Symmetry constraints in solving magnetic structures by neutron diffraction: representation analysis and Shubnikov groups

Vladimir Pomjakushin

Laboratory for Neutron Scattering, PSI

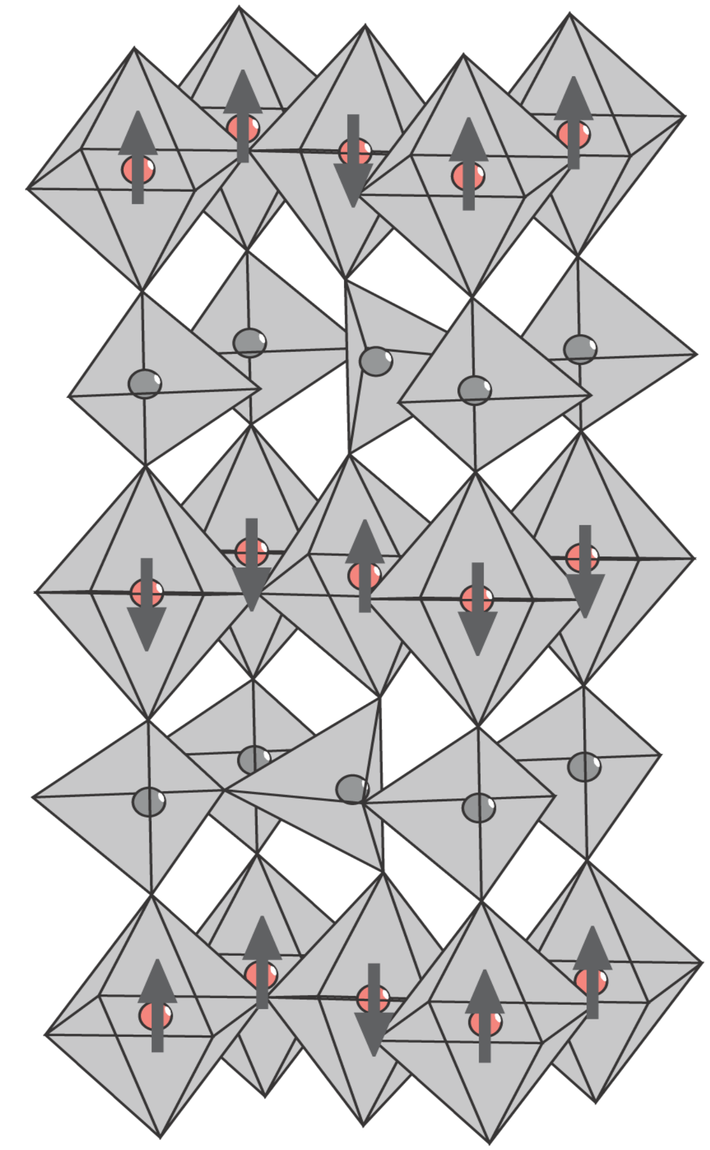
This lecture:

http://sinq.web.psi.ch/sinq/instr/hrpt/doc/magdif13.pdf

lecture from yesterday: Introduction to experimental neutron diffraction

http://sinq.web.psi.ch/sinq/instr/hrpt/doc/hrptdiff13.pdf

Purpose of this lecture is to show:



1. Basic principles of magnetic neutron diffraction.

2. Classification of the magnetic structures that are used in the literature, such as Shubnikov (or black-white) space groups and irreducible representation notations. Relation between two approaches.

3. How one can construct all possible symmetry adapted magnetic structures for a given crystal structure and a propagation vector (a point on the Brillouine zone) using *representation (rep) analysis of magnetic structures*. This way of description/construction is related to the Landau theory of second order phase transitions and applies not only to magnetic ordering, but generally to any type of phase transitions in crystals.

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.

Literature on (magnetic) symmetry and magnetic neutron diffraction

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

Yu. A. Izyumov, V. E. Naish and R. P. Ozerov,
"*Neutron diffraction of magnetic materials*", New York [etc.]: Consultants Bureau, 1981-1991.

Groups, representation analysis, and applications in physics

J.P Elliott and P.G. Dawber
"*Symmetry in physics*", vol. 1, 1979 The Macmillan press LTD

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,

- Bilbao Crystallographic Server
  bilbao crystallographic server http://www.cryst.ehu.es/

ISOTROPY Software Suite iso.byu.edu

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

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.
How to cite: ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

- ISODISTORT: Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- ISOSUBGROUP: Coming soon!
- ISOTROPY: Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- SMODES: Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smalle possible blocks.
- FROZSL: Calculate phonon frequencies and displacement modes using the method of frozen phonons.

Space groups and irreducible representations

- ISOCIF: Create or modify CIF files.
- FINDSYM: Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- **New!** ISO-IR: Tables of Irreducible Representations. The 2011 version of IR matrices.
- ISO-MAG: Tables of magnetic space groups, both in human-readable and computer-readable forms.

Superspace Groups

- ISO(3+d)D: (3+d)-Dimensional Superspace Groups for d=1,2,3
- ISO(3+1)D: Isotropy Subgroups for Incommensurately Modulated Distortions in Crystalline Solids: A Complete List for One-Dimensional Modulations
- FINDSSG: Identify the superspace group symmetry given a list of symmetry operators.
- TRANSFORMSSG: Transform a superspace group to a new setting.

Phase Transitions

- COPL: Find a complete list of order parameters for a phase transition, given the space-group symmetries of the parent and subgroup phases.
- INVARIANTS: Generate invariant polynomials of the components of order parameters.
- COMSUBS: Find common subgroups of two structures in a reconstructive phase transition

Linux

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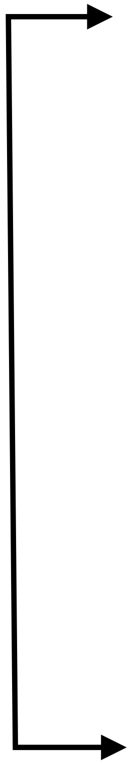
Computer programs to construct symmetry adapted magnetic structures and fit the experimental data.

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/`
- Wiesława Sikora et al, http://www.ftj.agh.edu.pl/~sikora/modyopis.htm
  `program MODY`
- Andrew S. Wills (UCL) http://www.ucl.ac.uk/chemistry/staff/academic_pages/andrew_wills
  `program SARAh`
- ...

Overview of Lecture



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- Principles of magnetic neutron scattering/diffraction. Long range magnetic order seen by ND with some simple examples. 8-22

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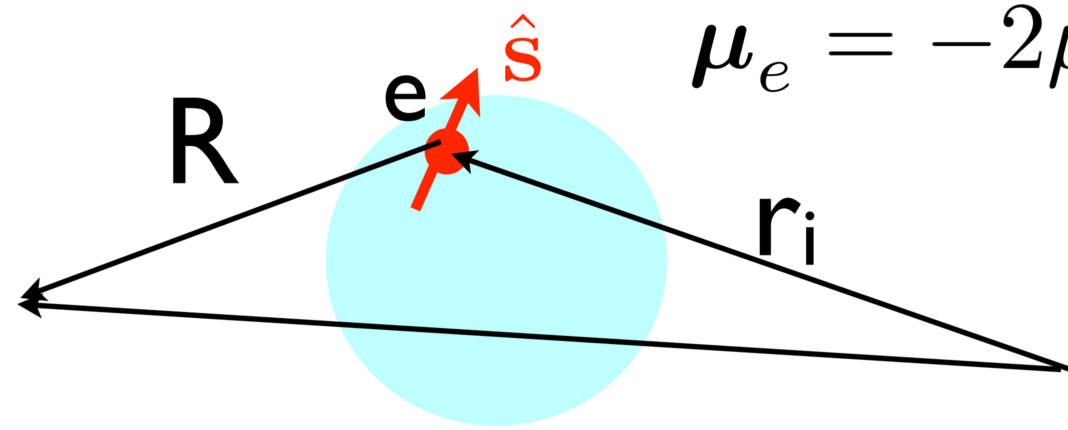
- Case study (experimental) of modulated magnetic structure determination using k-vector reps formalism for classifying symmetry adopted magnetic modes 66-

Magnetic neutron scattering on an atom



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

Magnetic neutron scattering on an atom

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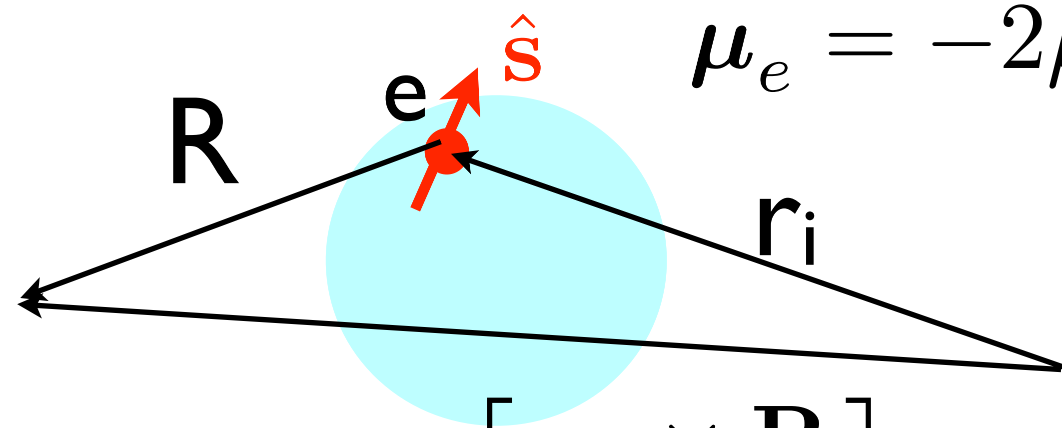
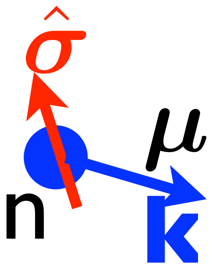
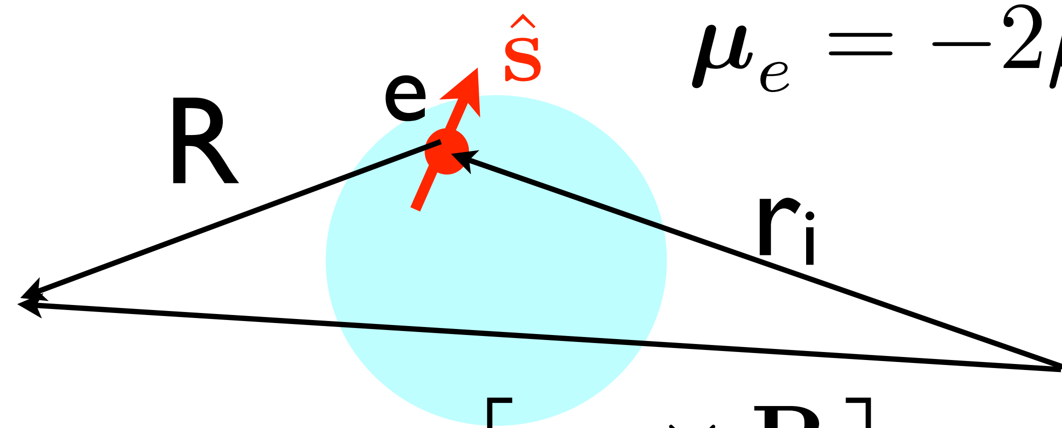


Magnetic field from an electron $$\mathbf{H}(\mathbf{R}) = -\mathrm{rot}\left[\frac{\boldsymbol{\mu}_e \times \mathbf{R}}{|\mathbf{R}|^3}\right] + \mathrm{transl.part}$$

Magnetic neutron scattering on an atom



$$\boldsymbol{\mu}_n = 2\gamma\mu_n\frac{\hat{\boldsymbol{\sigma}}}{2}$$



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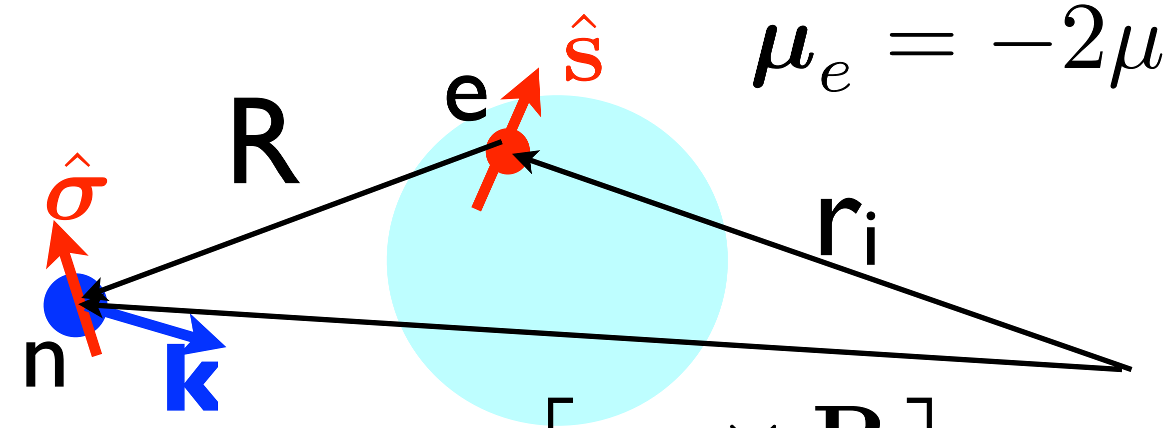

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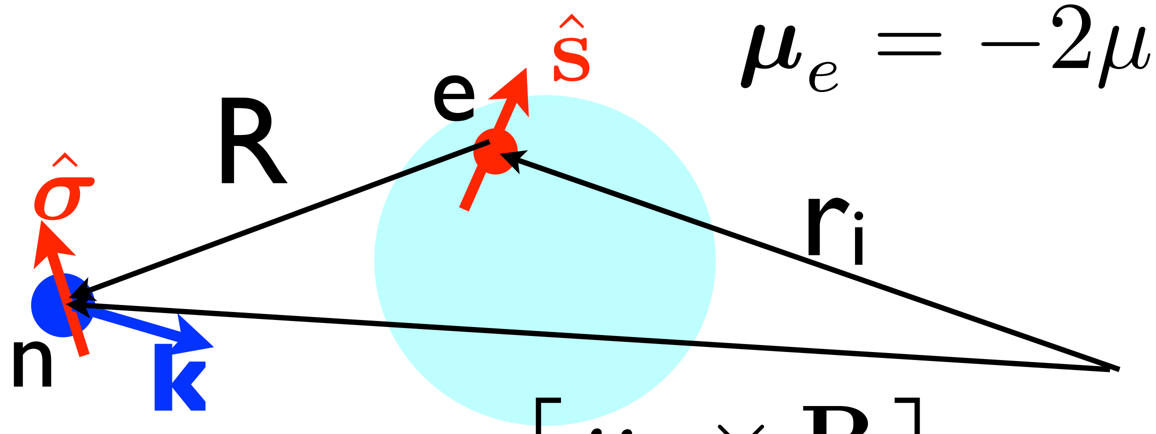

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averaging over neutron coordinates

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

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

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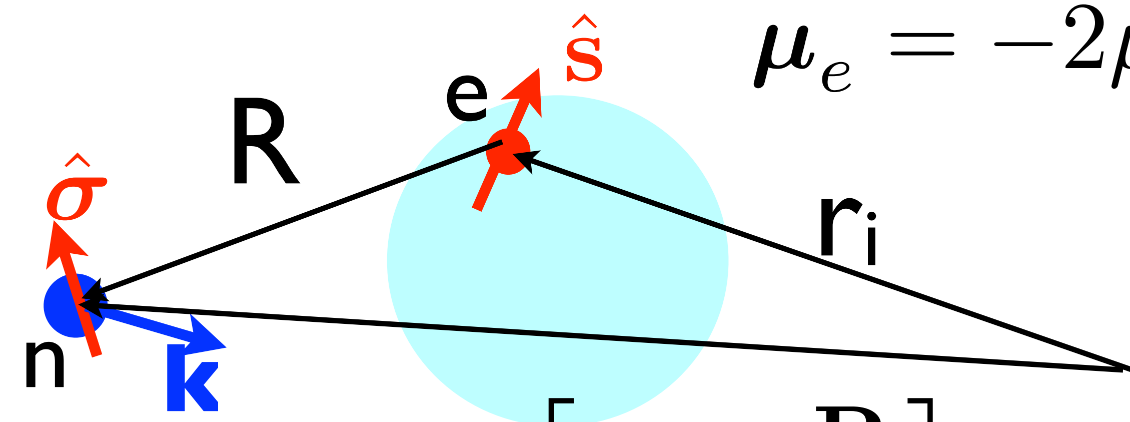

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magnetic interaction operator $\hat{\mathbf{Q}}_\perp$

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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neutron magnetic moment in μ_n -1.91 (→ γ)

classical electron radius $\frac{e^2}{mc^2}$ (→ r_e)

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

fm=fermi=10^{-13} cm

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x-ray scattering length: $Z r_e$

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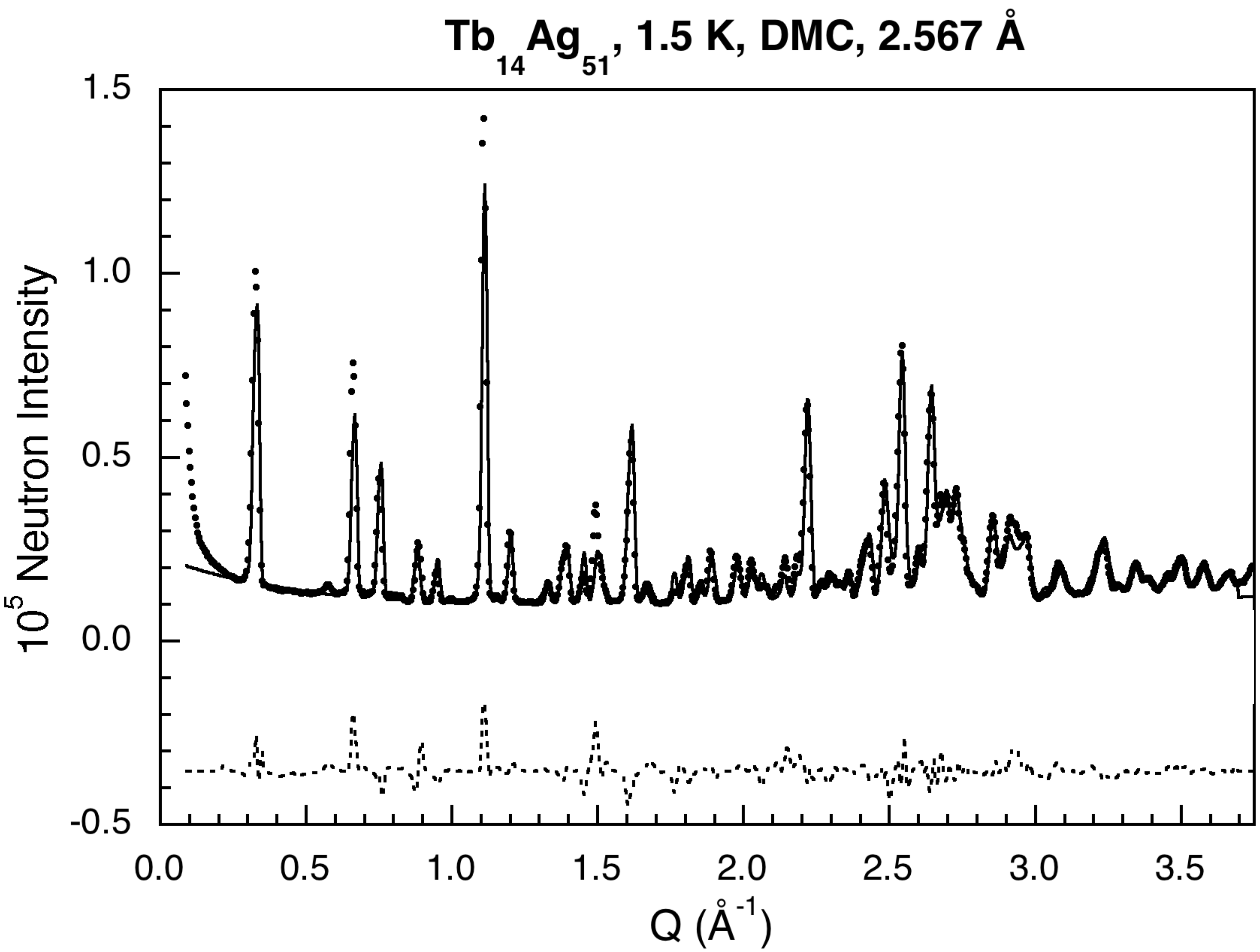
Comparison of neutron scattering lengths (fm)

magnetic

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

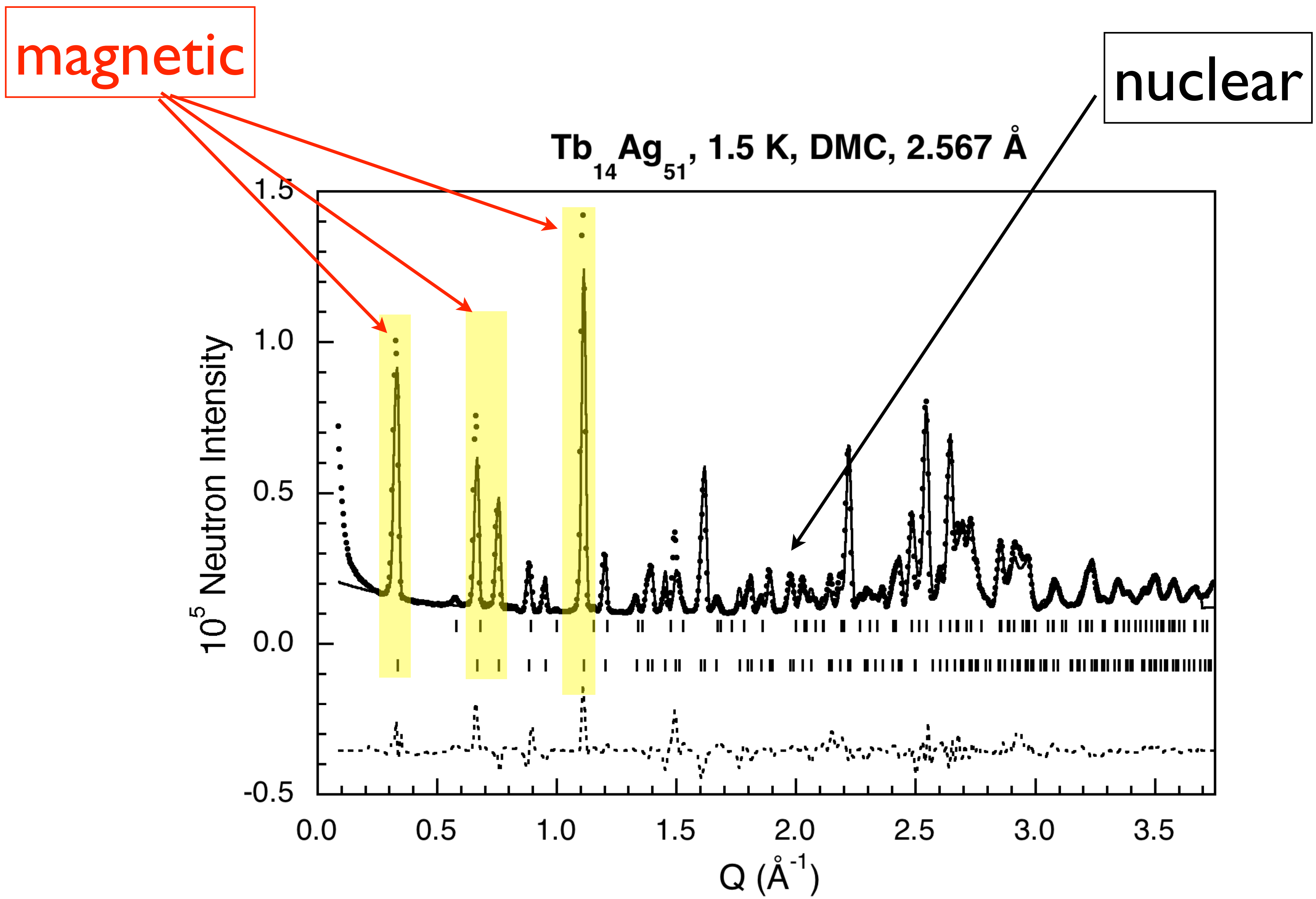
nuclear

Mn : -3.7, Cu: 7.7



Tb14Ag51, 1.5 K, DMC, 2.567 Å
10^5 Neutron Intensity
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
Q (Å^-1)

magnetic scattering intensity can be larger than the nuclear one



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Magnetic neutron scattering on an atom

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

Magnetic neutron scattering on an atom

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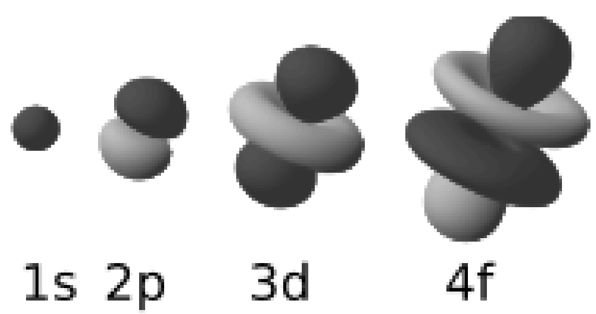
$$\left\langle \hat{\mathrm{Q}} \right\rangle = \left\langle \sum_i \hat{\mathbf{s}}_i e^{i\mathbf{q}\mathbf{r}_i} \right\rangle = \mathbf{S} \int d\mathbf{r} \rho_s(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}}$$



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

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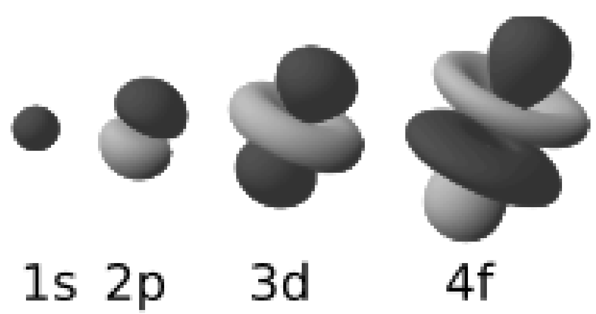

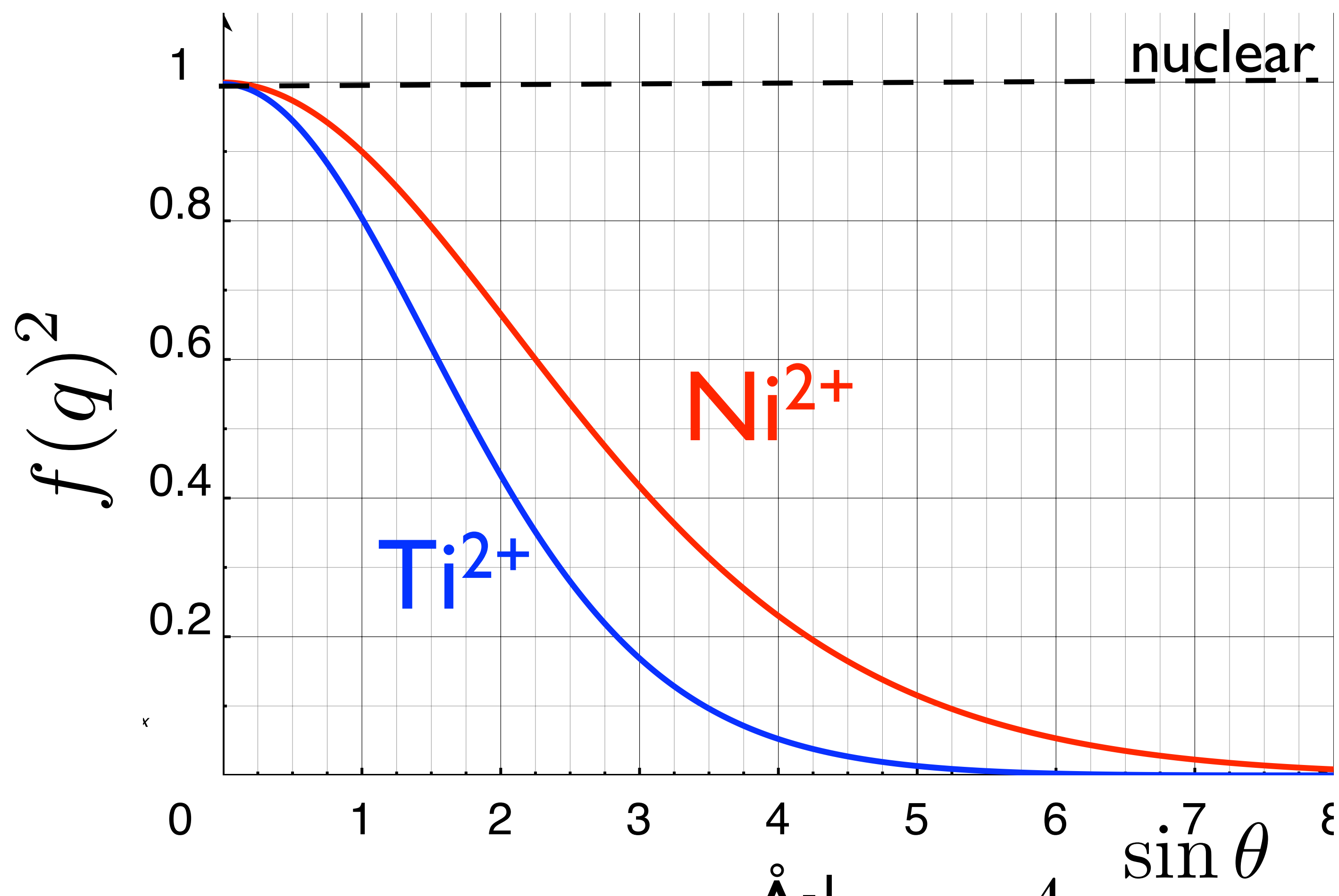

$$q = 4\pi \frac{\sin\theta}{\lambda}$$

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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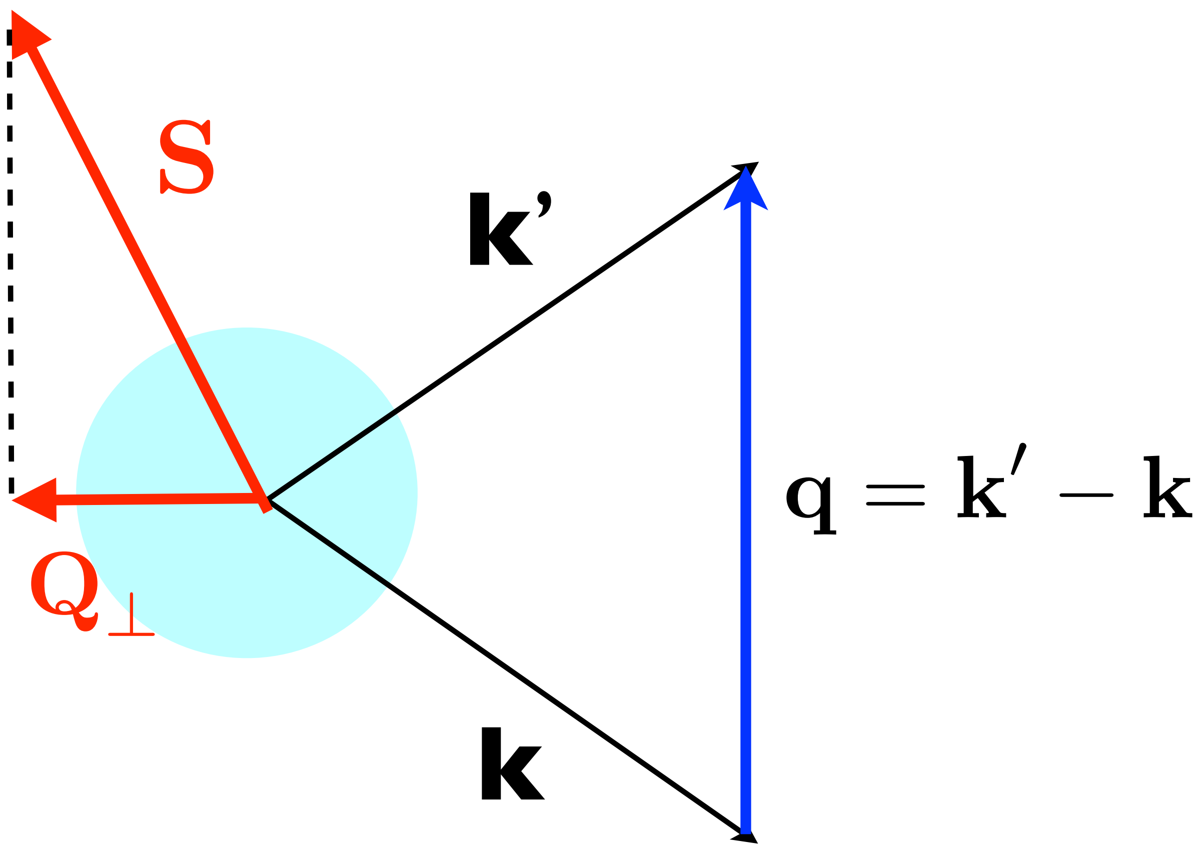

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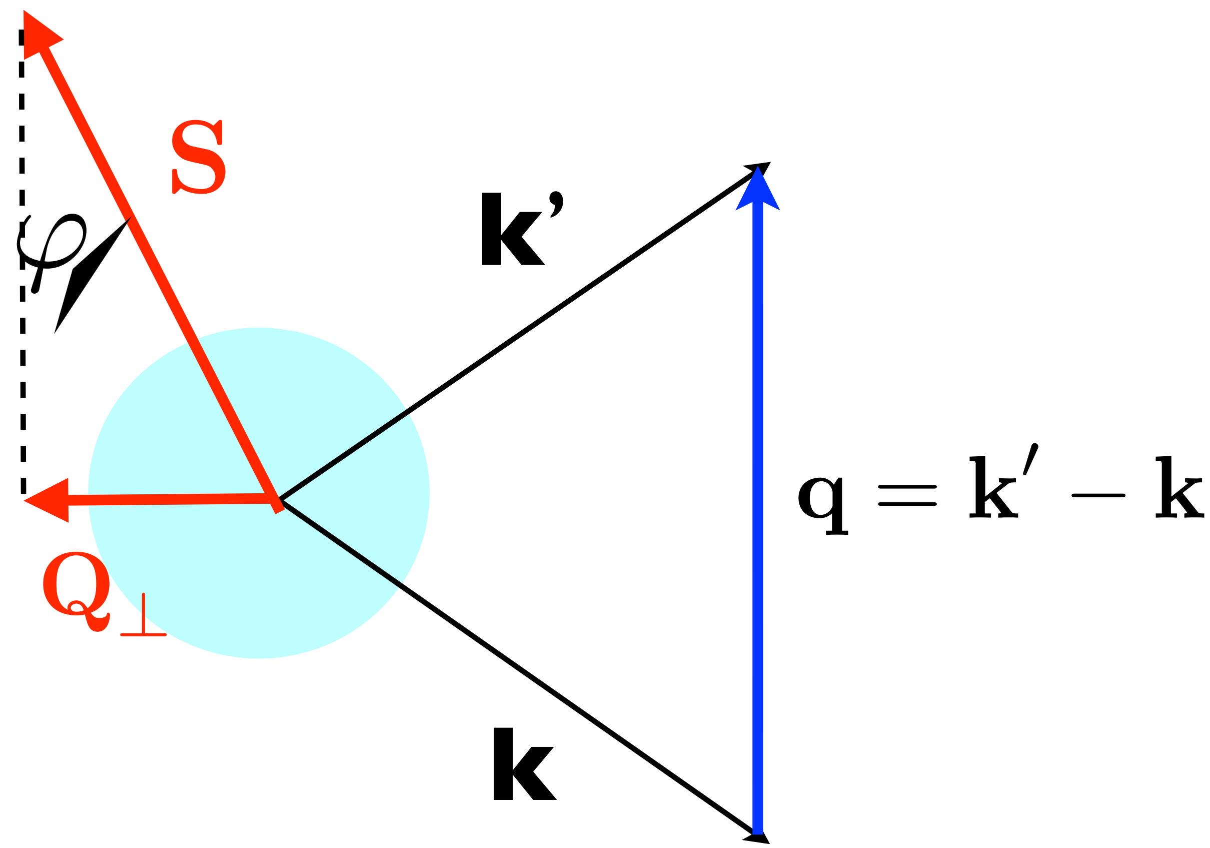


$$|\mathbf{Q}_\perp| = |\mathbf{S}| \sin(\varphi)$$

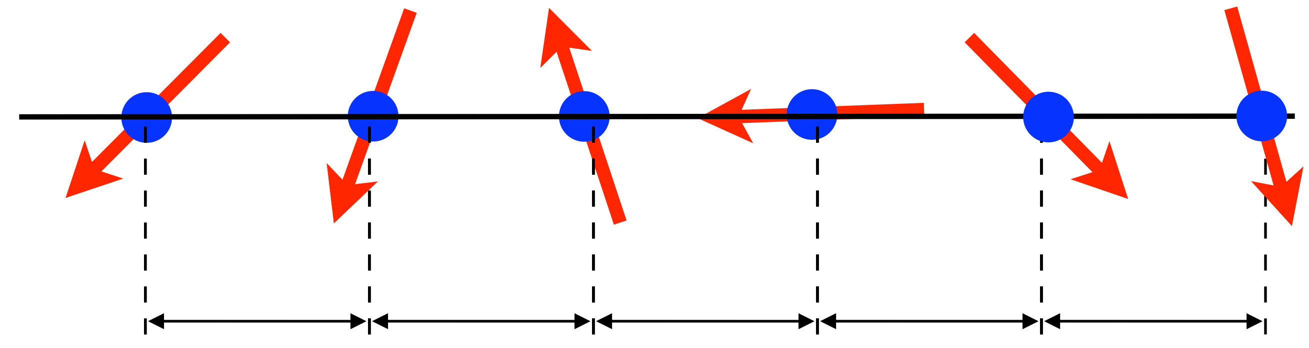
Elastic scattering intensity

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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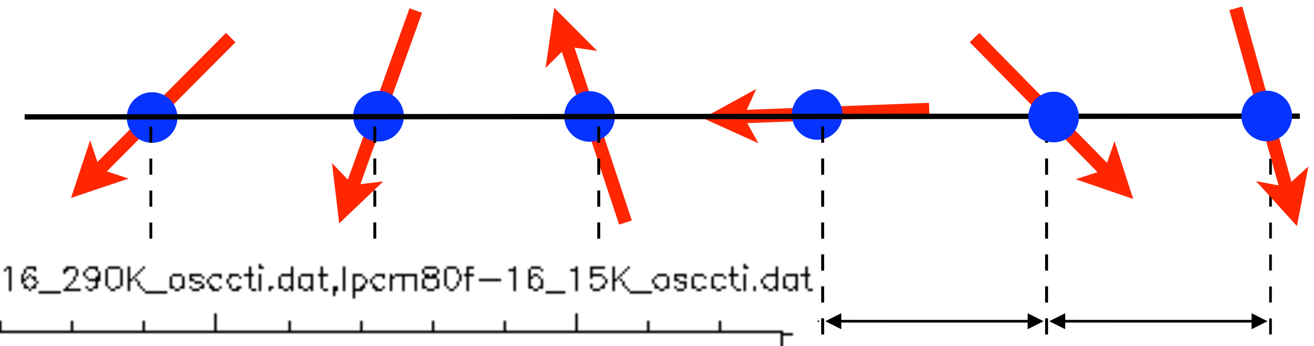
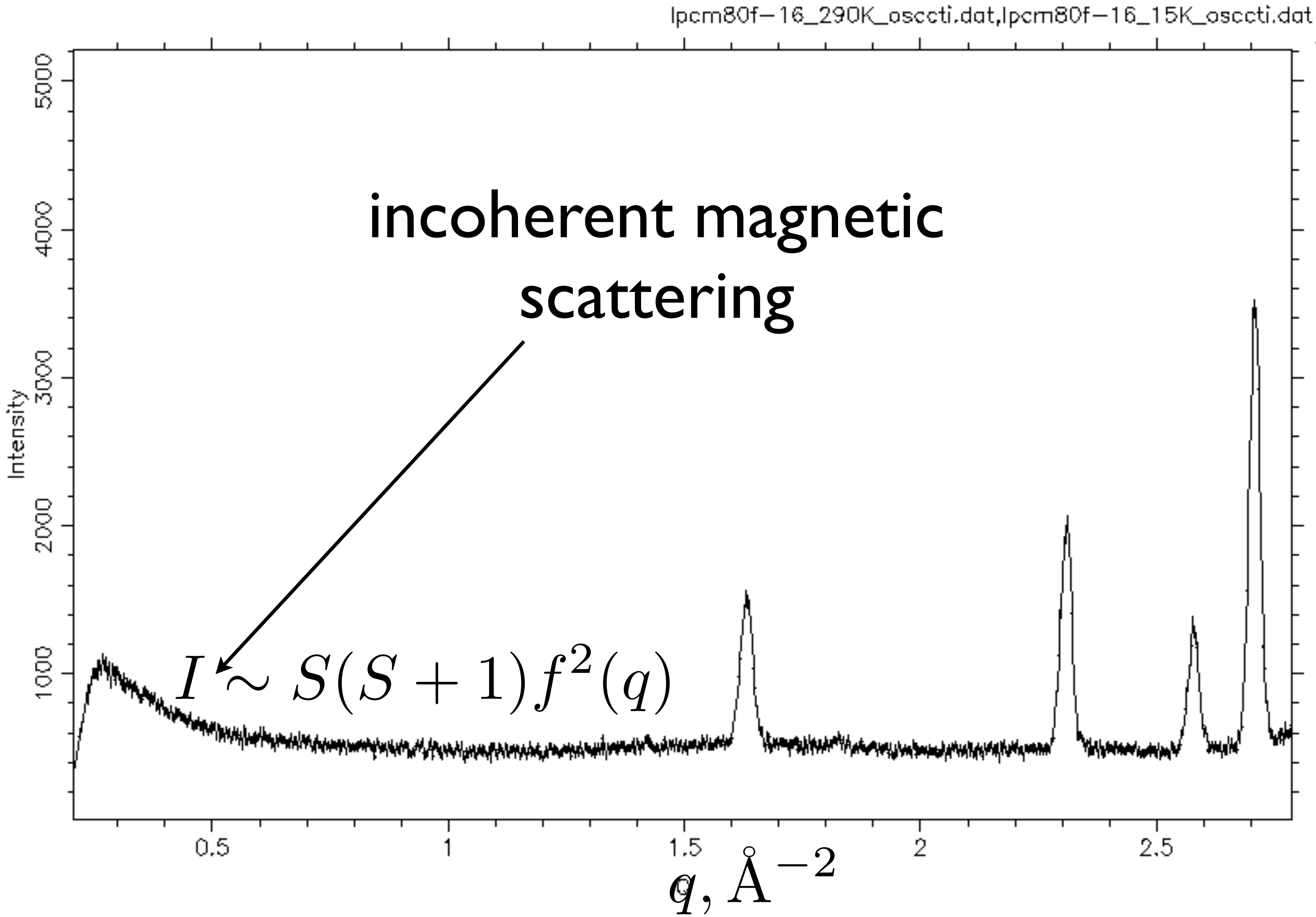


