetic objects neutrons sensitive to

sketch of multipole expansion, octupoles

Dipole approximation



anapole, toroidal multipole



Expansion of the scattering operator Q in powers of $(\mathbf{k} \cdot \mathbf{r})$. Splitting neutron and electron variables

We measure an expectation value of the scattering operator

$$Q_{\perp} = [\tilde{\kappa} \times Q \times \tilde{\kappa}]$$

electron neutron
↓ ↓
 $Q = \exp(i \mathbf{r} \cdot \mathbf{k}) [\mathbf{S} - (i/\hbar k)(\tilde{\kappa} \times \mathbf{p})], \quad \tilde{\kappa} = \mathbf{k}/k \text{ where } \mathbf{k} \text{ is the neutron scattering wavevector}$
spin momentum $\rightarrow L$

expectation value of Q is $\langle Q \rangle \equiv \langle \psi_{ATOM} | Q | \psi_{ATOM} \rangle$

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mathematical difficulty is related to the expansion of the exponent and further calculus

$$\exp(\mathbf{k} \cdot \mathbf{r}) = 4\pi \sum_{L=0}^{\infty} \sum_{M=-L}^L i^L j_L(\kappa r) Y_M^L(\Omega_r) Y_M^{L*}(\Omega_k),$$

will give
multipoles

use of Racah tensor-algebra, is required S.W. Lovesey, "Theory of Neutron Scattering from Condensed Matter", Oxford Univ. Press, 1987

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expectation value of Q is $\langle Q \rangle \equiv \langle \psi_{ATOM} | Q | \psi_{ATOM} \rangle$

We expand in powers of $(\mathbf{k} \cdot \mathbf{r})$, (i.e. Y_{L0})

$$e^{-i\kappa \cdot \mathbf{r}} = \sum_{n=0}^{\infty} (2n+1) (-i)^n j_n(\rho) P_n(\cos \theta)$$

$$\rho = \kappa r \text{ and } \cos \theta = \kappa \cdot \mathbf{r} / \rho,$$

Some mathematics...

Legendre polynomials

$$P_{n=0,1,2,3}(x) = \left[1, x, -\frac{1}{2} + \frac{3x^2}{2}, \frac{5}{2}x^3 - \frac{3}{2}x \right]$$

Spherical Bessel functions

$$j_{n=0,1,2}(x) = \left[\frac{\sin(x)}{x}, \frac{-\cos(x)x + \sin(x)}{x^2}, \frac{-\sin(x)x^2 - 3\cos(x)x + 3\sin(x)}{x^3} \right]$$

$$j_n(\rho) = \rho \{ j_{n-1}(\rho) + j_{n+1}(\rho) \} / (2n+1).$$

multipoles (parity even) Sketch of spin multipole expansion for $\mathbf{Q}$.

$$e^{-i\mathbf{\kappa} \cdot \mathbf{r}} = \sum_{n=0}^{\infty} (2n+1) (-i)^n j_n(\rho) P_n(\cos \theta) \quad \rho = \kappa r \text{ and } \cos \theta = \mathbf{\kappa} \cdot \mathbf{r} / \rho,$$

expansion $e^{-i\vec{k} \cdot \vec{r}}$ in powers of $(\vec{k} \cdot \vec{r})$

Legendre polynomials

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Spherical Bessel functions

$$j_{n=0,1,2}(x) = [\frac{\sin x}{x}, \cos x, -\frac{\sin x}{x}]$$

$$\langle \hat{Q}_i \rangle \approx \left(\underbrace{\hat{S}_i}_{\substack{\uparrow \\ \text{i-th component} \\ \text{of atom spin}}} \cdot \left(\dots j_0(\rho) + \dots \frac{1}{\rho^2} (\underbrace{\vec{k}}_{\substack{\uparrow \\ \text{neutron}}} \cdot \underbrace{\vec{r}}_{\substack{\uparrow \\ \text{atom}}})^2 j_2(\rho) + \dots \frac{1}{\rho^4} (\vec{k} \cdot \vec{r})^4 j_4(\rho) \dots \right) \right)$$

$\rho = |\vec{k}| |\vec{r}|$

multipoles (parity even) Sketch of spin multipole expansion for **Q**.

$$e^{-i\kappa \cdot \mathbf{r}} = \sum_{n=0}^{\infty} (2n+1) (-i)^n j_n(\rho) P_n(\cos \theta) \quad \rho = \kappa r \text{ and } \cos \theta = \kappa \cdot \mathbf{r} / \rho,$$

expansion $e^{-i\vec{k} \cdot \vec{r}}$ in powers of $(\vec{k} \cdot \vec{r})$

Legendre polynomials

$$P_{n=0,1,2,3}(x) = [1, x, \frac{3}{2}x^2 - \frac{1}{2}, \frac{5}{2}x^3 - \frac{3}{2}x]$$

Spherical Bessel functions

$$j_{n=0,1,2}(x) = [\frac{\sin x}{x}, \cos x, -\frac{\sin x}{x}]$$

$$\langle \hat{Q}_i \rangle \approx \left\langle \hat{\underline{S}}_i \cdot (\dots j_0(\rho) + \dots \frac{1}{\rho^2} (\underline{\vec{k}} \underline{\vec{r}})^2 j_2(\rho) + \dots \frac{1}{\rho^4} (\underline{\vec{k}} \underline{\vec{r}})^4 j_4(\rho) \dots) \right\rangle$$

i th component of atom spin

dipole

neutron

atom

$$\rho = |\underline{\vec{k}}| |\underline{\vec{r}}|$$

$$\langle \psi_{\text{atom}} | \hat{\underline{S}}_i | \psi_{\text{atom}} \rangle \langle j_0(\kappa) \rangle$$

$$\langle j_n(\kappa) \rangle = \int_0^\infty r^2 R^2(r) j_n(\kappa r) dr$$

multipoles (parity even) Sketch of spin multipole expansion for $\mathbf{Q}$.

$$e^{-i\mathbf{\kappa} \cdot \mathbf{r}} = \sum_{n=0}^{\infty} (2n+1) (-i)^n j_n(\rho) P_n(\cos \theta) \quad \rho = \kappa r \text{ and } \cos \theta = \mathbf{\kappa} \cdot \mathbf{r} / \rho,$$

Legendre polynomials

$$P_{n=0,1,2,3}(x) = [1, x, -\frac{3}{2}x^2 + \frac{1}{2}, \frac{5}{2}x^3 - \frac{3}{2}x]$$

Spherical Bessel functions

$$j_{n=0,1,2}(x) = [\frac{\sin x}{x}, \cos x, -\frac{\sin x}{x}]$$

expansion $e^{-i\mathbf{\tilde{k}} \cdot \mathbf{\tilde{r}}}$ in powers of $(\mathbf{\tilde{k}} \cdot \mathbf{\tilde{r}})$

$$\langle \hat{Q}_i \rangle \approx \left\langle \hat{\underline{S}}_i \cdot \left(\dots j_0(\rho) + \dots \frac{1}{\rho^2} (\mathbf{\tilde{k}} \cdot \mathbf{\tilde{r}})^2 j_2(\rho) + \dots \frac{1}{\rho^4} (\mathbf{\tilde{k}} \cdot \mathbf{\tilde{r}})^4 j_4(\rho) \dots \right) \right\rangle$$

$\uparrow$ $\uparrow$
*i*th component of atom spin neutron atom $\rho = |\mathbf{\tilde{k}}| |\mathbf{\tilde{r}}|$

$$\sum_{j \neq i} \underline{S}_i (\mathbf{\tilde{k}}_j \cdot \mathbf{\tilde{r}}_j) (\mathbf{\tilde{k}}_e \cdot \mathbf{\tilde{r}}_e) \cdot j_2(\rho)$$

$i, j, k = x, y, z$

$$\mathbf{\tilde{k}} = \mathbf{k}/k$$

$$\mathbf{\tilde{r}} = \mathbf{r}/r$$

we split neutron / atom

$$\langle Q_i \rangle \sim \sum_{j \neq i} (\mathbf{\tilde{k}}_j \mathbf{\tilde{k}}_e) \langle \psi_{\text{atom}} | \underline{S}_i \mathbf{\tilde{r}}_j \mathbf{\tilde{r}}_e | \psi_{\text{atom}} \rangle \langle j_2(k) \rangle$$

octupole

$$\langle Q_i \rangle \sim \sum_{j \neq i} (\mathbf{\tilde{k}}_j \mathbf{\tilde{k}}_e) \cdot \langle \hat{M}_{ije} \rangle \cdot \langle j_2(k) \rangle$$

contracting by $j \neq i \rightarrow \vec{Q}(|\vec{k}|, \Theta) \leftarrow \vec{k} \text{ octupole}$

Dipole approximation

We expand in powers of $(\mathbf{k} \cdot \mathbf{r})$, (i.e. Y_{L0})

$$e^{-i\boldsymbol{\kappa} \cdot \mathbf{r}} = \sum_{n=0}^{\infty} (2n+1) (-i)^n j_n(\rho) P_n(\cos \theta)$$

$$\simeq j_0(\rho) - 3i j_1(\rho) \cos \theta = \underbrace{j_0(\rho)}_{\text{even S}} - i\boldsymbol{\kappa} \cdot \mathbf{r} \underbrace{\{j_0(\rho) + j_2(\rho)\}}_{\text{odd L}}$$

$\rho = \kappa r$ and $\cos \theta = \boldsymbol{\kappa} \cdot \mathbf{r} / \rho$,

Dipole approximation

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$$e^{-i\mathbf{\kappa} \cdot \mathbf{r}} = \sum_{n=0}^{\infty} (2n+1) (-i)^n j_n(\rho) P_n(\cos \theta)$$

$$j_n(\rho) = \rho \{j_{n-1}(\rho) + j_{n+1}(\rho)\} / (2n+1).$$

$$\simeq j_0(\rho) - 3i j_1(\rho) \cos \theta = \boxed{j_0(\rho) - i\mathbf{\kappa} \cdot \mathbf{r} \{j_0(\rho) + j_2(\rho)\}}$$

$$\rho = \kappa r \text{ and } \cos \theta = \mathbf{\kappa} \cdot \mathbf{r} / \rho,$$

even S odd L

Dipole approximation

We expand in powers of ($\mathbf{k} \cdot \mathbf{r}$), (i.e. Y_{L0})

$$e^{-i\mathbf{\kappa} \cdot \mathbf{r}} = \sum_{n=0}^{\infty} (2n+1) (-i)^n j_n(\rho) P_n(\cos \theta)$$

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$$\rho = \kappa r \text{ and } \cos \theta = \mathbf{\kappa} \cdot \mathbf{r} / \rho,$$

even S odd L

$$\mathbf{Q} = \exp(i \mathbf{r} \cdot \mathbf{k}) [\mathbf{S} - (i/\hbar k)(\tilde{\mathbf{\kappa}} \times \mathbf{p})],$$

electron neutron
↓ ↓
spin momentum

is a term, which contains a linear combination of the spin and orbital angular moment of the magnetic ion, $\mathbf{S}$ and $\mathbf{L}$, respectively.

$$\frac{1}{2} \{ \langle j_0(\kappa) \rangle + \langle j_2(\kappa) \rangle \} \mathbf{1},$$

$$\boxed{\langle \mathbf{Q} \rangle = \frac{1}{2} \langle j_0(\kappa) \rangle (\mathbf{1} + 2\mathbf{s}) + \frac{1}{2} \langle j_2(\kappa) \rangle \mathbf{1}.}$$

$$\langle j_n(\kappa) \rangle = \int_0^{\infty} r^2 R^2(r) j_n(\kappa r) dr$$

$j_{n=0,1,2}(x) =$ Spherical Bessel functions

$$\left[\frac{\sin(x)}{x}, \frac{-\cos(x)x + \sin(x)}{x^2}, \frac{-\sin(x)x^2 - 3\cos(x)x + 3\sin(x)}{x^3} \right]$$

Examples of dipole and contribution to neutron scattering

assumed to be spin independent. In this case,

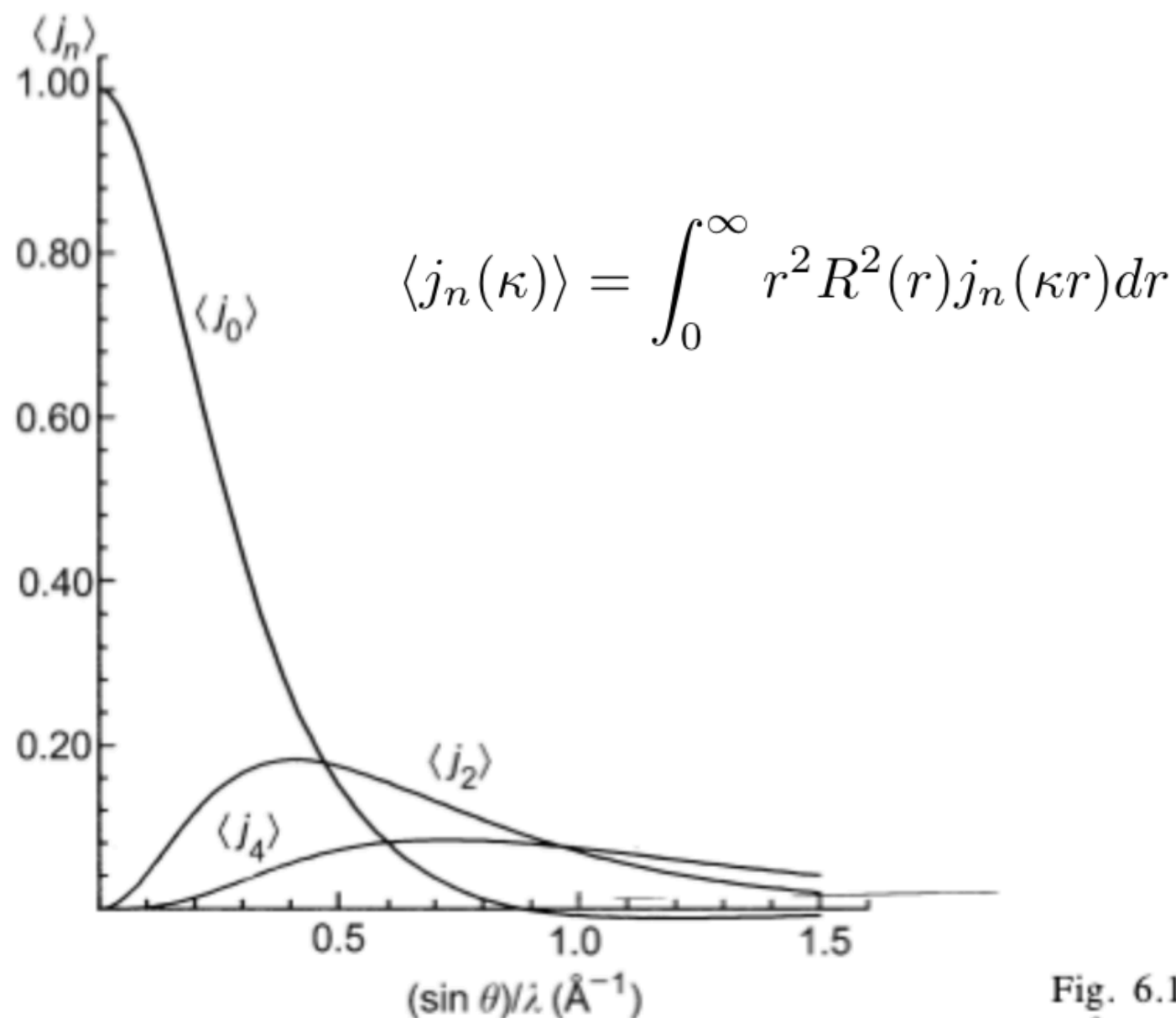


Fig. 6.1.2.1. The integrals $\langle j_0 \rangle$, $\langle j_2 \rangle$, and $\langle j_4 \rangle$ for the Fe²⁺ ion plotted against $(\sin \theta)/\lambda$. The integrals have been calculated from wavefunctions given by Clementi & Roetti (1974).

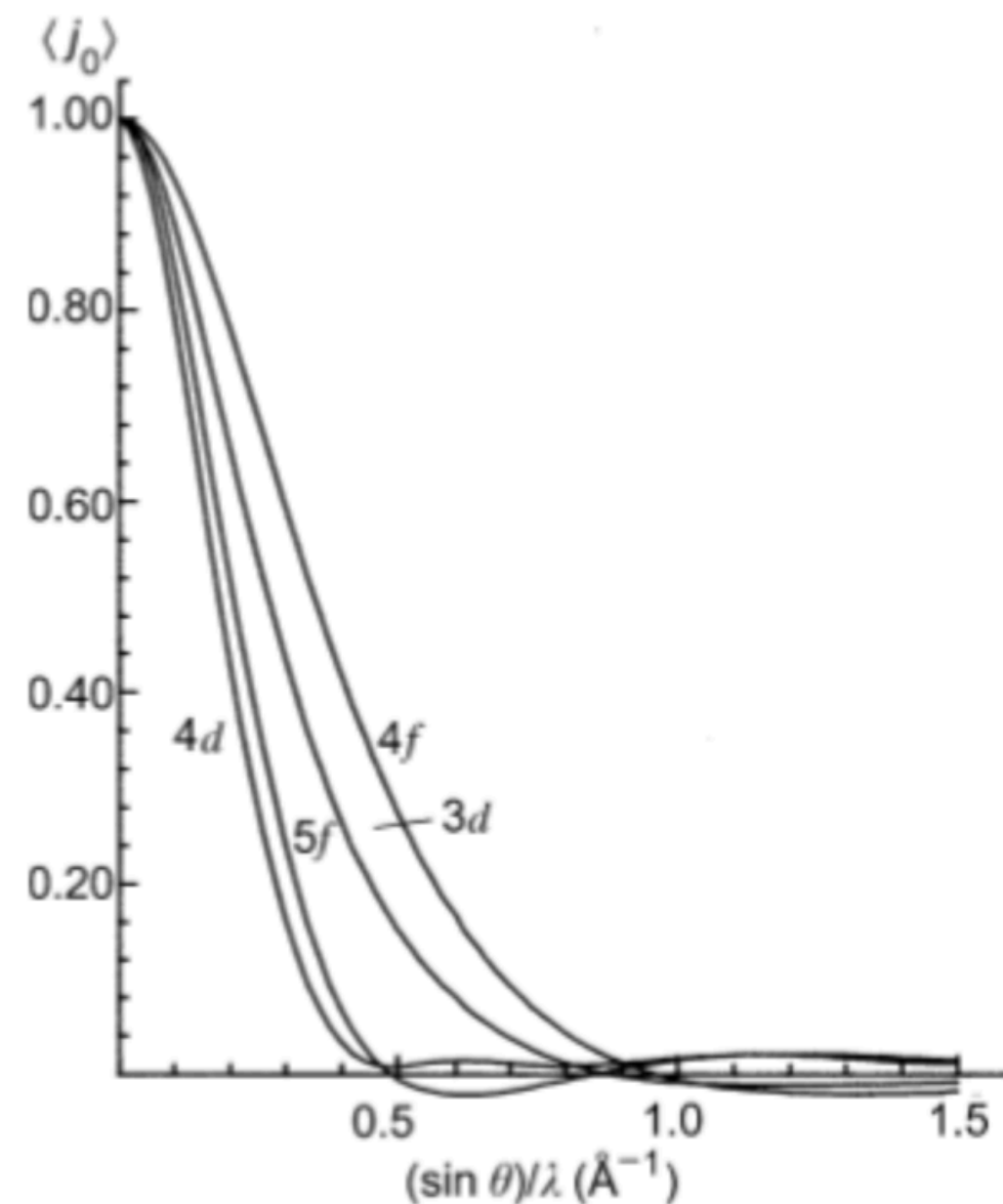
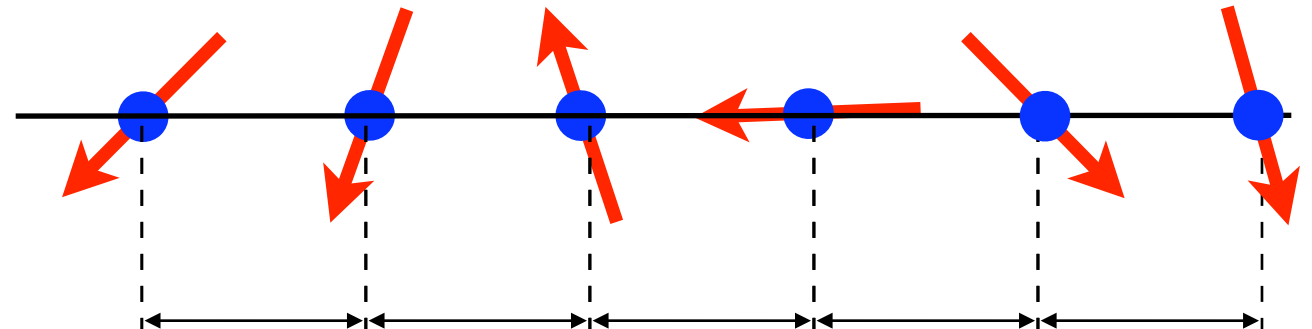


Fig. 6.1.2.2. Comparison of 3d, 4d, 4f, and 5f form factors. The 3d form factor is for Co, and the 4d for Rh, both calculated from wavefunctions given by Clementi & Roetti (1974). The 4f form factor is for Gd³⁺ calculated by Freeman & Desclaux (1972) and the 5f is that for U³⁺ given by Desclaux & Freeman (1978).

$$\text{Intensity} \sim \left| \frac{1}{2} \langle j_0(\kappa) \rangle (1 + 2s) + \frac{1}{2} \langle j_2(\kappa) \rangle 1 \right|^2$$

Experimental example of incoherent and coherent dipole magnetic scattering on a lattice of spins

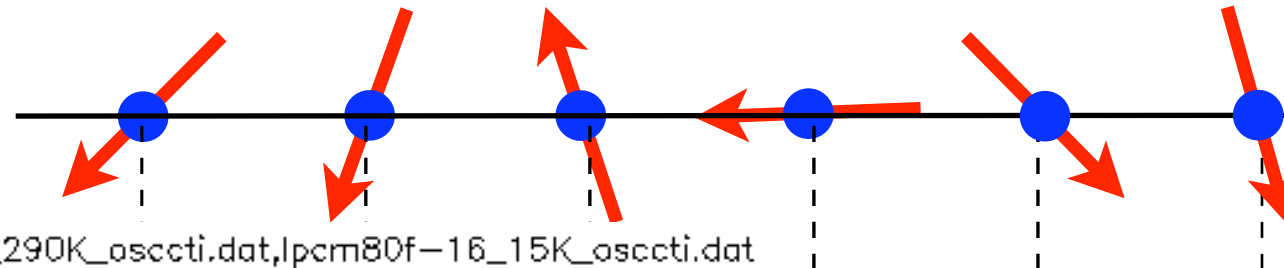
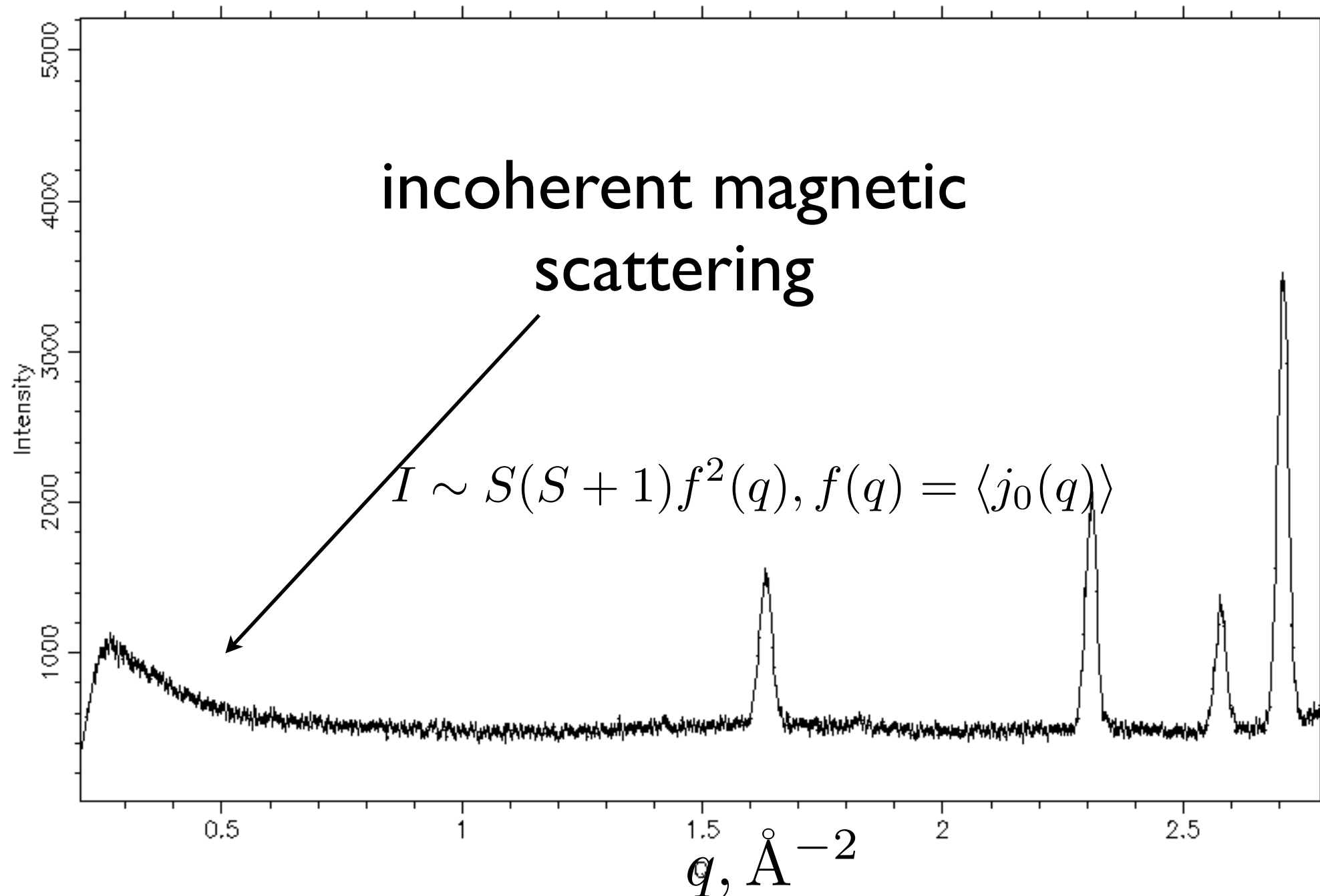
incoherent $I \sim \langle \hat{S}^2 \rangle = S(S + 1)$



The diagram illustrates a one-dimensional lattice of spins. A horizontal black line represents the lattice, with six blue circles placed at regular intervals along it. Each blue circle has a red arrow pointing in a different direction, representing the spin of the atom at that site. Below the lattice line, there are vertical dashed lines extending from each blue circle to a horizontal line. On this lower line, there are double-headed arrows indicating the distances between the vertical dashed lines, showing the periodicity of the lattice.

Experimental example of incoherent and coherent dipole magnetic scattering on a lattice of spins

incoherent $I \sim \langle \hat{S}^2 \rangle = S(S+1)$

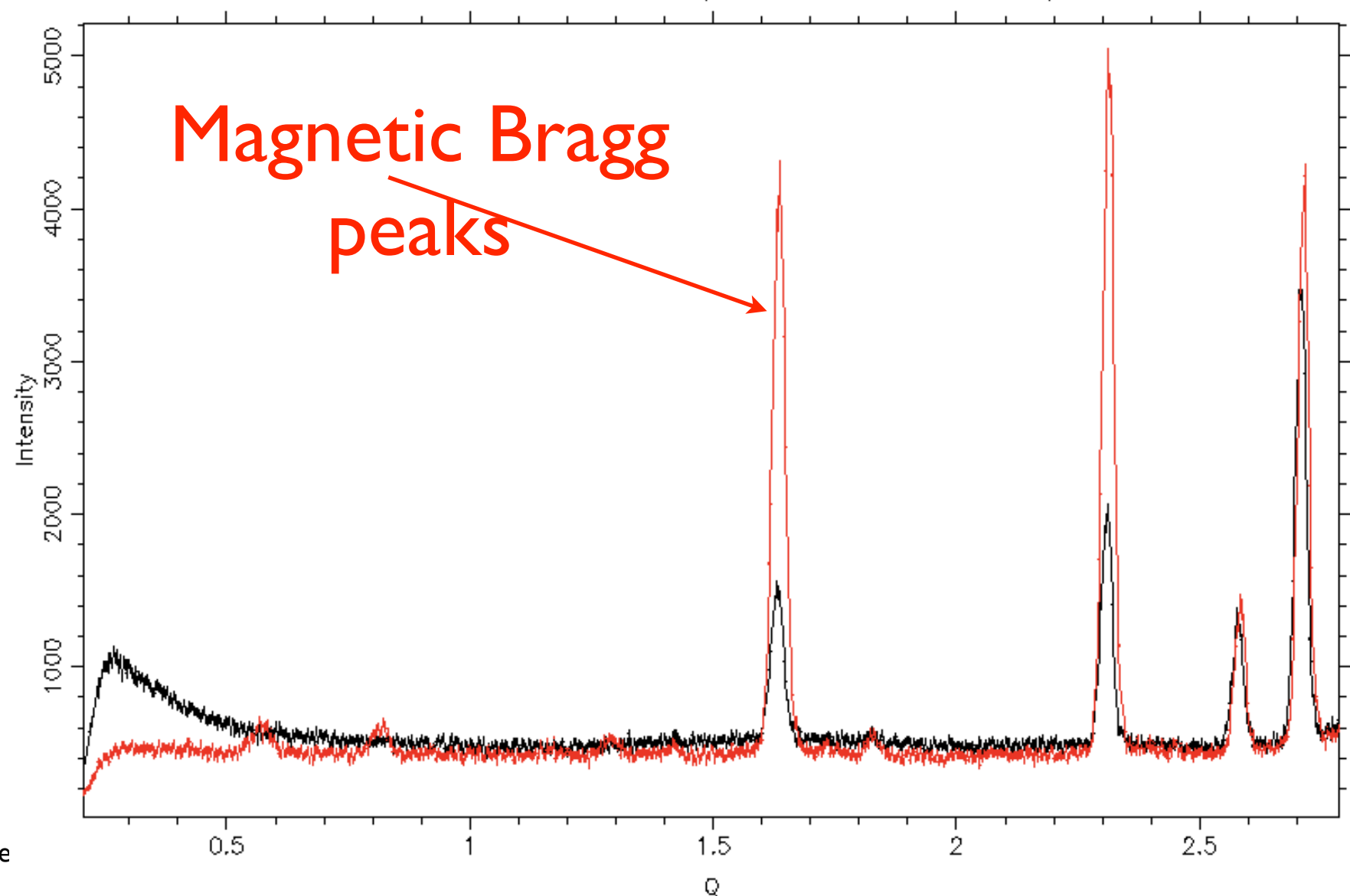
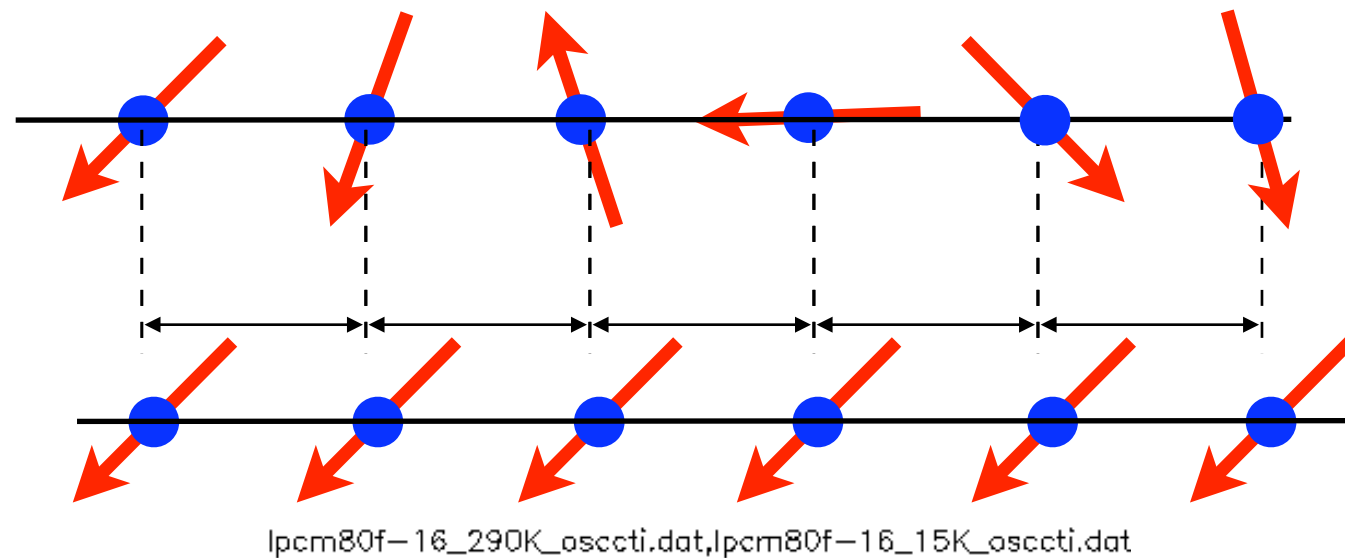



Experimental example of incoherent and coherent dipole magnetic scattering on a lattice of spins

