Determination of the magnetic structure from powder neutron diffraction

Vladimir Pomjakushin
Laboratory for Neutron Scattering, ETHZ and PSI

A Hands-on Workshop on X-rays, Synchrotron Radiation and Neutron Diffraction Techniques
June 18-22, 2008, Paul Scherrer Institut, Villigen, Switzerland

Lecture notes:
http://sinq.web.psi.ch/sinq/instr/hrpt/praktikum

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.

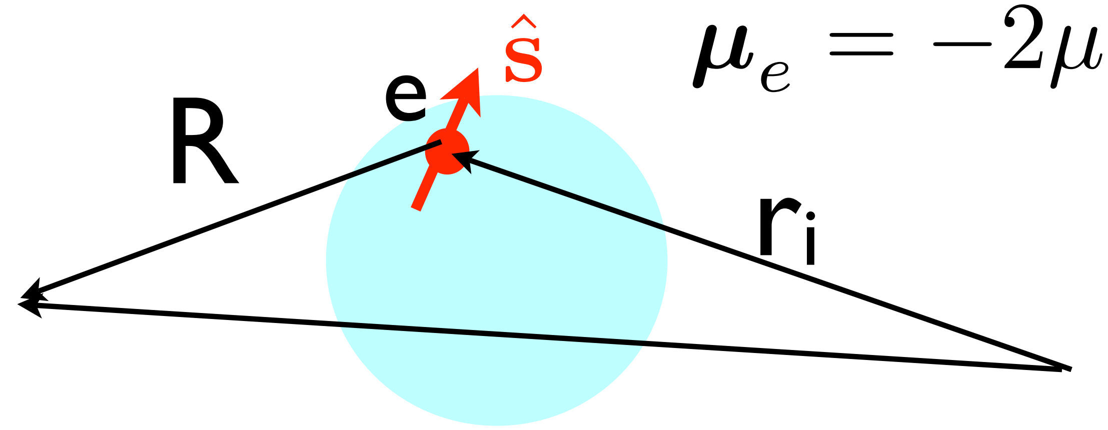
All you need to know about magnetic neutron diffraction. Symmetry, representation analysis

Yu. A. Izyumov, V. E. Naish and R. P. Ozerov, "*Neutron diffraction of magnetic materials*", New York [etc.]: Consultants Bureau, 1991.

Overview of Lecture

- Principles of magnetic neutron scattering/diffraction
- Types of magnetic structures
- Description of all possible magnetic structures. k-vector formalism for classifying the magnetic modes
- Real example of magnetic structure determination

Magnetic neutron scattering on an atom



$$\boldsymbol{\mu}_e = -2\mu_B \hat{\mathbf{s}}$$

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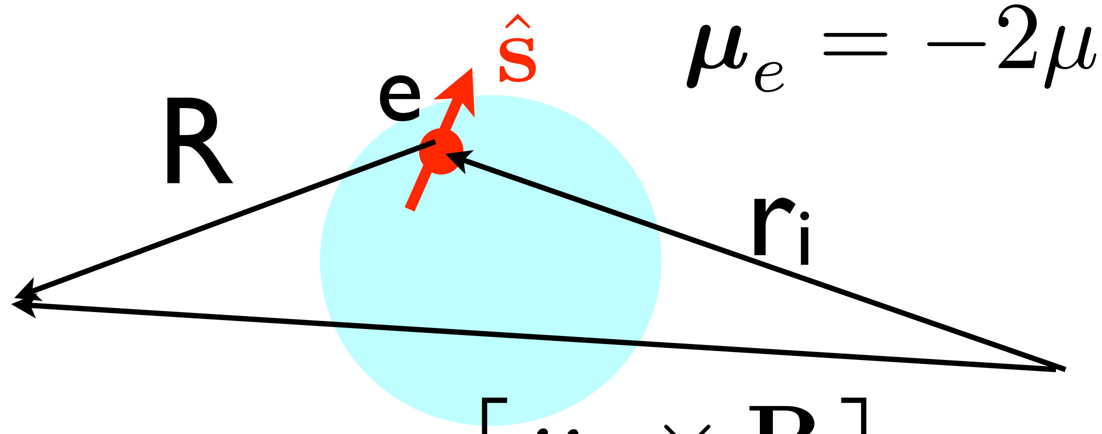

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Magnetic field from an electron $$\mathbf{H}(\mathbf{R}) = -\mathrm{rot}\left[\frac{\boldsymbol{\mu}_e \times \mathbf{R}}{|\mathbf{R}|^3}\right] + \mathrm{transl.part}$$

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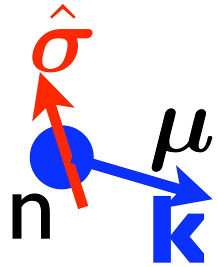

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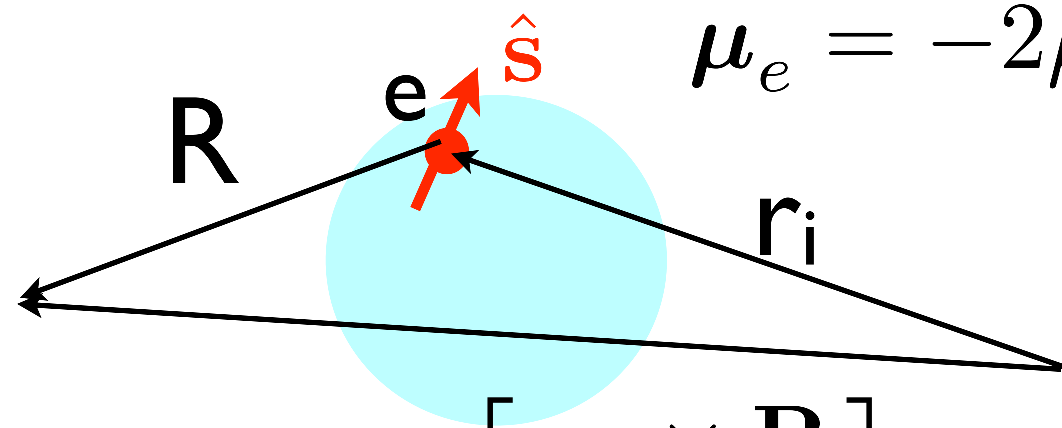

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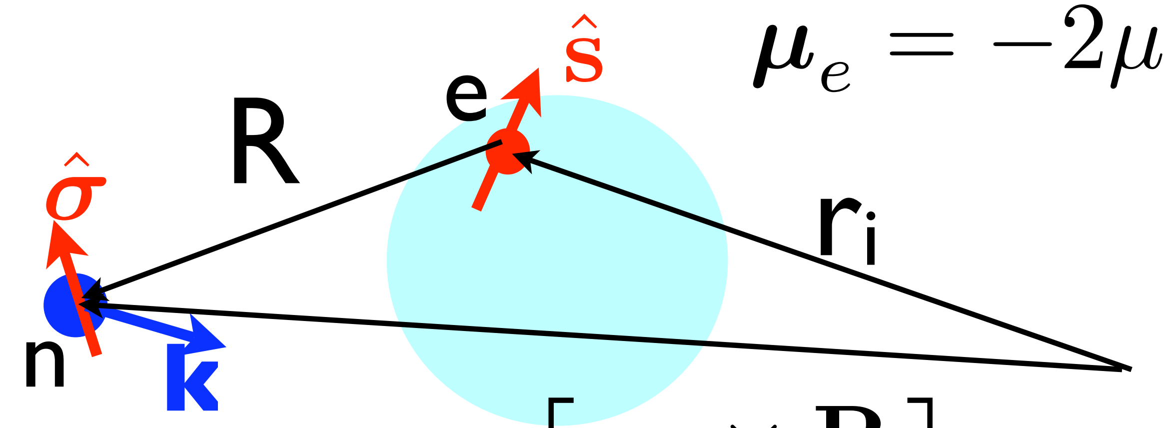

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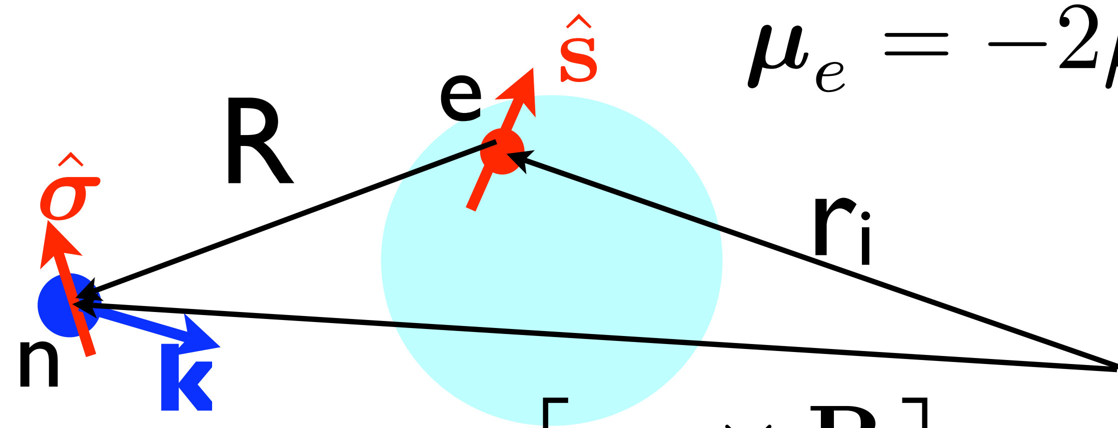

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averaging over neutron coordinates

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

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

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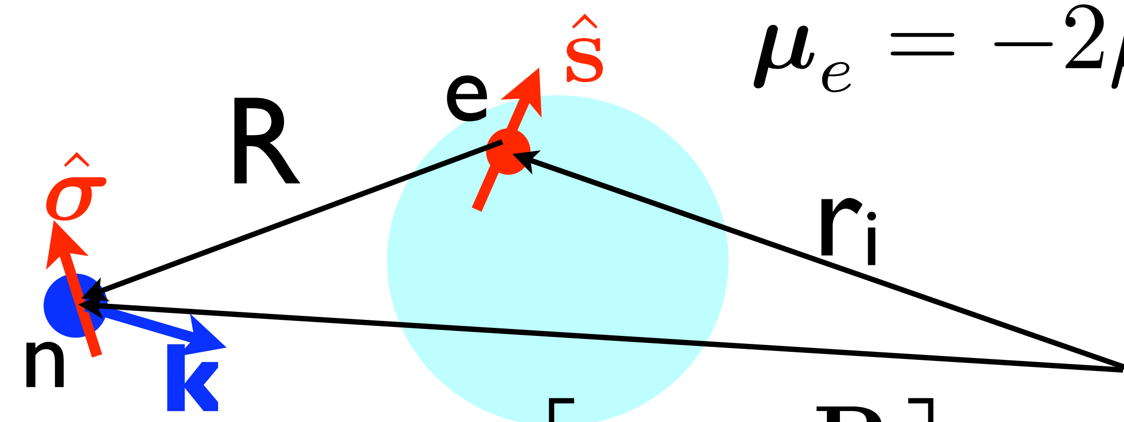

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magnetic interaction operator $\hat{\mathbf{Q}}_\perp$

Magnetic neutron scattering on an atom

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

Magnetic neutron scattering on an atom

1. The size

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neutron magnetic moment in μ_n -1.91

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

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x-ray scattering length: Zr_e

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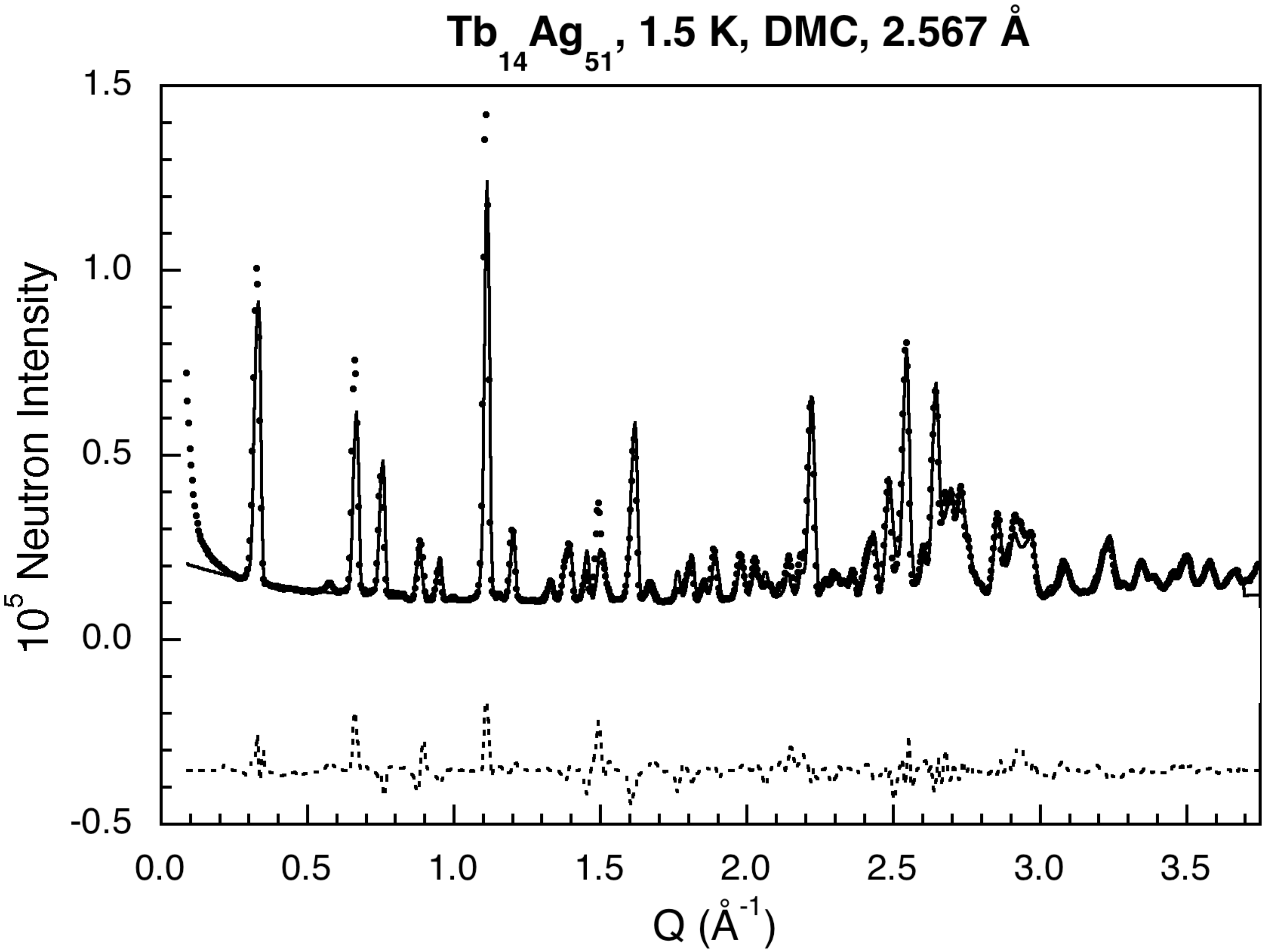
Comparison of neutron scattering lengths (fm)

magnetic

Mn^{3+} (S=2): -10.8, Cu^{2+} (S=½): -2.65

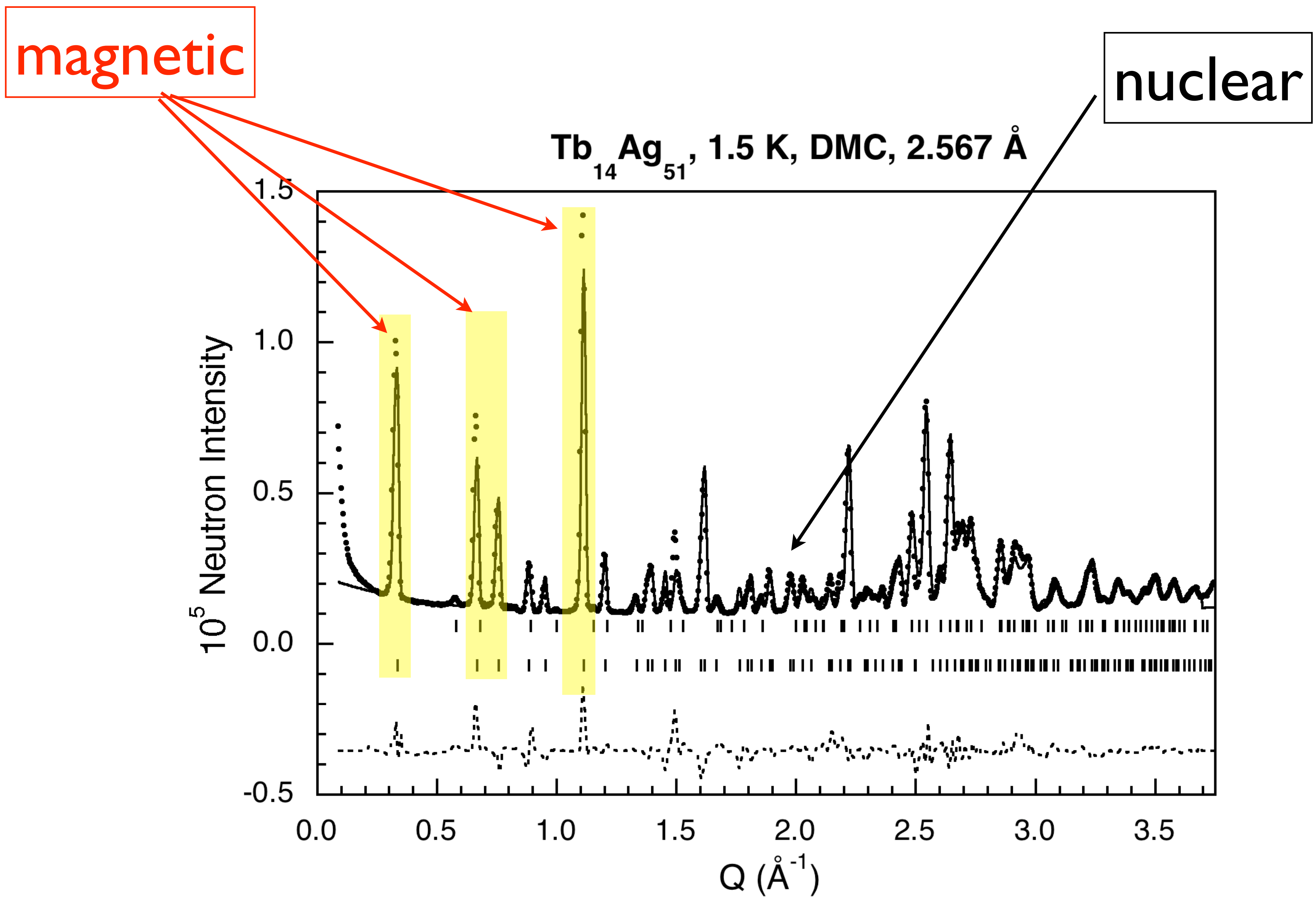
nuclear

Mn : -3.7, Cu: 7.7



Tb14Ag51, 1.5 K, DMC, 2.567 Å
10^5 Neutron Intensity
Q (Å^-1)
1.5
1.0
0.5
0.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5

magnetic scattering intensity can be larger than the nuclear one



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Magnetic neutron scattering on an atom

2. q-dependence

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$$\frac{1}{q^2}[\mathbf{q} \times \hat{\mathbf{Q}} \times \mathbf{q}]$$

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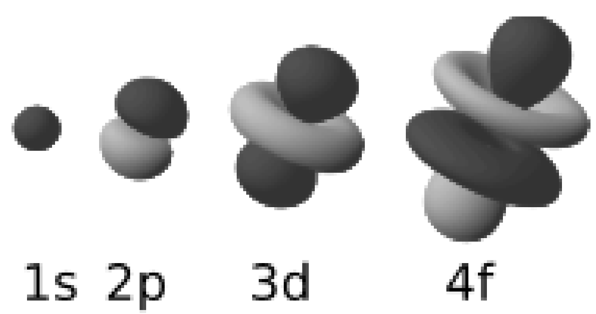
$$\left\langle \hat{\mathbf{Q}} \right\rangle = \left\langle \sum_i \hat{\mathbf{s}}_i e^{i\mathbf{q}\mathbf{r}_i} \right\rangle = \mathbf{S} \int d\mathbf{r} \rho_s(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}}$$



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

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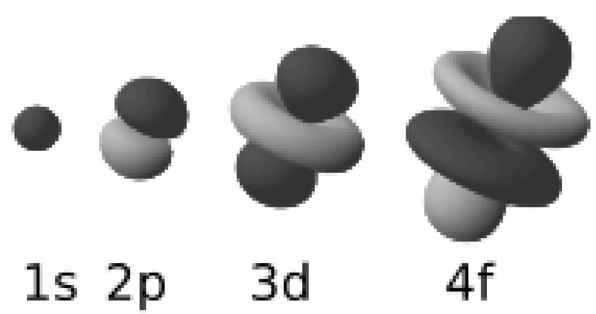

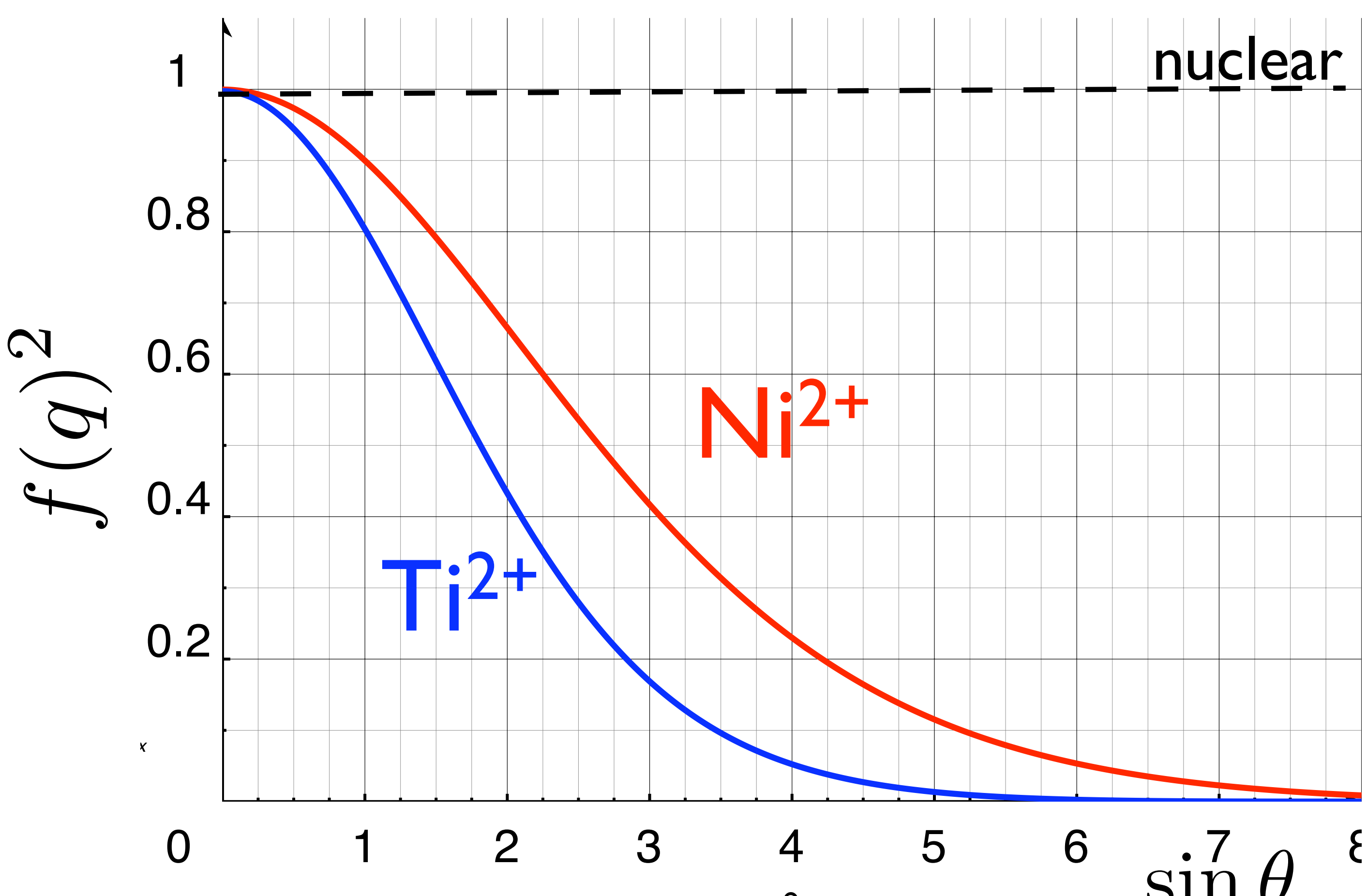

$$q = 4\pi \frac{\sin\theta}{\lambda}$$

Magnetic neutron scattering on an atom

$$\text{"magnetic scattering amplitude"} = \gamma r_e \left\langle \hat{\mathbf{Q}}_\perp \right\rangle$$

