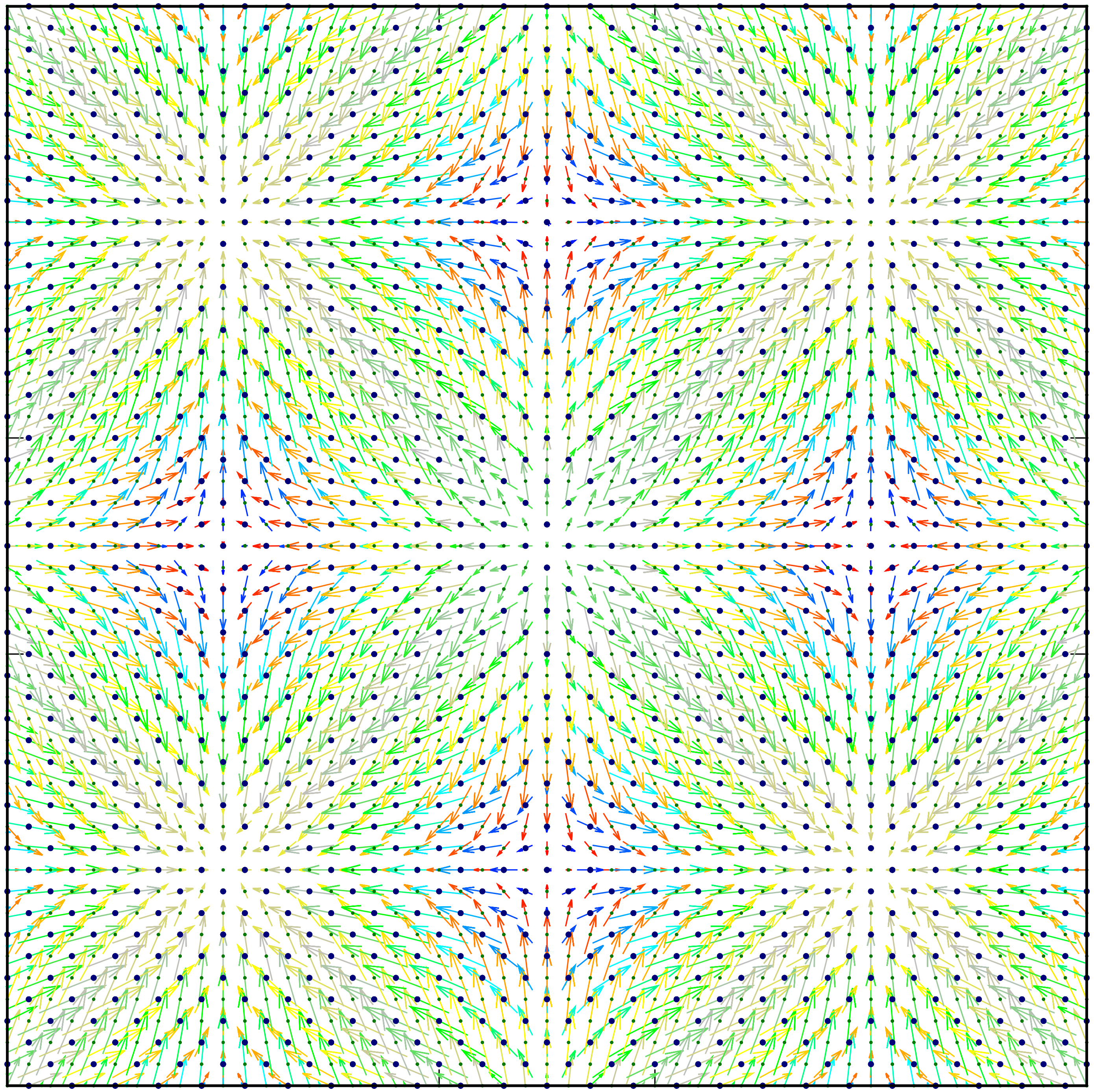
Magnetic symmetry for multi-k structure models