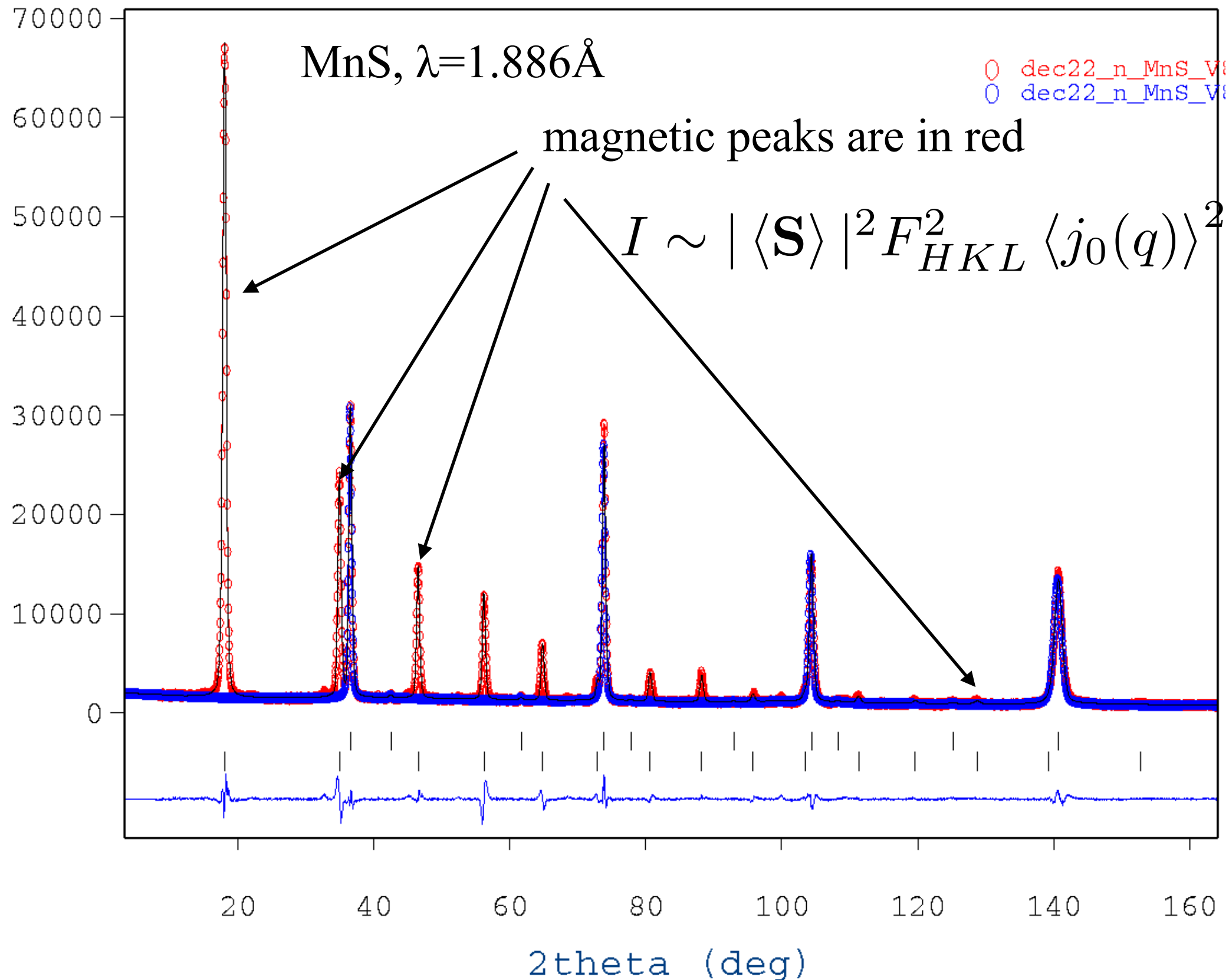
incoherent $I \sim \langle \hat{S}^2 \rangle = S(S+1)$

coherent Bragg scattering

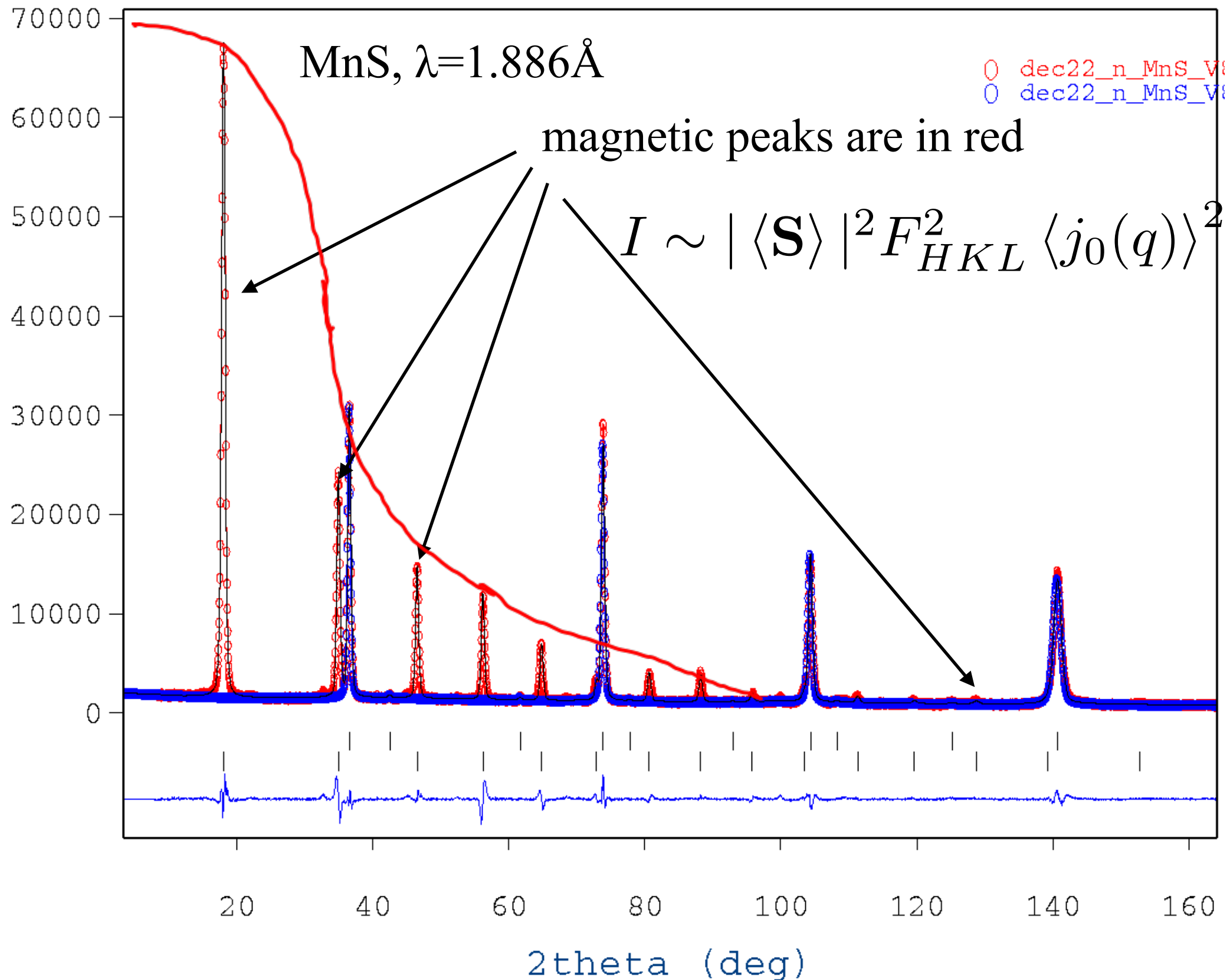
$$I \sim |\langle \mathbf{S} \rangle|^2 F_{HKL}^2 \langle j_0(q) \rangle^2$$



Experimental example of coherent dipole magnetic scattering MnS/MnO



Experimental example of coherent dipole magnetic scattering MnS/MnO



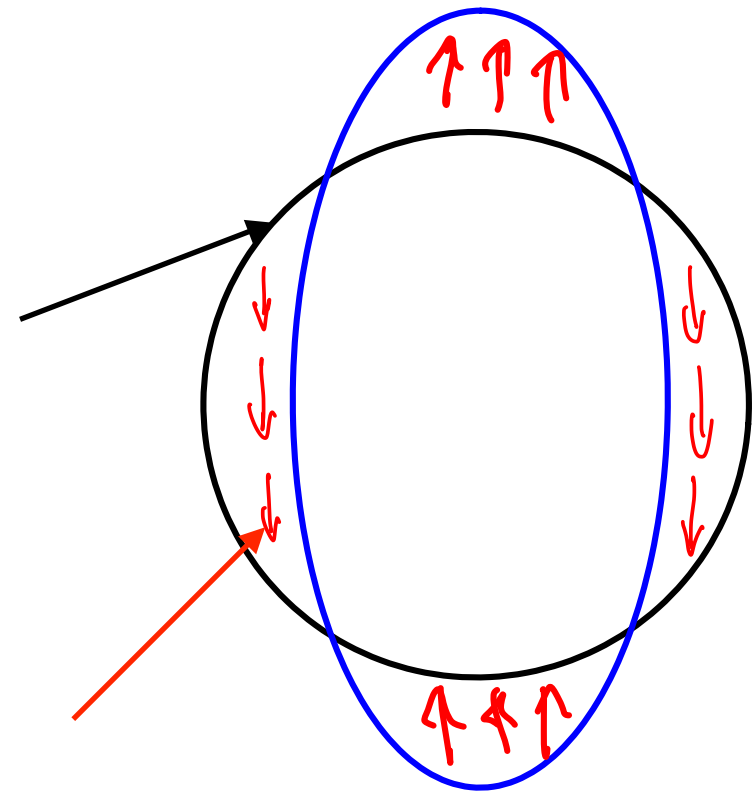
Conventional multipoles. Naive visualisations of octopole

magnetic multipoles == tensors of rank R

$$\hat{M}_{ijk\dots} = \hat{S}_i \underbrace{r_j r_k \dots}_R$$

electron spin or total **J** electron spin coordinates

$i, j, k\dots = 1, 2, 3(x, y, z)$



Conventional multipoles. Naive visualisations of octopole

magnetic multipoles == tensors of rank R

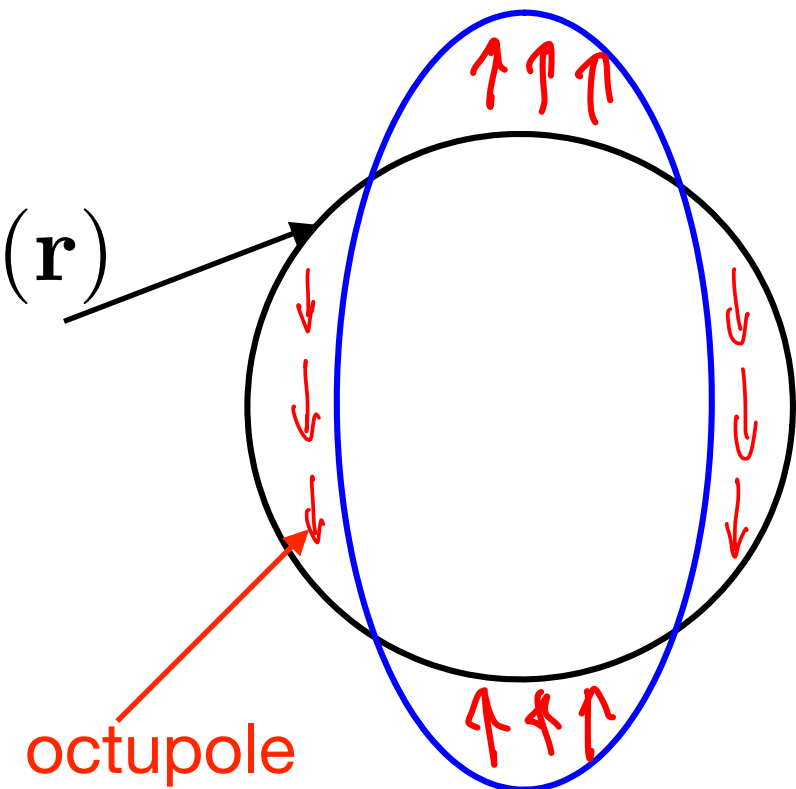
$$\hat{M}_{ijk\dots} = \underbrace{\hat{S}_i r_j r_k \dots}_{\text{electron spin or total } \mathbf{J}} \underbrace{\quad}_{\text{electron spin coordinates}} \quad i, j, k\dots = 1, 2, 3(x, y, z)$$

magnetic octopole: rank R=3 - operator in QM and has classical counterpart

$$\hat{O}_{ijk} = \hat{S}_i r_j r_k$$

Exp. value $\langle Q_{ijk} \rangle = \langle \psi | \hat{O}_{ijk} | \psi \rangle \longleftrightarrow O_{ijk}^c = \int M_i(\vec{r}) \cdot g(\vec{r}) r_j r_k d\vec{r}$

dipole $\rho(\mathbf{r})$



Conventional multipoles. Naive visualisations of octopole

magnetic multipoles == tensors of rank R

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$$\mathbf{L} + \mathbf{S} \sim [\mathbf{p} \times \mathbf{r}] = m \left[\frac{d\mathbf{r}}{dt} \times \mathbf{r} \right]$$

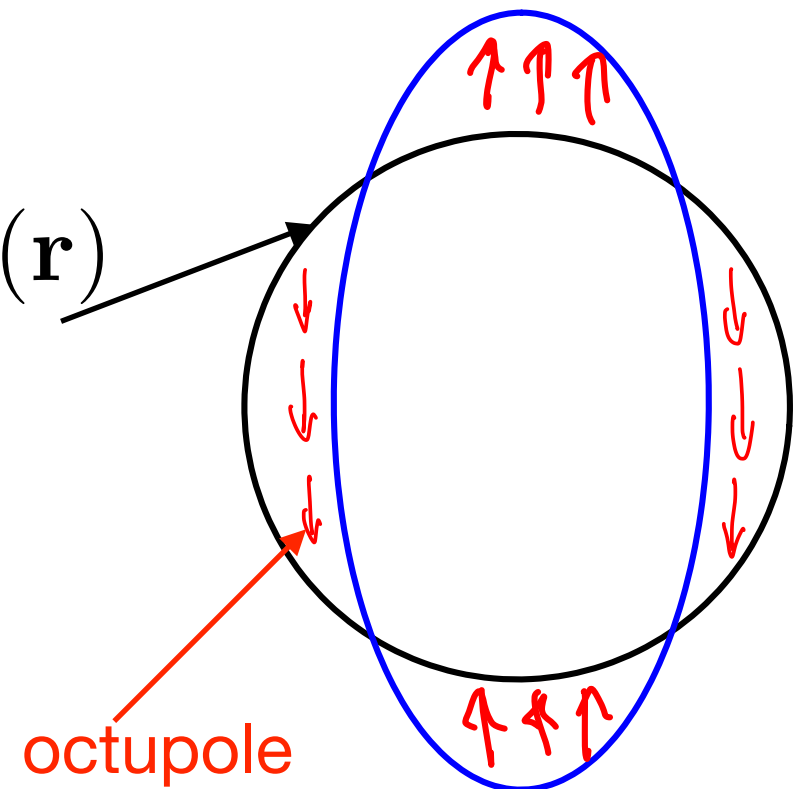
spin is **axial vector** = product of two polar vectors

time inversion (1') $\mathbf{S} = -\mathbf{S}$

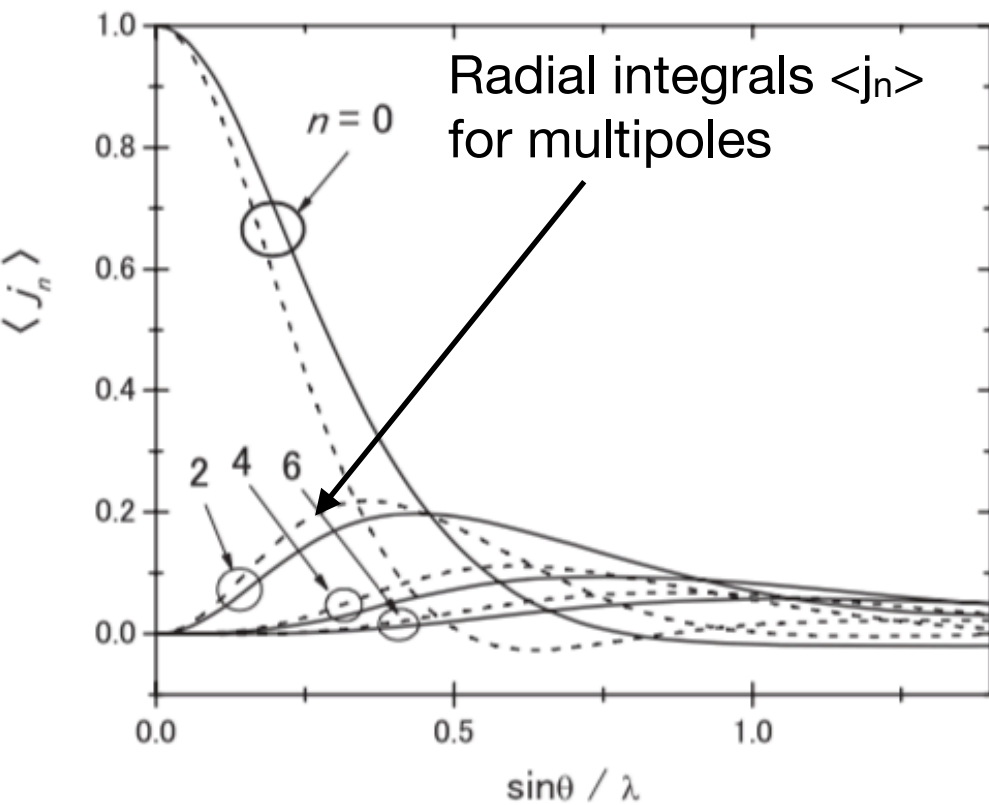
space inversion (-1) $\mathbf{S} = \mathbf{S}$

conventional odd-rank magnetic multipoles fulfil this: dipole (vector), octupole (rank-3 tensor),...

dipole $\rho(\mathbf{r})$

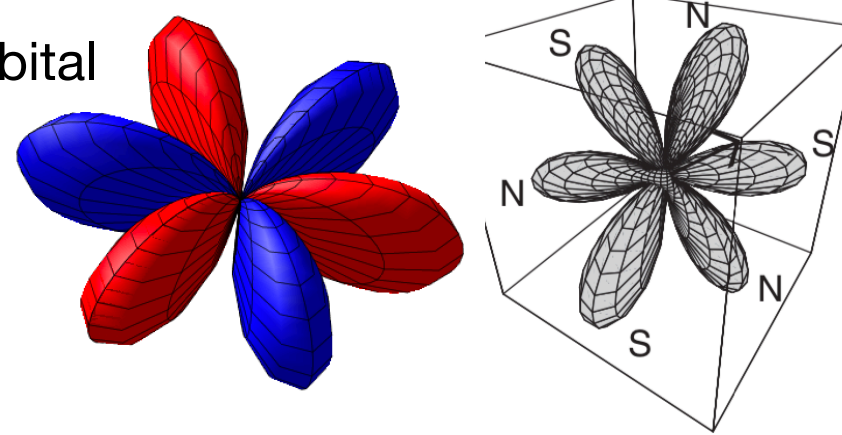


Multipole moments visualisation (qualitative, symmetry properties) and their q-dependence

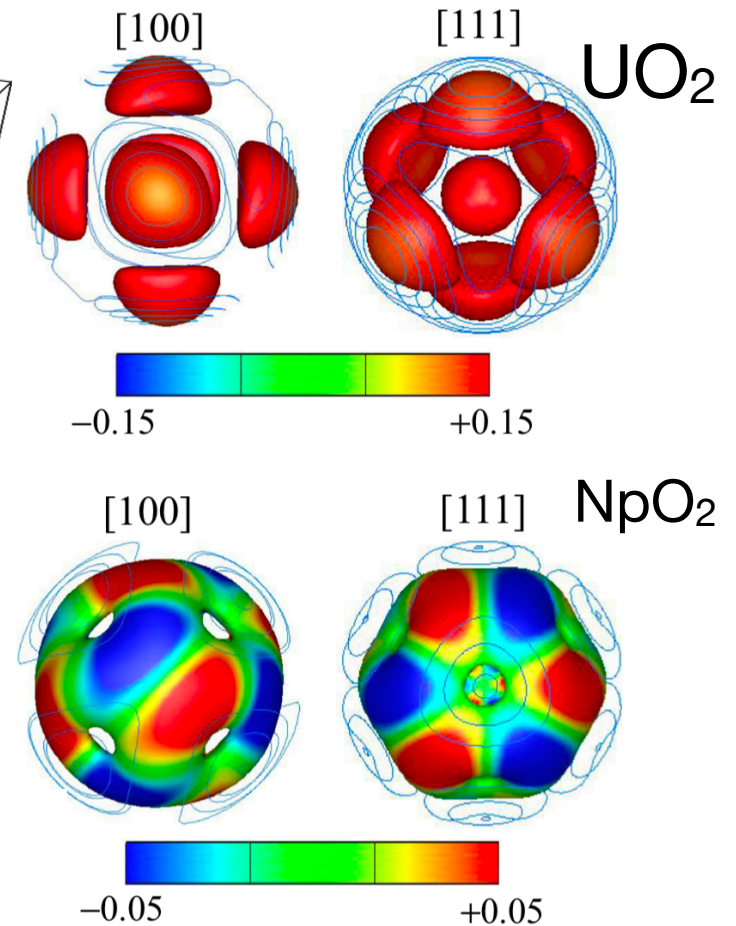


J. Phys. Soc. Jpn. 76, 094702 (2007)
J. Phys. Soc. Jpn. 80 (2011) SB008

f-orbital
 Y_{33}

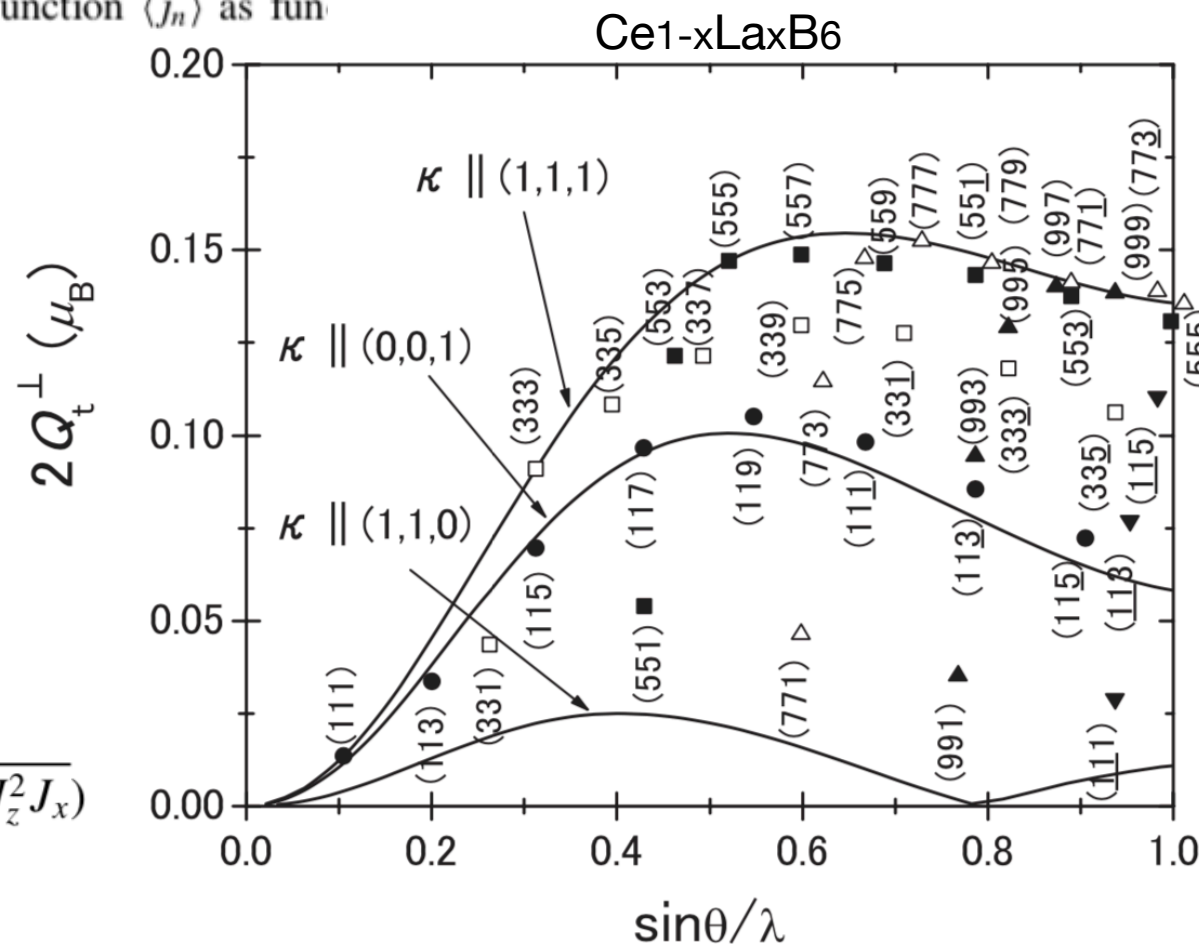


J. Phys. Soc. Jpn. 87, 041008 (2018)



Radial integrations of spherical Bessel function $\langle j_n \rangle$ as function of neutron momentum transfer $\sin\theta/\lambda$, and broken lines represent the re

$$T_x^\beta = \frac{\sqrt{15}}{6} (\overline{J_x J_z^2} - \overline{J_z^2 J_x})$$



Symmetry of multipoles

magnetic multipoles == tensors of rank R

$$\hat{M}_{ijk\dots} = \hat{S}_i \underbrace{r_j r_k \dots}_R$$

electron spin or total **J** electron spin coordinates

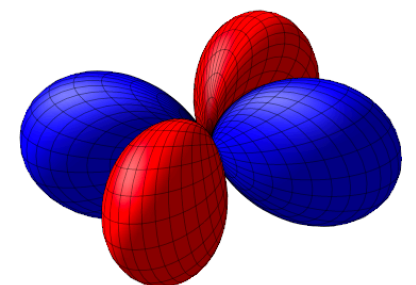
$i, j, k\dots = 1, 2, 3(x, y, z)$

1. Only **time reversal odd** multipoles
because of n-e interaction Hamiltonian

$$1' \cdot \hat{M}_{ijk\dots} = -\hat{M}_{ijk\dots}$$

one can construct multipoles
from pure J_x, J_y, J_z , angular
operators -> can be mapped to **Q**

$$Q = \exp(i\mathbf{R}_j \cdot \mathbf{k}) [s_j - (i/\hbar k)(\boldsymbol{\kappa} \times \mathbf{p}_j)]$$



Symmetry of multipoles

magnetic multipoles == tensors of rank R

$$\hat{M}_{ijk...} = \underbrace{\hat{S}_i r_j r_k ...}_R$$

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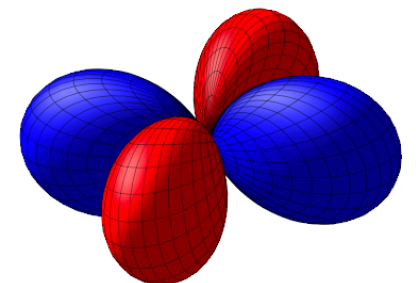
2. If wave function of unpaired electrons has definitive parity, i.e. under space inversion

$$\bar{1}|\psi\rangle = \pm|\psi\rangle \quad \langle\psi|\hat{M}_{ijk...}|\psi\rangle \neq 0$$

$$\bar{1} \cdot \hat{M}_{ijk...} = +\hat{M}_{ijk...}$$

conventional multipoles $R=1,3,... 2n+1$

we can have only **parity even** multipoles -> rank R -odd, e.g. no conventional quadrupoles



What are the magnetic objects neutrons sensitive to?

3. Dirac dipoles (anapoles) that are polar (parity odd) and magnetic (time odd).

Literature on neutron scattering on Dirac multipoles

S W Lovesey, “**Theory of neutron scattering by electrons in magnetic materials**”, Phys. Scr. 90 (2015) 108011. [Main paper](#)

S W Lovesey, “**Magneto-electric operators in neutron scattering from electrons**” J. Phys.: Condens. Matter 26 (2014) 356001

S W Lovesey and D D Khalyavin “**Neutron scattering by Dirac multipoles**”, J. Phys.: Condens. Matter 29 (2017) 215603

What are the magnetic objects neutrons sensitive to?

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If wave function of unpaired electrons has no parity we can have parity odd multipoles


$$|\psi\rangle = \left(a \left| s, +\frac{1}{2} \right\rangle |3d\rangle + b \left| s, -\frac{1}{2} \right\rangle |2p\rangle \right)$$

orbitals with opposite parities

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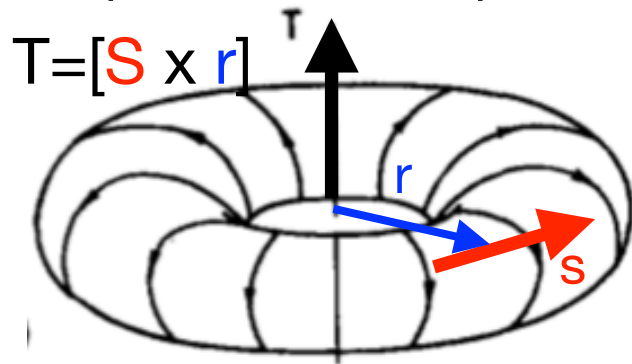
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$$\langle \psi | [\mathbf{S} \times \mathbf{n}] | \psi \rangle \neq 0, \mathbf{n} = \mathbf{r}/r$$

anapole, toroidal dipole moment



$$\mathbf{T}(\boldsymbol{\mu}) = \frac{1}{2} \int \mathbf{r} \times \boldsymbol{\mu}_{\perp} d^3r.$$

V.M. Dubovik and V.V. Tugushev, Toroid moments in electrodynamics and solid-state physics

$$|\psi\rangle = (a \left| s, +\frac{1}{2} \right\rangle |3d\rangle + b \left| s, -\frac{1}{2} \right\rangle |2p\rangle)$$

spinor

spinor

orbitals with opposite parities

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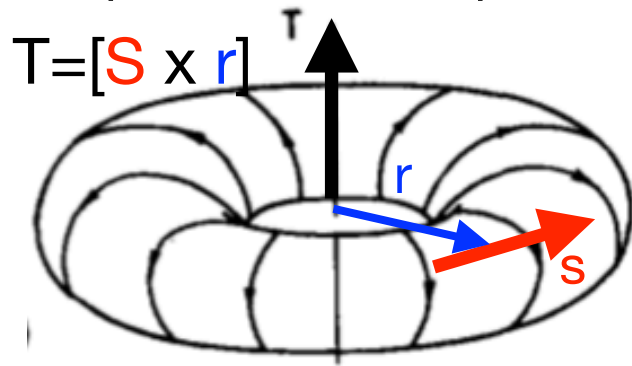
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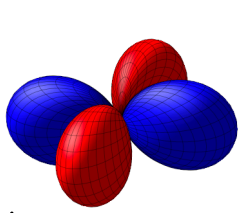
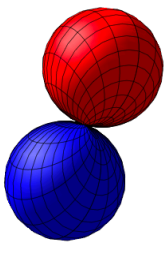
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spinor  spinor 

orbitals with opposite parities

$$\langle 2, 0 |_d \left\langle +\frac{1}{2} \right| (S_y n_z)_x \left| -\frac{1}{2} \right\rangle |1, 0\rangle_p \neq 0$$

Literature on neutron scattering on Dirac multipoles

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S W Lovesey, “**Magneto-electric operators in neutron scattering from electrons**” J. Phys.: Condens. Matter 26 (2014) 356001

S W Lovesey and D D Khalyavin “**Neutron scattering by Dirac multipoles**”, J. Phys.: Condens. Matter 29 (2017) 215603

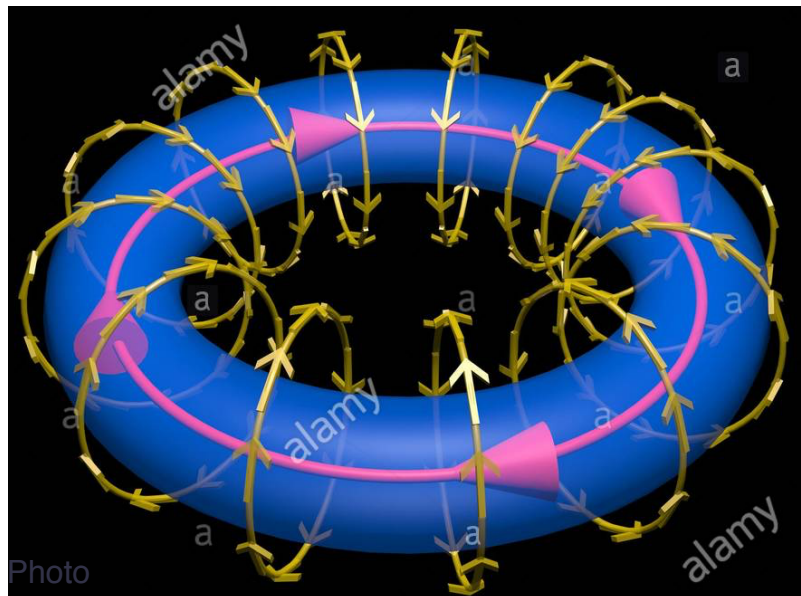
A zero-magnetization ferromagnet $\text{Sm}_{0.976}\text{Gd}_{0.024}\text{Al}_2$

S W Lovesey et al PRL 122, 047203 (2019). “Direct Observation of Anapoles by Neutron Diffraction”: Experiment & theory

Atomic wave functions are $4f^5-5d^1$

$$\Omega_S = [\mathbf{S} \times \mathbf{n}], \Omega_L = [\mathbf{L} \times \mathbf{n}] - [\mathbf{n} \times \mathbf{L}]$$

toroidal magnetic field is localised



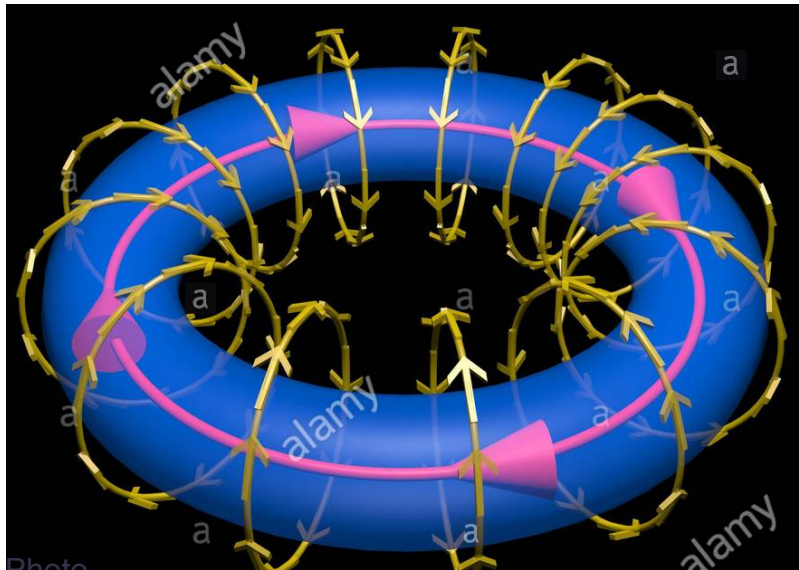
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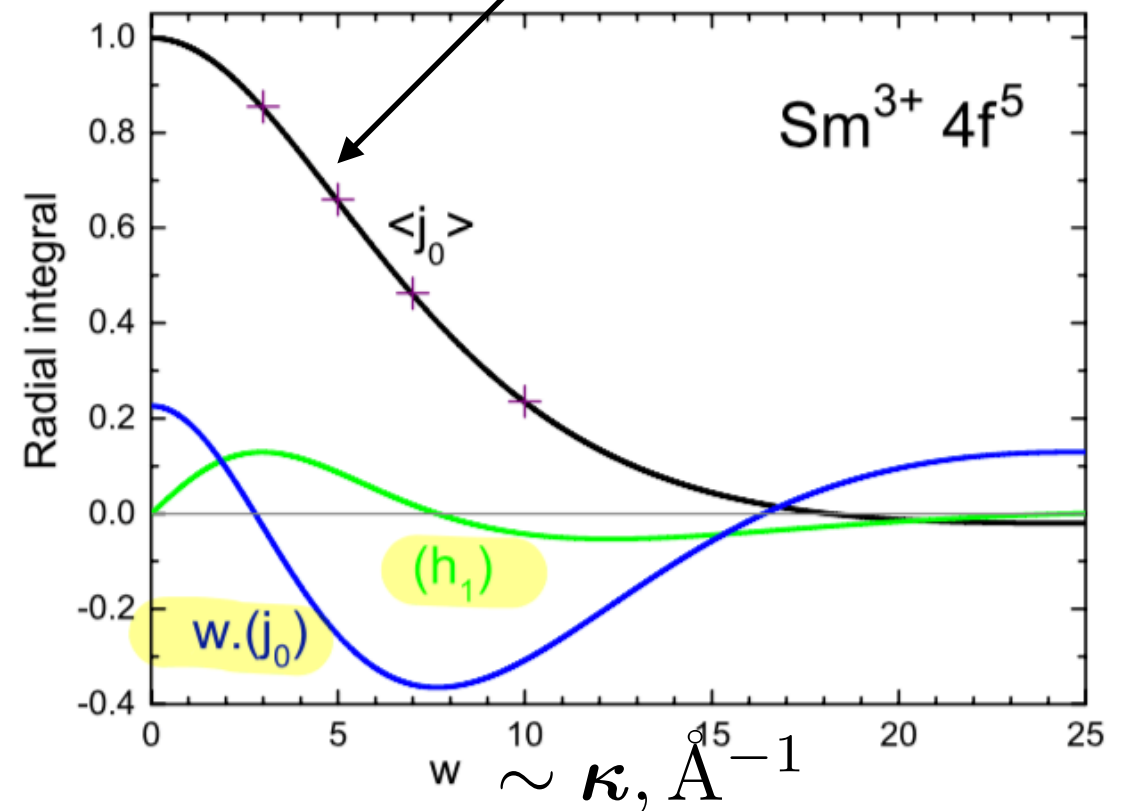


Alamy Stock Photo

FIG. 3. Radial integrals for Dirac multipoles that appear in Eq. (2) derived from an atomic code due to R. D. Cowan [22]. Dimensionless variable $w = 12\pi a_0 s$, where a_0 is the Bohr radius, while the standard variable for radial integrals s is derived from the Bragg angle and neutron wavelength $s = \sin \theta / \lambda$. Green curve shows (h_1) and blue shows $[w \times (j_0)]$. Note that (j_0) is proportional to $1/w$ as the wavevector approaches zero. Atomic wavefunctions are $4f^5-5d^1$. Also included in the figure is the standard radial integral $\langle j_0 \rangle$ that appears in the so-called dipole-approximation (Eq. 1) for diffraction by axial dipole moments. Results obtained with our $\text{Sm}^{3+} (4f^5)$ wavefunction are denoted by the continuous black curve, to which we added for comparison four values (+) derived from the standard interpolation formula [23].

magnetic dipole

$$\langle \mathbf{Q} \rangle = \frac{1}{2} \langle j_0(\kappa) \rangle (\mathbf{1} + 2\mathbf{s}) + \frac{1}{2} \langle j_2(\kappa) \rangle \mathbf{1}.$$