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

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

Magnetic neutron scattering on an atom

3. geometry

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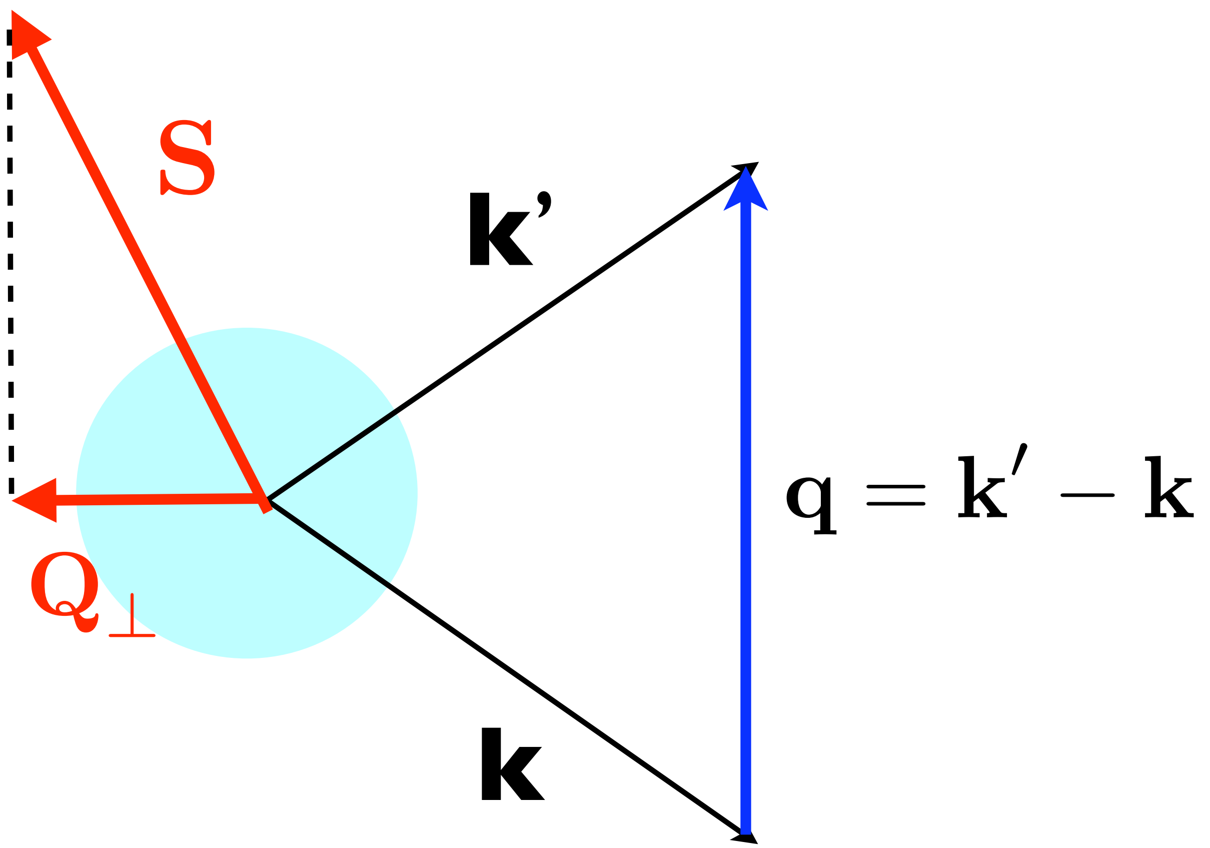

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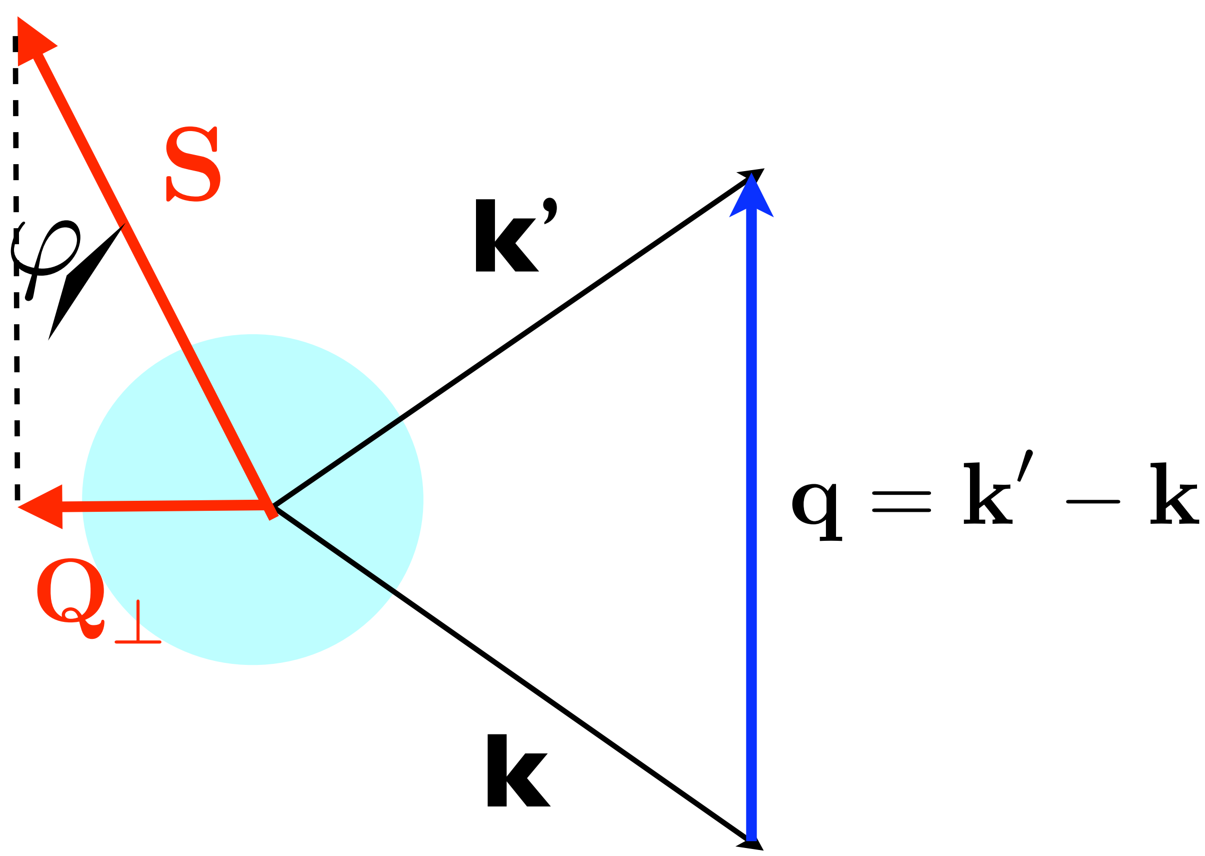


$$|\mathbf{Q}_\perp| = |\mathbf{S}| \sin(\varphi)$$

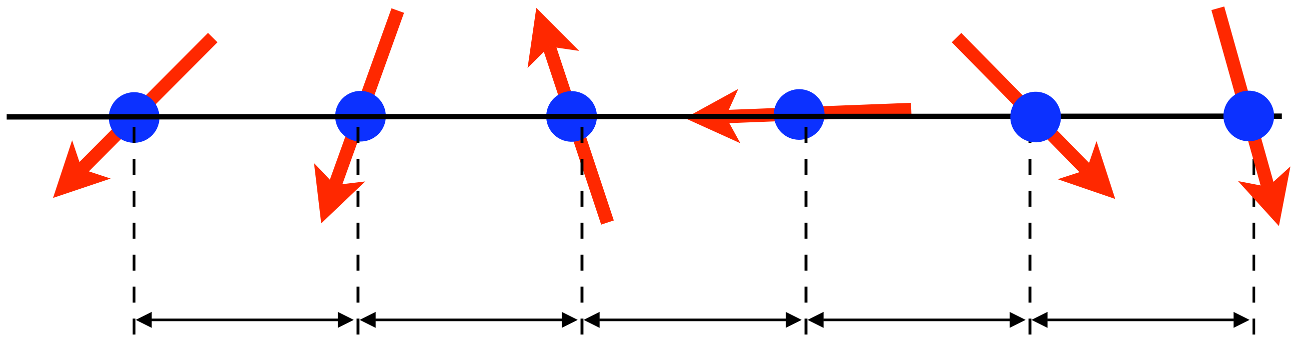
Elastic scattering intensity

Neutron scattering cross-section
(for unpolarized neutron beam)

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

Elastic scattering on a lattice of spins

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



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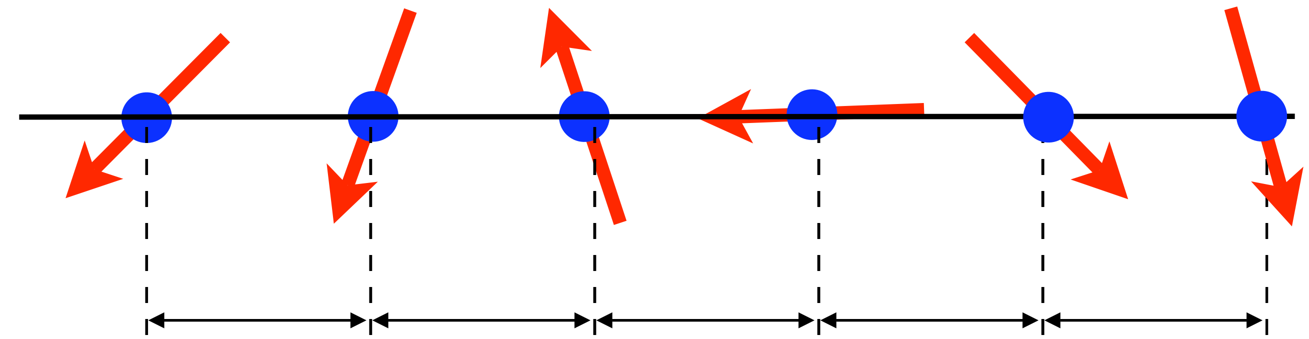

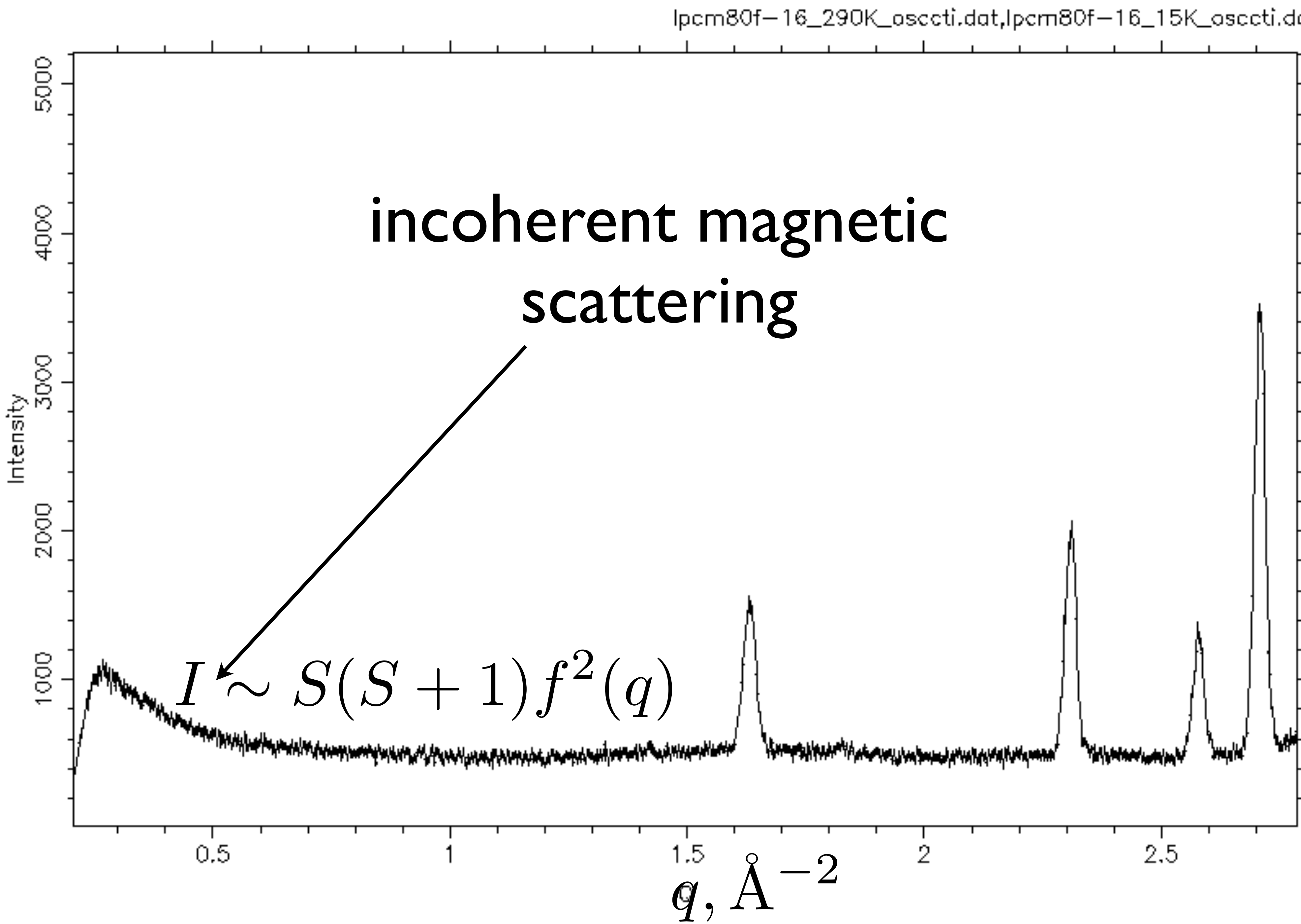

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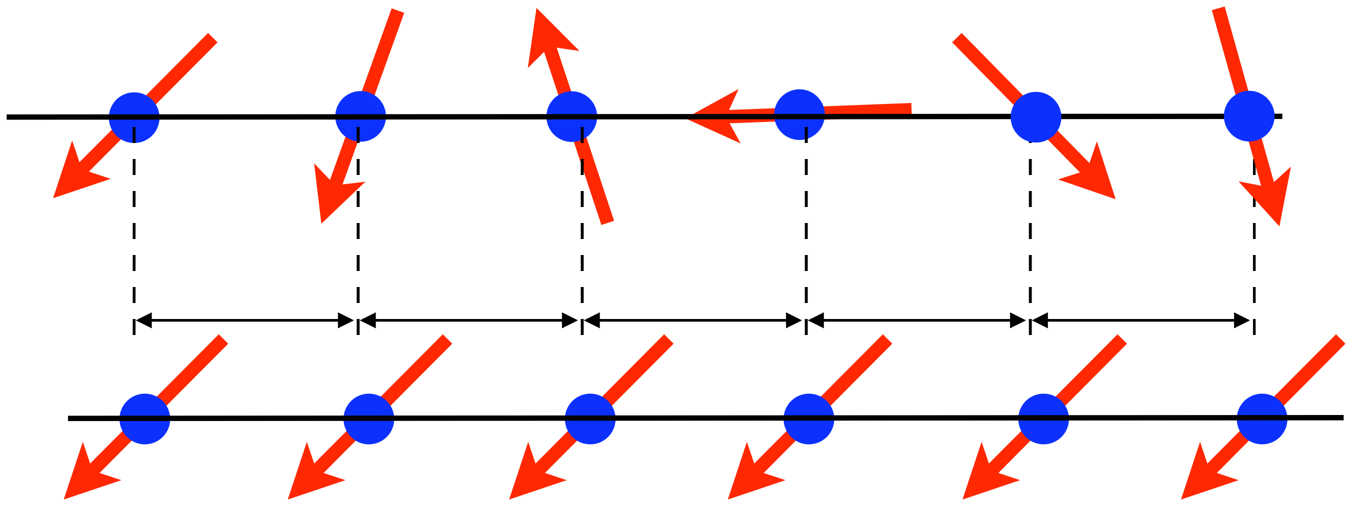

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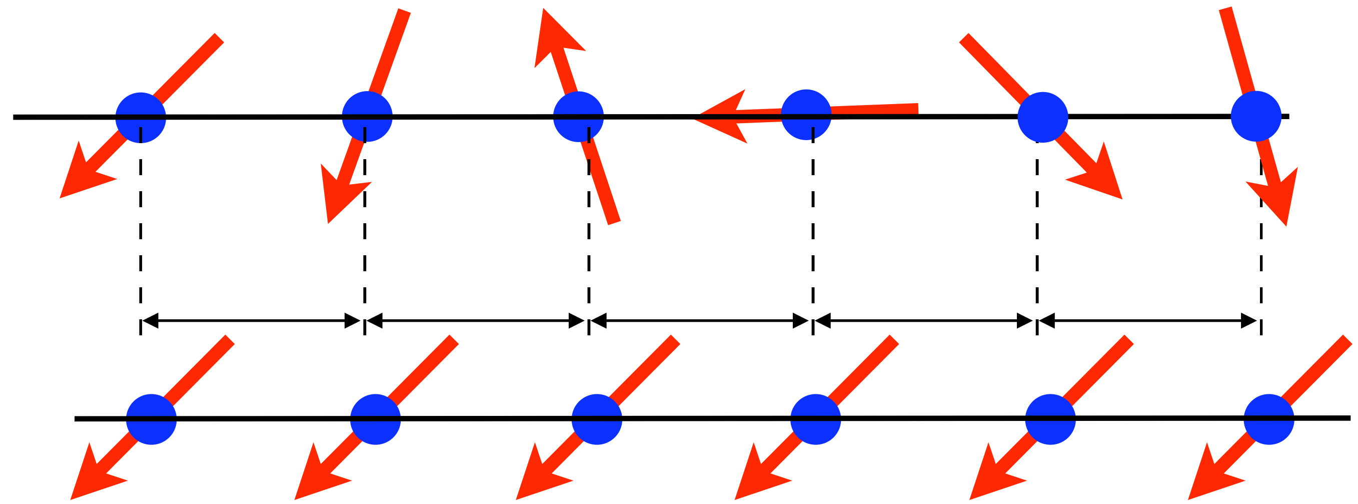

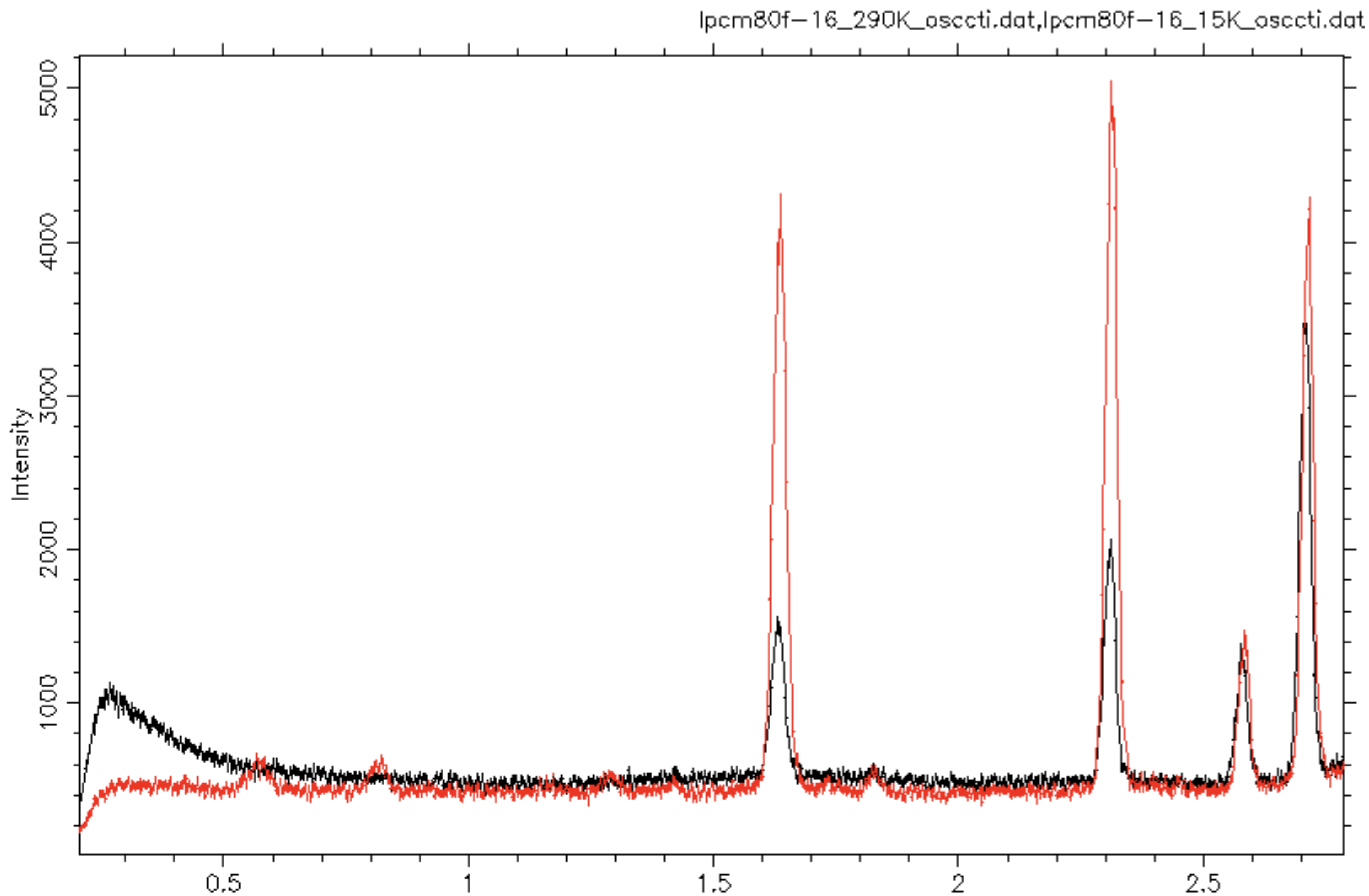

Non-polarized neutron diffraction

magnetic → $\mathbf{Q}_\perp$, nuclear → F

$$I^{++} \propto \left\langle |\mathbf{Q}_\perp \boldsymbol{\sigma}_n + F|^2 \right\rangle_{\sigma_n}$$

average over neutron polarization

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$$I \propto \langle (\mathbf{Q}_\perp \boldsymbol{\sigma}_n)(\mathbf{Q}_\perp^* \boldsymbol{\sigma}_n) + FF^* + \boldsymbol{\sigma}_n (F\mathbf{Q}_\perp^* + F^*\mathbf{Q}_\perp) \rangle_{\boldsymbol{\sigma}_n}$$

$\boldsymbol{\sigma}_n (F\mathbf{Q}_\perp^* + F^*\mathbf{Q}_\perp)$ → 0

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 Rietveld refinement

Interference between nuclear and magnetic scattering

General note:

When the magnetic unit cell is larger than the nuclear one (propagation vector $k \neq 0$) the interference between nuclear and magnetic scattering is absent in any (un)polarized neutron diffraction experiment.