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



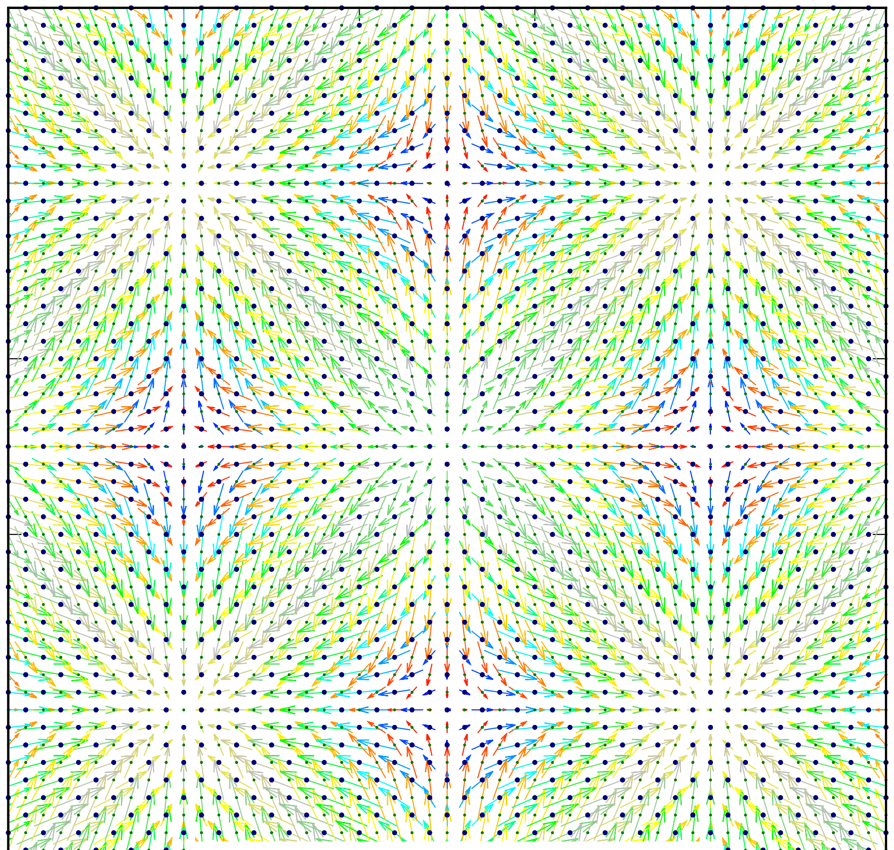
The pdf-file with this talk will be available at https://www.psi.ch/en/lns/people/vladimir-pomjakushin

or short link http://psi.ch/dKky

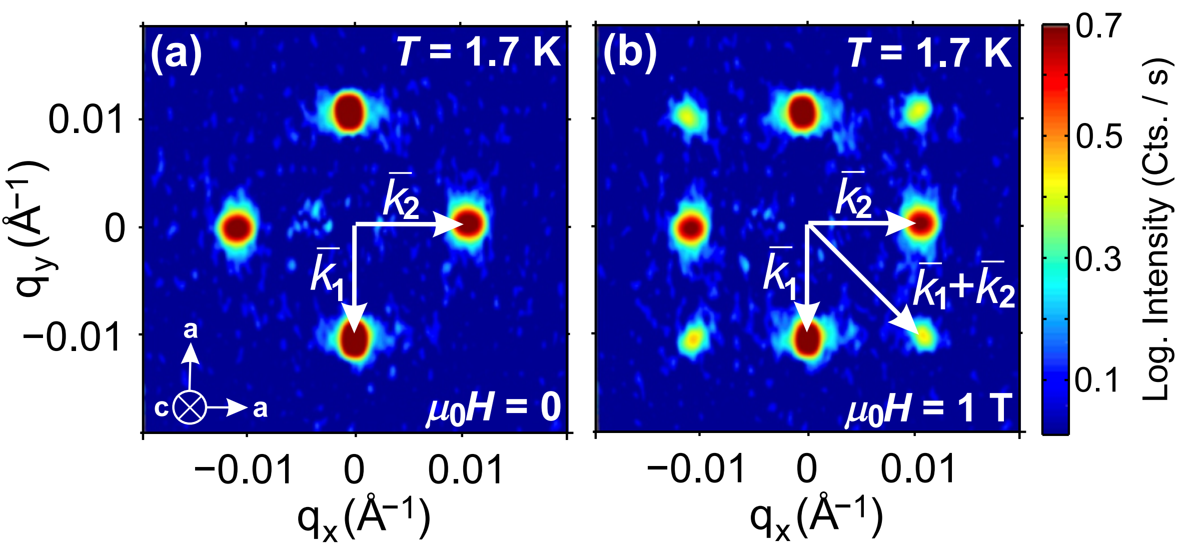
Magnetic symmetry for multi-k structure models

k1=[0,g,0], k2=[g,0,0]

wavevector or propagation vector of modulated magnetic structure $\sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$