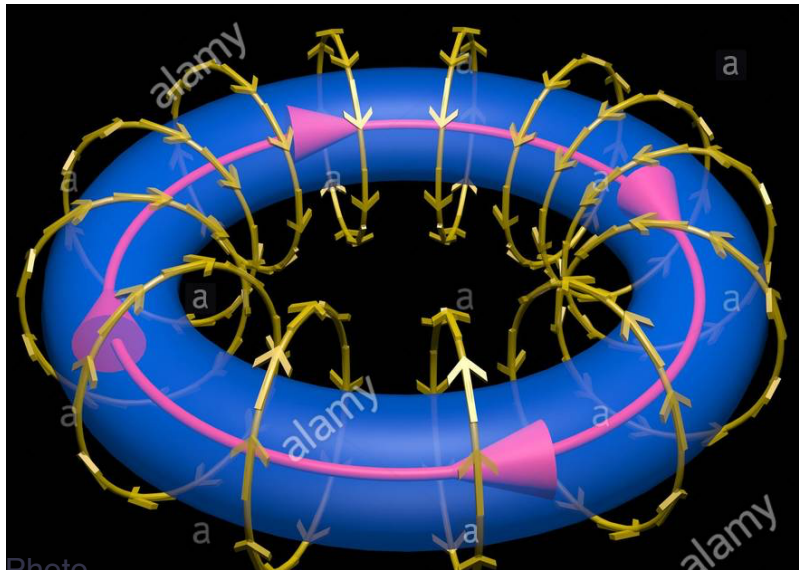
A zero-magnetization ferromagnet $\text{Sm}_{0.976}\text{Gd}_{0.024}\text{Al}_2$

S W Lovesey et al PRL 122, 047203 (2019). “Direct Observation of Anapoles by Neutron Diffraction”: Experiment & theory

Atomic wave functions are $4f^5-5d^1$

$$\Omega_S = [\mathbf{S} \times \mathbf{n}], \Omega_L = [\mathbf{L} \times \mathbf{n}] - [\mathbf{n} \times \mathbf{L}]$$

toroidal magnetic field is localised

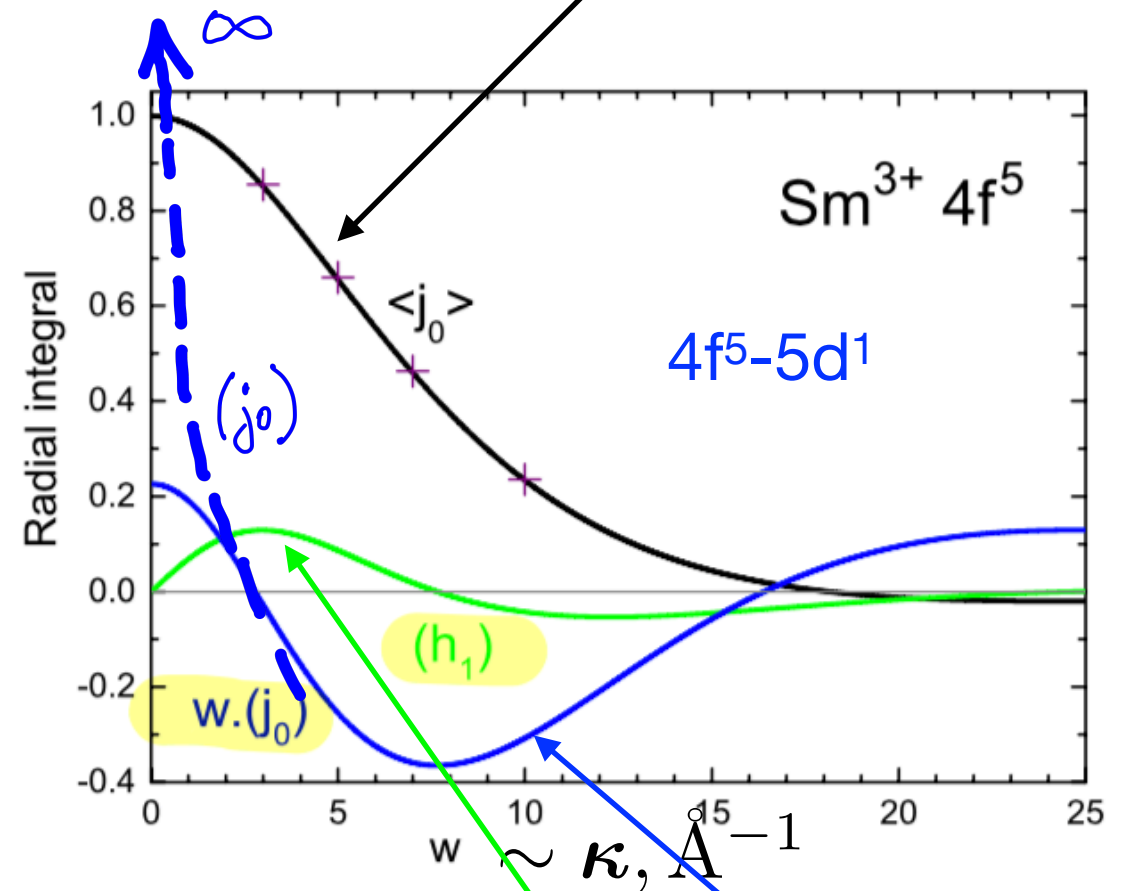


Alamy Stock Photo

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magnetic structure factor for ordered anapoles

$$F^{(-)} \approx -i \exp\left[\frac{i\pi}{4} (H_o - K_o - L_o)\right] \times \kappa_\zeta [3\langle \Omega_\eta \rangle_S (h_1) - \langle \Omega_\eta \rangle_L (j_0)],$$

1. Description of magnetic structures

1.1 How do we describe/classify/predict magnetic symmetries and structures?

1.2 How do we construct all symmetry allowed magnetic structures for a given crystal structure?

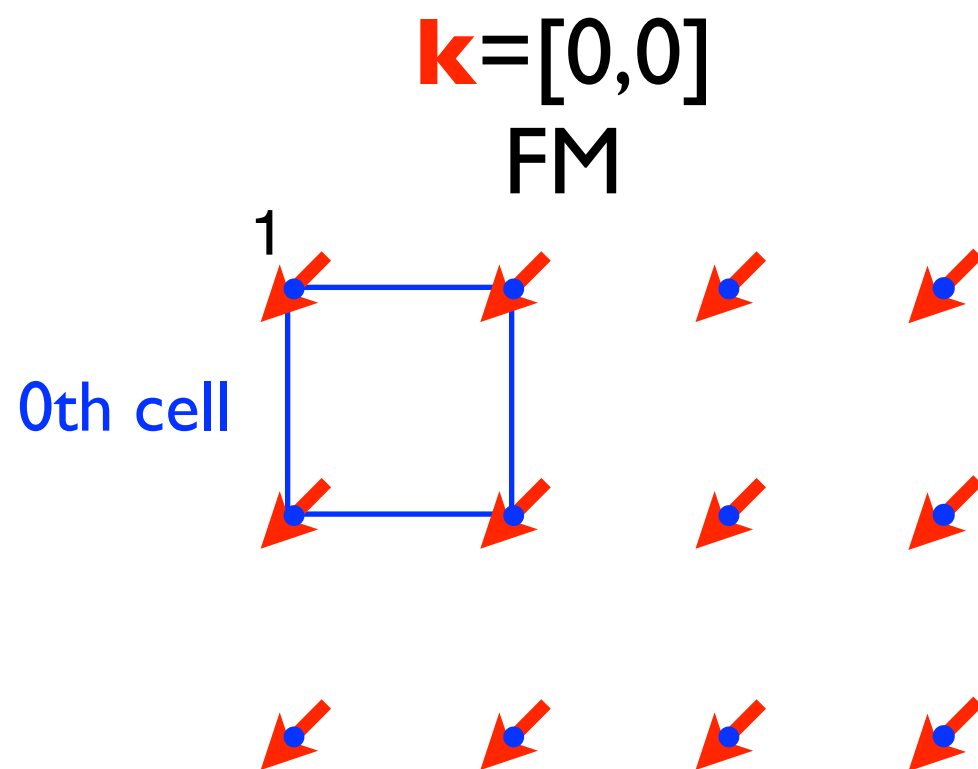
and

2. their determination by neutron diffraction

Magnetic structure factors, practical applications...

Magnetic structure

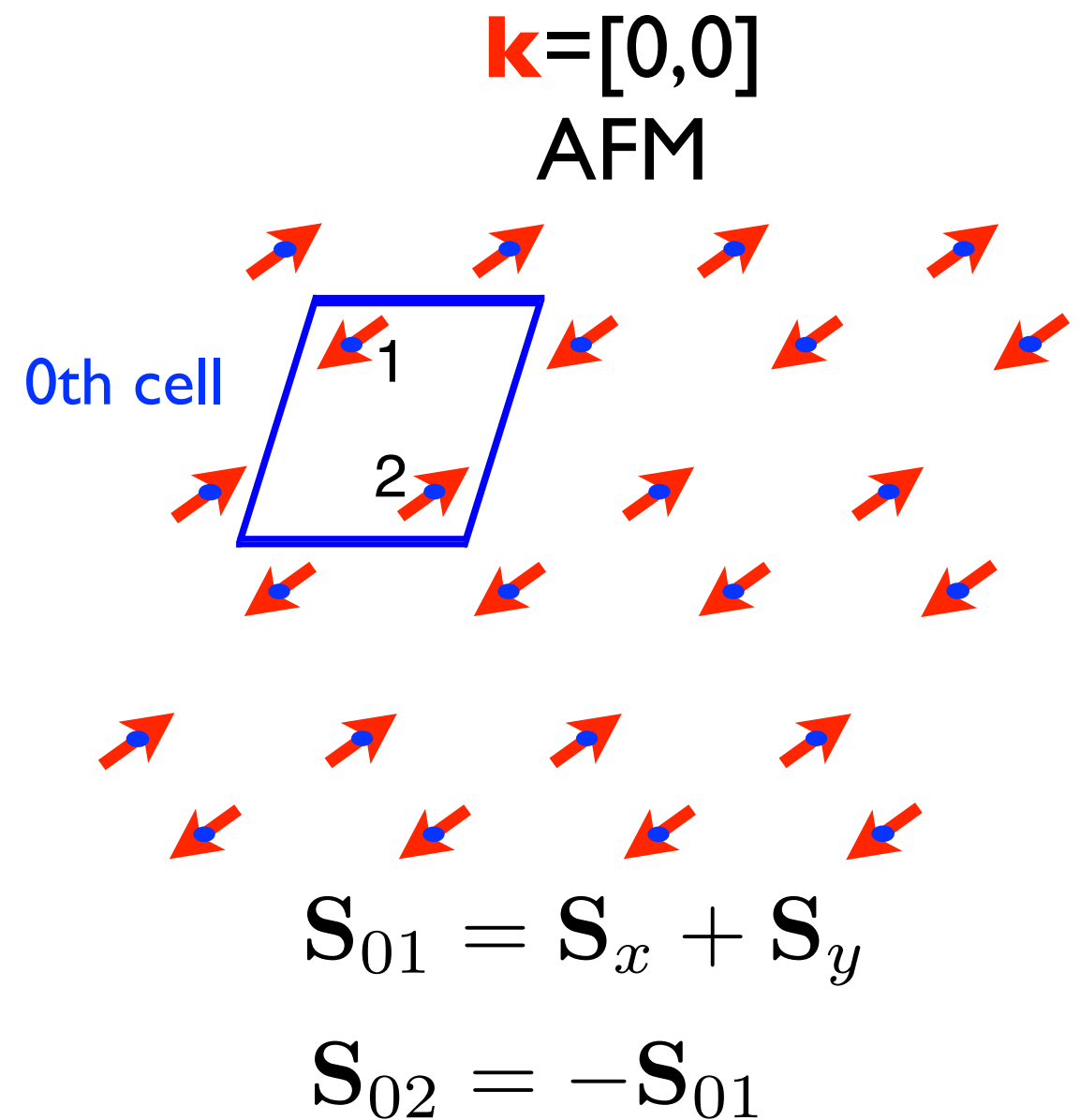
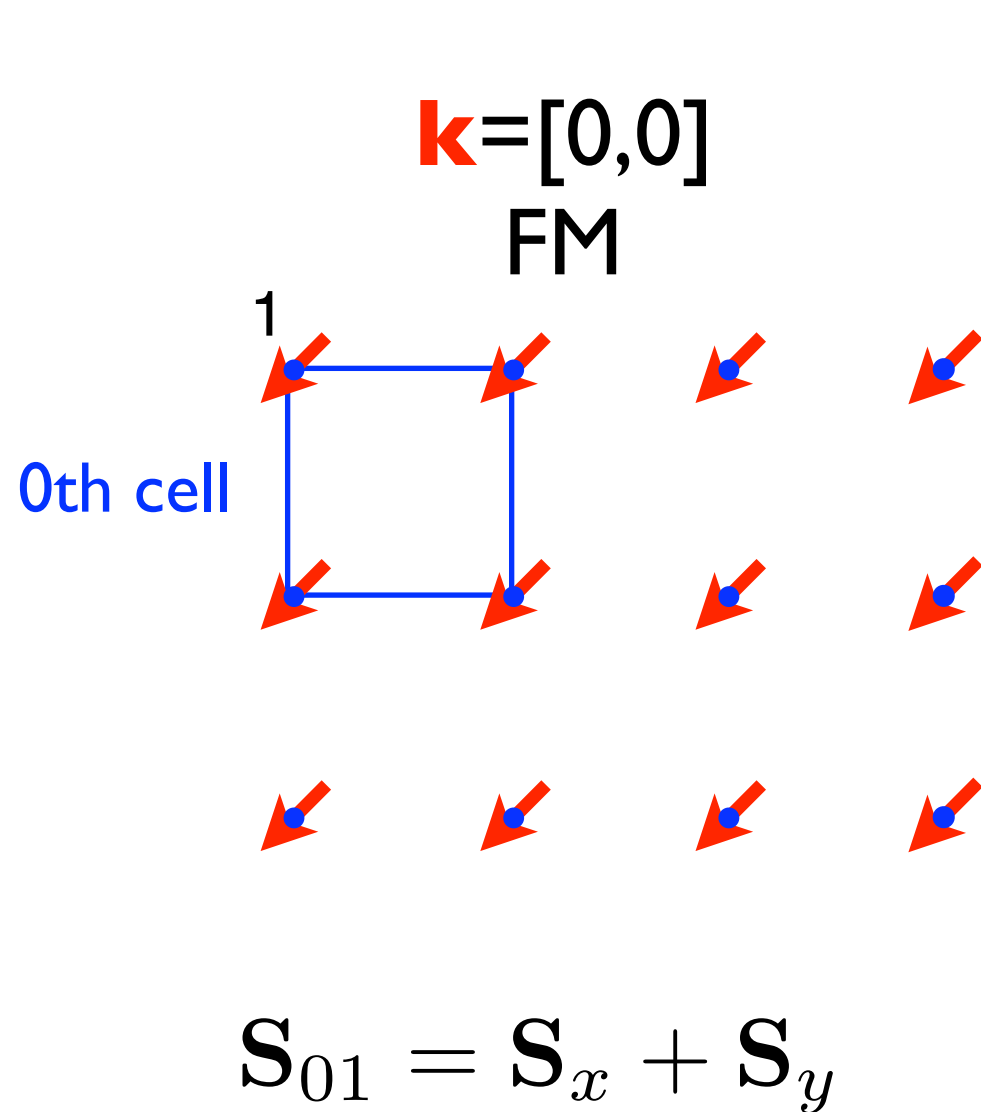
Examples



$$\mathbf{S}_{01} = \mathbf{S}_x + \mathbf{S}_y$$

Magnetic structure

Examples



Examples of magnetic structures.

Propagation vector formalism $\mathbf{k} \neq 0$.

position of spin in the lattice

Magnetic moment
is a real quantity

$$\mathbf{S}(\mathbf{t}_n) = \frac{1}{2} (\mathbf{S}_0 e^{+2\pi i \mathbf{t}_n \mathbf{k}} + \mathbf{S}_0^* e^{-2\pi i \mathbf{t}_n \mathbf{k}}) \equiv |S_{0\alpha}| \cos(2\pi \mathbf{t}_n \mathbf{k} + \phi_\alpha)$$

$\alpha = x, y, z$

Fourie amplitude is complex
(one can not avoid this)

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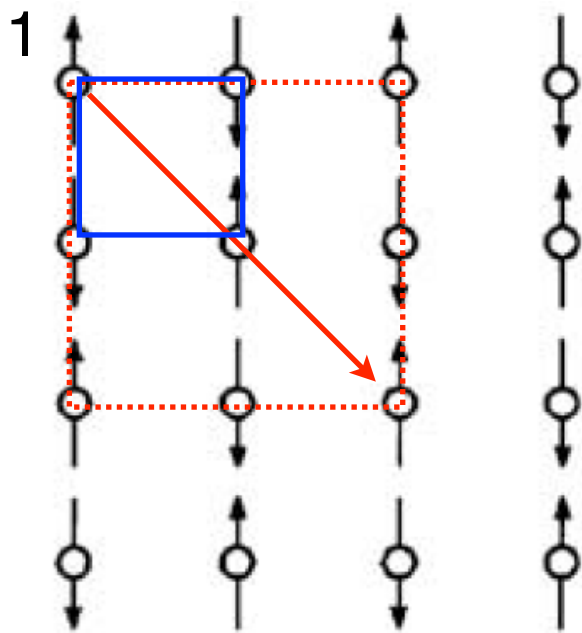
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$\mathbf{k} = [1/2, 1/2]$ AFM



$$\mathbf{S}_{01} = \mathbf{S}_y$$

$$\begin{aligned} \mathbf{S}(\mathbf{t}_n) &= \mathbf{S}_y \sin(2\pi \mathbf{t}_n \mathbf{k}) \\ &= \mathbf{S}_y \sin(\pi(t_{nx} + t_{ny})) \end{aligned}$$

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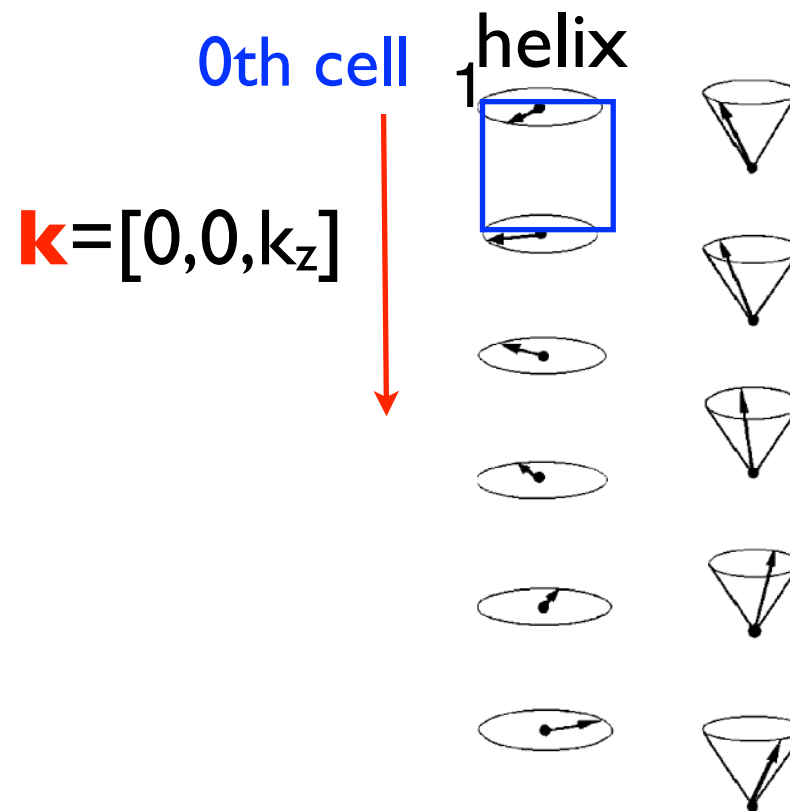
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modulated (in)commensurate



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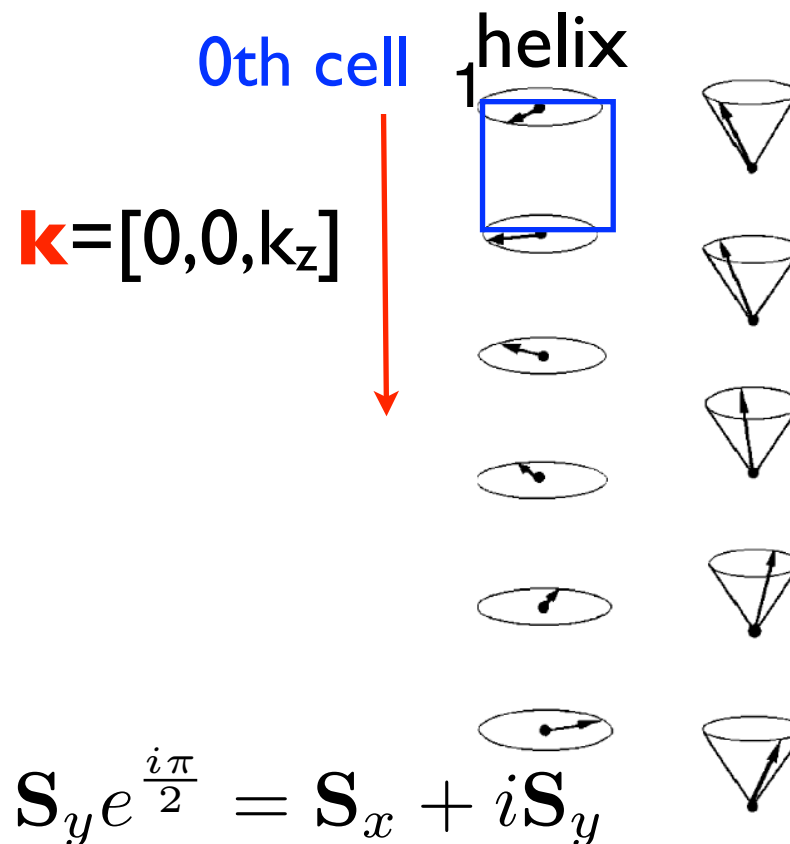
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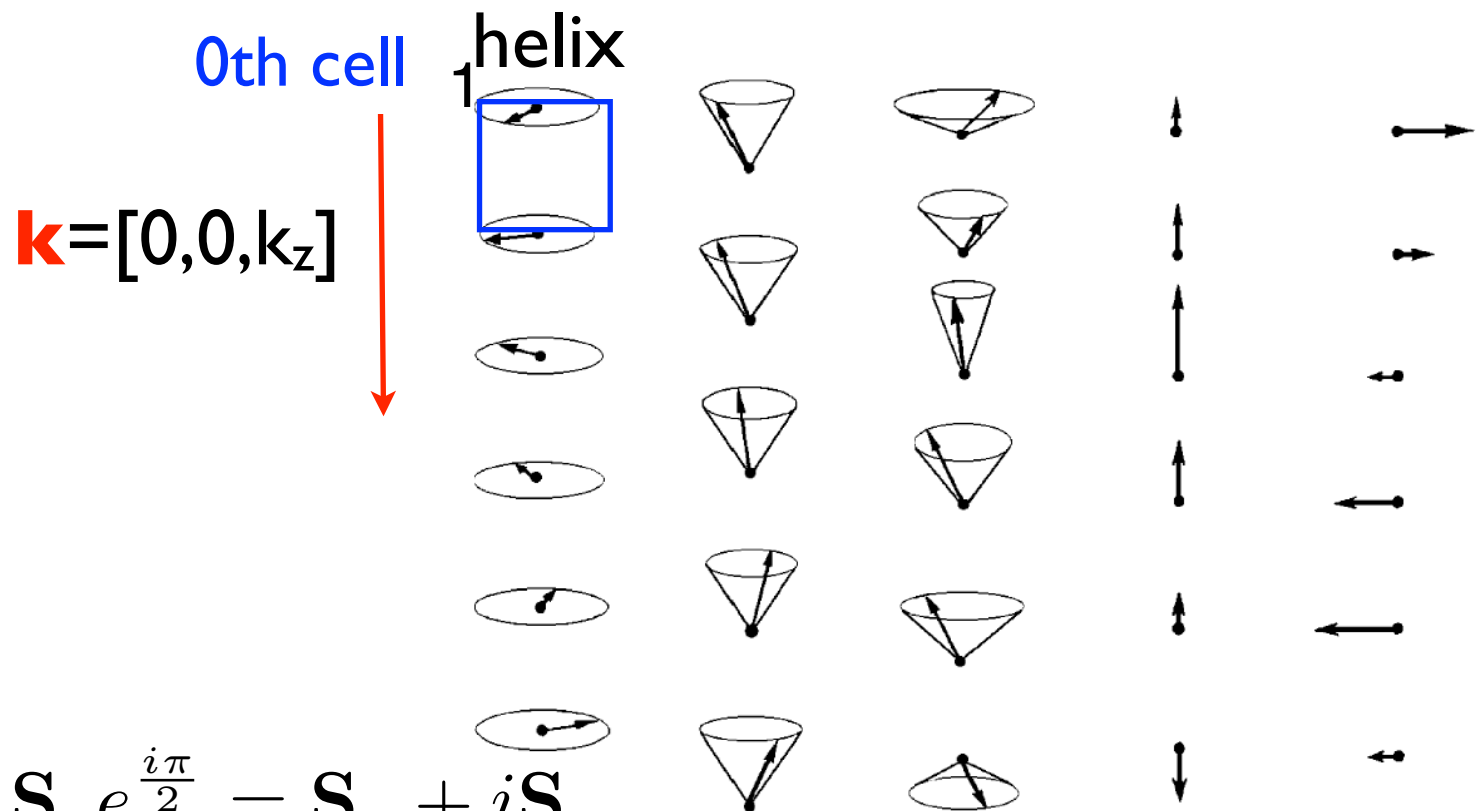
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cycloidal
spiral

SDW

Scattering from the lattice of spins.

Magnetic structure factor $\mathbf{F}(\mathbf{q})$

In ND experiment we measure correlators of Fourier transform of magnetic lattice

$$\frac{d\sigma}{d\Omega} \propto (\mathbf{Q}_{\perp}(\mathbf{q}) \cdot \mathbf{Q}_{\perp}^*(\mathbf{q}) + i\mathbf{P} \cdot [\mathbf{Q}_{\perp}(\mathbf{q}) \times \mathbf{Q}_{\perp}^*(\mathbf{q})]) \cdot \delta(\mathbf{H} \pm \mathbf{k} - \mathbf{q})$$

↑
structure factor

↑
polarized neutron
(chiral) term.

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Bragg peak at
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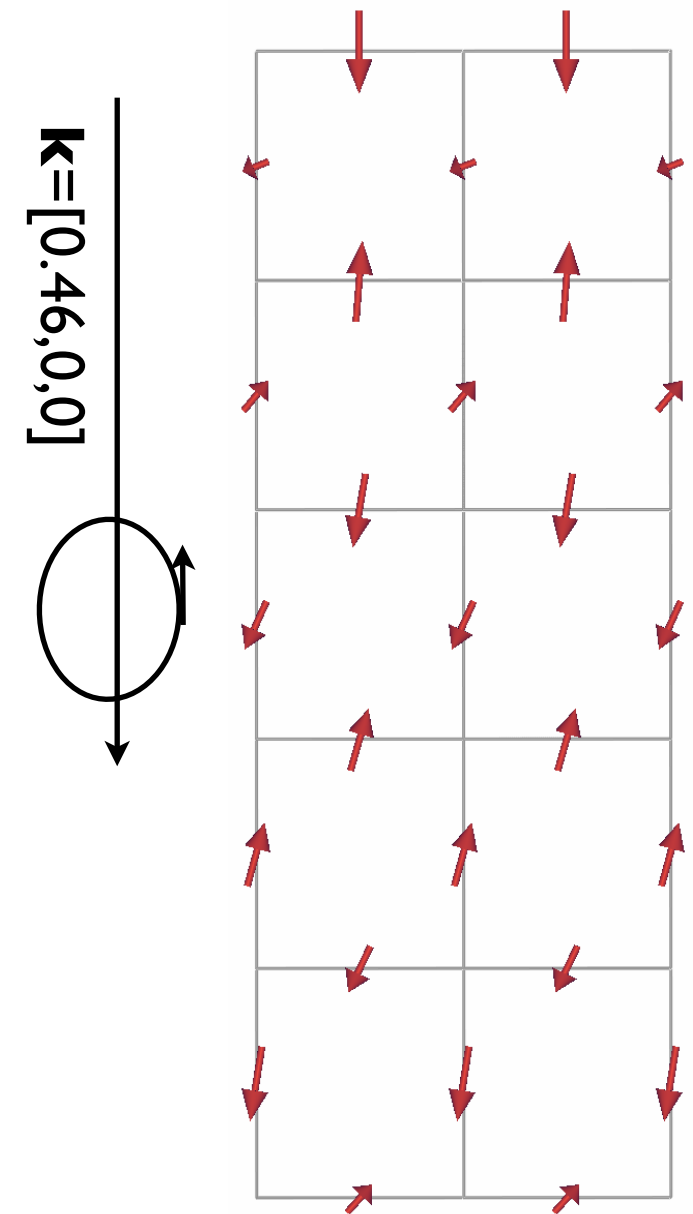
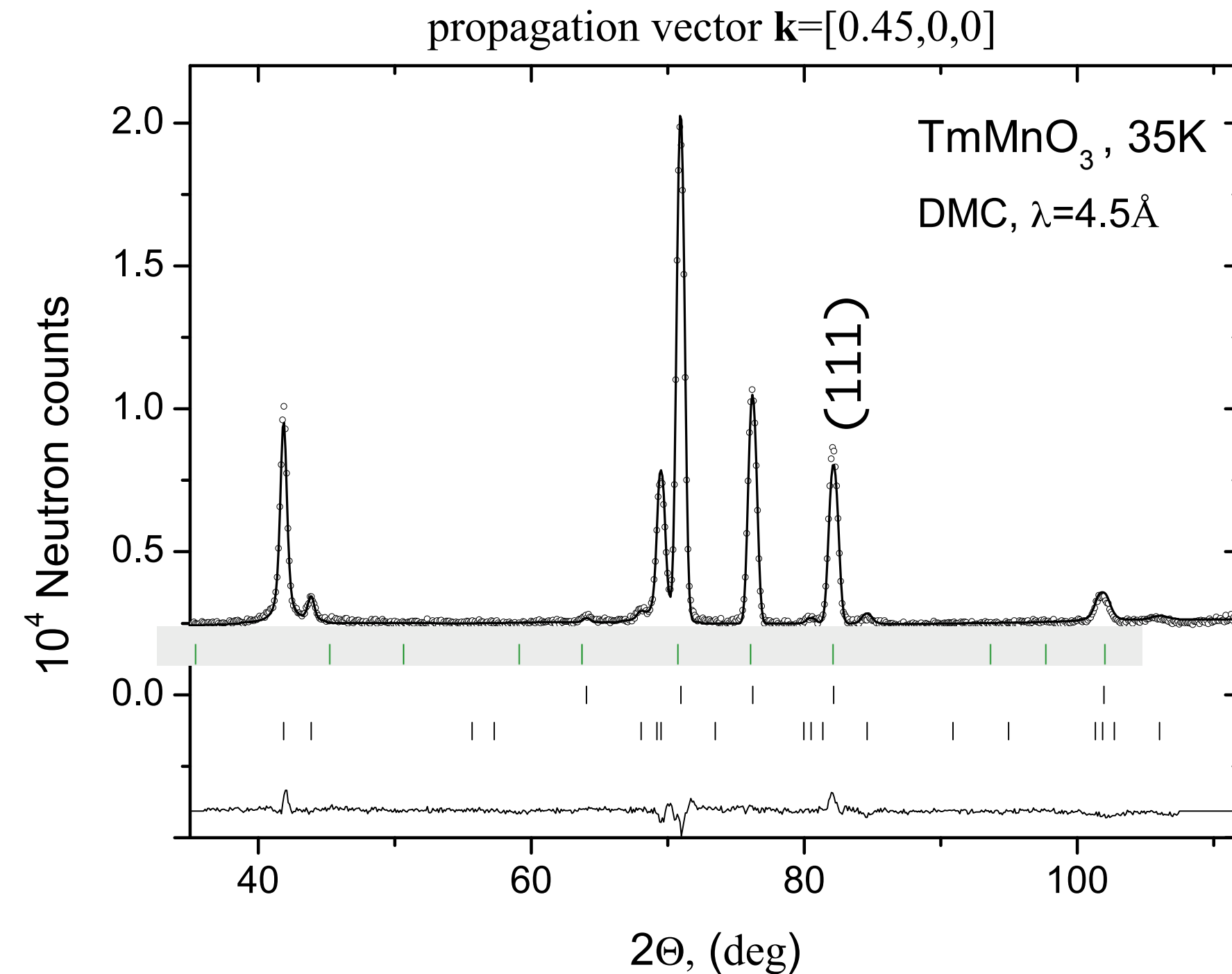
Sum runs over all atoms in zeroth cell

$$\mathbf{Q}_{\perp}(\mathbf{q})_{-k} = \sum_j \frac{1}{2} \mathbf{S}_{0j\perp} \cdot \exp(i\mathbf{r}_j \mathbf{q}) \quad \mathbf{Q}_{\perp}(\mathbf{q})_{+k} = \sum_j \frac{1}{2} \mathbf{S}_{0j\perp}^* \exp(i\mathbf{r}_j \mathbf{q})$$

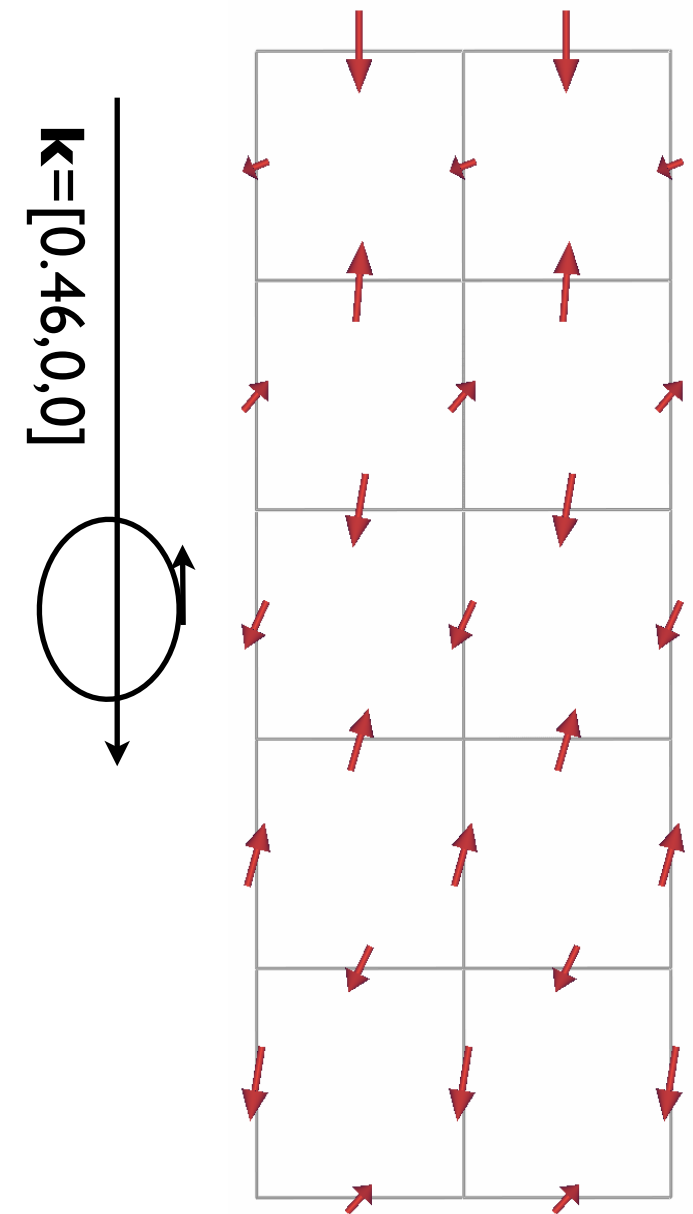
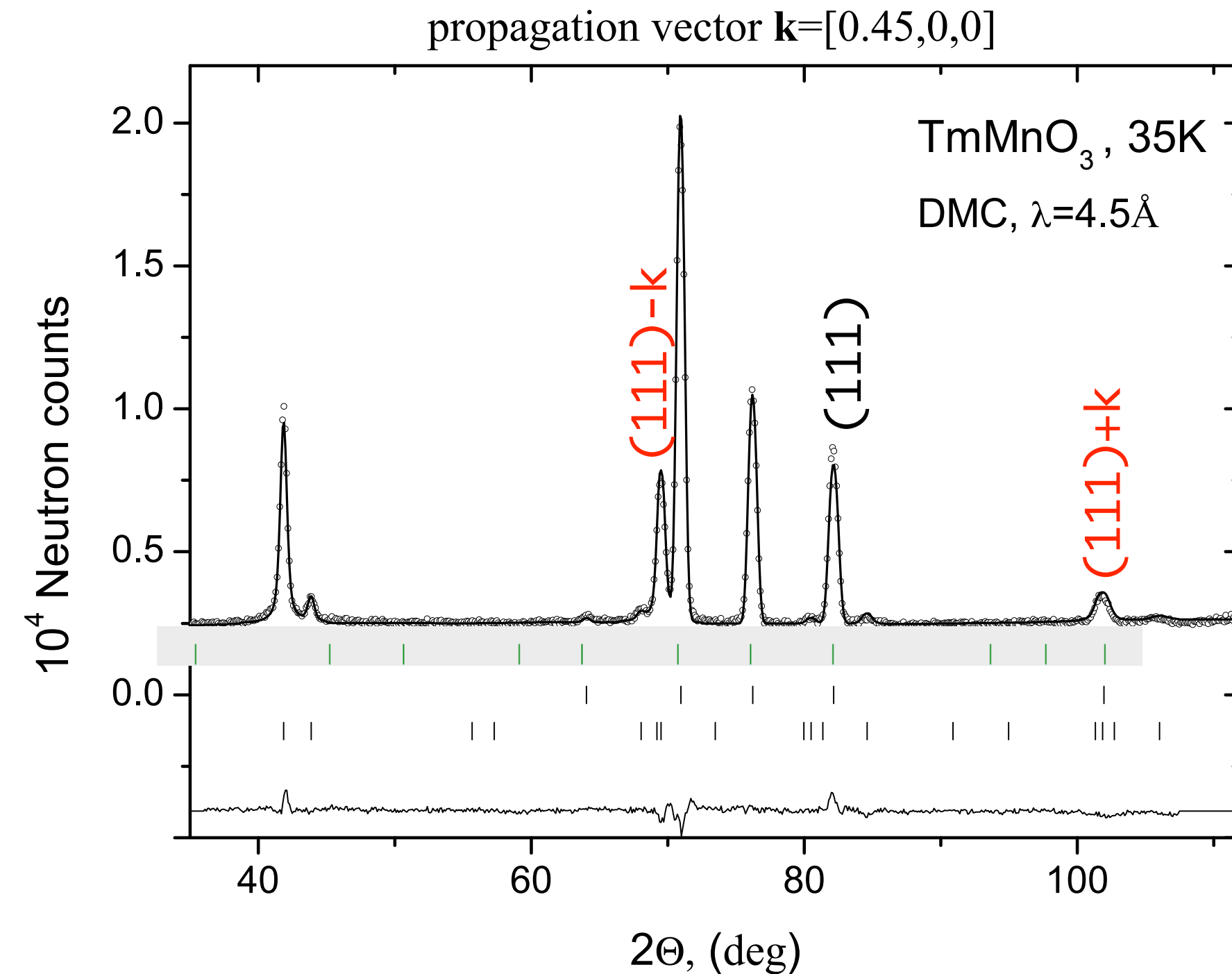
↑
Complex amplitude
of spin modulation
perpendicular to $\mathbf{q}$