Reason: Magnetic Bragg peaks appear at different positions in reciprocal space

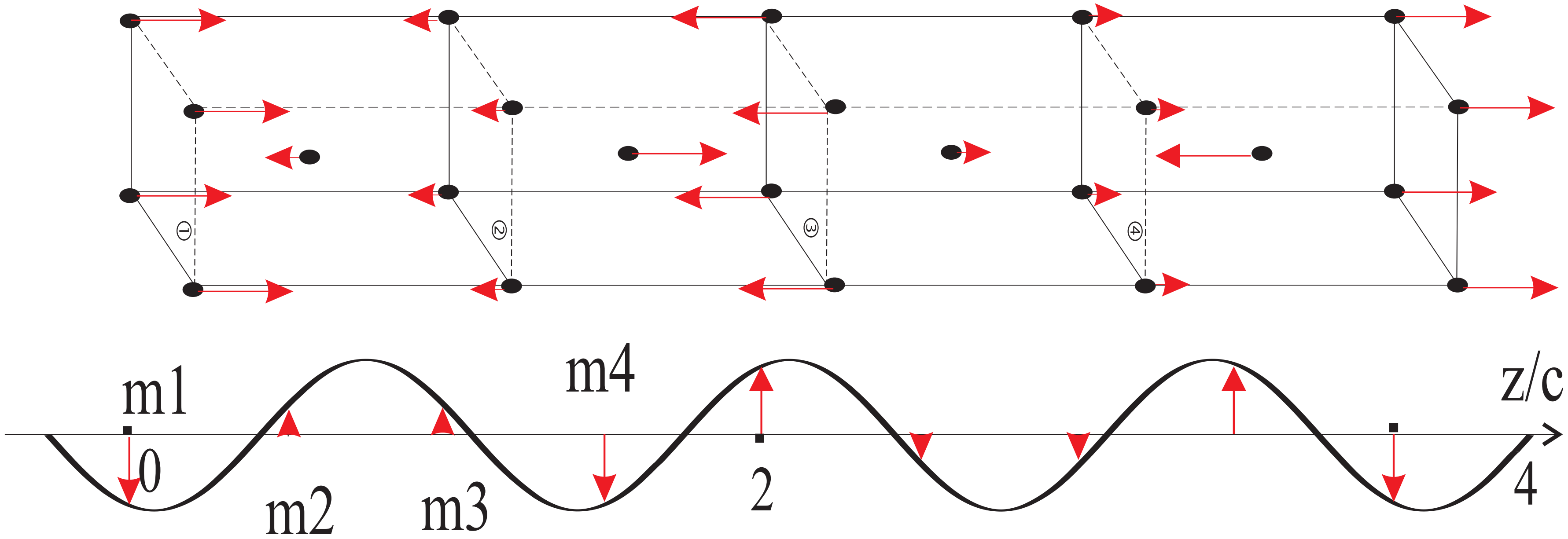
Only amplitudes can be determined

$$\mathbf{S} = \mathbf{S}_0 \cos(2\pi k z + \phi), k = \frac{3}{4}$$

Spin/atom magnetic moment

Amplitude

$\phi = 7\pi/8$



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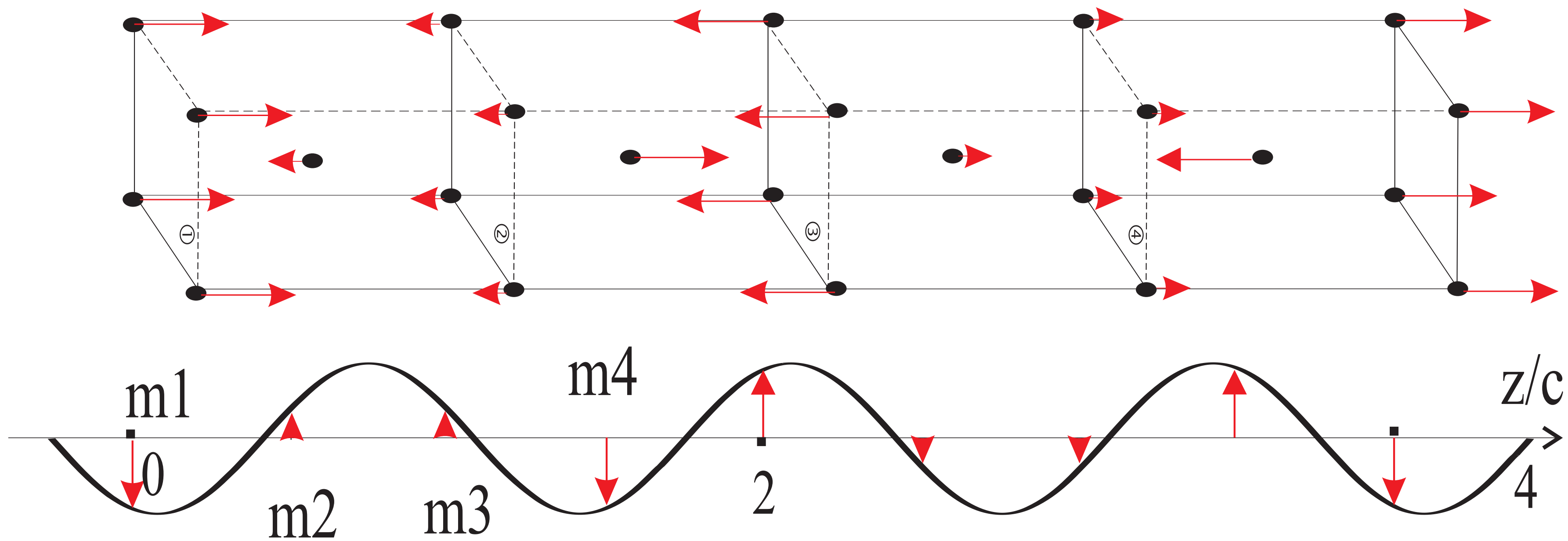

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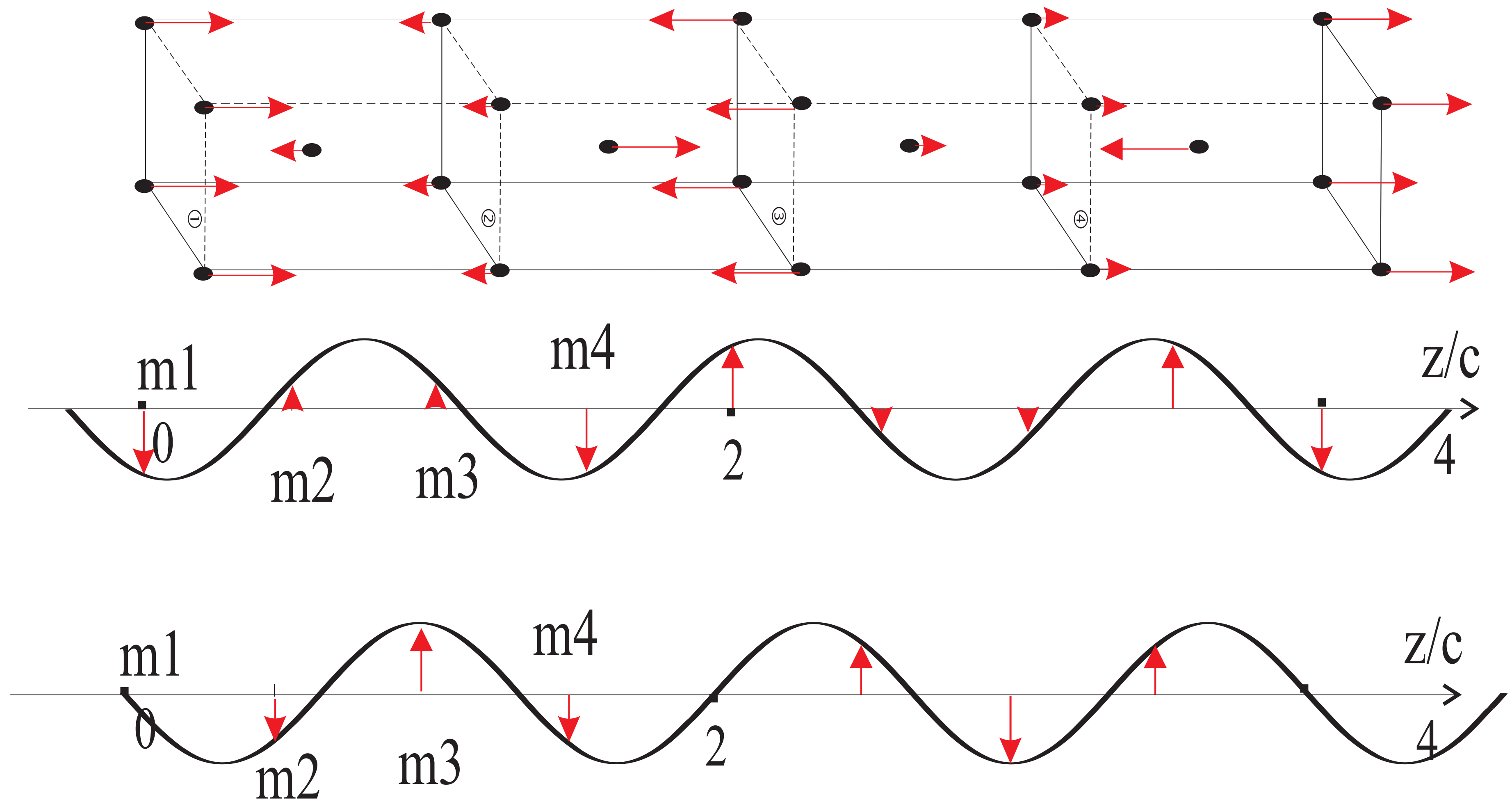
Spin/atom magnetic moment

Amplitude

$\phi = 7\pi/8$

$\phi = \pi/2$



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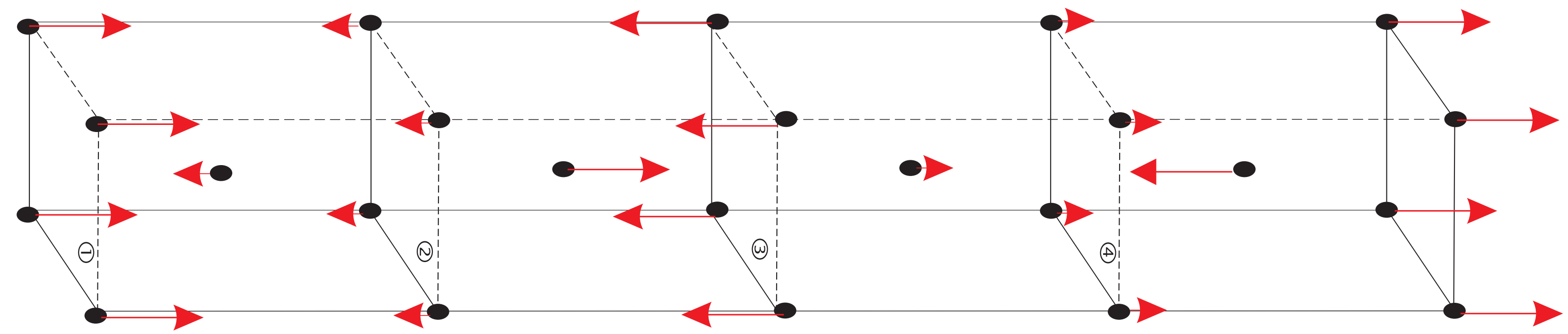

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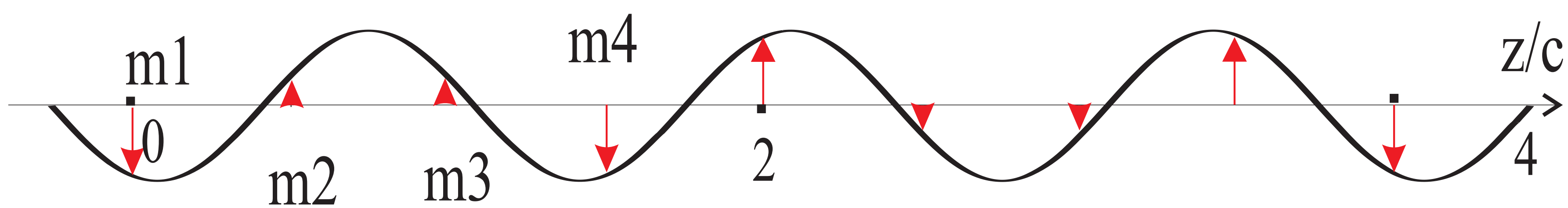
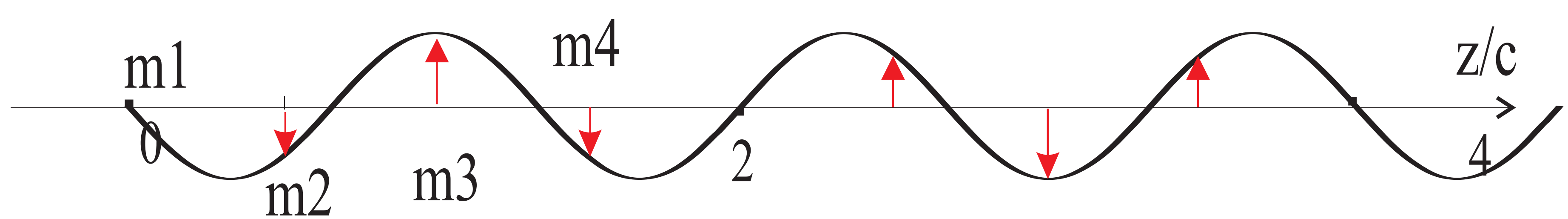


$\phi = \pi/2$



The phase *Φ* is not accessible and the magnetic moments on the atoms cannot be determined.

powder diffraction, + and −

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- \+ experimentally simple, full q-range is detected, no missed incommensurate satellites, better resolution
- \+ no difficult corrections, e.g. extinction, crystal shape
- \- peak overlapping/multiplicity in powder data puts a restriction on the determination of spin direction
- \- small spin components ($\sim 10^{-1}\mu_B$) are difficult to detect

Powder neutron diffractometers

European Portal for Neutron Scattering

http://pathfinder.neutron-eu.net

Powder neutron diffractometers

ILL, FR	D20, D2B, D1A
LLB, FR	G41, G42
ISIS, UK	GEM, HRPD, PEARL
FRM-II, DE	SPODI
FLNP/Dubna, RU	HRFD, DN2, DN12
SINQ/PSI, CH	DMC, HRPT, POLDI

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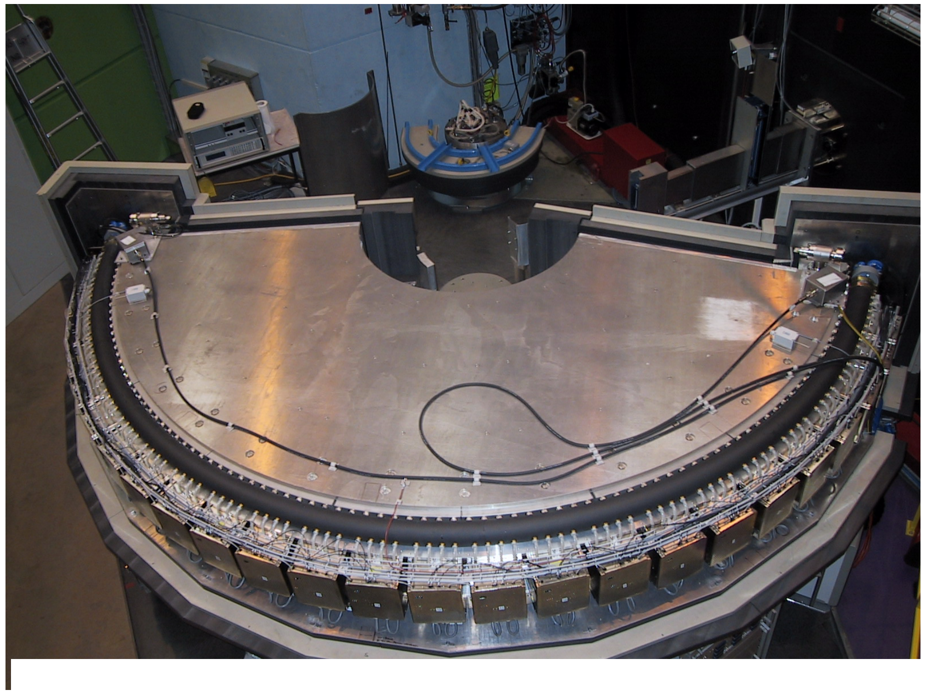
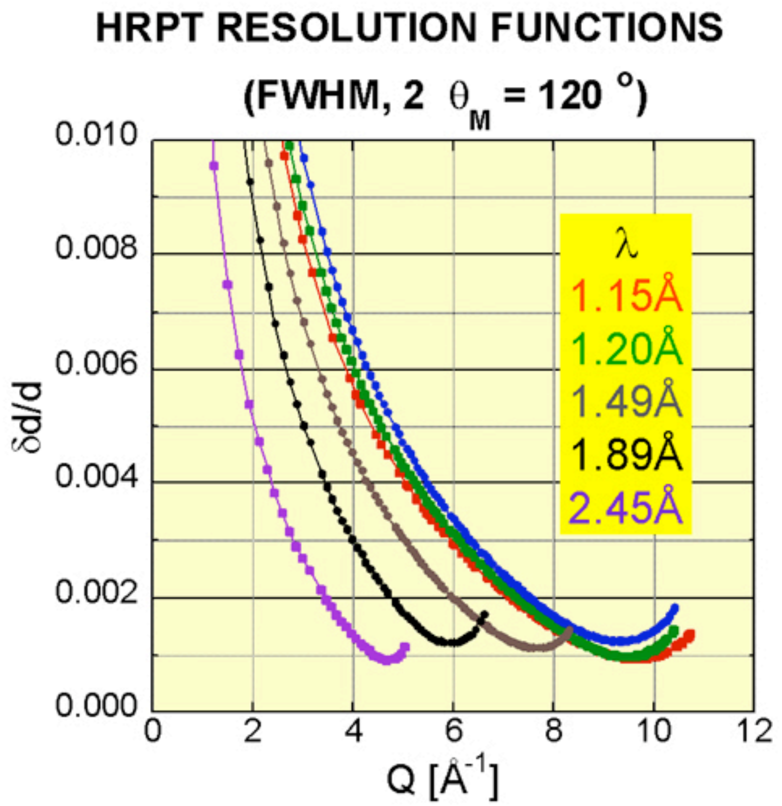
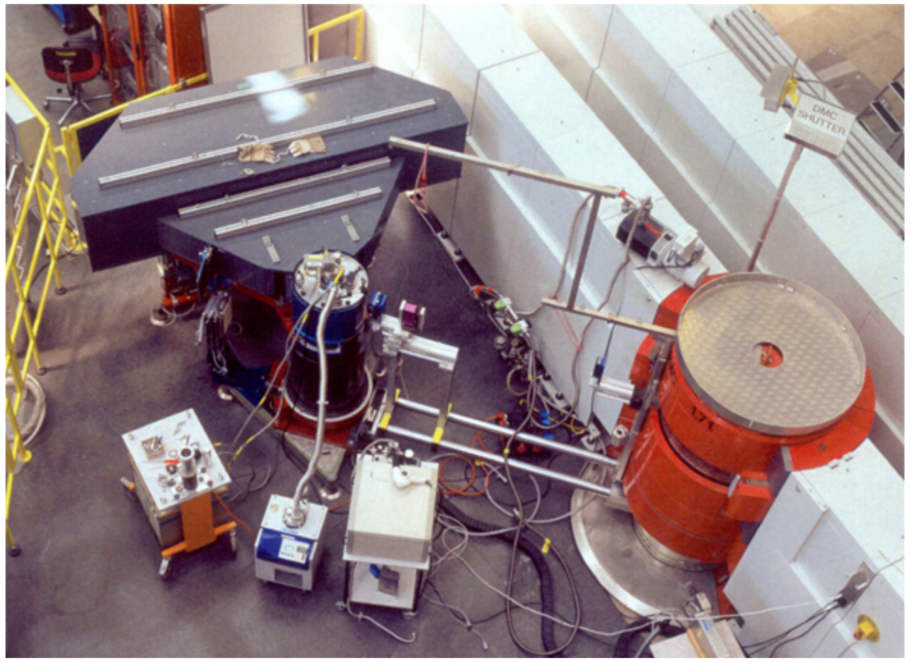
Powder ND at SINQ/PSI

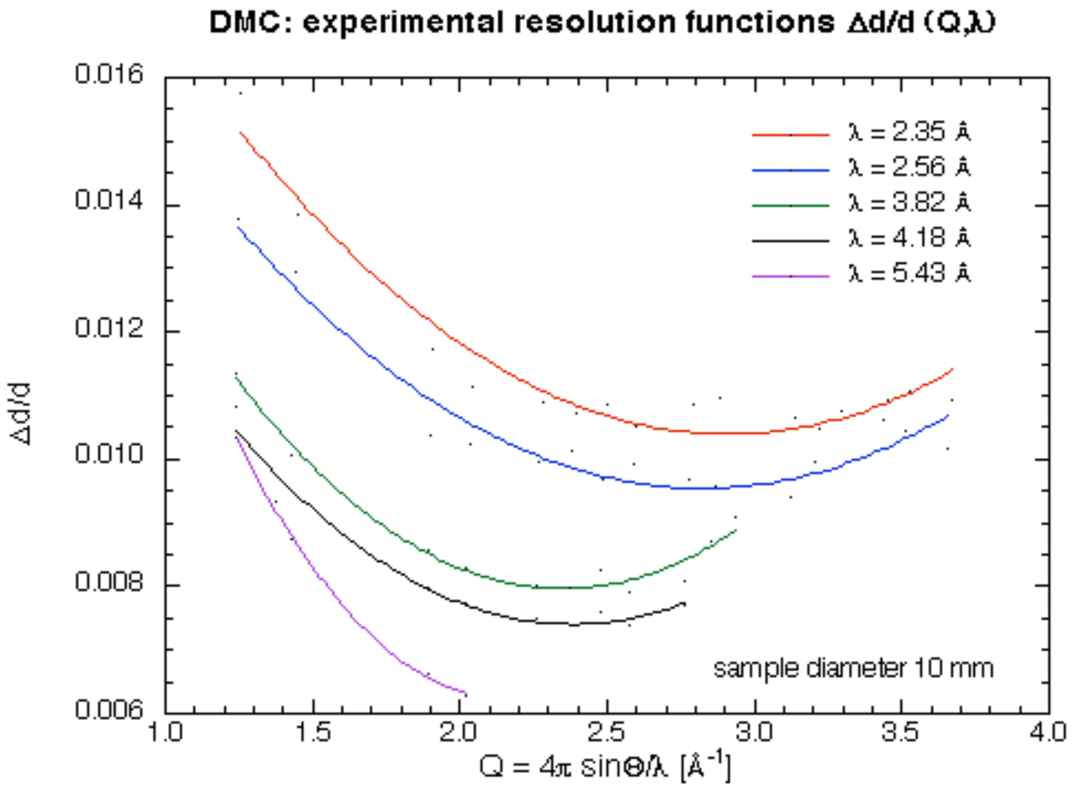
HRPT - High Resolution Powder Diffractometer for Thermal Neutrons at SINQ