Period about 15 cells, ~ 65 Å



multi-arm vs. multi-k

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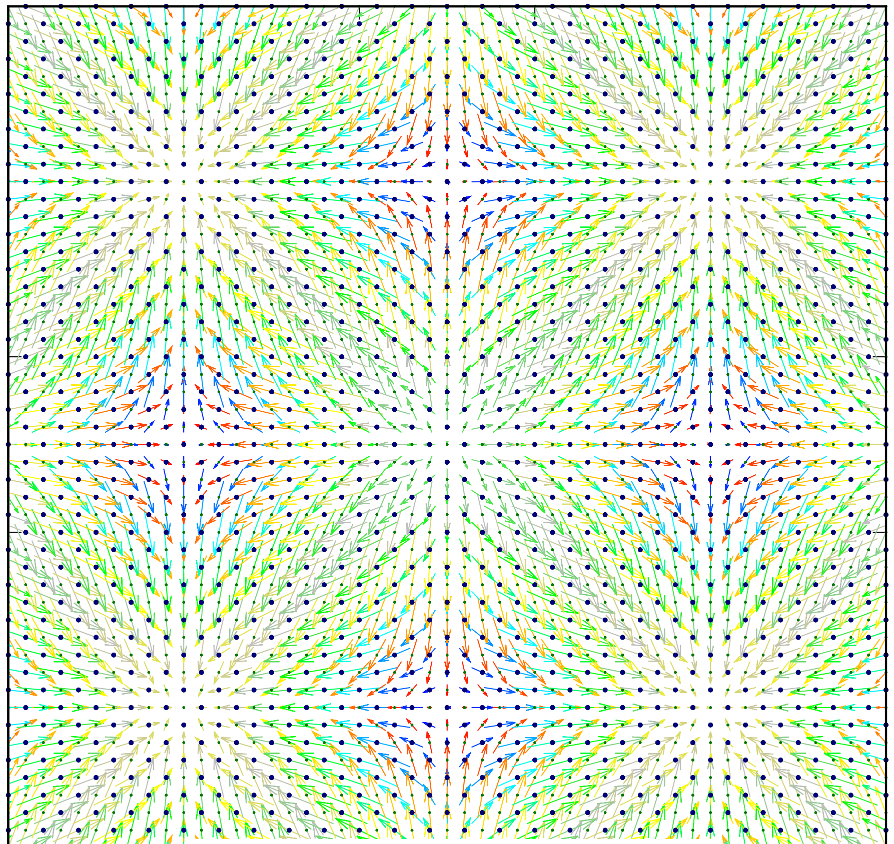
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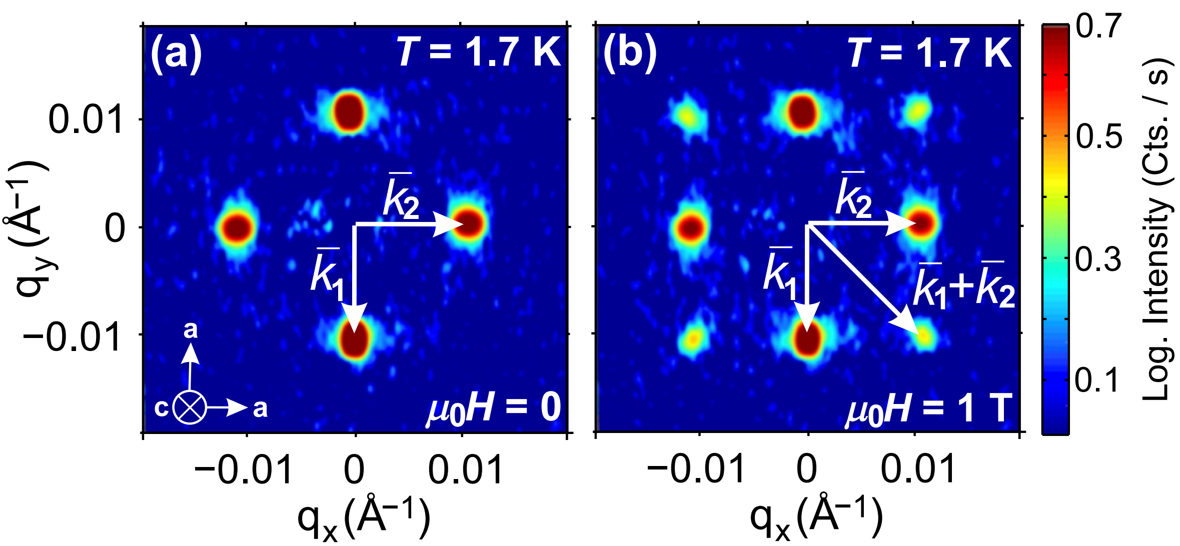
wavevector or propagation vector of modulated magnetic structure $\sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$

1. Multi-k structure is not very special case by magnetic symmetry

2. Symmetry analysis is done in a similar way for both multi-arm case and the case of multidimensional irreps (irreducible representations)

3. Multi-k/arm structures are special because only they can have non-trivial topological properties.



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

In 1960th-70th opposed

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

W. Opechovski, UBC, Vancouver
Shubnikov magnetic space groups

even until recent times RA was considered to be more powerful in neutron scattering community.*