↑
position of spin in
the zeroth cell

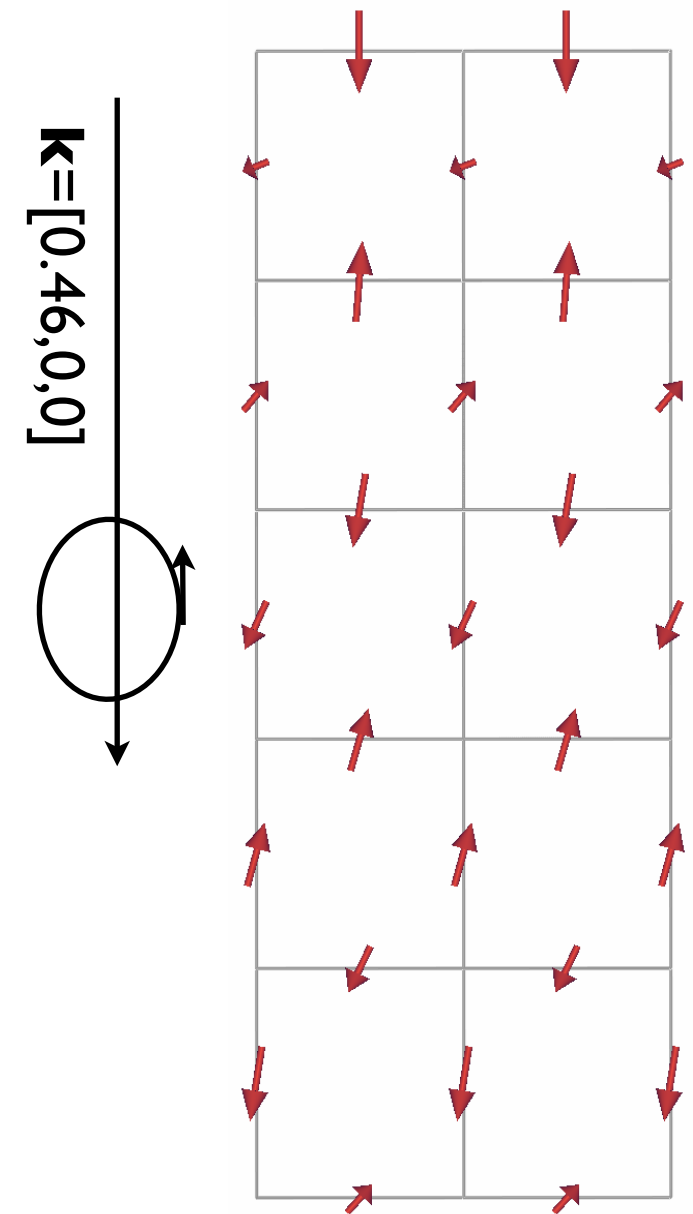
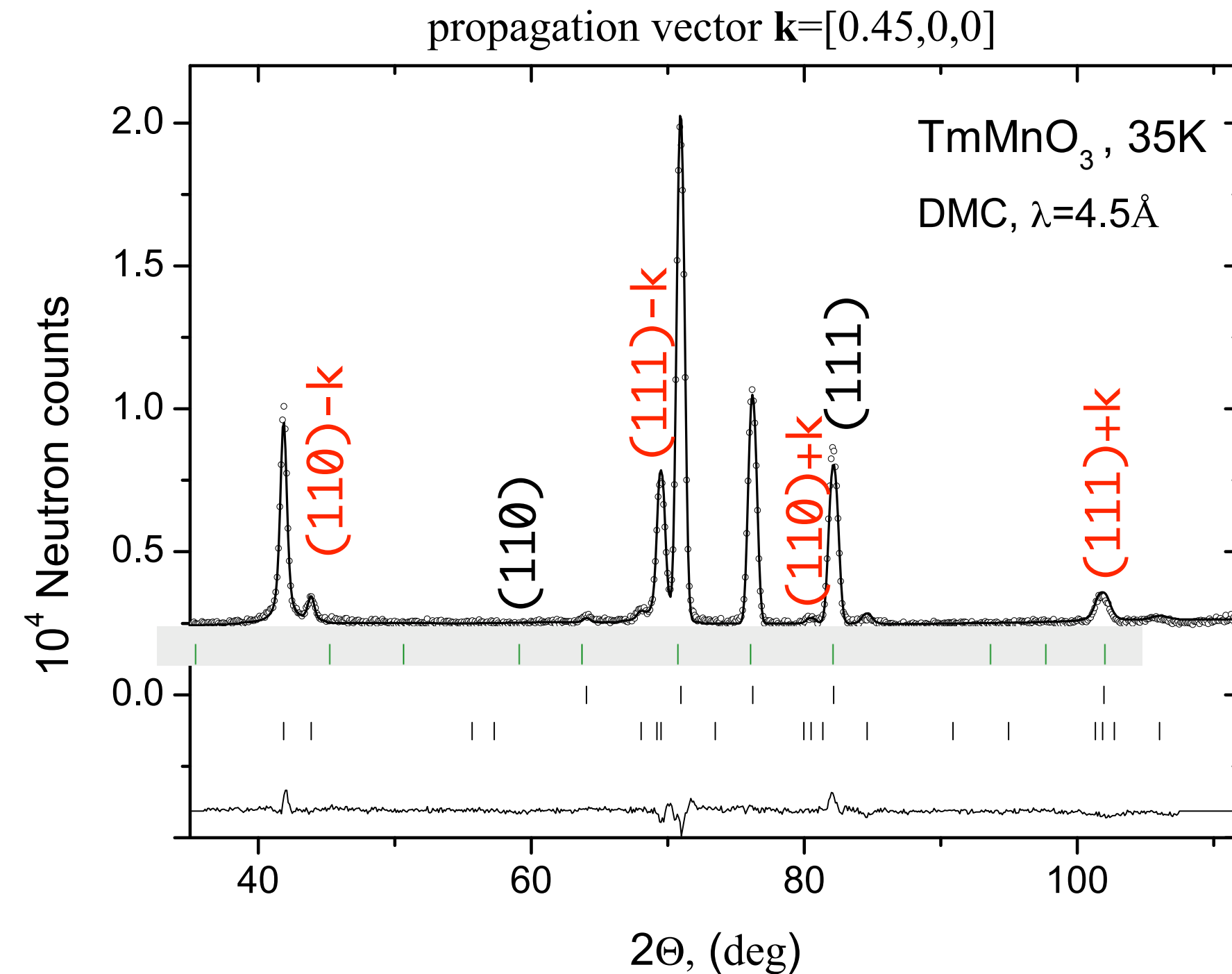
Example of modulated incommensurate structure and diffraction pattern



Example of modulated incommensurate structure and diffraction pattern



Example of modulated incommensurate structure and diffraction pattern



Example of commensurate magnetic structure

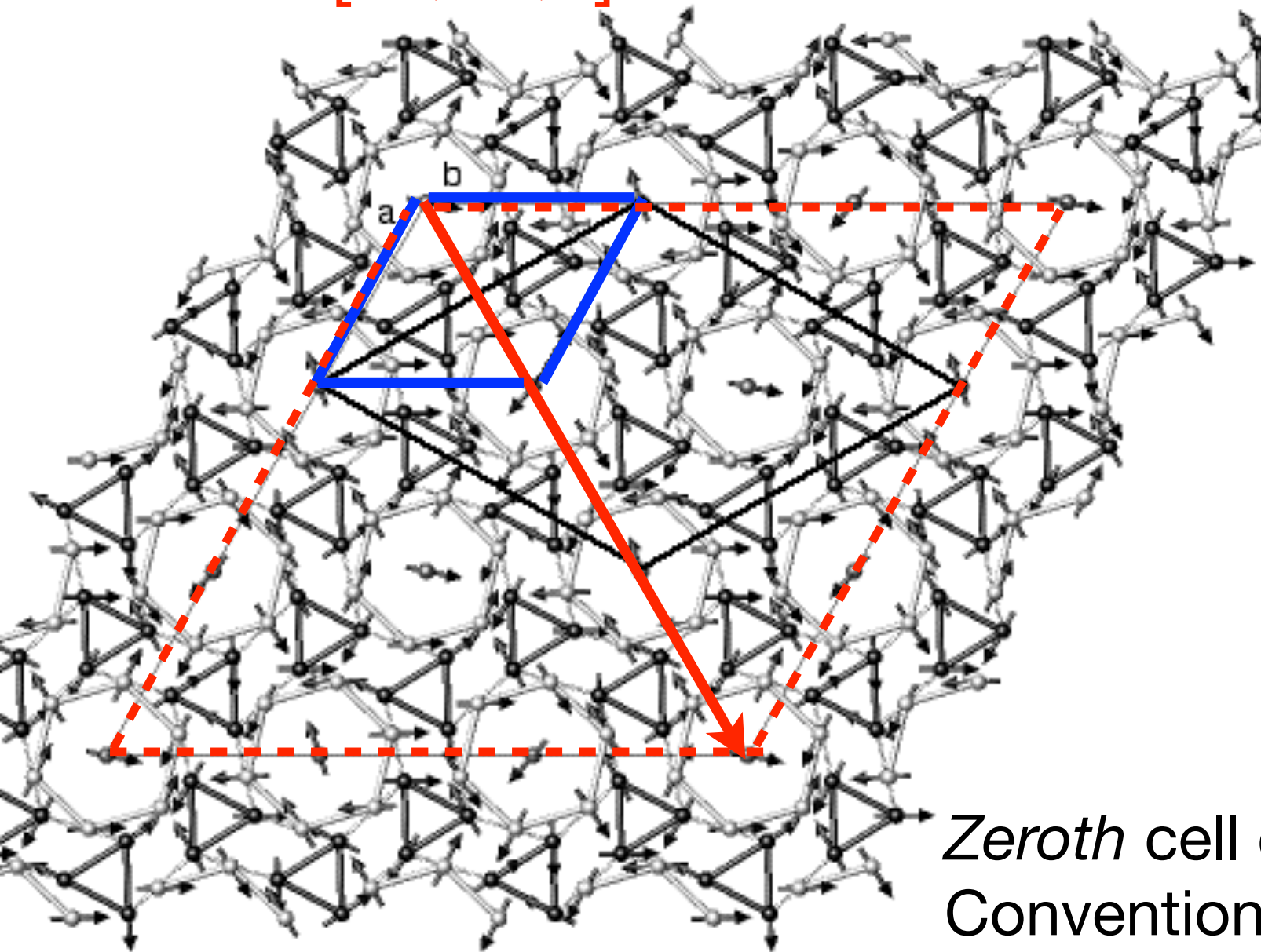
Antiferromagnetic (à la cycloidal spiral) three sub-lattice ordering in



commensurate: $k=m/n$, m,n : integers

P6/m

$k\text{-vector}=[1/3, 1/3, 0]$



Zeroth cell:

only **5 magnetic modes**, i.e.
5 mixing coefficients C to
find from experiment.

Zeroth cell contains 14 spins of Tb^{3+}
Conventional magnetic unit cell contains
126 spins of Tb^{3+} !!

Short note on non-polarized neutron diffraction

magnetic

nuclear

$$I^{++} \propto \langle |\vec{Q}_\perp \sigma_n + \vec{F}|^2 \rangle_{\sigma_n}$$

average over neutron polarization

Short note on non-polarized neutron diffraction

$$I^{++} \propto \langle |\mathbf{Q}_\perp \sigma_n + F|^2 \rangle_{\sigma_n}$$

magnetic nuclear
average over neutron polarization

$$I \propto \langle (\mathbf{Q}_\perp \sigma_n)(\mathbf{Q}_\perp^* \sigma_n) + FF^* + \cancel{\sigma_n(F\mathbf{Q}_\perp^* + F^*\mathbf{Q}_\perp)} \rangle_{\sigma_n}$$

no magnetic/nuclear interference

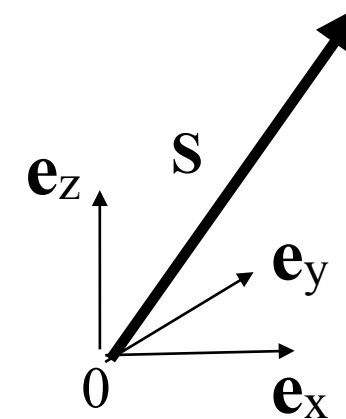
$$I \propto |\mathbf{Q}_\perp|^2 + |F|^2$$

Magnetic and nuclear scattering are completely independent and can be treated as two independent phases in the data analysis (Rietveld refinement)

Introduction to irreducible representations irreps and magnetic Shubnikov groups

Point groups. Magnetic moment rotations in 3D space. Notation of the group representation. Improper rotations.

3-dimensional vector space of $\mathbf{s}$ = $\sum_{j=x,y,z} s_j \mathbf{e}_j$
classical spin



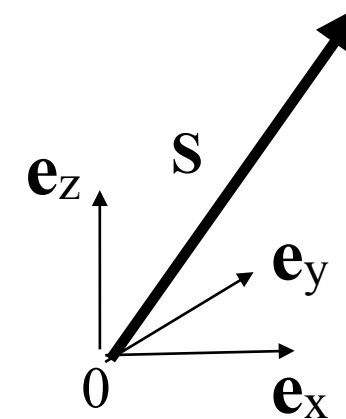
Rotation matrices can be used to construct **3-dimensional representation matrices** of proper rotations

$$\varphi_z \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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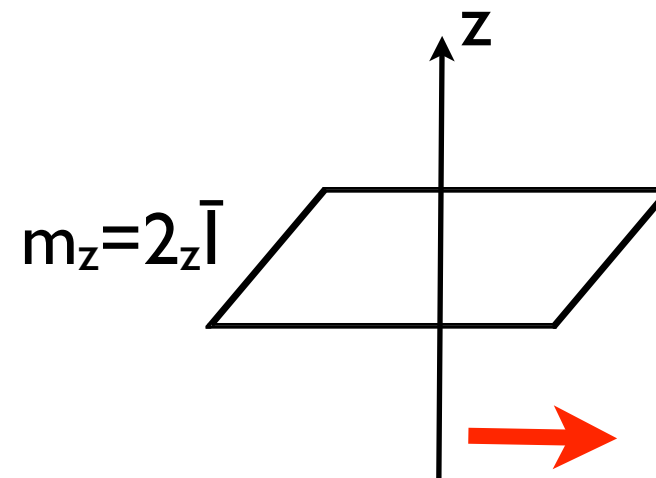
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Note: For improper rotations such as inversion (I) or mirror plane we should remember that spin is an axial vector.

$$\mathbf{S} = " [\mathbf{v} \times \mathbf{r}]"$$

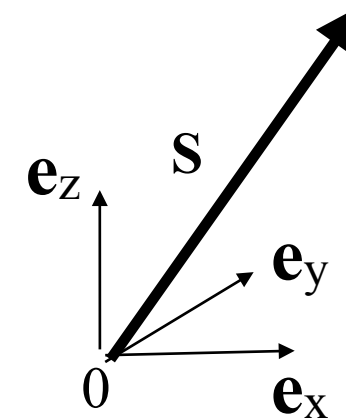
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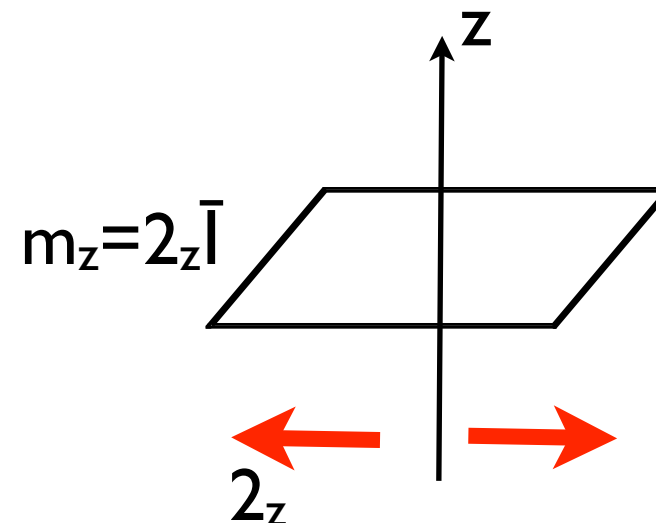
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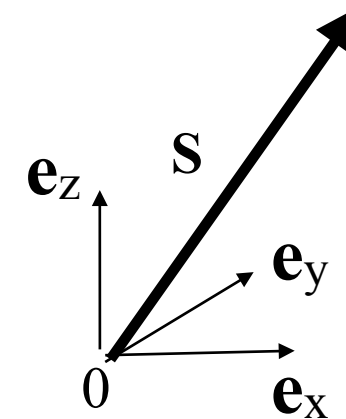
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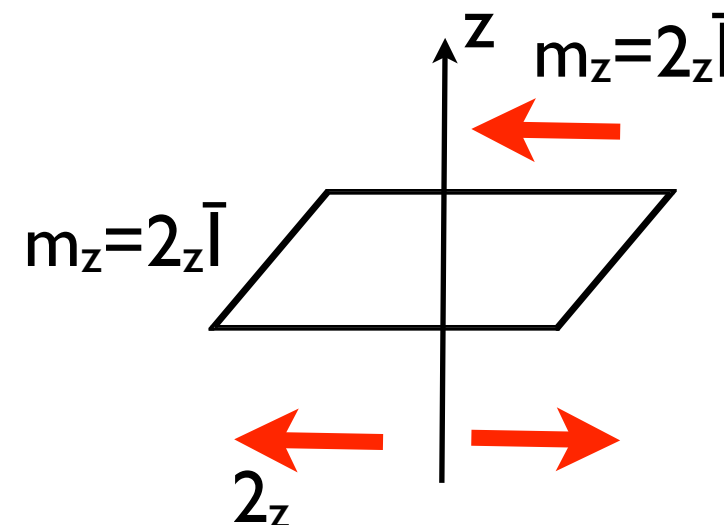
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Representation of point group 32 in 3D rotation space of spin **S**

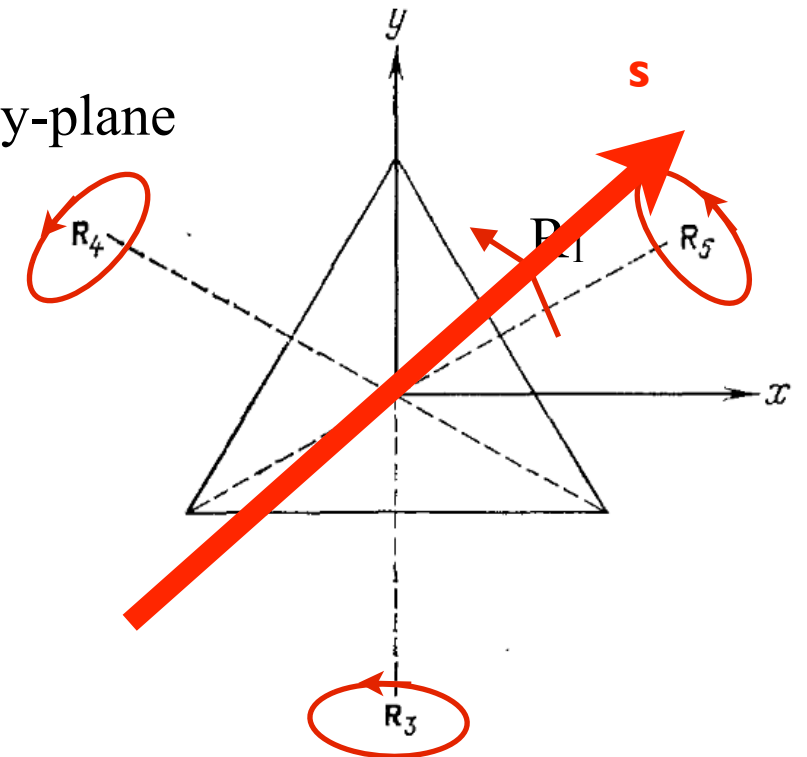
Example

6 symmetry elements (rotations):

$R_0=E$, $R_1=2\pi/3$, $R_2=4\pi/3$ around z , R_3 , R_4 , R_5 , $=\pi$ around resp. axes in xy -plane

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1. 3-dimensional representation



Representation of point group 32 in 3D rotation space of spin S

Example

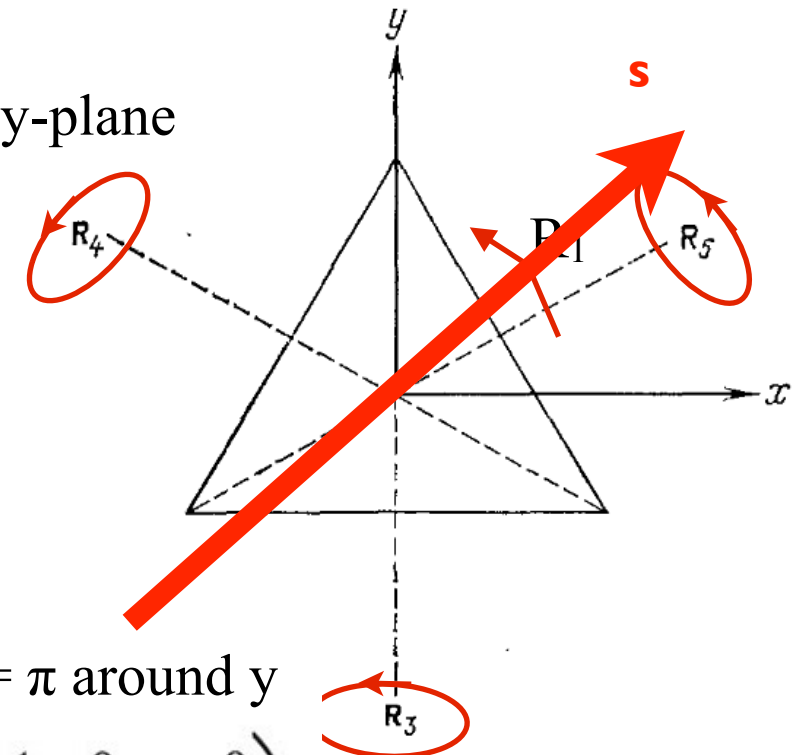
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1. 3-dimensional representation

$$\begin{array}{ccc} R_1=2\pi/3 & R_2=4\pi/3 \text{ around } z & R_3 = \pi \text{ around } y \\ T(R_1) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} & 0 \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} & T(R_2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} & 0 \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} & T(R_3) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \dots \text{etc} \end{array}$$



Representation of point group 32 in 3D rotation space of spin **S**

Example

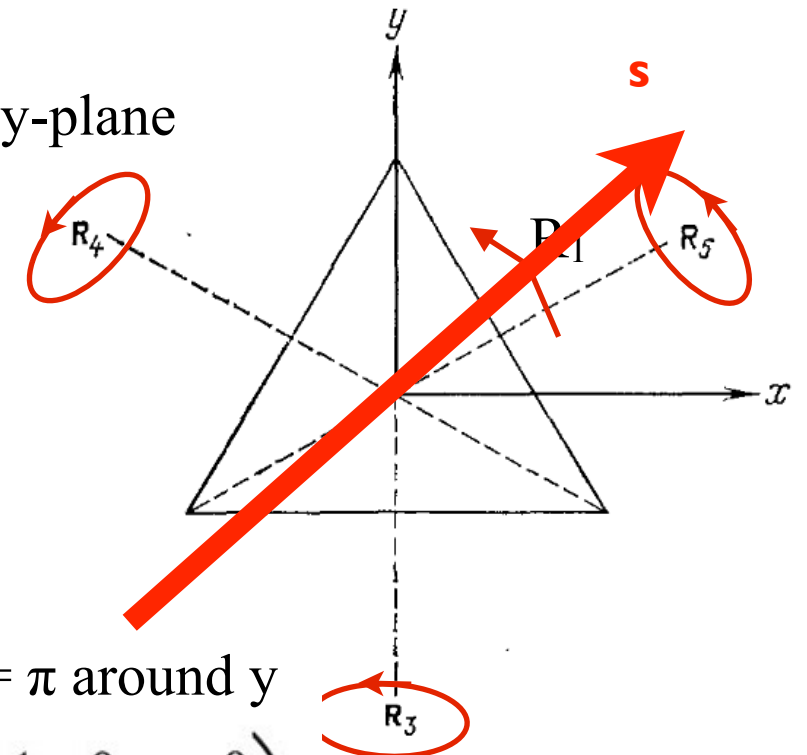
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2. By taking the one dimensional space of vector $\mathbf{e}_z$ alone we may generate very simple one-dimensional representation

$$T^{(2)}(R_1) = 1, T^{(2)}(R_2) = 1, T^{(2)}(R_3) = -1, T^{(2)}(R_4) = -1, T^{(2)}(R_5) = -1, T^{(2)}(E) = 1$$

Space group irreps, examples

dimensions up to 6 (cf. 3 for point groups)

Example 1

***Pnma* at X-point $[1/2, 0, 0]$ of BZ, two 2D-irreps, e.g. mX1**

g: Group elements, *G*: matrices or irreducible representation *irrep*

$$\begin{array}{l}
 g = \quad 1 \quad \quad 2_x \quad \quad 2_y \quad \quad 2_z \quad \quad -1 \quad \quad n \quad \quad m \quad \quad a \\
 G = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}
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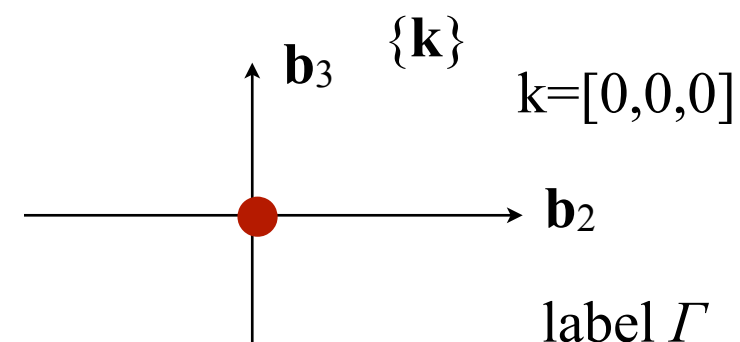
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Example 2

Pnma $k=[0,0,0]$, k19

irreps: eight 1D $\tau_1, \tau_2, \tau_3, \tau_4, \tau_5, \tau_6, \tau_7, \tau_8$

<i>g</i>	/2	/3	/4	/25	/26	/27	/28
$\hat{\tau}1$	1	1	1	1	1	1	1
$\tau 2$	1	1	1	-1	-1	-1	-1
$\hat{\tau}3$	1	-1	-1	1	1	-1	-1
$\hat{\tau}5$	-1	1	-1	1	-1	1	-1
$\hat{\tau}7$	-1	-1	1	1	-1	-1	1
$\hat{\tau}4 = \hat{\tau}3 \times \hat{\tau}2, \hat{\tau}6 = \hat{\tau}5 \times \hat{\tau}2, \hat{\tau}8 = \hat{\tau}7 \times \hat{\tau}2$							



$$G_k = G$$

Space group irreps, examples

dimensions up to 6 (cf. 3 for point groups)

Example 1

***Pnma* at X-point $[1/2, 0, 0]$ of BZ, two 2D-irreps, e.g. mX1**

g: Group elements, *G*: matrices or irreducible representation *irrep*

$$g = \quad 1 \quad 2_x \quad 2_y \quad 2_z \quad -1 \quad n \quad m \quad a$$

$$G = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

Example 2

Pnma $k=[0,0,0]$, k19

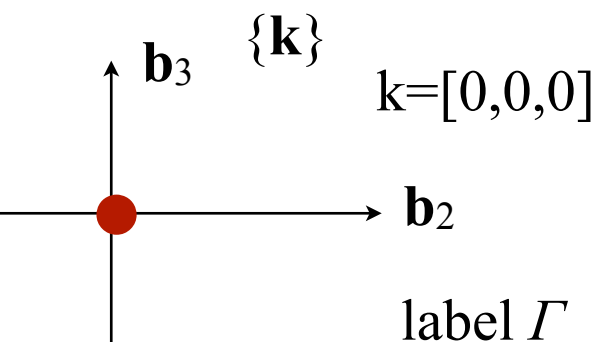
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Example 3

Higher dimensions: Ia3d (#230) $k=[1,0,0]$: 1(6D) $\oplus$ 3(2D)

$k=[1/2, 1/2, 1/2]$: 1(4D) $\oplus$ 2(2D)



$$G_k = G$$

Representation* Analysis (RA). Propagation vector $\mathbf{k}$ formalism. Magnetic mode $\mathbf{S}_0$ is specified in zeroth block of the cell == parent cell without centering translations

Magnetic moment
below a phase transition

$$\mathbf{S}(\mathbf{t}_n) = \text{Re} \left(C \mathbf{S}_0 e^{2\pi i \mathbf{t}_n \mathbf{k}} \right) \sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$$

amplitude or
mixing
coefficients

magnetic mode

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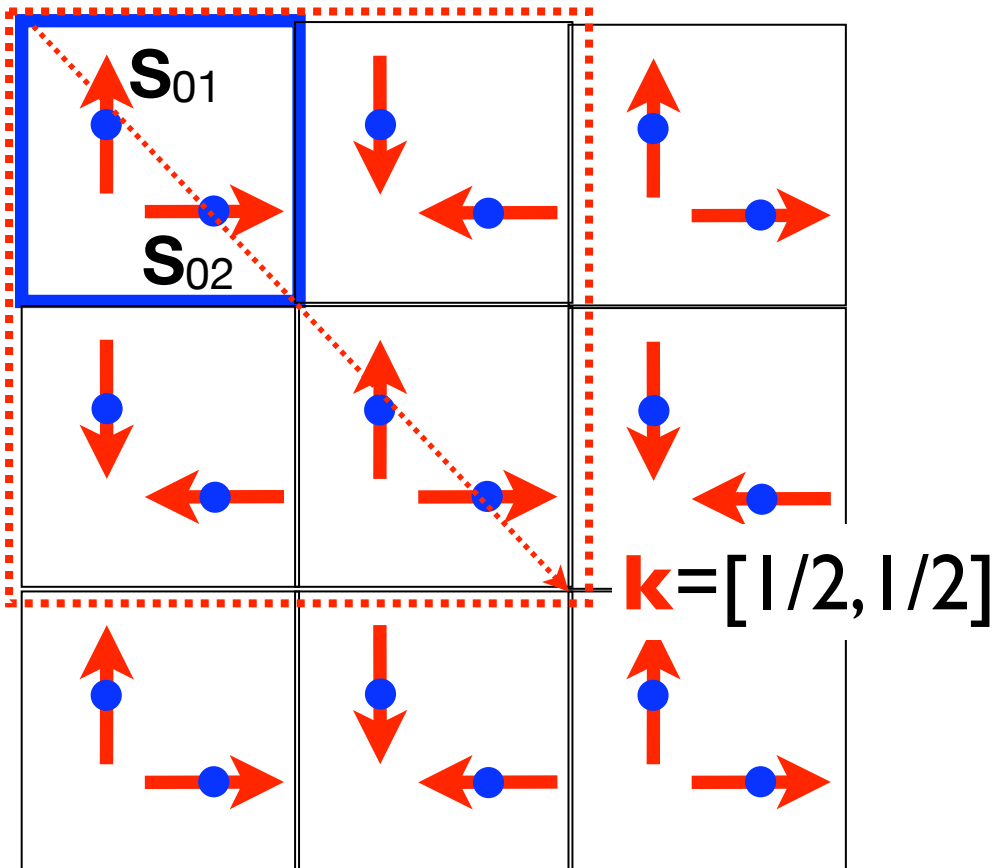
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0th cell with many atoms in general