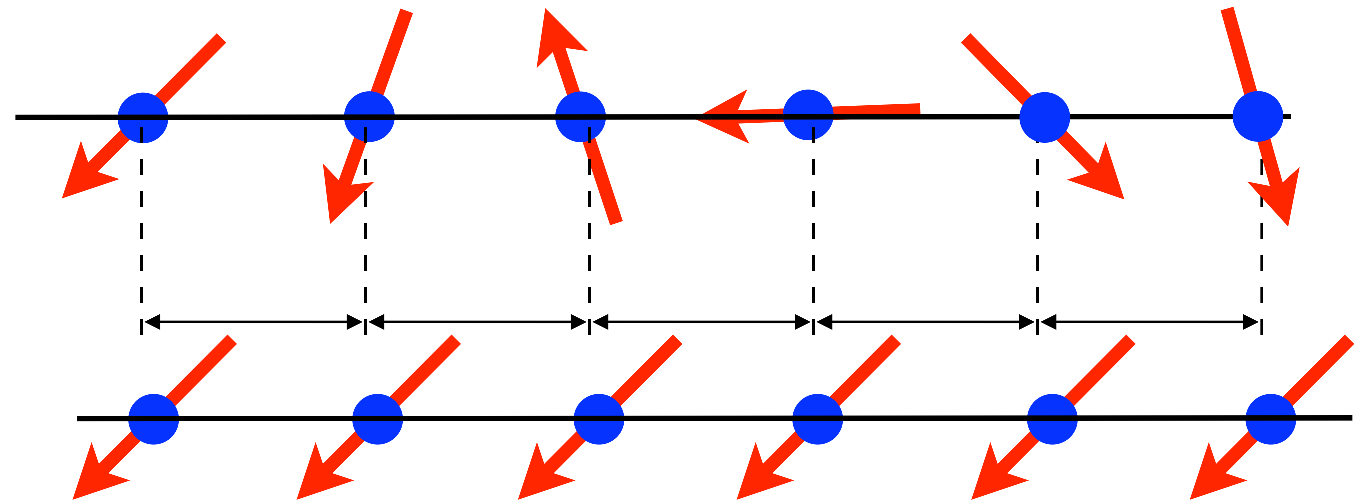


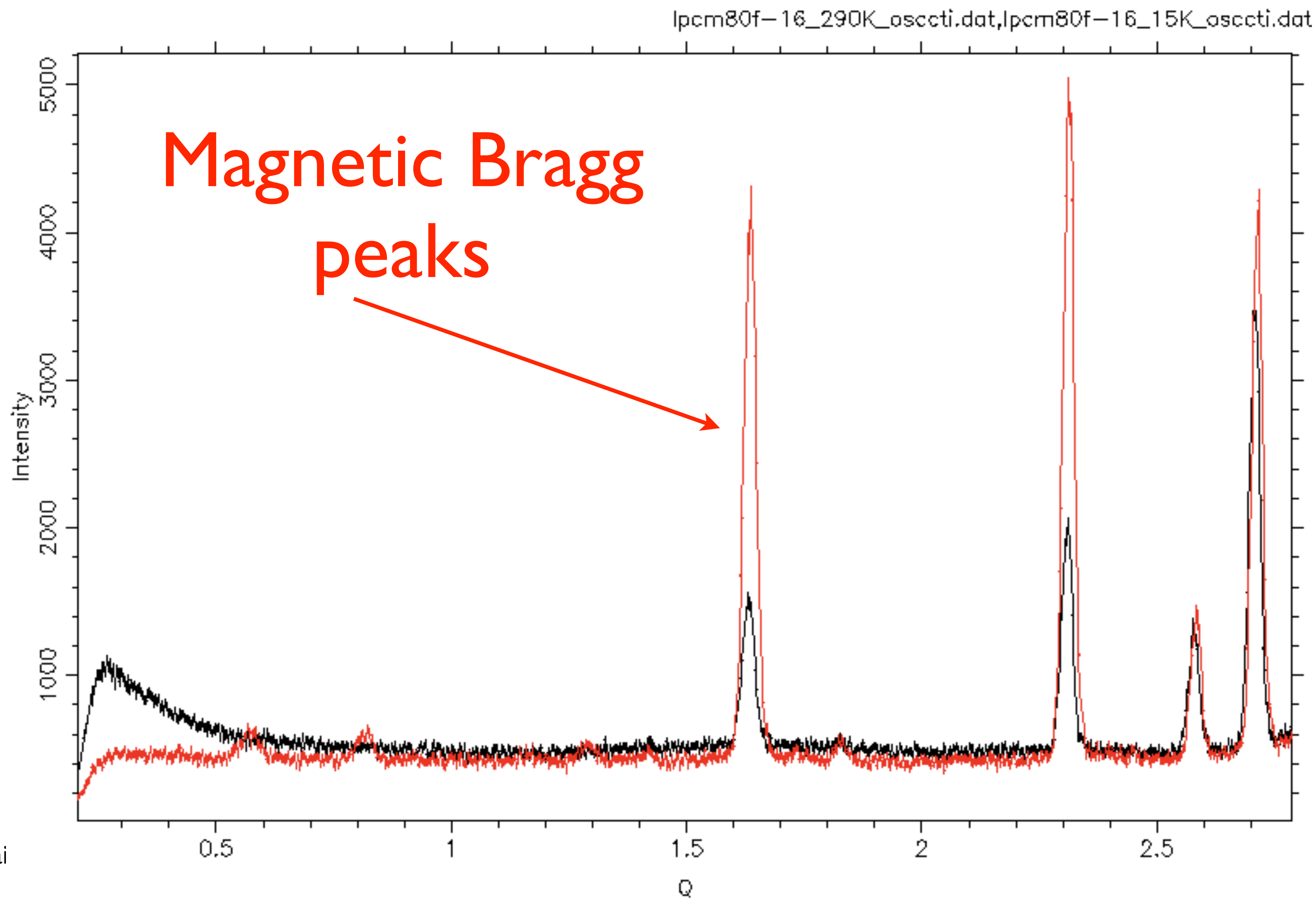
Elastic scattering on a lattice of spins

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

coherent Bragg scattering

$$I \sim |<\mathbf{S}>|^2 F_{HKL}^2$$

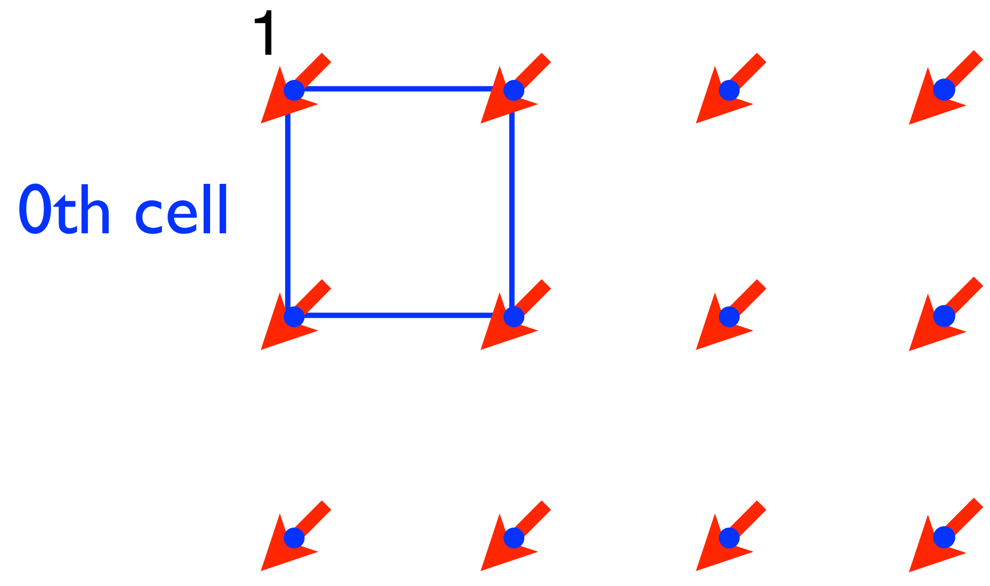




Magnetic structure

Examples

k=[0,0]
FM



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

Magnetic structure

Examples

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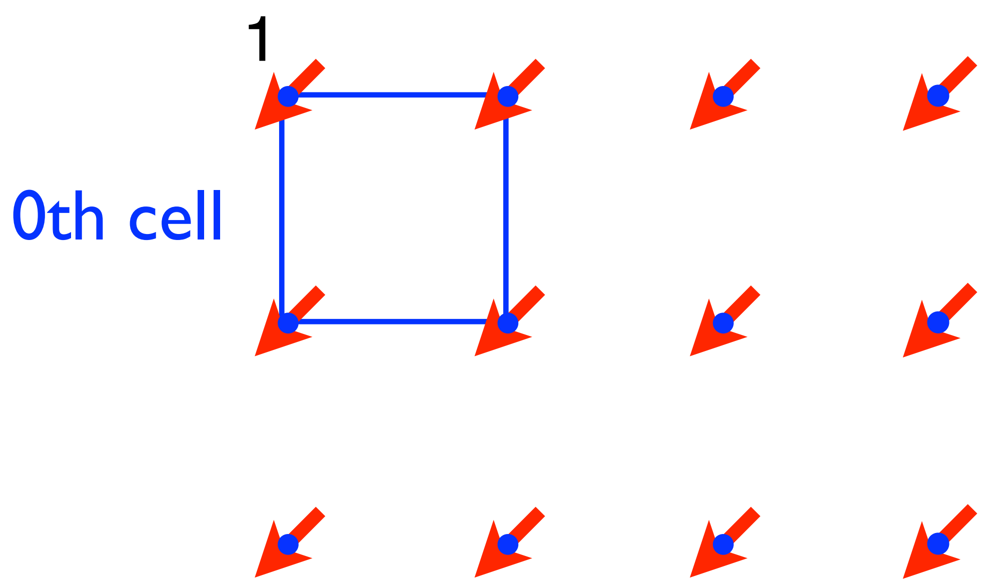
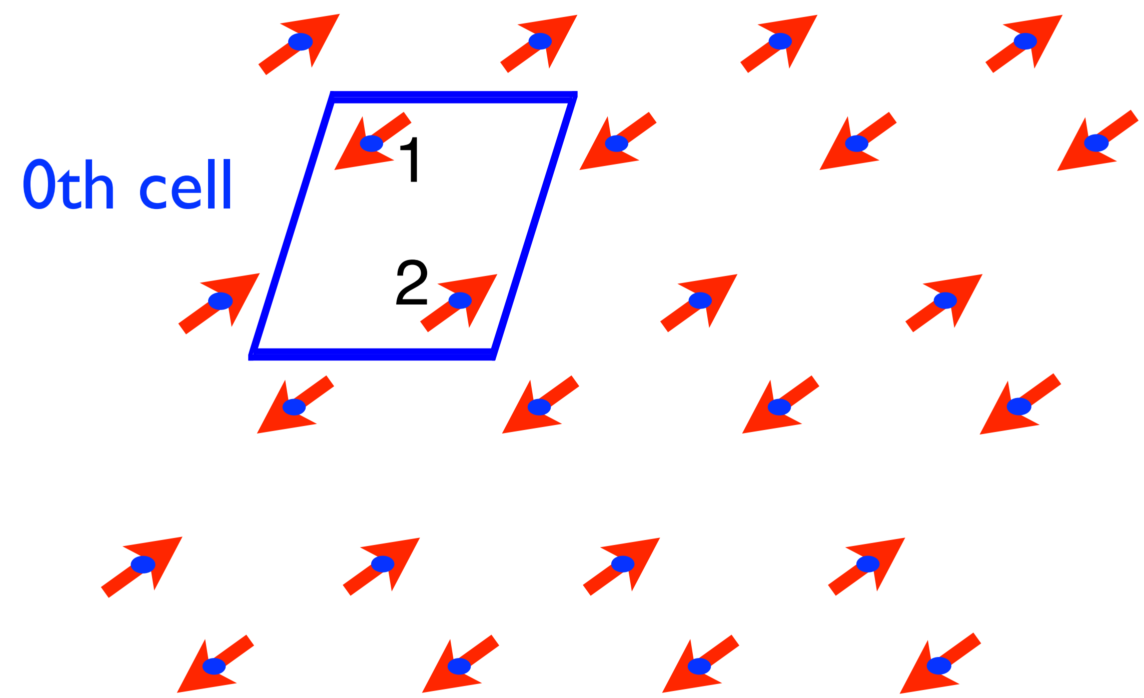
FM



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

k=[0,0]
AFM



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

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

Examples of magnetic structures. Propagation vector formalism k≠0

Magnetic moment is a real quantity

$$\mathbf{S}(\mathbf{t}_n) = \frac{1}{2}(\mathbf{S}_0 e^{+2\pi i \mathbf{t}_n \mathbf{k}} + \mathbf{S}_0^* e^{-2\pi i \mathbf{t}_n \mathbf{k}})$$

Bloch waves

Fourie amplitude is complex (one can not avoid this)

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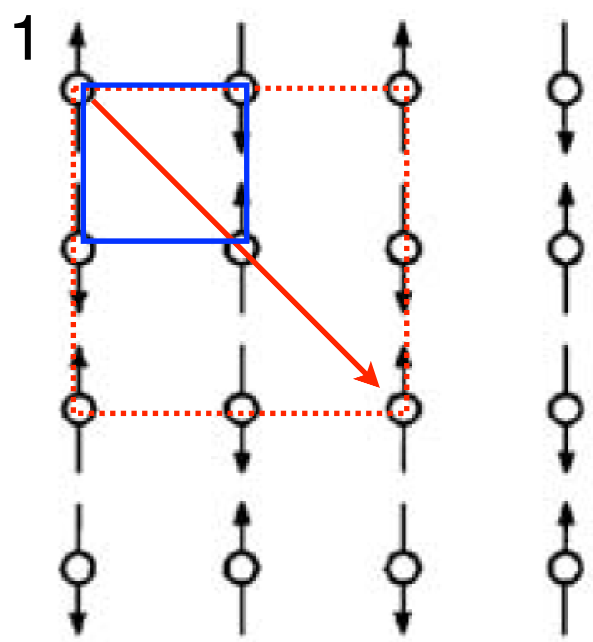
k=[1/2,1/2] AFM



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

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

Examples of magnetic structures.
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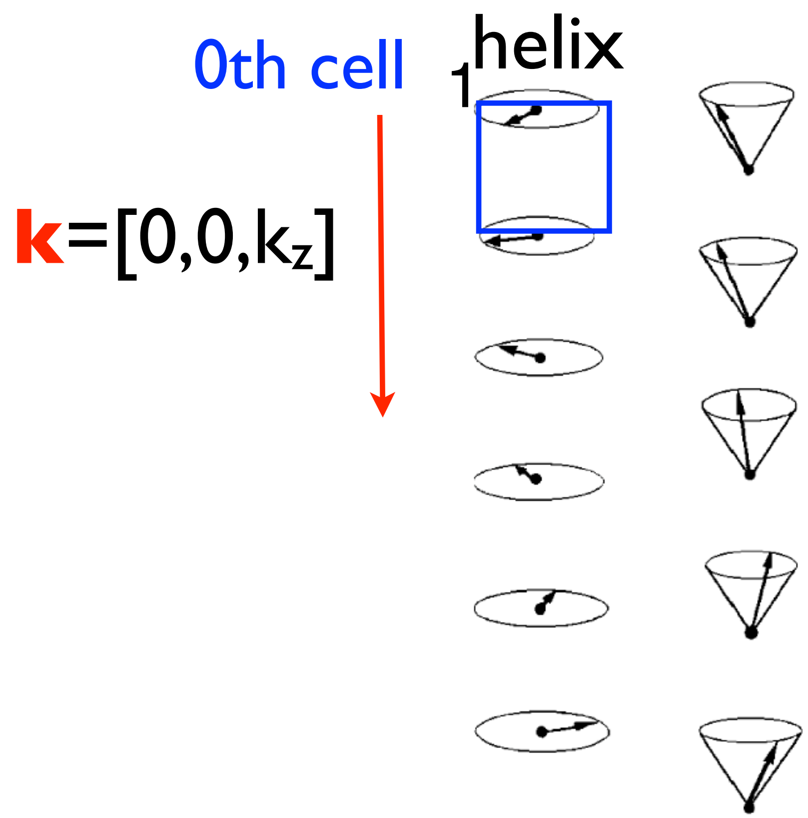
<u>modulated (in)commensurate</u>



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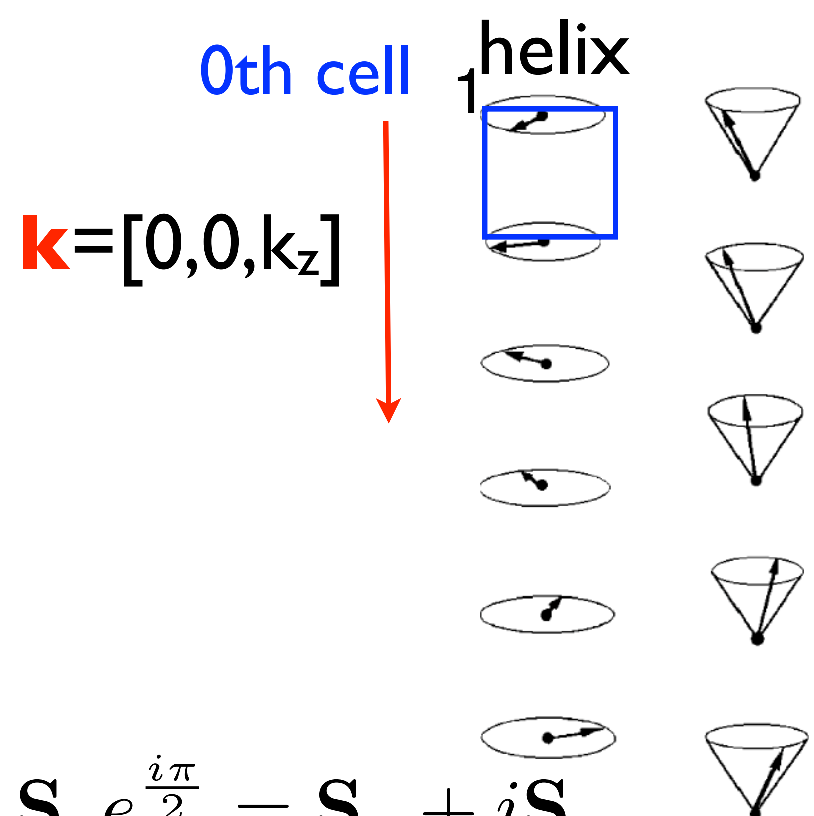

$$\mathbf{S}_{01} = \mathbf{S}_x + \mathbf{S}_y e^{\frac{i\pi}{2}} = \mathbf{S}_x + i\mathbf{S}_y$$

$$\varphi_n = 2\pi i \mathbf{t}_n \mathbf{k}$$

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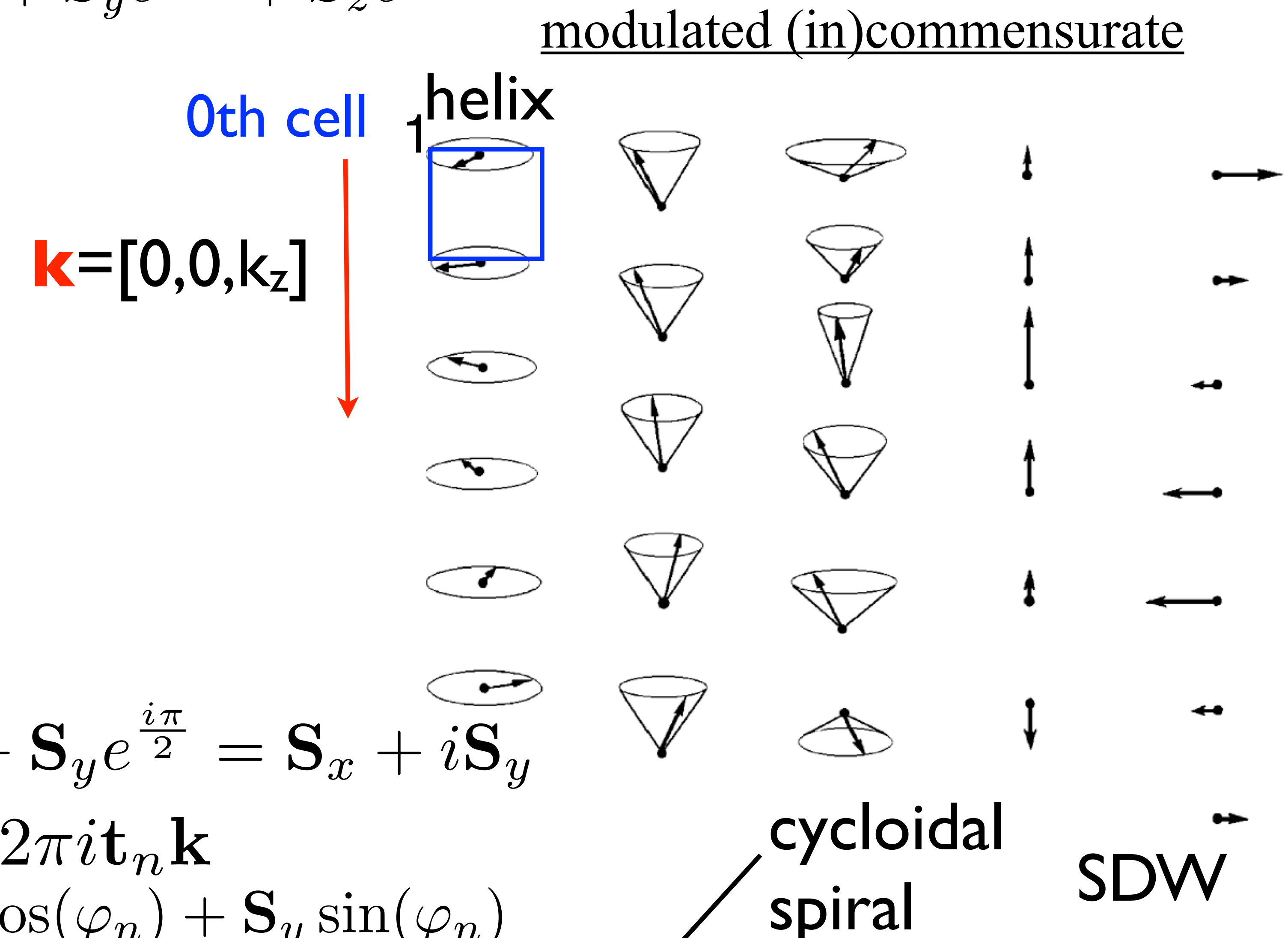

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Scattering from the lattice of spins. Structure factor F(q)

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

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

↑ structure factor

↑ polarized neutron (chiral) term.

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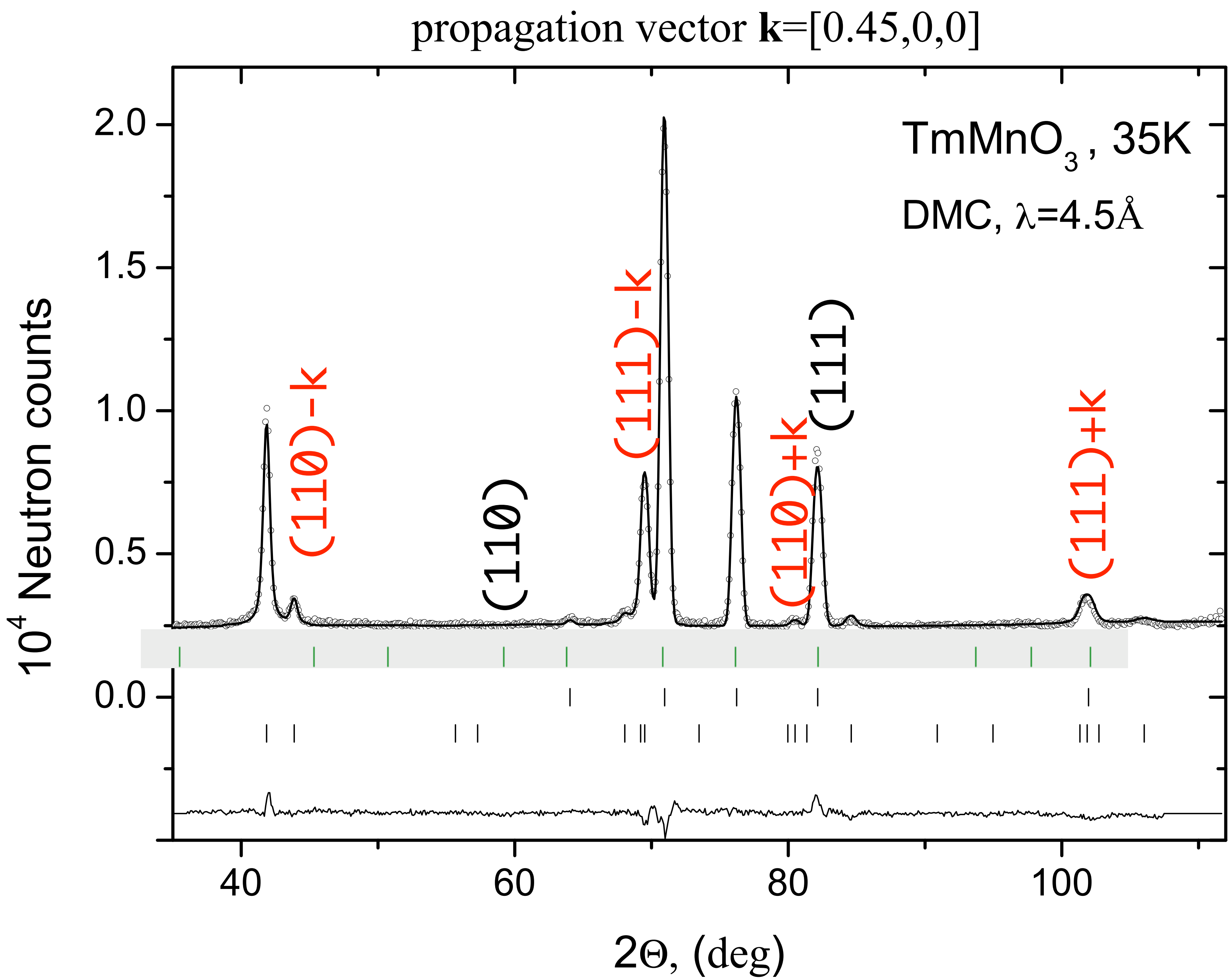
Sum runs over all atoms in zeroth cell

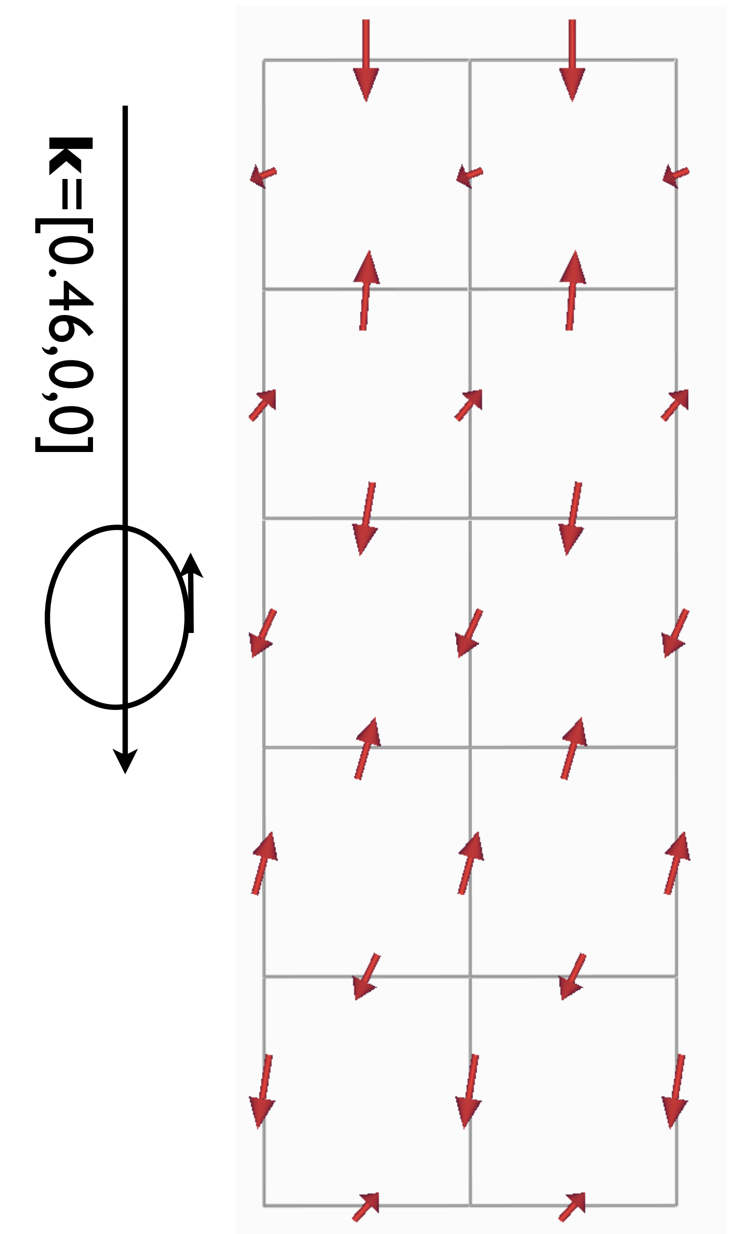
$$\mathbf{F}(\mathbf{q})_{-\boldsymbol{k}} = \sum_j \frac{1}{2}\mathbf{S}_{\perp 0j} \exp(i\mathbf{r}_j\mathbf{q}) \qquad \mathbf{F}(\mathbf{q})_{+\boldsymbol{k}} = \sum_j \frac{1}{2}\mathbf{S}^*_{\perp 0j} \exp(i\mathbf{r}_j\mathbf{q})$$

Complex amplitude of spin modulation perpendicular to **q**

position of spin in the zeroth cell

Example of modulated structure and diffraction pattern





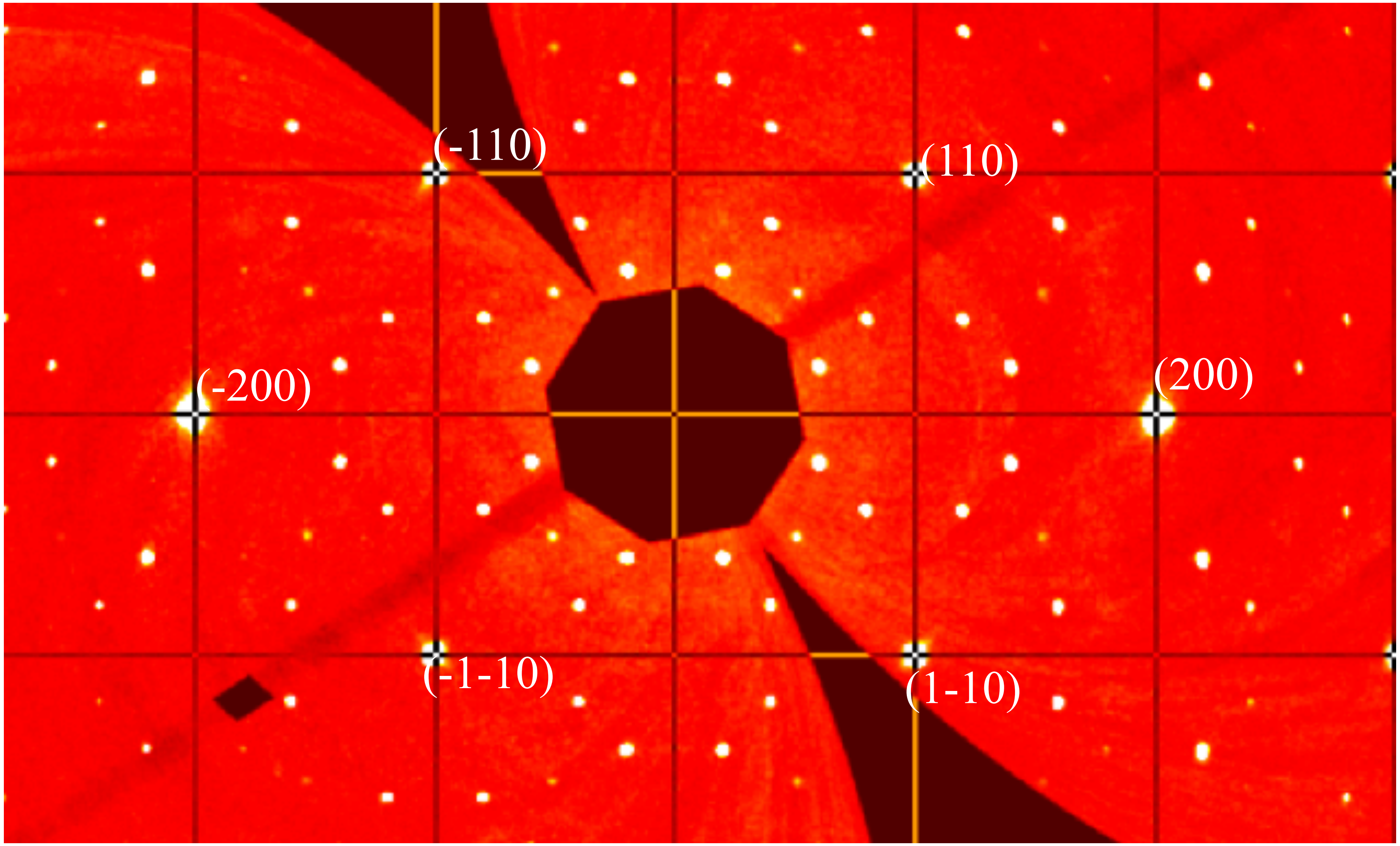
Example of modulated structure and single crystal diffraction

4-arms k-vector stars

$$\{\mathbf{k}_1\} = \{[\frac{2}{5}, \frac{1}{5}, 1]\}$$

$$\{\mathbf{k}_2\} = \{[\frac{1}{5}, \frac{2}{5}, \bar{1}]\}$$

superstructure satellites



the mesh is for the parent I4/mmm cell
T=300K, (hk0) plane of $Cs_yFe_{2-x}Se_2$

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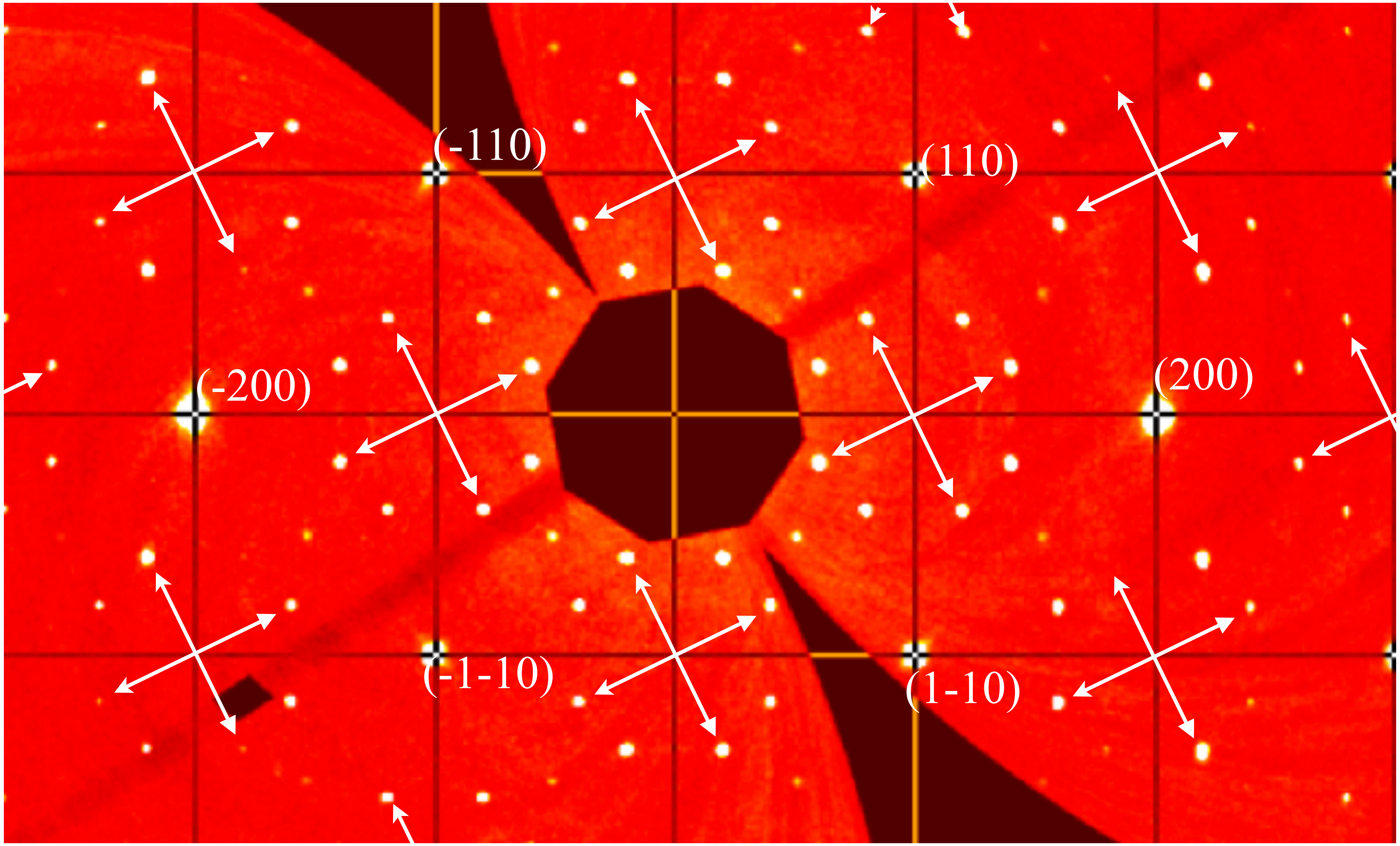

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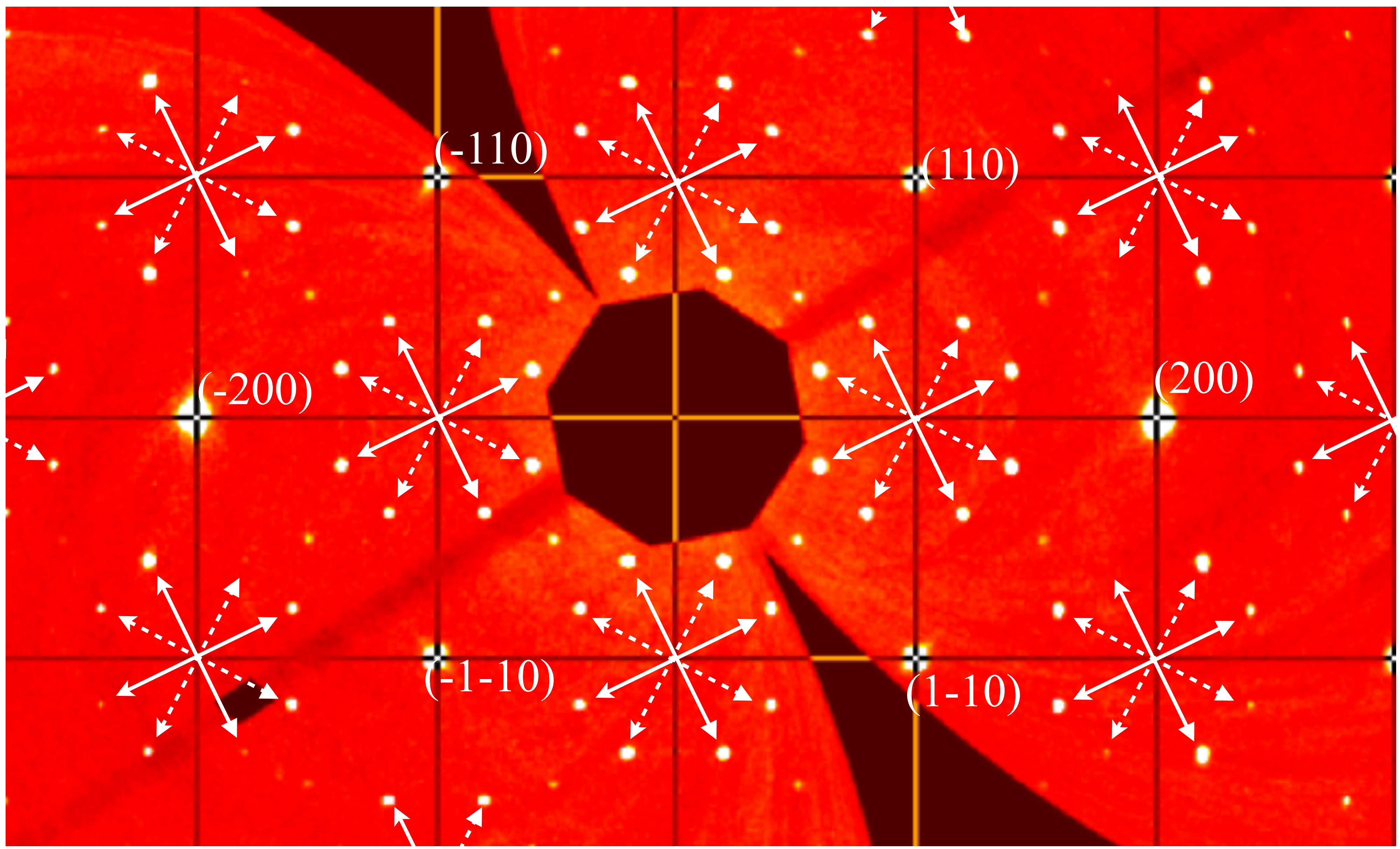

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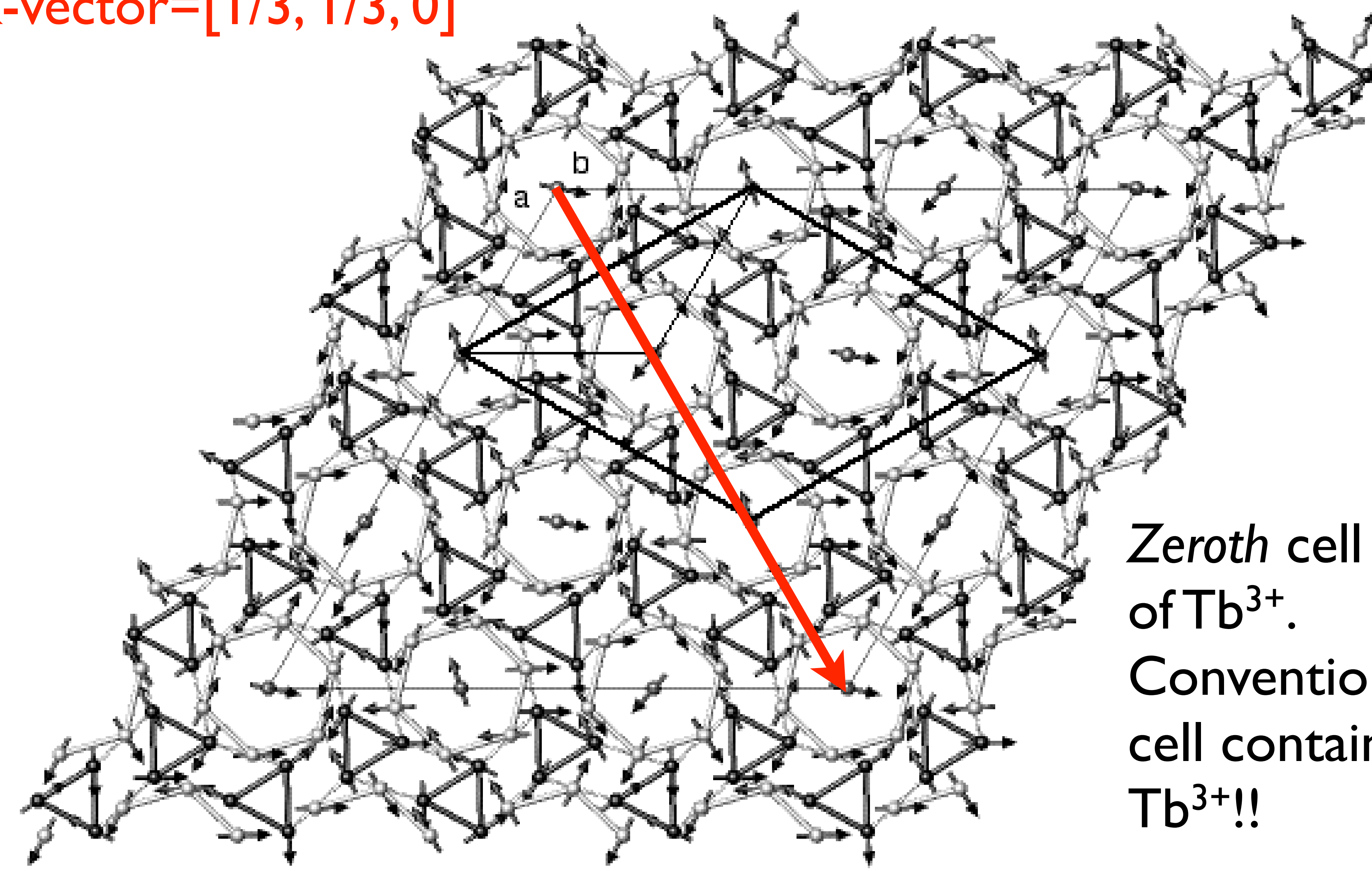
Example of complex magnetic structure

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+}!!