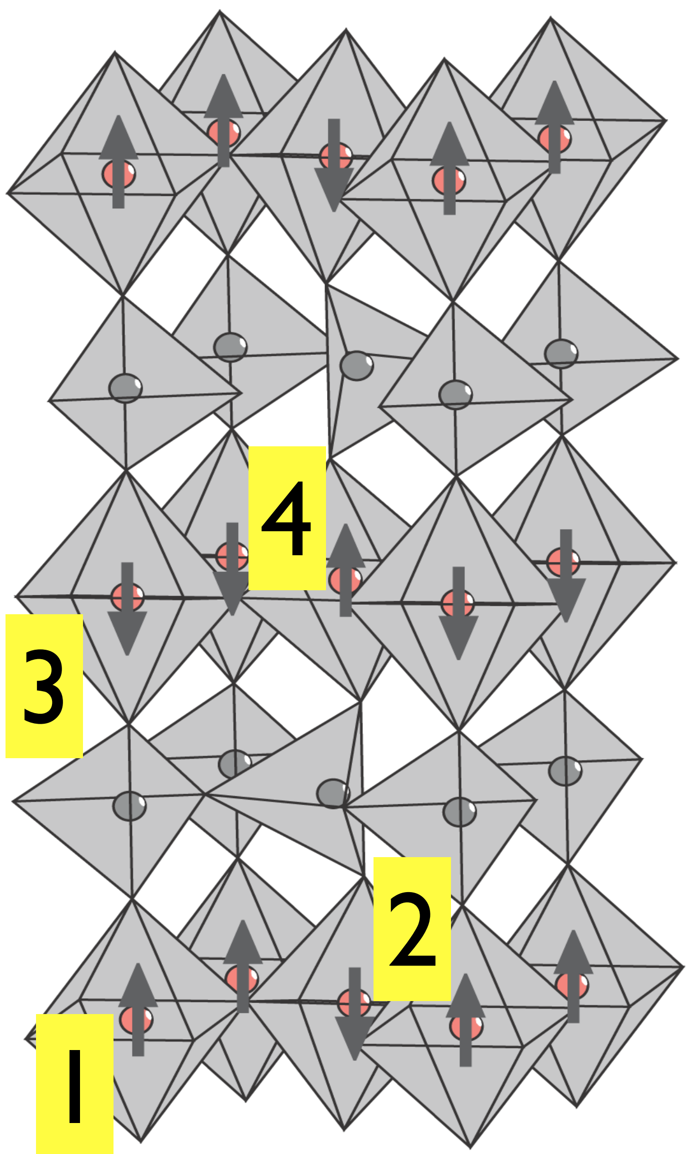
* Yu.A. Izyumov, V. E. Naish well known papers (1978-), book:, *"Neutron diffraction of magnetic materials"*, New York [etc.]: Consultants Bureau, 1991.

RA + symmetry for crystal structure
H. T. Stokes and D. M. Hatch (1988)

Two ways of description of magnetic structures

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

Crystal with space group *G*



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

   or

2. How can $\mathbf{S}(\mathbf{r})$ be transformed under elements of G ?
   $g\mathbf{S}(\mathbf{r}) = \mathbf{S}^{new}{}_{g}(\mathbf{r})$ to different functions for each $g \in G$

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Currently > 2010-…

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

IUCr Commission on Magnetic Structures

to establish standards for the description and dissemination of magnetic structures and their underlying symmetries…

http://magcryst.org

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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...

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

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

ISODISTORT: ISOTROPY Software Suite http://iso.byu.edu

ISOTROPY Software Suite

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

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

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

bilbao crystallographic server

Modern way of magnetic symmetry and representation analysis

Topical Review

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

"***MAGNDATA: towards a database of magnetic structures I & II***"
Gallego, Perez-Mato, Elcoro, Tasci, Hanson, Momma, Aroyo & Madariaga
JOURNAL OF APPLIED CRYSTALLOGRAPHY (2016) Volume: 49 Pages: 1750-1776, 1941-1956

"Tabulation of irreducible representations of the crystallographic space groups and their superspace extensions"
Harold T. Stokes, Branton J. Campbell and Ryan Cordes
Acta Cryst. (2013). A69, 388–395

Enumeration and tabulation of magnetic (3+d)-dimensional superspace groups
H. T. Stokes and B. J. Campbell
Acta Cryst. (2022). A78, 364-370

All that is needed to know about magnetic neutron diffraction. Symmetry, representation analysis

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

Propagation vector k formalism. Spin amplitudes S_0 are specified in zeroth block of the cell==parent cell w/o centering translations.