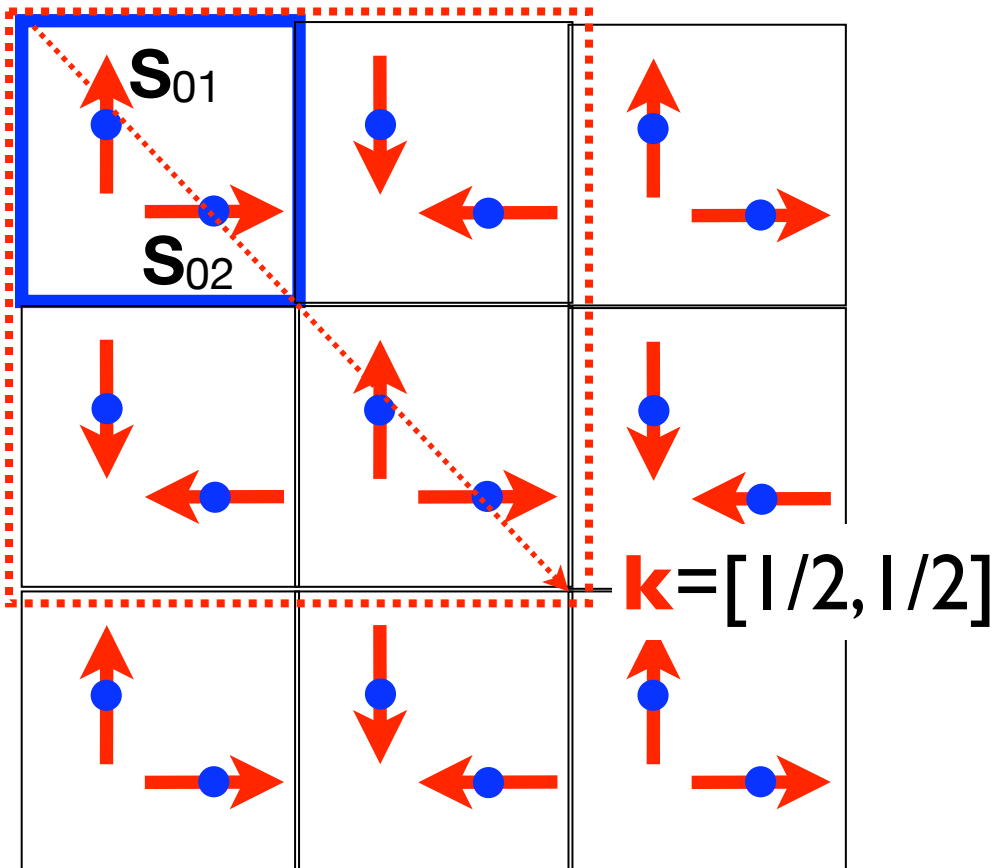


*irreducible representation irrep:
each group element $g \rightarrow$ matrix $\tau(g)$ that
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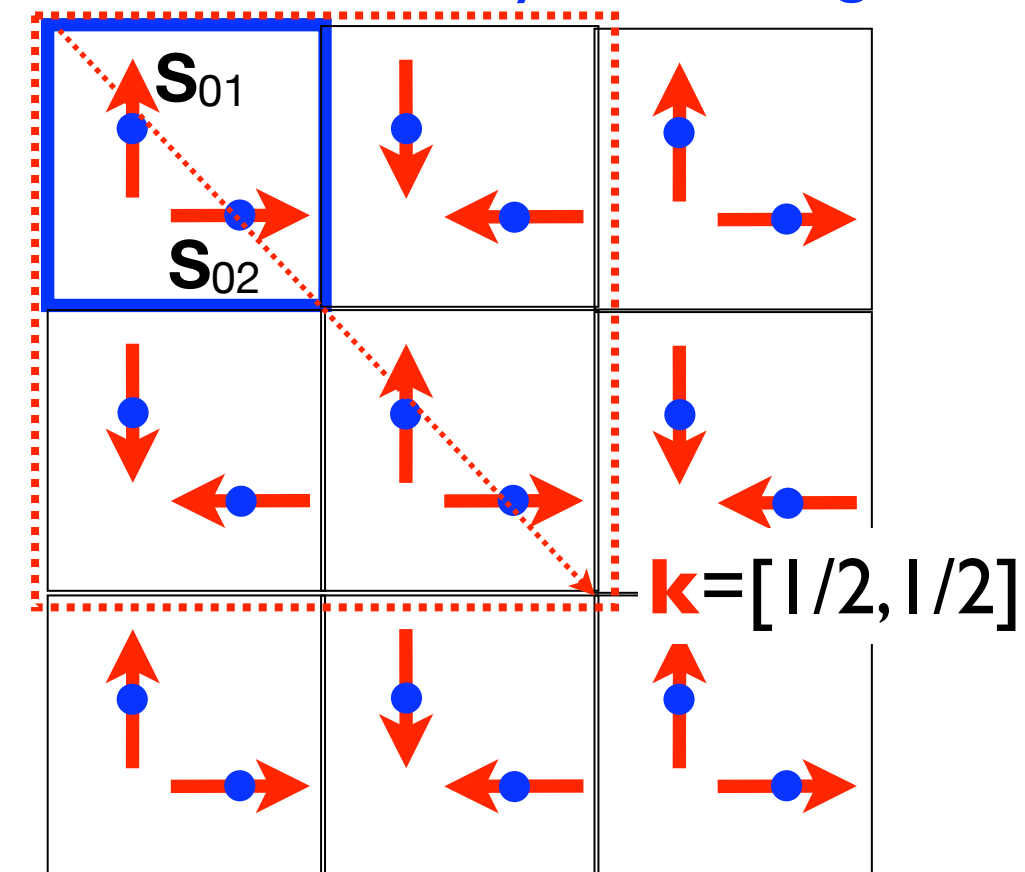
$$\longrightarrow \mathbf{S}_0 = \begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \dots \\ \dots \\ \dots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$$

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Magnetic moment below a phase transition

0th cell with many atoms in general



E.g., atom1 $\mathbf{S}_{01} = \mathbf{e}_y$

atom2 $\mathbf{S}_{02} = \mathbf{e}_x$

$$\mathbf{S}_1(\mathbf{t}_n) = C\mathbf{e}_y \cos(\pi(t_{nx} + t_{ny}))$$

$$\mathbf{S}_2(\mathbf{t}_n) = C\mathbf{e}_x \cos(\pi(t_{nx} + t_{ny}))$$

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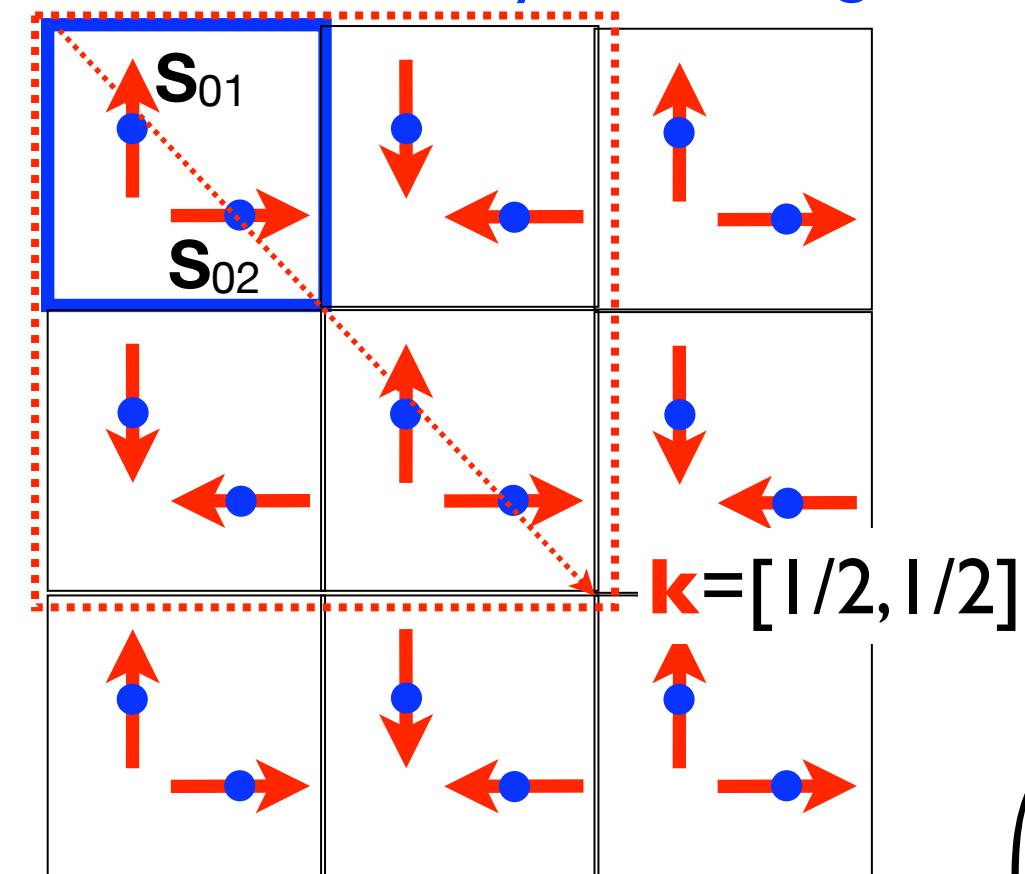
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$\mathbf{S}_0 =$

$$\begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

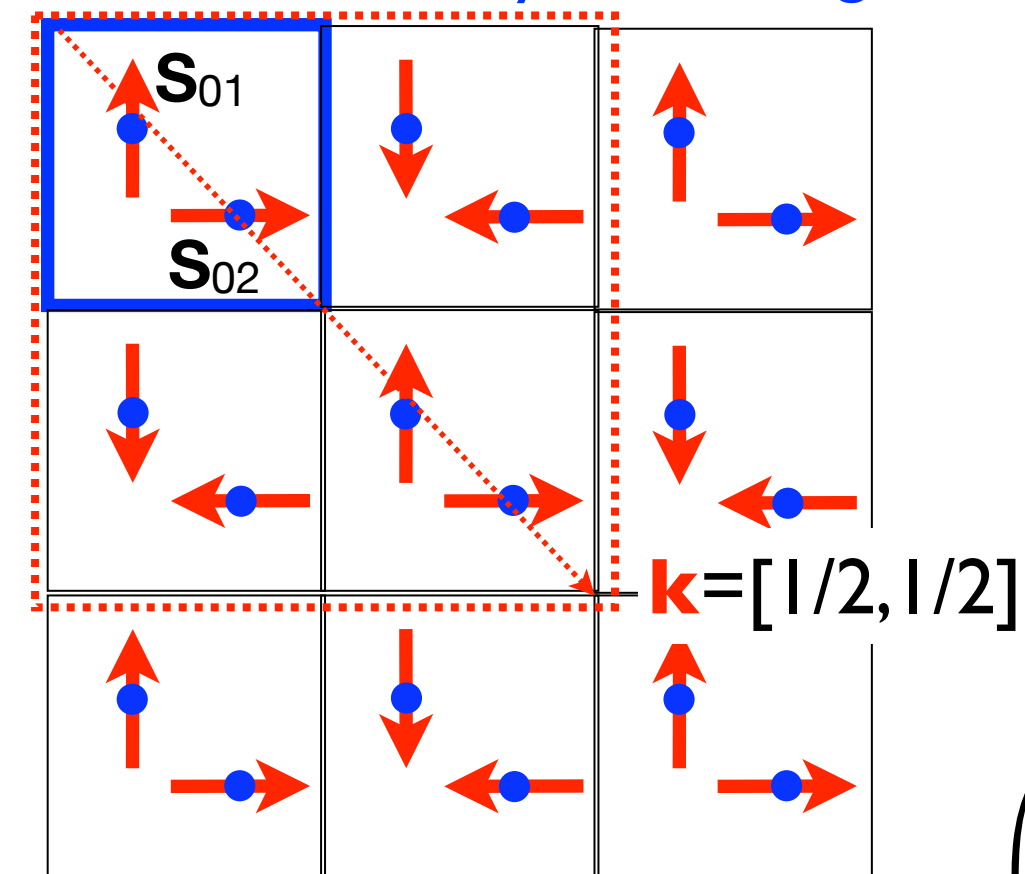
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$\mathbf{S}_0$ and $C = |C|e^{i\varphi}$ are
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$$s_{x1} = |s_{x1}| e^{i\phi_{x1}} \mathbf{e}_x$$

$$s_{y1} = |s_{y1}| e^{i\phi_{y1}} \mathbf{e}_y$$

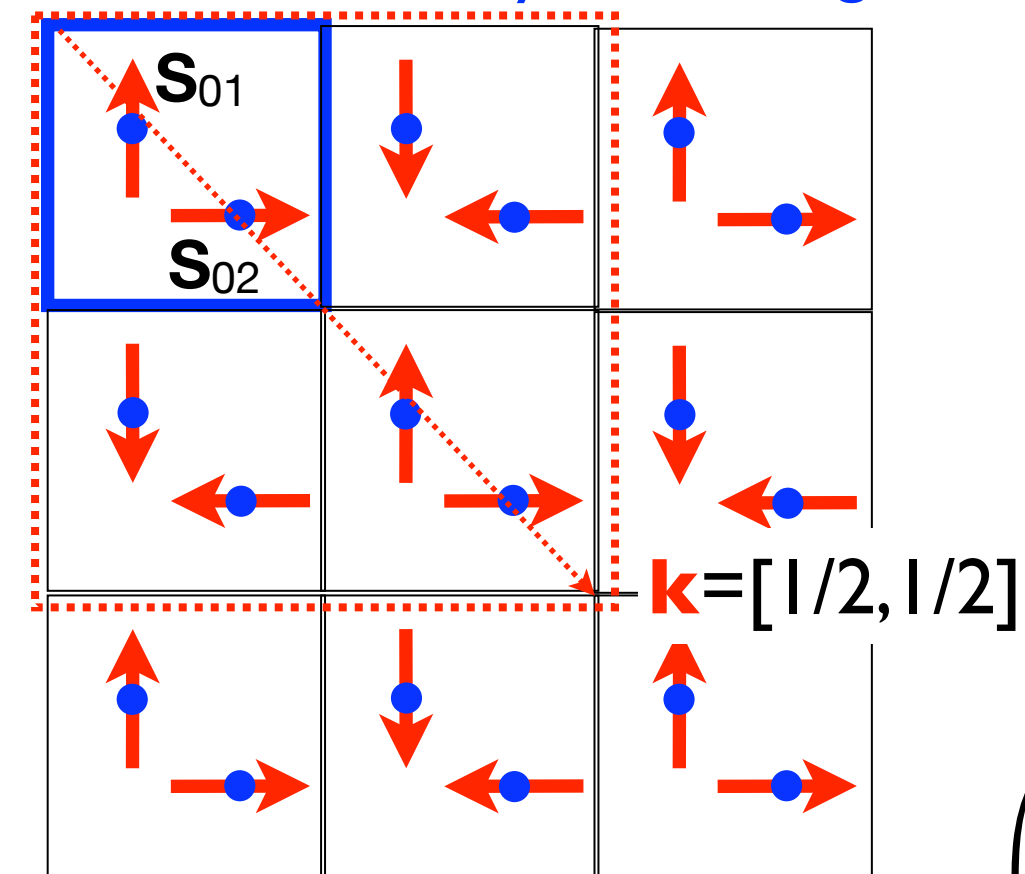
...

$$s_{zN} = |s_{zN}| e^{i\phi_{zN}} \mathbf{e}_z$$

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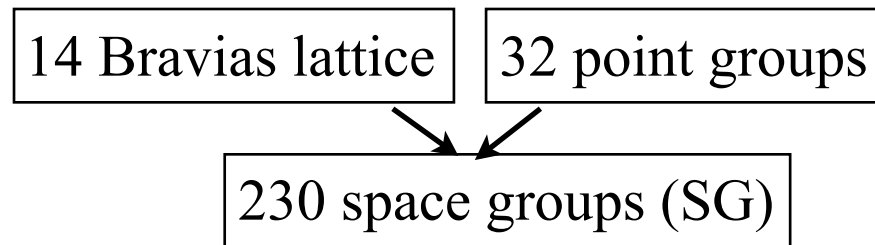
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...

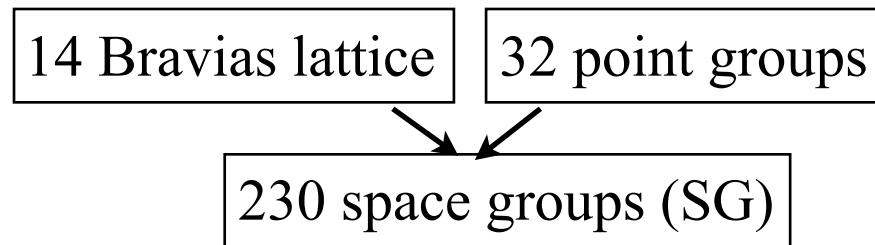
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Magnetic symmetry. 1651 3D-Shubnikov (Sh or $\mathbb{I}$) space groups



antisymmetry: Heesh (1929), Shubnikov (1945).
groups: Zamorzaev (1953, 1957); Belov, Neronova, Smirnova (1955)
spin reversal: Landau and Lifschitz (1957)

Magnetic symmetry. 1651 3D-Shubnikov (Sh or $\mathbb{M}$) space groups



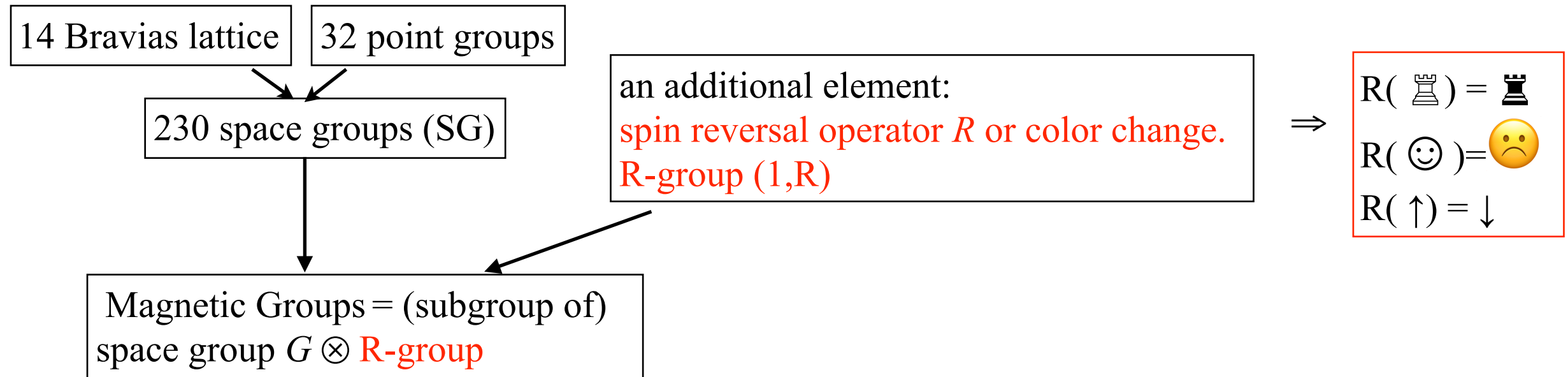
an additional element:
spin reversal operator R or color change.
 R -group $(1, R)$

$\Rightarrow$

$R(\text{♖}) = \text{♜}$
 $R(\text{☺}) = \text{☹}$
 $R(\uparrow) = \downarrow$

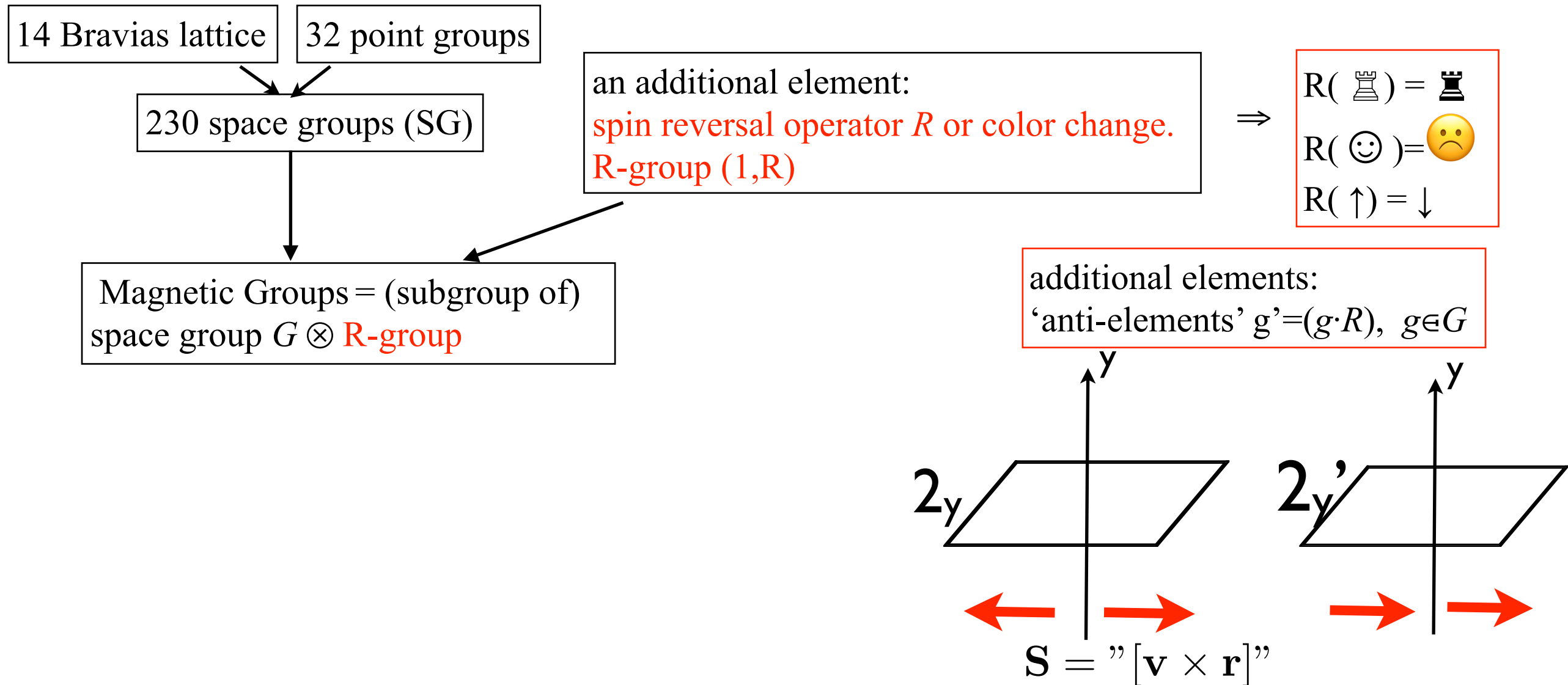
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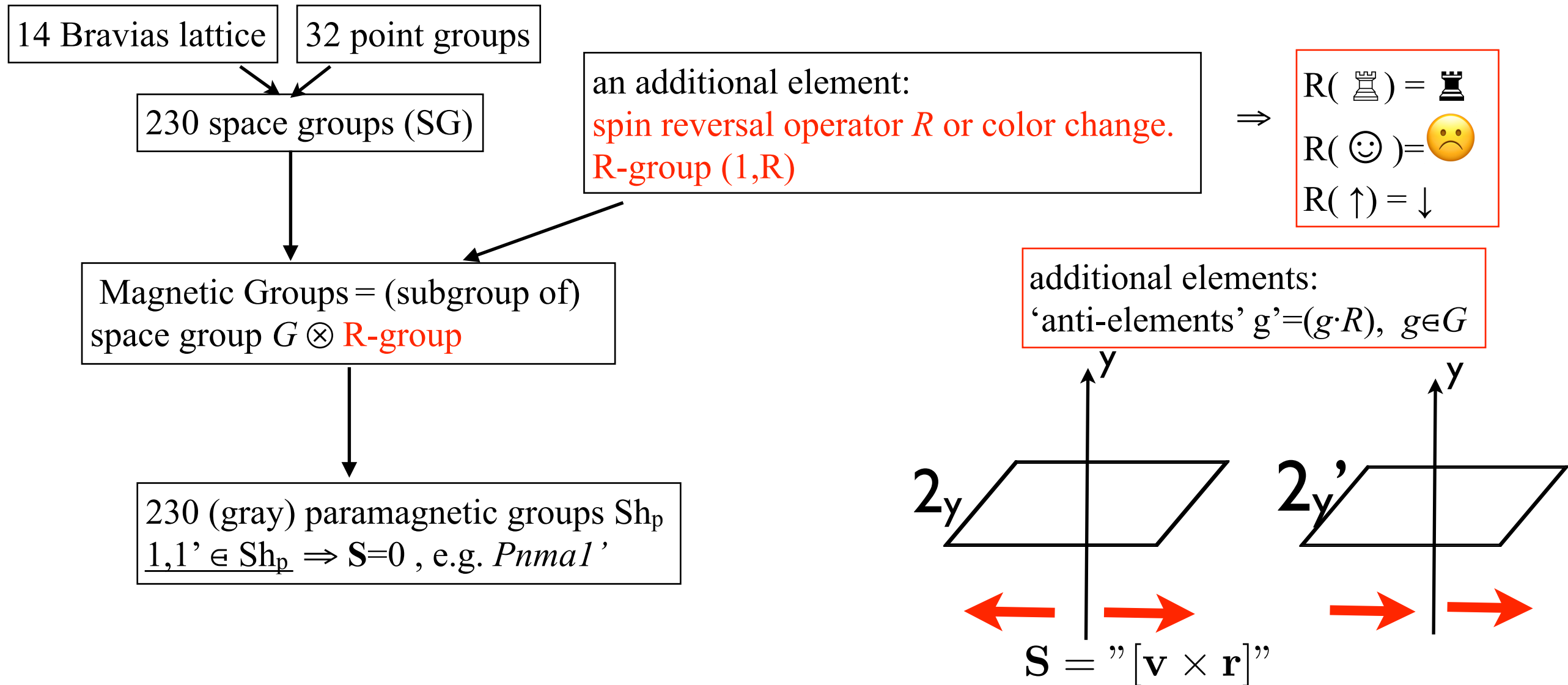
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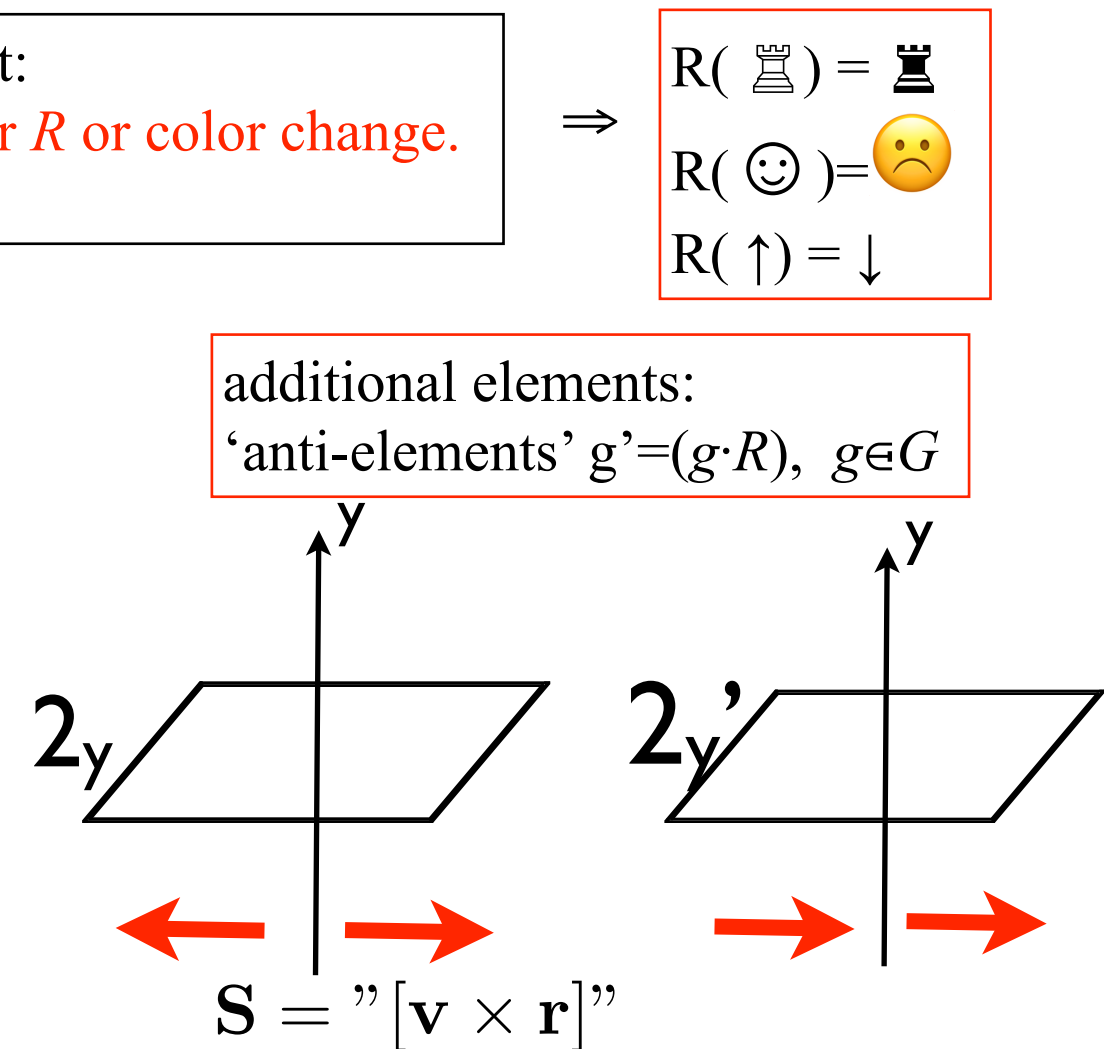
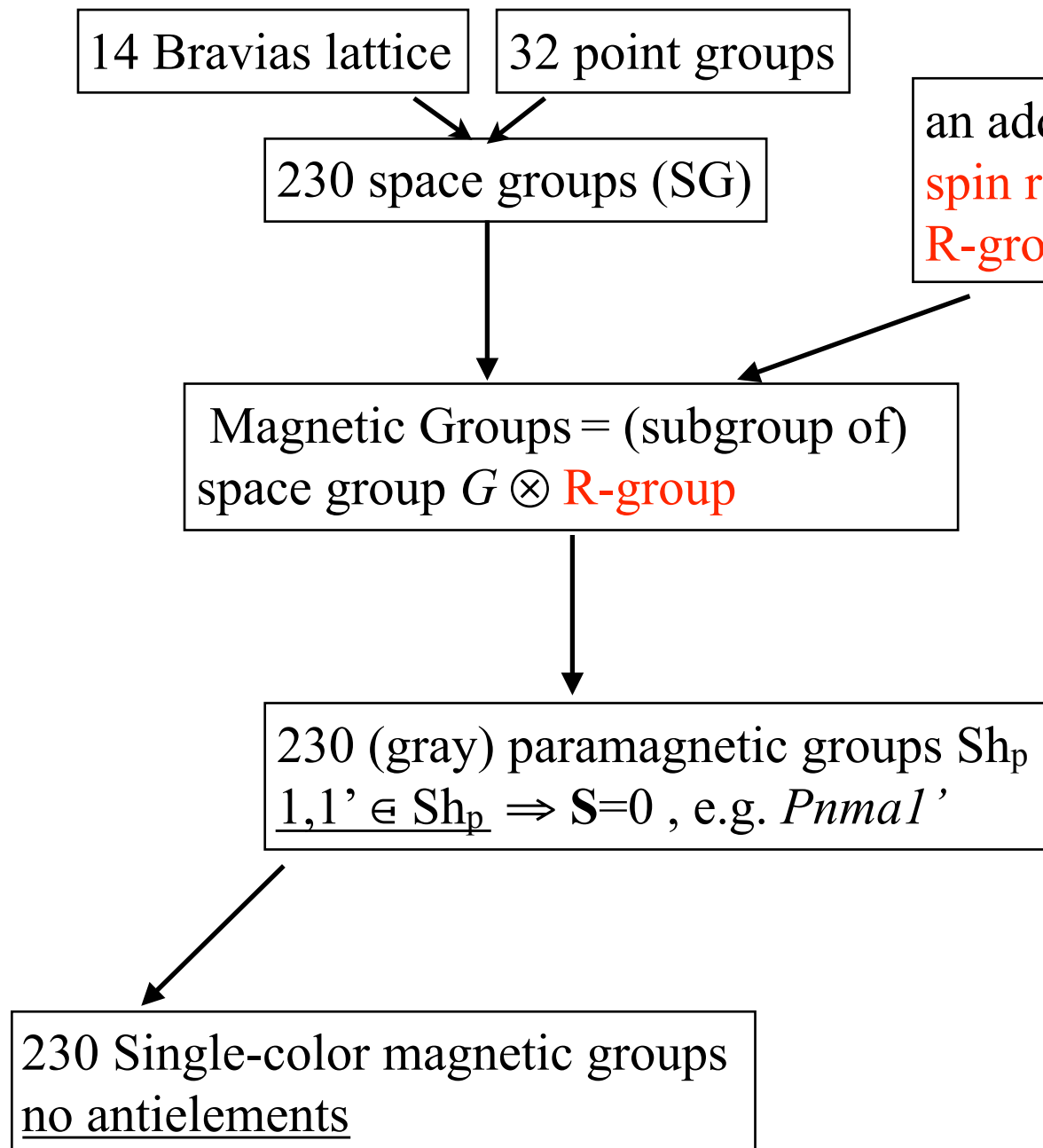
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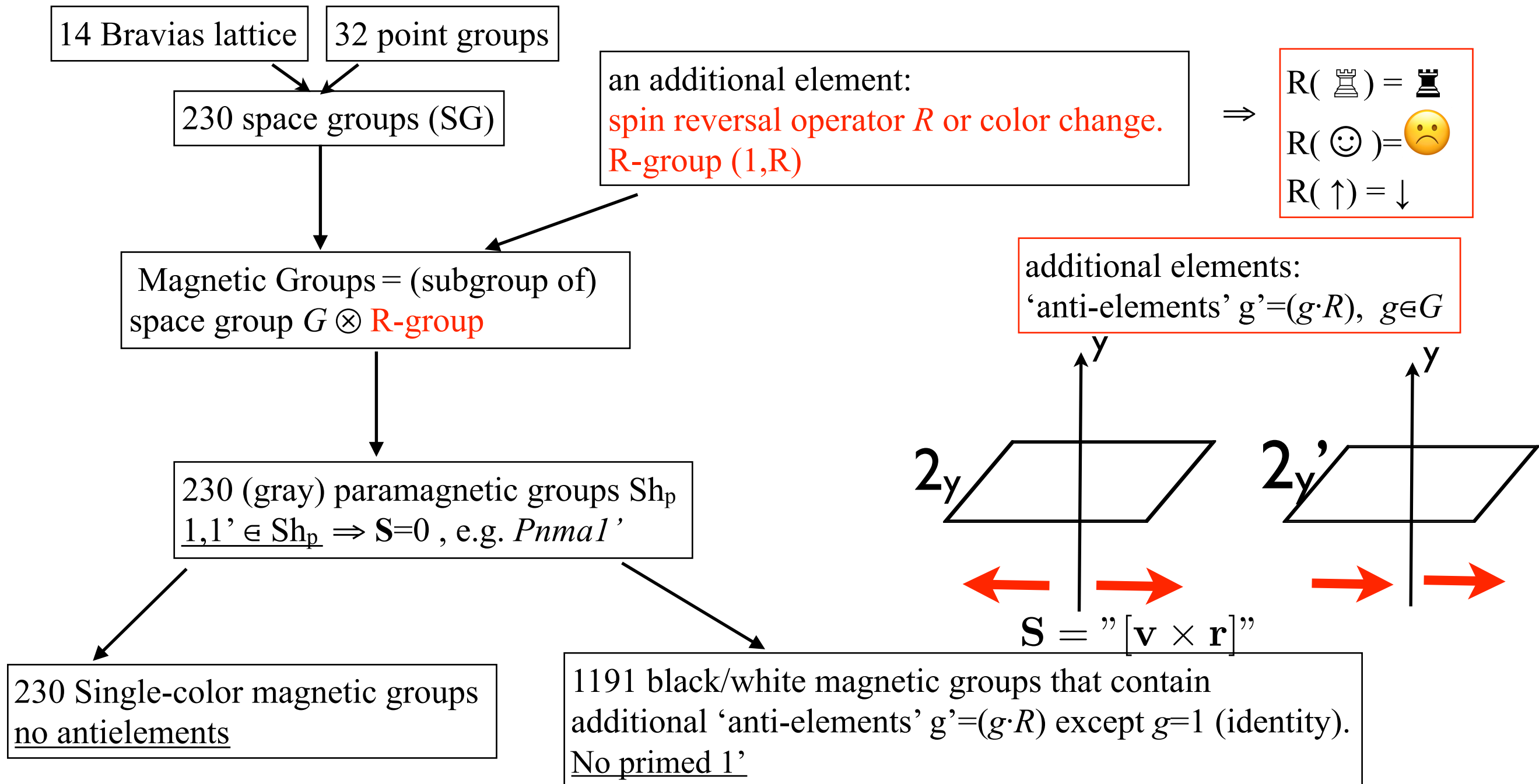
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Examples of Sh groups

59 *Pmmn*

Pm'mn

Pmmn'

**Pm'm'n*

**Pmm'n'*

Pm'm'n'

P_{2c}mmn

P_{2c}m'mn

P_{2c}m'm'n

62 *Pnma*

Pn'ma

Pnm'a

Pnma'

**Pn'm'a*

**Pnm'a'*

**Pn'ma'*

Pn'm'a'

Examples of Sh groups

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Pm'mn

Pmmn'

**Pm'm'n*

**Pmm'n'*

Pm'm'n'

P_{2c}mmn

P_{2c}m'mn

P_{2c}m'm'n

62 *Pnma*

Pn'ma

Pnm'a

Pnma'

**Pn'm'a*

**Pnm'a'*

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Pn'm'a'

Ferromagnetic groups: point symmetry allows FM orientation of spins
Only 275 FM groups out of 1651...