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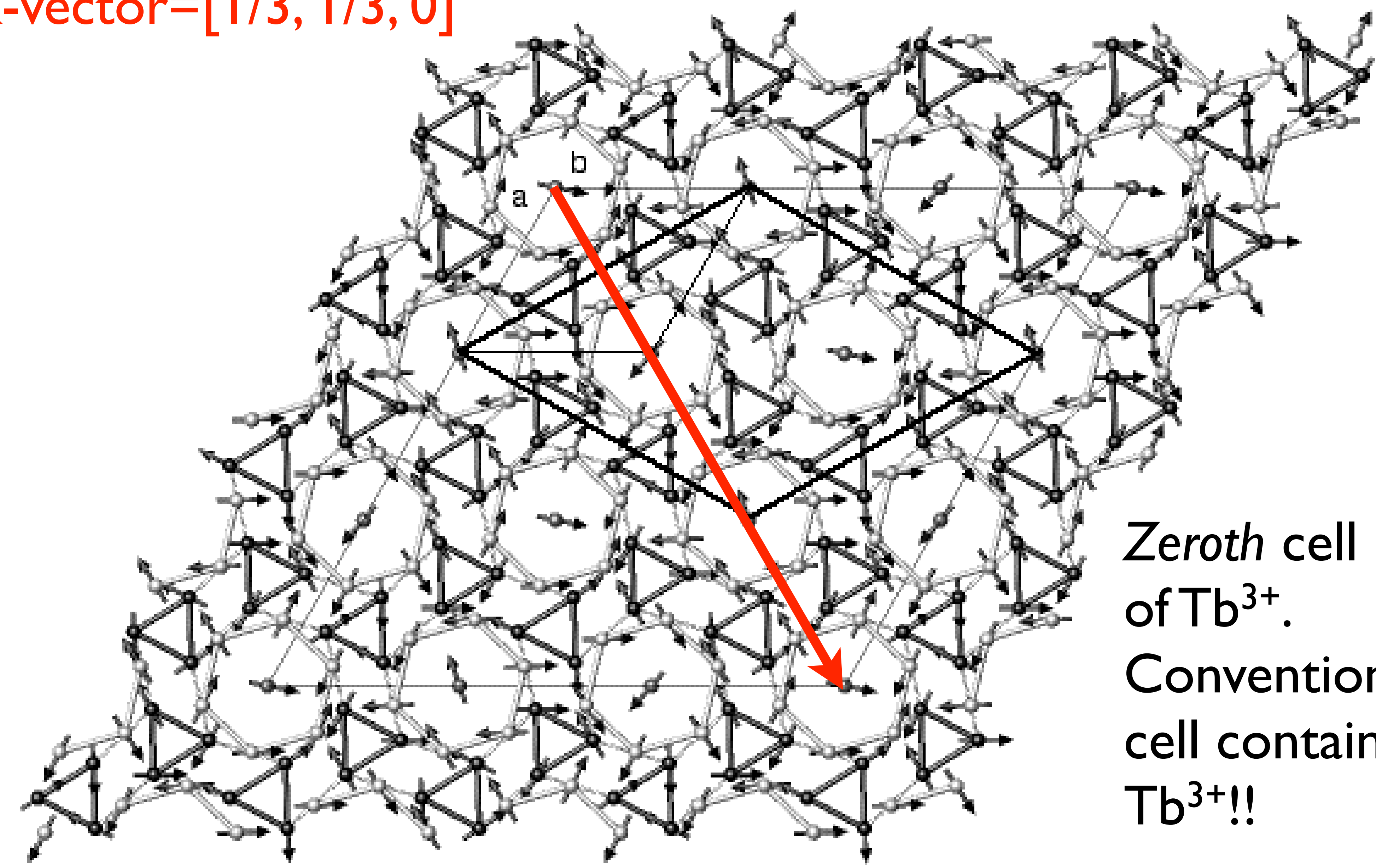

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PHYSICAL REVIEW B 72, 134413 (2005)

Some legitimate questions

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

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

Magnetic structure/symmetry seen by ND

Magnetic interactions are described by QM Hamiltonian with quantum spin operators

$$\hat{H} = -\sum_{i,j} J_{ij}\hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_j + \sum_i D_i \hat{s}_z^2 + \ldots$$

In a diffraction experiment the problem is reduced and we observe only the spin expectation values: <> averaging over all states (wave function ψ) of the scatterer.

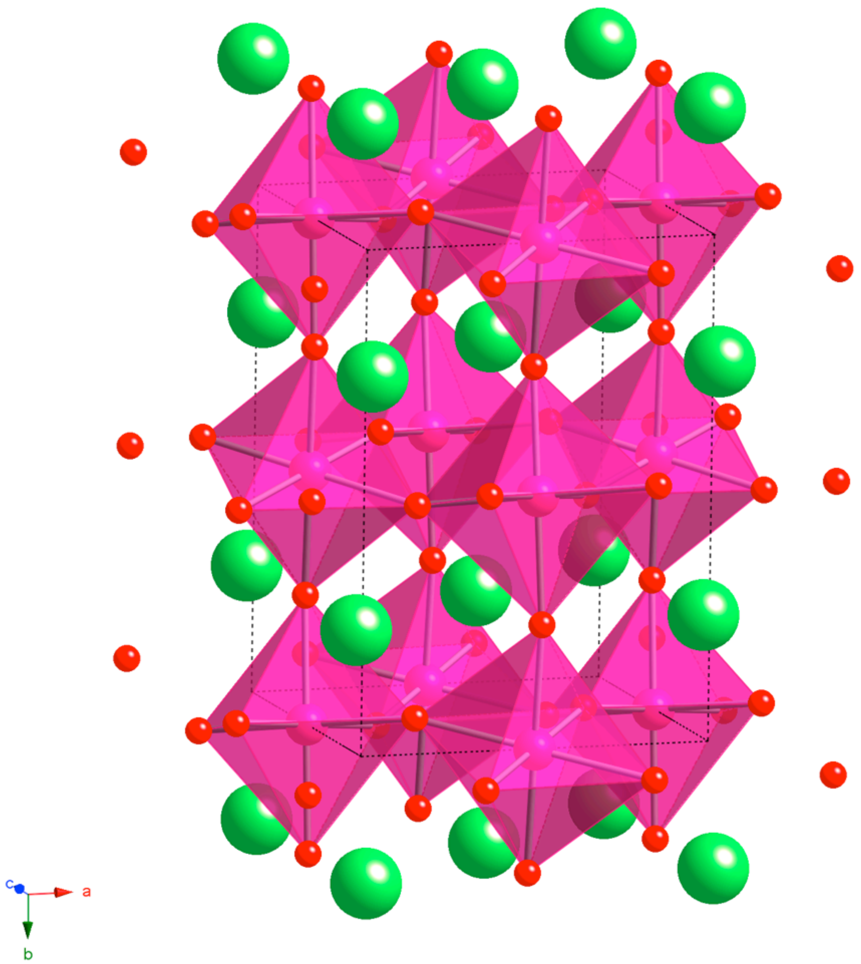
$$\mathbf{s}_i = \langle \hat{\mathbf{s}}_i \rangle = s_x \mathbf{e}_{\boldsymbol{x}} + s_y \mathbf{e}_{\boldsymbol{y}} + s_z \mathbf{e}_{\boldsymbol{z}} \qquad \langle \hat{s}_z \rangle, \langle \hat{\mathbf{s}}^2 \rangle$$

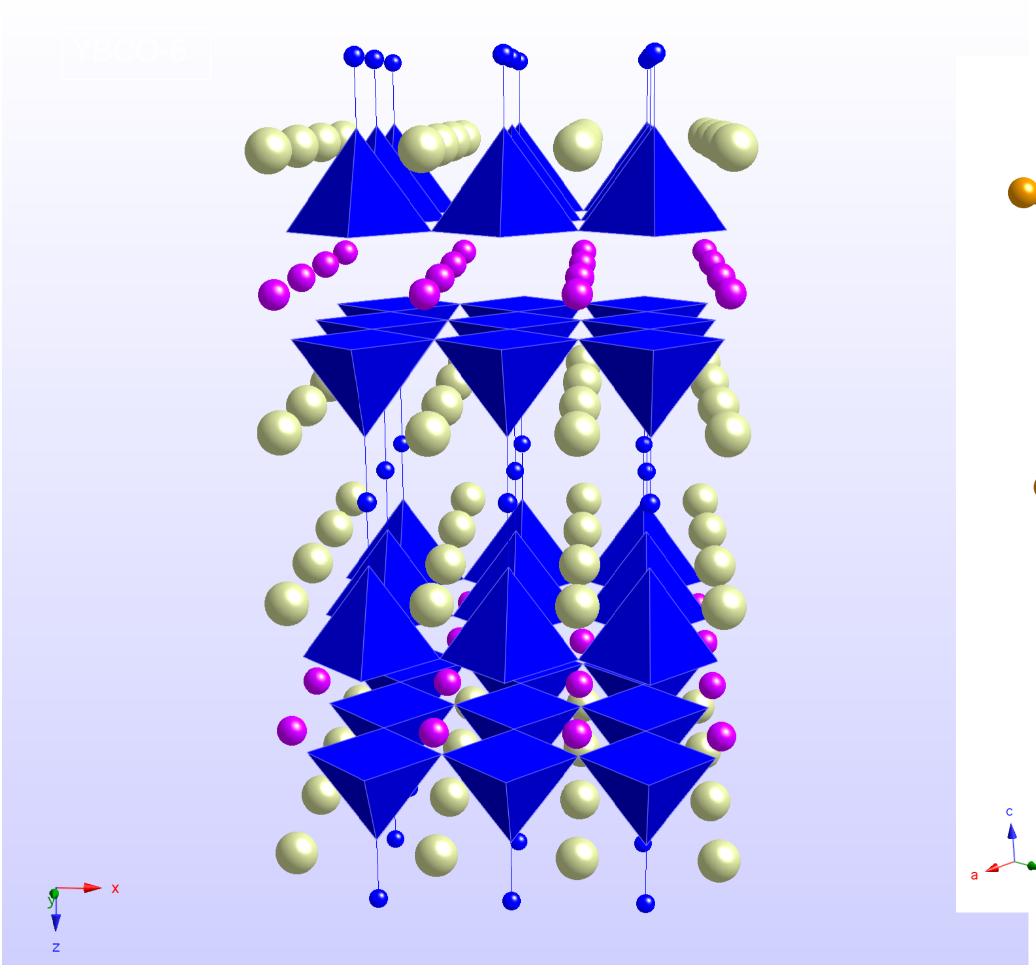
(the last two expressions are crossed out)

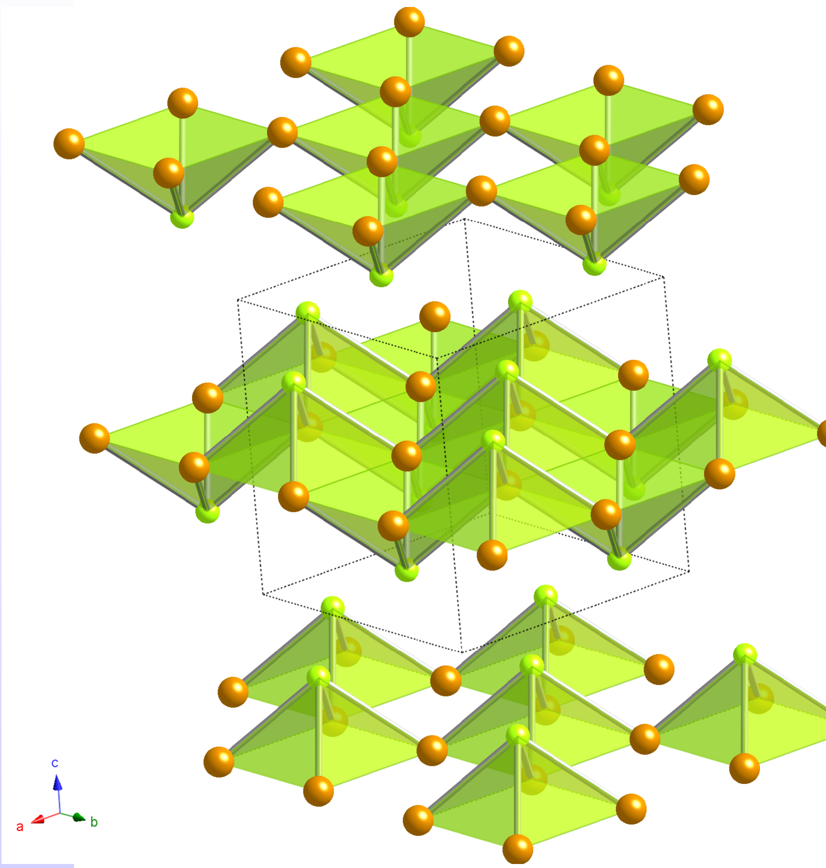
Magnetic structure that we observe by ND is an ordered set of ***classical*** axial vectors $\mathbf{s}_i = \langle \hat{\mathbf{s}}_i \rangle$ that can be directed at any angle with respect to crystal axes and field.

In the representation symmetry analysis we deal with the classical spins transforming as axial vectors under symmetry operations of **space groups** such as rotations, inversion, etc.

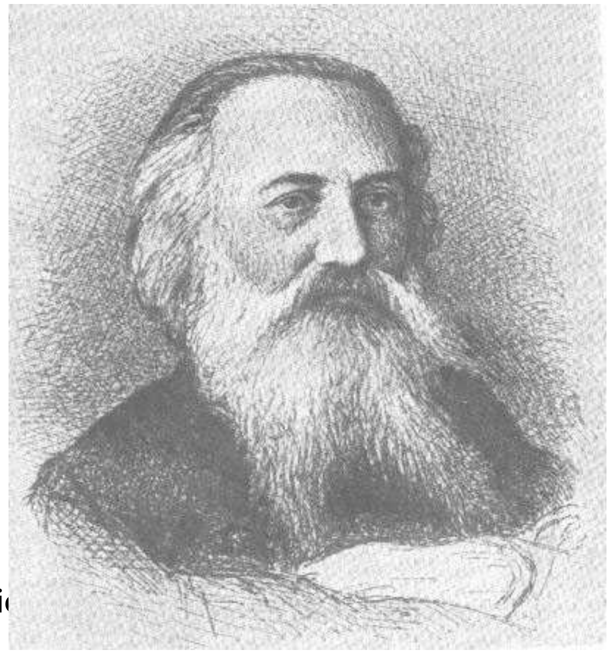
Atomic structure of any 3D crystal can be described by one of 230 3D Space* groups







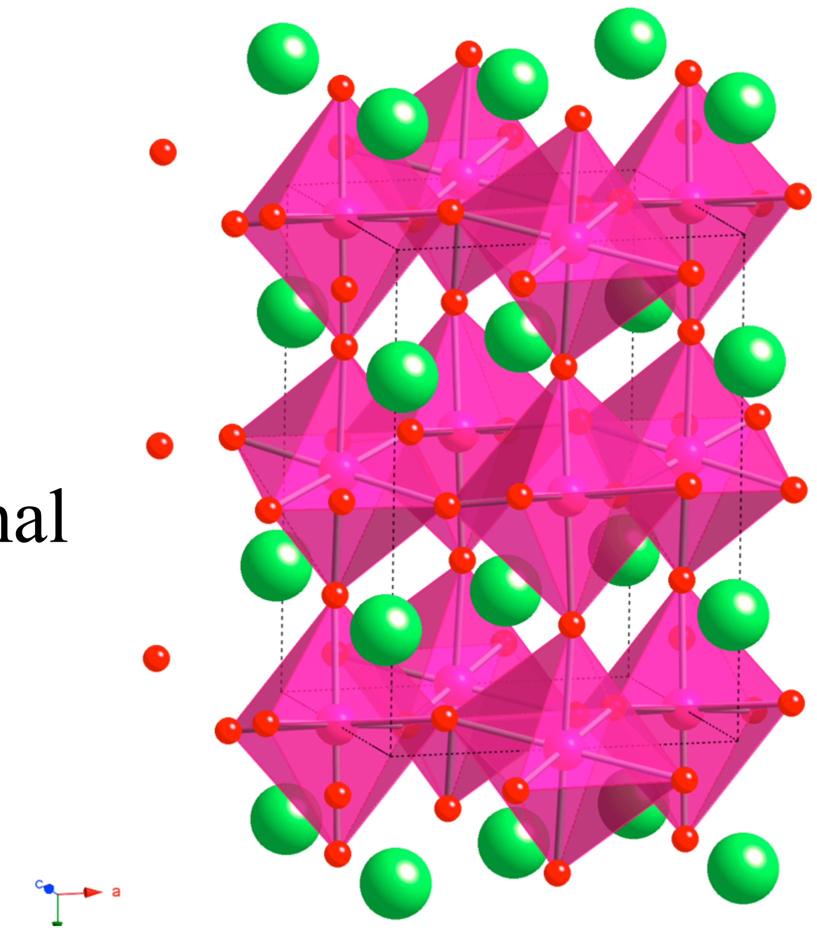
* E.S. Fedorov 1853 – 1919. "Symmetry of regular figures" (1890)



Artur Moritz Schöenflies 1853 – 1928. "Kristallsysteme Und Kristallstruktur" (1891)

Basic crystallography (3 slides)

230 3D Space* groups



Groups of transformations/motions of three dimensional homogeneous discreet space into itself

Two kinds of transformations/motions = 1. rotations (32 point groups)

e.g: 4_z^+ 2_z 4_z^- -1 -4_z^+ m_z -4_z^-

2. lattice translations $\mathbf{t} = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3$

(14 Bravias groups)

Space group ~ (semi)product point crystallographic group and Bravias group.

---

* E.S. Fedorov (1890) A.Schoenflies (1890)

230 space groups. New symmetry elements

Product of 32 point crystallographic groups and 14 Bravias groups

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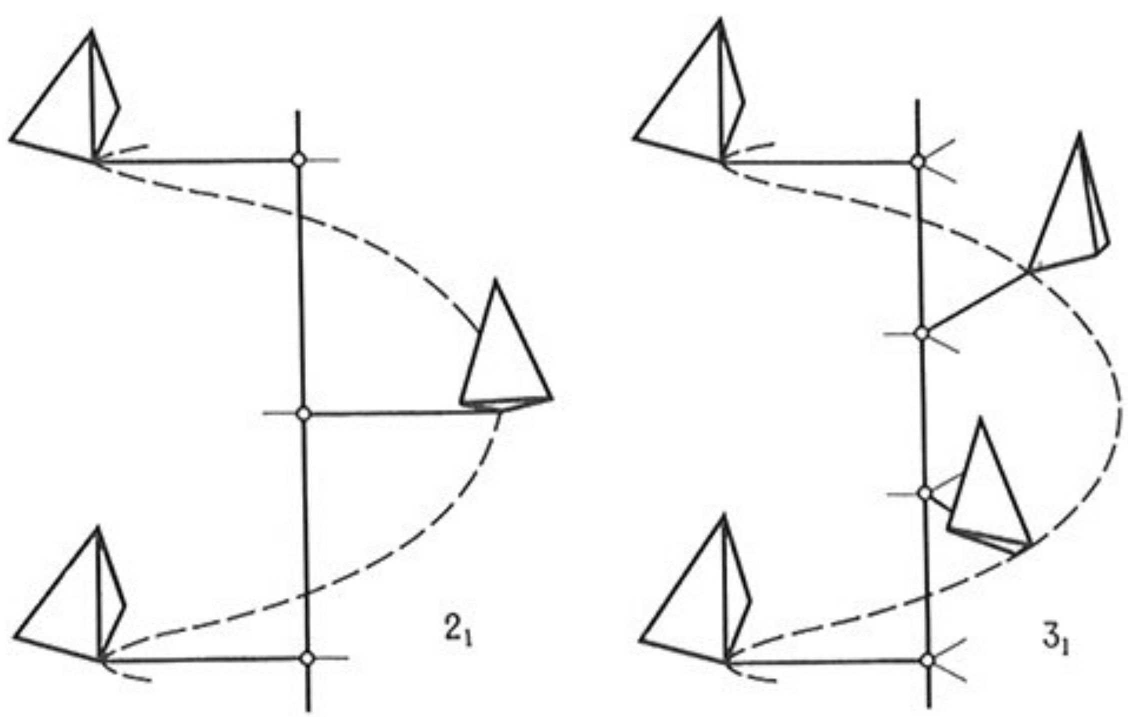
Screw axes or axes of screw rotations = rotation + translation. e.g. 2_1, 3_1,3_2, ...

$$\alpha_s = 2\pi/N,\ N = 2, 3, 4, 6,$$

$$t_s = \frac{q}{N}\, t, \quad q = 1, 2, 3, 4, 6.$$



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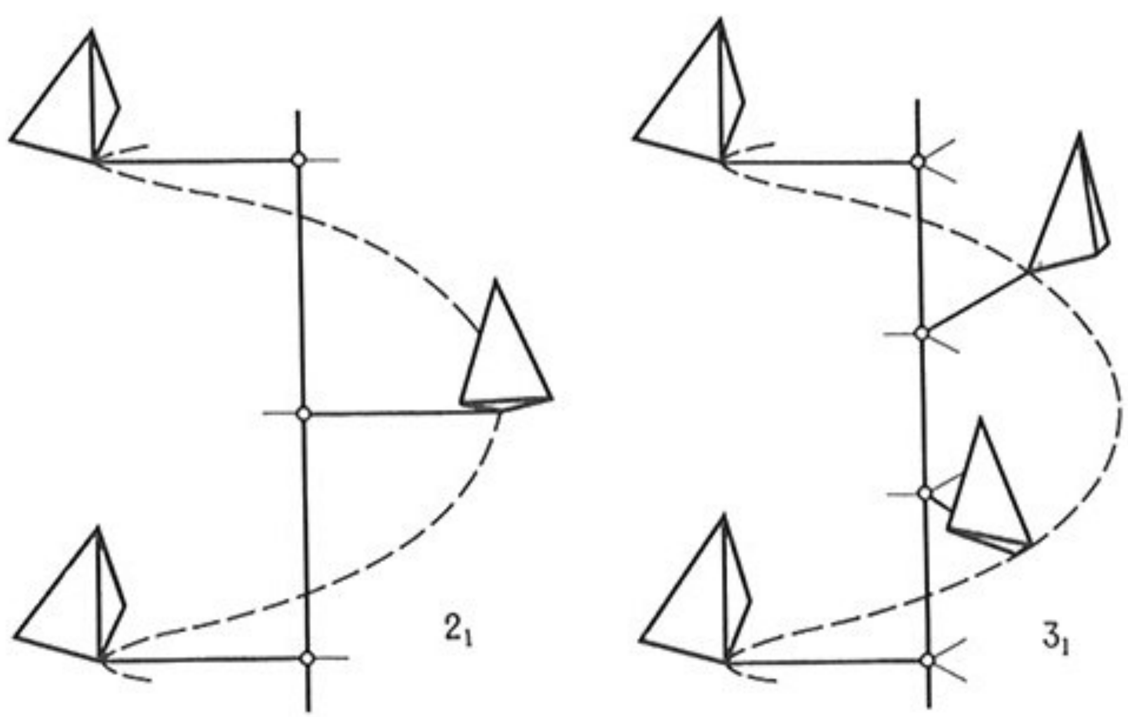
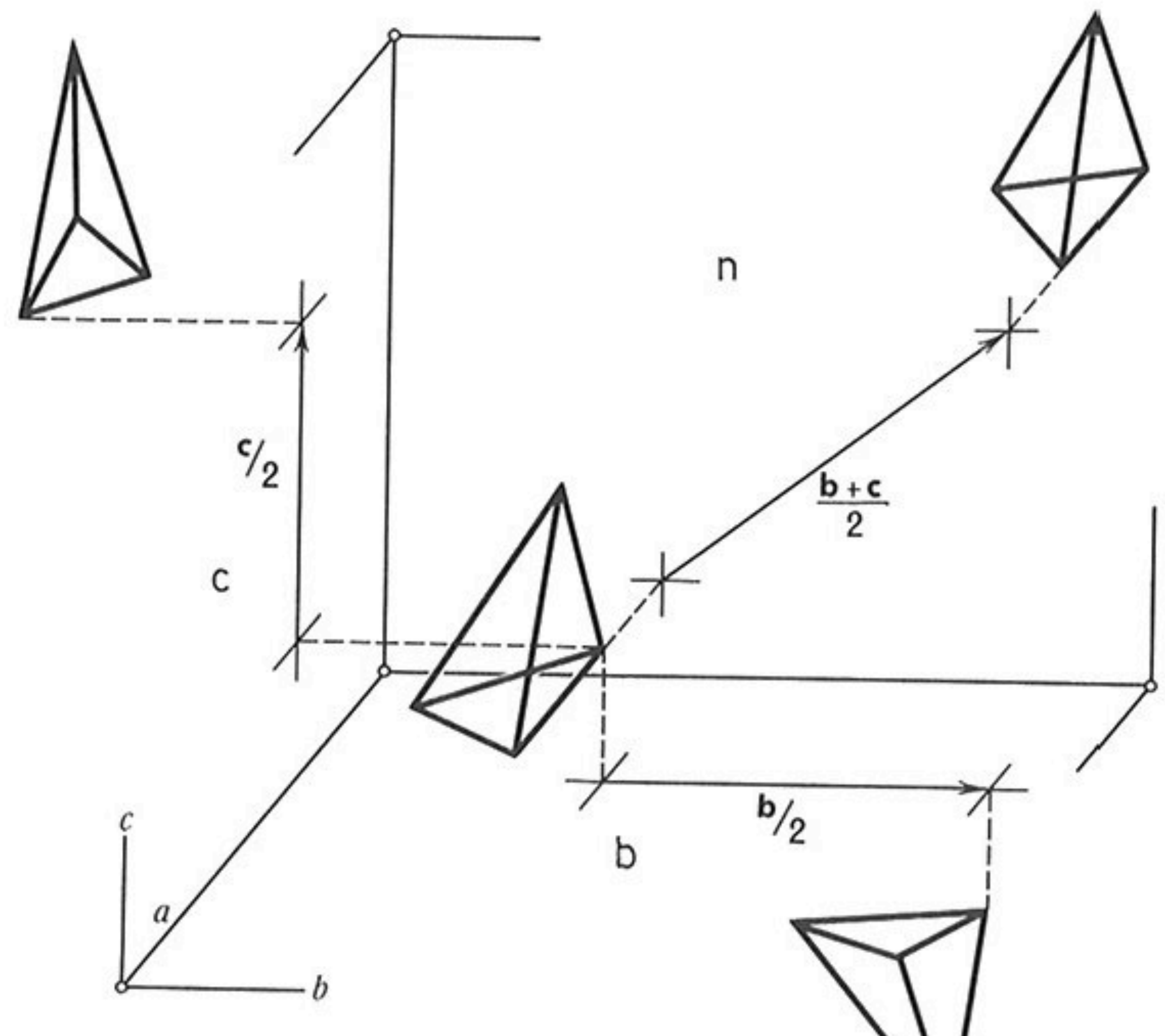


Glide-reflection planes =
mirror reflection *m* + translation by *t/2*,
a, *b*, *n*



International Tables

$Pnma$	D_{2h}^{16}	mmm	Orthorhombic
No. 62	$P\ 2_1/n\ 2_1/m\ 2_1/a$		Patterson symmetry $Pmmm$

Origin at $\bar{1}$ on $1\,2_1\,1$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+l,k=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+l,k=2n$

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International Tables

Hermann–Mauguin, short

$Pnma$	D_{2h}^{16}	Schoenflies symbol	mmm	Orthorhombic

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Hermann–Mauguin

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4 a $\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+l,k=2n$

International Tables

Hermann–Mauguin, short

$Pnma$ | D_{2h}^{16} Schoenflies symbol | mmm | Orthorhombic

No. 62 | $P\ 2_1/n\ 2_1/m\ 2_1/a$ | Patterson symmetry $Pmmm$

Hermann–Mauguin

Origin at $\bar{1}$ on $1 2_1 1$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

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

zeroth block of SG

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+l,k=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+l,k=2n$

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Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
8	d	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$00l$: $l=2n$
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4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
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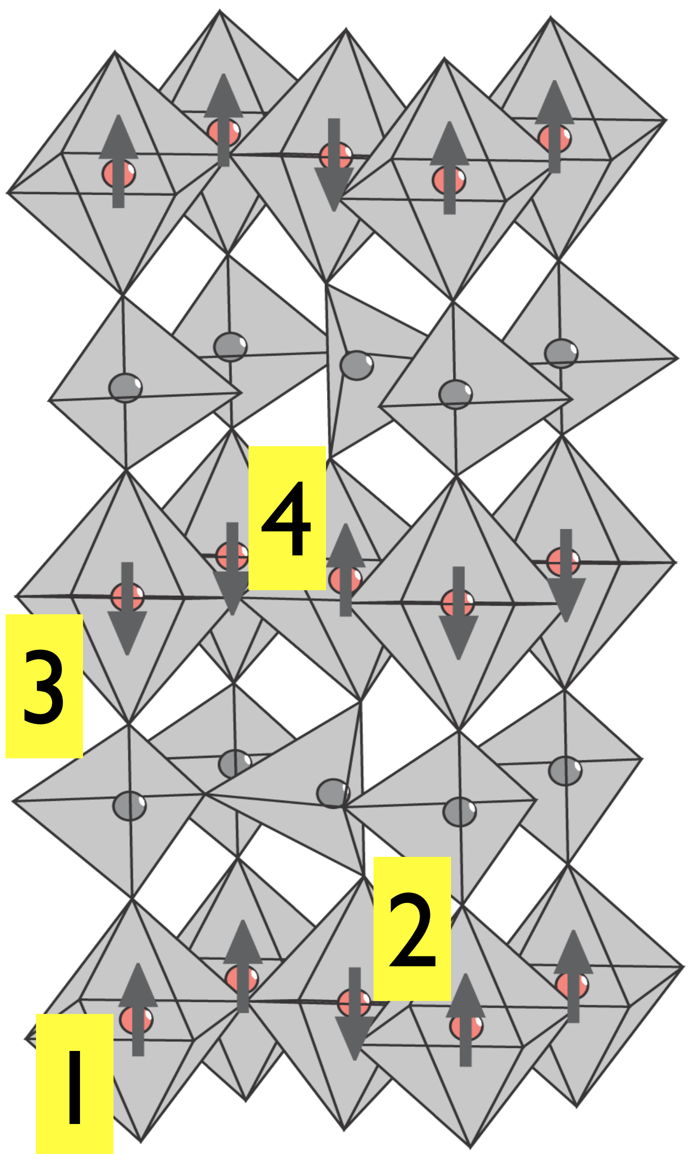
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+l,k=2n$

general position:
rotation matrix + translation
$\{h|\boldsymbol{\tau}_h\}$

Two ways of description of magnetic structures

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



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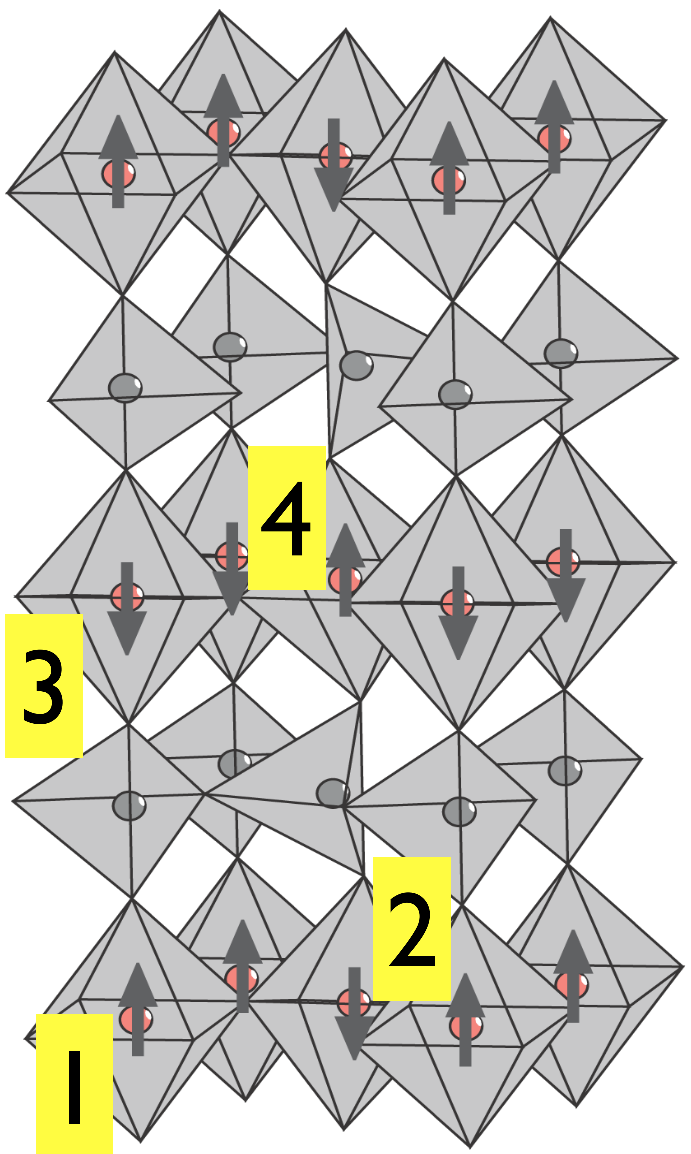

1. g**S**(**r**) = **S**(**r**) to itself, where g ∈ subgroup of SG⊗1’, 1’=spin/time reversal, SG (space group)

   or

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1. **Magnetic or Shubnikov groups MSG.** Historically the first way of description. A group that leaves **S(r)** invariant under a subgroup of G⊗1'. Identifying those symmetry elements that leave S(r) invariant.
   Similar to the space groups (SG 230). The MSG symbol looks similar to SG one, e.g. *I4/m'*

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MSG Example:

87.1.733	I4/m
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87.3.735	I4'/m
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S(**r**) is transformed to $\mathbf{S}^i(\mathbf{r})$ under $g \in G$ 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 space group G

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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

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

In 1960th-70th often opposed

E.F.Bertaut, CNRS, Grenoble
Representation Analysis

W.Opechovski, UBC, Vancouver
Shubnikov magnetic space groups

Nowdays

(Representation Analysis) and (Magnetic space groups) are complementary and in case k=0 or commensurate (e.g 1/2) provide identical description of magnetic symmetry.

Magnetic symmetry. 1651 3D-Shubnikov (Sh or Ш) space groups

14 Bravias lattice

32 point groups

230 space groups (SG)

antisymmetry: Heesh (1929), Shubnikov (1945).
groups: Zamorzaev (1953, 1957); Belov, Neronova, Smirnova (1955)
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R(♖) = ♜

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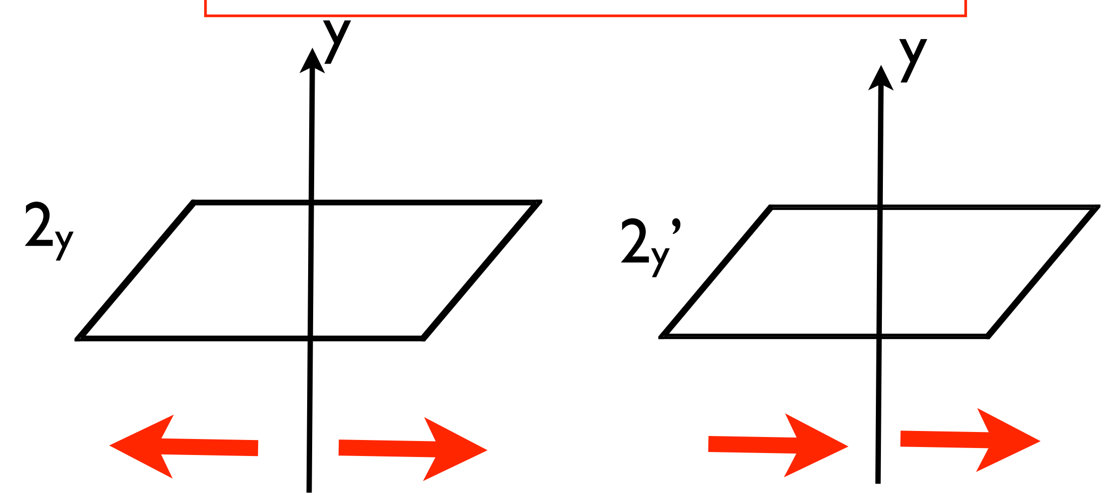

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230 (gray) paramagnetic groups Sh_p
$1,1' \in Sh_p \Rightarrow \mathbf{S}=0$, e.g. *Pnma1'*

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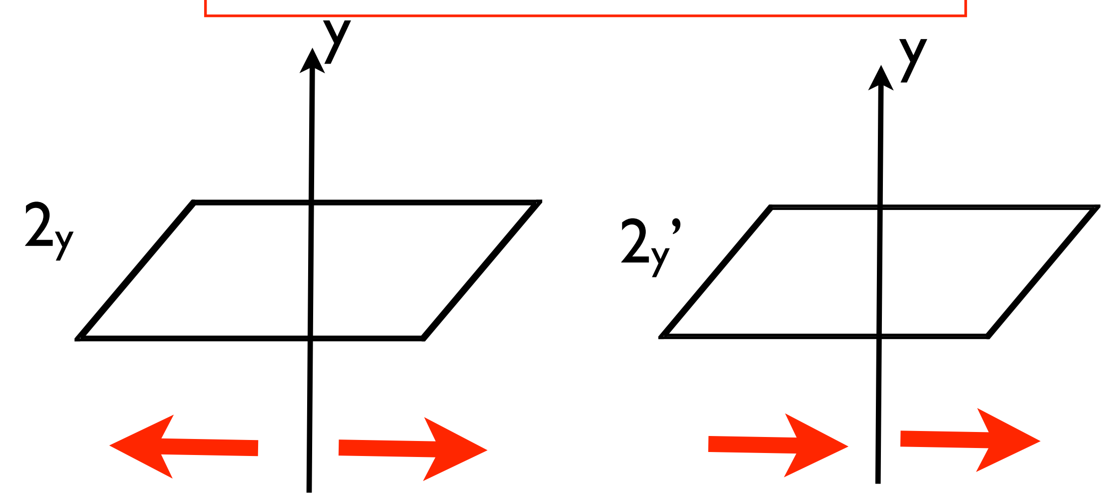

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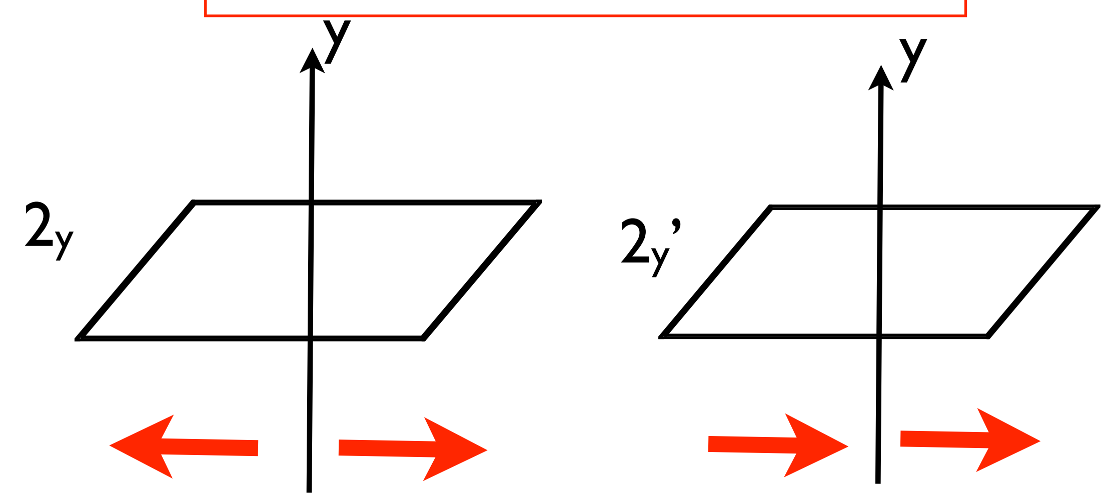

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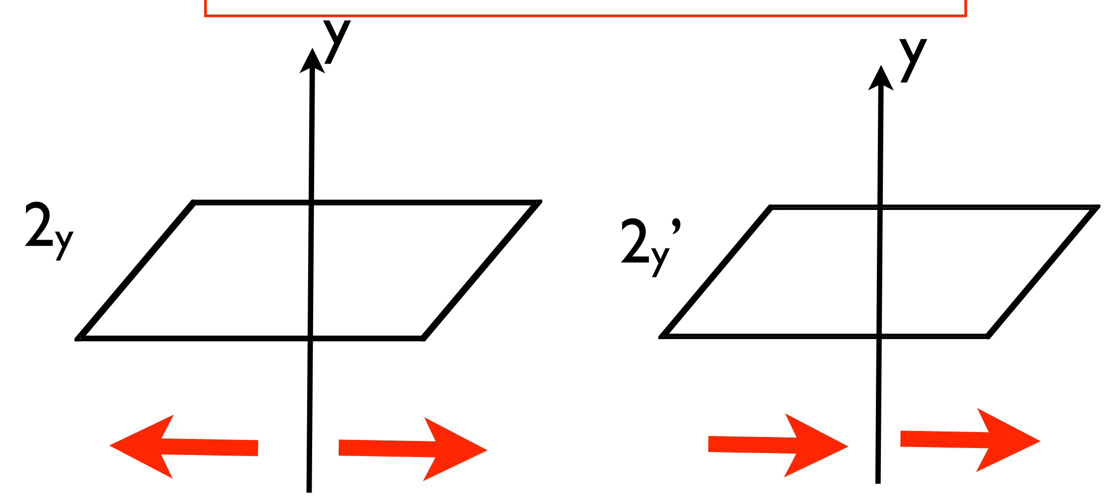

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1191 black/white magnetic groups that contain additional 'anti-elements' g'=($g \cdot R$) except g=1 (identity). <u>No primed 1'</u>

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Examples of Sh groups

59 <u>*Pmmn*</u>

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

62 <u>*Pnma*</u>

- $Pn'ma$
- $Pnm'a$
- $Pnma'$
- * $Pn'm'a$
- * $Pnm'a'$
- * $Pn'ma'$
- $Pn'm'a'$

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*$Pmm'n'$
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Ferromagnetic groups: point symmetry allows FM orientation of spins
Only 275 FM groups out of 1651...