All C, I, F, R –> Primitive

Magnetic moment below a phase transition

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

$$\equiv |S_{0\alpha}| \cos(2\pi \mathbf{t}_n \mathbf{k} + \phi_\alpha)$$
$$\alpha = x, y, z$$

Bragg peaks at

$$\mathbf{q} = \mathbf{H} \mp \mathbf{k}$$

In general
-k is nonequivalent to **+k**
i.e. **-k**≠**k**+'recip. latt. period'

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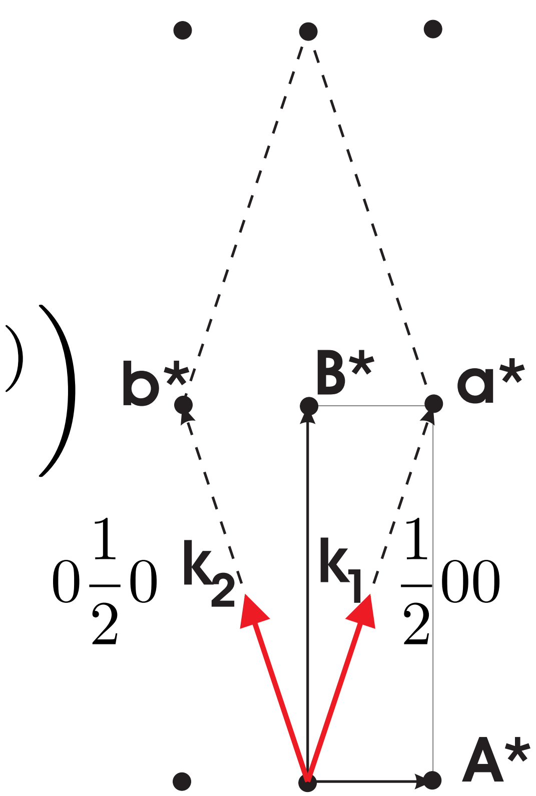
multi-**k** or multi-*arm*★ structure
(non-equivalent $\mathbf{k}_1$, $\mathbf{k}_2$, … $\mathbf{k}_m$).

$$\mathbf{S}(\mathbf{t}_n) = \sum_{l=1}^{m} \frac{1}{2}\left(\mathbf{S}_{0l} e^{2\pi i \mathbf{t}_n(+\mathbf{k}_l)} + \mathbf{S}_{0l}^* e^{2\pi i \mathbf{t}_n(-\mathbf{k}_l)}\right)$$



★One must distinguish between the *arms* and the *twin* domains

Representation analysis RA without symmetry

Representation★ Analysis (RA). Propagation vector k formalism.

Magnetic mode S_0 is specified in zeroth block of the cell == parent cell without centering translations

Magnetic moment
below a phase transition $\mathbf{S}(\mathbf{t}_n) = Re\left(C\mathbf{S}_0 e^{2\pi i \mathbf{t}_n \mathbf{k}}\right) \sim \cos(2\pi\mathbf{t}_n\mathbf{k} + \varphi)$

amplitude or mixing coefficients (→ C)

magnetic mode (→ $\mathbf{S}_0$)

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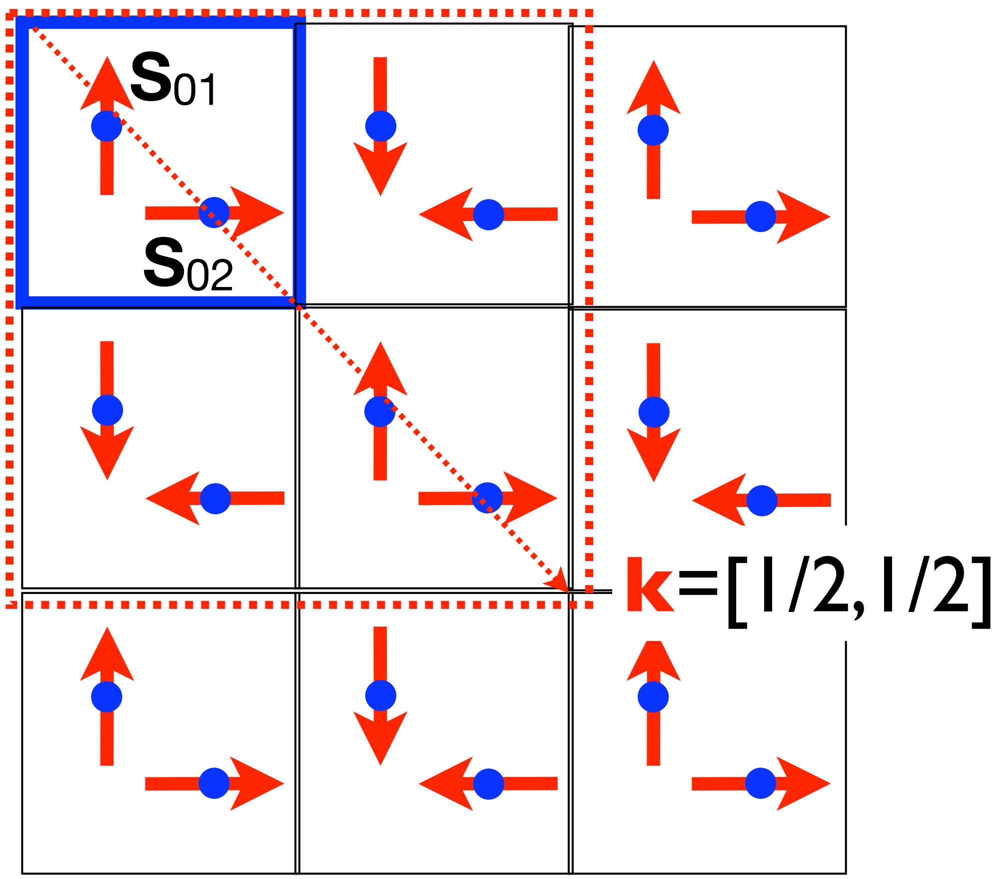
zeroth cell of parent space group