Examples of Sh groups

59 $Pmmn$

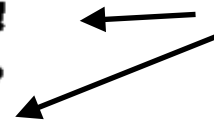
$Pm'mn$
 $Pmmn'$
 $*Pm'm'n$
 $*Pmm'n'$
 $Pm'm'n'$
 $P_{2c}mmn$
 $P_{2c}m'mn$
 $P_{2c}m'm'n$



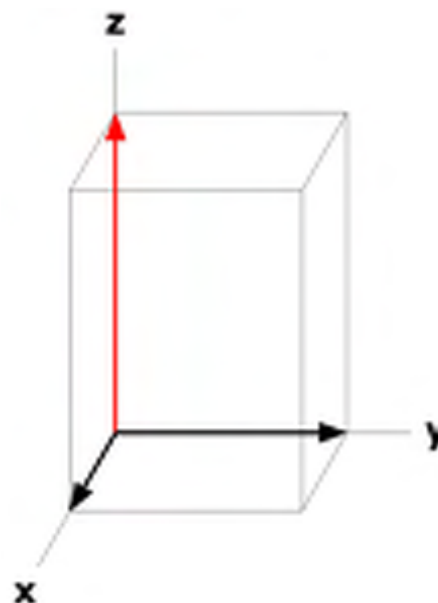
recap:
 for 'anti-elements' $g'=(g \cdot R)$, $g \in G$
 g can be a pure translation t , so t'
 gives centering/doubling

62 $Pnma$

$Pn'ma$
 $Pnm'a$
 $Pnma'$
 $*Pn'm'a$
 $*Pnm'a'$
 $*Pn'ma'$
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Ferromagnetic groups: point
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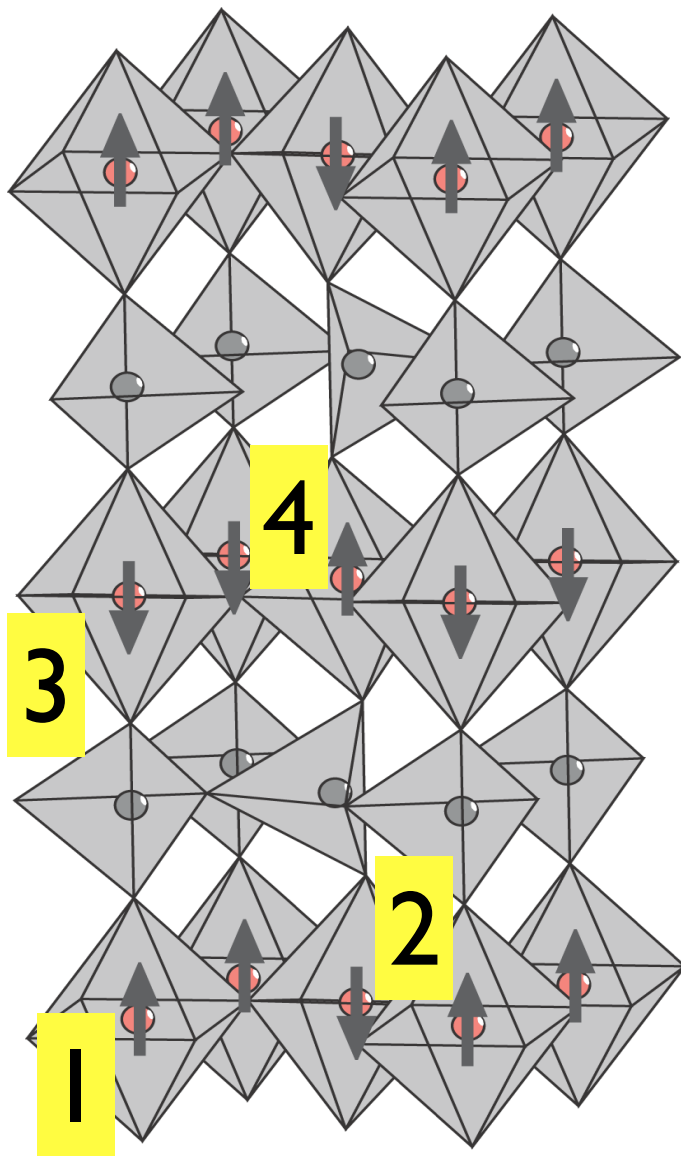
$$P_{2c} = P_{a,b,2c}$$

$$t_a = c = (0,0,1)$$

Two ways of description of magnetic structures

Magnetic structure is an axial vector function $\mathbf{S}(\mathbf{r})$ defined on the discrete system of points (atoms), e.g. $\mathbf{S}(\mathbf{r}) = \mathbf{s}(\mathbf{r}_1) \oplus \mathbf{s}(\mathbf{r}_2) \oplus \mathbf{s}(\mathbf{r}_3) \oplus \mathbf{s}(\mathbf{r}_4)$

Crystal with space group G

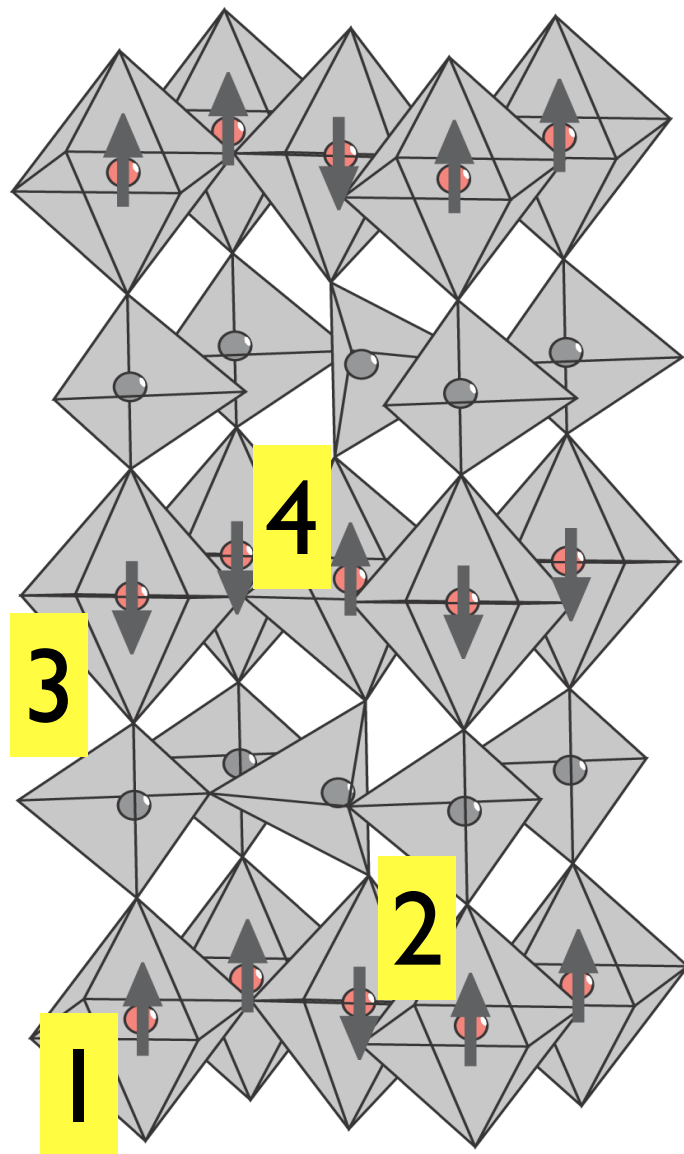


1. **How to make $\mathbf{S}(\mathbf{r})$ invariant? Find (new) symmetry elements.**
 $\mathbf{g}_{\text{new}} \mathbf{S}(\mathbf{r}) = \mathbf{S}(\mathbf{r})$ to itself, where $\mathbf{g}_{\text{new}} \in G_{\text{sh}}$ subgroup of PG
paramagnetic space group: $\text{PG} = G \otimes 1'$, where $1'$ = spin/time reversal, G (parent space group).

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or

2. **How should $\mathbf{S}(\mathbf{r})$ be transformed under elements of G ?**

$g\mathbf{S}(\mathbf{r}) = \mathbf{S}^{\text{new}}_g(\mathbf{r})$ to different functions for each $g \in G$

Two ways of description of magnetic structures

1. How to make $\mathbf{S}(\mathbf{r})$ invariant?
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MSG Example:

87.1.733	I4/m
87.2.734	I4/m1'
87.3.735	I4'/m
87.4.736	I4/m'
87.5.737	I4'/m'
87.6.738	I _P 4/m
87.7.739	I _P 4'/m
87.8.740	I _P 4/m'
87.9.741	I _P 4'/m'

1. **Magnetic or Shubnikov groups MSG.** Historically the first way of description (Landau, Lifshitz 1951). $\mathbf{S}(\mathbf{r})$ invariant under the Shubnikov subgroup G_{sh} of $G \otimes 1'$ ($1'$ = spin/time reversal).

Identifying those symmetry elements that leave $\mathbf{S}(\mathbf{r})$ invariant.

The MSG symbol looks similar to SG one, e.g. $I4/m'$

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VS.

2. **Representation analysis.** (Bertaut 1967) $\mathbf{S}(\mathbf{r})$ is transformed to $\mathbf{S}^i(\mathbf{r})$ under $g \in G$ (parent space group) according to a single irreducible representation τ_i of G .
Identifying/classifying all the functions $\mathbf{S}^i(\mathbf{r})$ that appears under all symmetry operators of the **same space group G with propagation vector $\mathbf{k}$**

*each group element $g \rightarrow$ matrix $\tau(g)$

Two ways of description of magnetic structures

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The MSG symbol looks similar to SG one, e.g. $I4/m'$

VS.

2. **Representation analysis.** (Bertaut 1967) $\mathbf{S}(\mathbf{r})$ is transformed to $\mathbf{S}^i(\mathbf{r})$ under $g \in G$ (parent space group) according to a single irreducible representation τ_i of G . Identifying/classifying all the functions $\mathbf{S}^i(\mathbf{r})$ that appears under all symmetry operators of the **same space group G with propagation vector $\mathbf{k}$**

irrep Example:

$I4/m$, $\mathbf{k}=0$ has 8 1D irreps $\tau_1, \dots, \tau_8$.

	h_1	h_{14}	h_4	h_{15}	h_{25}	h_{38}	h_{28}	h_{39}
τ, ψ	1	4_z^+	2_z	4_z^-	-1	-4_z^+	m_z	-4_z^-
τ_2	1	1	1	1	-1	-1	-1	-1
τ_3	1	i	-1	$-i$	1	i	-1	$-i$
τ_5	1	-1	1	-1	1	-1	1	-1
τ_7	1	$-i$	-1	i	1	$-i$	-1	i

*each group element $g \rightarrow$ matrix $\tau(g)$

Example of Shubnikov group. Magnetic structure of Iron based superconductor KFeSe

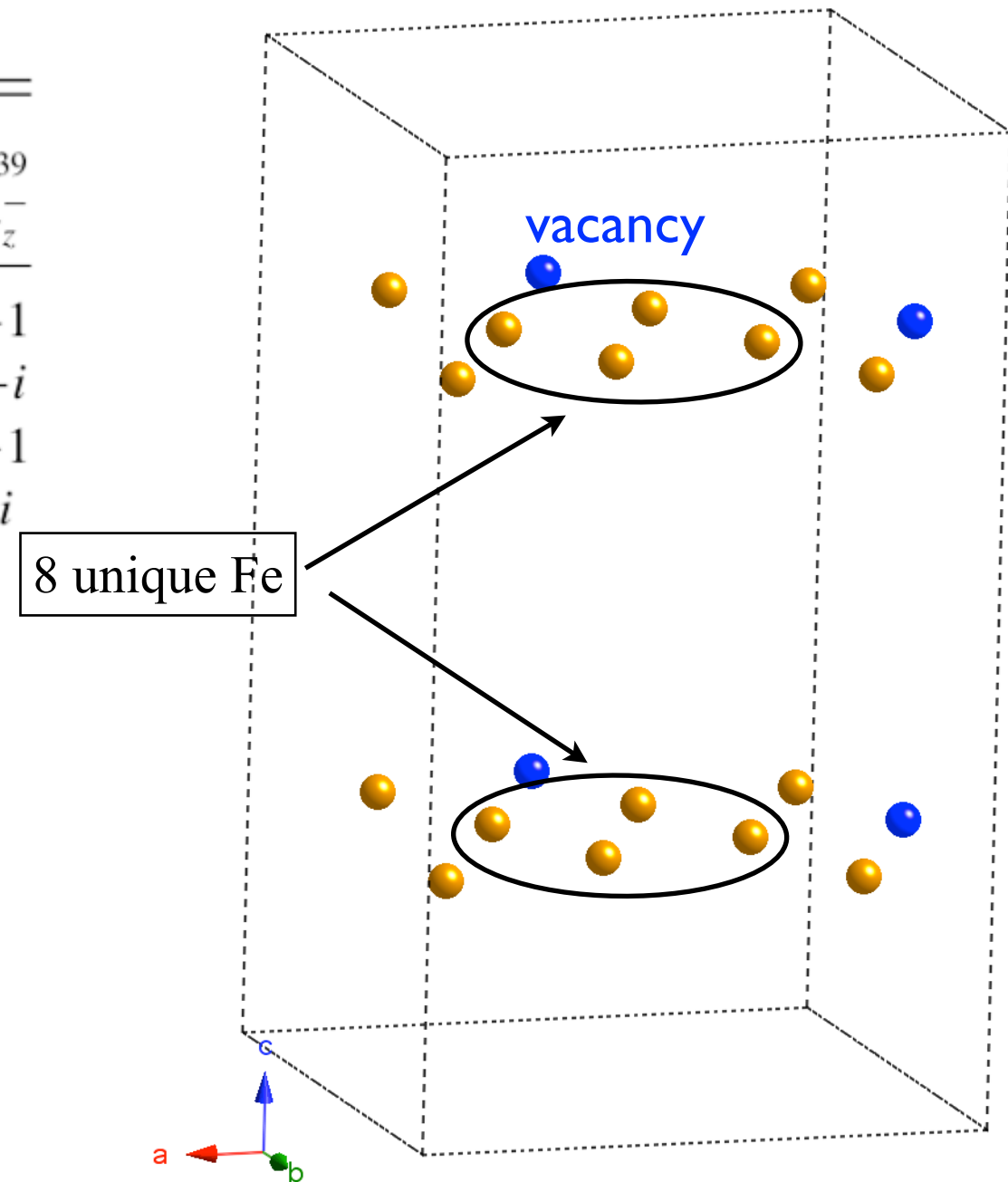
$I4/m$, $k=0$ has 8 1D irreps $\tau_1, \dots, \tau_8$.

4 real irreps $\leftrightarrow$ Shubnikov groups of $I4/m$

4 complex irreps

τ, ψ	h_1	h_{14}	h_4	h_{15}	h_{25}	h_{38}	h_{28}	h_{39}
	1	4_z^+	2_z	4_z^-	-1	-4_z^+	m_z	-4_z^-
$\tau_2 \ I4/m'$	1	1	1	1	-1	-1	-1	-1
τ_3	1	i	-1	$-i$	1	i	-1	$-i$
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One unit cell with 16 Fe



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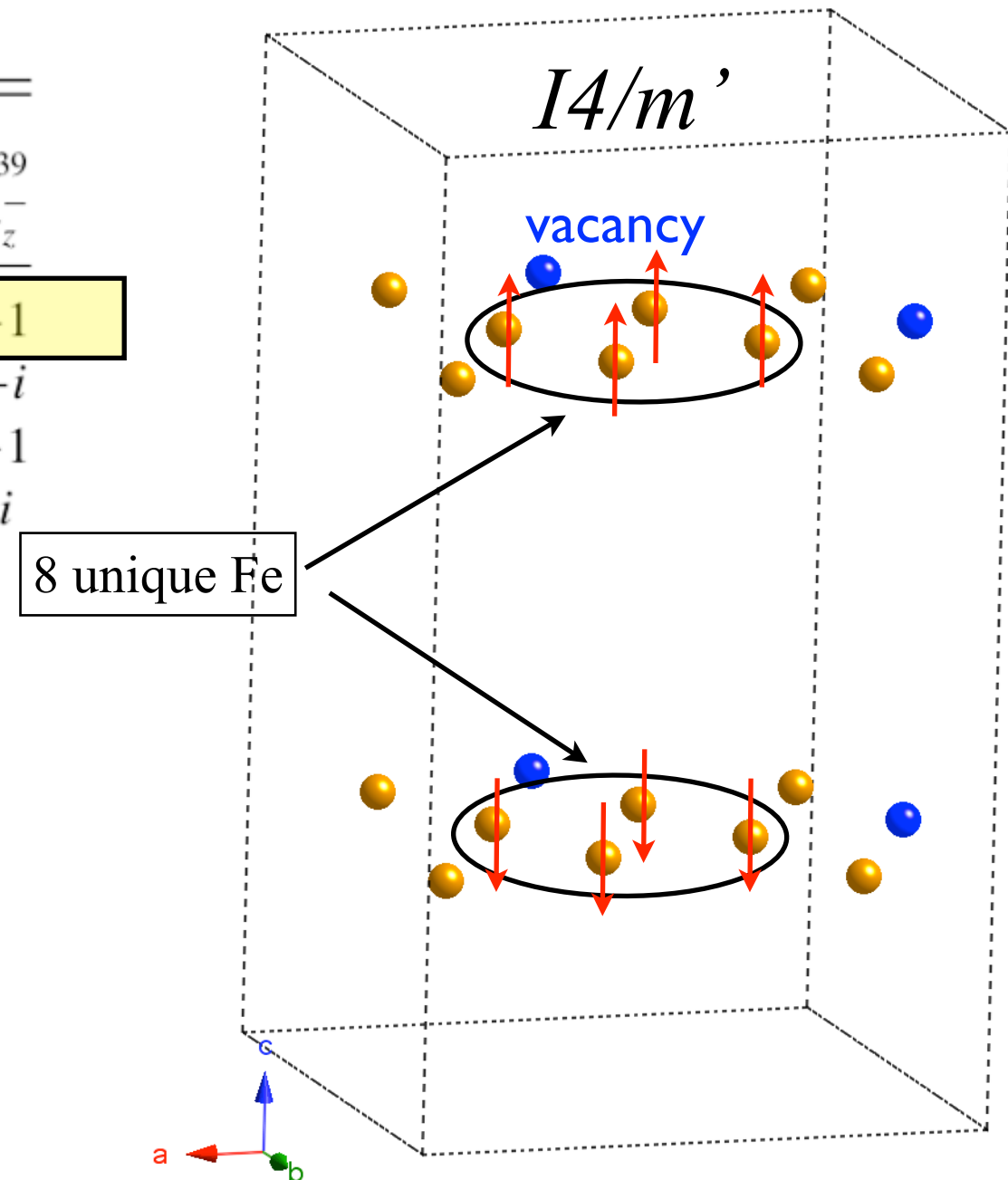
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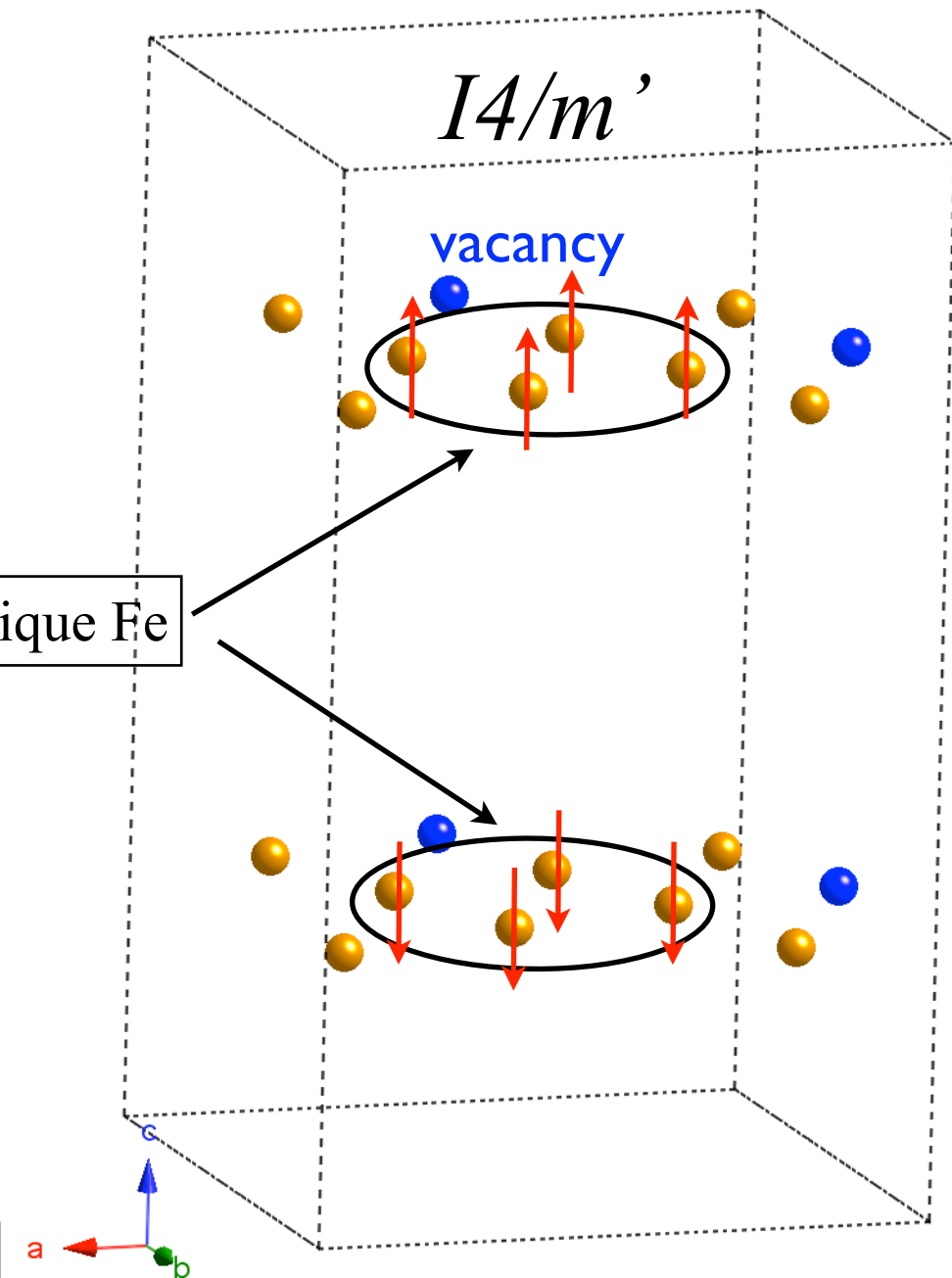
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8 unique Fe



Example of Shubnikov group. Magnetic structure of Iron based superconductor KFeSe

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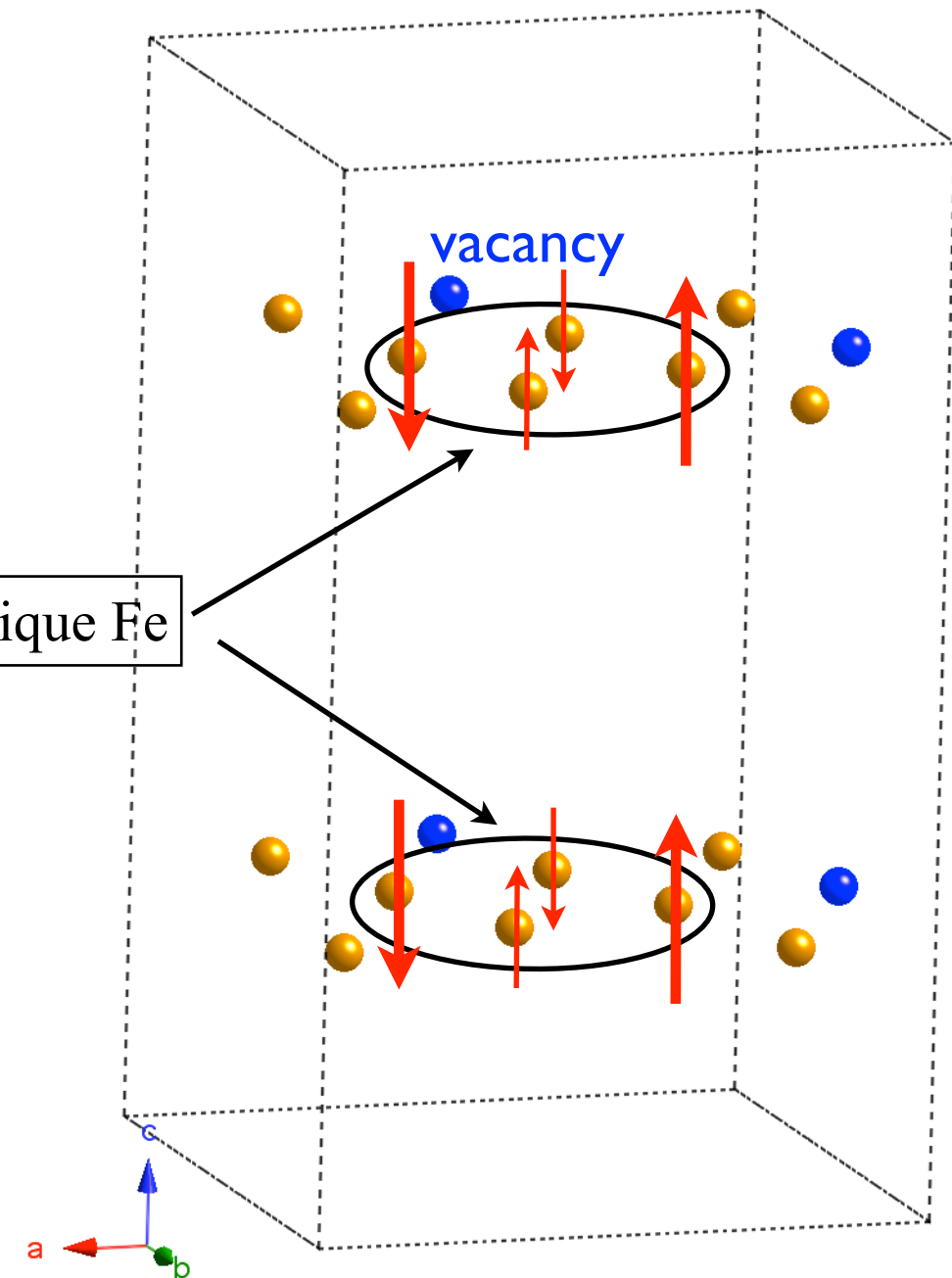
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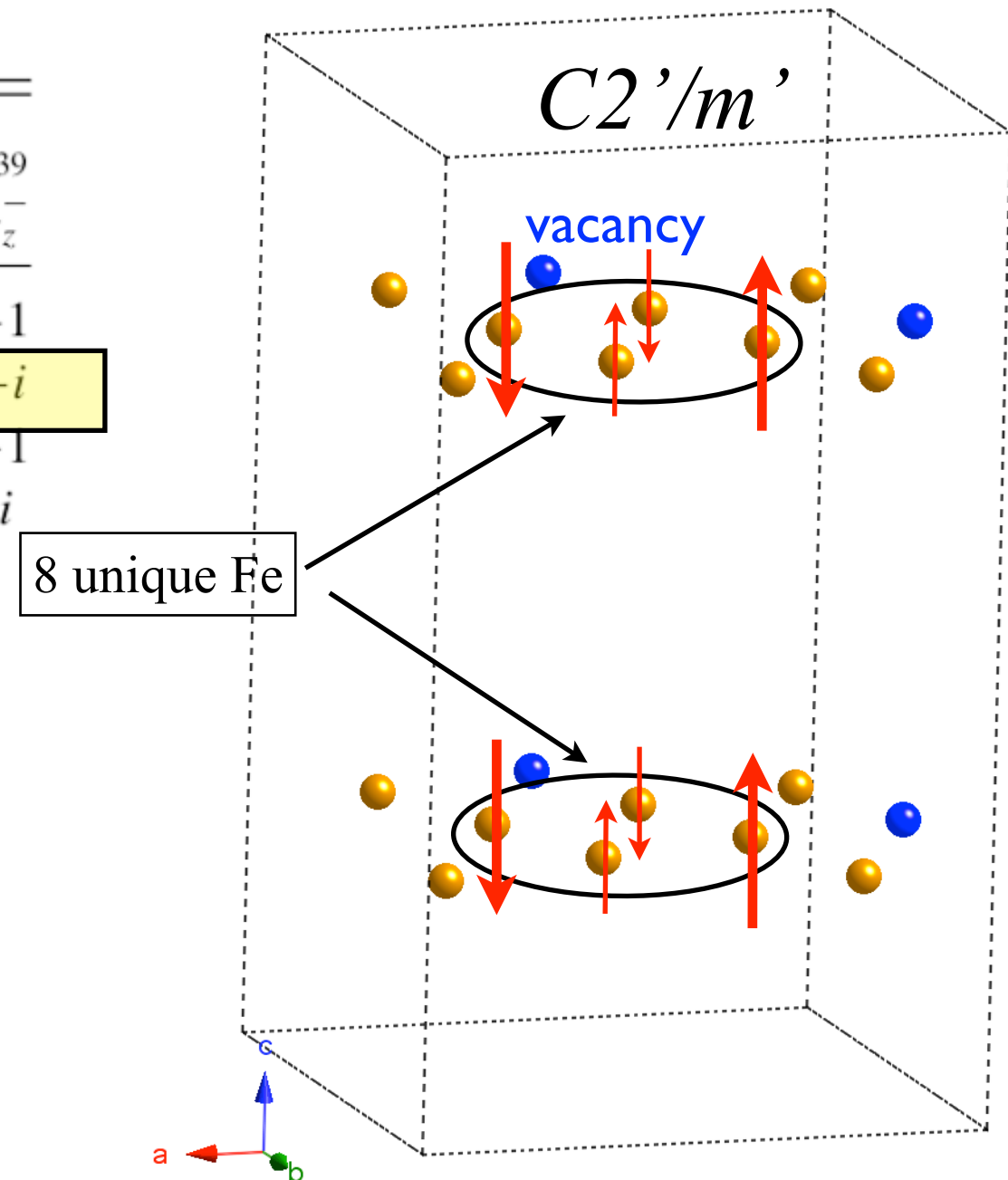
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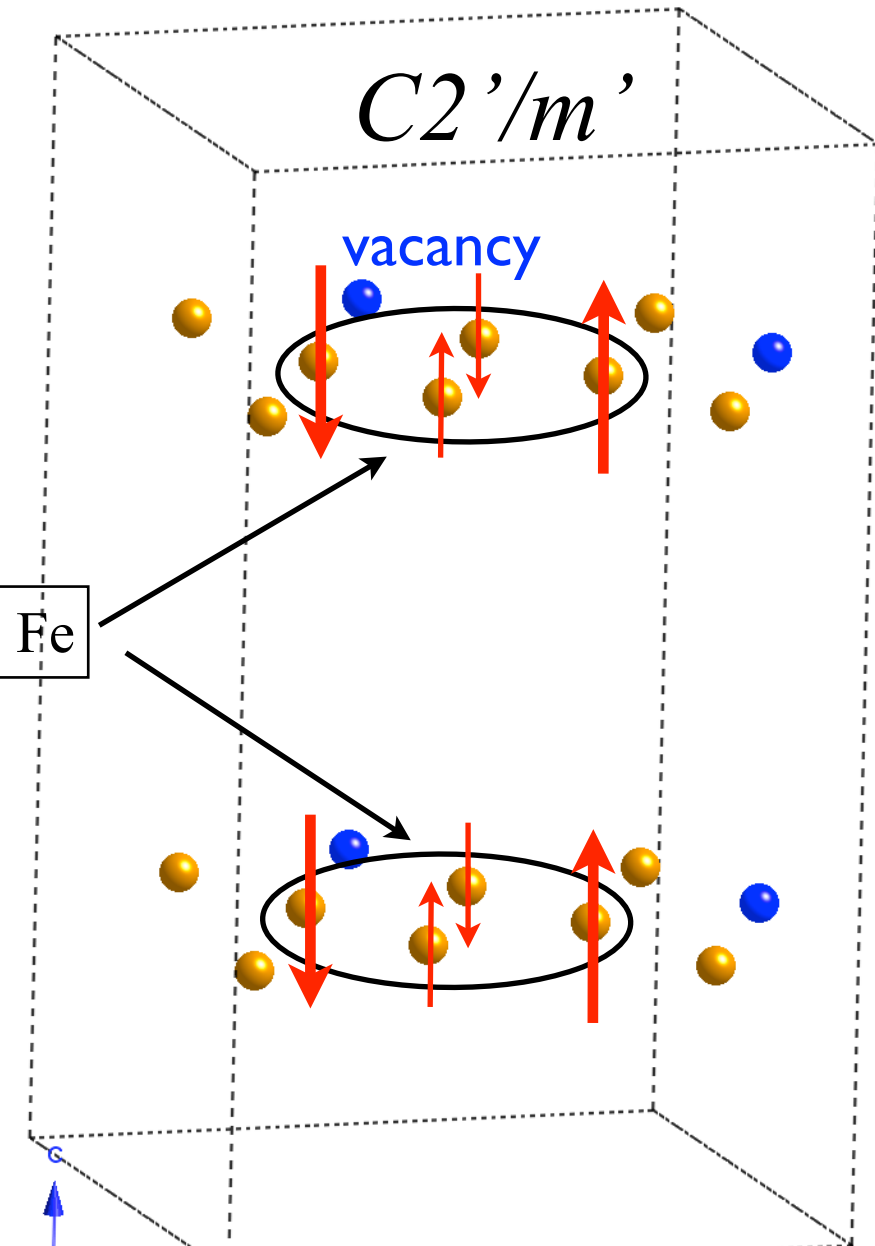
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$$\times |C| \exp(i\varphi) = \frac{1}{2} + i\frac{\sqrt{3}}{2}$$

Magnetic space groups and representation analysis: competing or friendly concepts?

In 1960th-70th opposed

E. F. Bertaut, CNRS, Grenoble
Representation Analysis (RA)*

W. Opechovski, UBC, Vancouver
Shubnikov magnetic space
groups

even until recent times RA was considered to be more
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Currently > 2010-...

(Representation Analysis) and (Magnetic space groups) are
complementary and **must** be used together to fully identify the
magnetic symmetry.

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“Old new” trends in magnetic structure determination from ND. **Currently there is solid understanding that both RA and Shubnikov magnetic symmetry should be used together.** Big progress in software tools during last years in this way of analysis ...



IUCr Commission on
Magnetic Structures



<http://magcryst.org>

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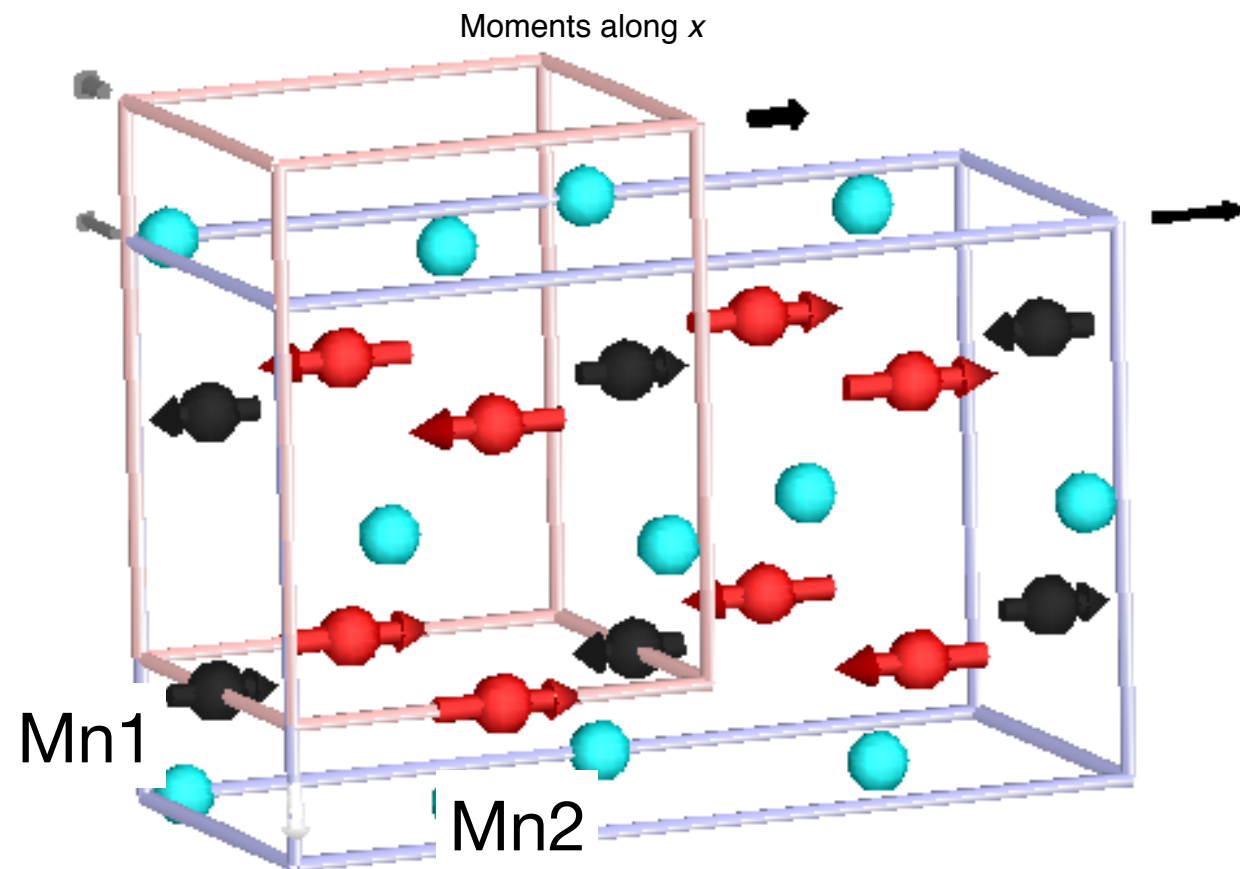
- In many (most) cases this allows one **to find a hidden symmetry**, which is not evident from the representation analysis alone.
- **Regular practice for crystal structure transitions:** This approach is routinely used by crystallographers in the analysis of crystal phase transition,
- **Magnetic transitions:** Usually, representation approach with a single arm and general direction of order parameter of propagation vector star. Possible high symmetry Shubnikov subgroups are lost.