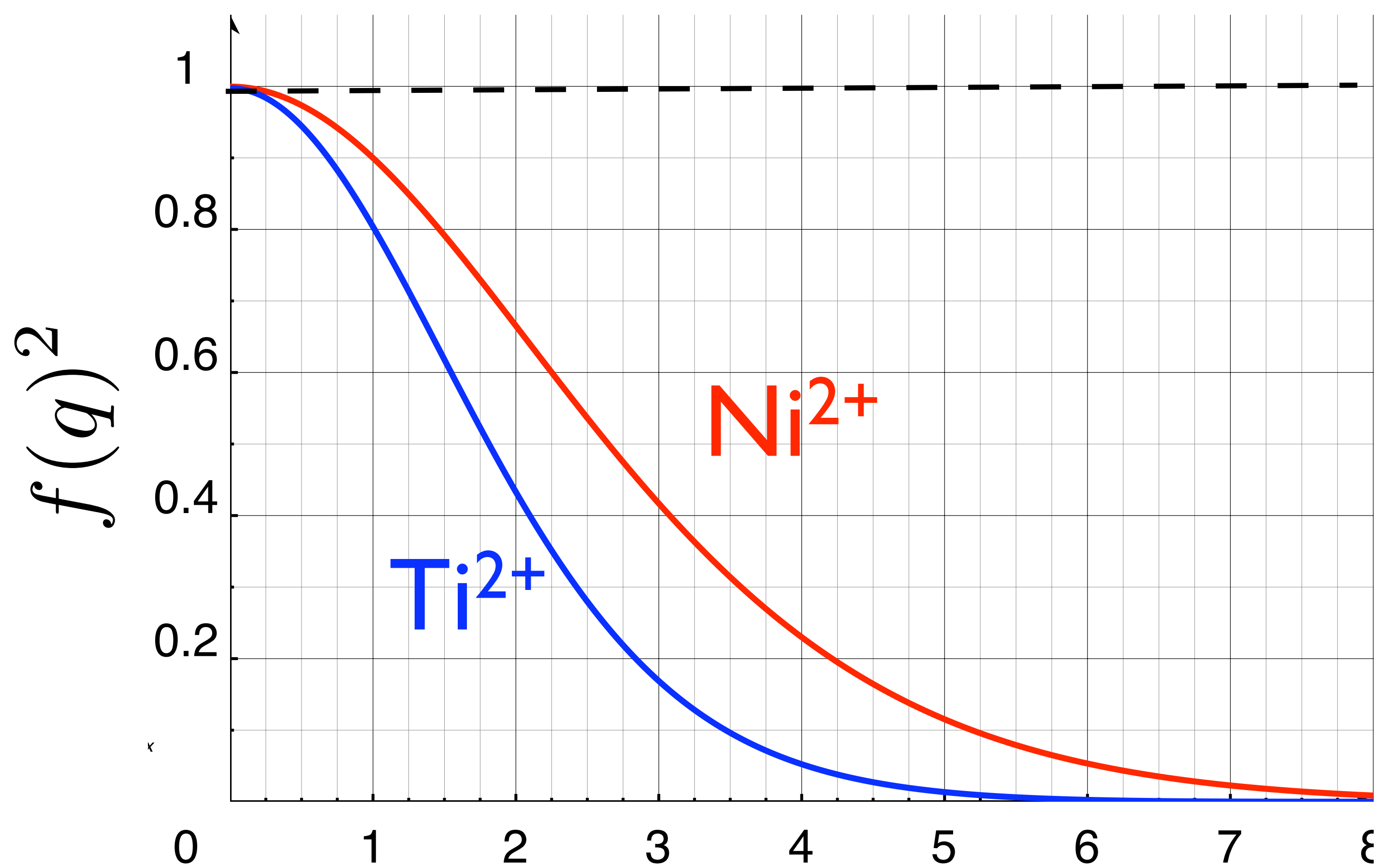


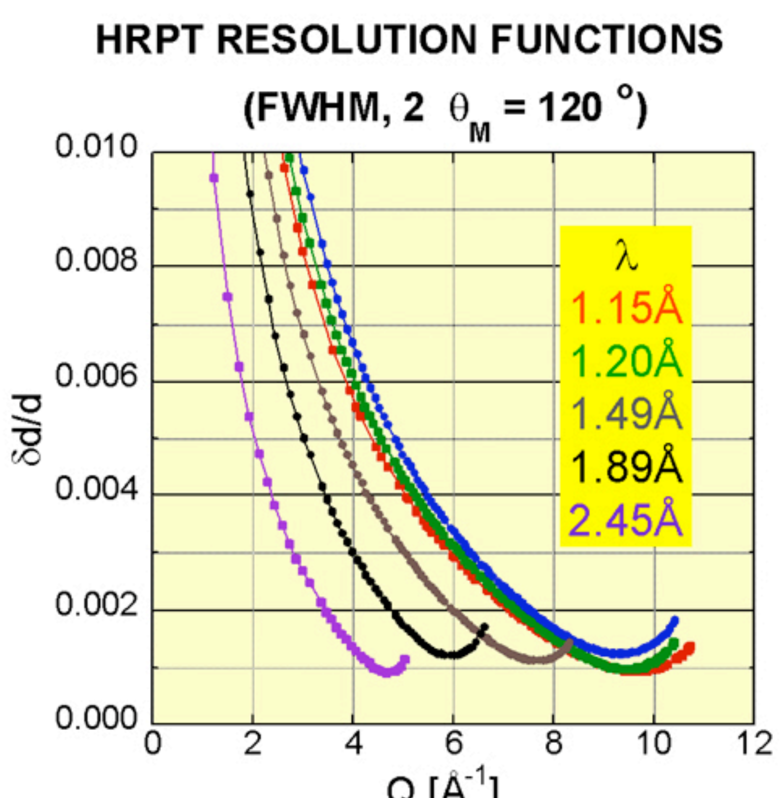
DMC - cold neutron powder diffractometer

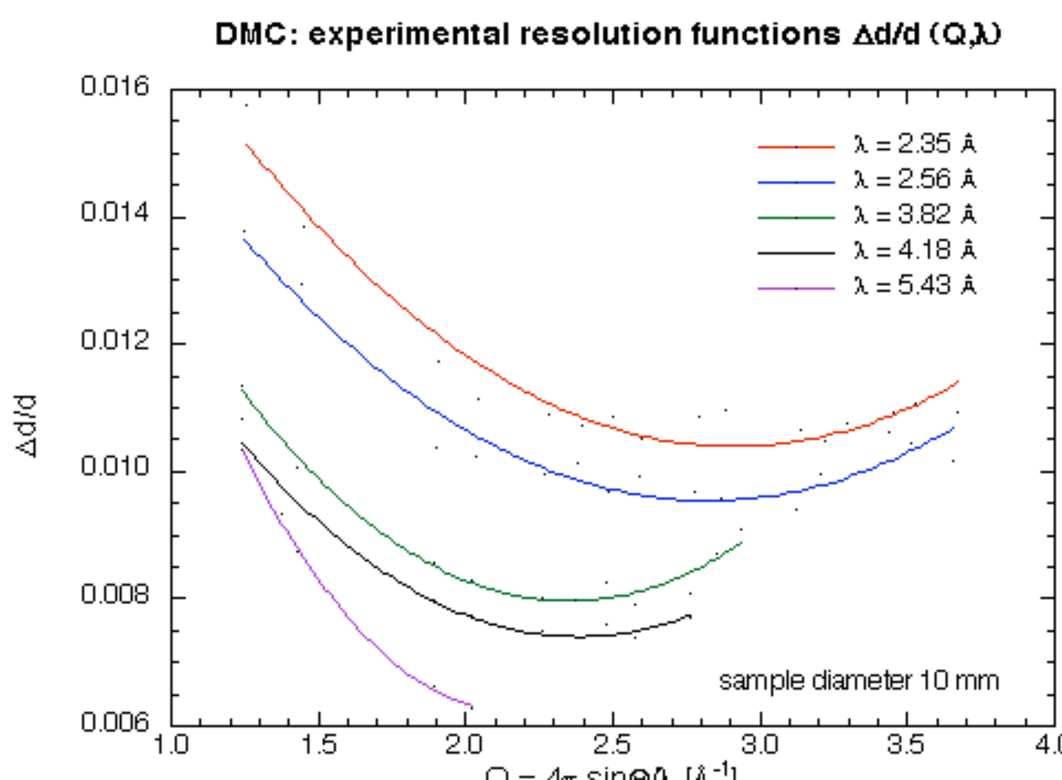




Powder ND at SINQ/PSI







Examples of magnetic structures.
Propagation vector k

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☺ Magnetic moment is a real quantity!

$$\mathbf{S}(\mathbf{r}_j) = Re(\mathbf{S}_0 e^{2\pi i \mathbf{r}_j \mathbf{k}}) = \frac{1}{2}(\mathbf{S}_0 e^{+2\pi i \mathbf{r}_j \mathbf{k}} + c.c.)$$

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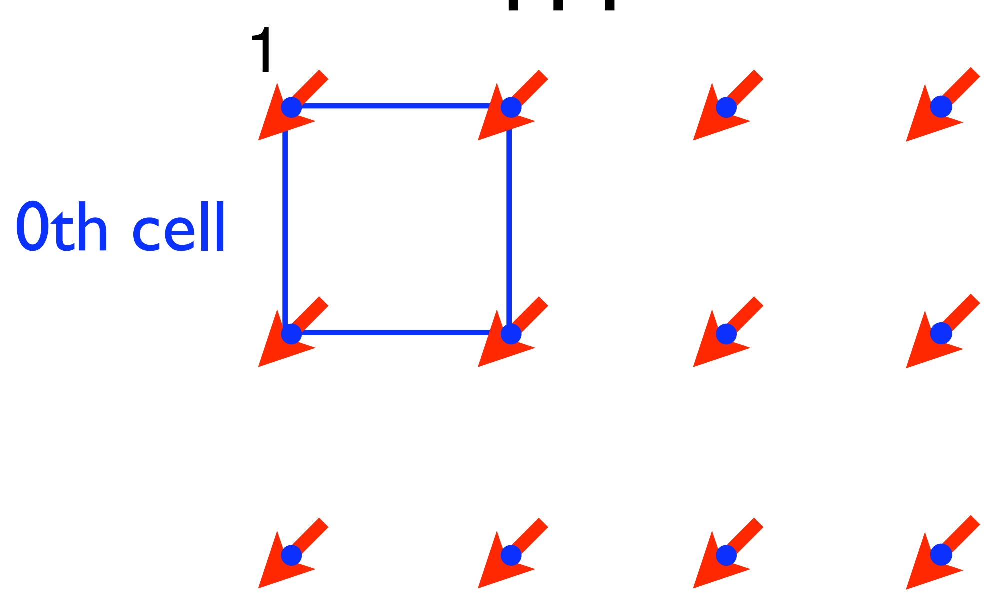
☹ Amplitude is complex $$\mathbf{S}_0 = \mathbf{S}_x e^{i\phi_x} + \mathbf{S}_y e^{i\phi_y} + \mathbf{S}_z e^{i\phi_z}$$

Examples of magnetic structures.
Propagation vector k

☺ Magnetic moment is a real quantity! $\mathbf{S}(\mathbf{r}_j) = Re(\mathbf{S}_0 e^{2\pi i \mathbf{r}_j \mathbf{k}}) = \frac{1}{2}(\mathbf{S}_0 e^{+2\pi i \mathbf{r}_j \mathbf{k}} + c.c.)$

☹ Amplitude is complex $\mathbf{S}_0 = \mathbf{S}_x e^{i\phi_x} + \mathbf{S}_y e^{i\phi_y} + \mathbf{S}_z e^{i\phi_z}$

k=[0,0]
FM



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

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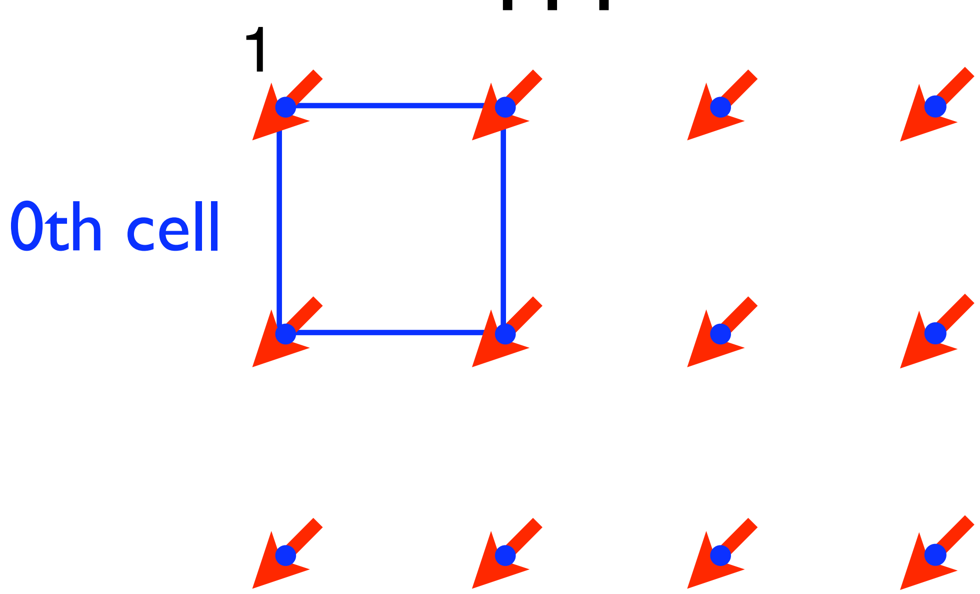

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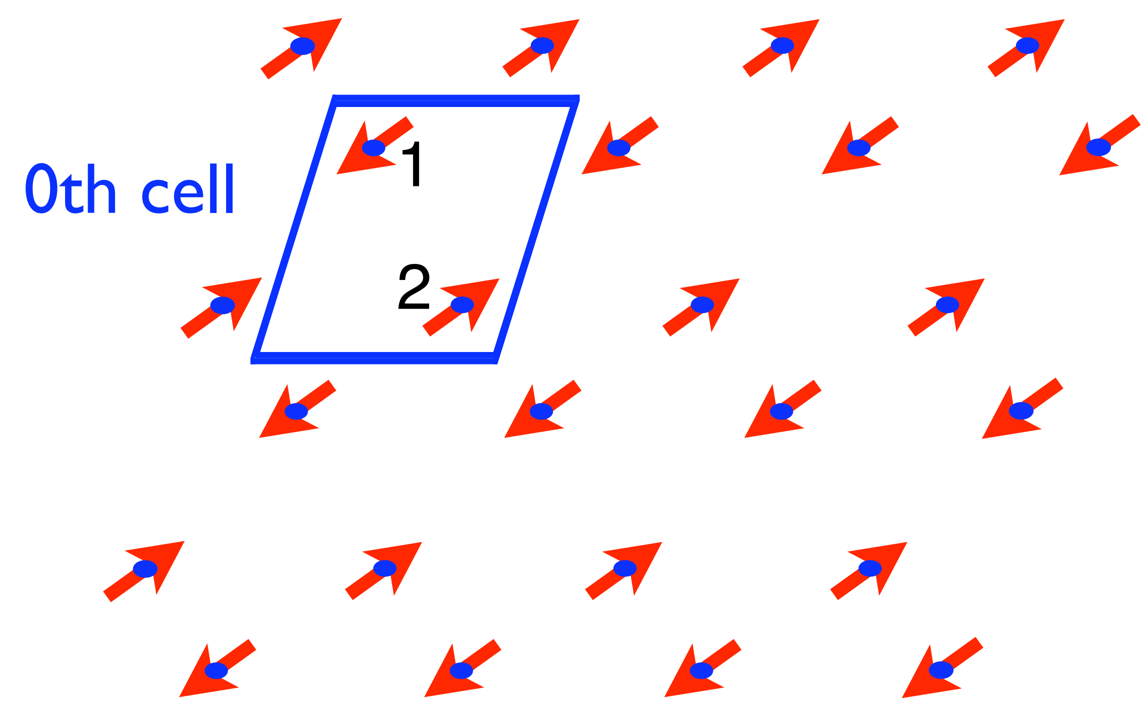
AFM



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

$$\mathbf{S}_{02} = -\mathbf{S}_{01}$$

Examples of magnetic structures.
Propagation vector k≠0

Magnetic moment is a real quantity!

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Amplitude is complex

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Examples of magnetic structures. Propagation vector k≠0

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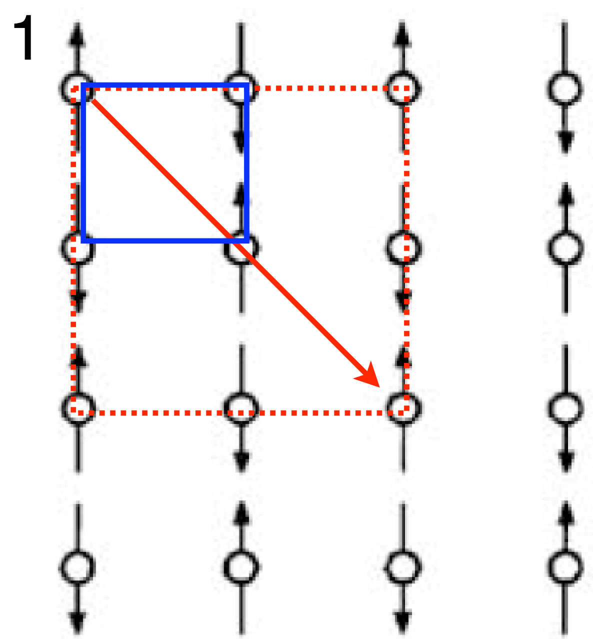
k=[1/2,1/2] AFM



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

Examples of magnetic structures. Propagation vector k≠0

Magnetic moment is a real quantity!

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Amplitude is complex

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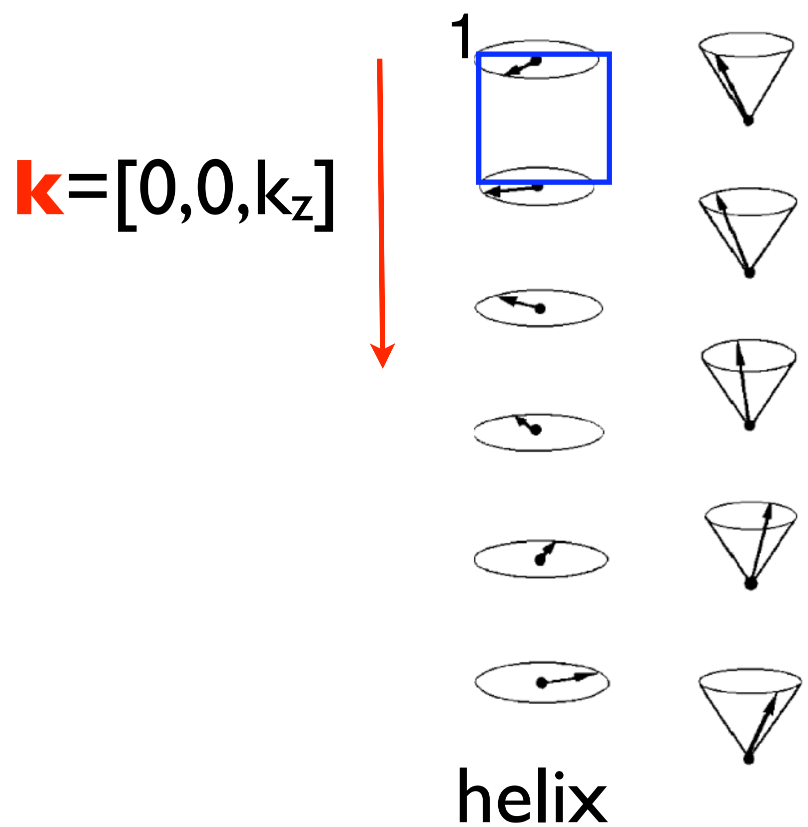
<u>modulated (in)commensurate</u>



Examples of magnetic structures. Propagation vector k≠0

Magnetic moment is a real quantity!

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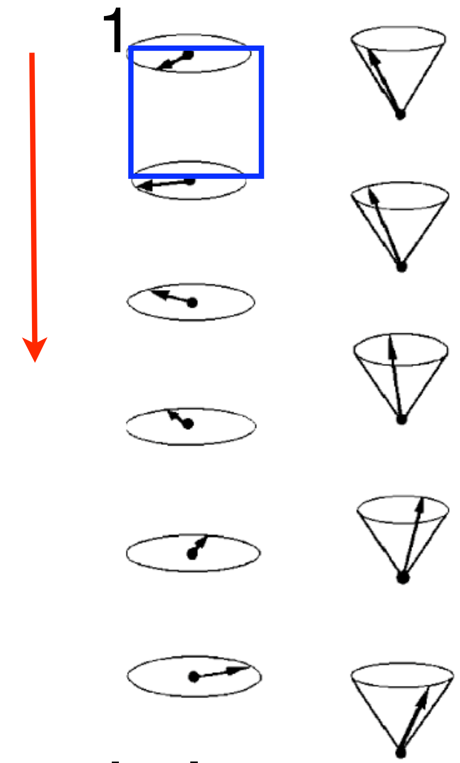
<u>modulated (in)commensurate</u>

k=[0,0,k_z]



helix

$$\mathbf{S}_{01} = \mathbf{S}_x + \mathbf{S}_y e^{\frac{i\pi}{2}} = \mathbf{S}_x + i\mathbf{S}_y$$

Examples of magnetic structures. Propagation vector k≠0

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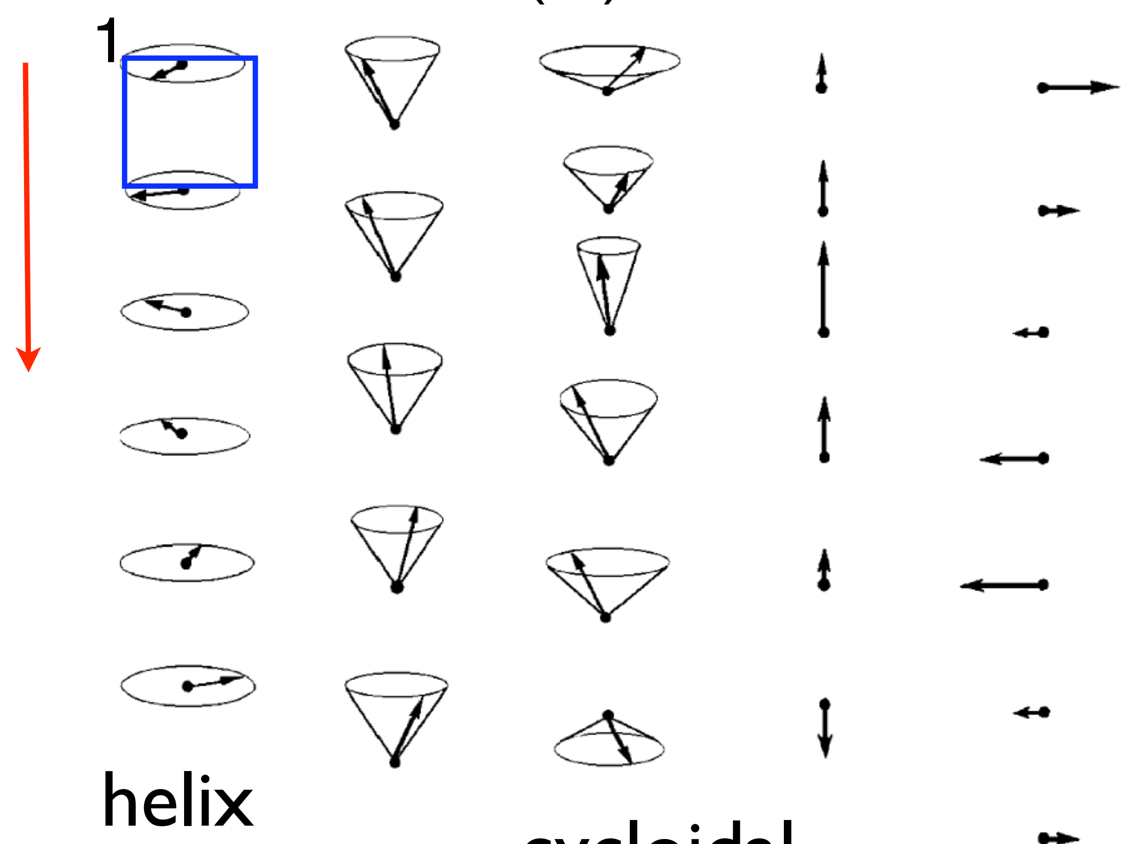

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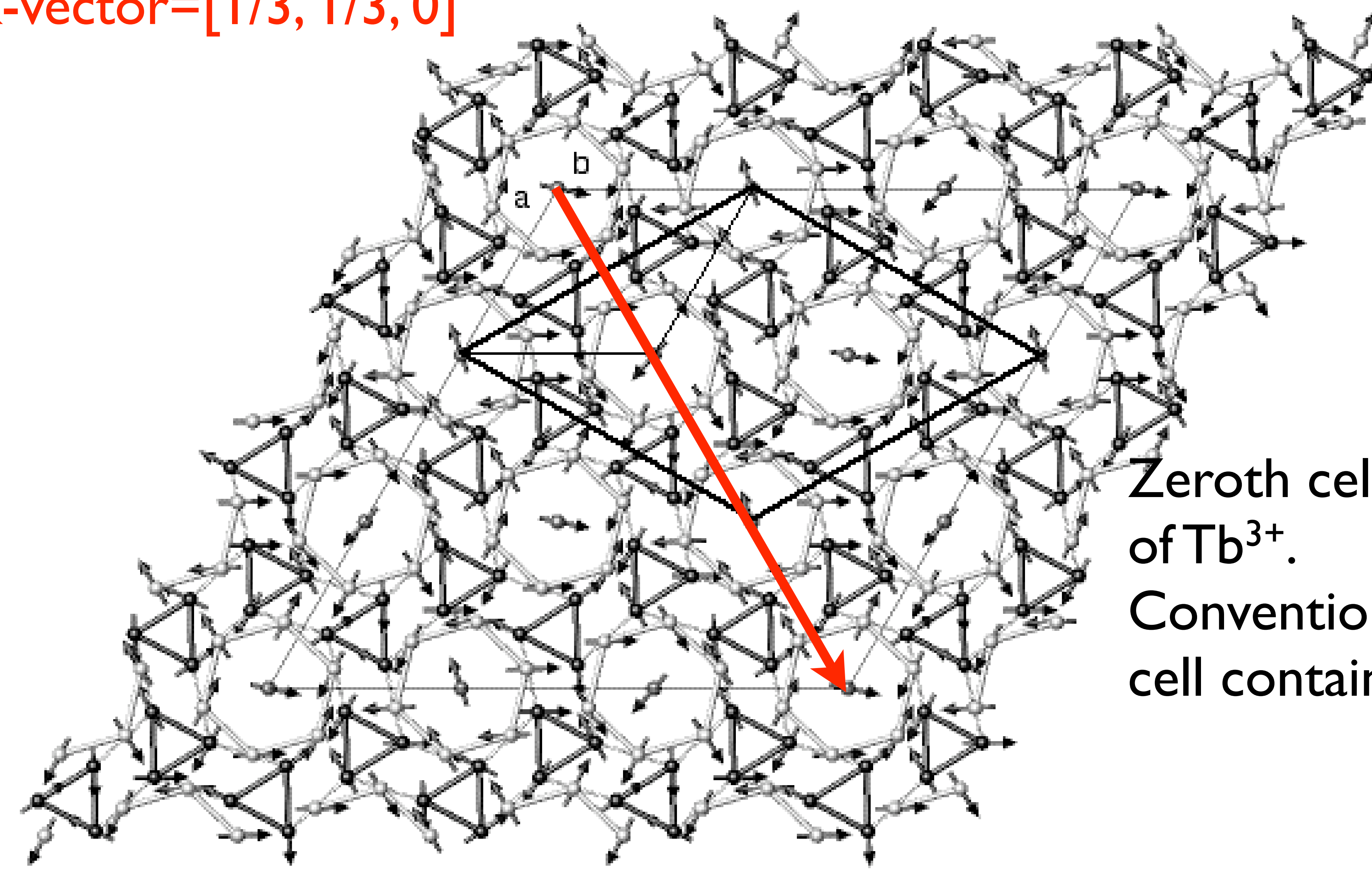
Example of complex magnetic structure

Example of complex magnetic structure

Antiferromagnetic three sub-lattice ordering in $Tb_{14}Au_{51}$

P6/m

k-vector=[1/3, 1/3, 0]



Zeroth cell contains 14 spins of Tb^{3+}.