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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′*
* *Pn′ma′*
Pn′m′a′

Ferromagnetic groups: point symmetry allows FM orientation of spins
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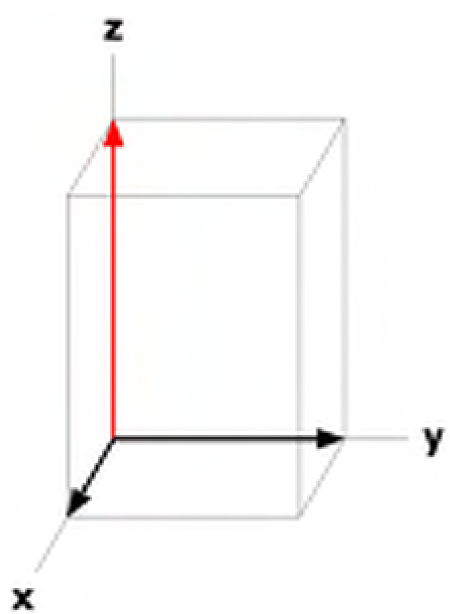
recap:
for ‘anti-elements’ g’=($g\cdot R$), $g\in G$
g can be a pure translation *t*, so *t’* gives centering/doubling



$P_{2c} = P_{a,b,2c}$
$t_\alpha = c = (0,0,1)$

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

I4/m, k=0 has 8 1D irreps τ_1,... τ_8.
4 real irreps <--> Shubnikov groups of *I4/m*
4 complex irreps

	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^-
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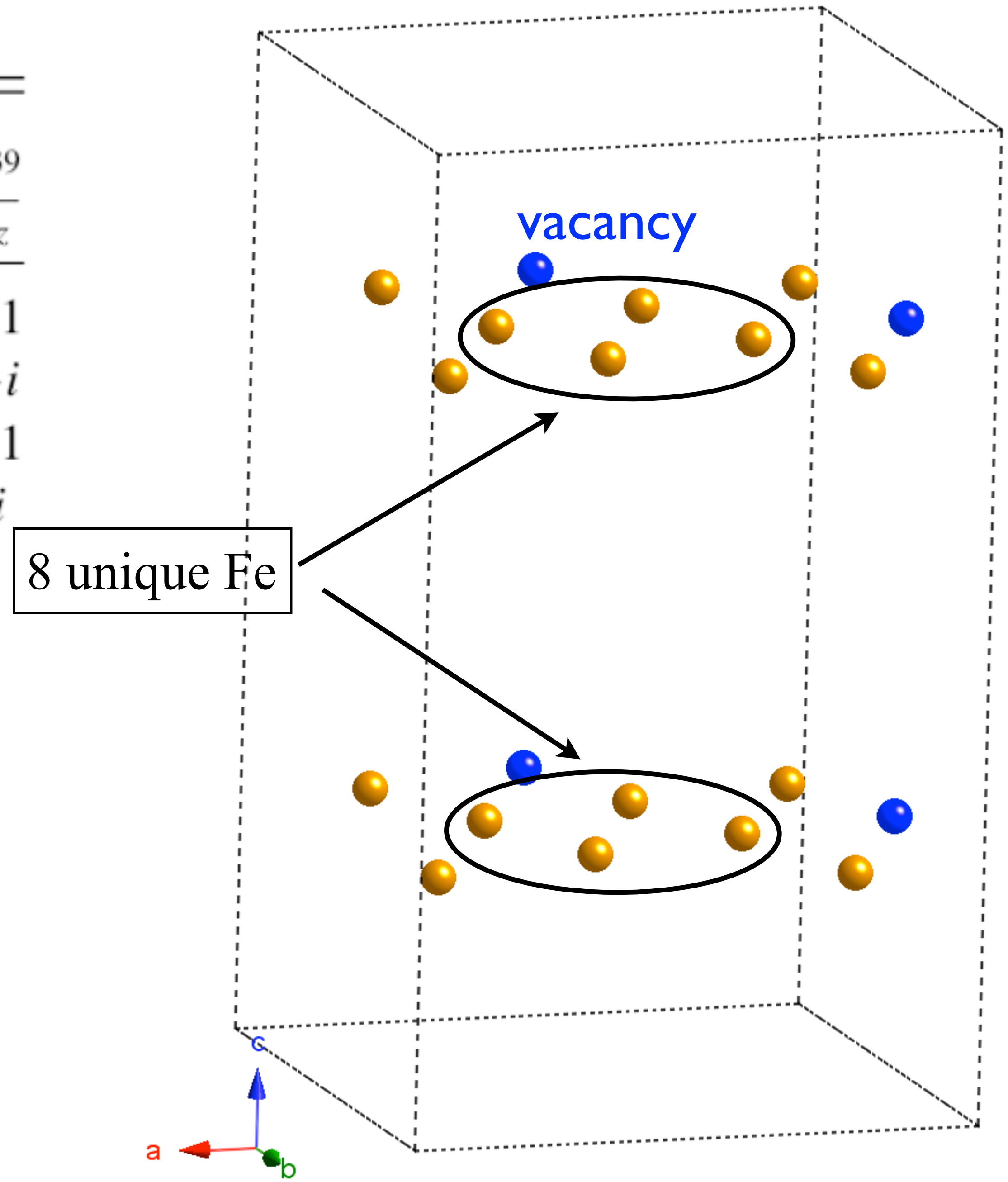
One unit cell with Fe



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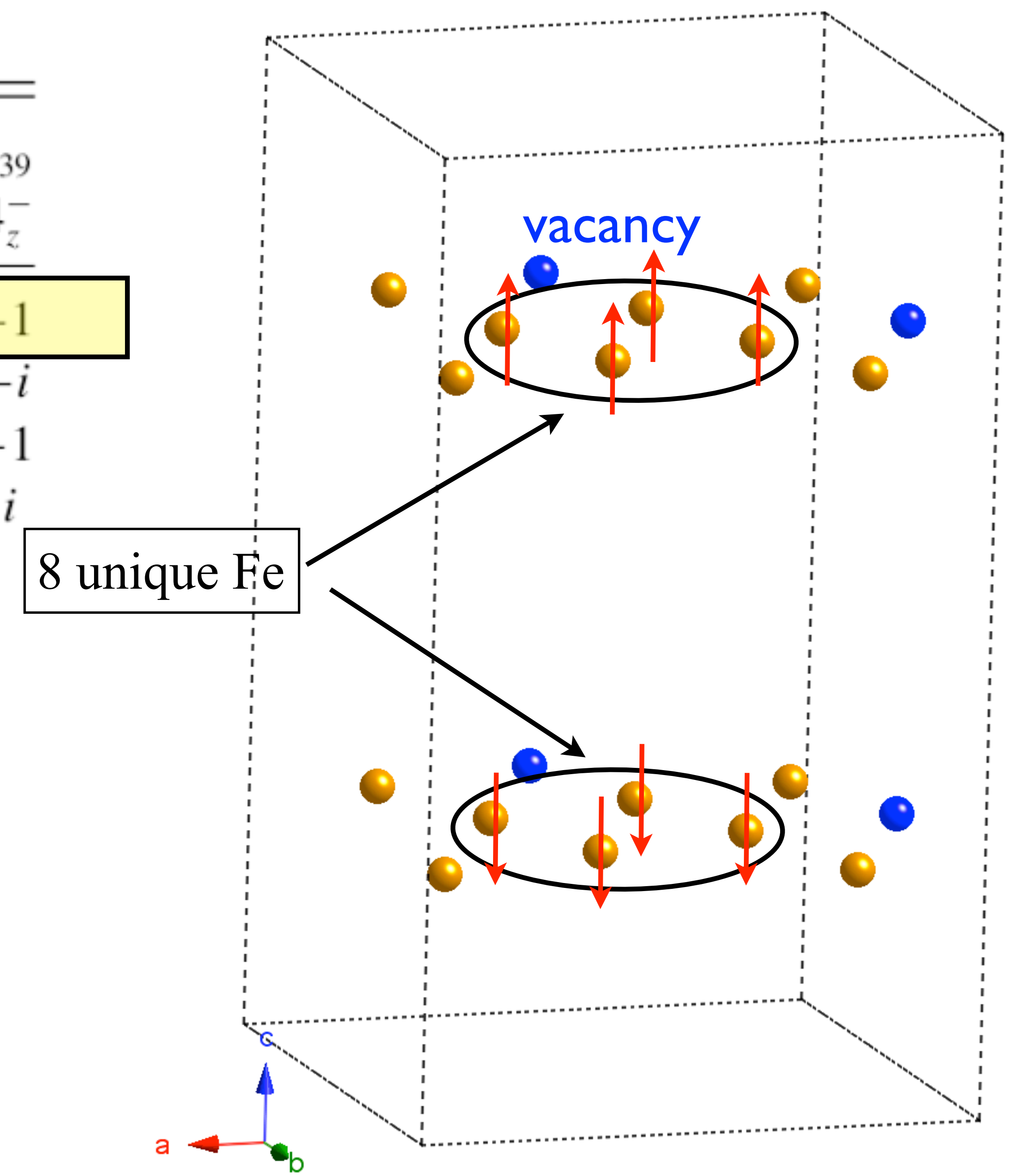

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there are no cubic ferromagnetic Sh-groups. "problems" with cubic ferromagnets Fe, Ni, EuO, EuS, ...
One can find lower symmetry ferromagnetic group, e.g. tetragonal Sh-group *I4/mm'm'* for Fe (*Im-3m*)

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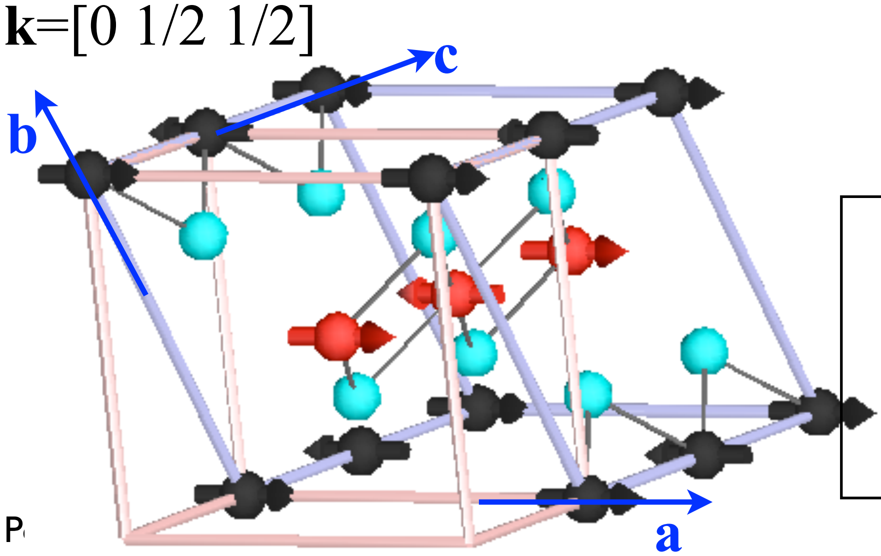
Example 2:
$CrCl_2$ orthorhombic space group: *Pnnm*.
No *Sh* group derived from *Pnnm* describes $CrCl_2$ magnetic structure
Cr-atoms in 2a-position
k=[0 1/2 1/2]

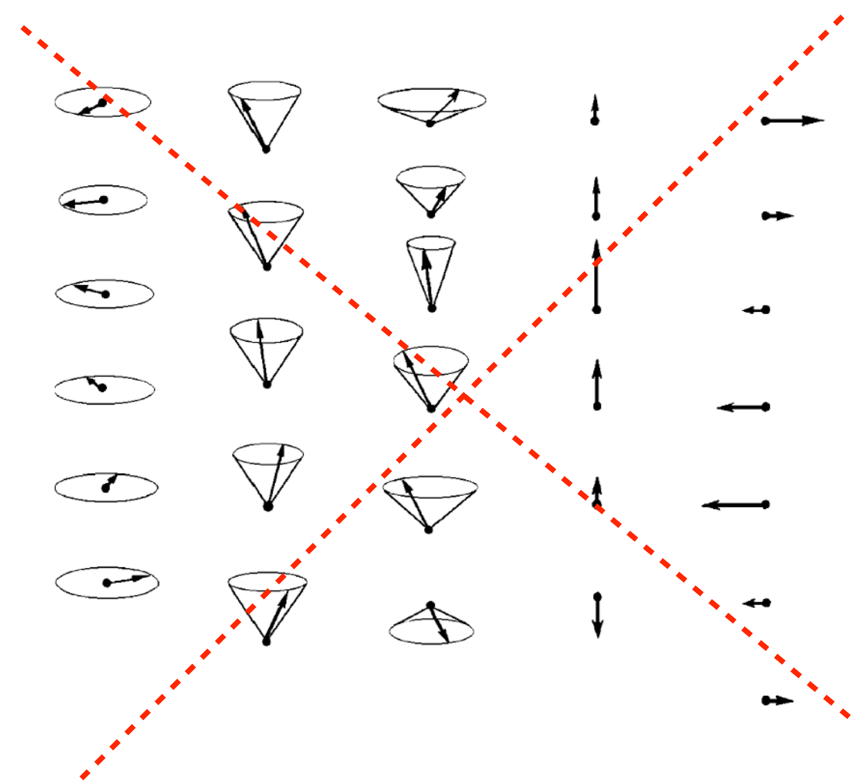


One can still find less symmetric *Sh* group triclinic $Sh^7_2=P_{2s}\bar{1}$;

~~“Disadvantages”~~ Specifics of Shubnikov Sh-group description

Specifics 1: *Sh* group that describes the magnetic structure is not necessarily made from the parent *G*.
Thus, it is not an ultimately practical...

Specifics 2: 3D *Sh* do not describe modulated structures.
* No rotations on non-crystallographic angle - no helix
* Linear orthogonal transformations preserve the spin size - no SDW



Example 1:
there are no cubic ferromagnetic Sh-groups. “problems” with cubic ferromagnets Fe, Ni, EuO, EuS, ...
One can find lower symmetry ferromagnetic group, e.g. tetragonal Sh-group *I4/mm’m’* for Fe (*Im-3m*)

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$CrCl_2$ orthorhombic space group: *Pnnm*.
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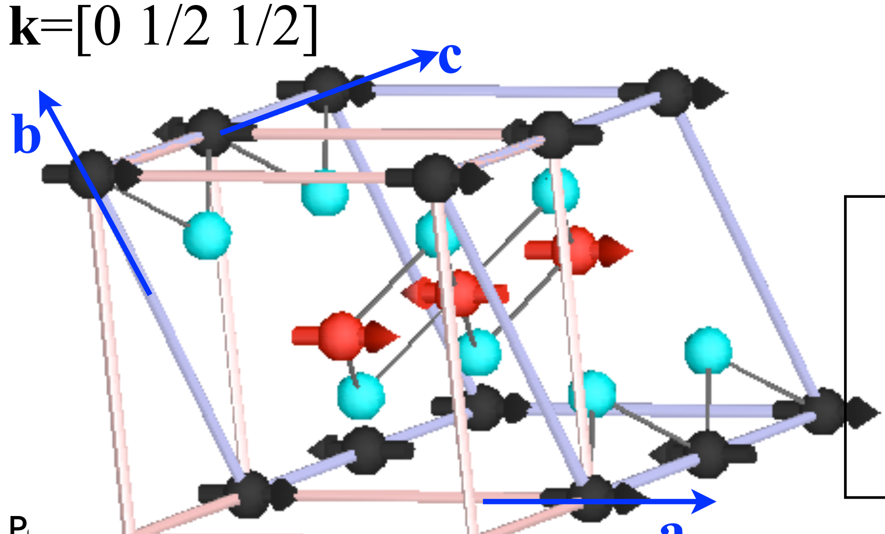

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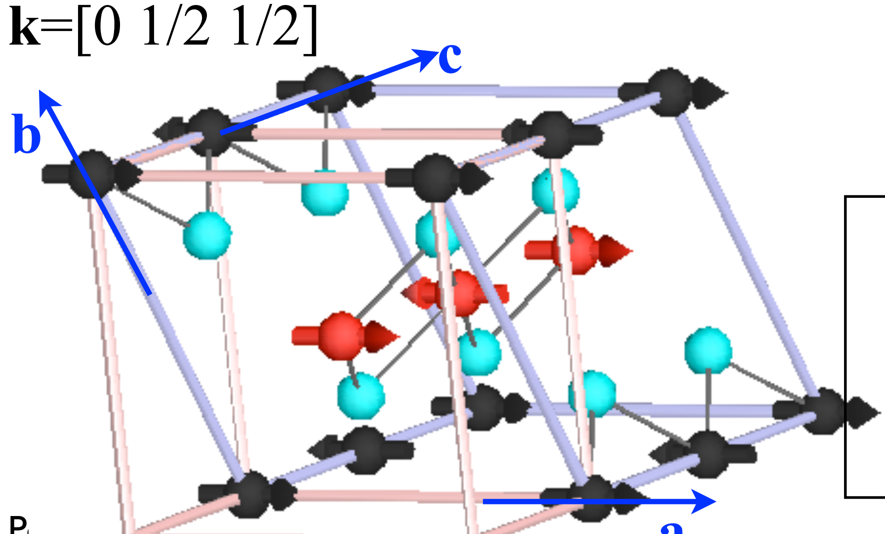

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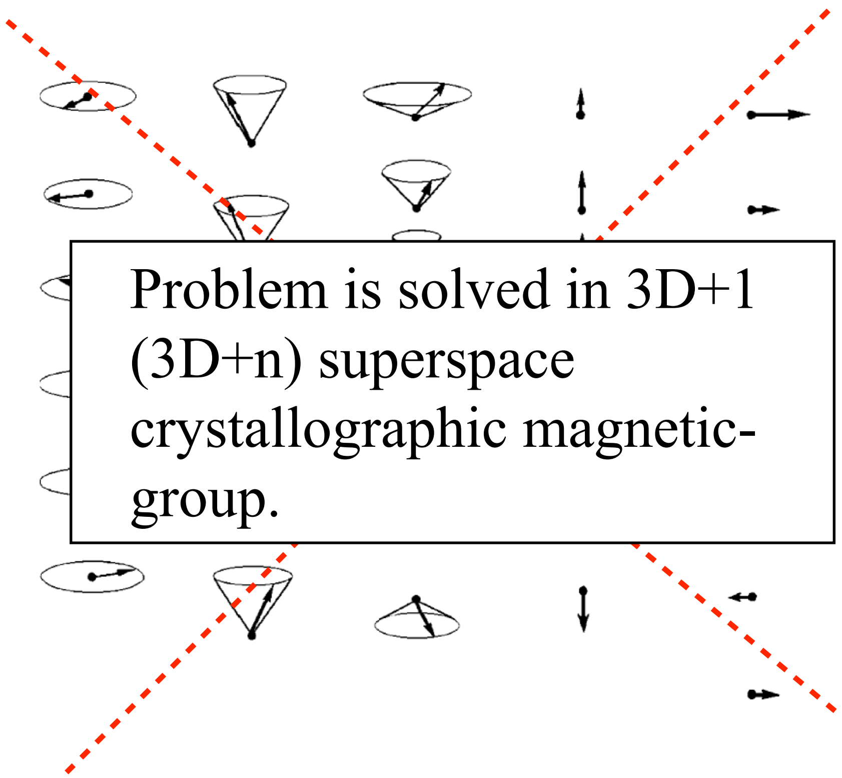

Problem is solved in 3D+1 (3D+n) superspace crystallographic magnetic-group.

Introduction to representation theory with relatively simple example of magnetic representation. Classification of magnetic structures by irreducible representations irreps of group

Why irreducible representations of space group is so important for magnetic structure?

Symmetry in QM

$\hat{H}(\mathbf{r})$, $\mathbf{r} = (r_1, r_2, r_3, \ldots r_n)$, vector space with dimension n
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$$\hat{H}\psi_v = E_v\psi_v \quad \Rightarrow E_v,\ \psi_v{}^1,\ \psi_v{}^2,\ \ldots\ \psi_v{}^{l_v}$$

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E_v, $\psi_v^{\,lv}$ can be classified by irreps $\tau_{ij}^{\,v}$ degeneracy l_v is ≥ dimension of $\tau_{ij}^{\,v}$

!

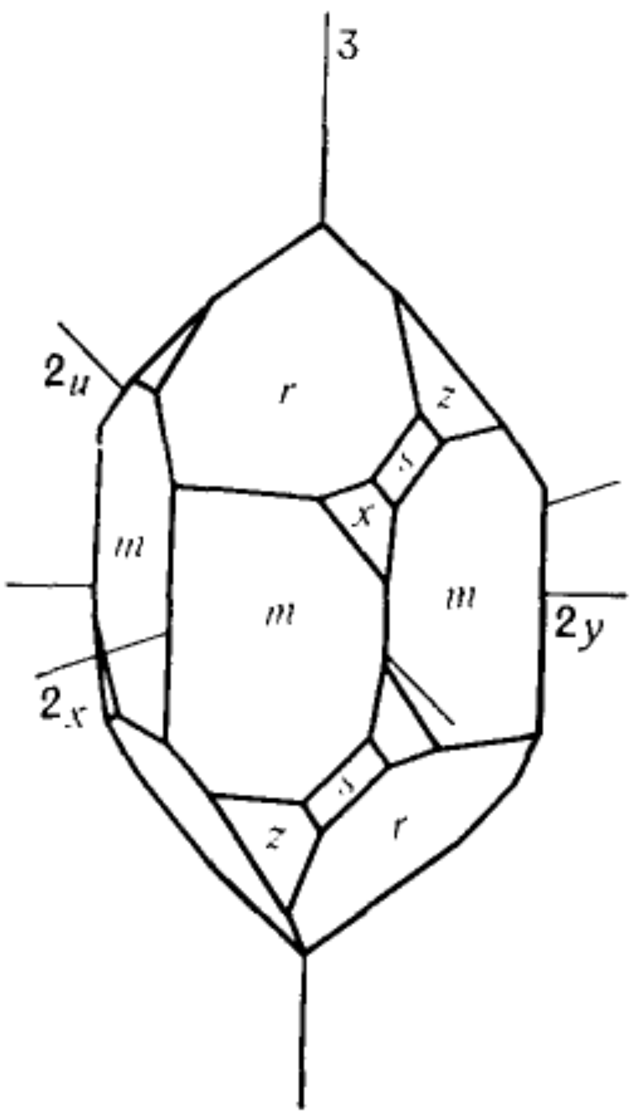
For example:
* Crystal field splitting
* Molecular vibrations
* Phonons
* Magnetic structure
... e.v.

rep $\Rightarrow_{\Sigma_\oplus}$ irreps: $T_{ij} = \sum_{\oplus} n_\nu \tau_{ij}^{\nu}$

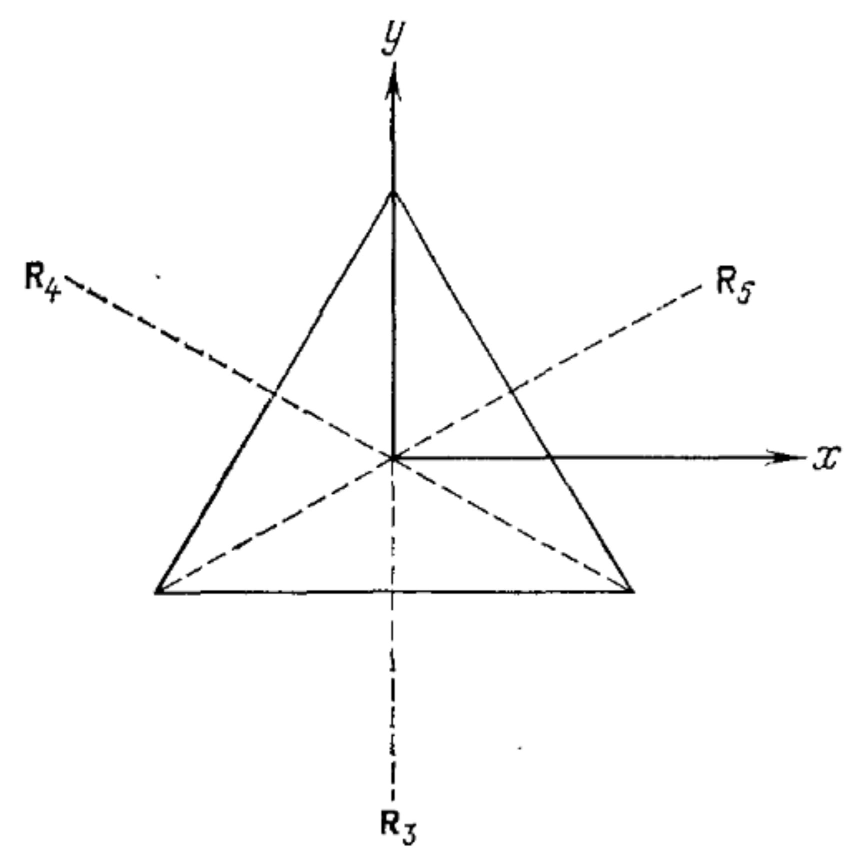
τ_{ij}^1	0	0	0
0	τ_{ij}^1	0	0
0	0	τ_{ij}^2	0
0	0	0	...

Example: point group 32

Point group Hermann–Mauguin symbol *32* (D_3 Schoenflies symbol)
e.g Quartz



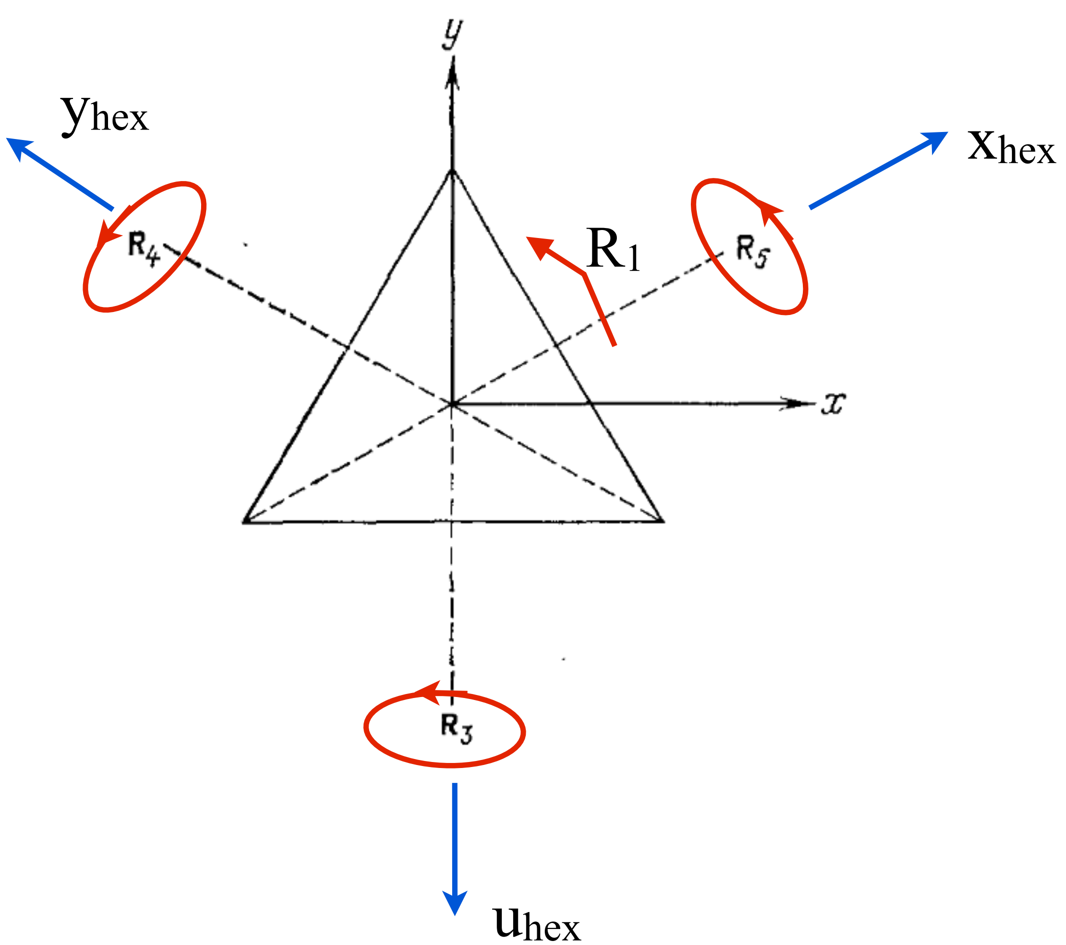
or regular triangle



Multiplication table, isomorphism

Point group 32 (D_3 Schoenflies symbol)
e.g regular triangle

6 symmetry elements (rotations):
R0=E, $R_1=2\pi/3$, $R_2=4\pi/3$ around z, R_3, R_4, R_5, = π around resp.
hex ⟶ 1 3^1 3^2 2_u 2_y 2_x axes in xy-plane



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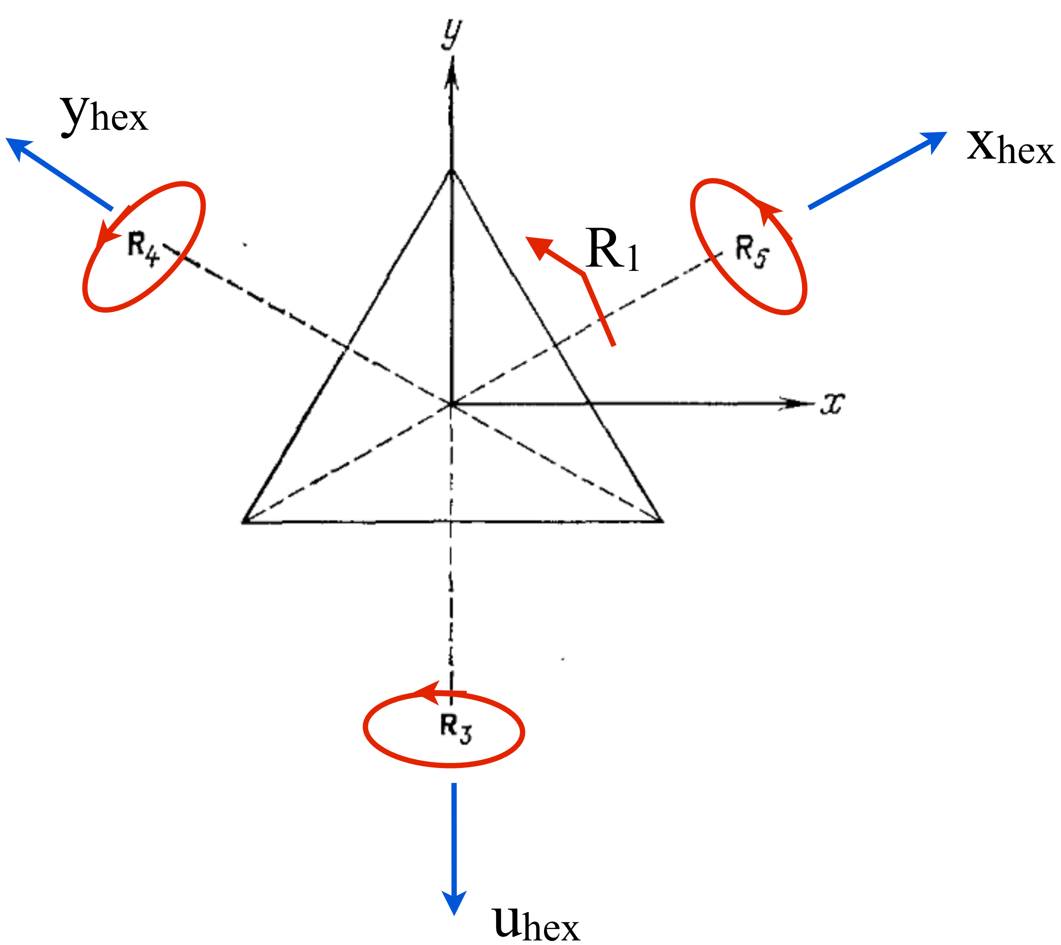

multiplication table

	g_1	g_2	$\cdots$	g_n
g_1	g_1^2	g_1g_2	$\cdots$	g_1g_n
g_2	g_2g_1	g_2^2	$\cdots$	g_2g_n
$\vdots$	$\vdots$	$\vdots$		$\vdots$
g_n	g_ng_1	g_ng_2		g_n^2

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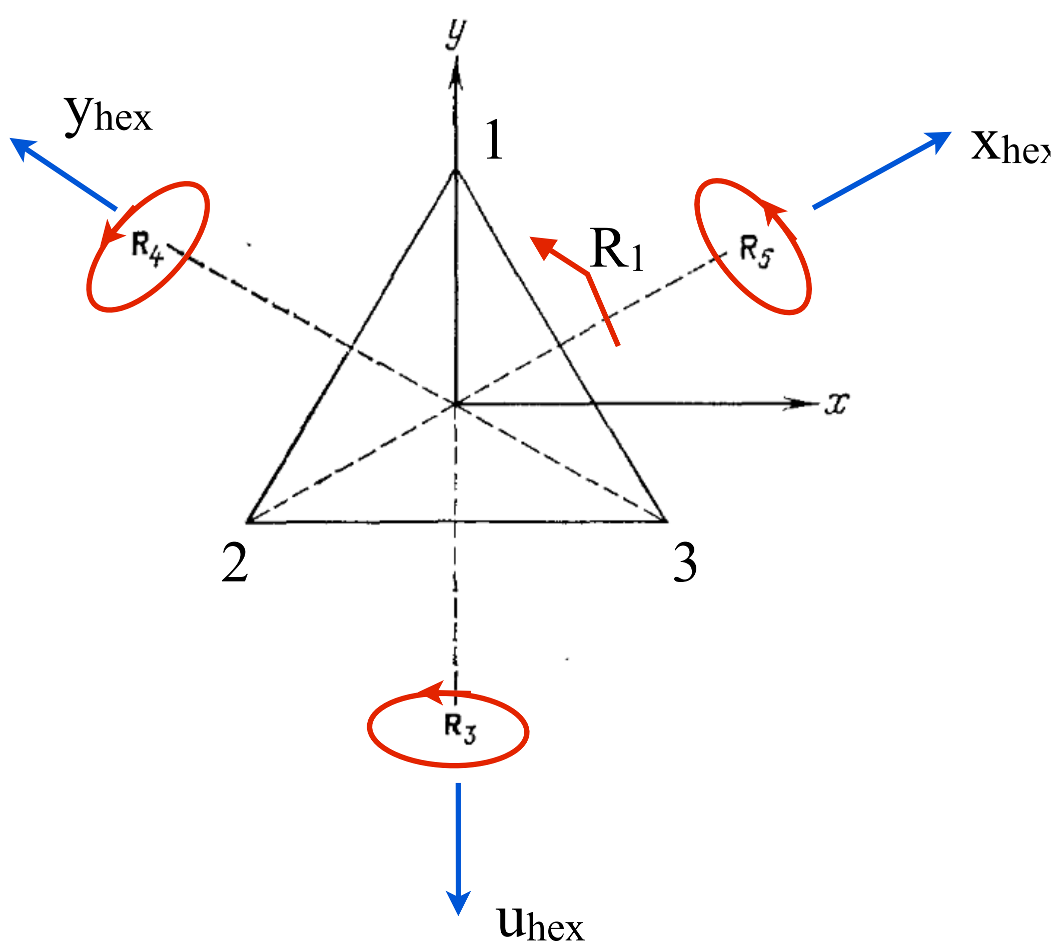
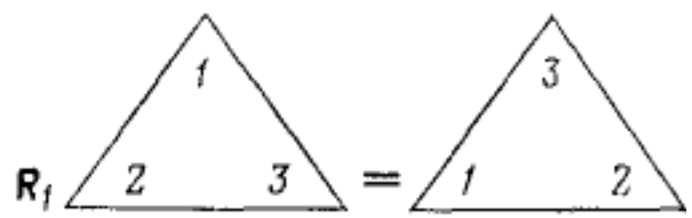
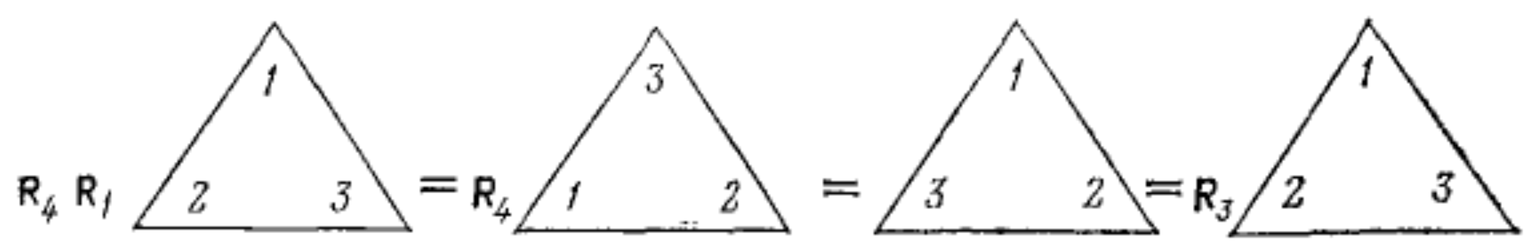
hex $\longrightarrow$ 1 3^1 3^2 2_u 2_y 2_x

multiplication table

	g_1	g_2	$\cdots$	g_n
g_1	g_1^2	$g_1 g_2$	$\cdots$	$g_1 g_n$
g_2	$g_2 g_1$	g_2^2	$\cdots$	$g_2 g_n$
$\vdots$	$\vdots$	$\vdots$		$\vdots$
g_n	$g_n g_1$	$g_n g_2$		g_n^2







$R_4 R_1 = R_3$

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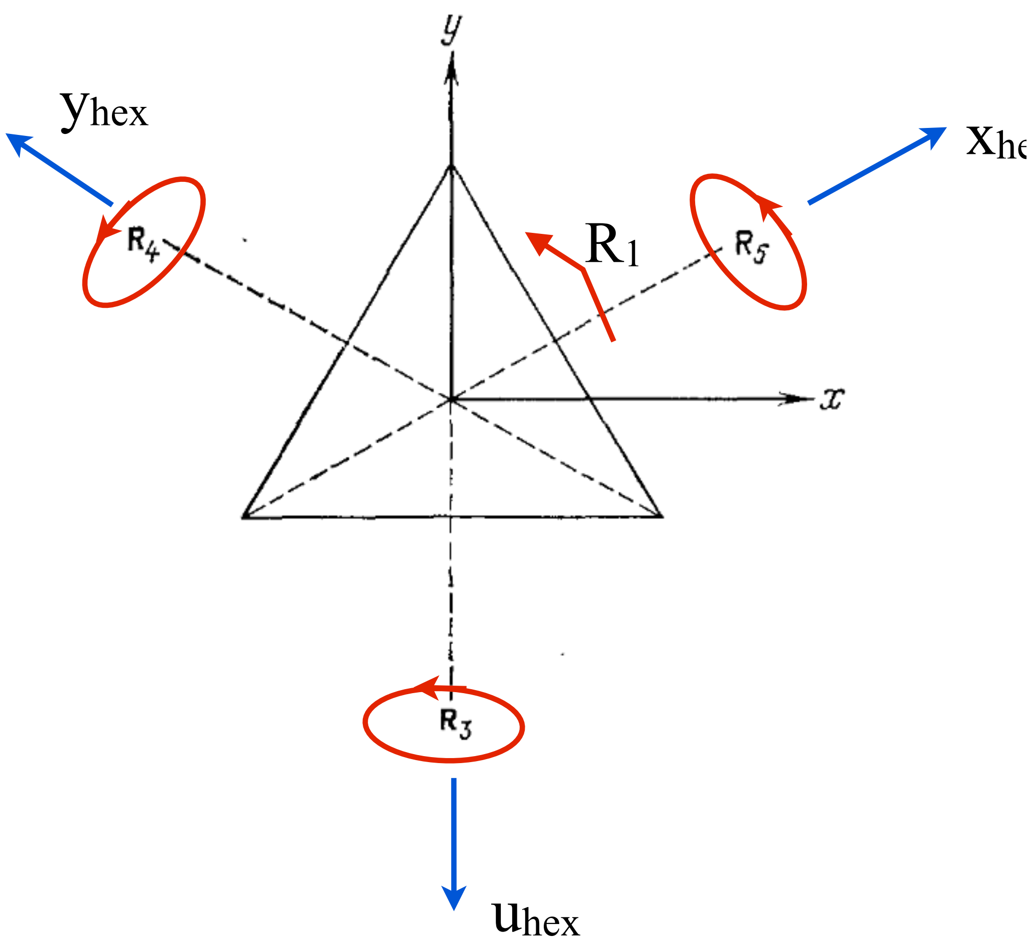

hex →	1	3^1	3^2	2_u	2_y	2_x
G_a \ G_b	E	R_1	R_2	R_3	R_4	R_5
E	E	R_1	R_2	R_3	R_4	R_5
R_1	R_1	R_2	E	R_4	R_5	R_3
R_2	R_2	E	R_1	R_5	R_3	R_4
R_3	R_3	R_5	R_4	E	R_2	R_1
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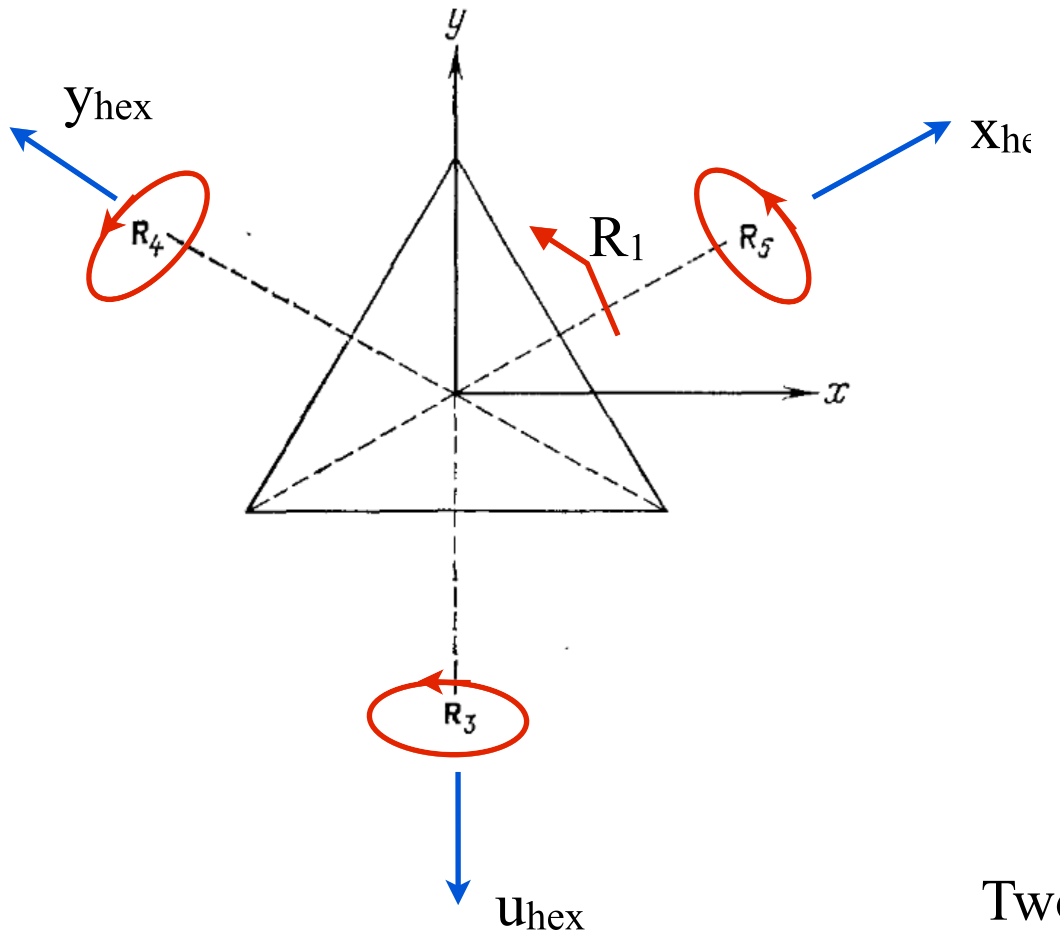

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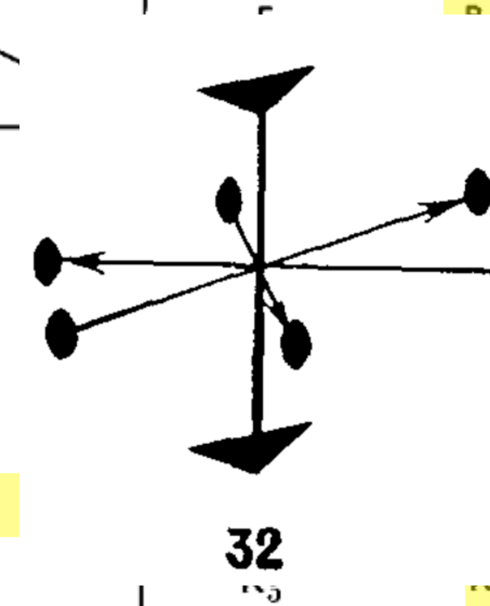
G_a \ G_b	E	R_1	R_2	R_3	R_4	R_5
E	[illegible]	[illegible]	[illegible]	[illegible]	R_4	R_5
R_1	[illegible]	[illegible]	[illegible]	[illegible]	R_5	R_3
R_2	[illegible]	[illegible]	[illegible]	[illegible]	R_3	R_4
R_3	[illegible]	[illegible]	[illegible]	[illegible]	R_2	R_1
R_4	[illegible]	[illegible]	[illegible]	[illegible]	E	R_2
R_5	R_5	R_4	R_3	R_2	R_1	E



Two groups are **isomorphous** if they have the same multiplication table
Quartz *32* D_3
Ammonia molecule *3m* C_{3v}

Group representations: formal definition

If we can find **a set of square matrices** (in general linear operators) T(g_a) in a **vector space *L*,** which correspond to the elements g_a of group *G* and have the same multiplication table, i.e. T(g_a) T(g_b)= T(g_a g_b) then this set of matrices is said to form a matrix **'representation'** of the group *G* in space *L*.

n matrices *l*x*l*. *n* is order of *G*

multiplication table

	g_1	g_2	$\cdots$	g_n
g_1	g_1^2	g_1g_2	$\cdots$	g_1g_n
g_2	g_2g_1	g_2^2	$\cdots$	g_2g_n
$\cdot$	$\cdot$	$\cdot$		$\cdot$
$\cdot$	$\cdot$	$\cdot$		$\cdot$
$\cdot$	$\cdot$	$\cdot$		$\cdot$
g_n	g_ng_1	g_ng_2		g_n^2

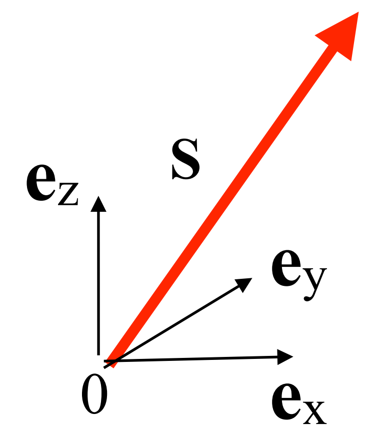
$$T(g_1) = \begin{pmatrix} t^1_{11} & t^1_{12} & t^1_{13} & \ldots & t^1_{1l} \\ t^1_{21} & t^1_{22} & t^1_{23} & \ldots & t^1_{2l} \\ . & . & . & & . \\ . & . & . & & . \\ . & . & . & & . \\ t^1_{l1} & t^1_{l2} & t^1_{l3} & \ldots & t^1_{ll} \end{pmatrix}, T(g_2) = \begin{pmatrix} t^2_{11} & t^2_{12} & t^2_{13} & \ldots & t^2_{1l} \\ t^2_{21} & t^2_{22} & t^2_{23} & \ldots & t^2_{2l} \\ . & . & . & & . \\ . & . & . & & . \\ . & . & . & & . \\ t^2_{l1} & t^2_{l2} & t^2_{l3} & \ldots & t^2_{ll} \end{pmatrix}, T(g_3) = \ldots$$

Dimension of representation is equal to the dimension of the vector space

Linear vector spaces

3-dimensional space of particle displacement (or magnetic moment)

$$\mathbf{s} = \sum_{j=x,y,z} s_j \mathbf{e}_j$$



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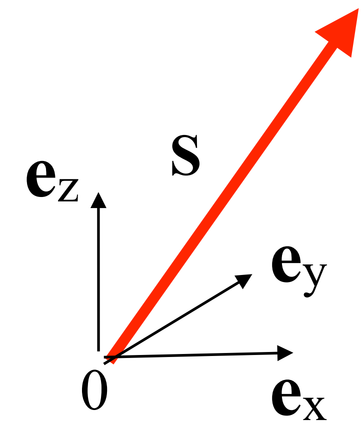
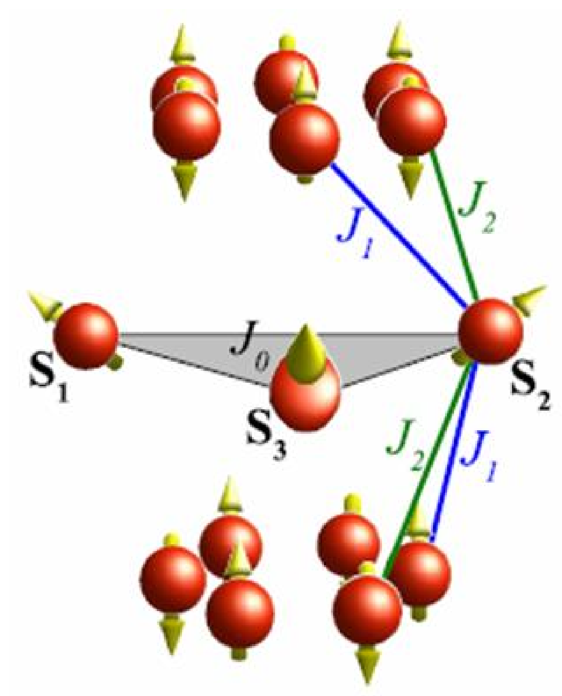


3N-dimensional space of all possible displacements (or magnetic moments)
Function ψ is defined on N discreet points

$$\psi = \sum_{n=1}^{N} \sum_{j=x,y,z} s_{jn} \mathbf{e}_{jn}$$

$$\begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \cdots \\ \cdots \\ \cdots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$$



Induced representation of group in "magnetic" linear space.

To construct the representation one has to know the rules of transformations of the vector in LS under group symmetry elements.

3N-dimensional space of magnetic moments defined on N discreet points

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3N by 3N matrices given by group transformations different ψ-vectors form a magnetic representation of group.