Two examples of magnetic structures

multiferroic TmMnO_3

one-arm two dimensional irrep $\mathbf{k}=[1/2,0,0]$.

Ferro-electric phase polar magnetic group P_bmn2_1



V. Yu. Pomjakushin, et al New Journal of Physics vol. 11, 043019 (2009)

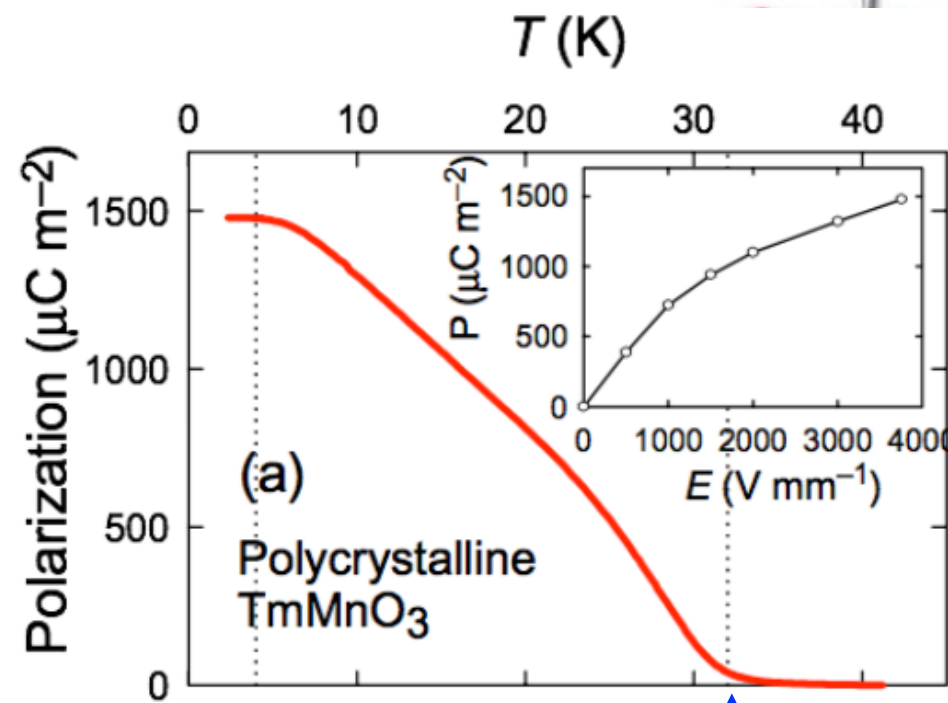
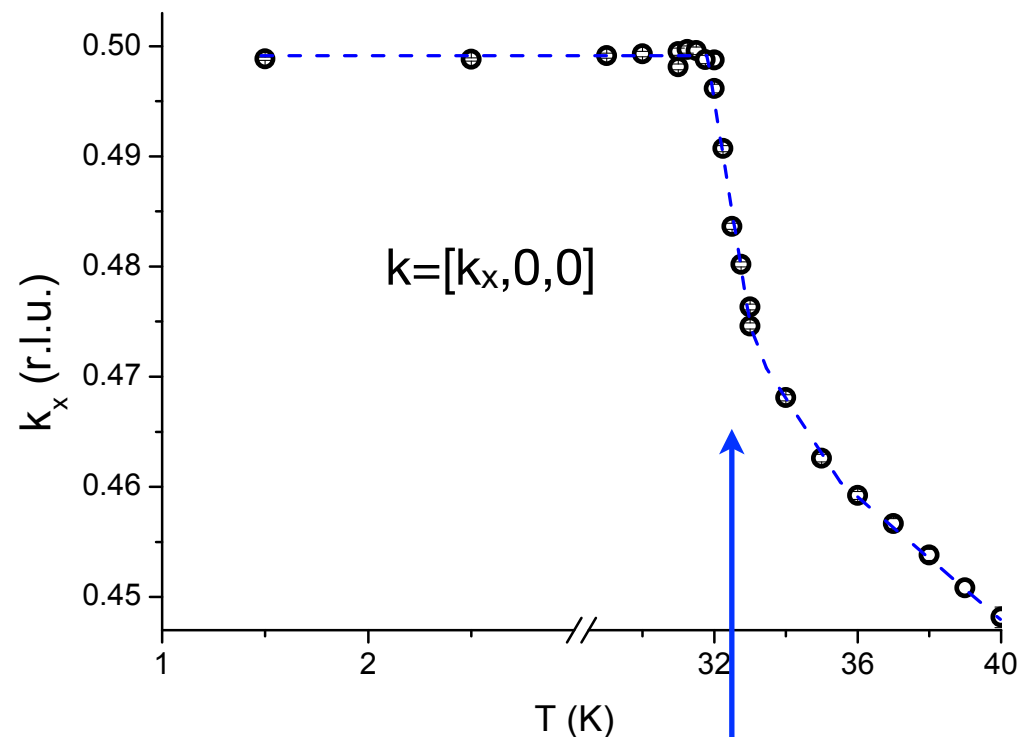
magnetic Weyl semimetal CeAlGe

Topologically nontrivial magnetisation textures in real-space

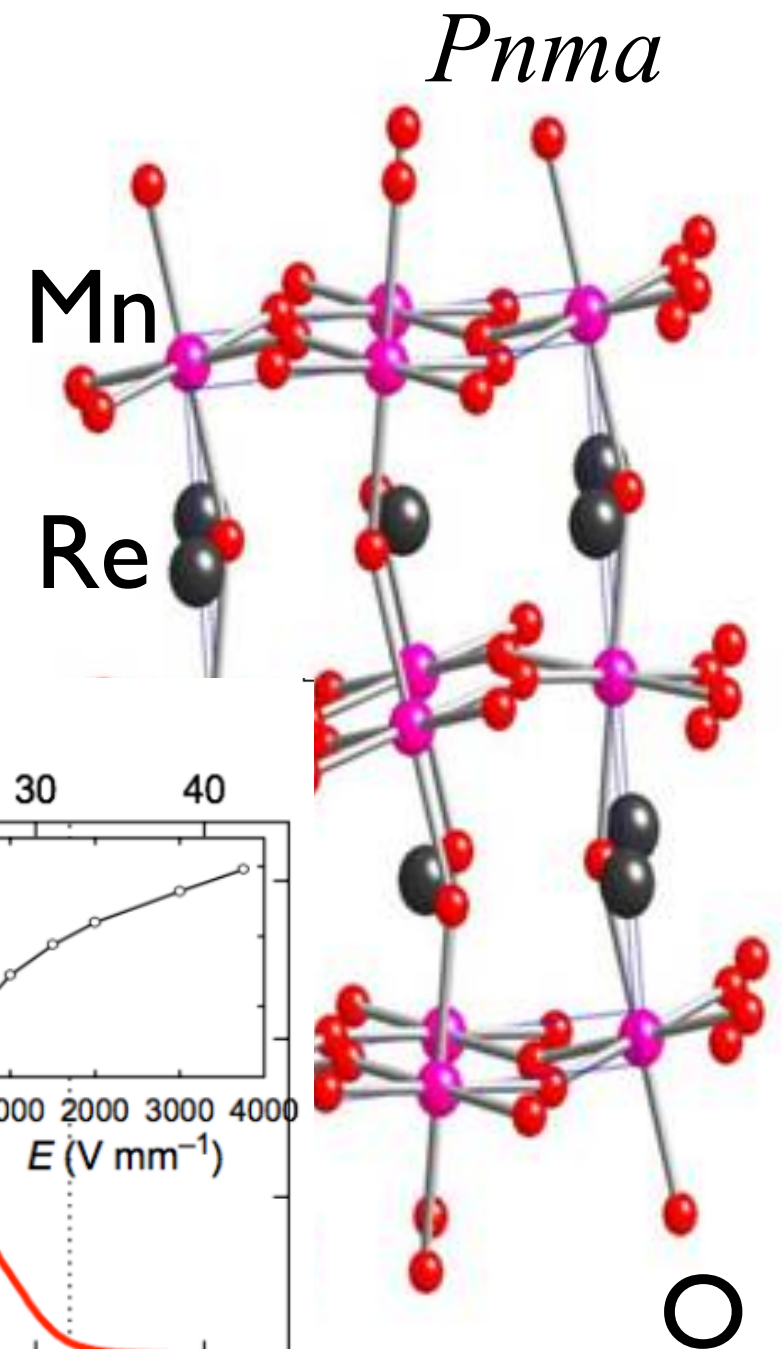
to be updated later

Antiferromagnetic order in orthorhombic multiferroic TmMnO_3

- one-arm two dimensional irrep $\mathbf{k}=[1/2,0,0]$.
Ferro-electric phase polar magnetic group P_bmn2_1
- Constraints on basis functions vs. superspace for the incommensurate two arm $\mathbf{k}=[1/2\pm\delta,0,0]$. $\{\mathbf{k}\}=\{-\mathbf{k},+\mathbf{k}\}$.
Para-electric phase (3D+1) superspace magnetic group $Pmcn1'(00g)000s [Pnma, bca]$



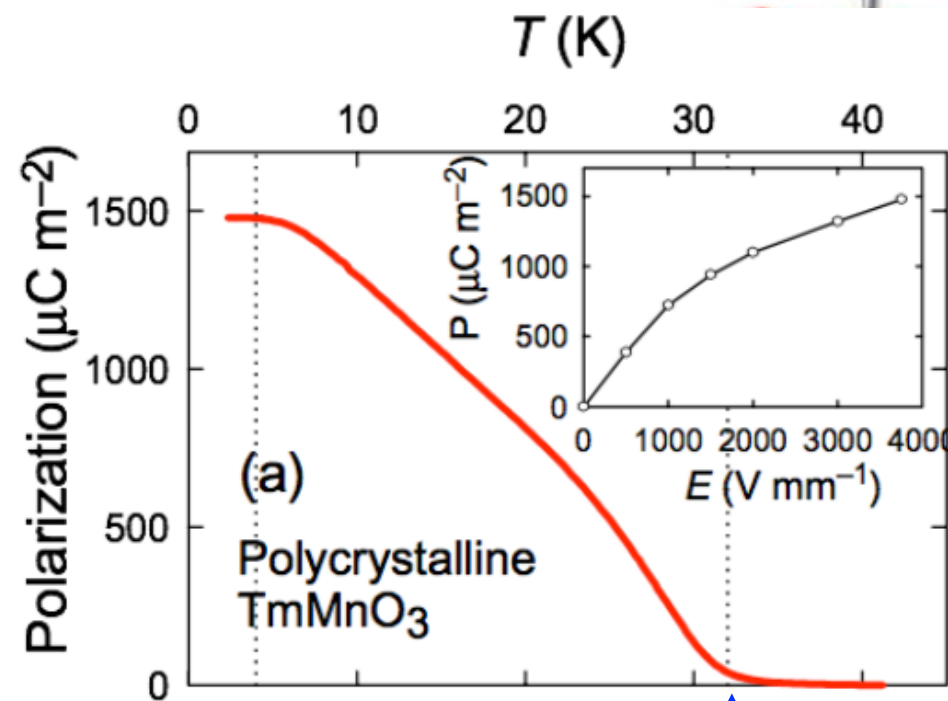
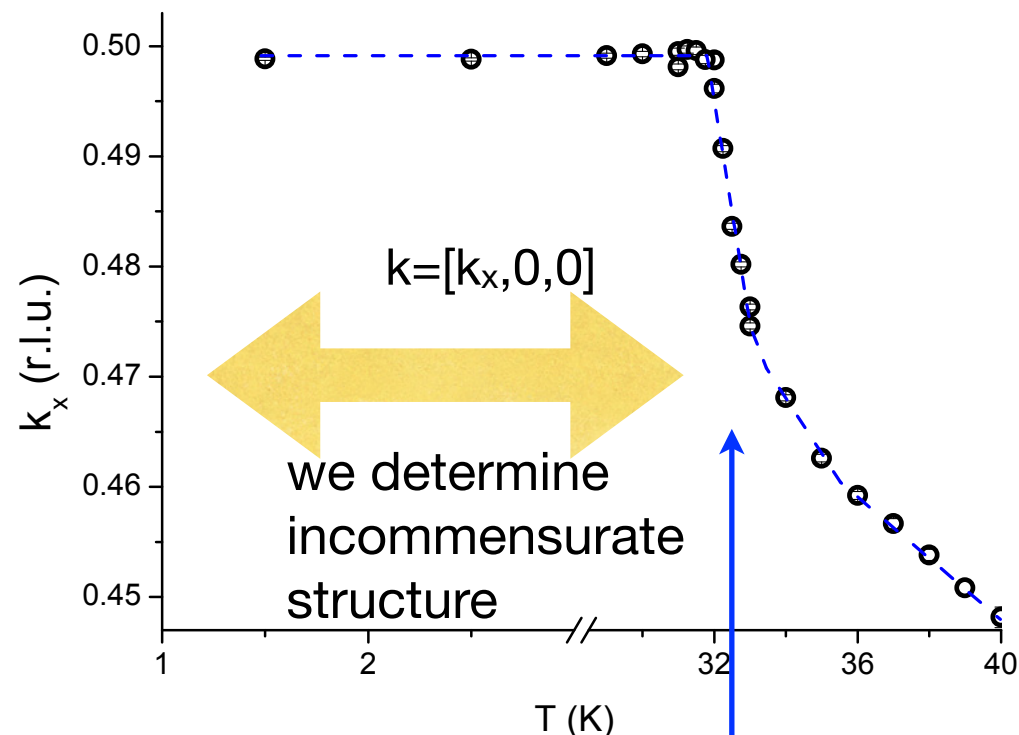
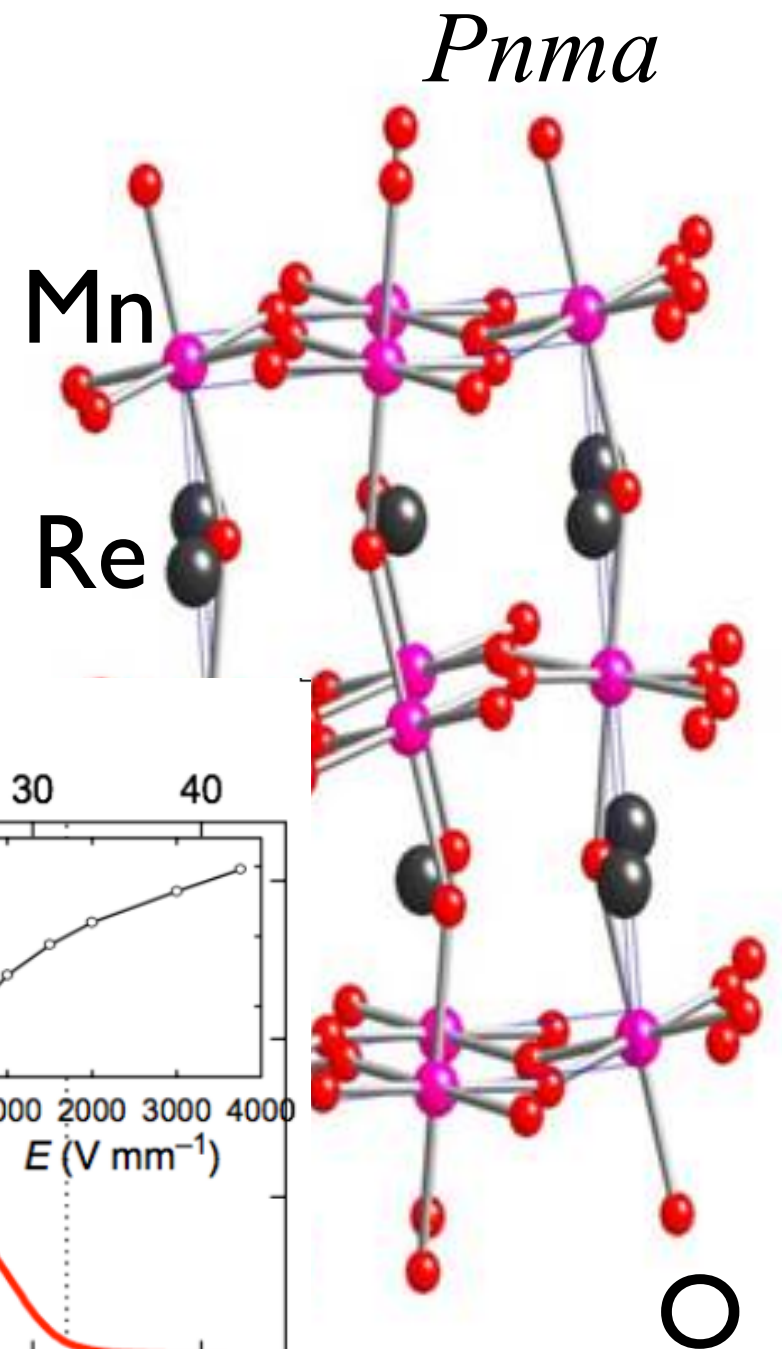
magnetic $T_{\text{Néel}}$ & electric: T_C



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magnetic $T_{\text{Néel}}$ & electric: T_C

New Journal of Physics 11, 043019 (2009)

TmMnO₃

Two magnetic modes E_1 and E_2 along x.

Mn-position (1) $0, 0, \frac{1}{2}$ (2) $\frac{1}{2}, \frac{1}{2}, 0$ (3) $0, \frac{1}{2}, \frac{1}{2}$ (4) $\frac{1}{2}, 0, 0$

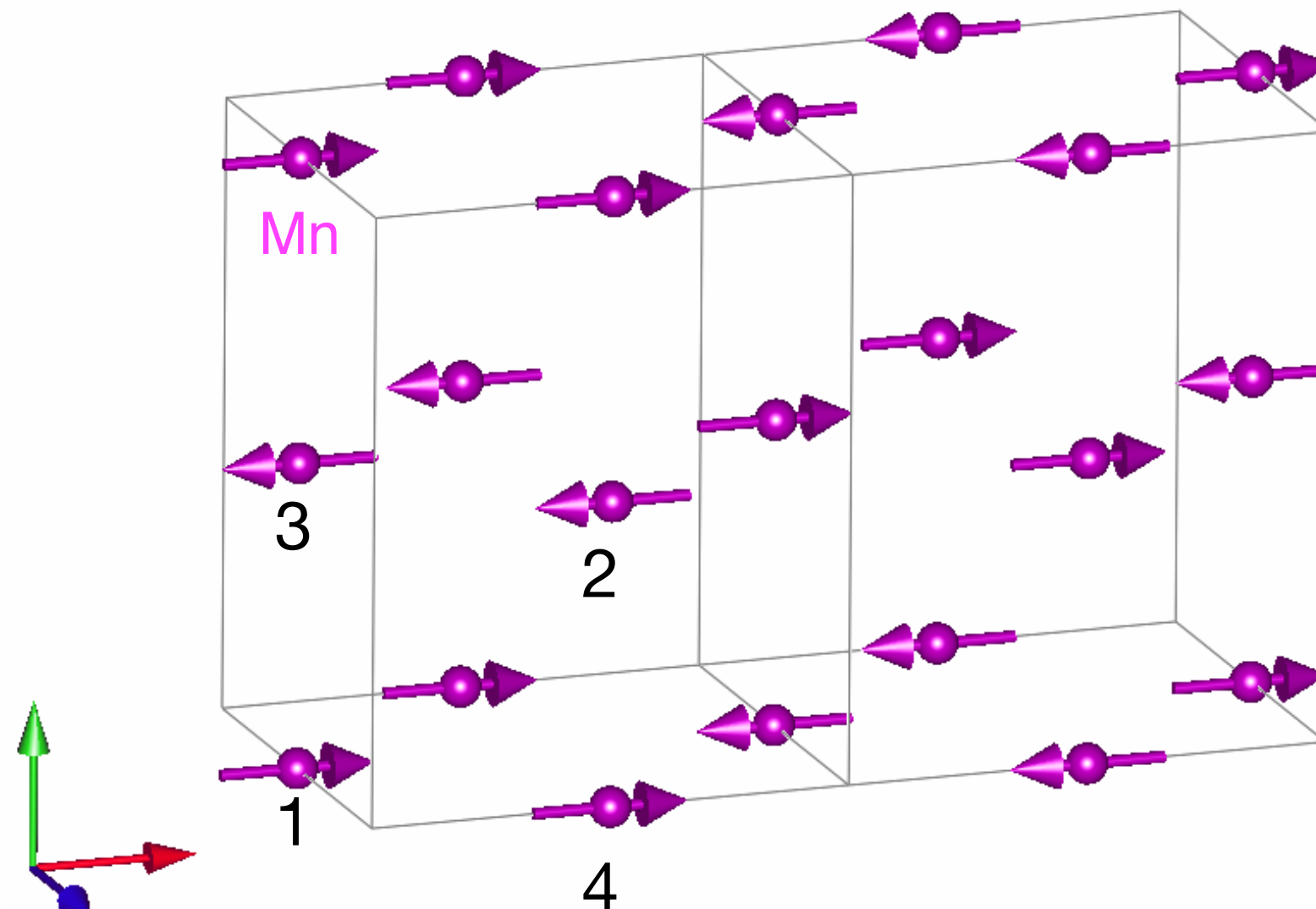
$$S_0^1 == E_1 = +1 \quad +1 \quad -1 \quad -1$$

$$S_0^2 == E_2 = +1 \quad -1 \quad -1 \quad +1$$

Pnma $k=[1/2, 0, 0]$, $k20$, X

irreps: two **2D** τ_1, τ_2

Mn $m\Gamma$: $3\tau_1 \oplus 3\tau_2$



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$$S_0^1 == E_1 = +1 \quad +1 \quad -1 \quad -1$$

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Any linear combination, in general

$$C_1 E_1 + C_2 E_2 = C_1 + C_2 \quad C_1 - C_2 \quad -C_1 - C_2 \quad C_1 + C_2$$

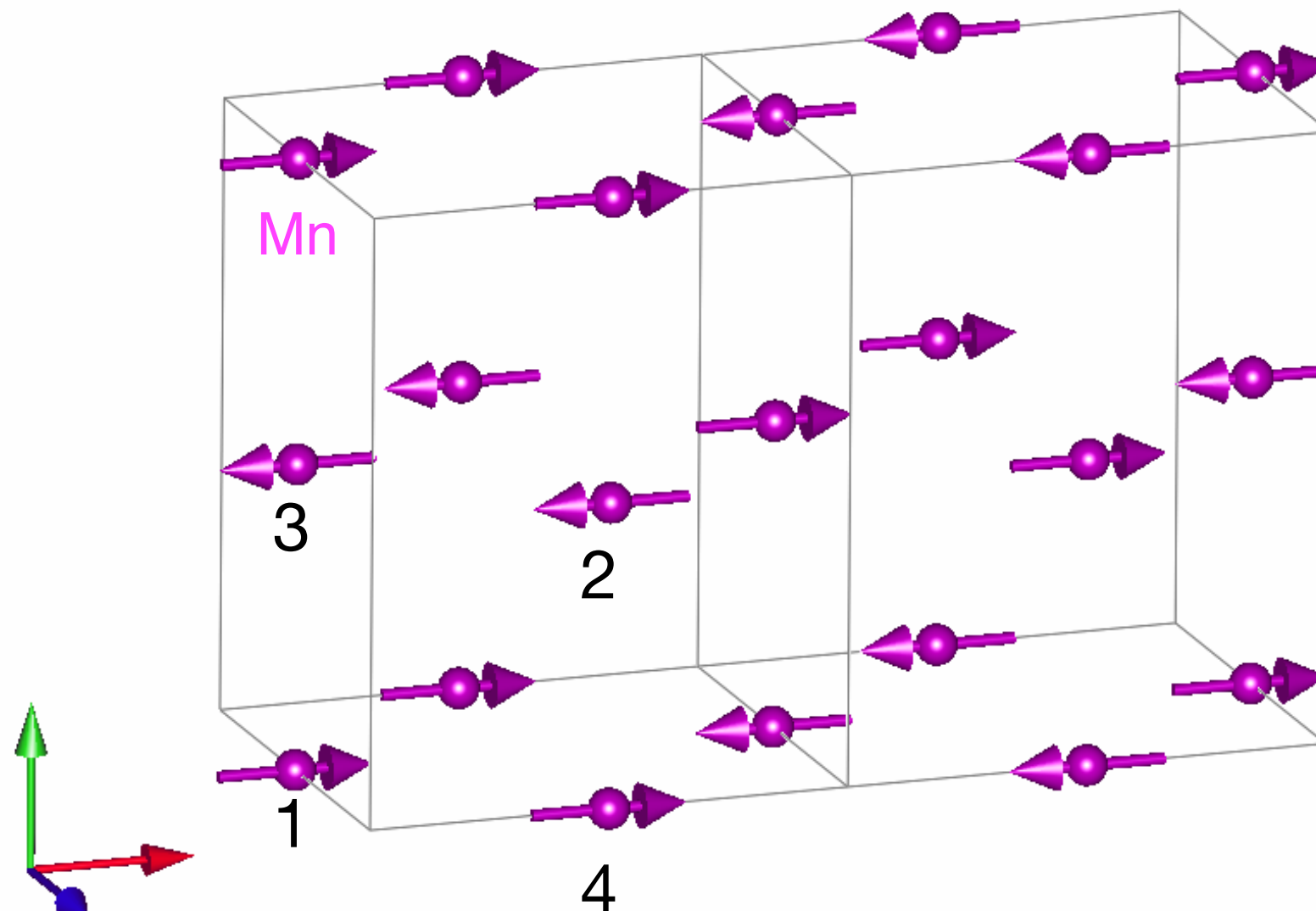
$$(E_1 + E_2)/2 = +1 \quad 0 \quad -1 \quad 0$$

$$(E_1 - E_2)/2 = 0 \quad +1 \quad 0 \quad -1$$

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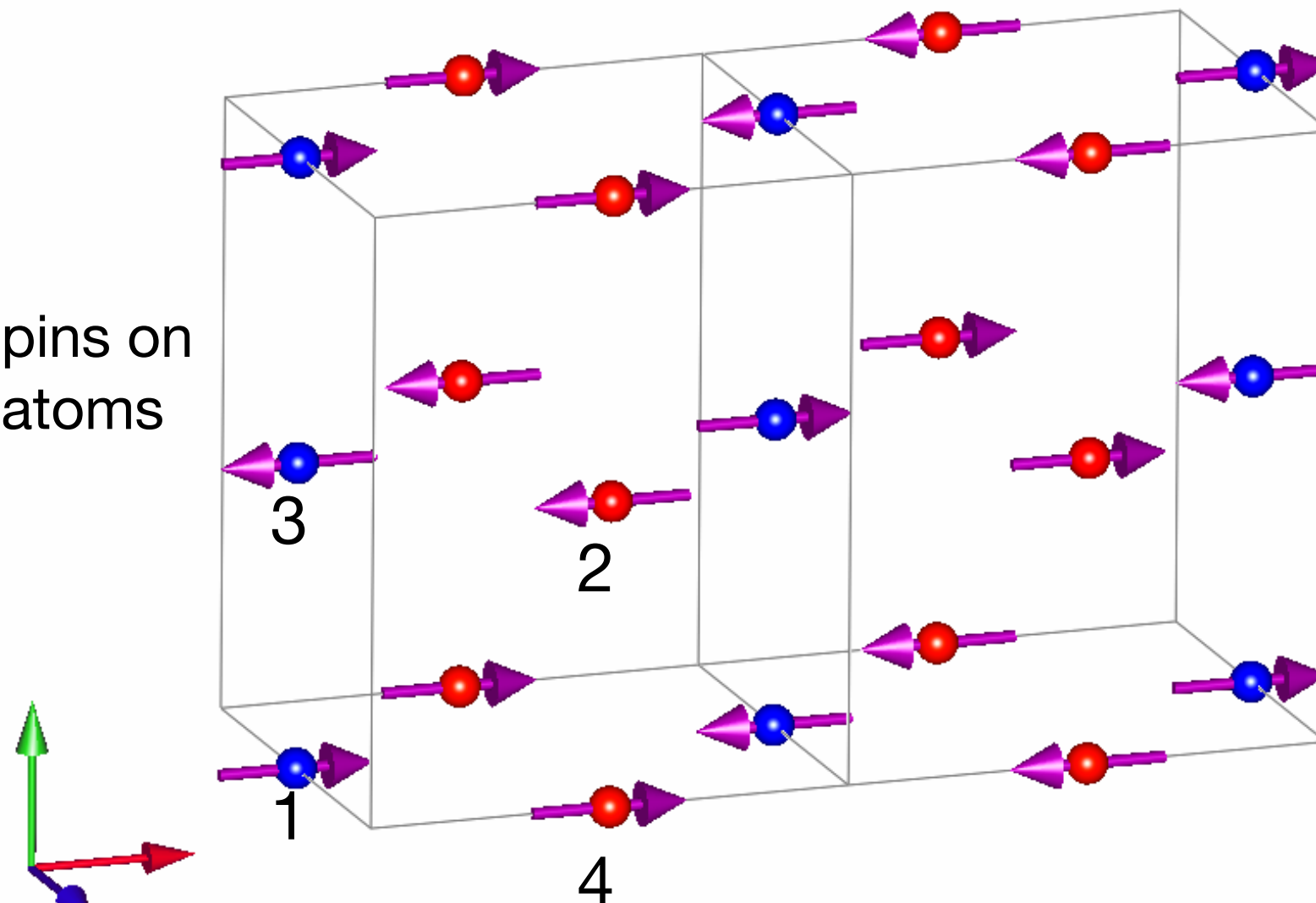
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independent spins on
red and blue atoms

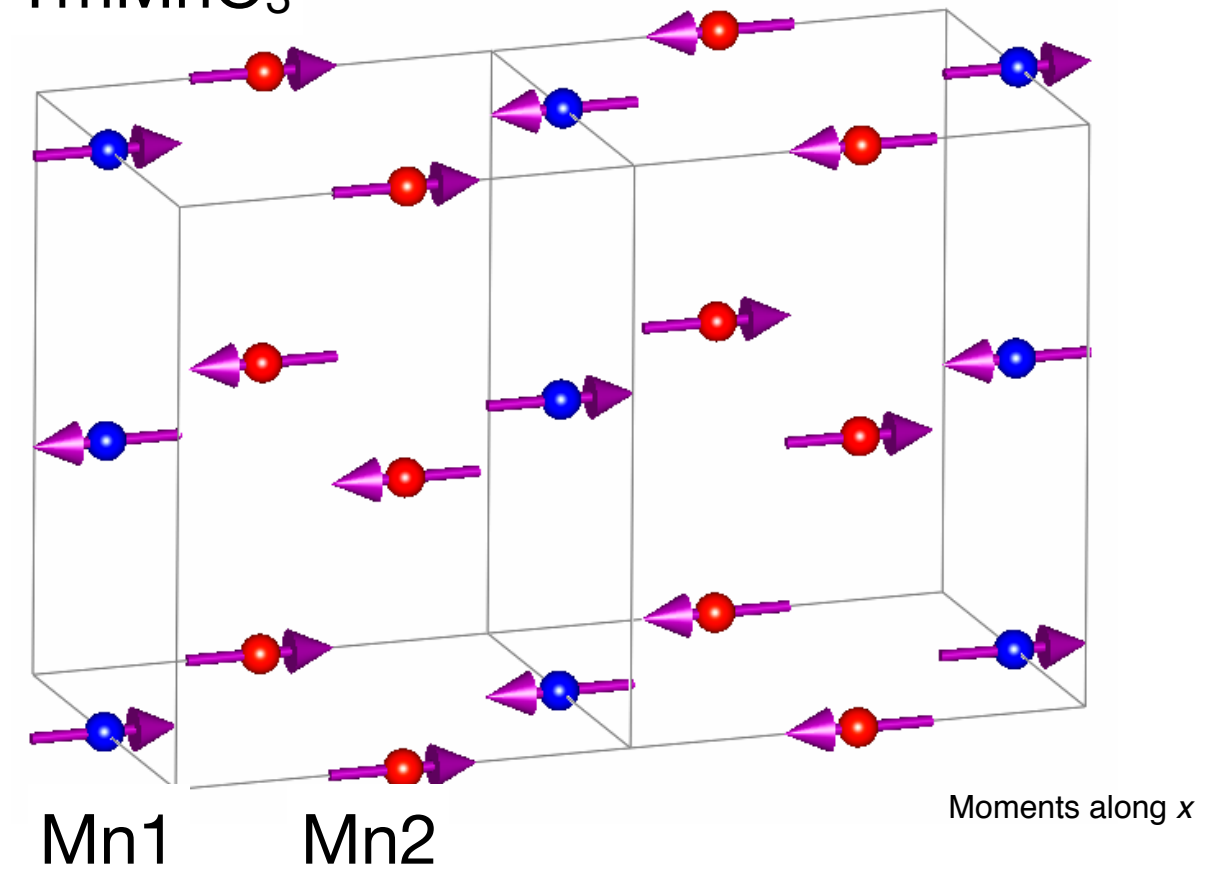


Symmetry analysis using both RA and magnetic subgroups

$Pnma$ $k=[1/2,0,0]$, irrep: $2D_{mX1}(\tau_1)$

RA with arbitrary mixing coefficients gives different spin sizes for the same type of spins. Symmetry?