Conventional magnetic unit cell contains 126 spins of Tb^{3+}.

Analysis of magnetic neutron diffraction: computer programs and tutorials/notes

- INDEXING, K-VECTOR: programs distributed with FullProf Suite [1]
- SYMMETRY: BasIreps[1], SARAh[2], MODY[3]
- SOLUTION: FullProf [1] (simulated annealing)
- REFINEMENT: FullProf, GSAS [4]
- Visualization: FPStudio [1]

REFERENCES

1. **Juan Rodríguez-Carvajal (ILL) et al,** http://www.ill.fr/sites/fullprof/
2. **Andrew S. Wills (UCL)** http://www.chem.ucl.ac.uk/people/wills/magnetic_structures/magnetic_structures.html
3. **Wieslawa Sikora et al,** http://www.ftj.agh.edu.pl/~sikora/modyopis.htm
4. **Bob Von Dreele (ANL) et al,** http://www.ncnr.nist.gov/programs/crystallography/software/gsas.html

Description of magnetic structures

Description of magnetic structures

Magnetic symmetry

1651 3D magnetic Shubnikov (*Sh*) space groups. Derived from 230 space groups *G* and an additional element: spin inversion operator *R*. *Sh* groups contain additional 'antielements' g'=(*g* · *R*), *g*∈*G* (except 1) e.g. Pnnm'

R= time reversal
changes **S** to -**S**

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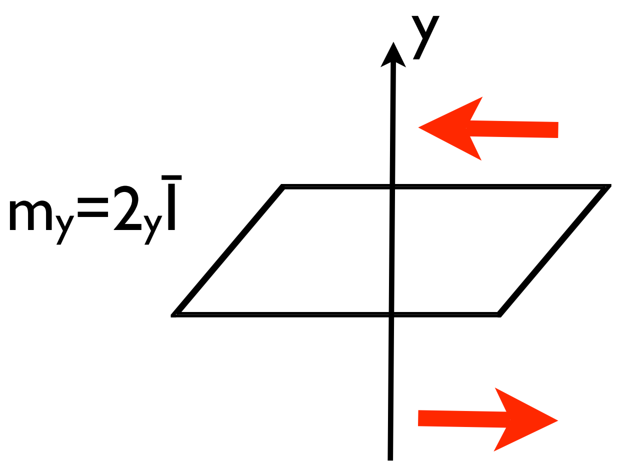

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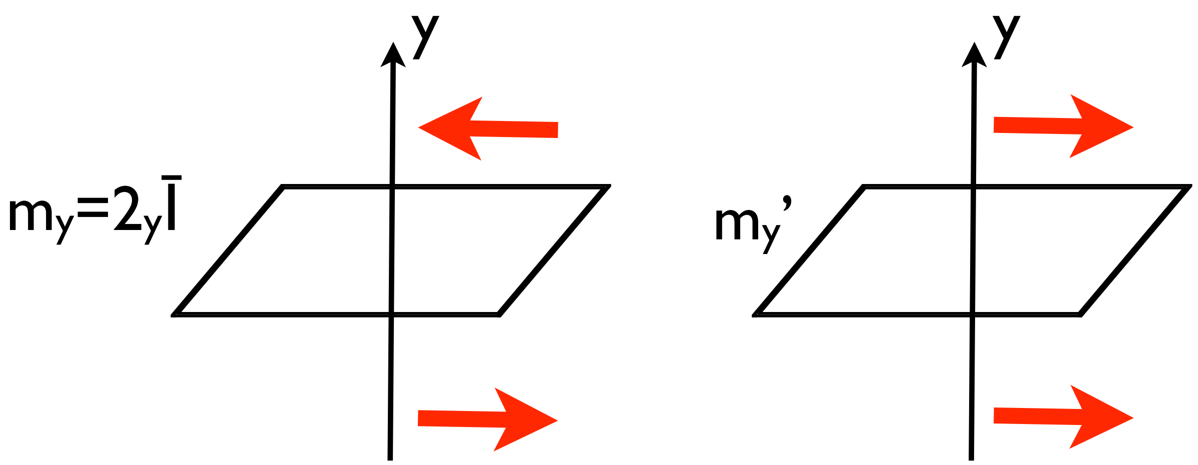

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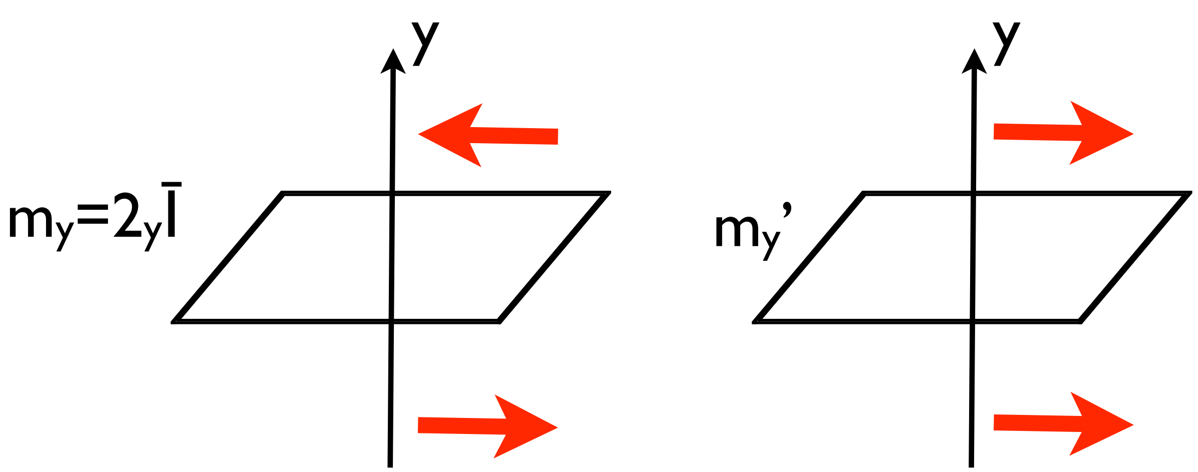

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Disadvantages:

- *Sh* group is not necessarily made from the parent *G*. Thus, it is not an ultimate practical tool for obtaining all allowed spin configurations

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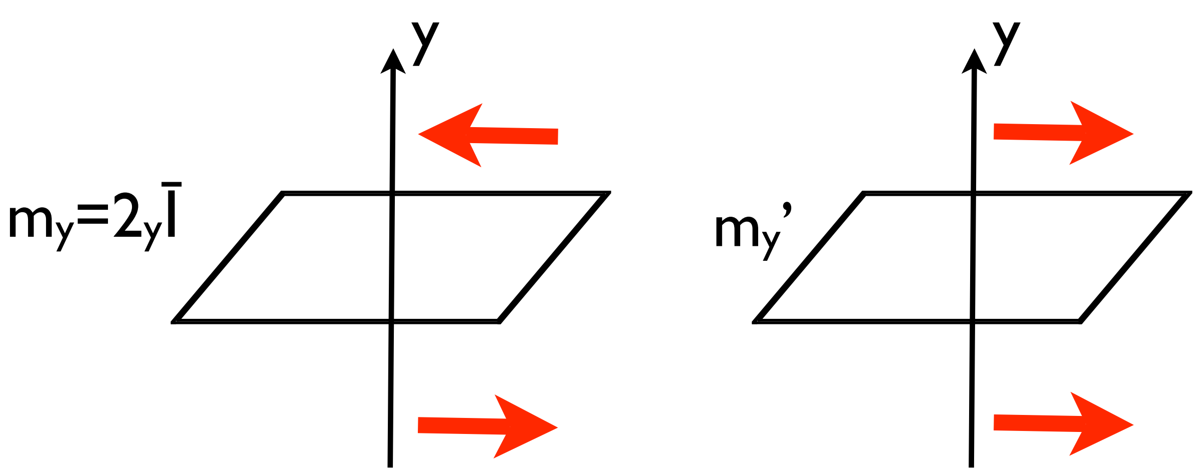
For example:
$CrCl_2$ space group: *Pnnm*
Possible *Sh groups* derived from the parent space group are: *Pnnm Pn'nm, Pnnm', Pn'n'm, Pnn'm', Pn'n'm'*



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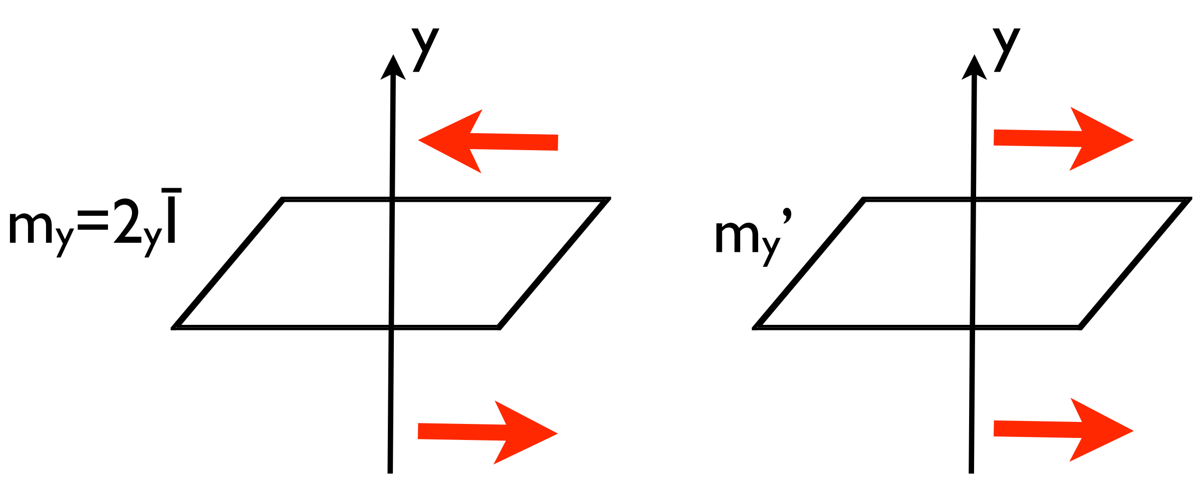

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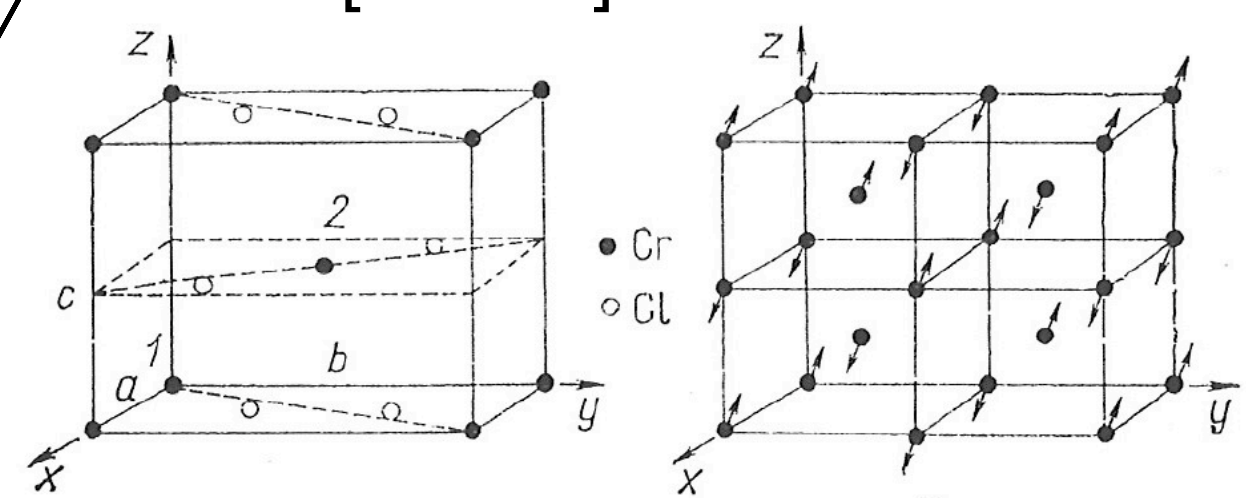
No one describes $CrCl_2$ magnetic structure

Cr-atoms in 2(a)-position

Cr-spins are antiparallel in 0th cell

k=[0 1/2 1/2]



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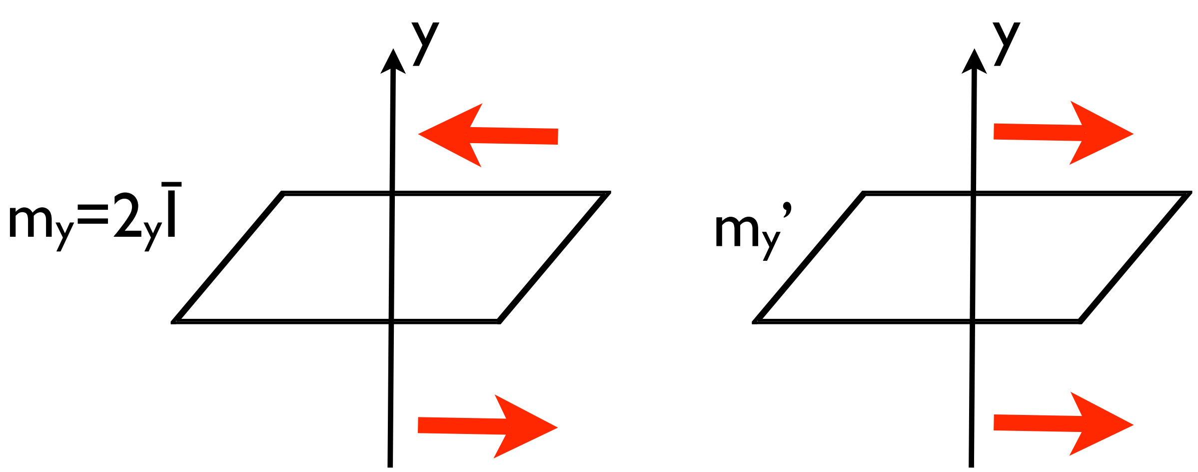

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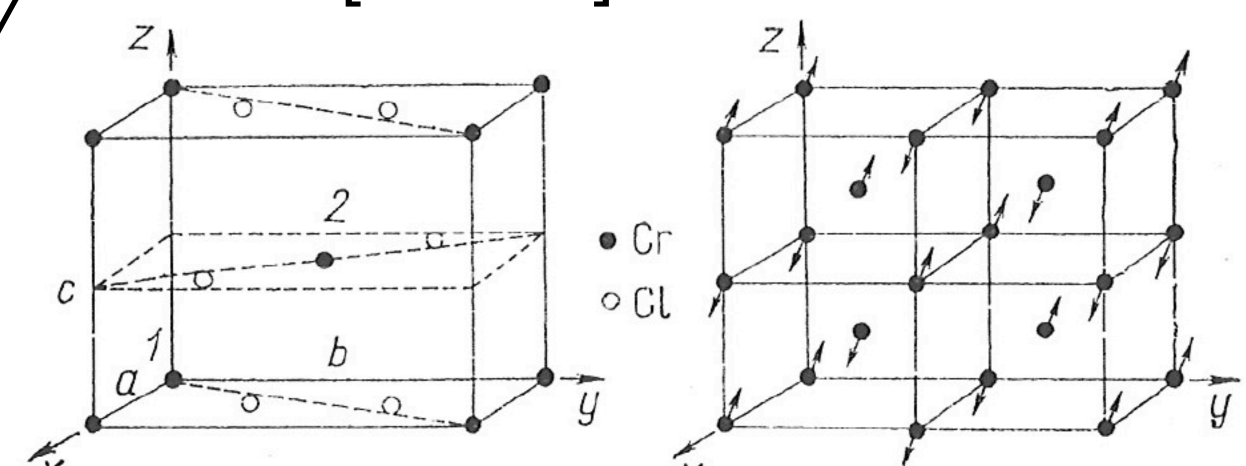

One can still find less symmetric *Sh* group

Magnetic symbol

{*Pnnm;* 2(a) $Sh^7_2=P_s\bar{1}$;

$\mathbf{S}_1$=(uvw), $\mathbf{S}_2$=(-u-v-w)}

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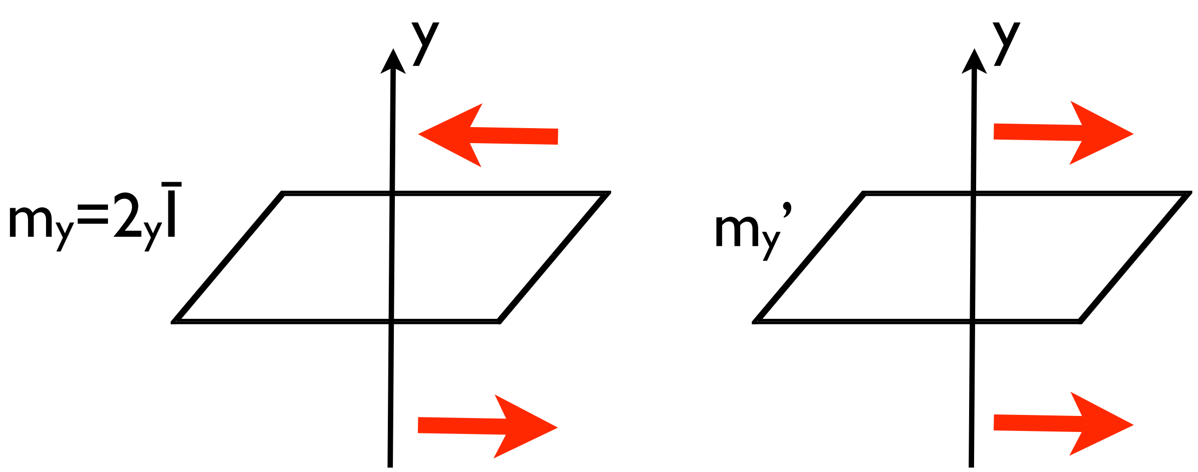

$$\mathbf{S} = "[\mathbf{v} \times \mathbf{r}]"$$

Disadvantages:

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- Do not describe modulated structures. No rotations on non-crystallographic angle - no helix. Linear orthogonal transformations preserve the spin size - no SDW

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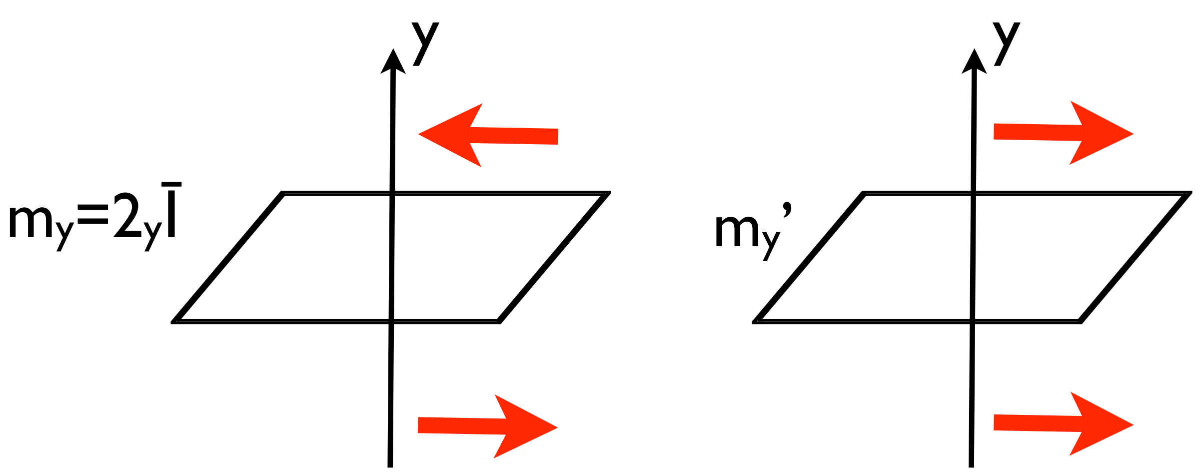

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Representation analysis

A universal technique of finding all possible symmetry adapted spin configurations for the given space group *G* and the propagation vector **k.**

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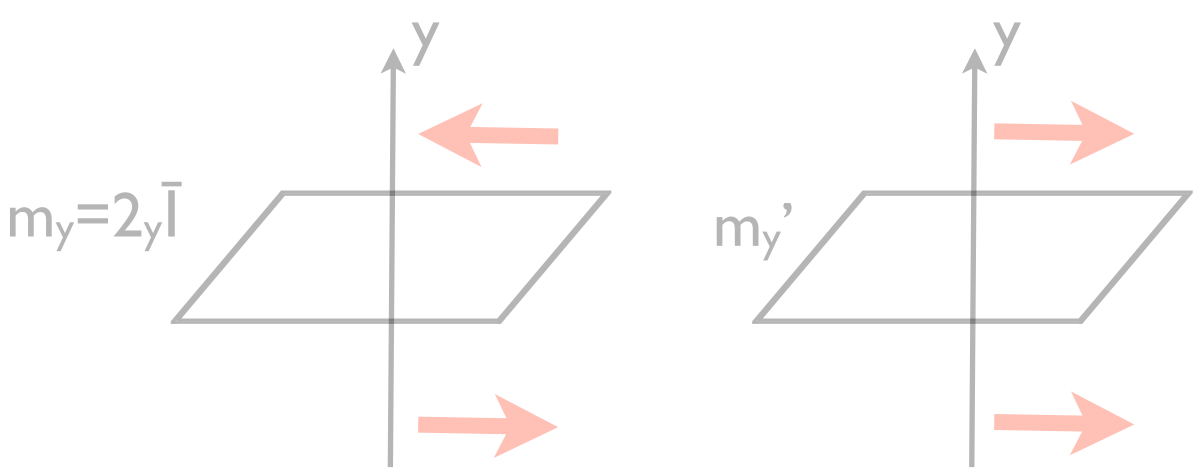