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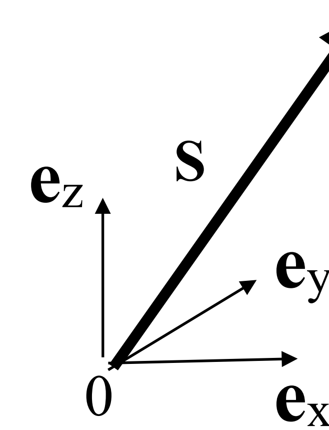
<u>We split the problem:</u>

1. 3D space of spin rotations
2. N-dimentional space of positions/sites

Point groups. Classical spin rotations in 3D space

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



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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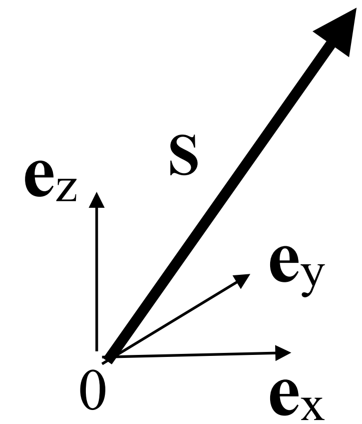

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For improper rotations such as inversion (I) or mirror plane we should remember that spin is an axial vector.

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

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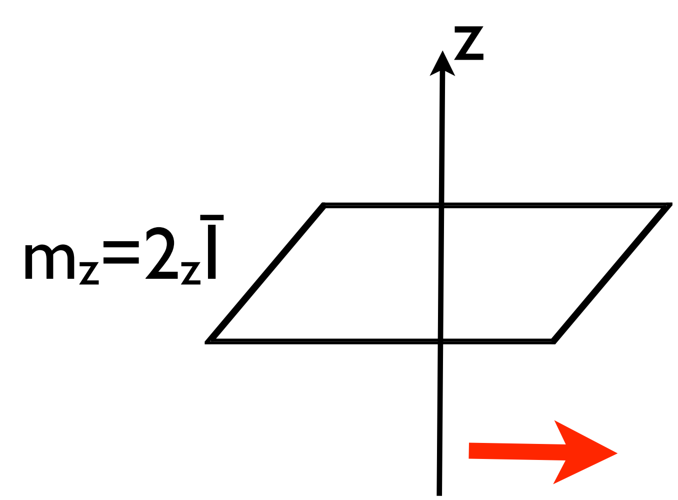

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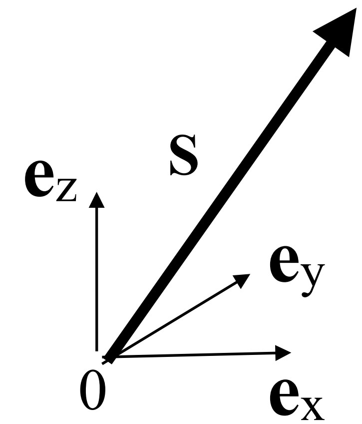

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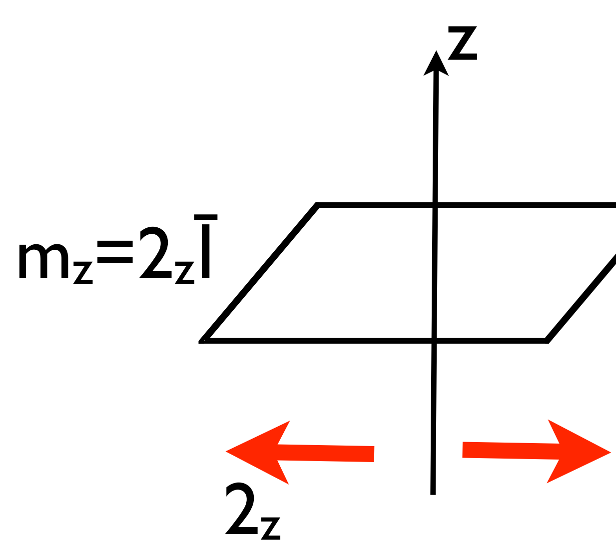

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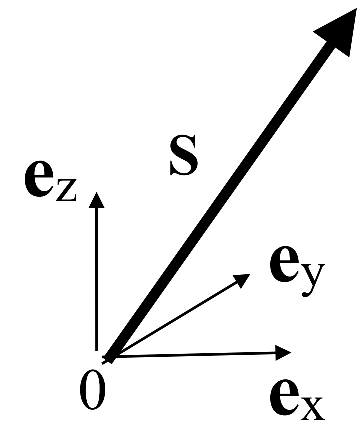

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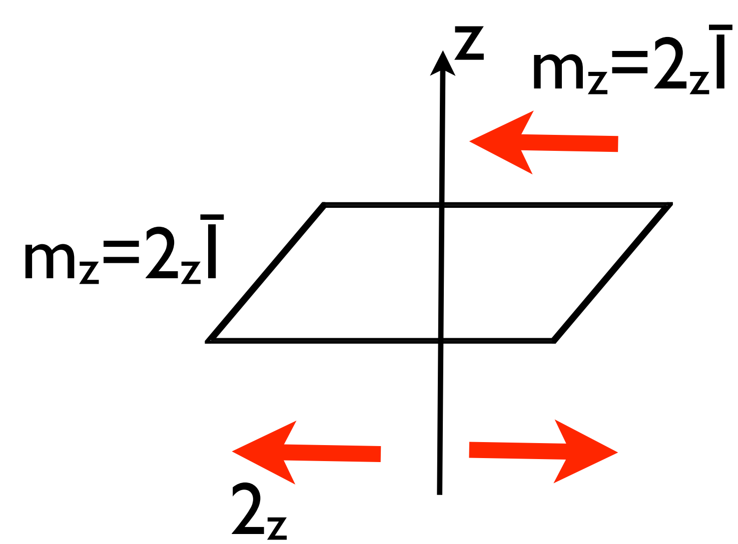
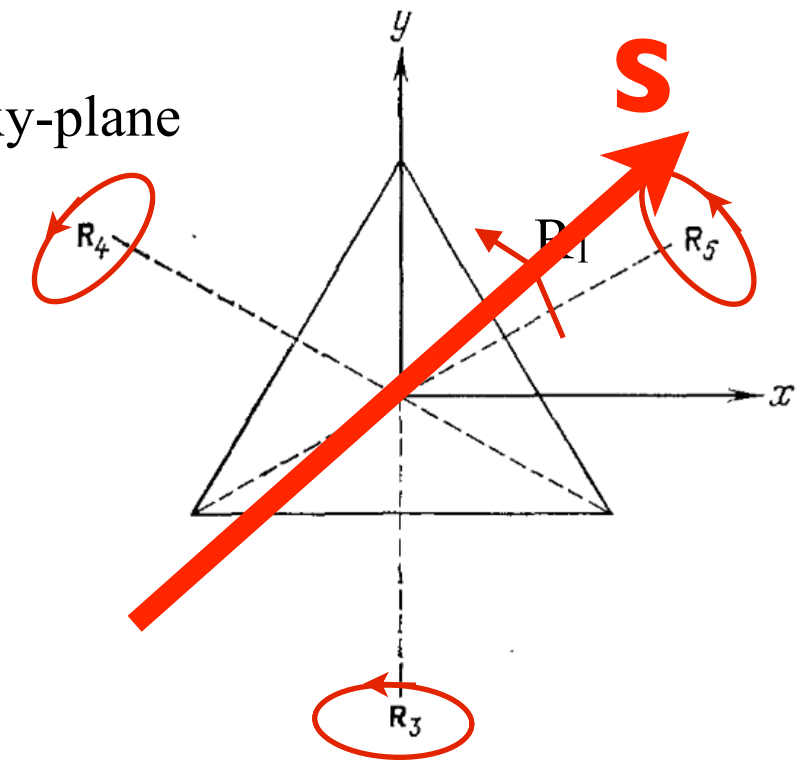


Induced representation of Point group 32 in 3D rotation space of spin S

6 symmetry elements (rotations):
R0=E, $R_1=2\pi/3$, $R_2=4\pi/3$ around z, R_3, R_4, R_5, = π around resp. axes in xy-plane



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1. **3-**dimensional representation

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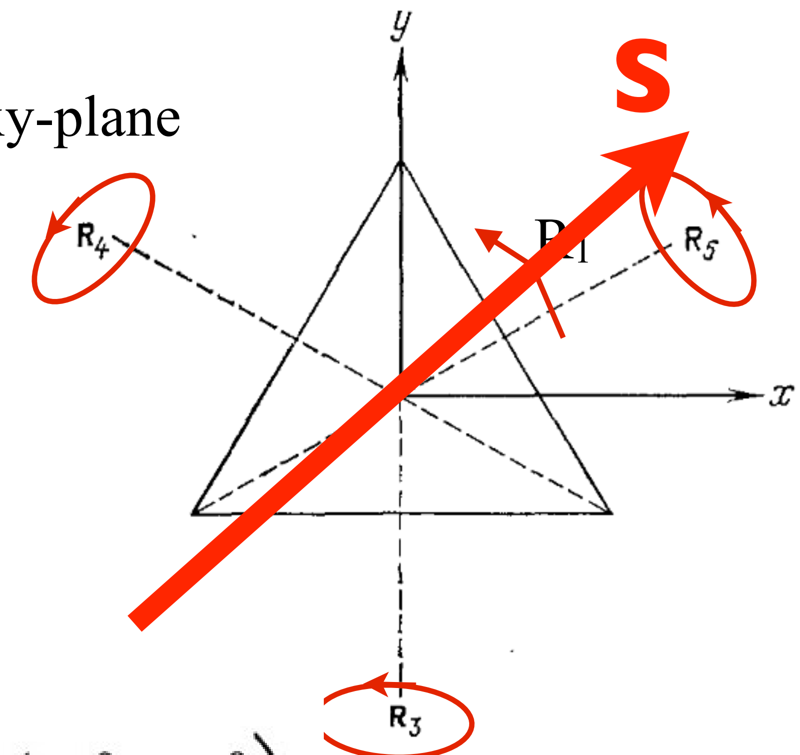


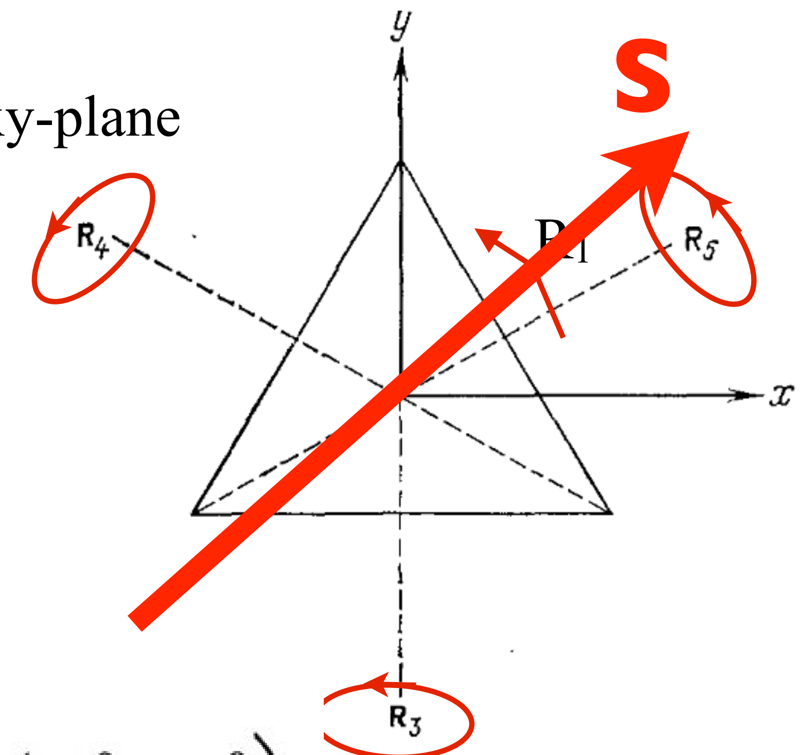
$$\varphi_z \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

1. **<u>3-</u>**dimensional representation

$$T(R_1) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} & 0 \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(R_2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} & 0 \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(R_3) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \text{ ... etc}$$

Induced representation of Point group 32 in 3D rotation space of spin S

6 symmetry elements (rotations):
R0=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



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

1. **3-**dimensional representation

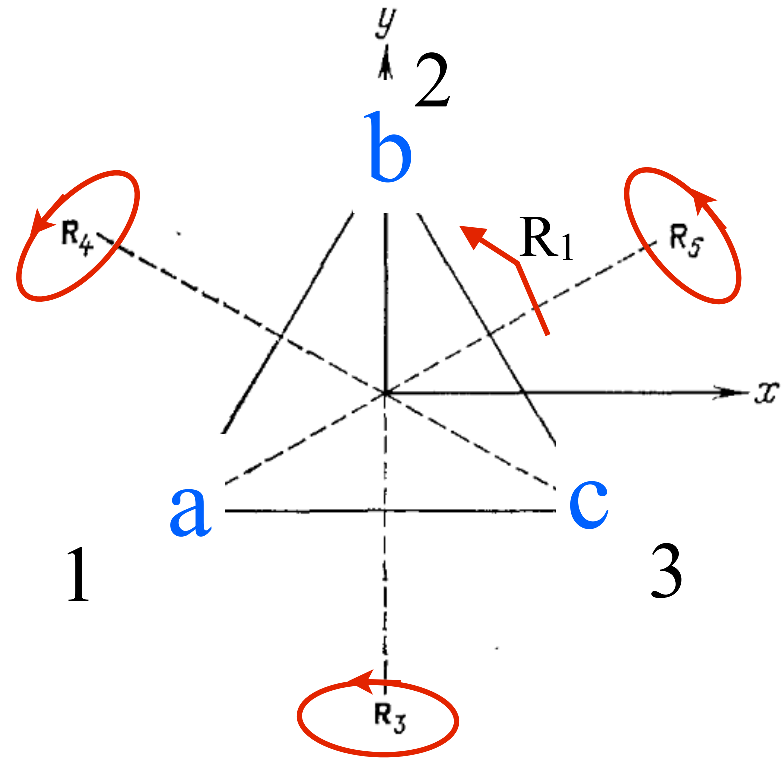
$$T(R_1) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} & 0 \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(R_2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} & 0 \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(R_3) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \text{ ... etc}$$

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

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

Representation in sites space for point group 32

6 symmetry elements (rotations):
R0=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-plar



Let us assume we have 3 atoms/spins a, b, c in the sites 1,2,3
3-dimensional linear space of atom/spin sites.
Note, not the 3D xyz, but labeled sites.

Representation in sites space for point group 32

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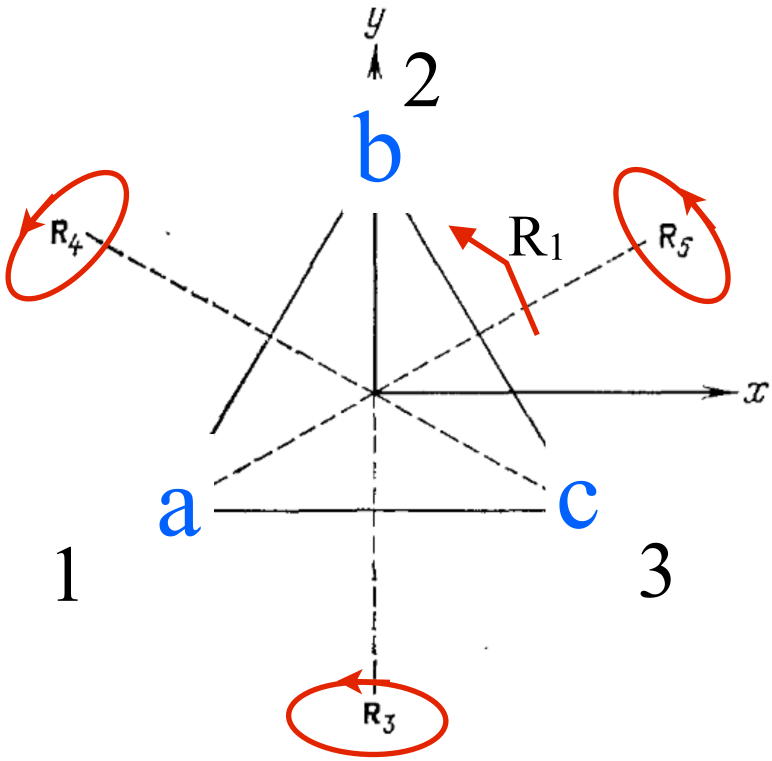

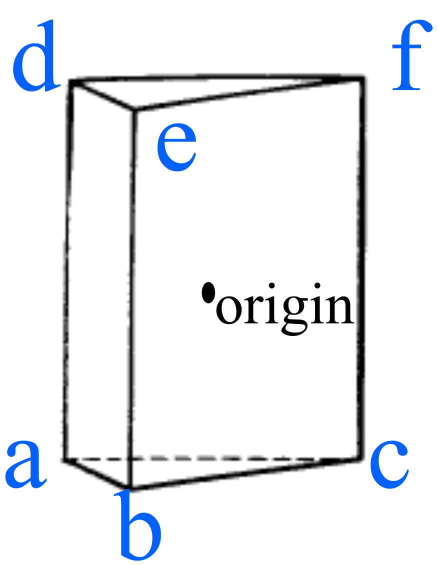

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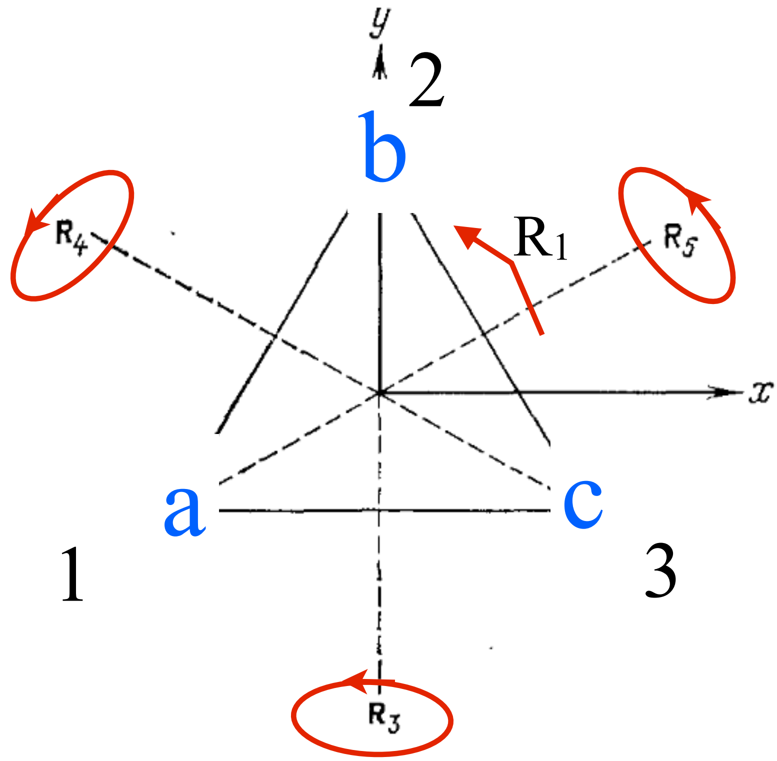

element R_1 permutes the atoms

$b \Rightarrow a$

$c \Rightarrow b$

$a \Rightarrow c$

Representation in sites space for point group 32

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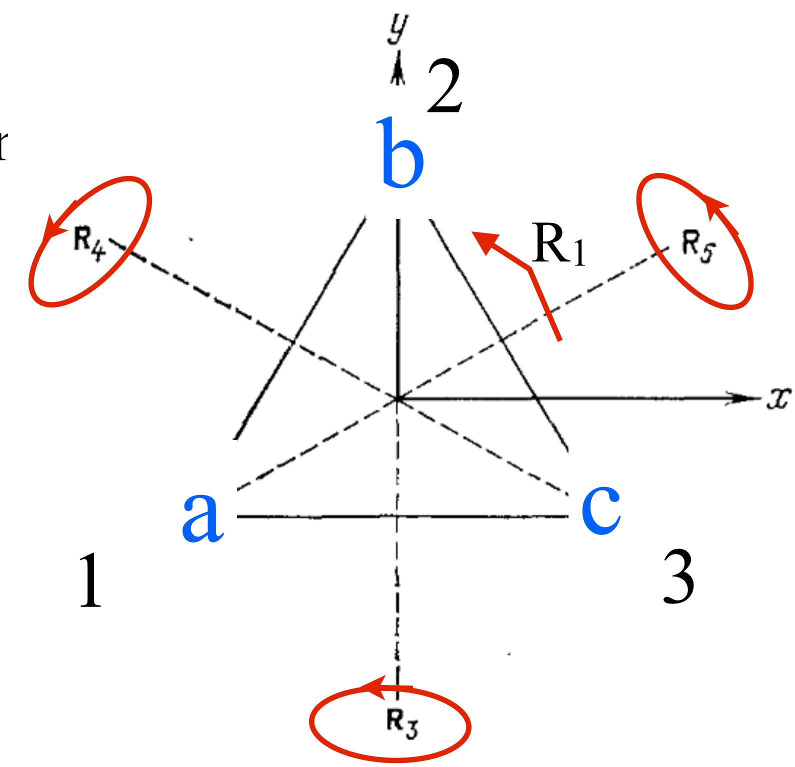

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b ⇒ a
c ⇒ b
a ⇒ c

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

Representation in sites space for point group 32

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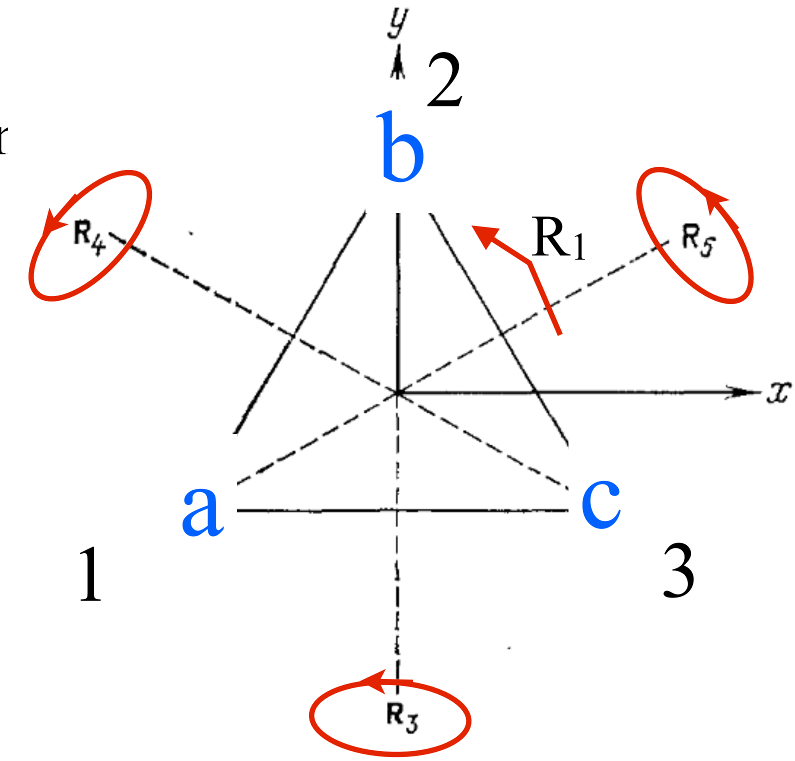

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b ⇒ a
c ⇒ b
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$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} b \\ c \\ a \end{pmatrix}$$

Representation in sites space for point group 32

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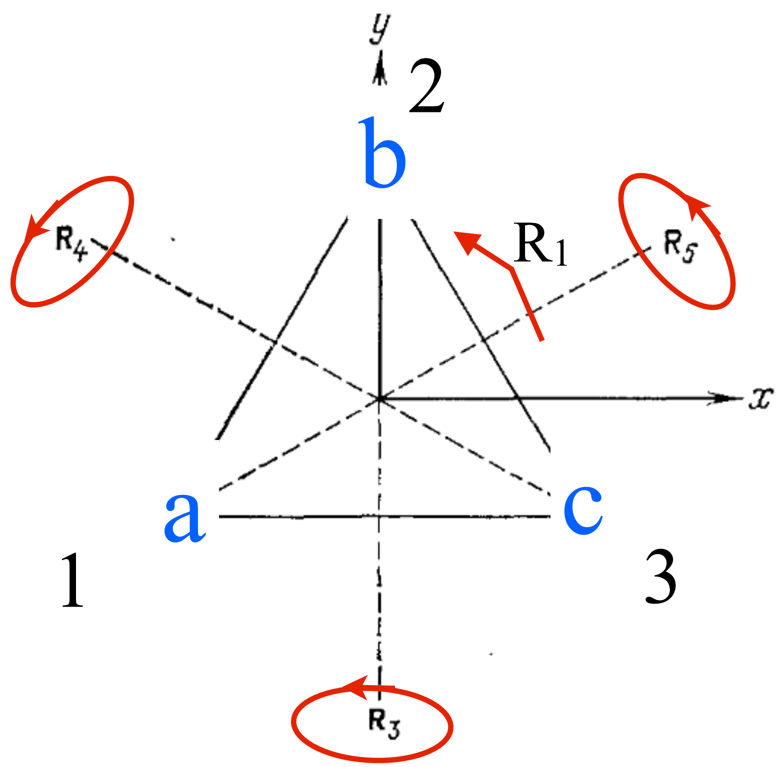

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$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} b \\ c \\ a \end{pmatrix}$$

permutation (n=3) representation of group 32

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Product of two representations of group

Direct (tensor) matrix product

$$U \otimes V = \begin{bmatrix} u_{1,1}V & u_{1,2}V & \cdots \\ u_{2,1}V & u_{2,2}V & \\ \vdots & & \ddots \end{bmatrix} = \begin{bmatrix} u_{1,1}v_{1,1} & u_{1,1}v_{1,2} & \cdots & u_{1,2}v_{1,1} & u_{1,2}v_{1,2} & \cdots \\ u_{1,1}v_{2,1} & u_{1,1}v_{2,2} & & u_{1,2}v_{2,1} & u_{1,2}v_{2,2} & \\ \vdots & & \ddots & & & \\ u_{2,1}v_{1,1} & u_{2,1}v_{1,2} & & & & \\ u_{2,1}v_{2,1} & u_{2,1}v_{2,2} & & & & \\ \vdots & & & & & \end{bmatrix}.$$

(U: dimension m; V: n)

gives a new rep with dimension m×n and new vector space!

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dimension *m* (of U), *n* (of V)

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$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

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$$\begin{bmatrix} 1&0&0\\0&1&0\\0&0&1 \end{bmatrix} \begin{bmatrix} 0&1&0\\0&0&1\\1&0&0 \end{bmatrix} \begin{bmatrix} 0&0&1\\1&0&0\\0&1&0 \end{bmatrix} \begin{bmatrix} 0&1&0\\1&0&0\\0&0&1 \end{bmatrix} \begin{bmatrix} 0&0&1\\0&1&0\\1&0&0 \end{bmatrix} \begin{bmatrix} 1&0&0\\0&0&1\\0&1&0 \end{bmatrix}$$

$\otimes$

Rotation matrices for point group 32

$$T(R_1) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} & 0 \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(R_2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} & 0 \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(R_3) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

... etc

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dimension *m* (U), *n* (V)

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$$\begin{bmatrix} 1&0&0\\0&1&0\\0&0&1 \end{bmatrix} \begin{bmatrix} 0&1&0\\0&0&1\\1&0&0 \end{bmatrix} \begin{bmatrix} 0&0&1\\1&0&0\\0&1&0 \end{bmatrix} \begin{bmatrix} 0&1&0\\1&0&0\\0&0&1 \end{bmatrix} \begin{bmatrix} 0&0&1\\0&1&0\\1&0&0 \end{bmatrix} \begin{bmatrix} 1&0&0\\0&0&1\\0&1&0 \end{bmatrix}$$

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... etc

= 9 by 9 matrices: 9 dimensional representation in LS

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

Reducibility

A study of possible representations of even a simple group like D_3 seems to be a scaring task...

$$T(R_1) = \begin{pmatrix} 0 & 0 & 0 & -1/2 & -1/2\sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2\sqrt{3} & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1/2 & -1/2\sqrt{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/2\sqrt{3} & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -1/2 & -1/2\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/2\sqrt{3} & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad T(R_3) = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Reducibility

A study of possible representations of even a simple group like D_3 seems to be a scaring task...

BUT!

All representations can be built up from a finite number of ‘distinct‘ irreducible representations. There is an easy way of finding the decomposition.

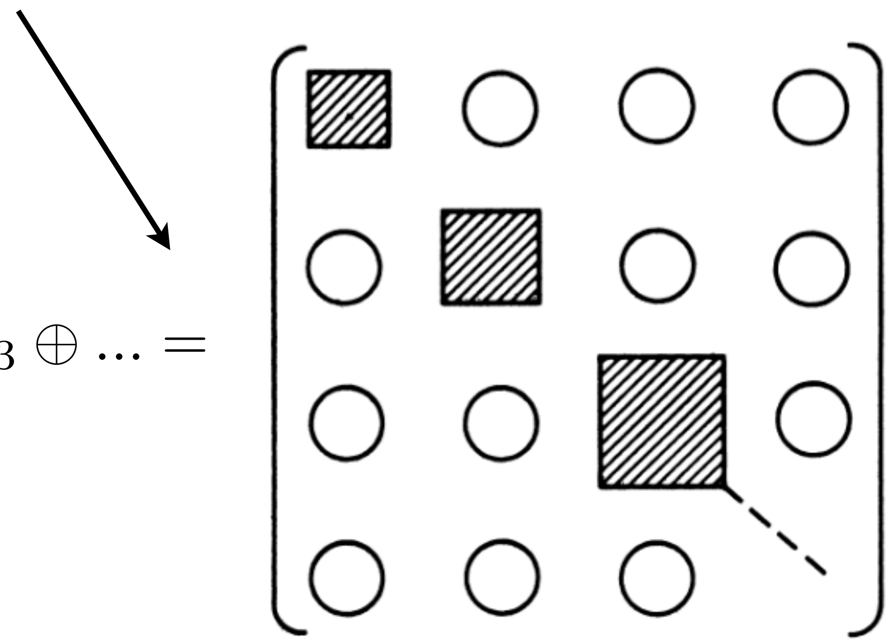
$$T(R_1) = \begin{pmatrix} 0 & 0 & 0 & -1/2 & -1/2\sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2\sqrt{3} & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1/2 & -1/2\sqrt{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/2\sqrt{3} & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -1/2 & -1/2\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/2\sqrt{3} & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad T(R_3) = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

representation is reducible!

Reduction of any representation of group to block diagonal shape

Representation (dimension=n) of a group G in linear space L is reducible to a block-diagonal shape that is a direct sum of irreducible square matrices τ_1, τ_2, ... For each element G_a the representation has the shape:

$$\tau_1 \oplus \tau_2 \oplus \tau_3 \oplus ... =$$



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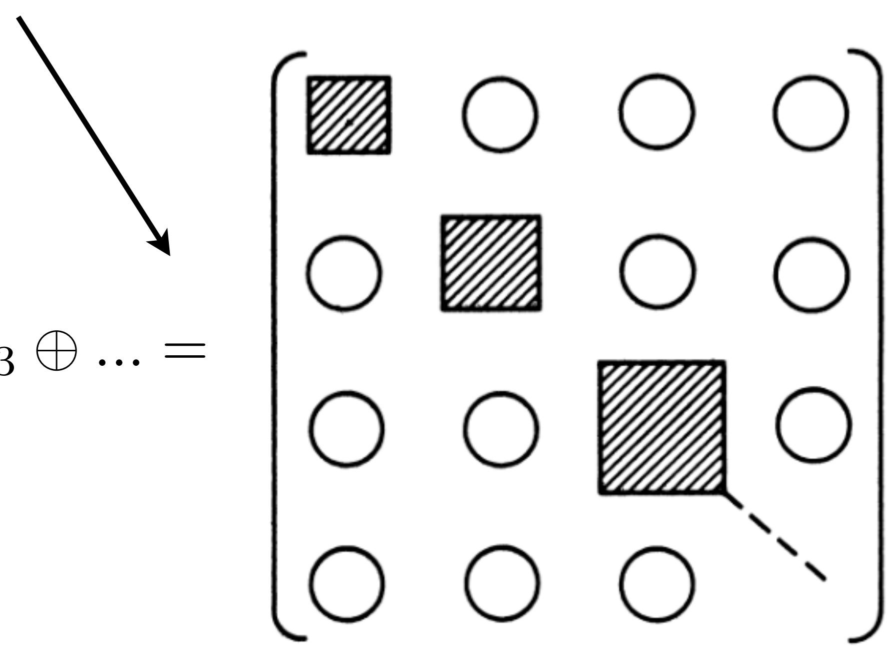
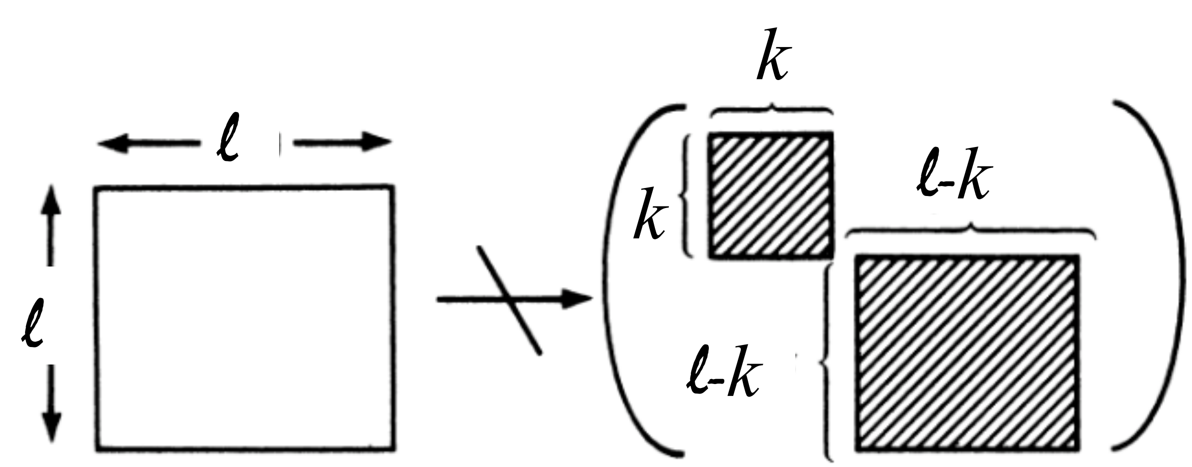


τ_i is irreducible if: It is impossible to find a new basis such that non-diagonal elements of any τ_i in the new basis are zero for all elements G_a.



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One can divide space L into the sum of subspaces L_i each of which is invariant and irreducible. $S_{\tau i}$ is a vector from L_i and is transformed by matrices $\tau_i(G_a)$.

$S_{\tau i}$ are linear combinations of n basis functions of L with some coefficients

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

$$S_{\tau 1}(1) = \sum_{j=1}^{n} c_j^{\tau 1}(1)\mathbf{e}_j$$

$l_{\tau 1}$ dim of τ •••

$$S_{\tau 1}(l_{\tau 1}) = \sum_{j=1}^{n} c_j^{\tau 1}(l_{\tau 1})\mathbf{e}_j$$

Reduction of any representation of group to block diagonal shape

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group G | space L under actions of Ga

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$S_{\tau i}$ are linear combinations of n basis functions of L with some coefficients

group G

τ_1, τ_2, τ_3 ...

structures of these matrixes depend solely on group G and are independent on the choice of L.

space L under actions of Ga

Irreducible representations (irreps) of point group 32 (D_3)

Representation \ Group element G_a	1 E	3^1 R_1	3^2 R_2	2_u R_3	2_y R_4	2_x R_5
τ_1	1	1	1	1	1	1
τ_2	1	1	1	−1	−1	−1
τ_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & -\sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$

Irreducible representations (irreps) of point group 32 (D_3)

Group element G_a / Representation	1 E	3^1 R_1	3^2 R_2	2_u R_3	2_y R_4	2_x R_5
τ_1	1	1	1	1	1	1
τ_2	1	1	1	−1	−1	−1
τ_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & -\sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$

Our magnetic 9x9 representation splits up in:

rep $\Rightarrow_{\sum_{\oplus}}$ irreps:

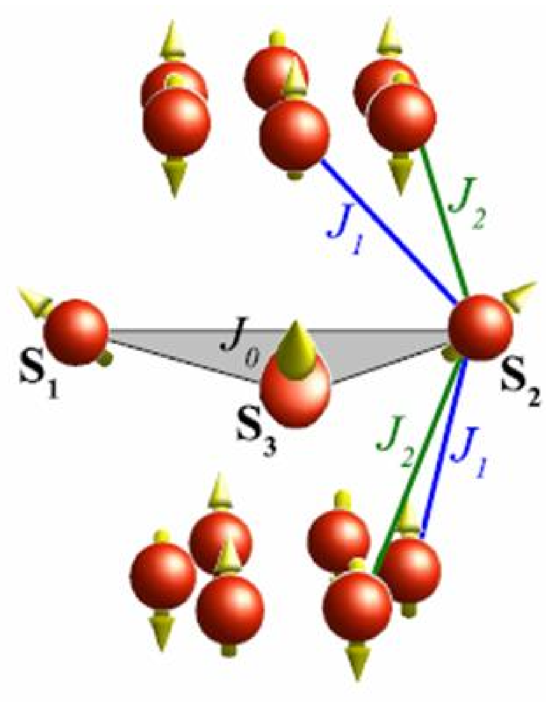
$$T_{ij} = \sum_{\oplus} n_\nu \tau^\nu_{ij} = \tau_1 \oplus 2\tau_2 \oplus 3\tau_3 = \begin{pmatrix} \tau_1 & 0 & 0 & \dots & 0 \\ 0 & \tau_2 & 0 & \dots & 0 \\ 0 & 0 & \tau_2 & \dots & 0 \\ . & . & . & . & \\ . & . & . & . & \\ 0 & 0 & 0 & & \end{pmatrix}$$

$$n_\nu = \frac{1}{n(G)} \sum_{g \subset G} \chi(g) \chi^{*\nu}(g)$$

Classification of normal modes of a magnet

The crystal has symmetry group G

$$H = \sum_{\mathbf{R},\mathbf{R}',\alpha,\beta} J_{\alpha,\beta}(\mathbf{R},\mathbf{R}')s_\alpha(\mathbf{R})s_\beta(\mathbf{R}') \quad (\alpha,\beta = x,y,z)$$



$$\begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \dots \\ \dots \\ \dots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$$

3N-dimensional space of expectation values of the spins $<\psi|\mathbf{s}|\psi>$ defined on N discreet points

induced magnetic representation of group G

$$\sum_{n=1}^{N} \sum_{\alpha=x,y,z} s_{\alpha n}\mathbf{e}_{\alpha n}$$

$$T_{ij}(G_a)$$

is decomposed into independent normal modes $S_{\tau 1}$, $S_{\tau 2}$, ...
(specific vectors from 3N-dimensional space of spins)

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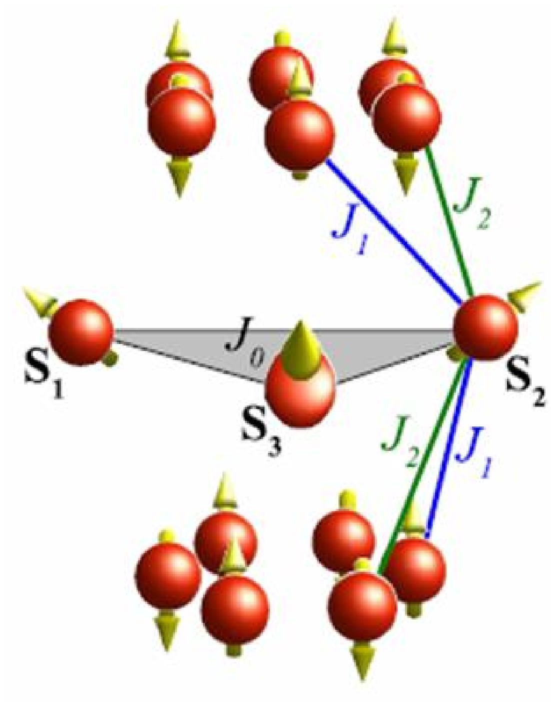

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$S_{\tau i}$ called normal modes or basis functions, corresponding to E_ν, $\psi_\nu{}^{l\nu}$ can be classified by irreps τ^ν of group G

rep $\Rightarrow_{\Sigma_\oplus}$ irreps: $T_{ij} = \sum_{\oplus} n_\nu \tau^\nu_{ij}$

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

Normal modes of magnetic configurations for spins sitting on the triangle corners

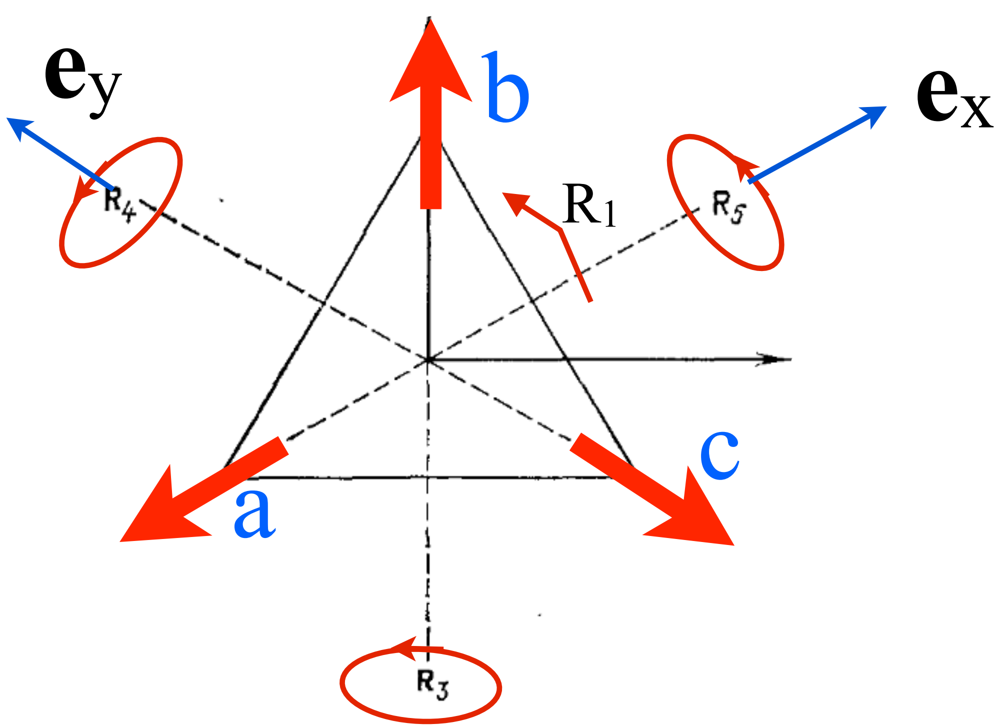
Point group *32*

irrep τ1

1D linear subspace of 9-dimensional space

$$S_{\tau 1} = -1 \cdot \mathbf{e}_{xa} + 1 \cdot \mathbf{e}_{xb} + 1 \cdot \mathbf{e}_{yb} - 1 \cdot \mathbf{e}_{yc}$$

Normal mode for irrep τ1



One parameter instead of 9 is enough to describe the structure!