$TmMnO_3$



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$Pnma$ $k=[1/2,0,0]$, *irrep*: **2D** $mX1(\tau_1)$

<http://stokes.byu.edu/iso/>

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA,

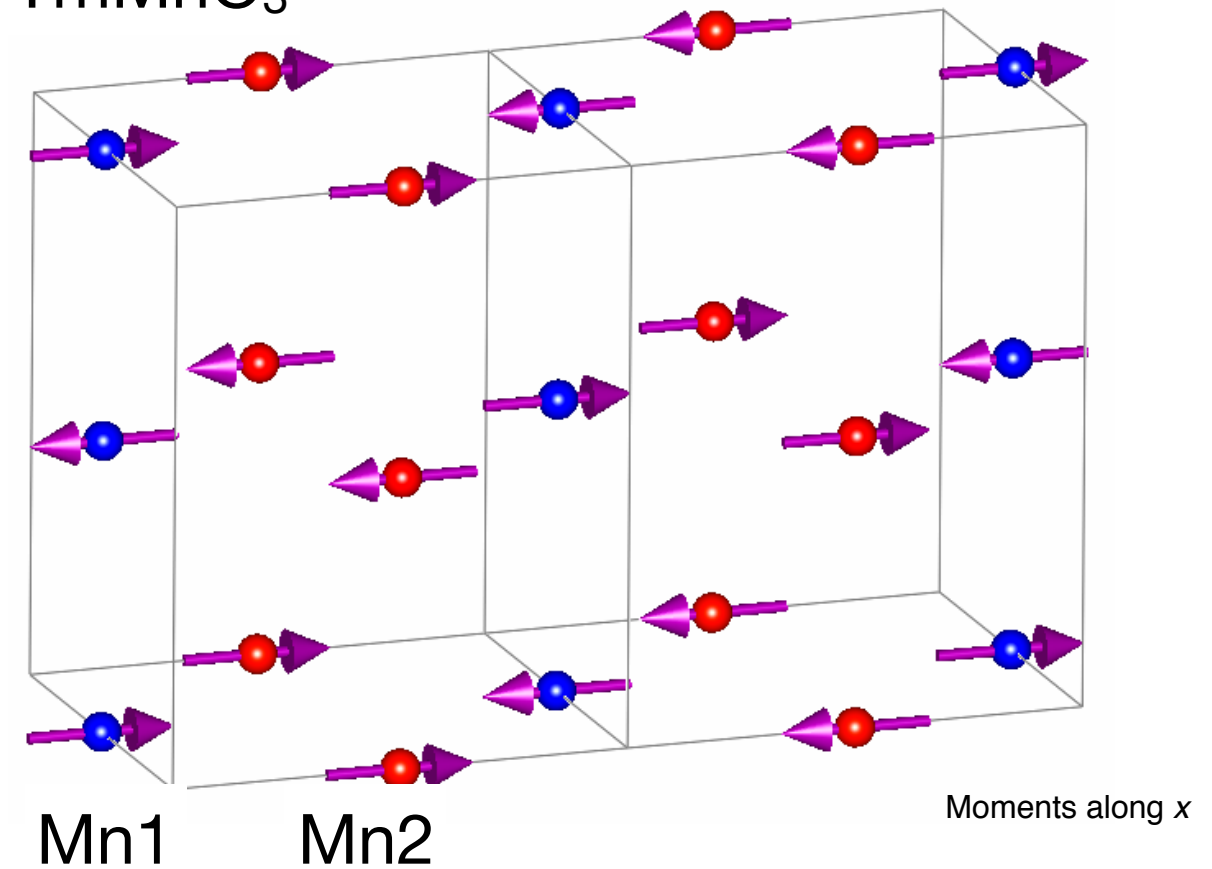
ISODISTORT

Version 6.1.8, November 2014

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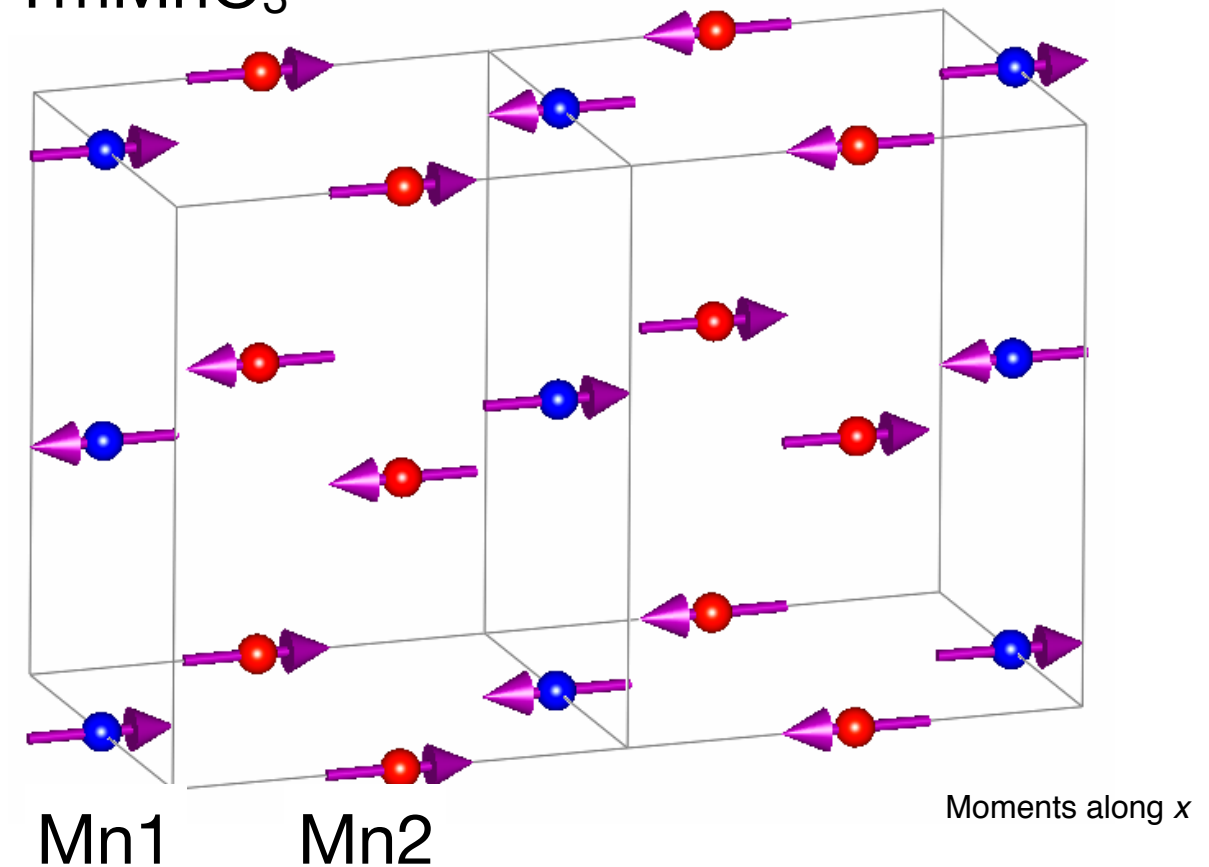
P1 (a,0) 11.55 P_a2_1/m, basis={ (2,0,0), (0,1,0), (0,0,1) }, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,0,0)
 P3 (a,a) 31.129 P_bmn2_1, basis={ (0,1,0), (2,0,0), (0,0,-1) }, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)
 C1 (a,b) 6.21 P_am, basis={ (2,0,0), (0,1,0), (0,0,1) }, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

Order parameter
direction

Magnetic Shubnikov
Space group

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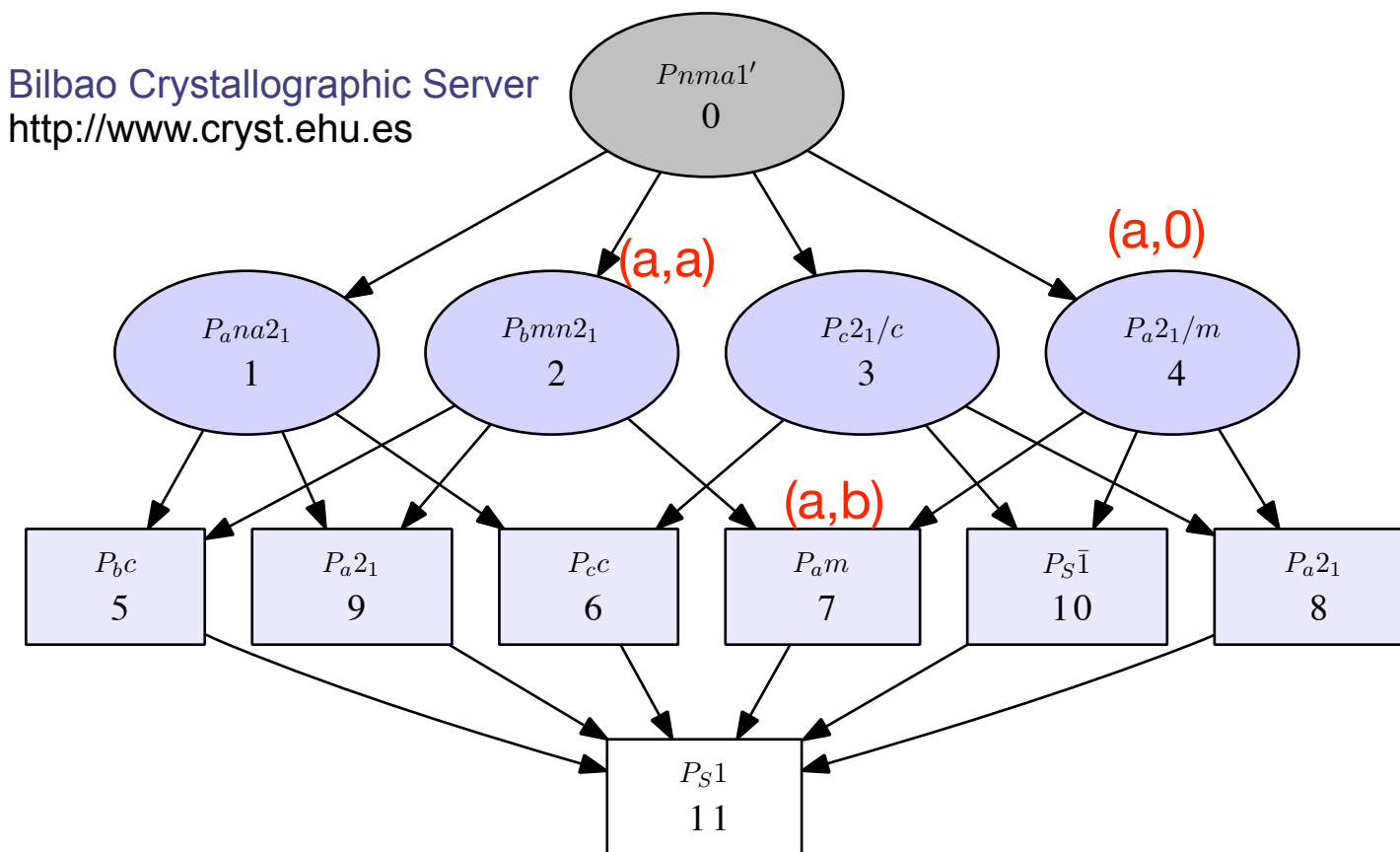
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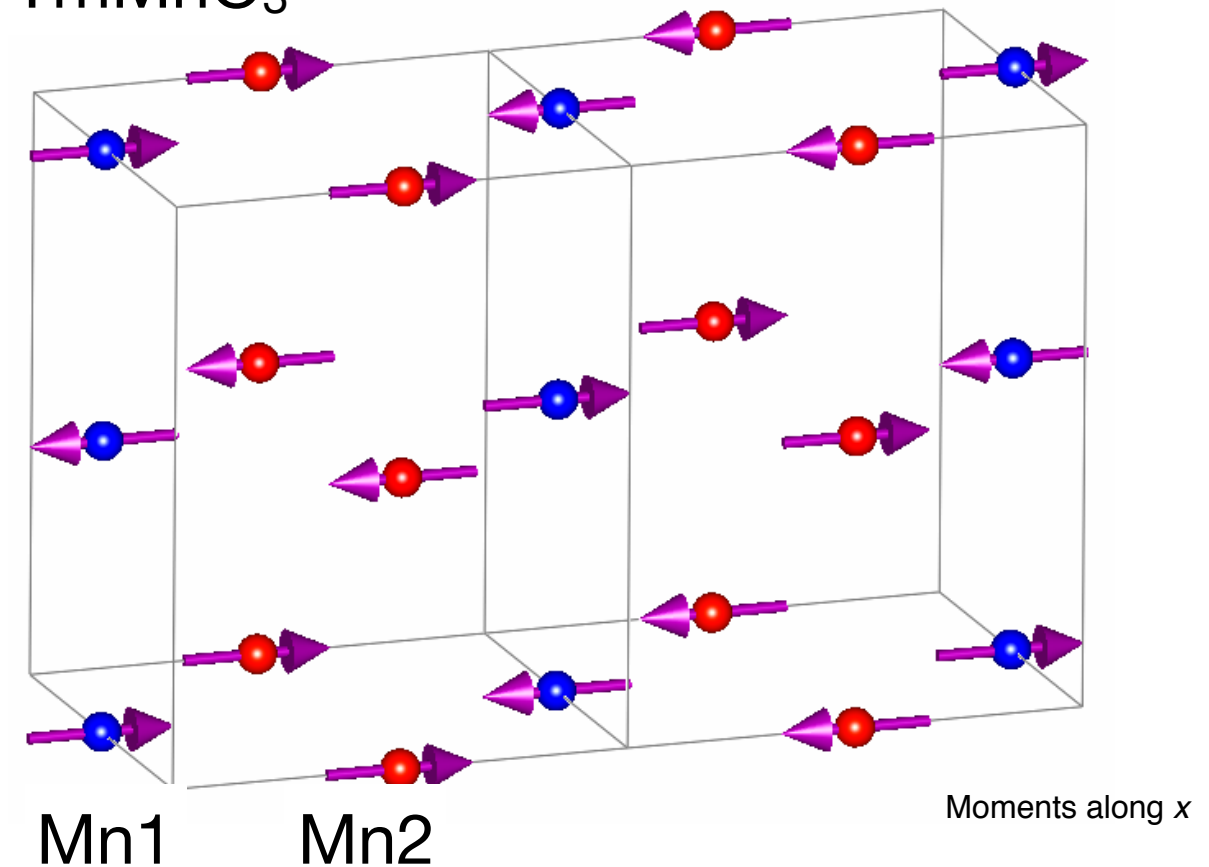
Order parameter direction
 Magnetic Shubnikov Space group

Bilbao Crystallographic Server
<http://www.cryst.ehu.es>



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$TmMnO_3$



Case 1: magnetic mode E1 -> most symmetric maximal subgroup of $Pnma1'$

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Solution!

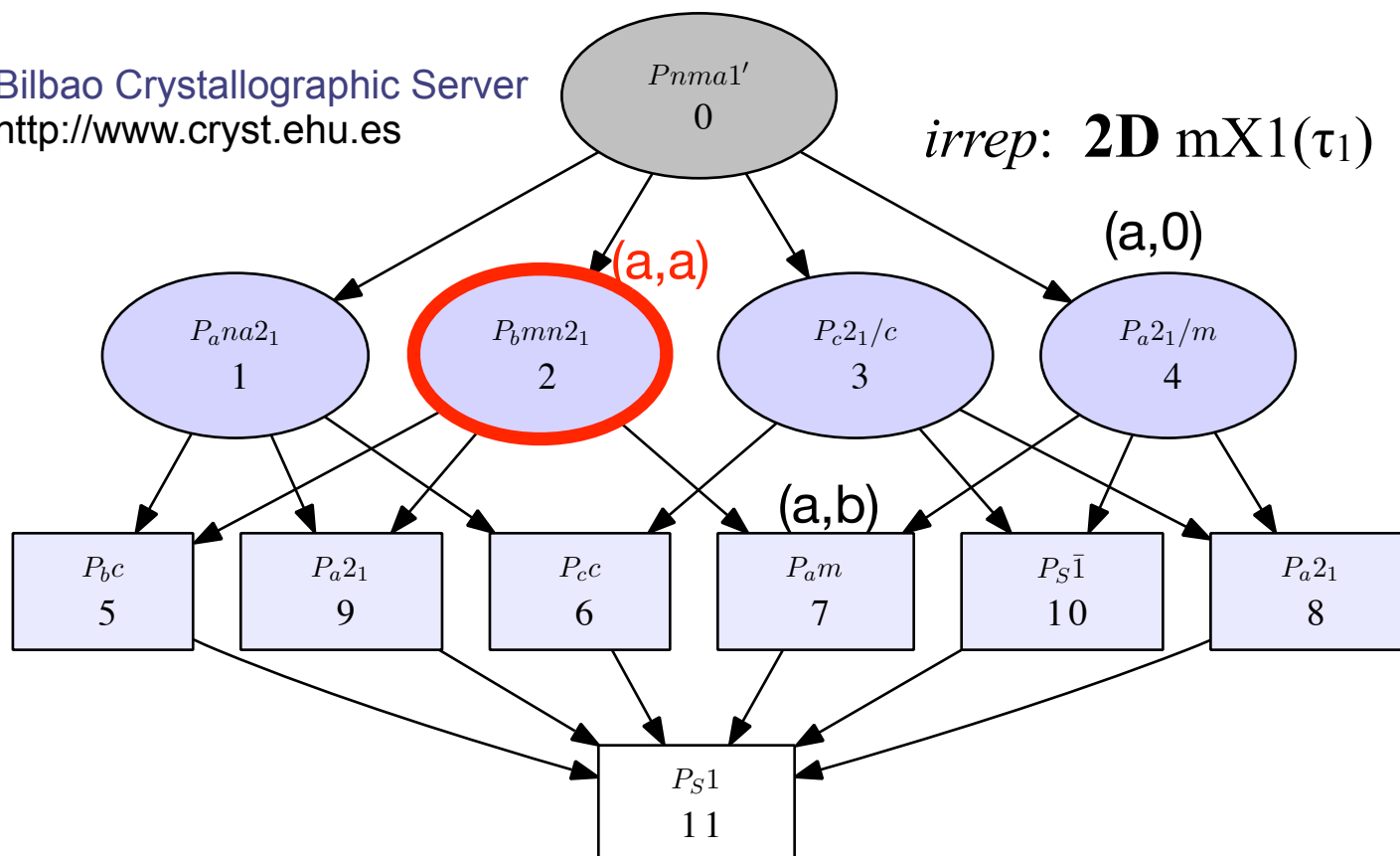
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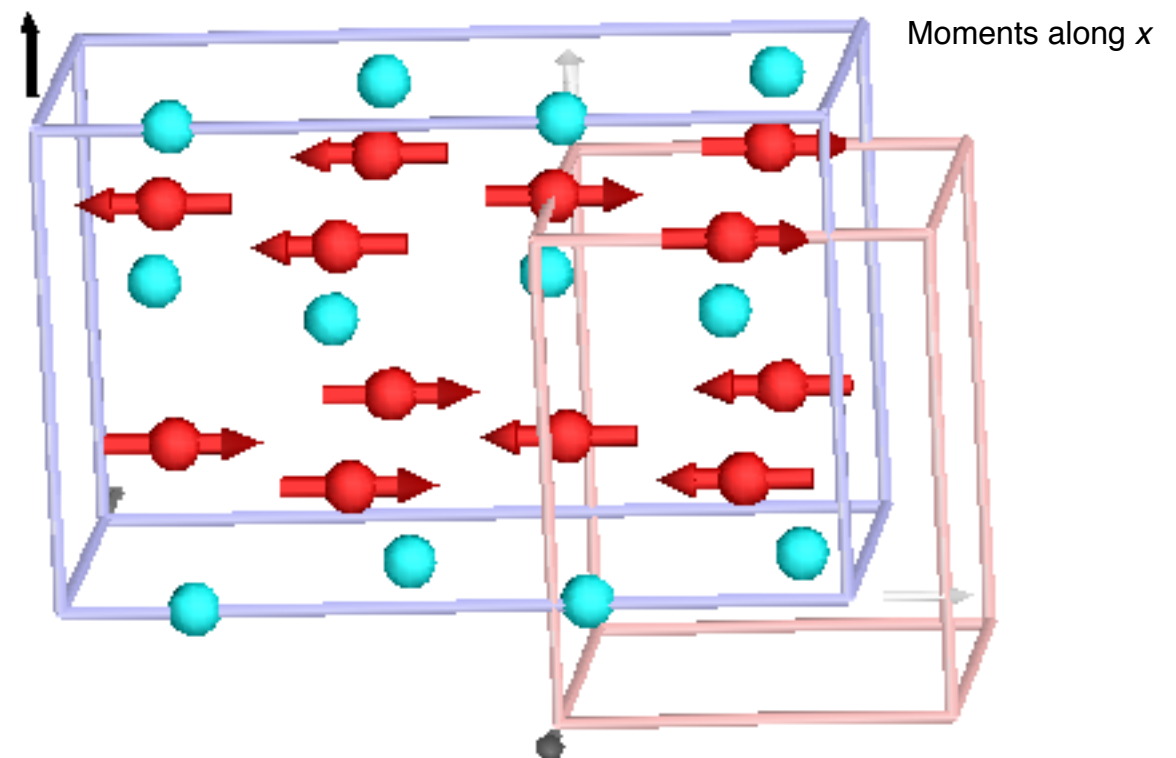
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 C1 (a,b) 6.21 P_am, basis={ (2,0,0), (0,1,0), (0,0,1) }, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

Solution!

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orthorhombic $Pmn2_1$

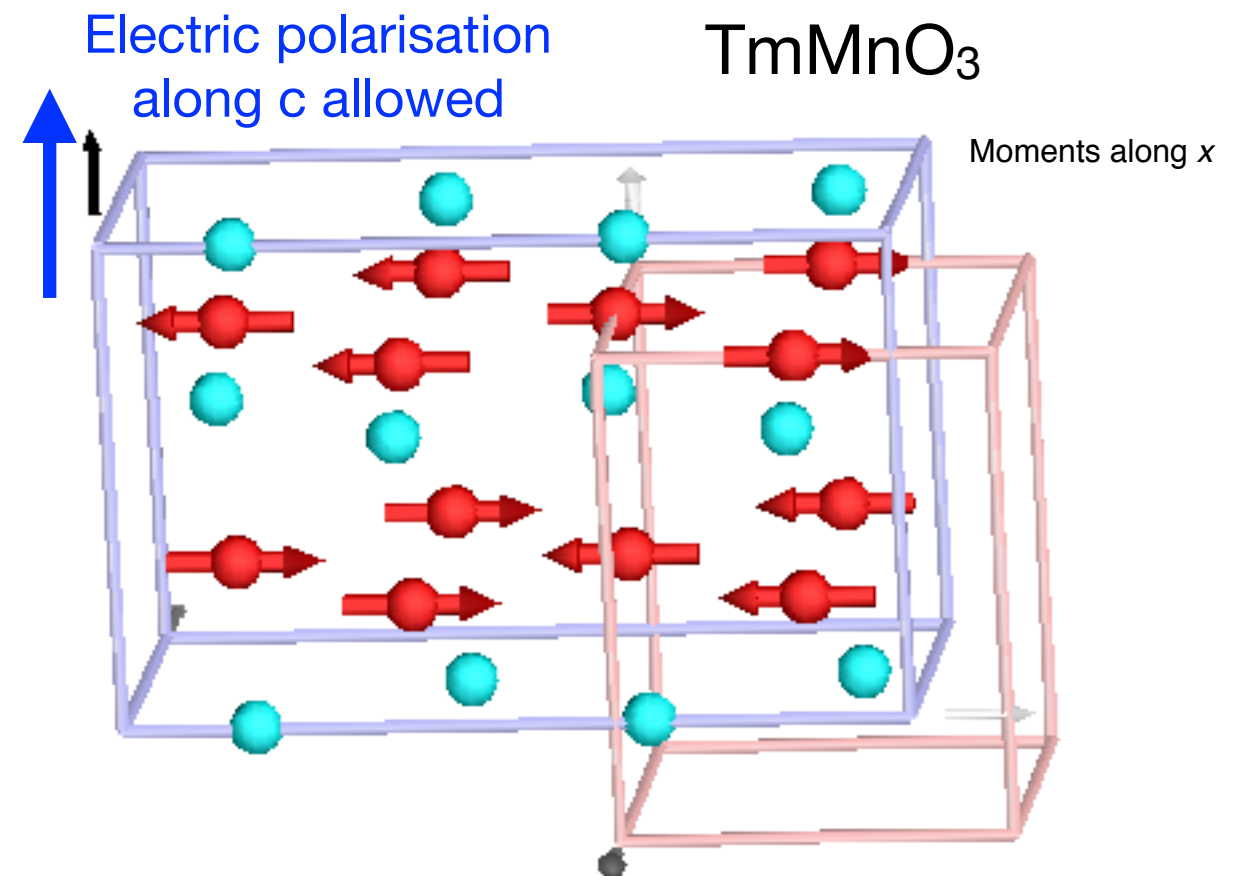
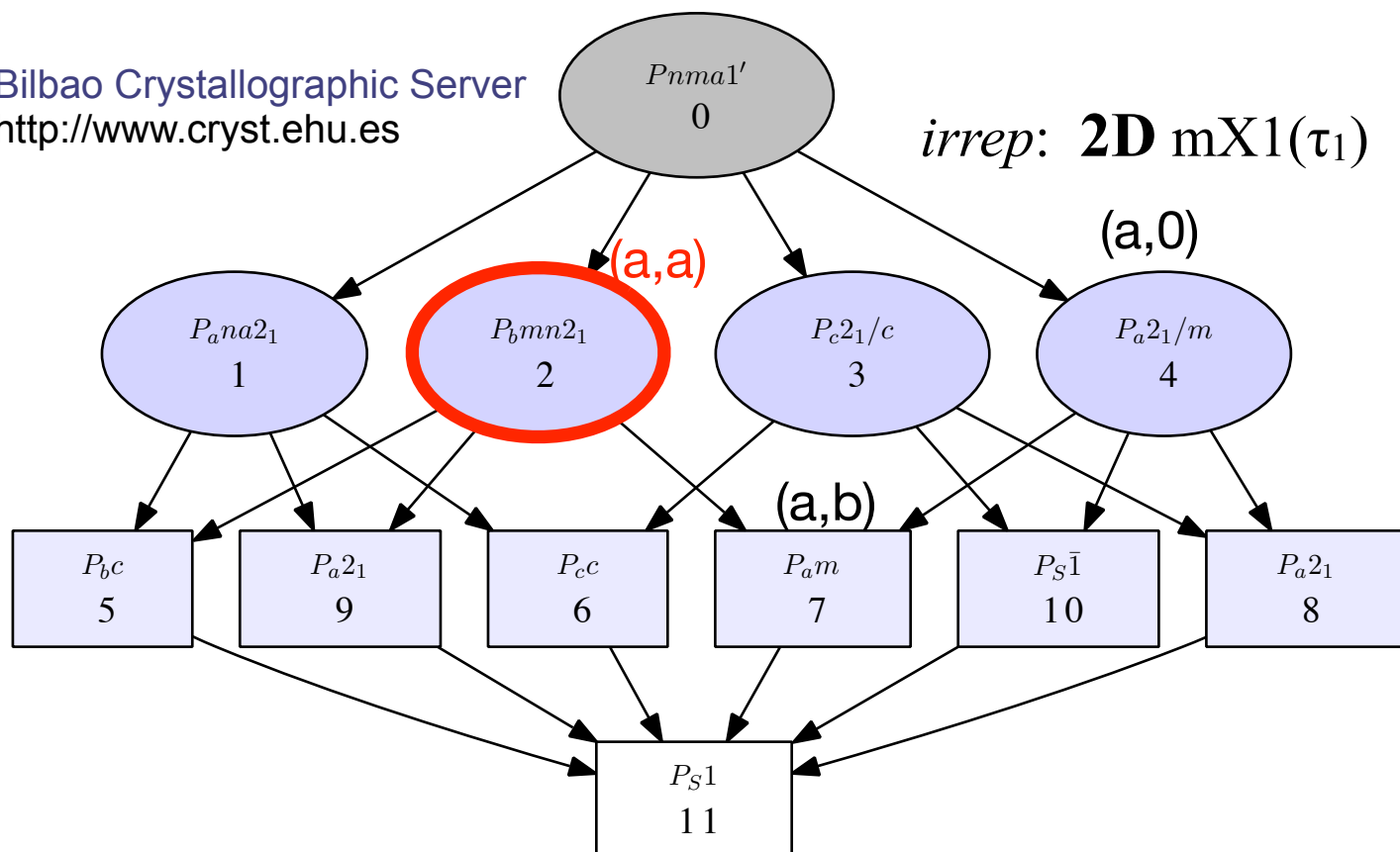
(1) 1
(5) $\bar{1}$ 0,0,0

(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(6) a $x,y,\frac{1}{4}$

(3) $2(0,\frac{1}{2},0)$ $0,y,0$
(7) m $x,\frac{1}{4},z$

(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Case 2: General solution in RA -> low symmetry non-maximal subgroup

Order parameter
direction

Magnetic Shubnikov
Space group

P1 (a,0) 11.55 P_a2_1/m, basis={ (2,0,0), (0,1,0), (0,0,1) }, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,0,0)
P3 (a,a) 31.129 P bmn2 1, basis={ (0,1,0), (2,0,0), (0,0,-1) }, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)
 C1 (a,b) 6.21 P_am, basis={ (2,0,0), (0,1,0), (0,0,1) }, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

conventional general solution in RA: lowest symmetry for the given irrep

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(1) 1
(5) $\bar{1}$ 0,0,0

(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(6) a $x,y,\frac{1}{4}$

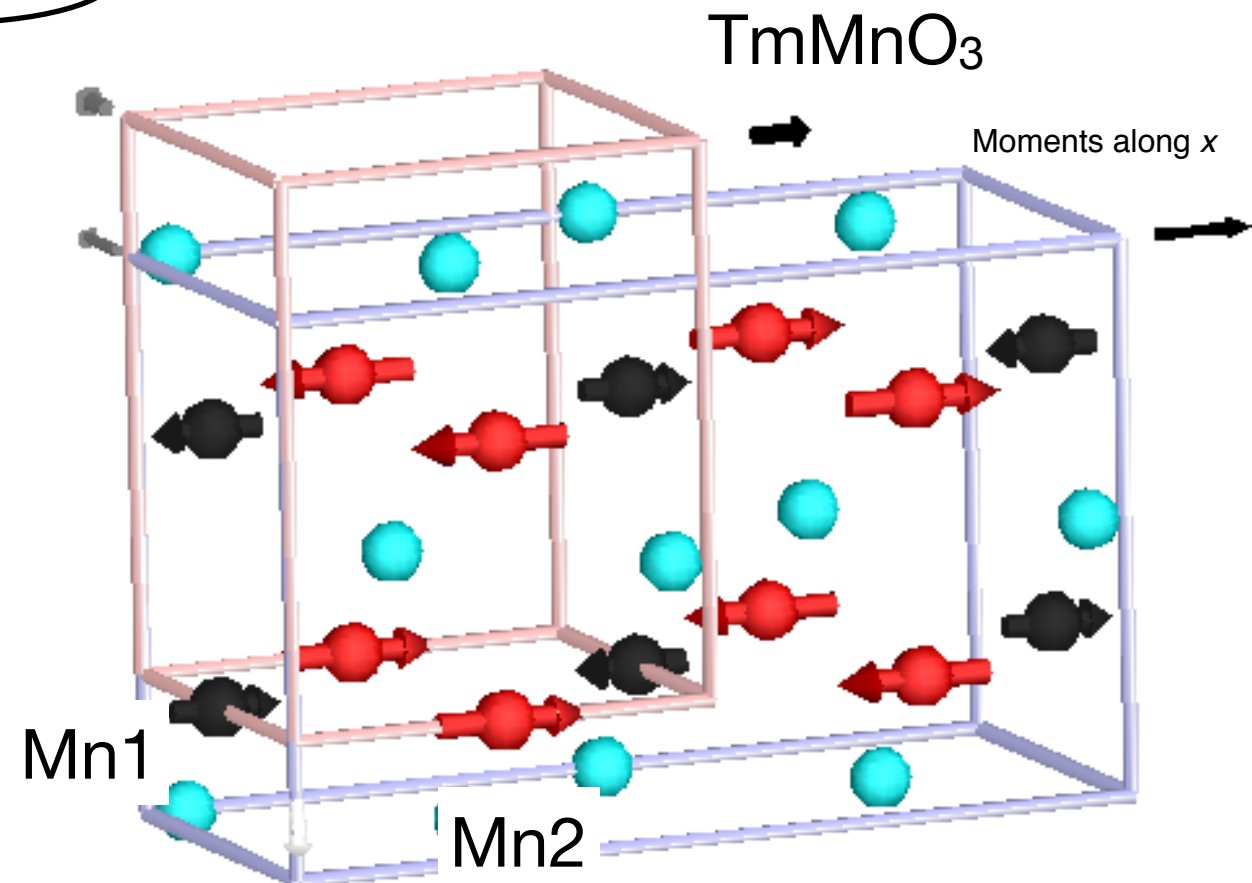
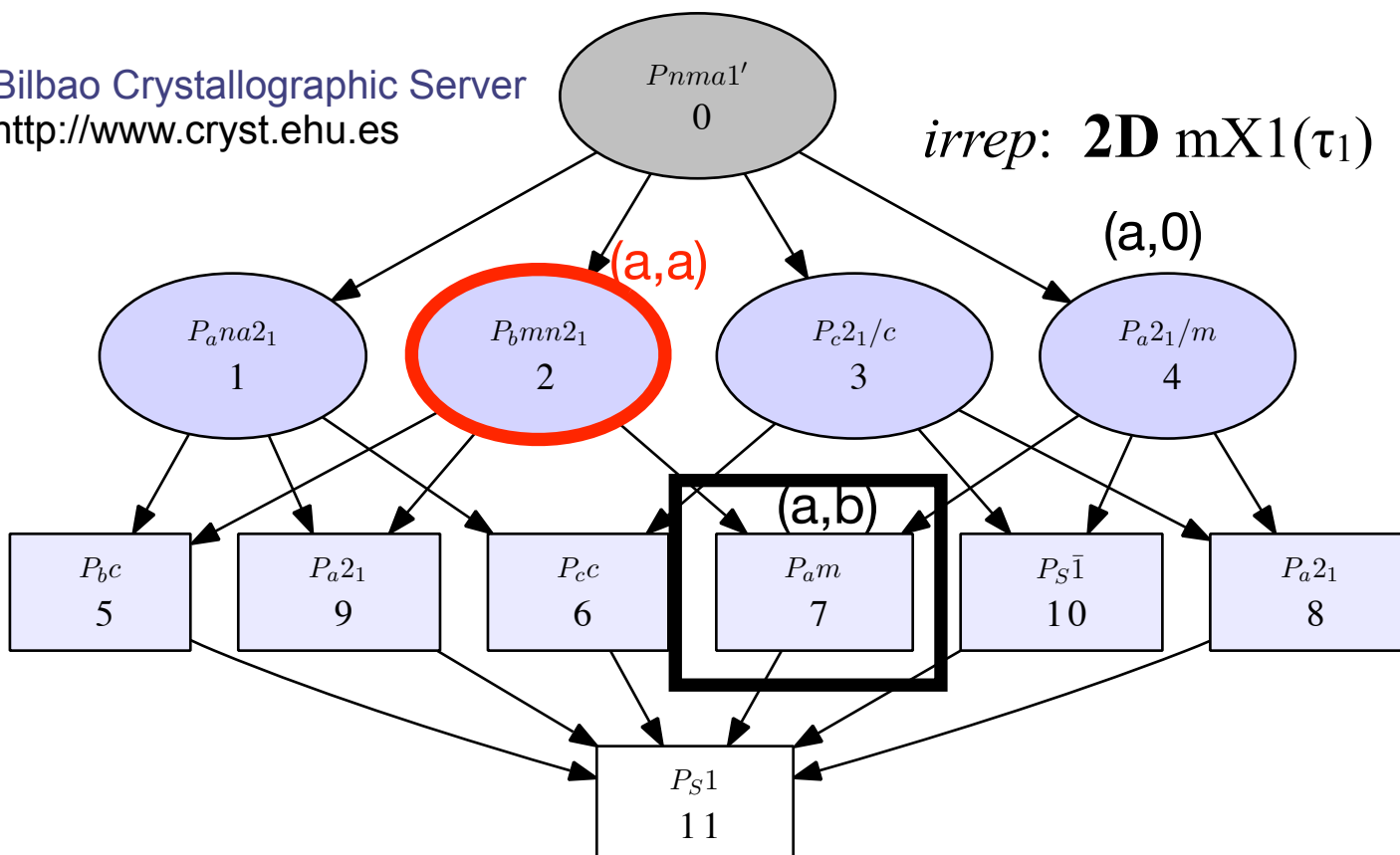
(3) $2(0,\frac{1}{2},0)$ $0,y,0$
(7) m $x,\frac{1}{4},z$

(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},v,z$

monoclinic Pm

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irrep: **2D mX1(τ_1)**



Purpose of this lecture is to show:

The pdf-file with this talk will be available at
<https://www.psi.ch/en/sinq/hrpt/talks>

or short link
<http://psi.ch/node/29534>

1. Introduction to magnetic neutron diffraction (1-13)
 - 1.1. General. Intro. Experimental technics for magnetic diffraction
 - 1.2. Examples of instruments at PSI
 - 1.3. Literature, computer and web-resources related to magnetic diffraction
2. Basic principles of magnetic neutron diffraction. (15-32)
 - 2.1. Master formulae for the scattering. neutron-electron interaction Hamiltonian. Scattering Q-operator (15-20)
 - 2.2. Magnetic order parameters overview. Magnetic multipoles (22-27)
 - 2.3. Magnetic form-factors (what are neutrons sensitive to?) Expansion of Q [exp(i $\mathbf{k}\mathbf{r}$) series] (29-40)
 - 2.3.1. Dipole approximation. Examples.
 - 2.3.2. Multipole approximation, parity even, time odd. Symmetry of multipoles.
 - 2.3.3. Anapole (toroidal moment) and other parity-odd modern exotics (theory: Lovesey)
3. Description and determination of magnetic structure (41-72)
 - 3.1. Introduction to propagation vector(s) formalism star/arm (42,43,51)
 - 3.2. Magnetic structure factors. General formula 44-47
 - 3.3. Commensurate vs. incommensurate case's examples.
 - 3.4. Introduction to irreps (48-50)
 - 3.5. Magnetic Shubnikov groups (52-53)
4. Classification of the magnetic structures that are used in the literature, such as Shubnikov (or Magnetic) space groups, 3D+n superspace groups and irreducible representation (irrep) notations. Relation between two approaches. A bit of history. (54-59)
5. How can one construct all possible symmetry adapted magnetic structures for a given crystal structure and a propagation vector (a point on the Brillouine zone) by the combined use of irrep and the magnetic symmetry? A real case study of:
 - 5.1. multiferroic TmMnO₃: 2D irrep $\mathbf{k}=[1/2,0,0]$. Ferro-electric phase polar magnetic group Pbm_n21 (61-65)
 - 5.2. Topologically nontrivial skyrmionic incommensurate magnetic structure. Superspace. (66-72)