★irreducible representation irrep:
each group element *g* --> *matrix τ(g)* that

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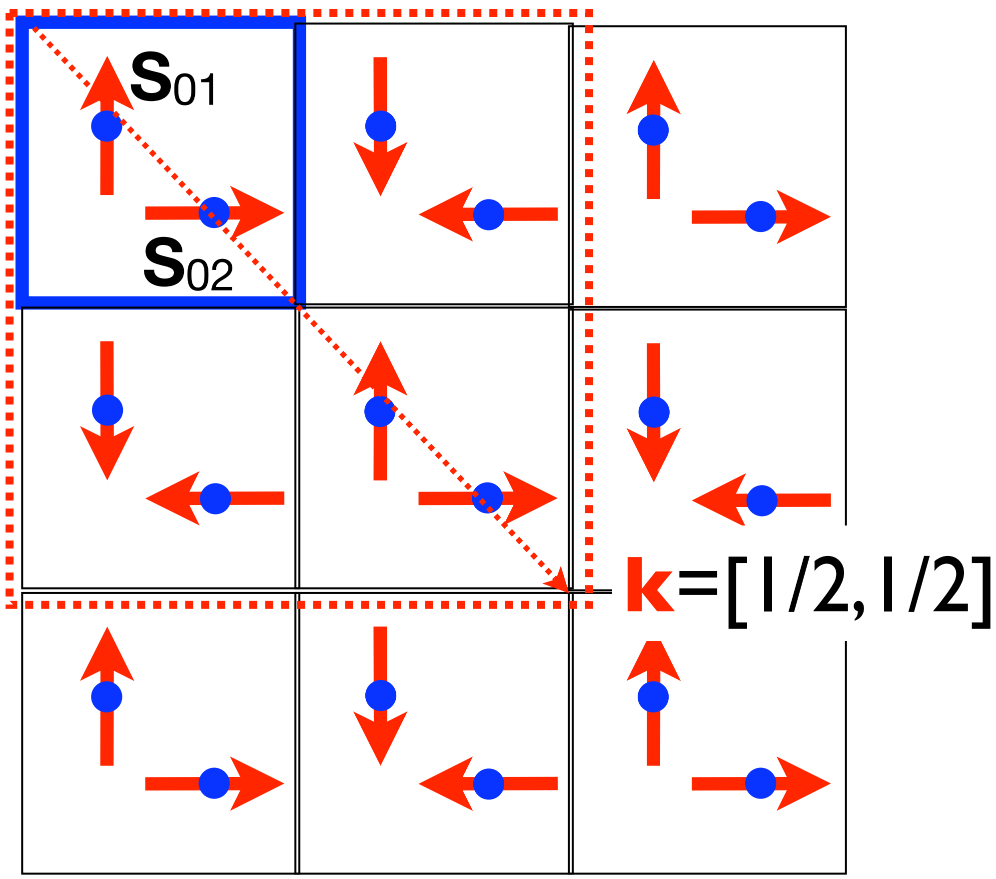

magnetic mode $\mathbf{S}_0$ for chosen irrep★ specifies magnetic configuration of all spins in zeroth cell

$$\mathbf{S}_0 = \begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \cdots \\ \cdots \\ \cdots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$$