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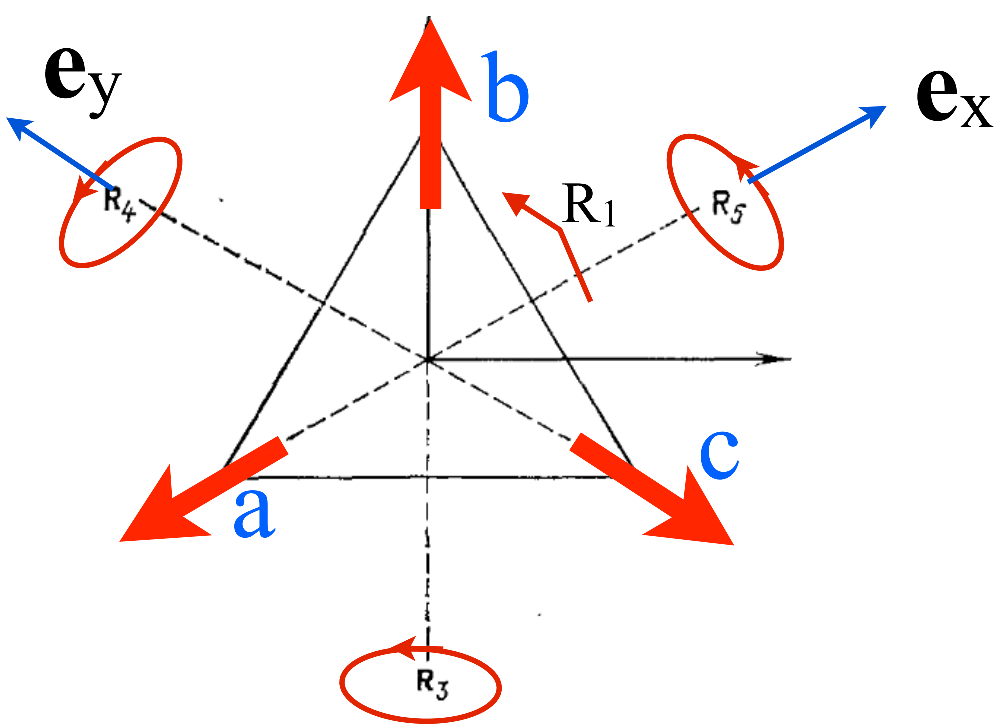
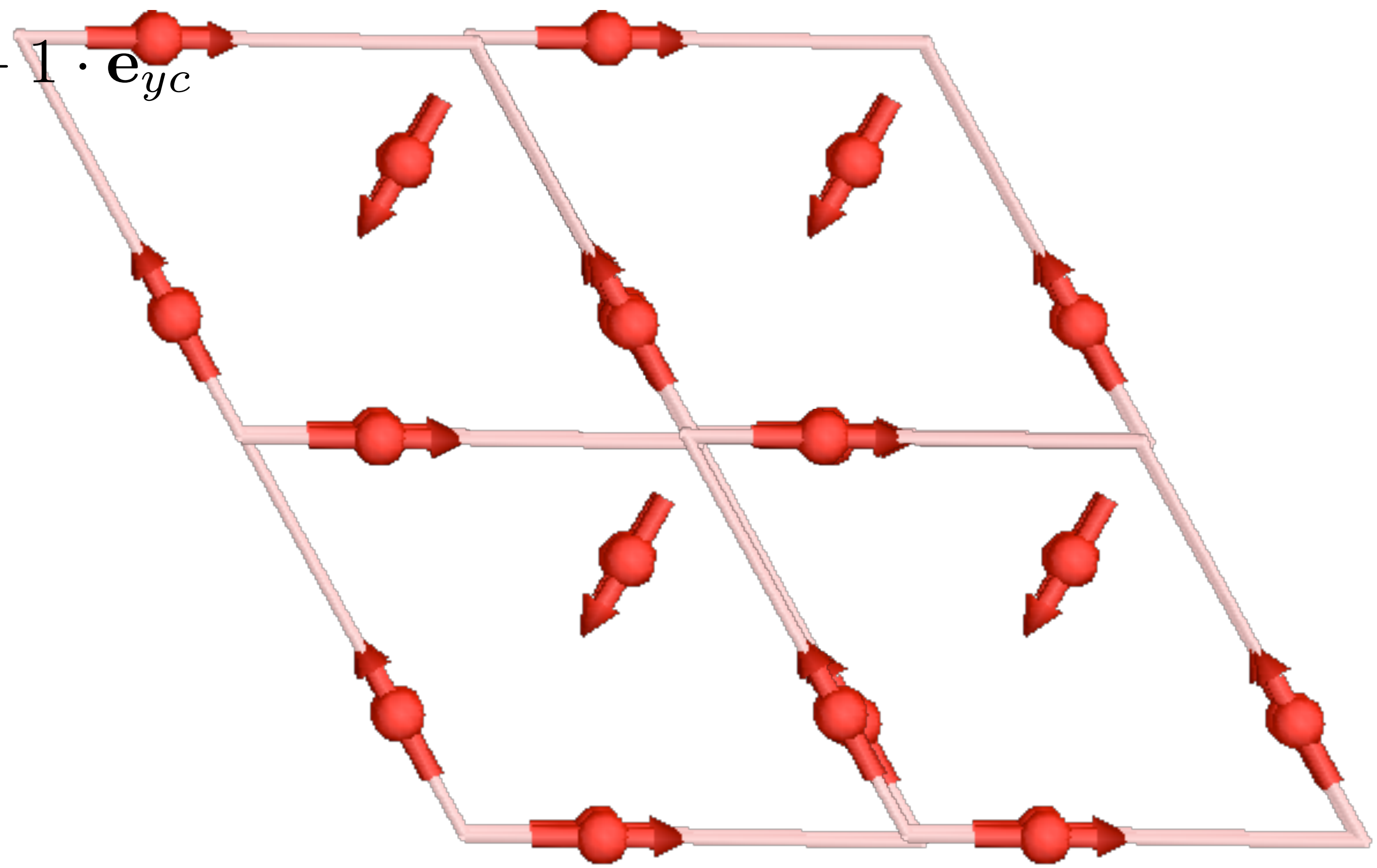
Space group *P321*, no. 150





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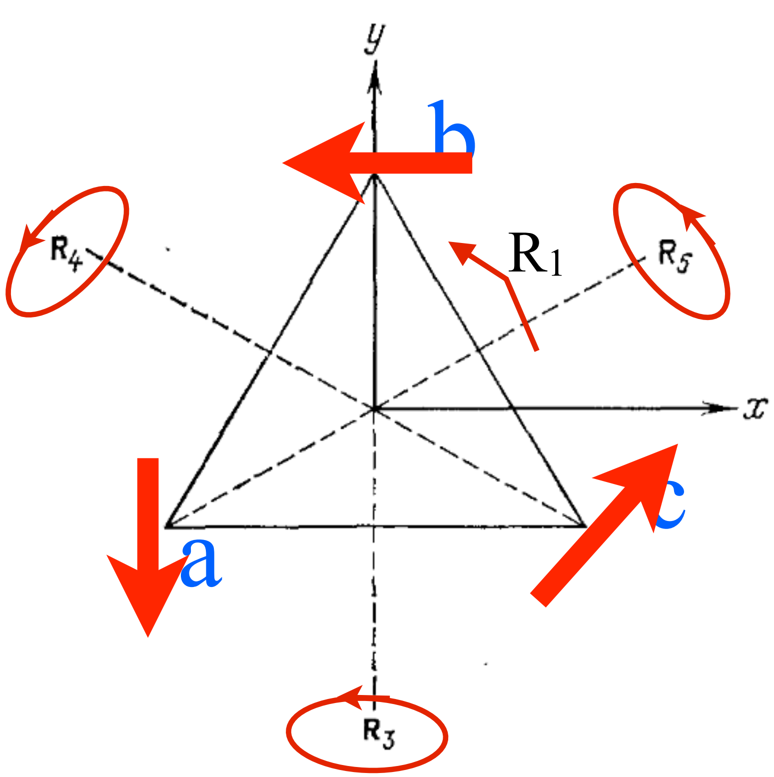
Normal modes of magnetic configurations for spins sitting on the triangle corners

Point group *32*

τ_2 enters 2 times

Normal mode 1



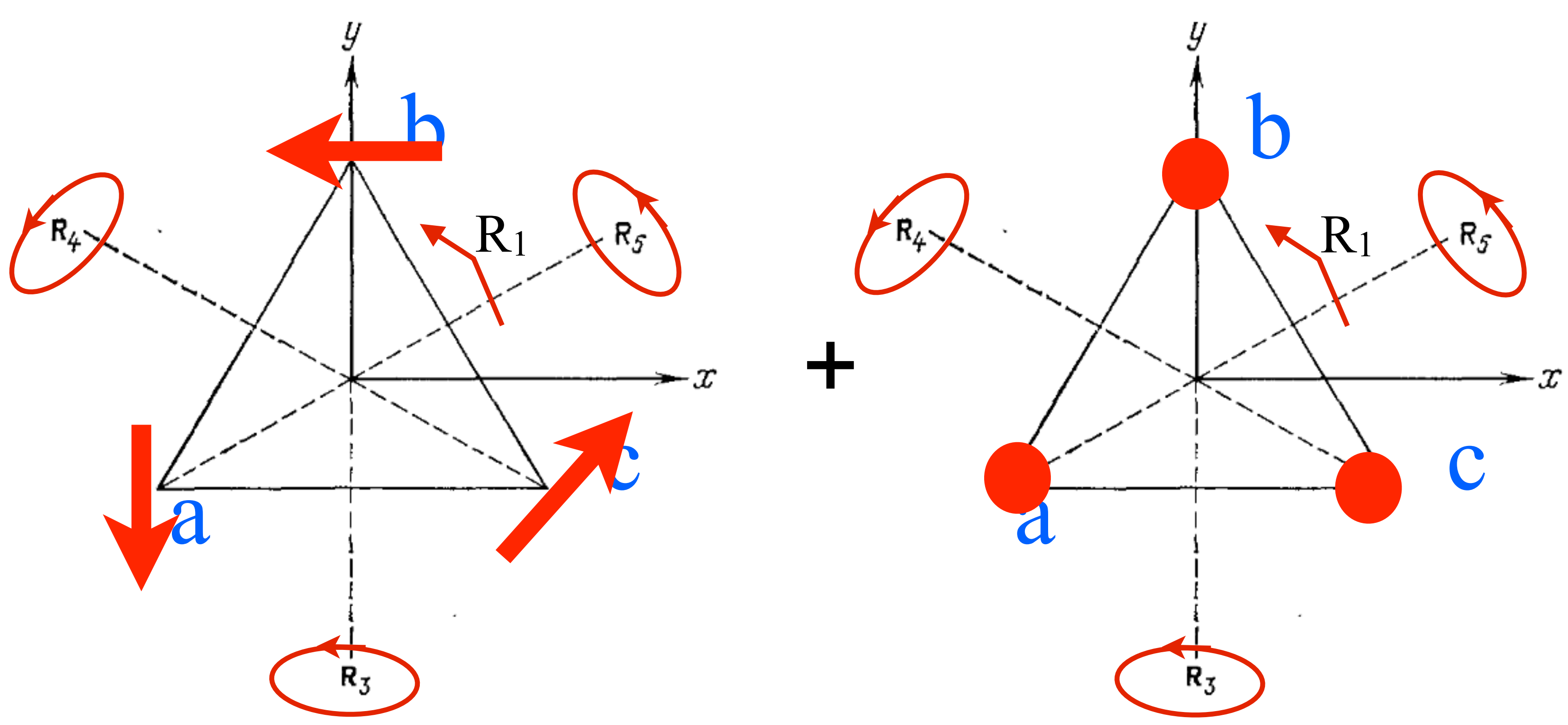
Normal mode 2

Normal modes of magnetic configurations for spins sitting on the triangle corners

Point group *32*

τ_2 enters 2 times

Normal mode 1 + Normal mode 2



Normal modes of magnetic configurations for spins sitting on the triangle corners

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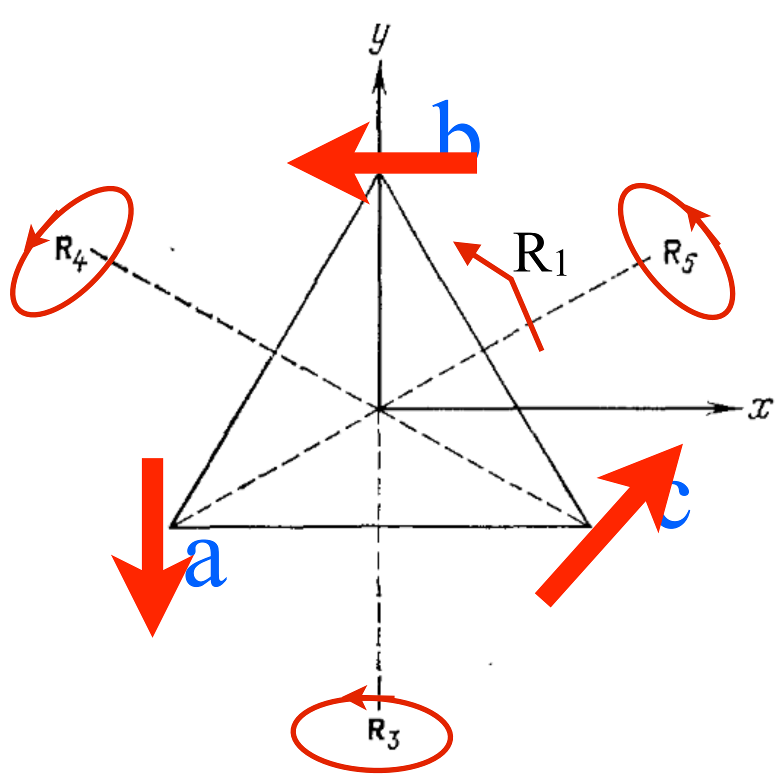
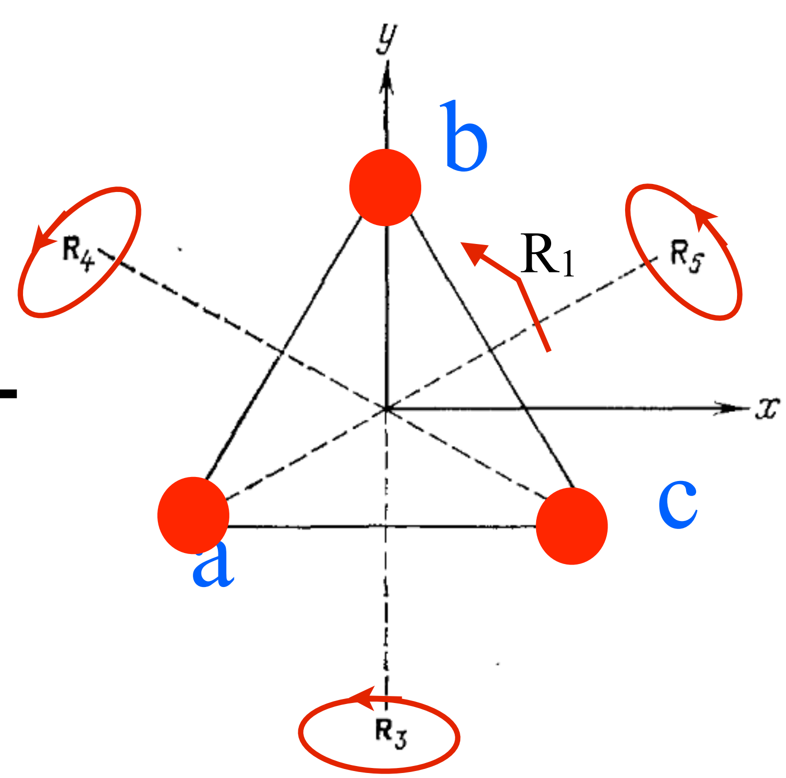
Space group *P321*, no. 150

Normal mode 1

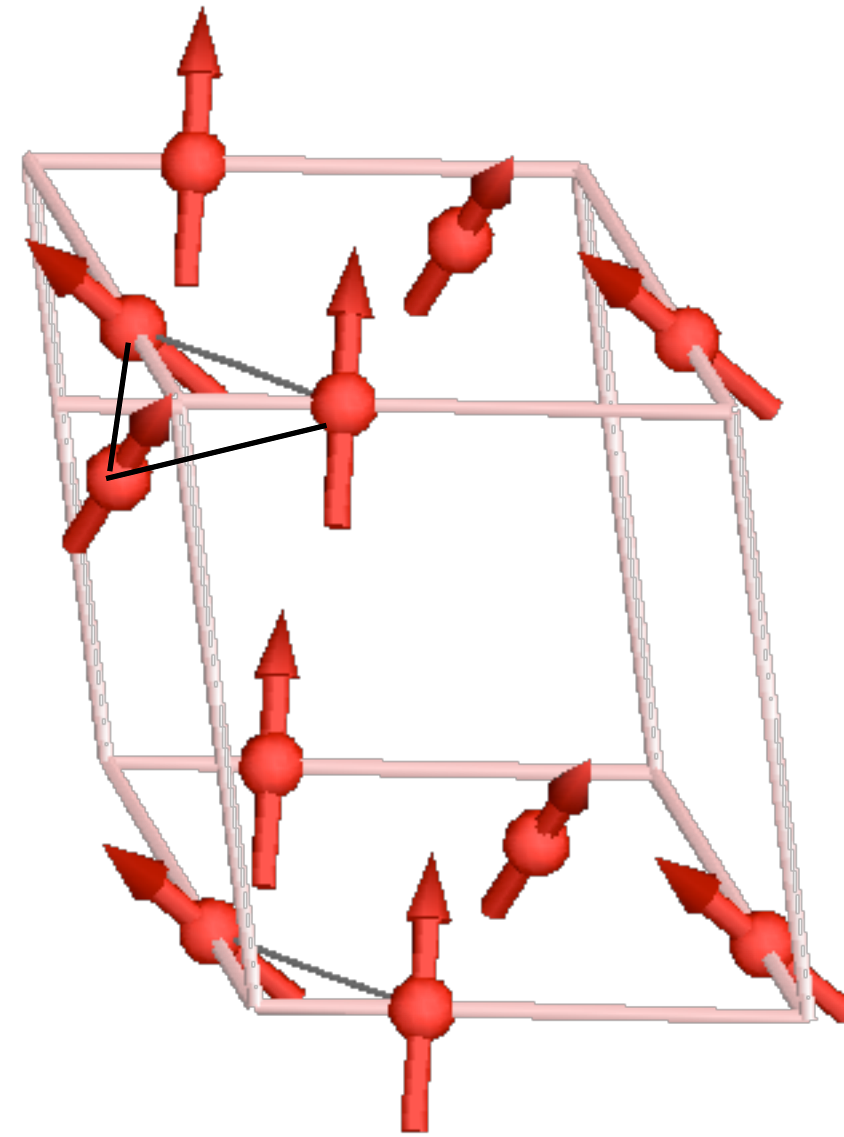


+

Normal mode 2



=



Landau theory of phase transitions says that only one irrep (+c.c.) is becoming critical and is needed to describe the ordered structure

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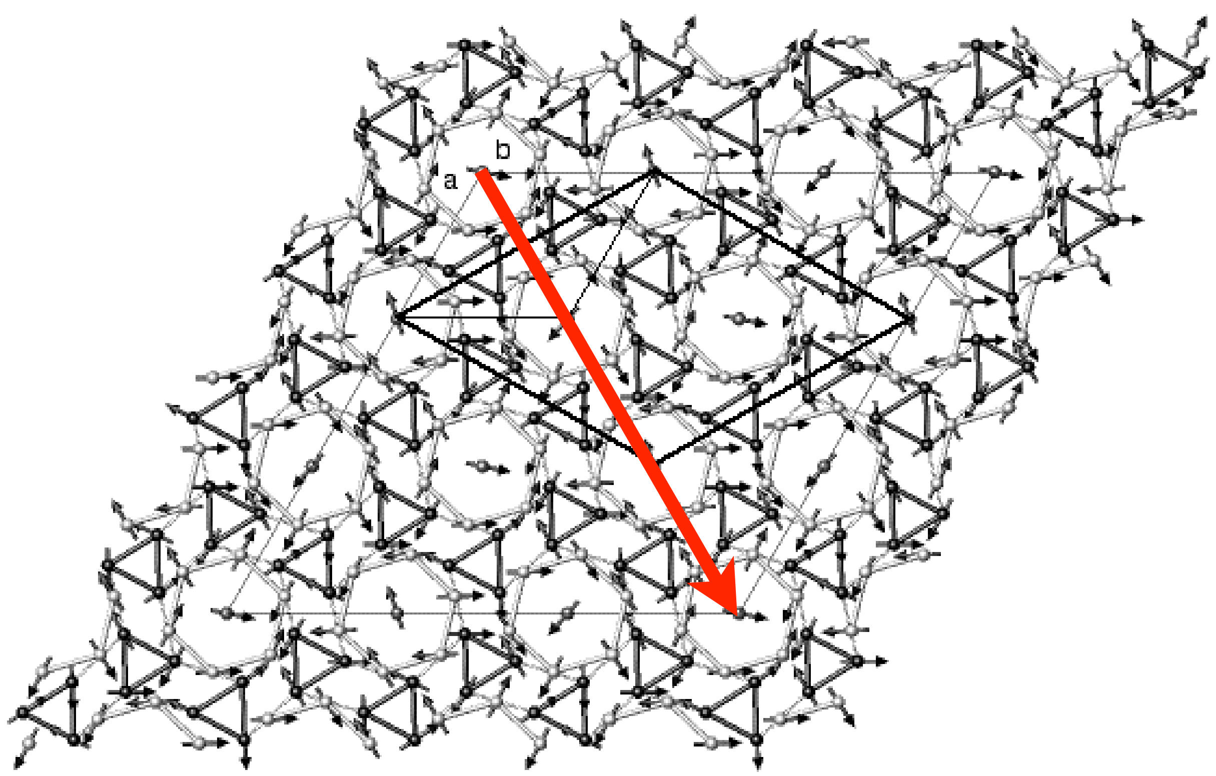
Real example: Antiferromagnetic three sub-lattice ordering in $Tb_{14}Au_{51}$

Great simplification!



PHYSICAL REVIEW B 72, 134413 (2005)

Zeroth cell contains **14** spins
=> 14*3=42 parameters.

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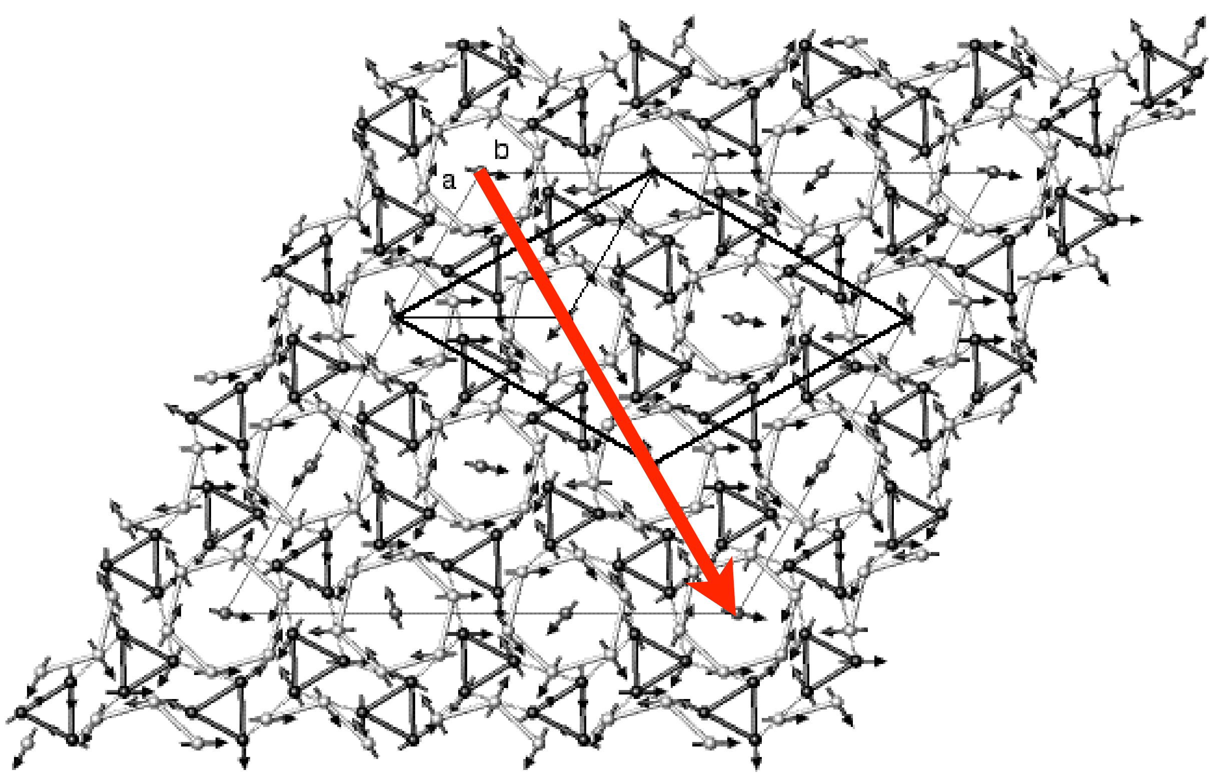

PHYSICAL REVIEW B 72, 134413 (2005)

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one irrep

Only 3 independent spins are needed!

irreps of space groups SG. Some history and an introduction

O. V. Kovalev, *"Representations of the Crystallographic Space Groups: irreducible representations, induced representations, and corepresentations" 1961-* (Gordon and Breach Science Publishers, 1993), 2nd ed.

S.C. Miller and W.F Love, *"Tables of Representations of the Crystallographic Space Groups and corepresentations of Magnetic space groups* (Colorado, 1967)

Harold T. Stokes and Dorian M. Hatch, "Isotropy Subgroups of the 230 Space Groups," (World Scientific, Singapore, 1988).

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,

http://stokes.byu.edu/iso

Bloch waves, irreps of Bravias Lattice group

Space group G contains translation (t) BL group T. $\mathbf{t} = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3$

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$$\mathbf{S}(\mathbf{t}_n) = \frac{1}{2}(\mathbf{S}_0 e^{i\mathbf{t}_n\mathbf{k}} + \mathbf{S}_0^* e^{-i\mathbf{t}_n\mathbf{k}})$$

three ψ(**r**) can describe magnetic structure S_x(**r**), S_y(**r**), S_z(**r**); u(r) <-> zeroth cell
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Representation theory

wave vector or *propagation vector* $\mathbf{k} = (p_1\mathbf{b}_1 + p_2\mathbf{b}_2 + p_3\mathbf{b}_3)$

sort out/enumerate all irreps of $T \in G$

Matrices of irrep number **k:** $D^{\mathbf{k}}(\mathbf{t}) = \exp(-i\mathbf{k}\mathbf{t})$ $\quad T(\mathbf{t}) \rightarrow \exp(-i\mathbf{k}\mathbf{t})$

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Bloch wave ψ(**r**) is a basis function of irrep **k** of BL translation group

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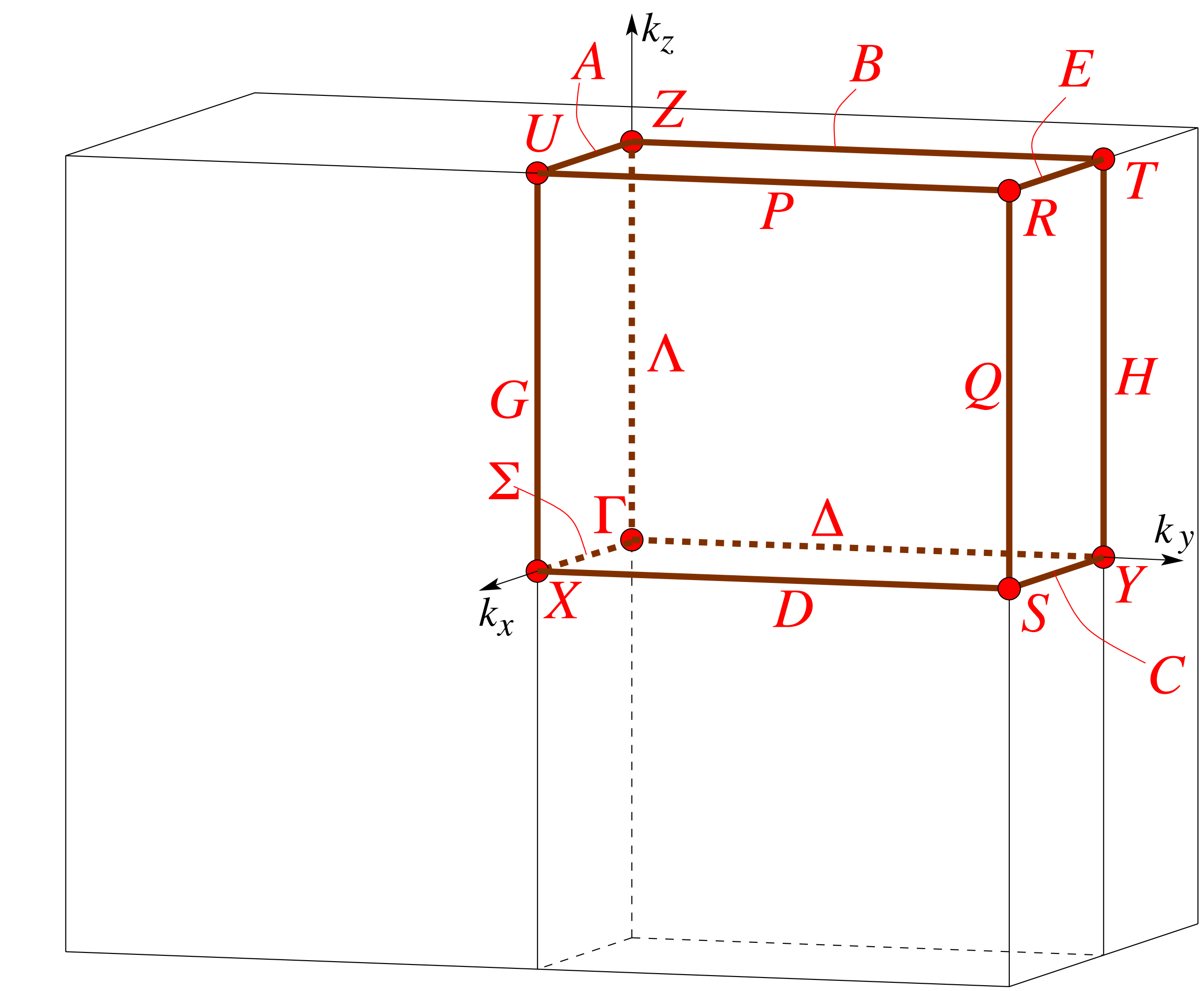
The k-vector types and Brillouin zones of the space groups

propagation vector = a point on/inside Brillouine zone

Brillouine zone of *Pmmm* (Γ_0)



Kovalev	k-vector label		Wyckoff position		
	CDML		ITA		
k_{19}	GM	0,0,0	1	a	mmm
k_{20}	X	1/2,0,0	1	b	mmm
k_{22}	Z	0,0,1/2	1	c	mmm
k_{24}	U	1/2,0,1/2	1	d	mmm
k_{21}	Y	0,1/2,0	1	e	mmm
k_{25}	S	1/2,1/2,0	1	f	mmm
…	T	0,1/2,1/2	1	g	mmm
…	R	1/2,1/2,1/2	1	h	mmm
	SM	u,0,0	2	i	2mm
	A	u,0,1/2	2	j	2mm
	C	u,1/2,0	2	k	2mm
	E	u,1/2,1/2	2	l	2mm
	DT	0,u,0	2	m	m2m
	B	0,u,1/2	2	n	m2m
	D	1/2,u,0	2	o	m2m
	P	1/2,u,1/2	2	p	m2m
	LD	0,0,u	2	q	mm2
	H	0,1/2,u	2	r	mm2
	G	1/2,0,u	2	s	mm2
	Q	1/2,1/2,u	2	t	mm2
	K	0,u,v	4	u	m..

A.P. Cracknell, B.L. Davis, S.C. Miller and W.F. Love (1979) (abbreviated as **CDML**)

Kovalev O.V (1986) (1993) *Representations of the Crystallographic Space Groups* (London: Gordon and Breach)

Basis functions of space group irrep

Propagation vector **k**
+
Space group elements *g* in zeroth cell

→

irrep with number ν: $\tau^{\mathbf{k}\nu}$
symmetry elements g are represented by matrixes $d^{\mathbf{k}\nu}(g)$
($l_\nu \times l_\nu$ matrixes) with dim=l_ν

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Its basis: l_ν functions with the same **k**

$$\psi_\lambda^{\mathbf{k}\nu} = u_\lambda^{\mathbf{k}\nu}(\mathbf{r})e^{i\mathbf{k}\mathbf{r}}$$
$$(\lambda = 1, ..., l_\nu)$$

→

$$\begin{pmatrix} \psi_1^{\mathbf{k}\nu} \\ \psi_2^{\mathbf{k}\nu} \\ \cdots \\ \cdots \\ \cdots \\ \psi_{l_\nu}^{\mathbf{k}\nu} \end{pmatrix}$$

that are transformed by symmetry elements g by matrixes $d^{\mathbf{k}\nu}(g)$

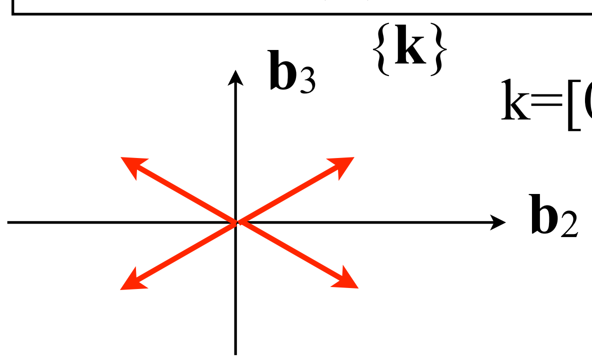
Symmetry group of propagation vector, examples of star {k}

Pnma	D_{2h}^{16}	*mmm*	Orthorhombic
No. 62	$P\ 2_1/n\ 2_1/m\ 2_1/a$		Patterson symmetry *Pmmm*

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	$+T(n_1\mathbf{t}_1+n_2\mathbf{t}_2+n_3\mathbf{t}_3)$
(5) $\bar{1}$ 0,0,0	(6) a $x,y,\frac{1}{4}$	(7) m $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	

Manyfold of all non-equivalent $h\mathbf{k}$ = propagation vector star $\{\mathbf{k}\}$



k=[0,u,v]

label *K*

Little group $G_k \in G$ leave ***k*** *invariant*

(1) 1

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G_k = '*P1n1*'

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$+T(n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3)$

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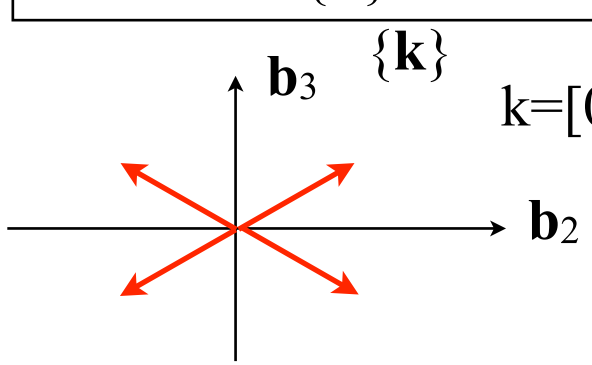

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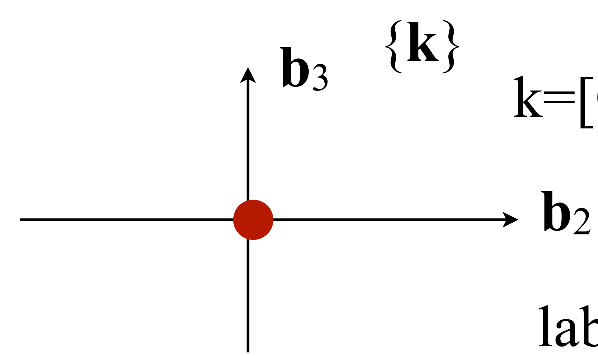

k=[0,0,0]

label *Γ*

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$G_k = G$

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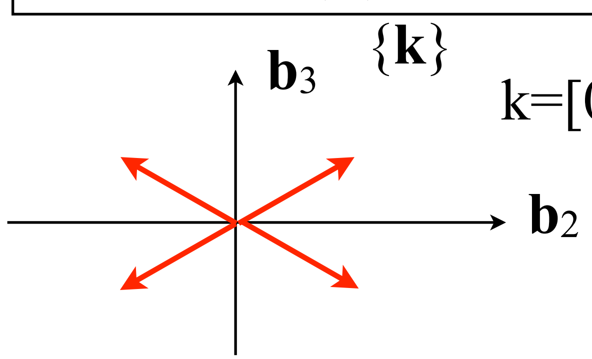

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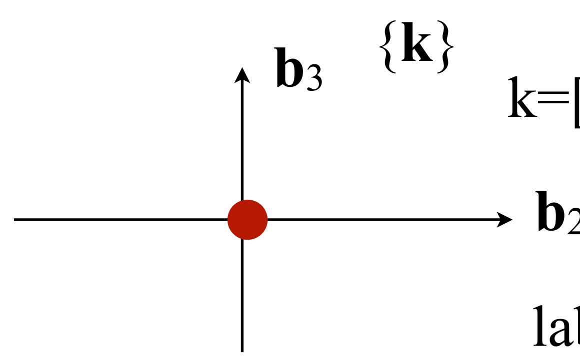
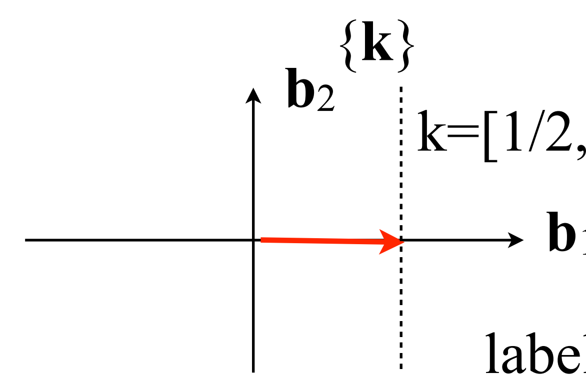
label *K*



k=[0,0,0]

label *Γ*



k=[1/2,0,0]

label *X*

Little group $G_k \in G$ leave ***k*** *invariant*

(1) 1

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

G_k = '*P1n1*'

$G_k = G$

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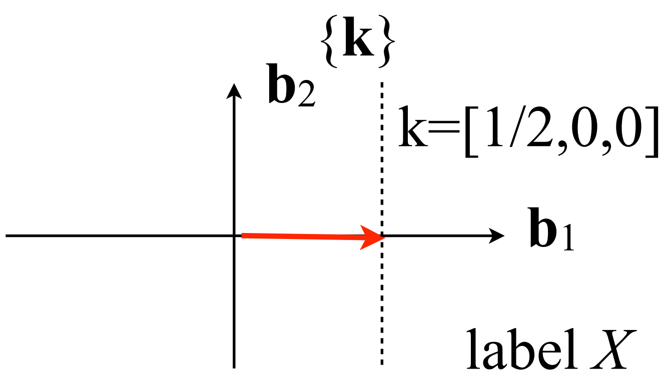
Space group irreps, examples
dimensions up to 6 (cf. 3 for point groups)



Example 1 *Pnma* k=[1/2,0,0], k20

irreps: two 2D τ_1, τ_2

$d^{\mathbf{k}\nu}(g)$

g	/2	/3	/4	/25	/26	/27	/28
$\hat{\tau}1$	$\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix}$	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$
$\hat{\tau}2 = \hat{\tau}1 \times$	1	1	1	-1	-1	-1	-1

$G_k = G$

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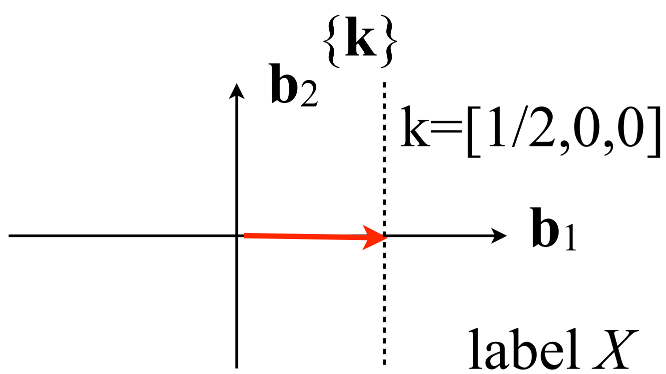

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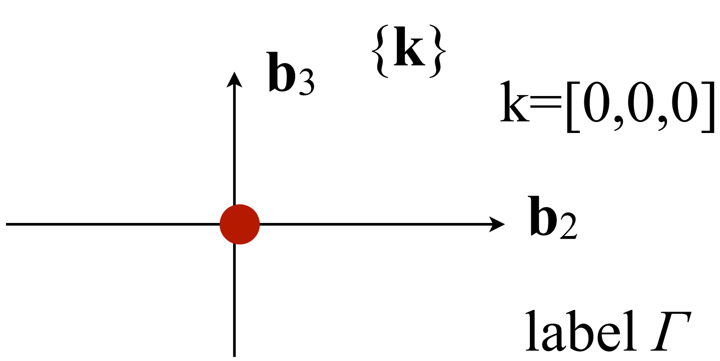

Example 2 *Pnma* k=[0,0,0], k19

irreps: eight 1D τ_1, τ_2, τ_3, τ_4, τ_5, τ_6, τ_7, τ_8

$d^{\mathbf{k}\nu}(g)$

g	/2	/3	/4	/25	/26	/27	/28
$\hat{\tau}1$	1	1	1	1	1	1	1
$\hat{\tau}2$	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

$\hat{\tau}4 = \hat{\tau}3 \times \hat{\tau}2,\ \hat{\tau}6 = \hat{\tau}5 \times \hat{\tau}2,\ \hat{\tau}8 = \hat{\tau}7 \times \hat{\tau}2$

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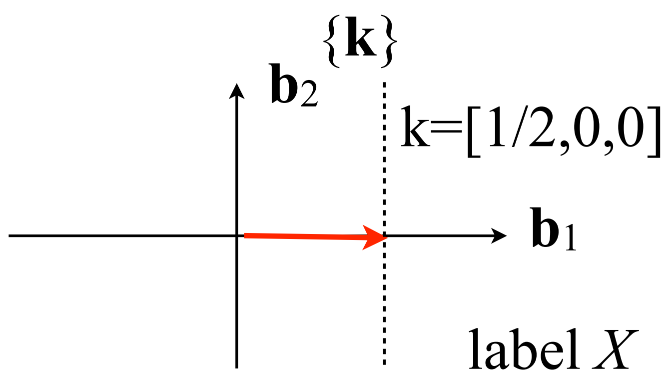
Space group irreps, examples
dimensions up to 6 (cf. 3 for point groups)



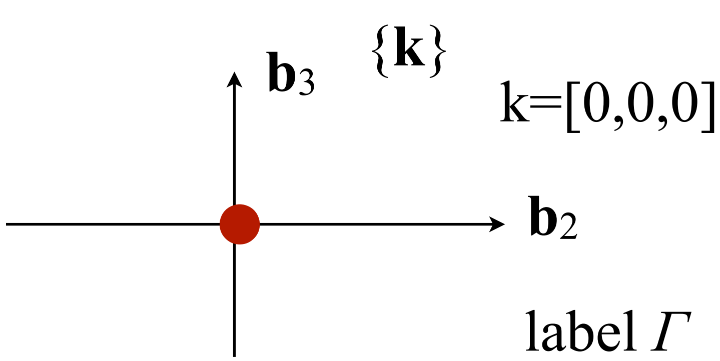
$G_k = G$

Example 1 *Pnma* k=[1/2,0,0], k20

irreps: two 2D τ_1, τ_2

$d^{\mathbf{k}\nu}(g)$

g	/2	/3	/4	/25	/26	/27	/28
$\hat{\tau}1$	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$
$\hat{\tau}2 = \hat{\tau}1 \times$	1	1	1	-1	-1	-1	-1



$G_k = G$

Example 2 *Pnma* k=[0,0,0], k19

irreps: eight 1D τ_1, τ_2, τ_3, τ_4, τ_5, τ_6, τ_7, τ_8

$d^{\mathbf{k}\nu}(g)$

g	/2	/3	/4	/25	/26	/27	/28
$\hat{\tau}1$	1	1	1	1	1	1	1
$\hat{\tau}2$	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

$\hat{\tau}4 = \hat{\tau}3 \times \hat{\tau}2,\ \hat{\tau}6 = \hat{\tau}5 \times \hat{\tau}2,\ \hat{\tau}8 = \hat{\tau}7 \times \hat{\tau}2$

Example 3

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

k=[1/2,1/2,1/2]: 1(4D) ⊕ 2(2D)

Relation of magnetic Shubnikov symmetry and irreducible representation of space group

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

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magnetic symmetry

representation

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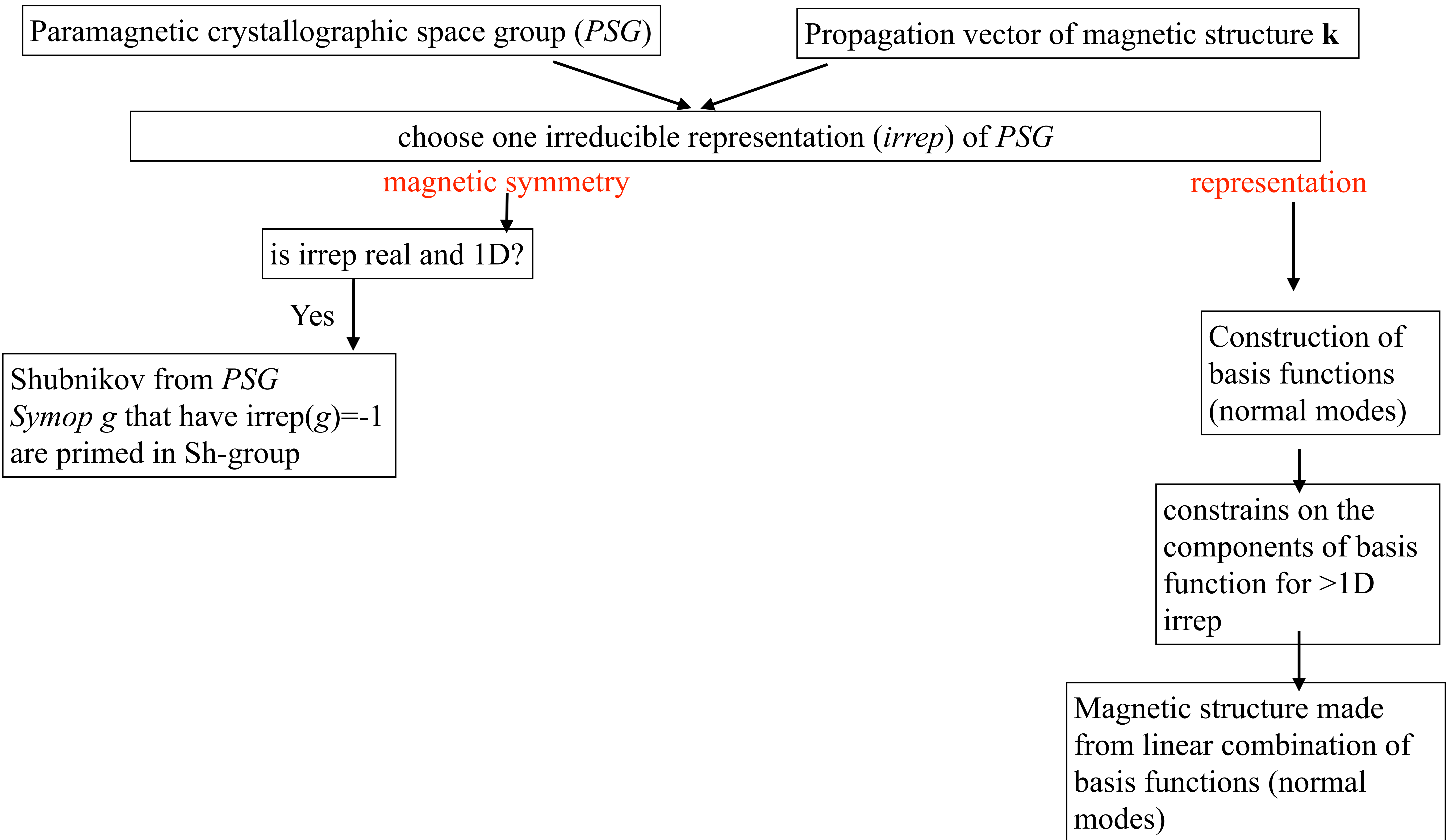

Relation of magnetic Shubnikov symmetry and irreducible representation of space group

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

choose one irreducible representation (*irrep*) of *PSG*

magnetic symmetry

is irrep real and 1D?