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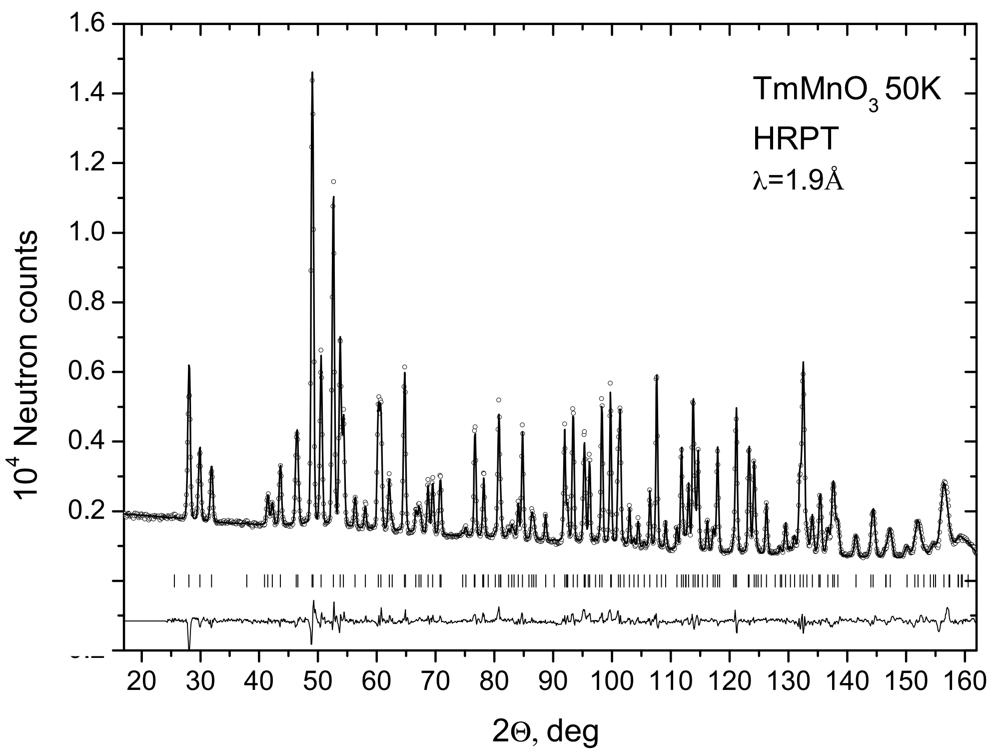
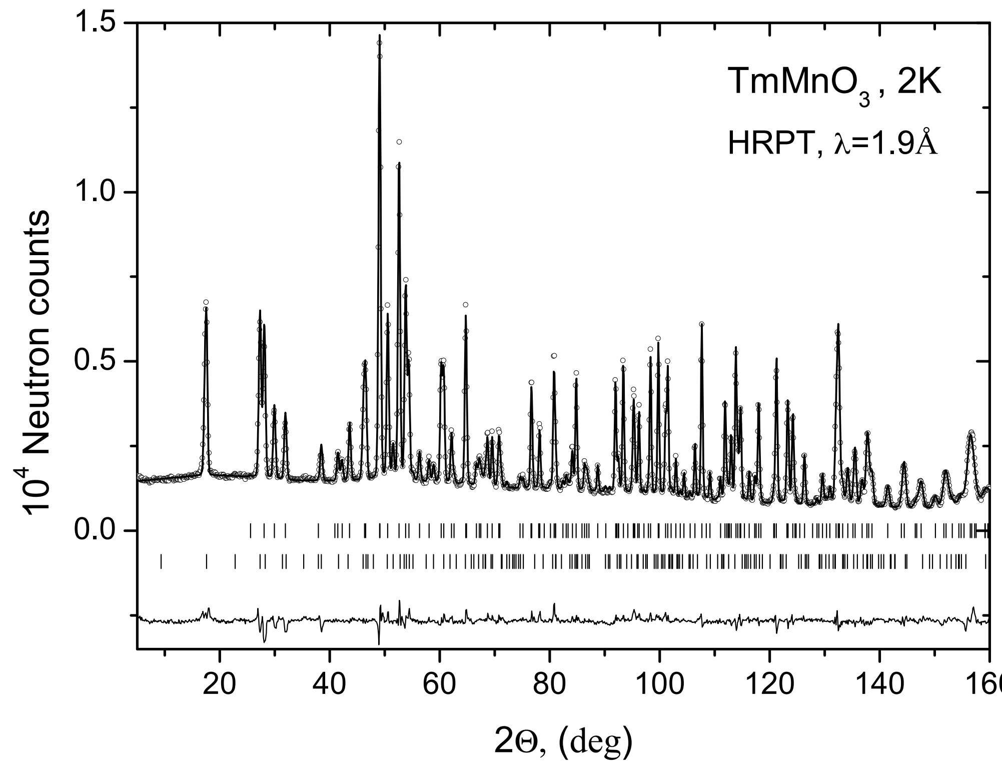
Case study. Antiferromagnetic order in orthorhombic $TmMnO_3$

Step 1

Experiment. q-range/resolution.

Patterns, 1.9Å HRPT and 4.5Å DMC





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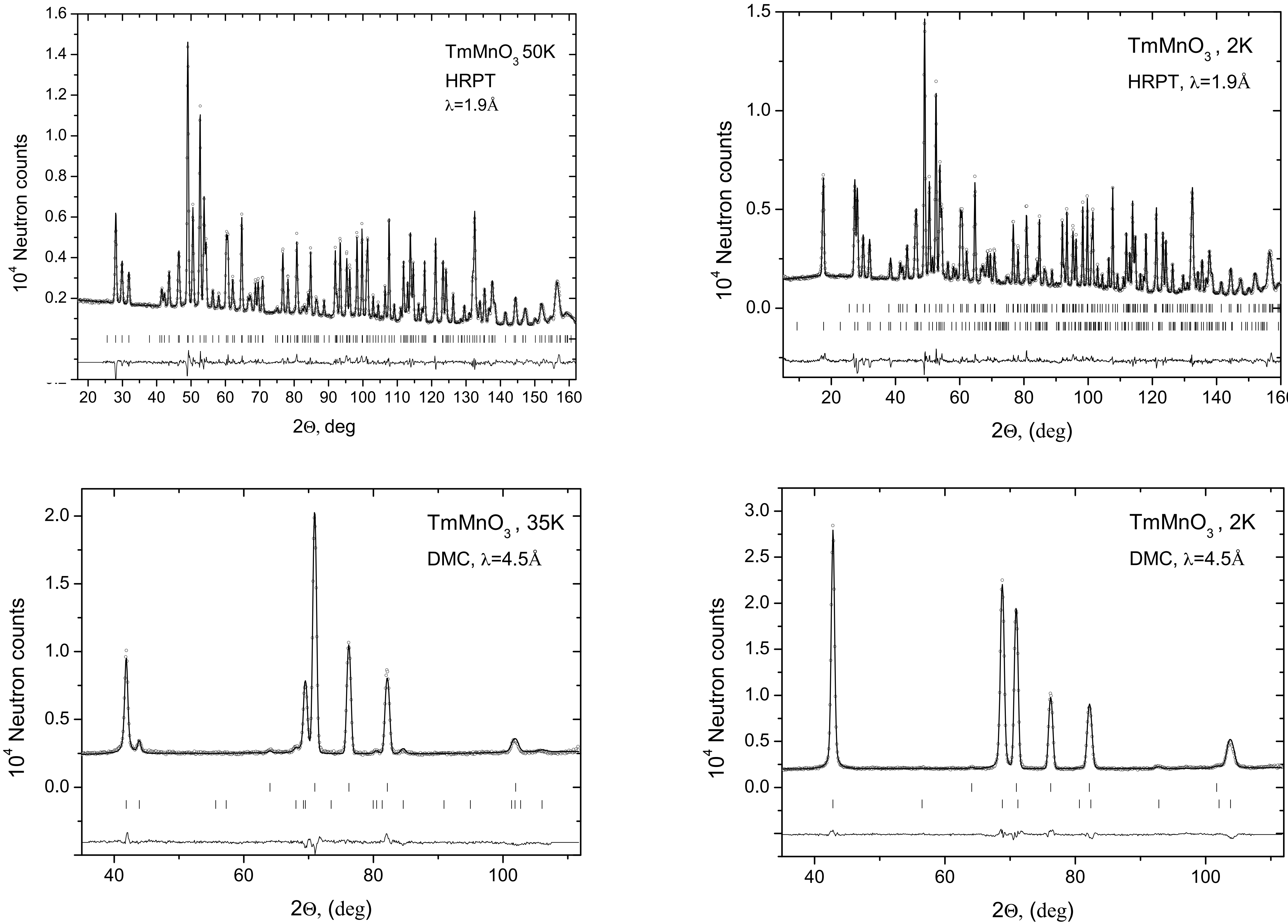
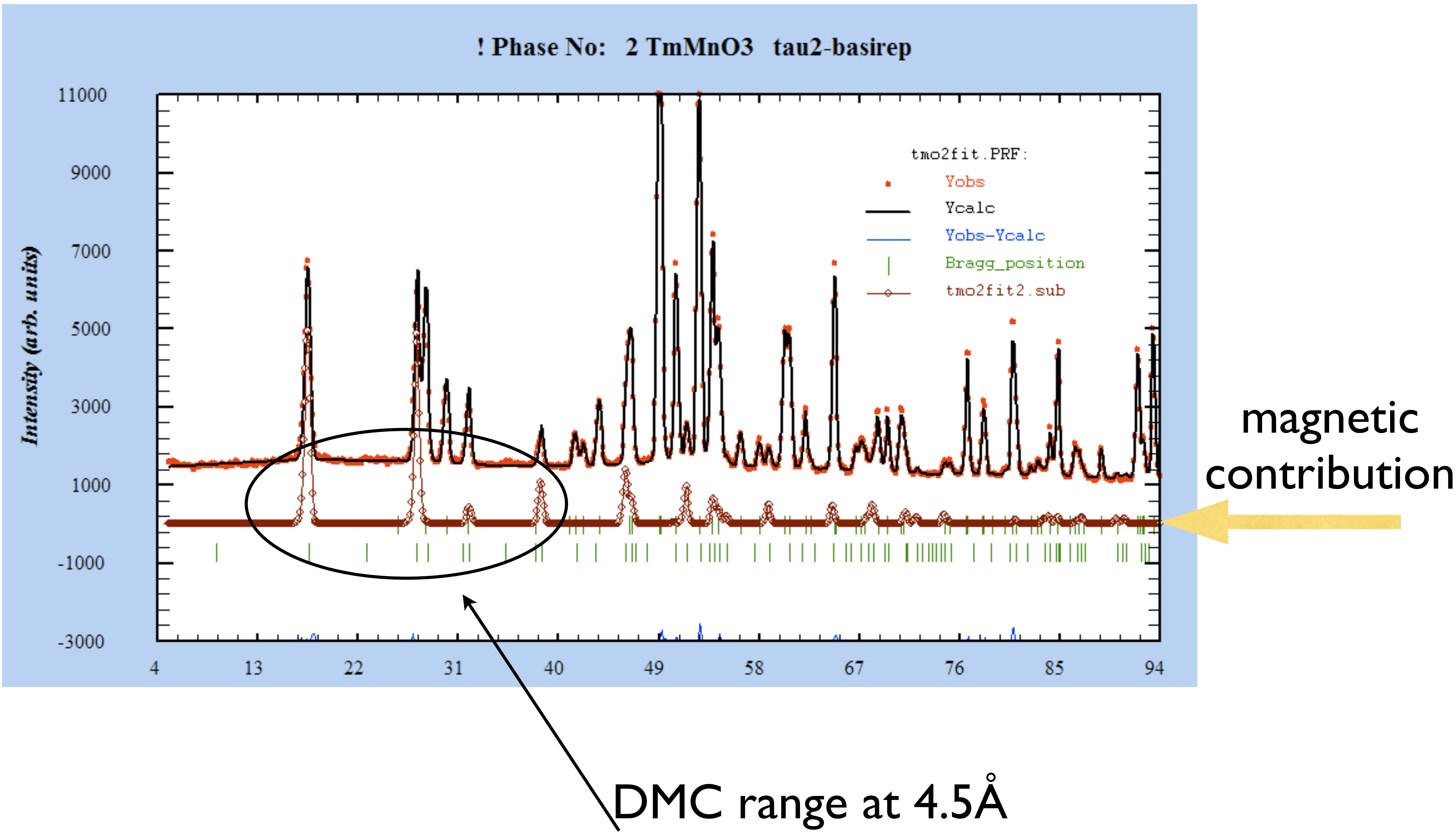
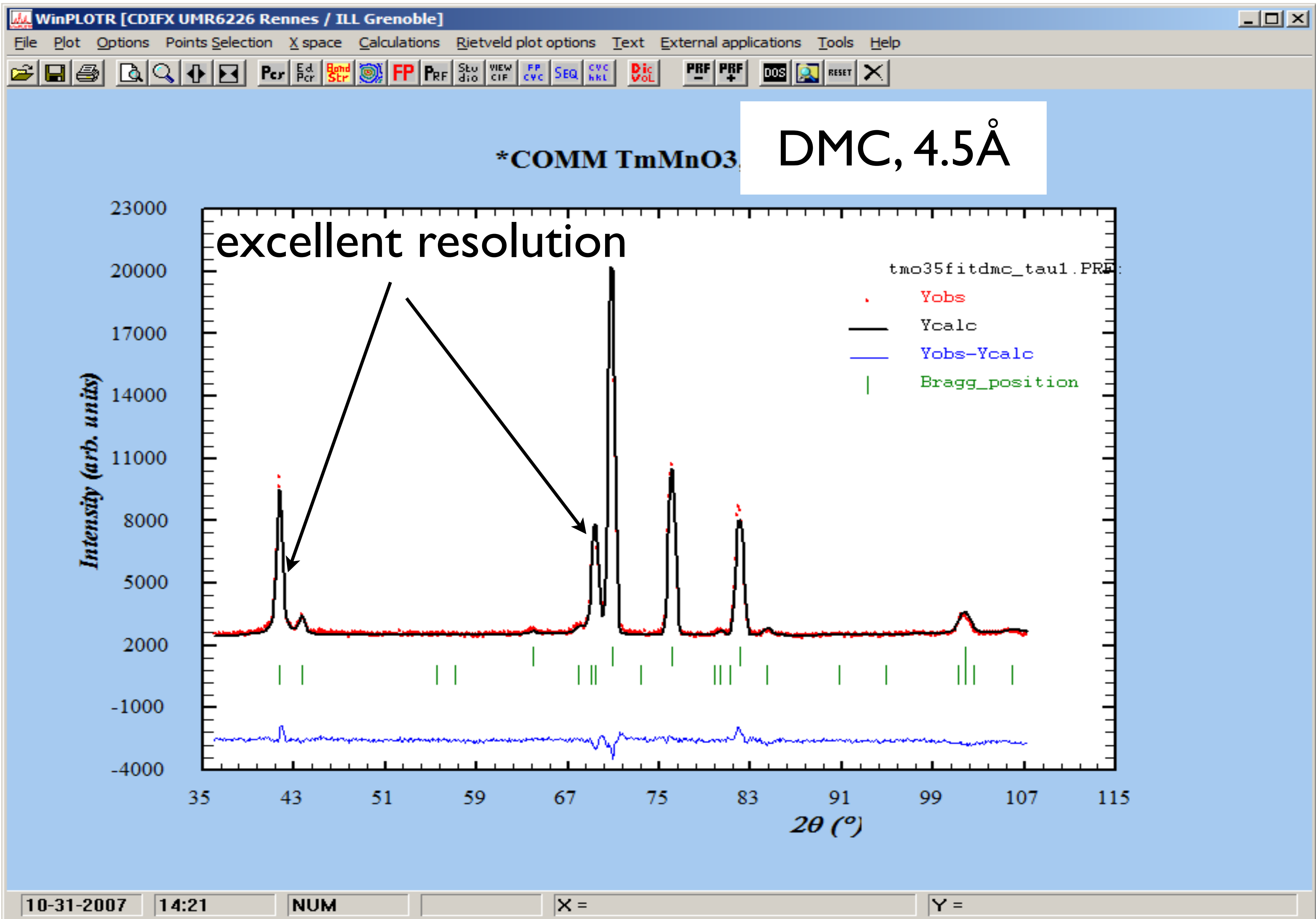


cf. resolution/q-range

HRPT 1.9Å



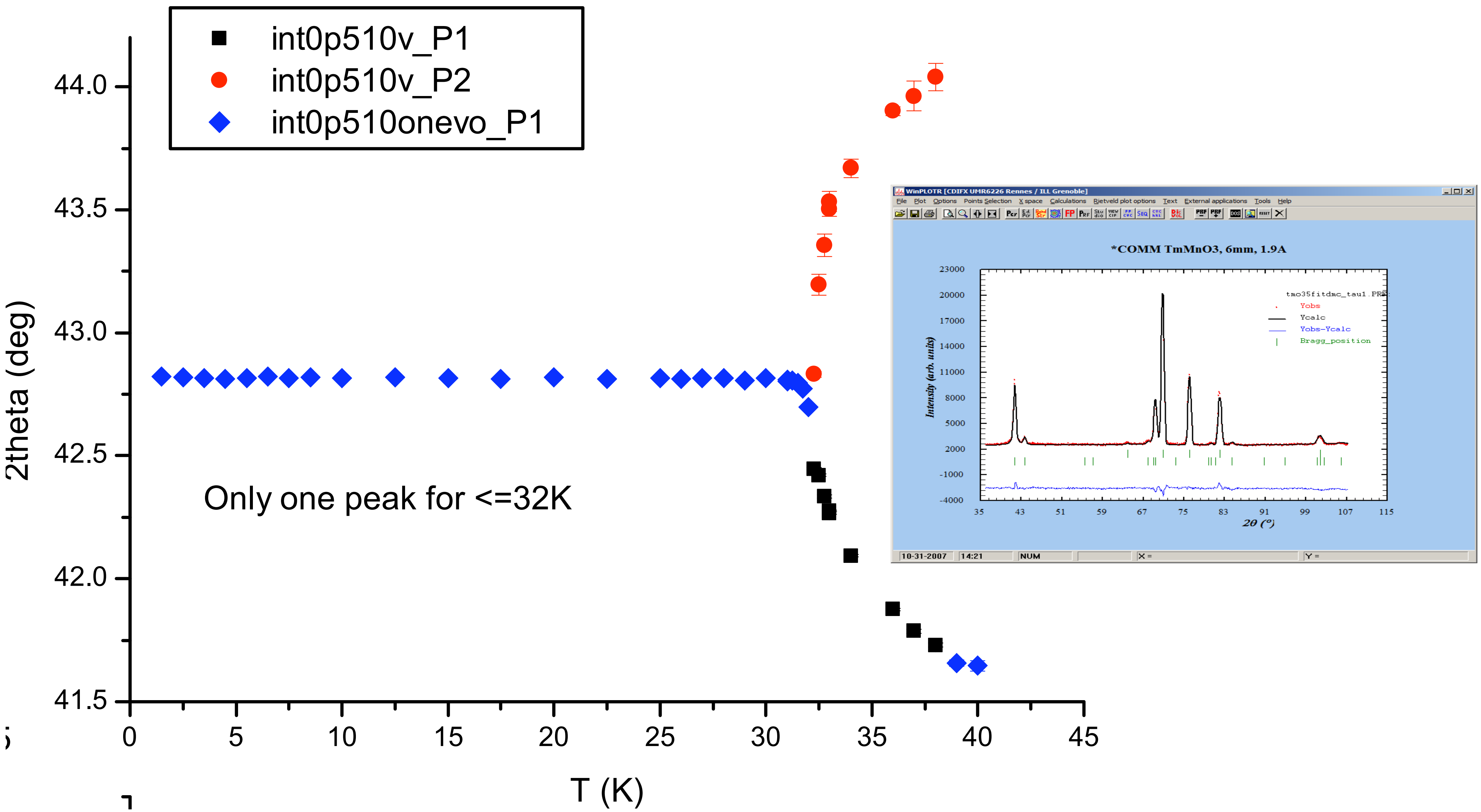
Cf. resolution/q-range



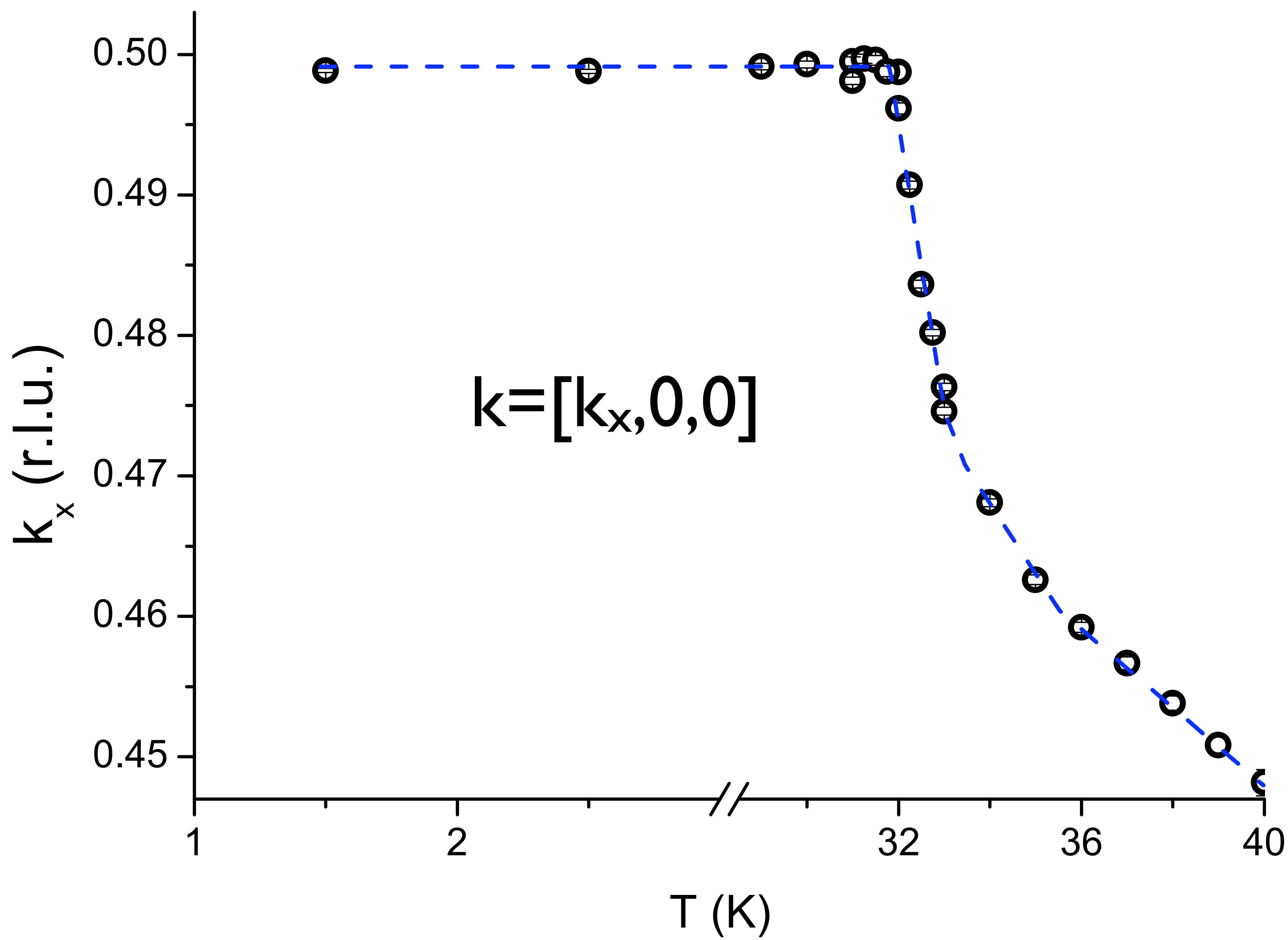
Step 2

Finding the propagation vector of magnetic structure (k-vector).
Le Bail profile matching fit.