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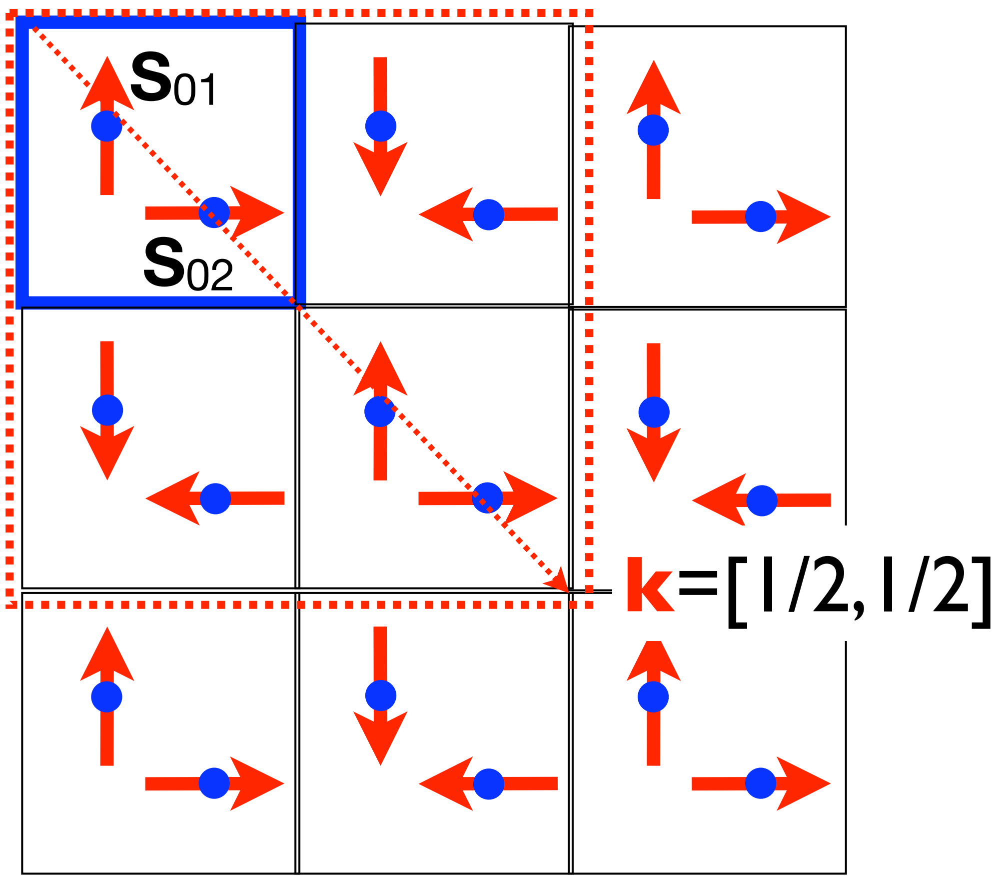
amplitude or mixing coefficients (points to C)

magnetic mode (points to $\mathbf{S}_0$)

zeroth cell of parent space group



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

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

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

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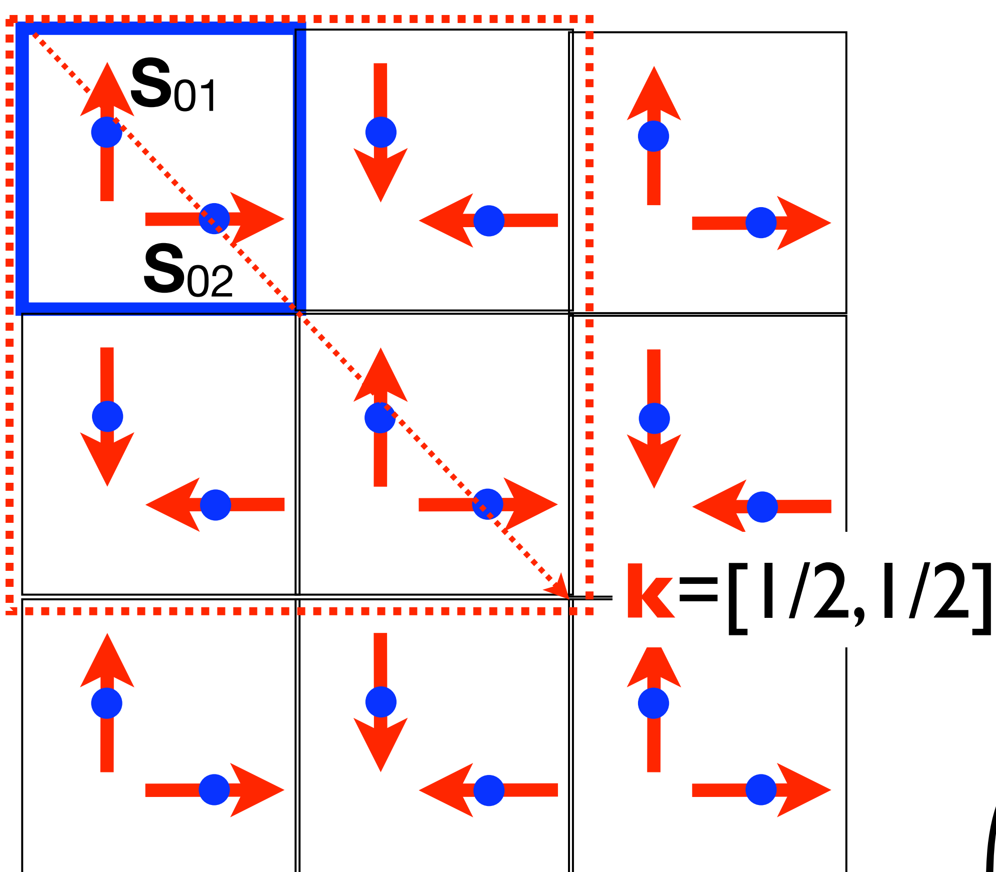