Yes

Shubnikov from *PSG*
Symop g that have irrep(*g*)=-1
are primed in Sh-group

Magnetic structure made from admissible spin directions in Sh-group

representation

Construction of basis functions (normal modes)

constrains on the components of basis function for >1D irrep

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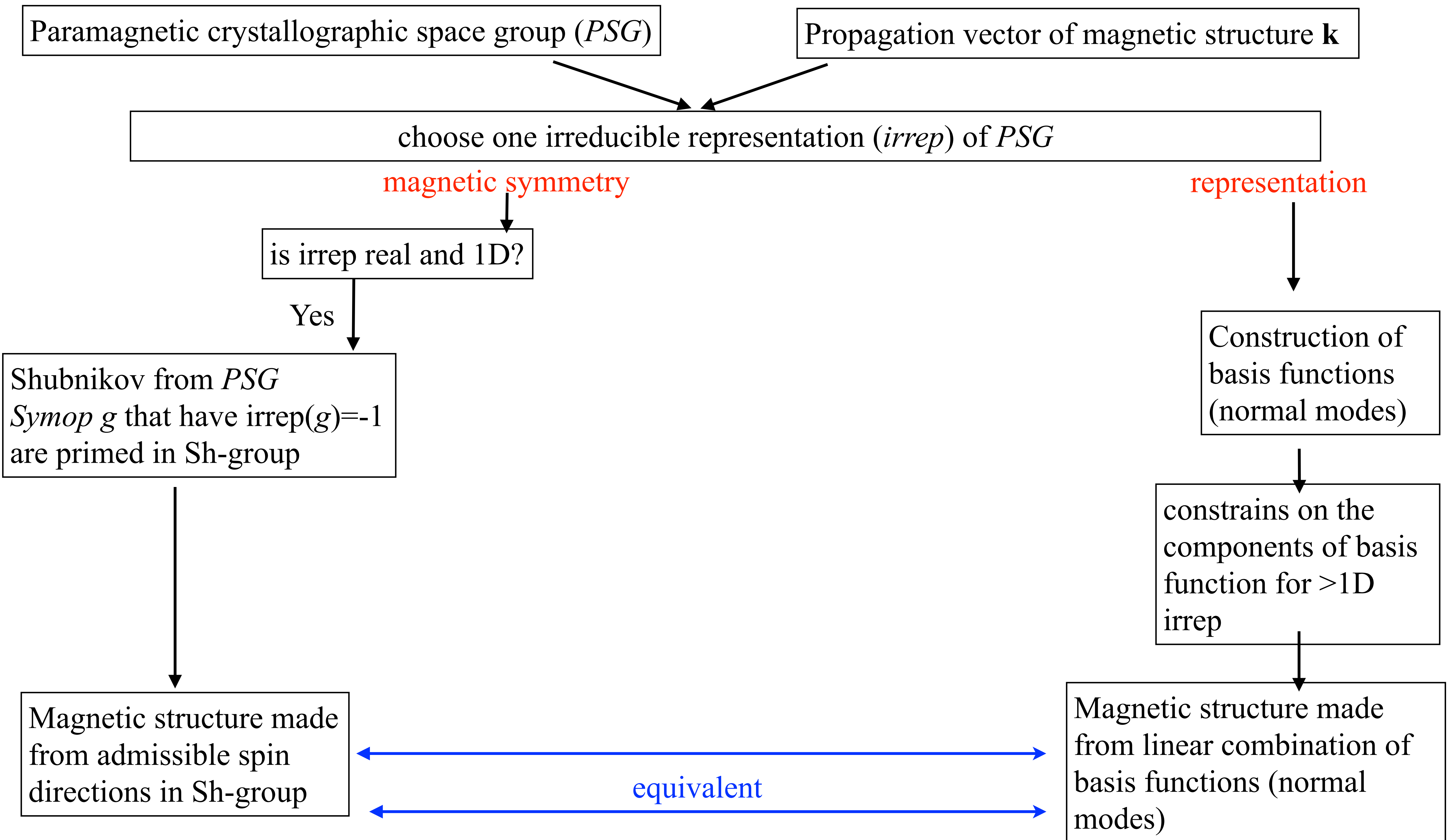

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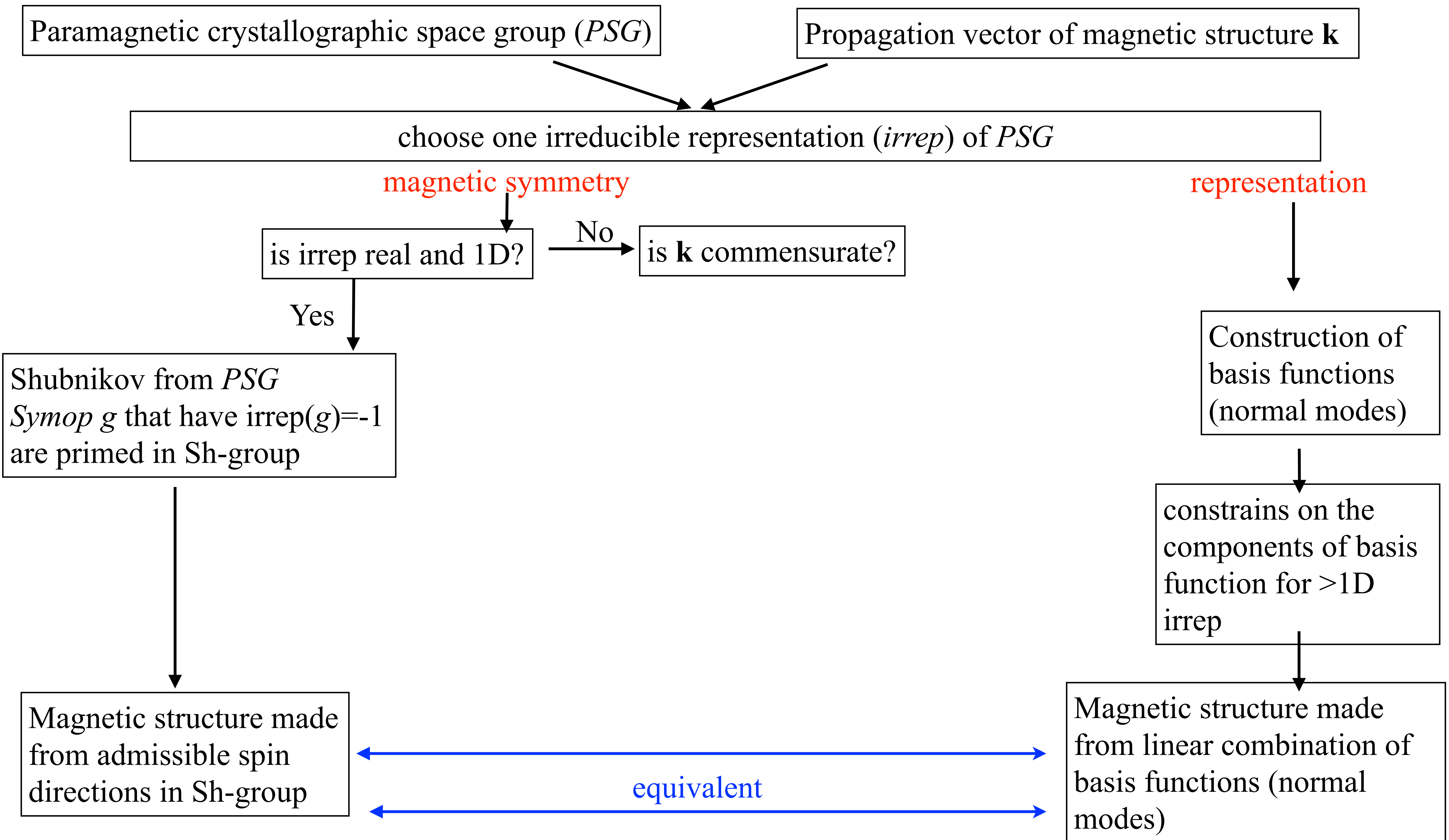

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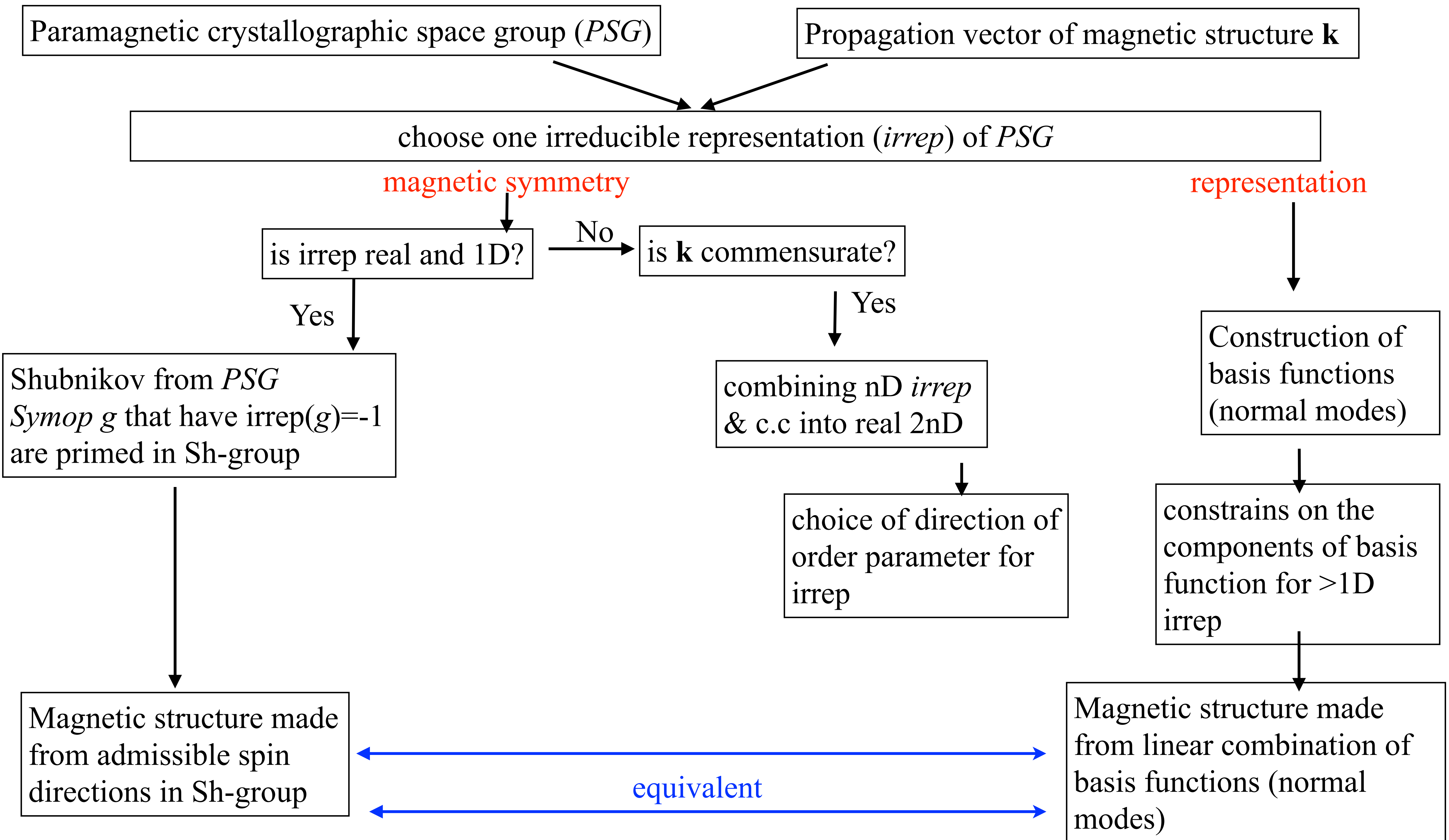

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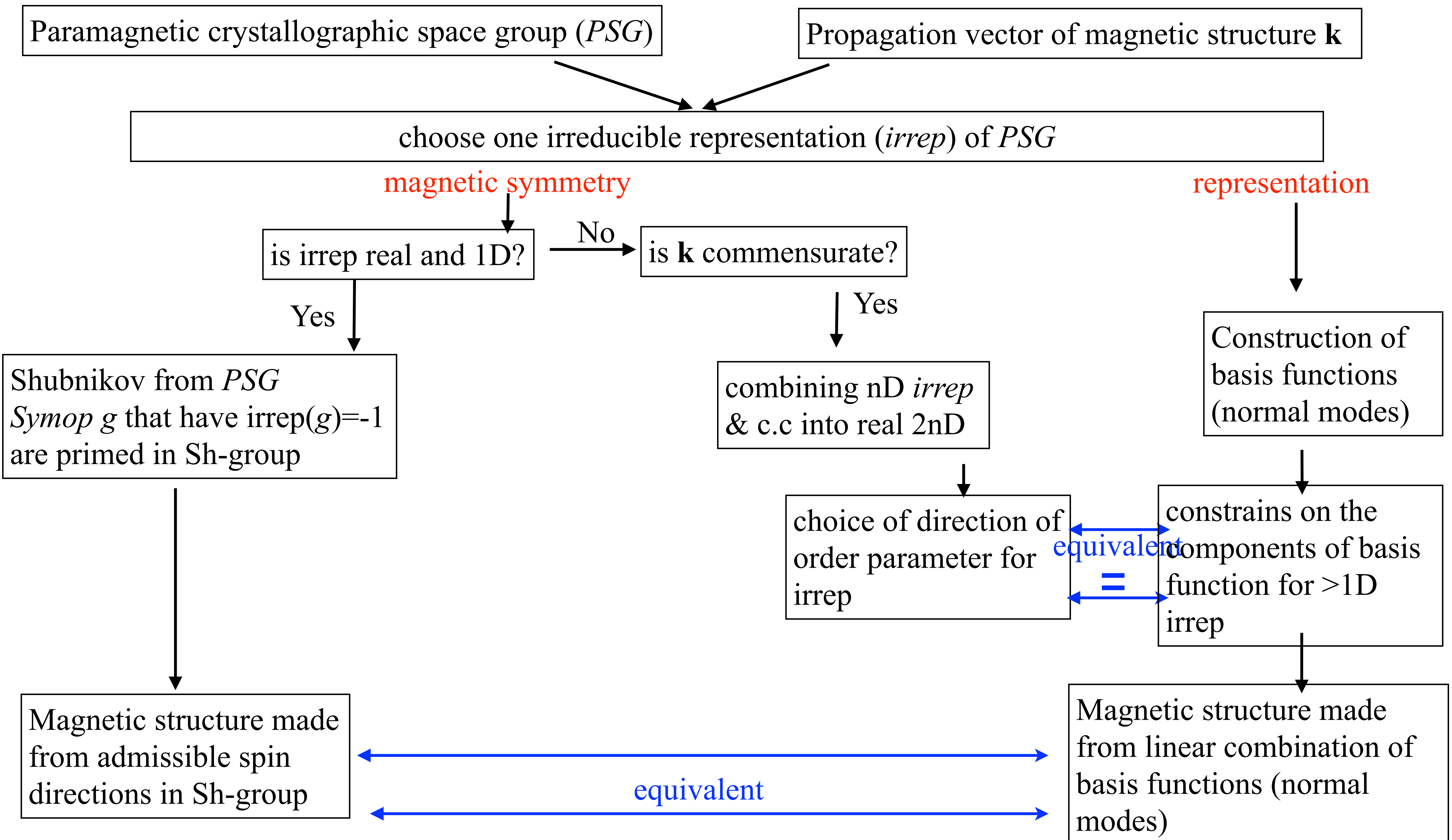

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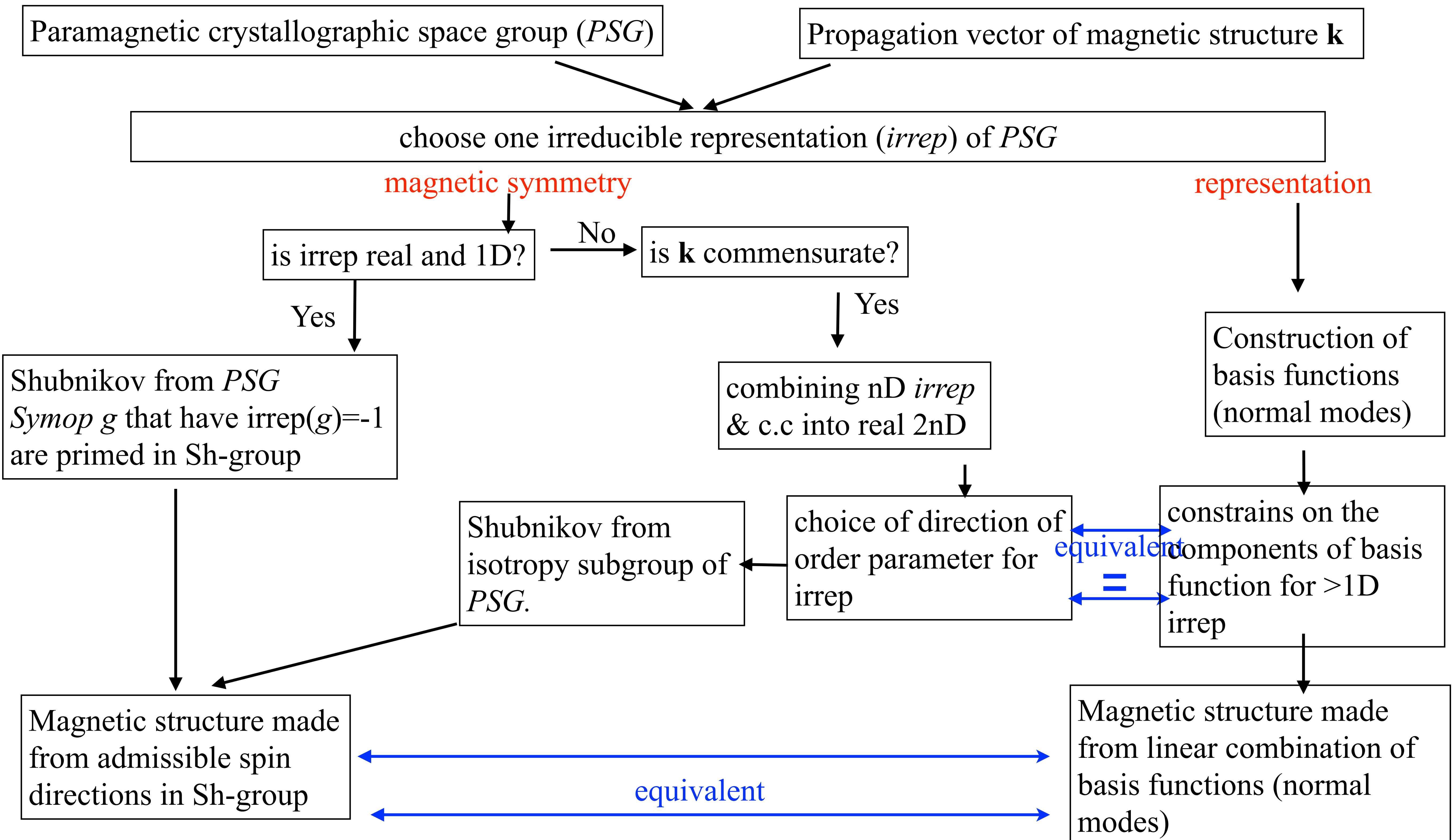

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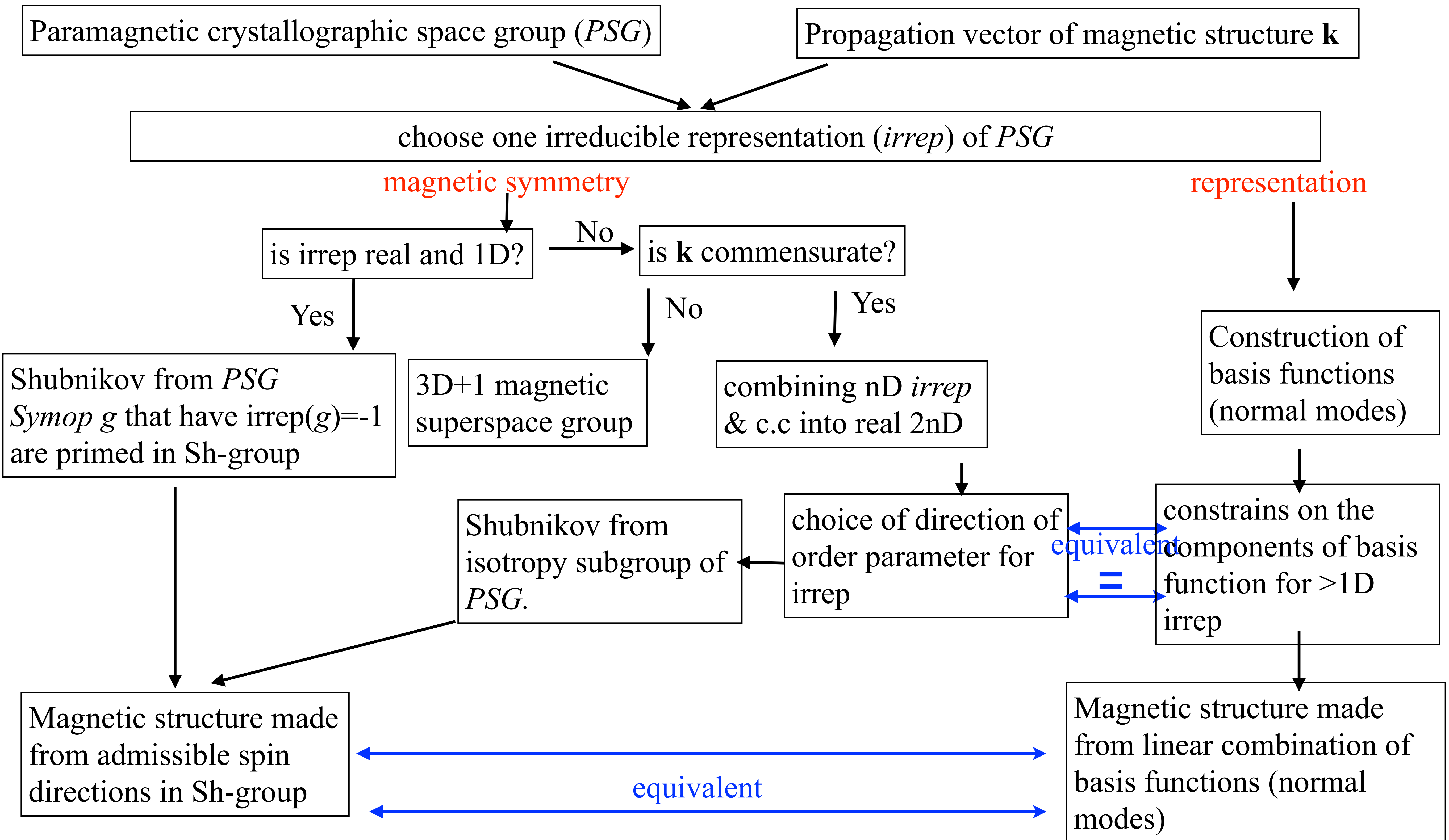

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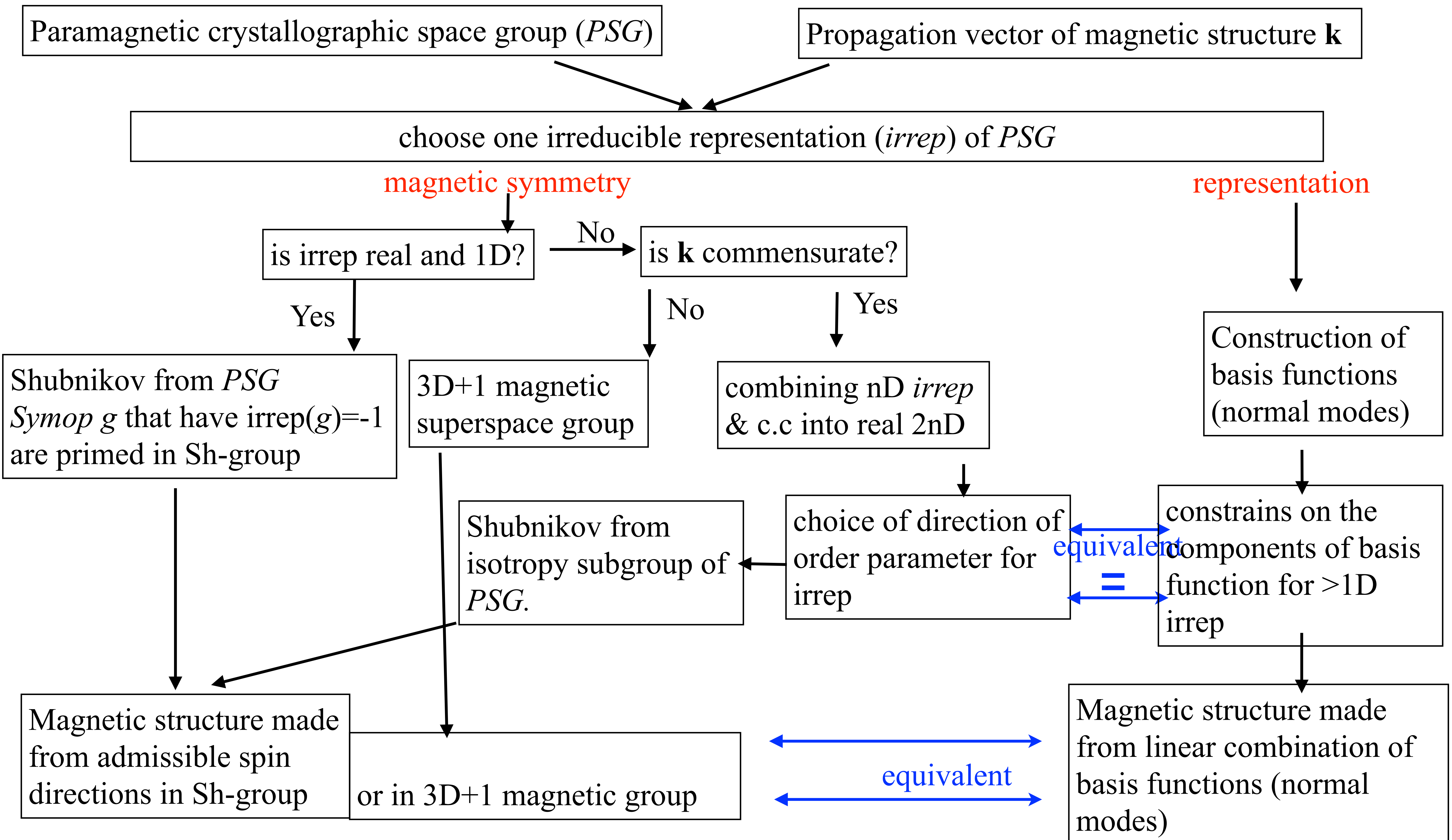


Comparison of Shubnikov and representation analysis: same symmetry adapted solutions.

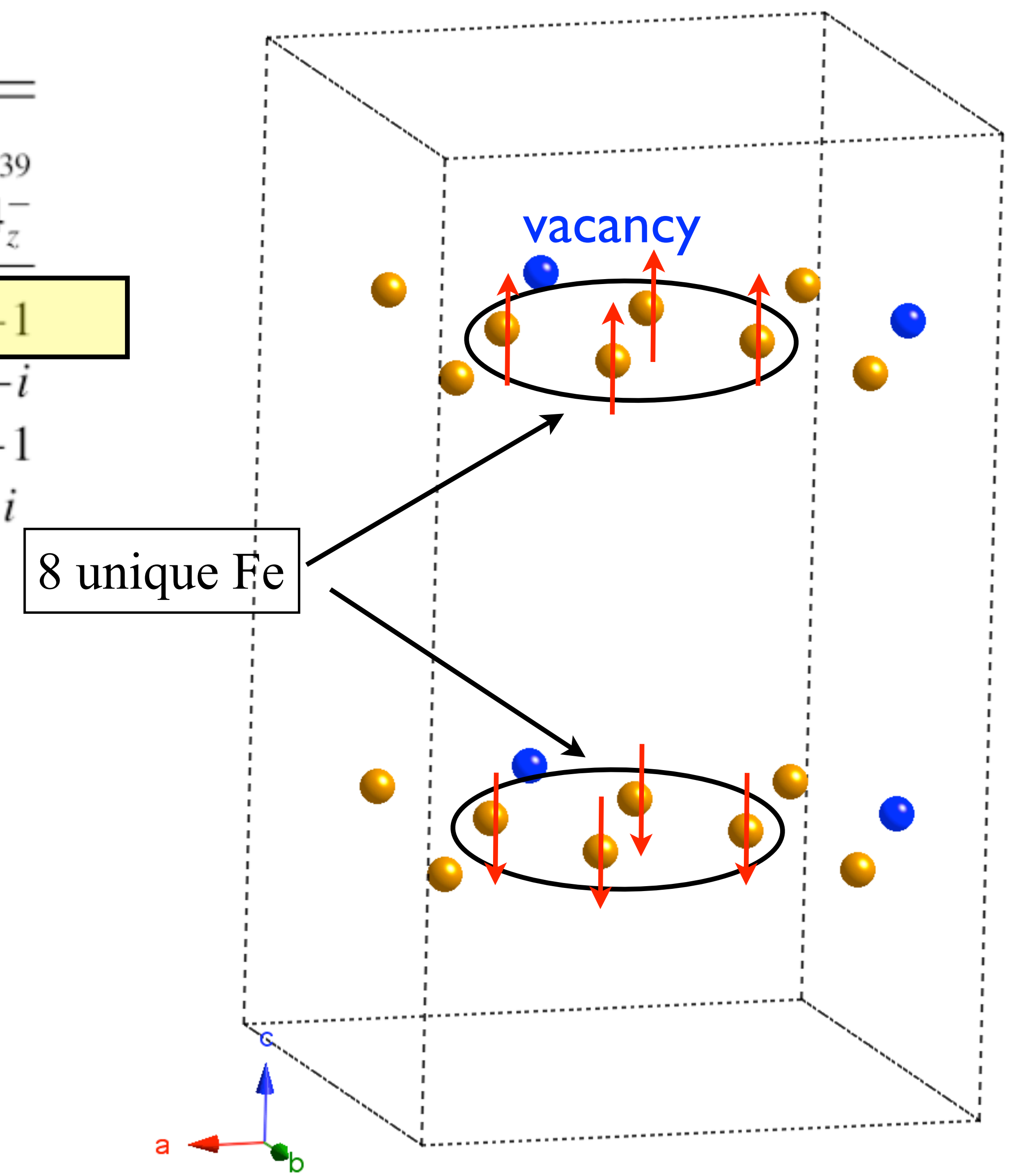
I4/m, k=0 has 8 1D irreps $\tau_1, \dots \tau_8$.
4 real irreps <--> Shubnikov groups of *I4/m*
4 complex irreps

	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 *I4/m'*	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

Fe Magnetic representation
(16i) (x,y,z): all eight irreps

$$\Gamma = 3\tau_1 \oplus 3\tau_2 \oplus 3 \dots \oplus 3\tau_8$$

One unit cell with Fe



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τ_2 *I4/m'*	1	1	1	1	-1	-1	-1	-1
τ_3 *C2'/m'*	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

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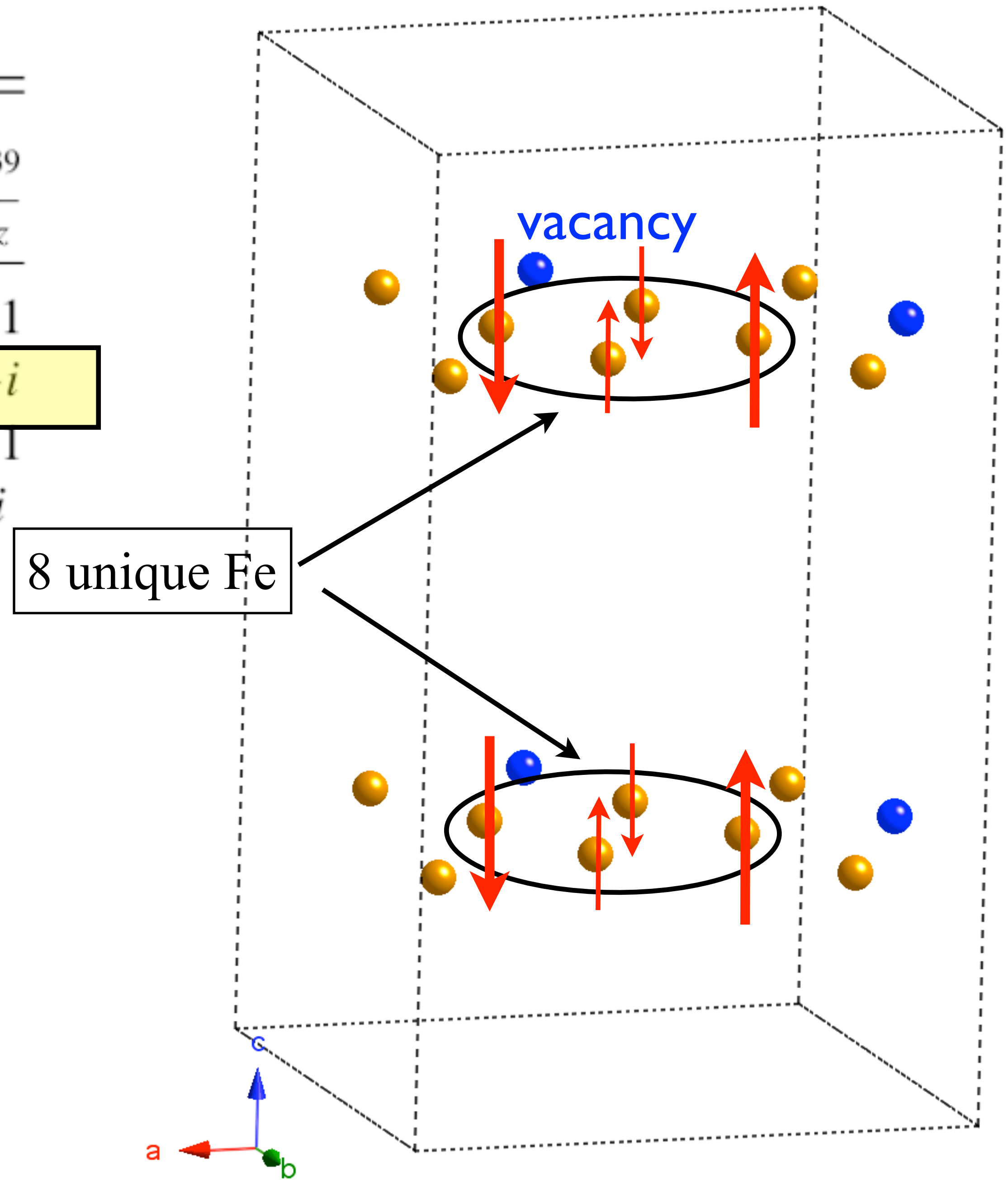

Fe — Magnetic representation (16i) (x,y,z): all eight irreps

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

- 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,

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

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

This lecture:

http://sinq.web.psi.ch/sinq/instr/hrpt/doc/magdif13.pdf

Case study. Antiferromagnetic order in orthorhombic multiferroic $TmMnO_3$

steps in magnetic structure determination

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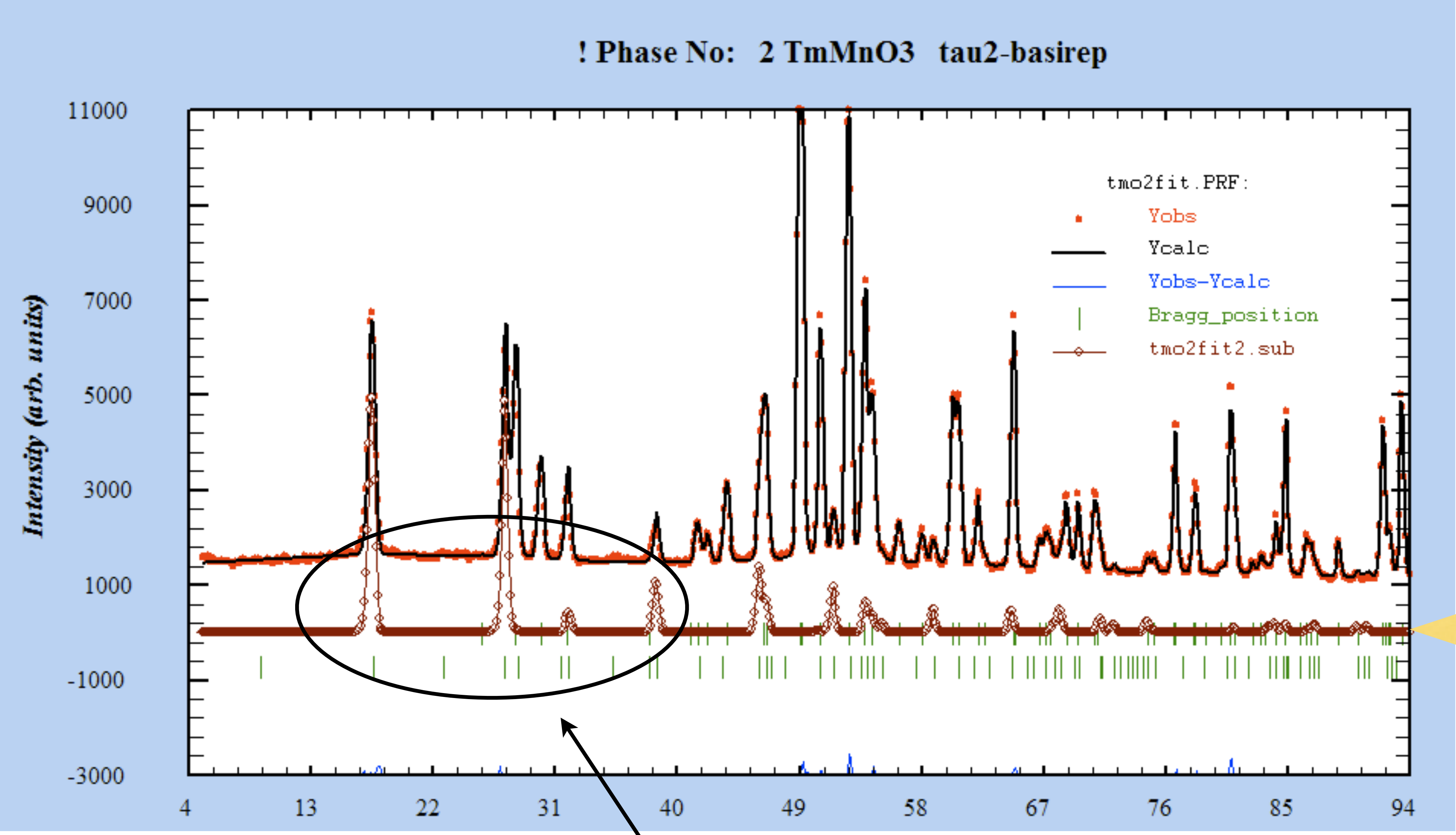
4. Fitting the data. In difficult cases 'simulated annealing' search of the solution is needed

Step 1

Experiment. q-range/resolution.