T-dependence of Bragg peak positions



Refining the propagation k-vector from profile matching fit



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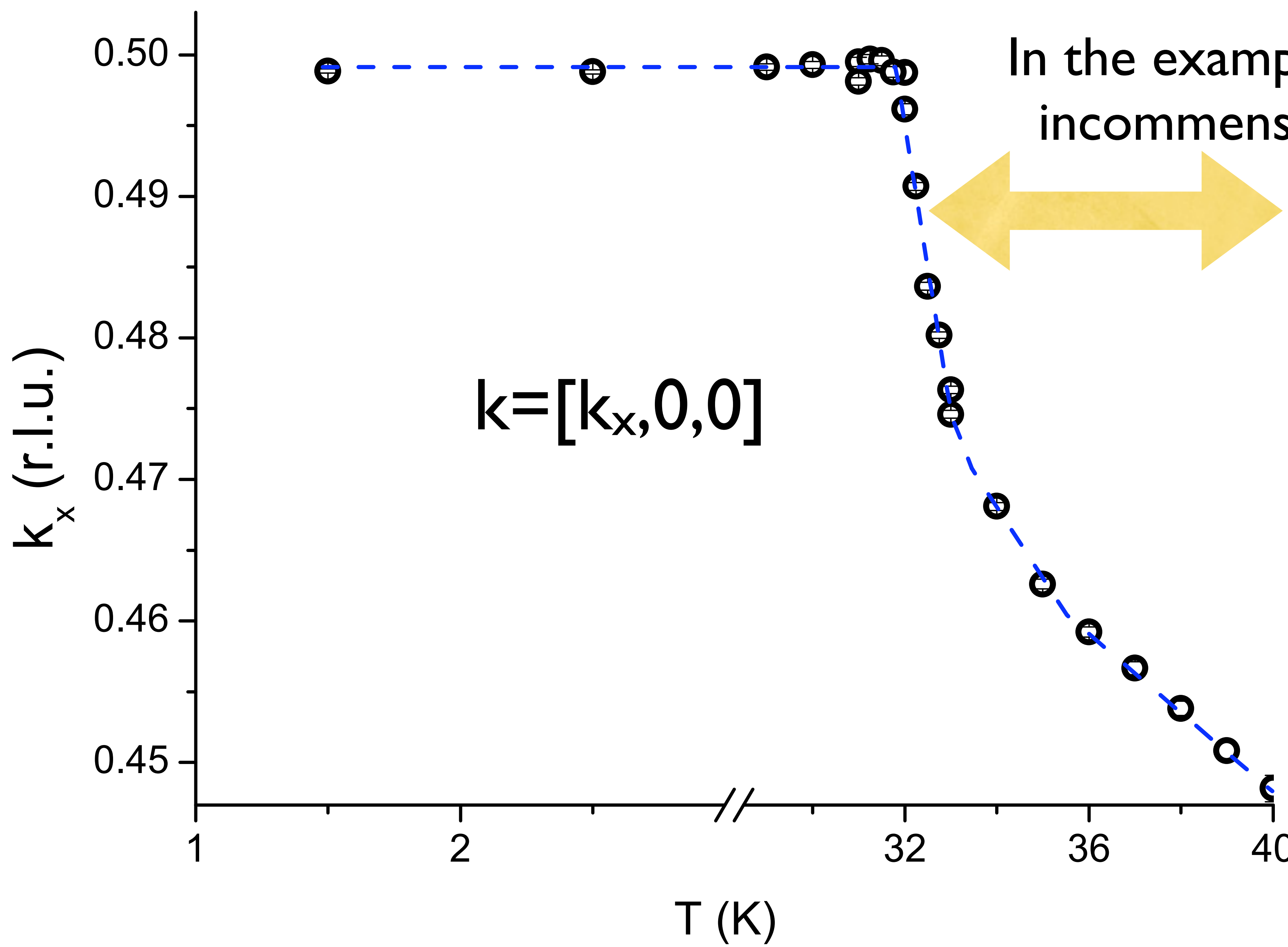

In the example we determine incommensurate structure

Step 3

Symmetry analysis.
Classifying possible magnetic structures

Classifying possible magnetic structures

k-vector group

Group *G: Pnma*, no.62: 8 symmetry operators

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $m\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Classifying possible magnetic structures

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Little group G_k, k=[0.45,0,0]=[q,0,0]

Little group of propagation vector G_k contains only the elements of *G* that do not change **k**

Classifying possible magnetic structures

k-vector group

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(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) m $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Little group of propagation vector *G*$_k$ contains only the elements of *G* that do not change **k**

$P2_1ma$ ($Pmc2_1$, 26)

(1) x,y,z (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$

rotation+ translation

$$E\begin{pmatrix}100\\010\\001\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}\quad 2_x\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}\quad m_y\begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix}\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}\quad m_z\begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$$

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix} 100 \\ 010 \\ 001 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	$2_x \begin{pmatrix} 100 \\ 0\bar{1}0 \\ 00\bar{1} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$	$m_y \begin{pmatrix} 100 \\ 0\bar{1}0 \\ 001 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$	$m_y \begin{pmatrix} 100 \\ 010 \\ 00\bar{1} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}$
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$
position number	a	b	c	d

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix} \begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix} \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$
position number	a	b	c	d

Permutation representation

Classifying possible magnetic structures

Magnetic representation

	g_1	g_2	g_3	g_4
group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix} \begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix} \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$
position number	a	b	c	d

Permutation representation

element g_2 changes atomic position:

a $\Rightarrow$ b

b $\Rightarrow$ a

c $\Rightarrow$ d

d $\Rightarrow$ c

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix} \begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix} \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$
position number	a	b	c	d

Permutation representation

element g_2 is represented by 4x4 matrix

$$\begin{pmatrix}0100\\1000\\0001\\0010\end{pmatrix} \begin{pmatrix}a\\b\\c\\d\end{pmatrix} = \begin{pmatrix}b\\a\\d\\c\end{pmatrix}$$

Classifying possible magnetic structures

Magnetic representation

	g_1	g_2	g_3	g_4
group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix} \begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix} \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
position number	a	b	c	d

Permutation representation

element g_2 is represented by 4x4 matrix

$$\begin{pmatrix}0100\\1000\\0001\\0010\end{pmatrix} \begin{pmatrix}a\\b\\c\\d\end{pmatrix} = \begin{pmatrix}b\\a\\d\\c\end{pmatrix}$$

in addition, element g_2 sometimes moves the atom outside of the *zero*cell. We have to return the atom back with $-\mathbf{a}_p$:

	$-\mathbf{a}_p$
a $\Longrightarrow$ b	(000)
b $\Longrightarrow$ a	(-100)
c $\Longrightarrow$ d	(000)
d $\Longrightarrow$ c	(-100)

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix} \begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix} \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
position number	a	b	c	d

Permutation representation

in addition, element g_2 sometimes moves the atom outside of the *zero*cell.
We have to return the atom back with $-\mathbf{a}_p$:

	$-\mathbf{a}_p$
a $\Longrightarrow$ b	(000)
b $\Longrightarrow$ a	(-100)
c $\Longrightarrow$ d	(000)
d $\Longrightarrow$ c	(-100)

$$\mathbf{S}(\mathbf{r}_j) = \mathbf{S}_0 e^{2\pi i \mathbf{r}_j \mathbf{k}}$$

element g_2 is represented by 4x4 matrix

$$\begin{pmatrix}0100\\b000\\0001\\00b0\end{pmatrix}\begin{pmatrix}a\\b\\c\\d\end{pmatrix} = \begin{pmatrix}b\\a\\d\\c\end{pmatrix}$$

$$b = e^{2\pi i(\mathbf{k}\mathbf{a}_p)} \simeq e^{-0.9\pi i}$$

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E\begin{pmatrix}100\\010\\001\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y\begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix}\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y\begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
position number	a	b	c	d

Permutation representation

4x4 matrices (P)	$\begin{pmatrix}1000\\0100\\0010\\0001\end{pmatrix}$	$\begin{pmatrix}0100\\b000\\0001\\00b0\end{pmatrix}$	$\begin{pmatrix}0010\\0001\\1000\\0100\end{pmatrix}$	$\begin{pmatrix}0001\\00b0\\0100\\b000\end{pmatrix}$

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix} \begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix} \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$
position number	a	b	c	d

Permutation representation

4x4 matrices (P)	$\begin{pmatrix}1000\\0100\\0010\\0001\end{pmatrix}$	$\begin{pmatrix}0100\\b000\\0001\\00b0\end{pmatrix}$	$\begin{pmatrix}0010\\0001\\1000\\0100\end{pmatrix}$	$\begin{pmatrix}0001\\00b0\\0100\\b000\end{pmatrix}$

Axial vector (spin) representation

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix} 100 \\ 010 \\ 001 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	$2_x \begin{pmatrix} 100 \\ 0\bar{1}0 \\ 00\bar{1} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$	$m_y \begin{pmatrix} 100 \\ 0\bar{1}0 \\ 001 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$	$m_y \begin{pmatrix} 100 \\ 010 \\ 00\bar{1} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}$
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$
position number	a	b	c	d

Permutation representation

4x4 matrices (P)	$\begin{pmatrix} 1000 \\ 0100 \\ 0010 \\ 0001 \end{pmatrix}$	$\begin{pmatrix} 0100 \\ b000 \\ 0001 \\ 00b0 \end{pmatrix}$	$\begin{pmatrix} 0010 \\ 0001 \\ 1000 \\ 0100 \end{pmatrix}$	$\begin{pmatrix} 0001 \\ 00b0 \\ 0100 \\ b000 \end{pmatrix}$

Axial vector (spin) representation

For instance:
rotational part of element g_2: $R(g_2)$ changes
atomic spin direction:

$$\begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} = \begin{pmatrix} S_x \\ -S_y \\ -S_z \end{pmatrix}$$

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix}\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$
position number	a	b	c	d

Permutation representation

4x4 matrices (P)	$\begin{pmatrix}1000\\0100\\0010\\0001\end{pmatrix}$	$\begin{pmatrix}0100\\b000\\0001\\00b0\end{pmatrix}$	$\begin{pmatrix}0010\\0001\\1000\\0100\end{pmatrix}$	$\begin{pmatrix}0001\\00b0\\0100\\b000\end{pmatrix}$

Axial vector (spin) representation

For instance:
rotational part of element g_2: $R(g_2)$ changes
atomic spin direction:

element g_2 is represented by 3x3 matrix

$$R(g_2)\times\det(R) \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}S_x\\S_y\\S_z\end{pmatrix} = \begin{pmatrix}S_x\\-S_y\\-S_z\end{pmatrix}$$

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix} \begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix} \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix} \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$
Mn-position	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
position number	a	b	c	d

Permutation representation

4x4 matrices (P)	$\begin{pmatrix}1000\\0100\\0010\\0001\end{pmatrix}$	$\begin{pmatrix}0100\\1000\\0001\\0010\end{pmatrix}$	$\begin{pmatrix}0010\\0001\\1000\\0100\end{pmatrix}$	$\begin{pmatrix}0001\\0010\\0100\\1000\end{pmatrix}$

Axial vector (spin) representation

3x3 matrices (A) *R(g₂)×det(R)*	$\begin{pmatrix}100\\010\\001\end{pmatrix}$	$\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}00\\010\\00\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}00\\0\bar{1}0\\001\end{pmatrix}$

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$
position number	a	b	c	d
spin	**S_1**	**S_2**	**S_3**	**S_4**

Permutation representation

4x4 matrices (P)

$$\begin{pmatrix}1000\\0100\\0010\\0001\end{pmatrix} \quad \begin{pmatrix}0100\\b000\\0001\\00b0\end{pmatrix} \quad \begin{pmatrix}0010\\0001\\1000\\0100\end{pmatrix} \quad \begin{pmatrix}0001\\00b0\\0100\\b000\end{pmatrix}$$

Axial vector (spin) representation

3x3 matrices (A)

$R(g_2)$×$det(R)$

$$\begin{pmatrix}100\\010\\001\end{pmatrix} \quad \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix} \quad \begin{pmatrix}\bar{1}00\\010\\00\bar{1}\end{pmatrix} \quad \begin{pmatrix}\bar{1}00\\0\bar{1}0\\001\end{pmatrix}$$

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4	
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	
position number	a	b	c	d	
spin	$\mathbf{S_1}$	$\mathbf{S_2}$	$\mathbf{S_3}$	$\mathbf{S_4}$	Vector spaces

Permutation representation

4x4 matrices (P)	$\begin{pmatrix}1000\\0100\\0010\\0001\end{pmatrix}$	$\begin{pmatrix}0100\\1000\\0001\\0010\end{pmatrix}$	$\begin{pmatrix}0010\\0001\\1000\\0100\end{pmatrix}$	$\begin{pmatrix}0001\\0010\\0100\\1000\end{pmatrix}$	$\begin{pmatrix}a\\b\\c\\d\end{pmatrix}$

Axial vector (spin) representation

3x3 matrices (A) *R(g2)×det(R)*	$\begin{pmatrix}100\\010\\001\end{pmatrix}$	$\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}00\\010\\00\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}00\\0\bar{1}0\\001\end{pmatrix}$	$\begin{pmatrix}S_x\\S_y\\S_z\end{pmatrix}$

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
Mn-position	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
position number	a	b	c	d
spin	**S_1**	**S_2**	**S_3**	**S_4**

Vector spaces

Permutation representation

4x4 matrices (P)	$\begin{pmatrix}1000\\0100\\0010\\0001\end{pmatrix}$	$\begin{pmatrix}0100\\1000\\0001\\0010\end{pmatrix}$	$\begin{pmatrix}0010\\0001\\1000\\0100\end{pmatrix}$	$\begin{pmatrix}0001\\0010\\0100\\1000\end{pmatrix}$	$\begin{pmatrix}a\\b\\c\\d\end{pmatrix}$

Axial vector (spin) representation

3x3 matrices (A) *R(g2)×det(R)*	$\begin{pmatrix}100\\010\\001\end{pmatrix}$	$\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}00\\010\\00\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}00\\0\bar{1}0\\001\end{pmatrix}$	$\begin{pmatrix}S_x\\S_y\\S_z\end{pmatrix}$

Magnetic representation

direct (tensor) product
P⊗A
12x12 matrices

Classifying possible magnetic structures

Magnetic representation

group element	g_1	g_2	g_3	g_4
Mn-position	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
position number	a	b	c	d
spin	S_1	S_2	S_3	S_4

Vector spaces

Permutation representation

4x4 matrices (P) $\begin{pmatrix}1000\\0100\\0010\\0001\end{pmatrix}$ $\begin{pmatrix}0100\\b000\\0001\\00b0\end{pmatrix}$ $\begin{pmatrix}0010\\0001\\1000\\0100\end{pmatrix}$ $\begin{pmatrix}0001\\00b0\\0100\\b000\end{pmatrix}$ $\begin{pmatrix}a\\b\\c\\d\end{pmatrix}$

Axial vector (spin) representation

3x3 matrices (A)
R(g2)×det(R) $\begin{pmatrix}100\\010\\001\end{pmatrix}$ $\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}$ $\begin{pmatrix}\bar{1}00\\010\\00\bar{1}\end{pmatrix}$ $\begin{pmatrix}\bar{1}00\\0\bar{1}0\\001\end{pmatrix}$ $\begin{pmatrix}S_x\\S_y\\S_z\end{pmatrix}$

Magnetic representation

direct (tensor) product
P⊗A
12x12 matrices

e.g. for group element g_2

$$\begin{pmatrix}0100\\b000\\0001\\00b0\end{pmatrix}\otimes\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}=\begin{pmatrix}0&0&0&1&0&0&0&0&0&0&0&0\\0&0&0&0&\bar{1}&0&0&0&0&0&0&0\\0&0&0&0&0&\bar{1}&0&0&0&0&0&0\\1&0&0&0&0&0&0&0&0&0&0&0\\0&\bar{b}&0&0&0&0&0&0&0&0&0&0\\0&0&\bar{b}&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&1&0&0\\0&0&0&0&0&0&0&0&0&0&\bar{1}&0\\0&0&0&0&0&0&0&0&0&0&0&\bar{1}\\0&0&0&0&0&0&1&0&0&0&0&0\\0&0&0&0&0&0&0&\bar{b}&0&0&0&0\\0&0&0&0&0&0&0&0&\bar{b}&0&0&0\end{pmatrix}$$

Classifying possible magnetic structures
Reducing magnetic representation

	g_1	g_2	g_3	g_4
group element				
rotation+ translation	$E\begin{pmatrix}100\\010\\001\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y\begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix}\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y\begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$

Matrix of magnetic representation acts on 12 dimensional vector

4x3=12 spin components

E.g. for the element g_2
M=P⊗A

$$\begin{pmatrix}
0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&\bar{1}&0&0&0&0&0&0&0\\
0&0&0&0&0&\bar{1}&0&0&0&0&0&0\\
1&0&0&0&0&0&0&0&0&0&0&0\\
0&\bar{b}&0&0&0&0&0&0&0&0&0&0\\
0&0&\bar{b}&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&\bar{1}&0\\
0&0&0&0&0&0&0&0&0&0&0&\bar{1}\\
0&0&0&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&\bar{b}&0&0&0&0\\
0&0&0&0&0&0&0&0&\bar{b}&0&0&0
\end{pmatrix}
\begin{pmatrix}
s_{x1}\\s_{y1}\\s_{z1}\\s_{x2}\\s_{y2}\\s_{z2}\\s_{x3}\\s_{y3}\\s_{z3}\\s_{x4}\\s_{y4}\\s_{z4}
\end{pmatrix}$$

Classifying possible magnetic structures
Reducing magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E\begin{pmatrix}100\\010\\001\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y\begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix}\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y\begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$

Matrix of magnetic representation acts on 12 dimensional vector

4x3=12 spin components

E.g. for the element g_2
M=P⊗A

$$\begin{pmatrix}
0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&\bar{1}&0&0&0&0&0&0&0\\
0&0&0&0&0&\bar{1}&0&0&0&0&0&0\\
1&0&0&0&0&0&0&0&0&0&0&0\\
0&\bar{b}&0&0&0&0&0&0&0&0&0&0\\
0&0&\bar{b}&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&\bar{1}&0\\
0&0&0&0&0&0&0&0&0&0&0&\bar{1}\\
0&0&0&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&\bar{b}&0&0&0&0\\
0&0&0&0&0&0&0&0&\bar{b}&0&0&0
\end{pmatrix}
\begin{pmatrix}
s_{x1}\\s_{y1}\\s_{z1}\\s_{x2}\\s_{y2}\\s_{z2}\\s_{x3}\\s_{y3}\\s_{z3}\\s_{x4}\\s_{y4}\\s_{z4}
\end{pmatrix}$$

Classifying possible magnetic structures
Reducing magnetic representation

group element	g_1	g_2	g_3	g_4
rotation+ translation	$E \begin{pmatrix}100\\010\\001\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}$	$2_x \begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$	$m_y \begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix}\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$	$m_y \begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$

Matrix of magnetic representation acts on 12 dimensional vector

4x3=12 spin components

E.g. for the element g_2
M=P⊗A

$$\begin{pmatrix}
0&0&0&1&0&0&0&0&0&0&\text{[illegible]}&0\\
0&0&0&0&\bar{1}&0&0&0&0&\text{[illegible]}&0&0\\
0&0&0&0&0&\bar{1}&0&0&\text{[illegible]}&\text{[illegible]}&0&0\\
1&0&0&0&0&0&0&\text{[illegible]}&\text{[illegible]}&0&0&0\\
0&\bar{b}&0&0&0&0&0&\text{[illegible]}&0&0&0&0\\
0&0&\bar{b}&0&0&0&\text{[illegible]}&0&0&0&0&0\\
0&0&0&0&0&\text{[illegible]}&0&0&0&1&0&0\\
0&0&0&0&\text{[illegible]}&\text{[illegible]}&0&0&0&0&\bar{1}&0\\
0&0&0&\text{[illegible]}&\text{[illegible]}&0&0&0&0&0&0&\bar{1}\\
0&0&0&\text{[illegible]}&0&0&1&0&0&0&0&0\\
0&0&\text{[illegible]}&0&0&0&0&\bar{b}&0&0&0&0\\
0&\text{[illegible]}&0&0&0&0&0&0&\bar{b}&0&0&0
\end{pmatrix}
\begin{pmatrix}
s_{x1}\\s_{y1}\\s_{z1}\\s_{x2}\\s_{y2}\\s_{z2}\\s_{x3}\\s_{y3}\\s_{z3}\\s_{x4}\\s_{y4}\\s_{z4}
\end{pmatrix}$$

Magnetic representation is reducible!

Classifying possible magnetic structures
Reducing magnetic representation

group element	g_1	g_2	g_3	g_4
Mn-position	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$

Magnetic representation is reducible to a block-diagonal shape that is a direct sum of irreducible square matrices τ_1, τ_2, ... (dimensions can be from 1 to 6.)

$$\tau_1 \oplus \tau_2 \oplus \tau_3 \oplus ... = \begin{pmatrix} \tau_1 & 0 & 0 & ... & 0 \\ 0 & \tau_2 & 0 & ... & 0 \\ 0 & 0 & \tau_3 & ... & 0 \\ . & . & . & . & \\ . & . & . & . & \\ 0 & 0 & 0 & & \end{pmatrix} \begin{pmatrix} S_{\tau 1} \\ S_{\tau 2} \\ S_{\tau 3} \\ . \\ . \\ \\ \end{pmatrix}$$

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each componet of $S_{\tau1}$ is a linear combinations of 12 spin components

$$\begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ s_{x3} \\ s_{y3} \\ s_{z3} \\ s_{x4} \\ s_{y4} \\ s_{z4} \end{pmatrix}$$

Landau theory of phase transitions says that only one irreducible representation is needed to describe the structure

Why the Landau theory does work for magnetic phase transition is a separate topic.

Classifying possible magnetic structures basis vectors/functions $S_{\tau 1}$, $S_{\tau 2}$, $S_{\tau 3}$, ...

Pnma, k=[0.45,0,0]
Mn in (4a)-position

Magnetic representation is reduced to four one-dimensional irreps

$$3\tau_1 \oplus 3\tau_2 \oplus 3\tau_3 \oplus 3\tau 4$$

	g_1	g_2	g_3	g_4
τ_1	1	a	1	a
τ_2	1	a	-1	$-a$
τ_3	1	$-a$	1	$-a$
τ_4	1	$-a$	-1	a

$$a = e^{\pi i k_x}$$

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Mn-position	1	2	3	4

$$S'_{\tau 3} = +1\mathbf{e}_{1x} - a^*\mathbf{e}_{2x} - 1\mathbf{e}_{3x} + a^*\mathbf{e}_{4x}$$
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Assuming that the phase transition goes according to one irreducible representation τ3 the spins of all four atoms are set only by 3 variables instead of 12!

$$C_1 S'_{\tau 3} + C_2 S''_{\tau 3} + C_3 S'''_{\tau 3}$$

Steps 3-4 in practice

Solving/refining the magnetic structure by using one irreducible representation

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1. construct basis functions for single irreducible representation irrep (use BasIreps, SARAh, MODY)

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Steps 3-4 in practice

Solving/refining the magnetic structure by using one irreducible representation

1. construct basis functions for single irreducible representation irrep (use BasIreps, SARAh, MODY)
2. plug them in the FULLPROF and try to fit the data. In difficult cases the Monte-Carlo simulated annealing search is required
3. If the fit is bad go to 1 and choose different irrep. If the fit is good it is still better to sort out all irreps.