cf. resolution/q-range

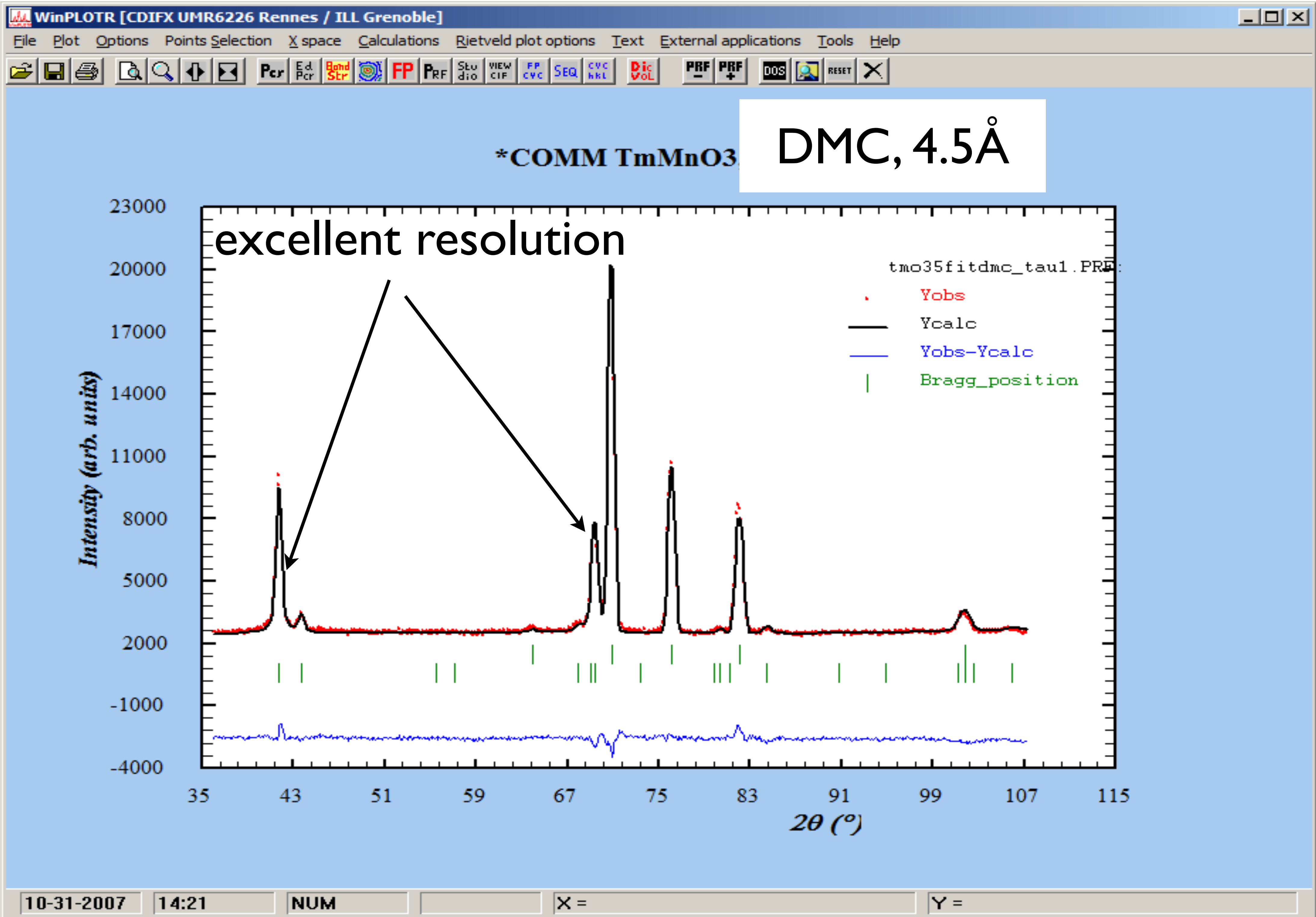
HRPT 1.9Å



magnetic contribution

DMC range at 4.5Å

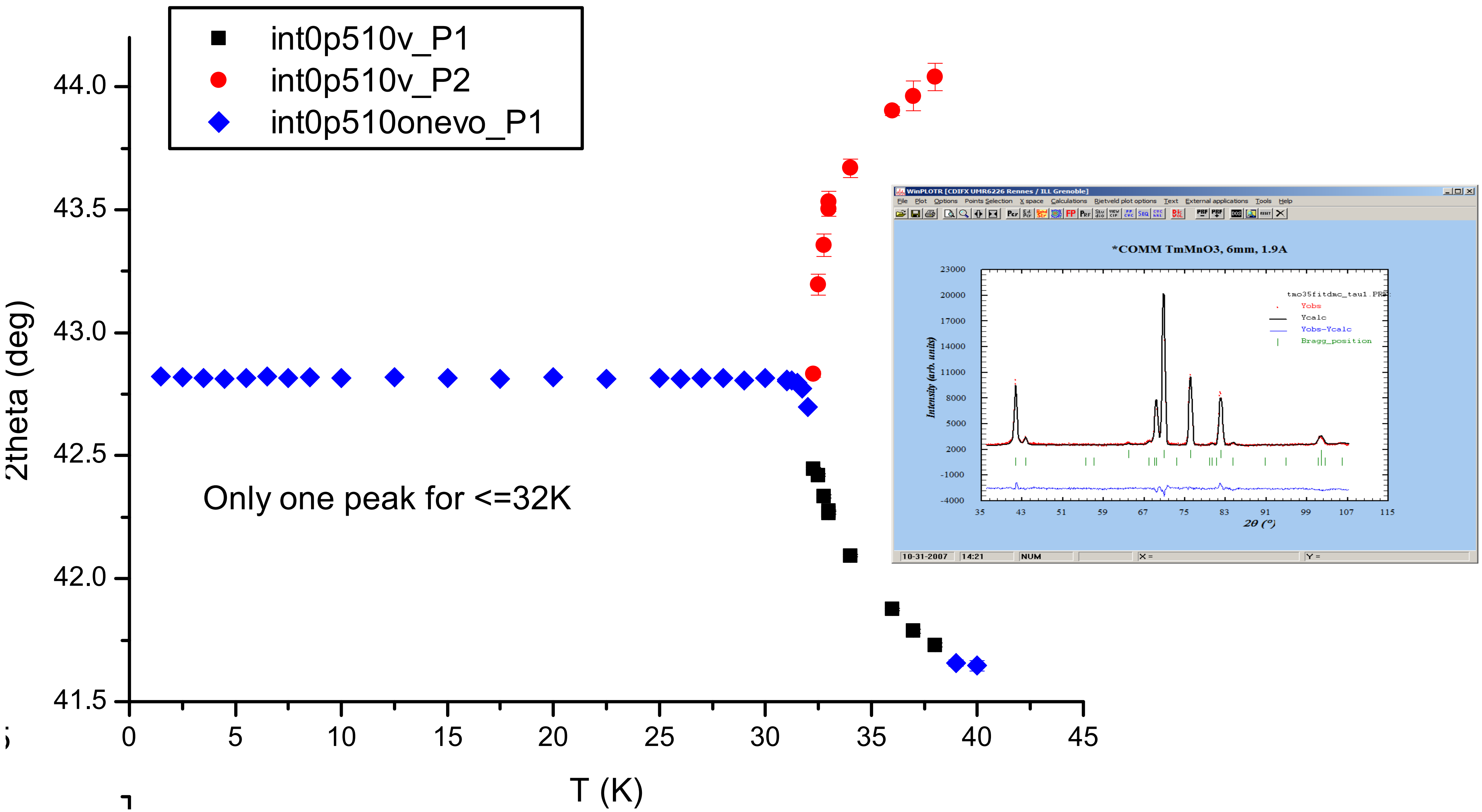
Cf. resolution/q-range



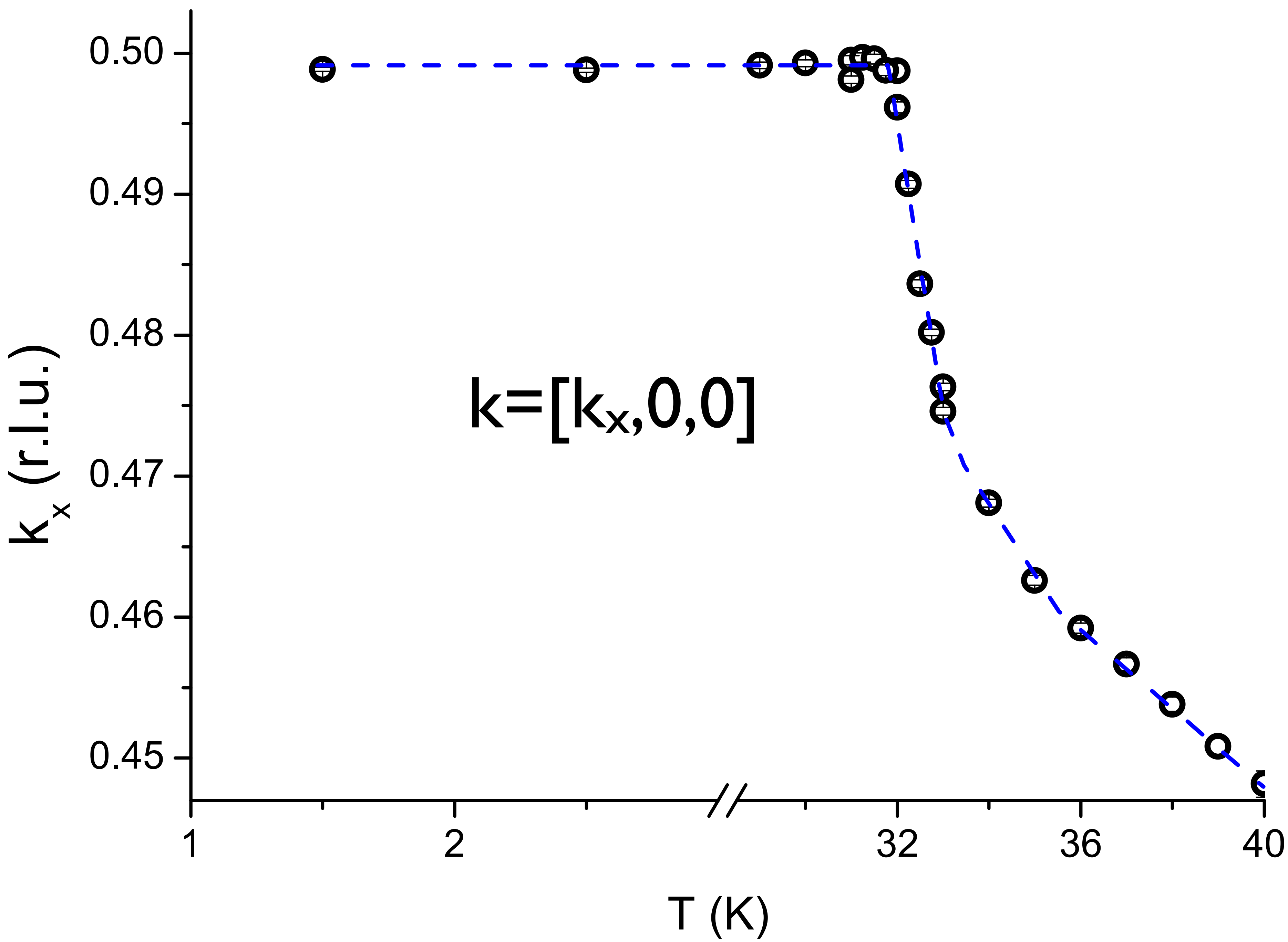
Step 2

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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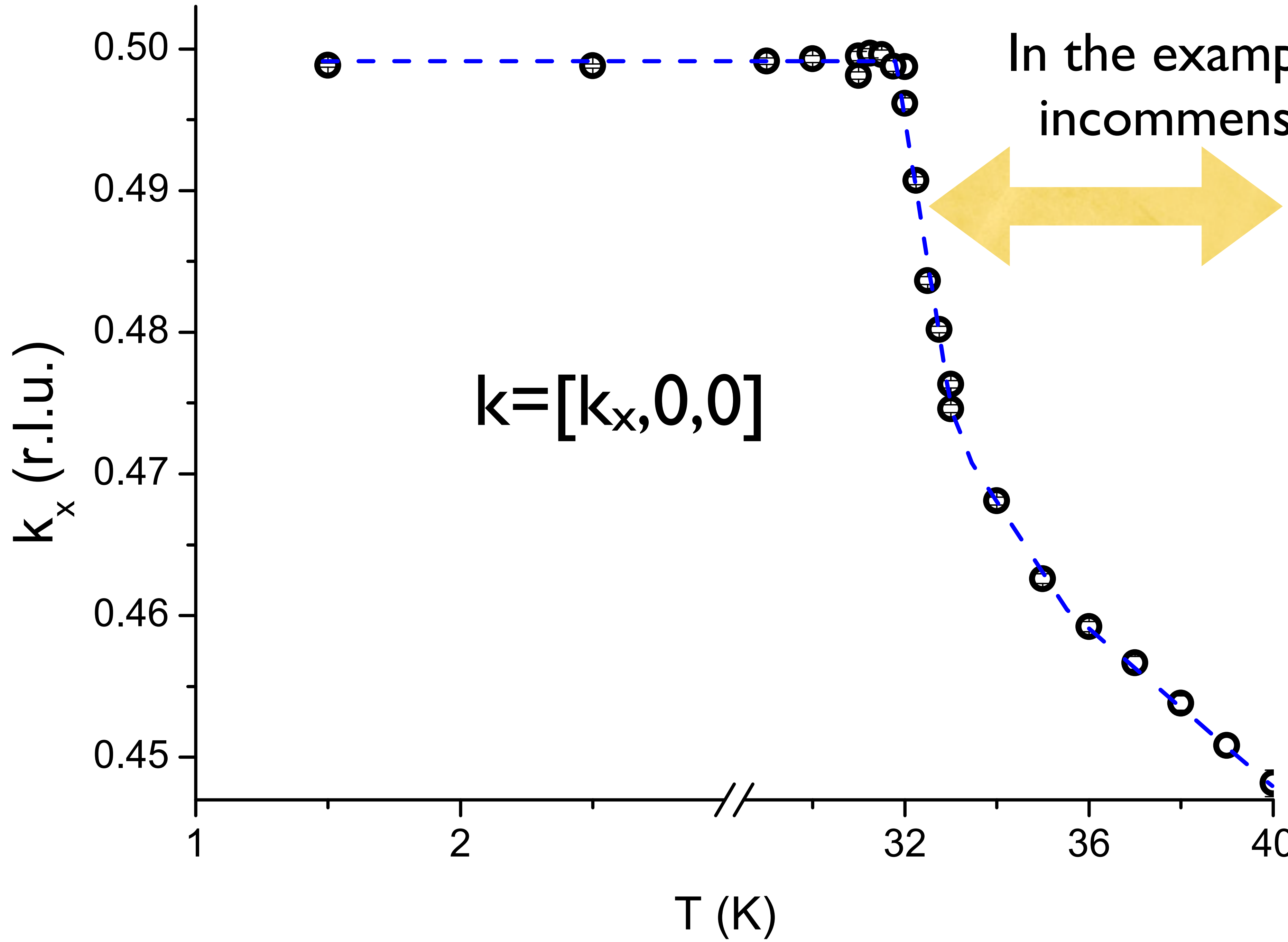


In the example we determine incommensurate structure

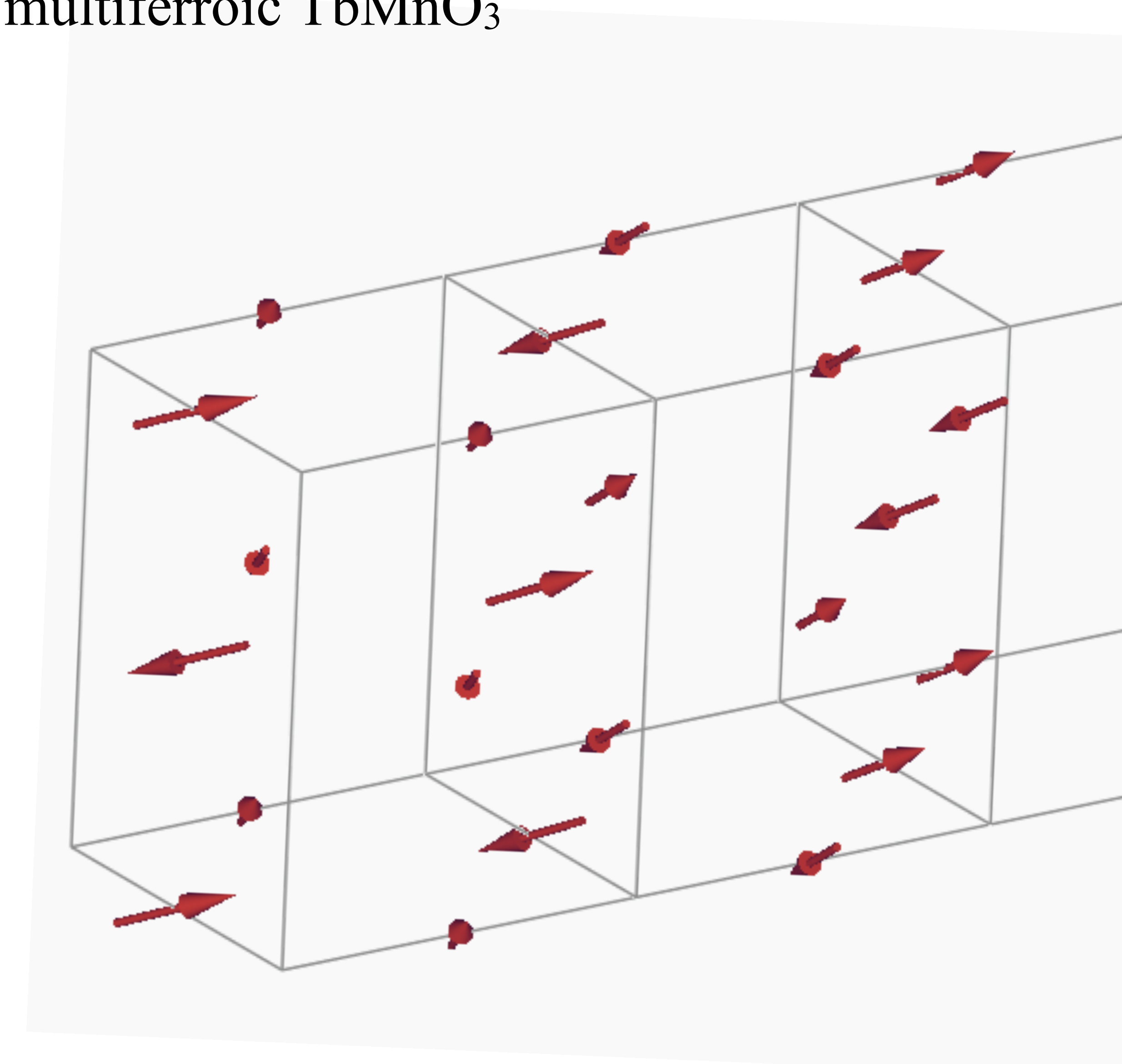
Step 3

Symmetry analysis.
Classifying possible magnetic structures

Constructing of normal modes of magnetic structure from irreps

Case study of magnetic structure of multiferroic $TbMnO_3$

Space Group *G: Pnma,* no.62
propagation vector k=[μ,0,0]



New Journal of Physics 11, 043019 (2009)

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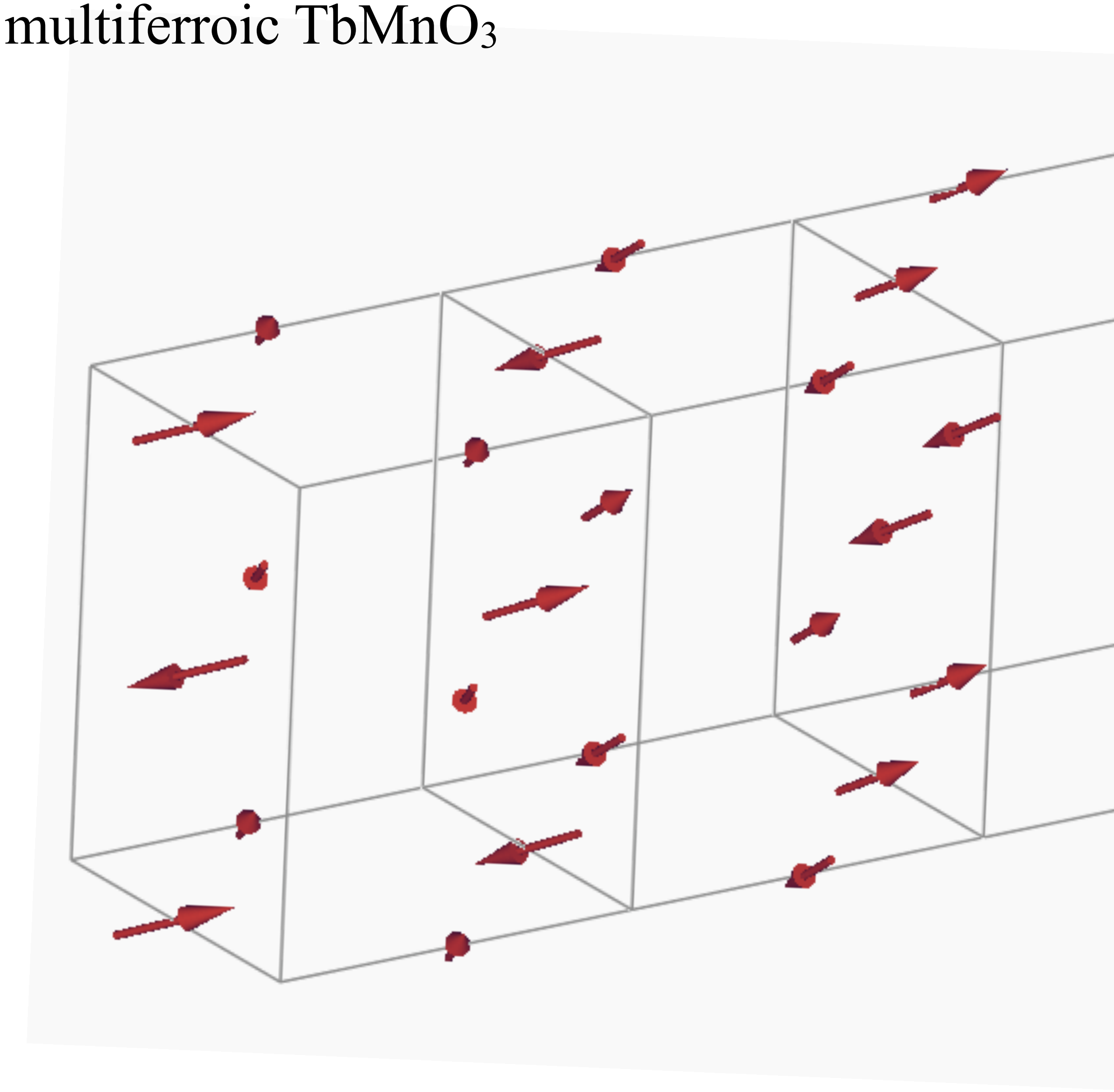
has 4 1D irreducible representations



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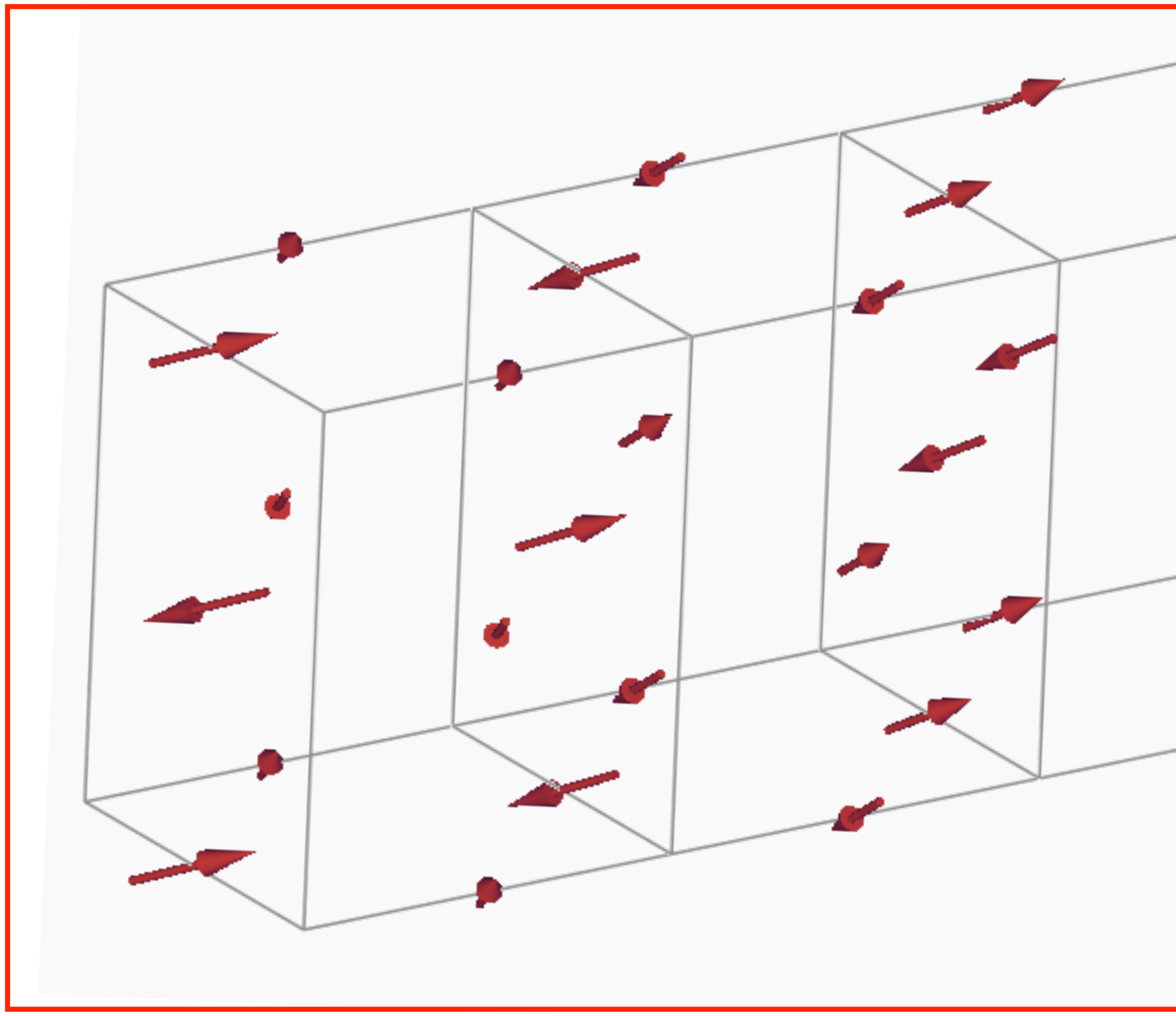

symmetry irreps ⟷ linear space spanned by Mn spins

New Journal of Physics 11, 043019 (2009)

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

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

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

	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
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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 τ3

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

k=[0.45,0,0]

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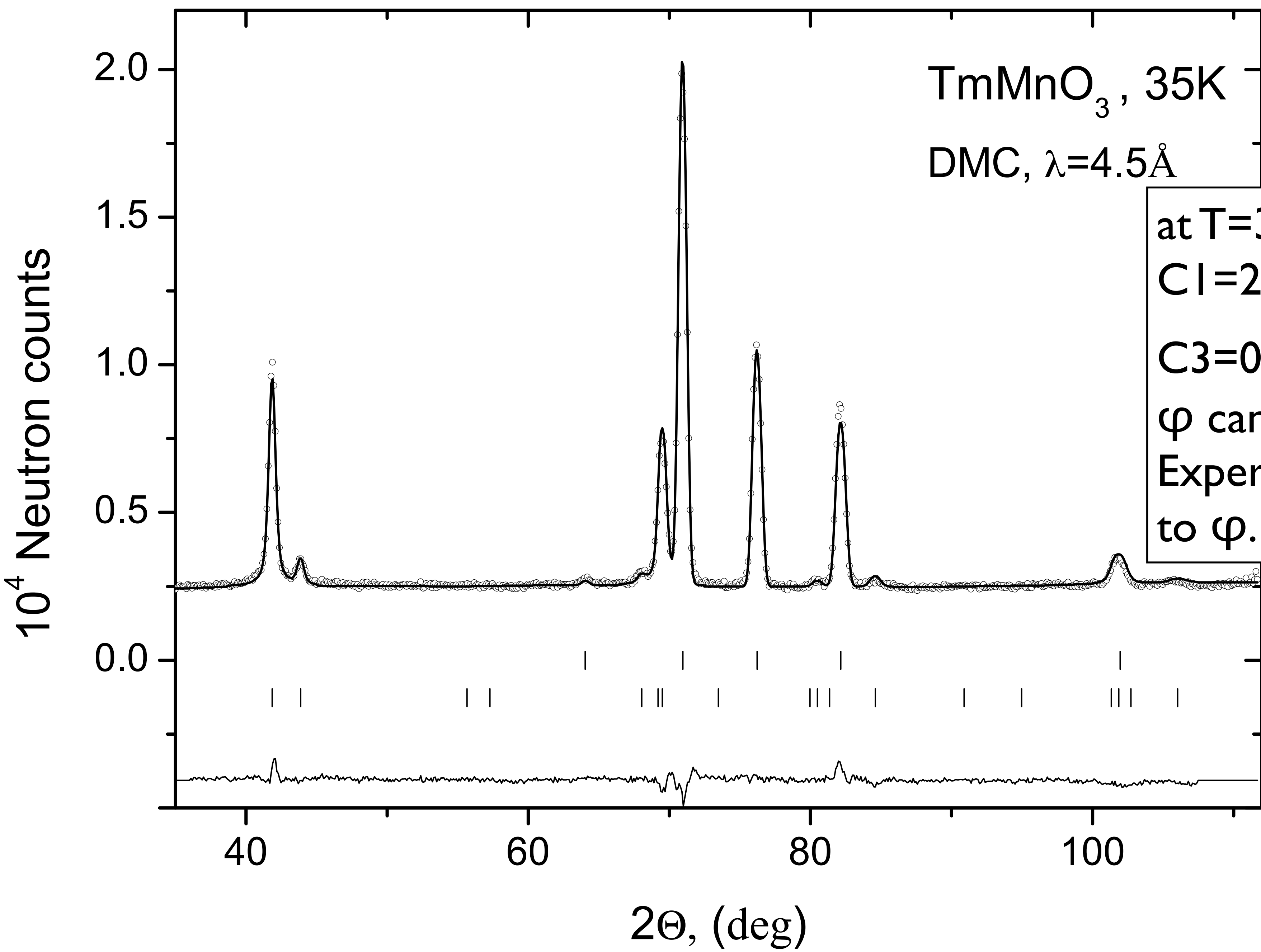

at T=35K
C1=2.11(1)μ_B, C2=0,
C3=0.67(2) $e^{i\varphi}$ μ_B
φ can be fixed to any value.
Experiment data are insensitive to φ.

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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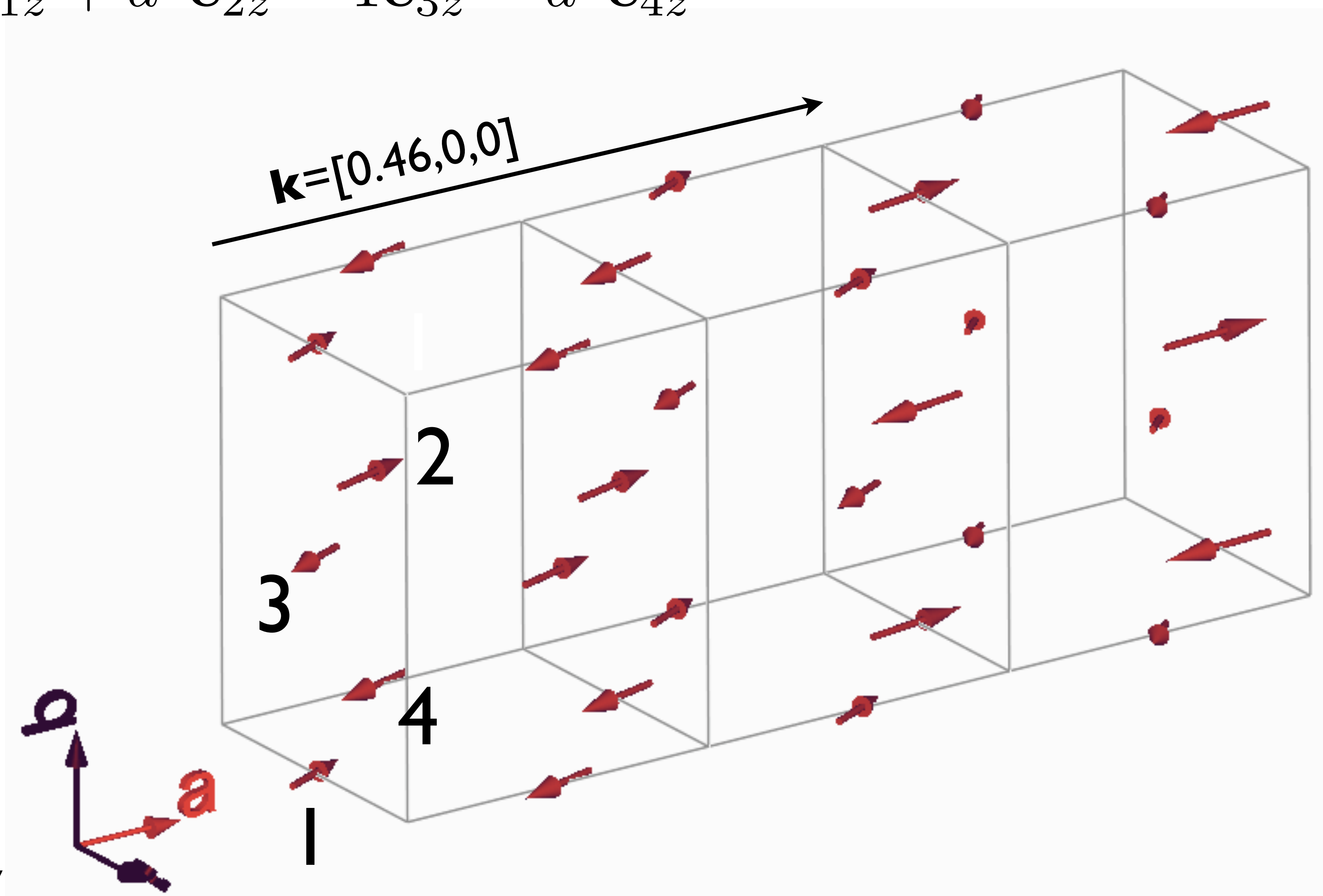

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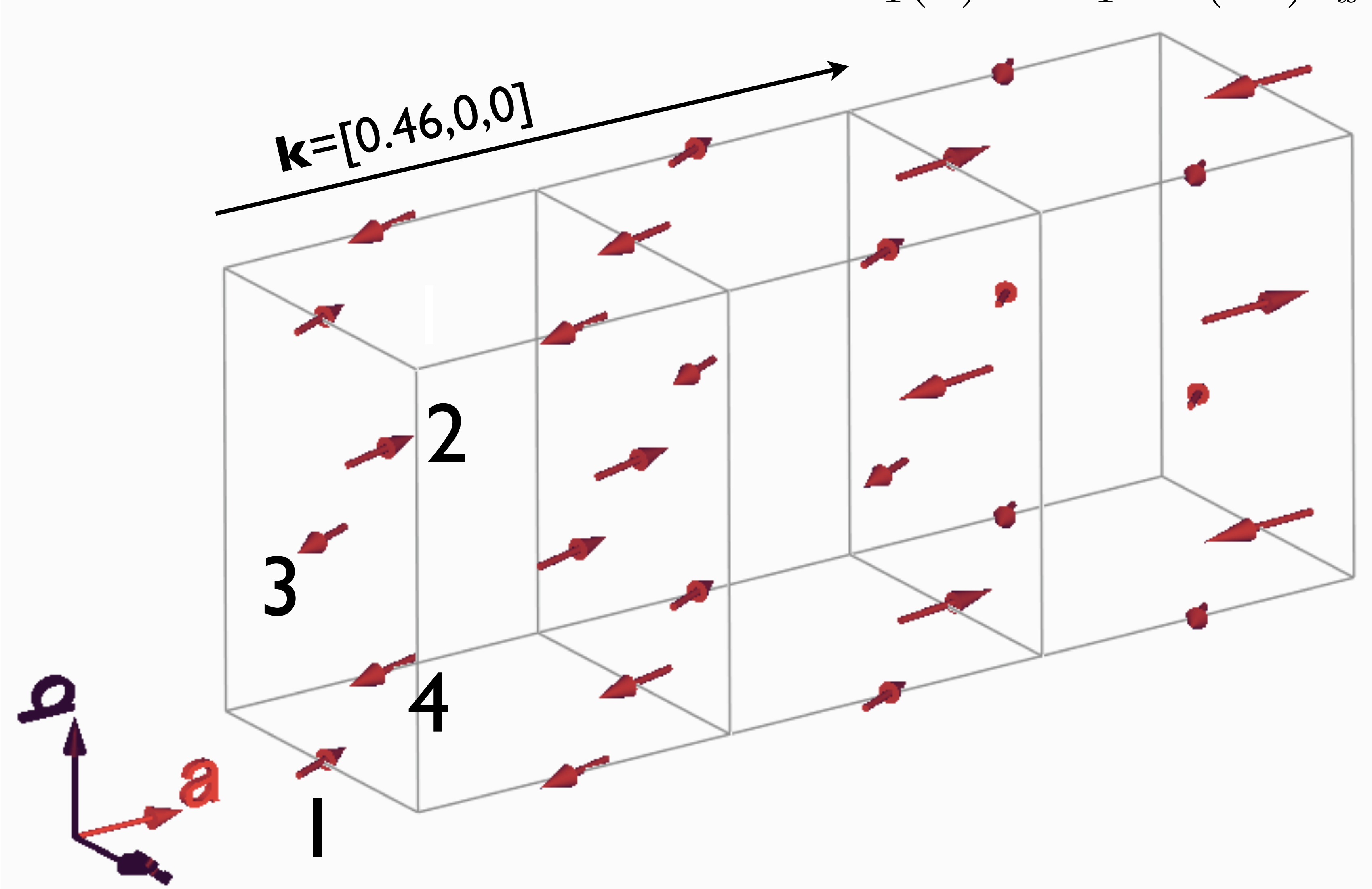
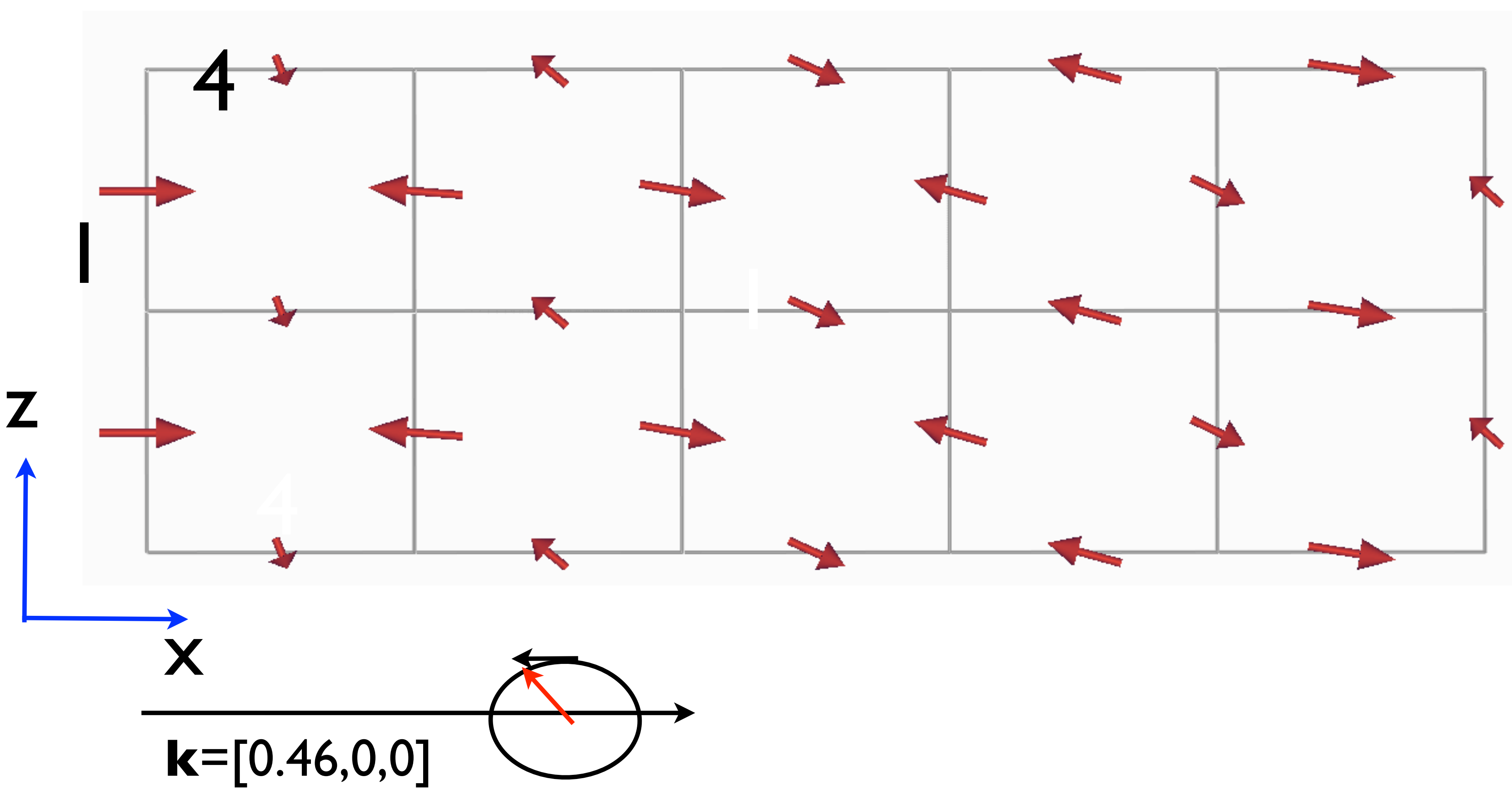
Propagation of the spin, e.g. for atom no. 1

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



Visualization of the magnetic structure: xz-projection

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



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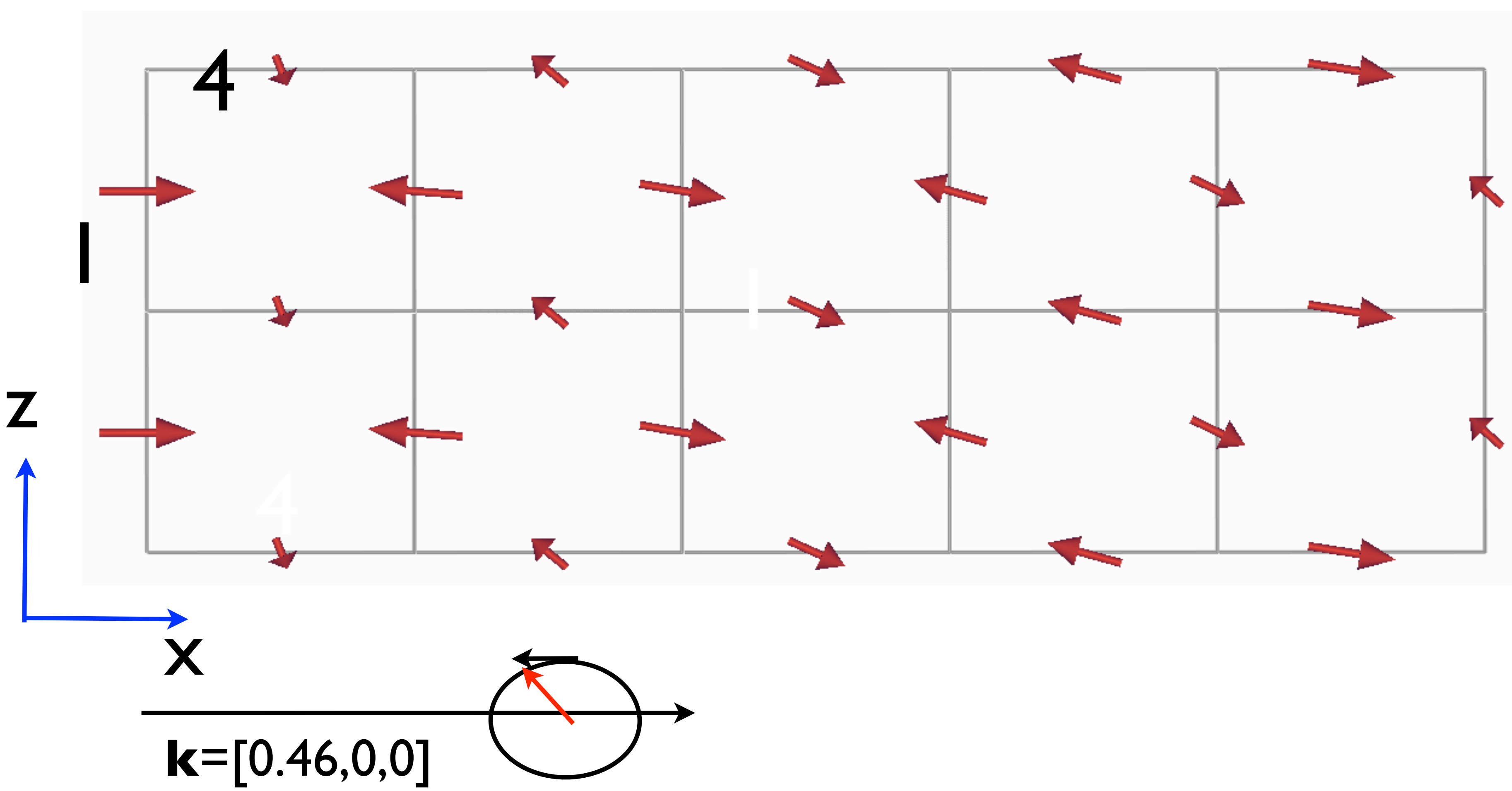
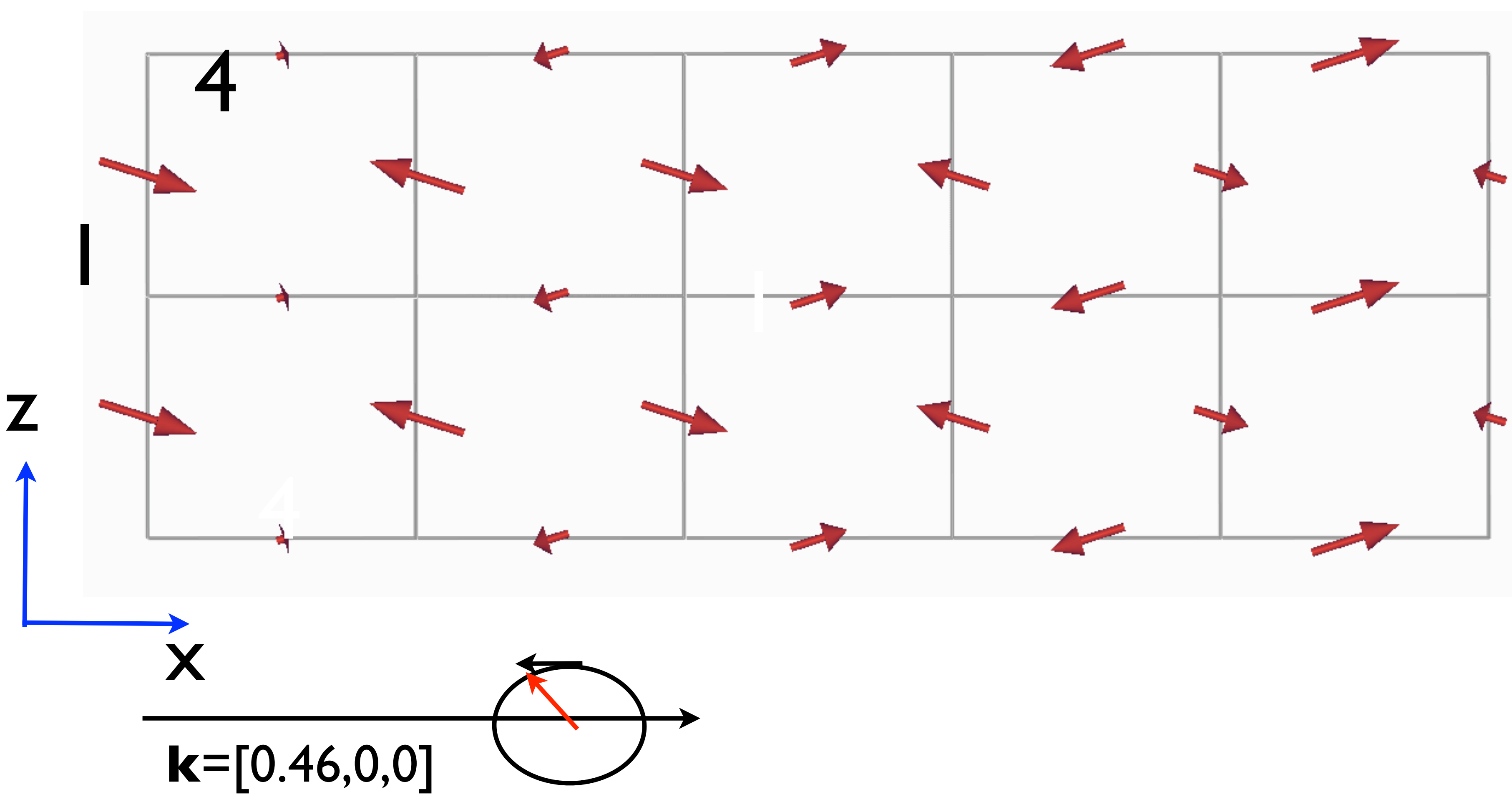


Visualization of the magnetic structure: xz-projection

for $\varphi=0$:
only the size of S_1 are changed

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

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



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

- 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,

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

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

This lecture:

http://sinq.web.psi.ch/sinq/instr/hrpt/doc/magdif13.pdf

further complications

further complications

1. several irreps involved, e.g. exchange multiplet
2. multi-k structures
3. spin domains, k-domains, chiral domains for single crystal data