Refinement of the data for τ_3

$$\mathbf{S}(\mathbf{r}) = \frac{1}{2}(C_1 S'_{\tau 3} + C_2 S''_{\tau 3} + C_3 S'''_{\tau 3}) e^{2\pi i \mathbf{k} \boldsymbol{r}} + c.c.$$

k=[0.45,0,0]

$$S'_{\tau 3} = +1\mathbf{e}_{1x} - a^*\mathbf{e}_{2x} - 1\mathbf{e}_{3x} + a^*\mathbf{e}_{4x}$$

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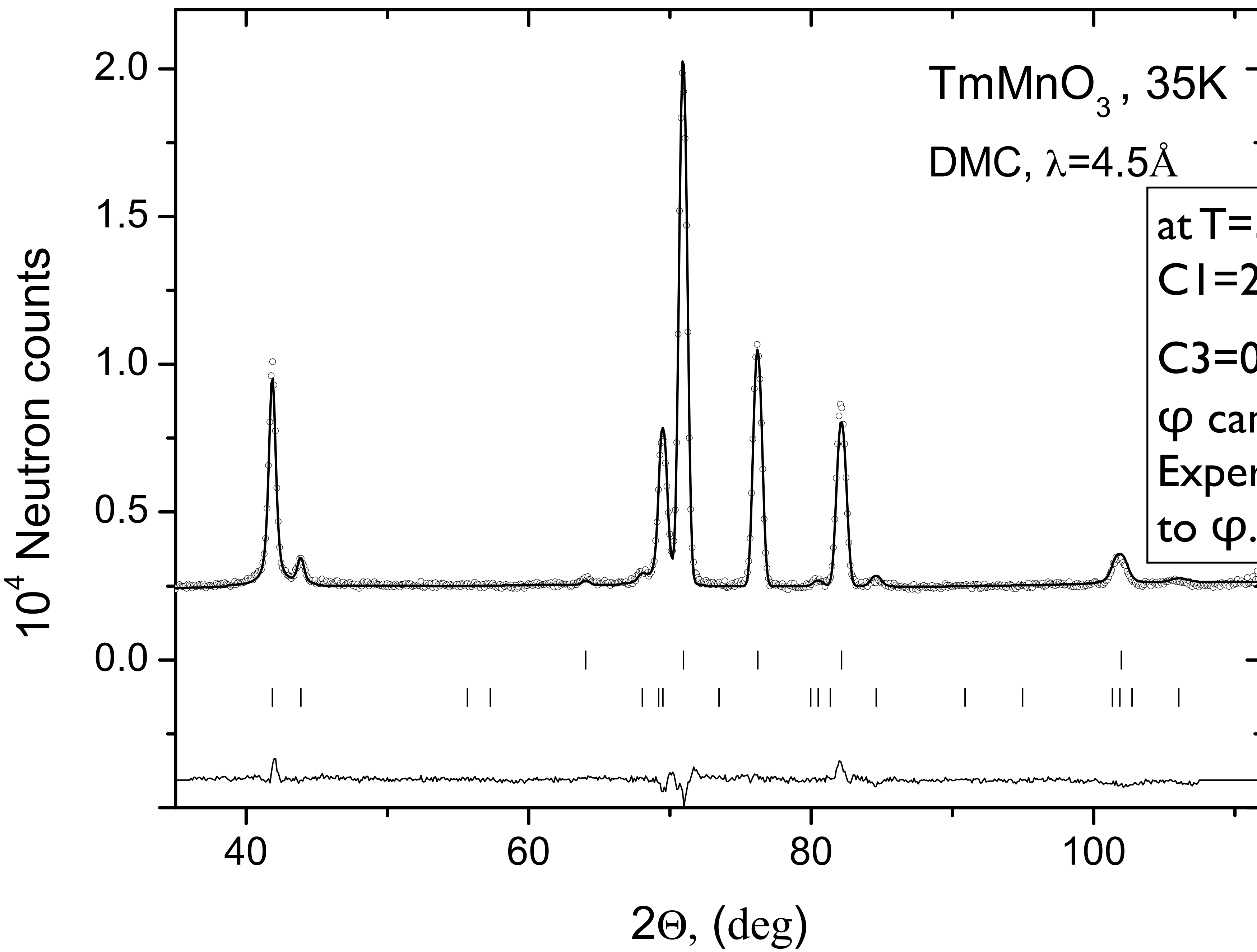

at T=35K
C1=2.11(1)μ_B, C2=0,
C3=0.67(2) $e^{i\varphi}$ μ_B
φ can be fixed to any value.
Experiment data are insensitive to φ.

Visualization of the magnetic structure

a cycloid structure propagating along x-direction

$$\mathbf{S}(\mathbf{r}) = Re\left[(C_1 S'_{\tau 3} + |C_3| \exp(i\varphi) S'''_{\tau 3}) \exp(2\pi i \mathbf{k}\boldsymbol{r})\right]$$

$$S'_{\tau 3} = +1\mathbf{e}_{1x} - a^*\mathbf{e}_{2x} - 1\mathbf{e}_{3x} + a^*\mathbf{e}_{4x}$$

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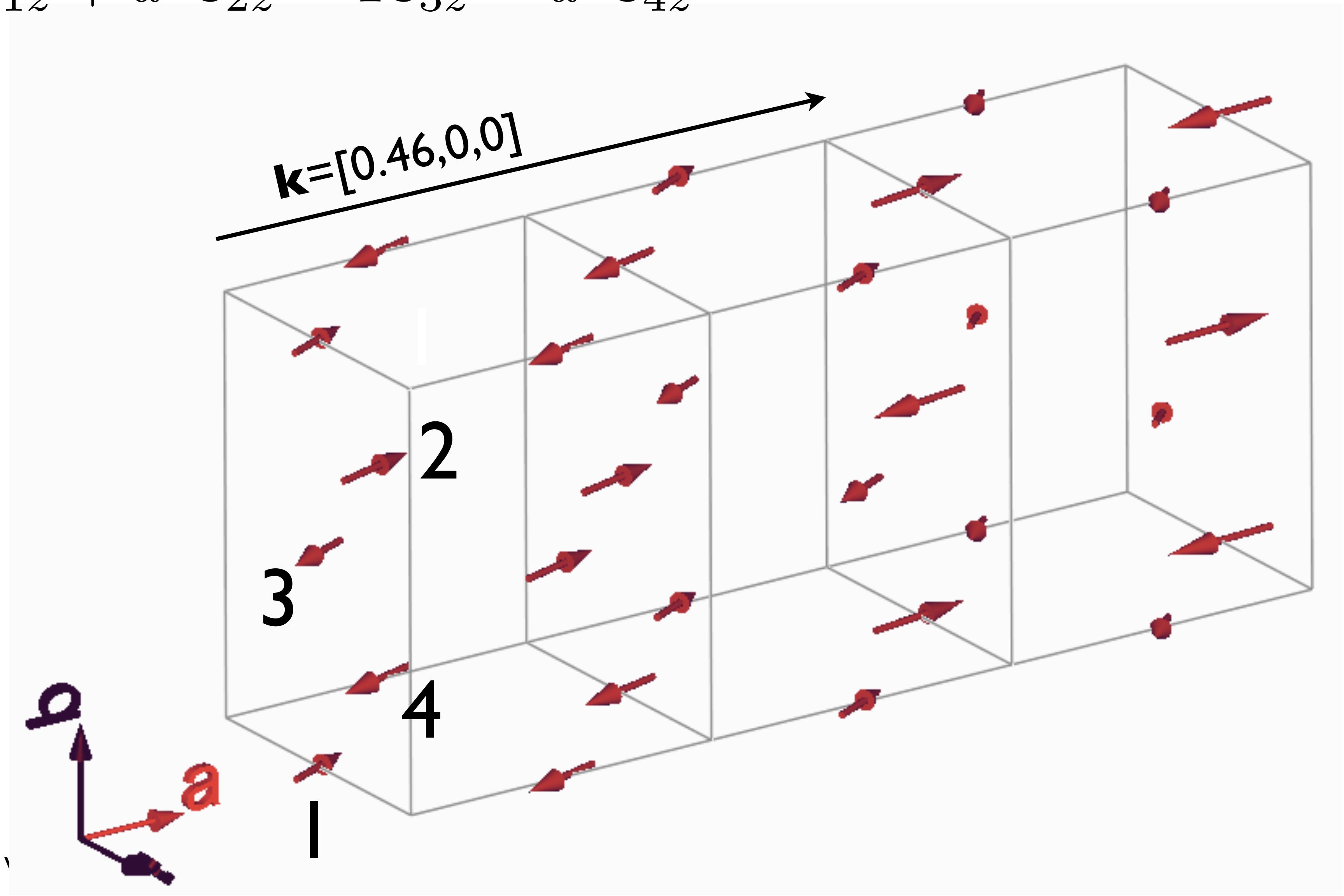

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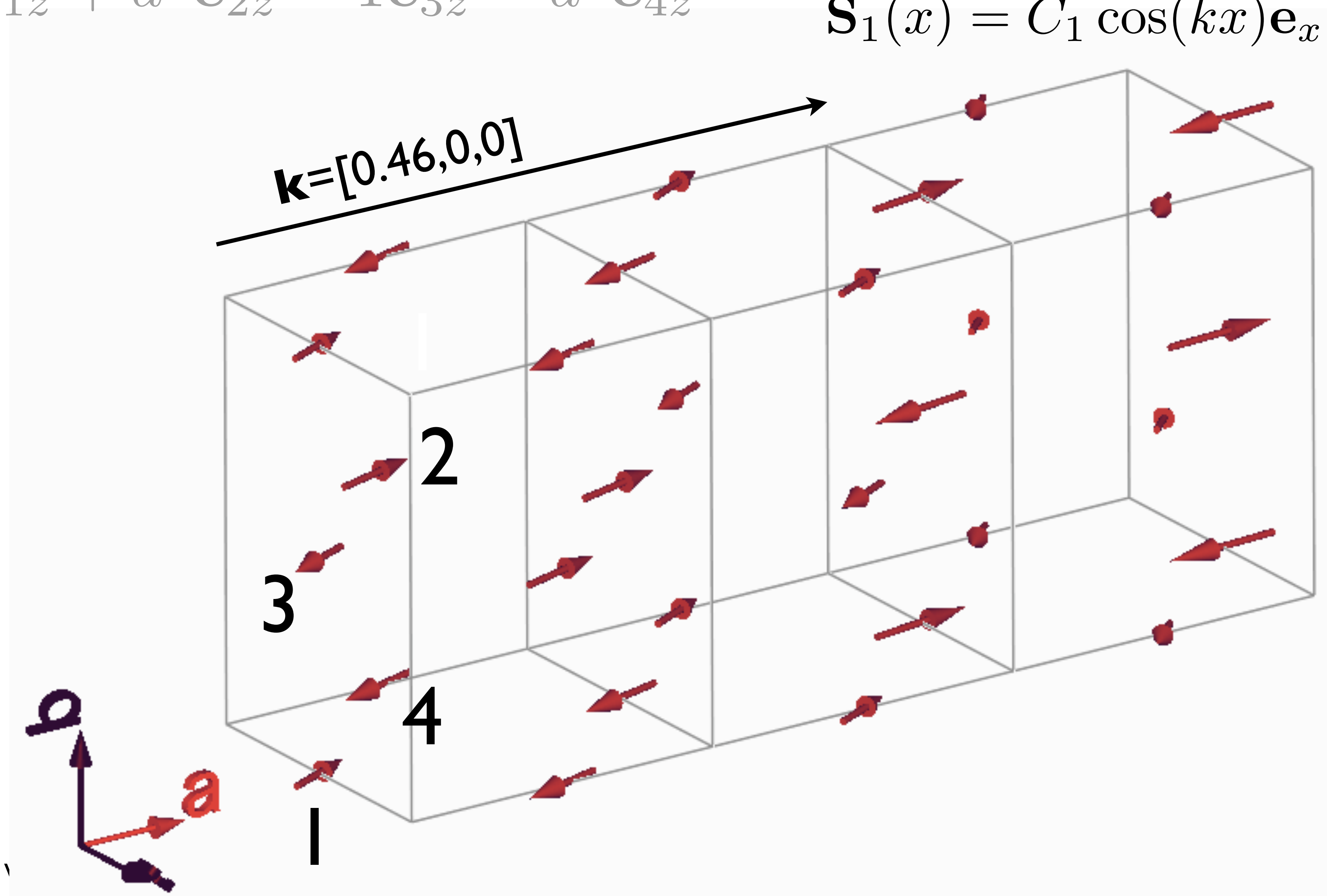
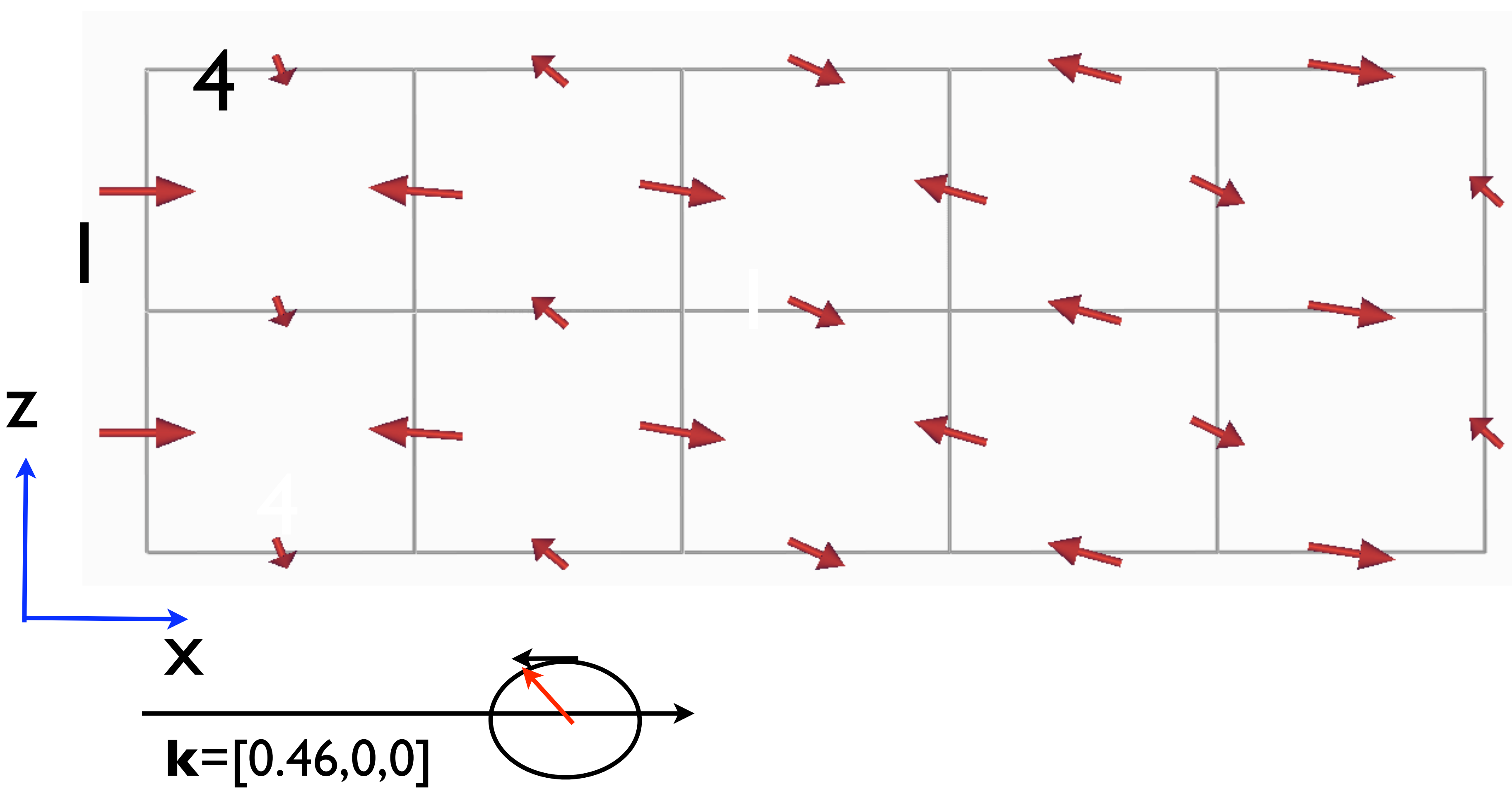
Propagation of the spin, e.g. for atom no. 1

$$\mathbf{S}_1(x) = C_1 \cos(kx)\mathbf{e}_x + |C_3| \cos(kx + \varphi)\mathbf{e}_z$$



Visualization of the magnetic structure: xz-projection

for arbitrary φ:
both direction and size of S_l are changed



Visualization of the magnetic structure: xz-projection

for arbitrary φ:
both direction and size of S_1 are changed

Propagation of the spin, e.g. for atom no. 1

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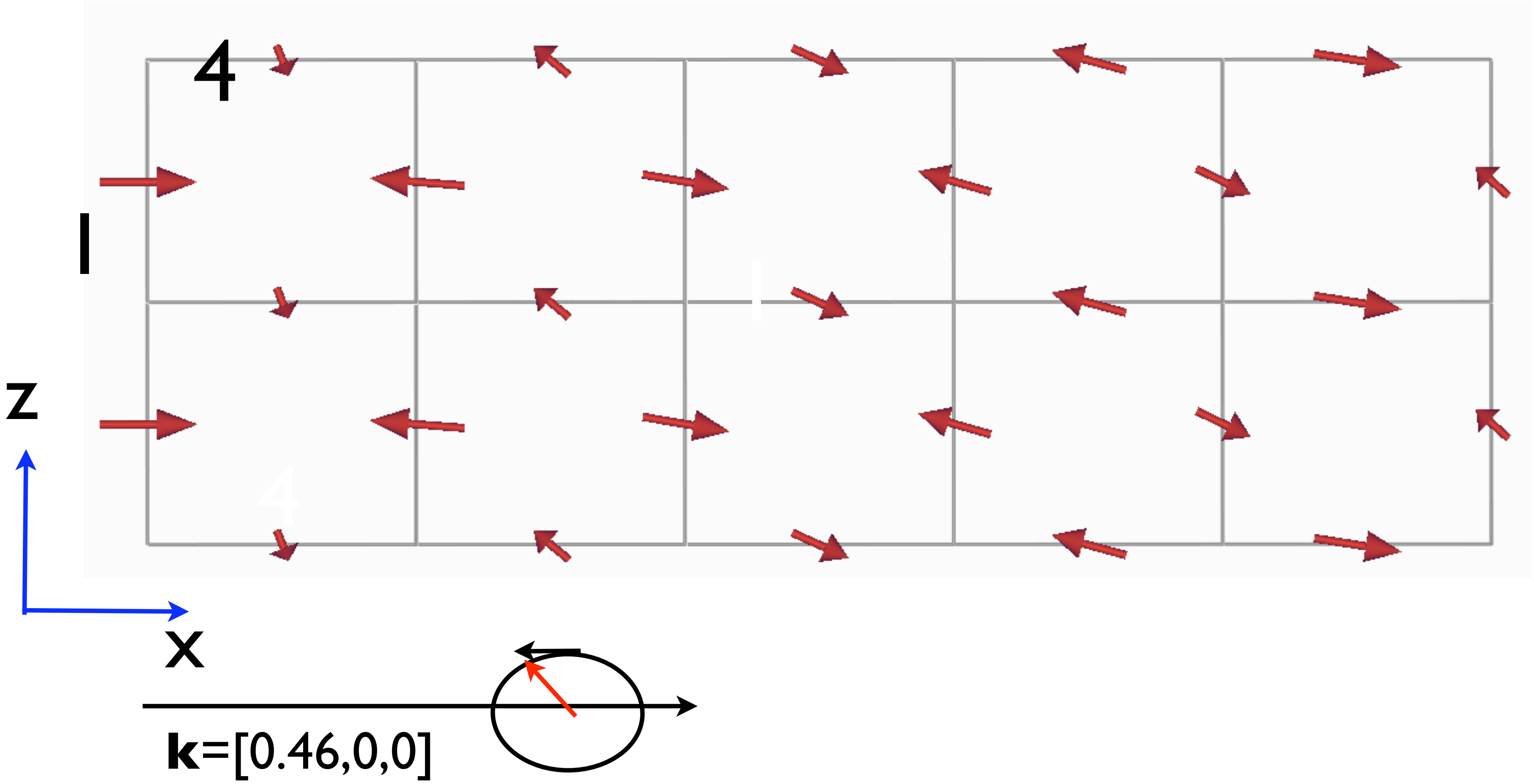
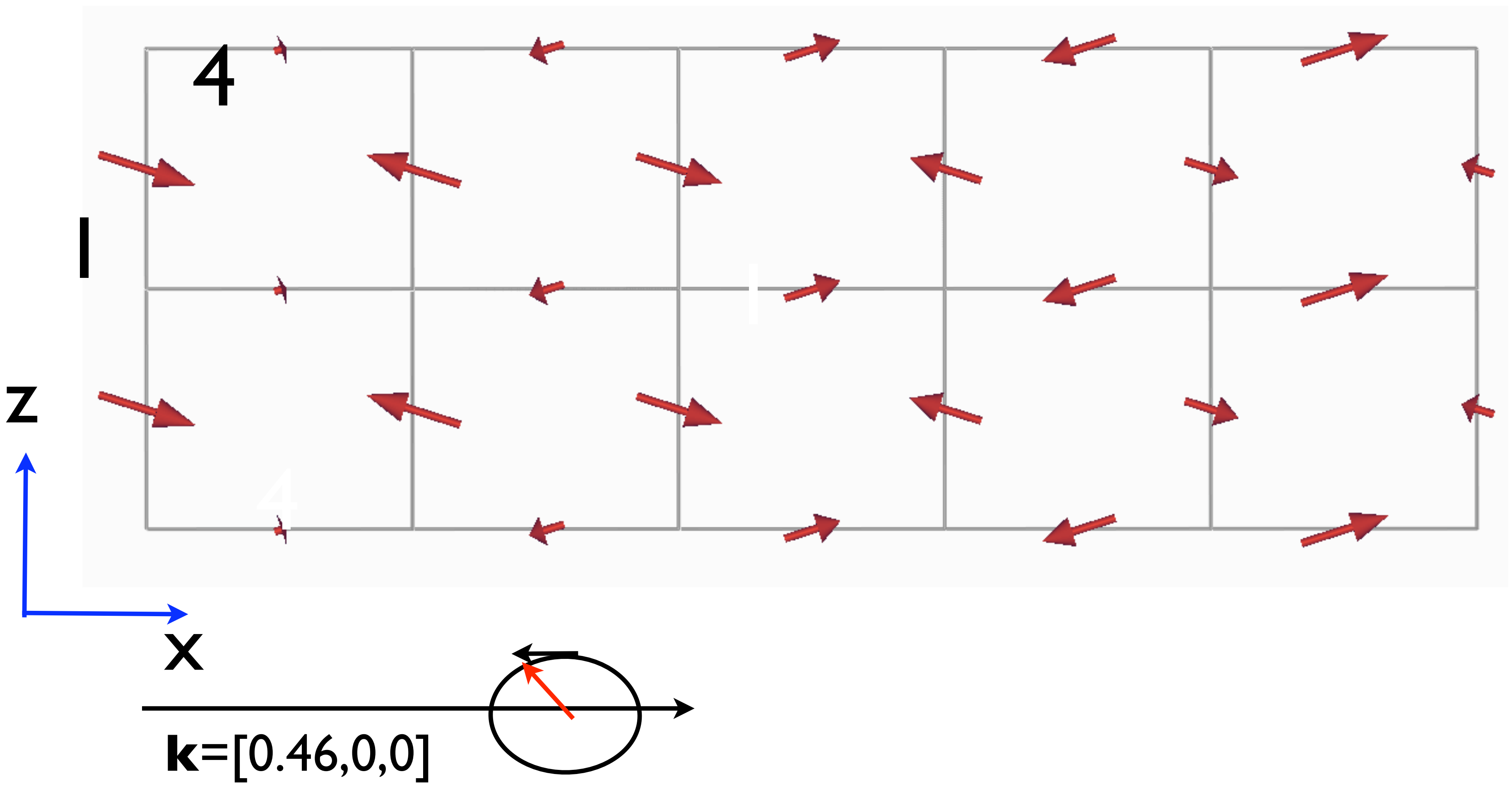


Visualization of the magnetic structure: xz-projection

for φ=0:
only the size of S_I are changed

Propagation of the spin, e.g. for atom no. I

$$\mathbf{S}_1(x) = (C_1\mathbf{e}_x + |C_3|\mathbf{e}_z)\cos(kx)$$



literature, programs and tutorials/notes

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.

COMPUTER PROGRAMS, TUTORIALS

1. Juan Rodríguez-Carvajal (ILL) et al, http://www.ill.fr/sites/fullprof/
2. Andrew S. Wills (UCL) http://www.chem.ucl.ac.uk/people/wills/magnetic_structures/magnetic_structures.html
3. Wieslawa Sikora et al, http://www.ftj.agh.edu.pl/~sikora/modyopis.htm

This lecture
http://sinq.web.psi.ch/sinq/instr/hrpt/praktikum