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C: amplitude or mixing coefficients

$\mathbf{S}_0$: magnetic mode

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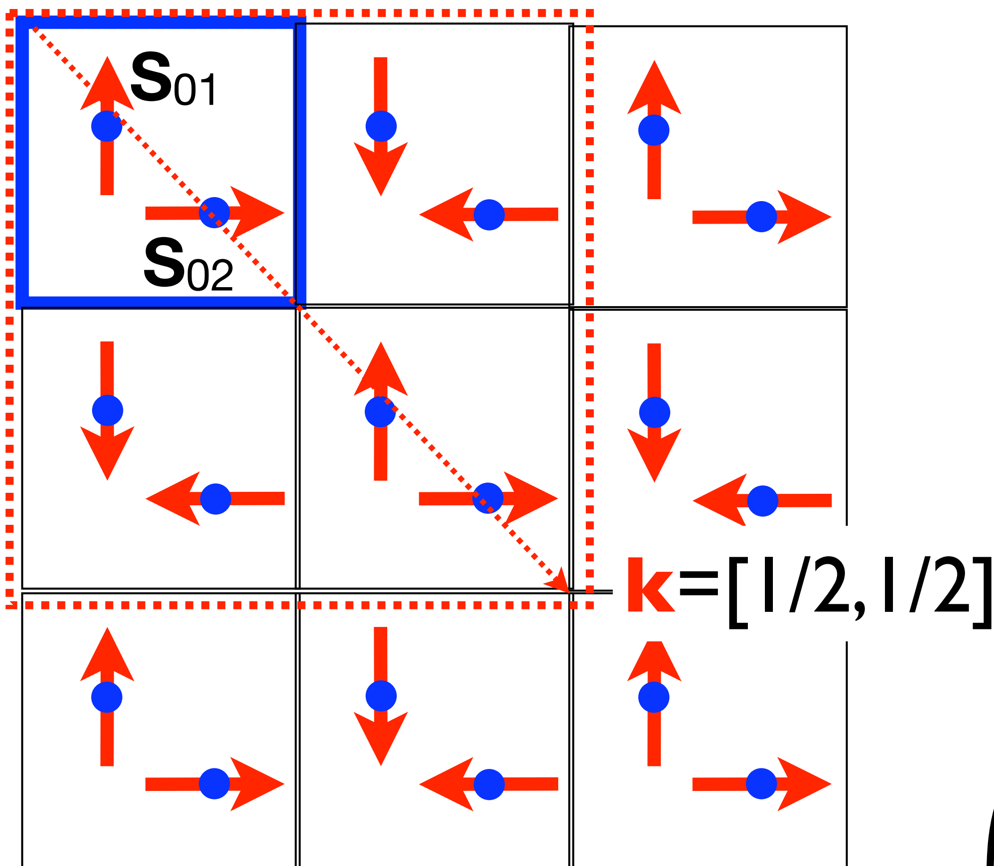

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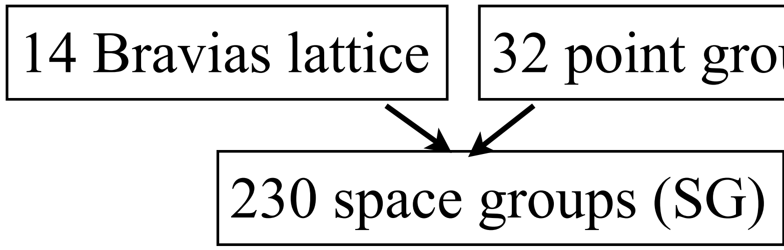
$\mathbf{S}_0$ and $C = |C|e^{i\varphi}$ are complex quantities

$$s_{x1} = |s_{x1}|e^{i\phi_{x1}}\mathbf{e}_x$$
$$s_{y1} = |s_{y1}|e^{i\phi_{y1}}\mathbf{e}_y$$
$$\cdots$$
$$s_{zN} = |s_{zN}|e^{i\phi_{zN}}\mathbf{e}_z$$

Magnetic symmetry without irreducible representations

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



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

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

14 Bravias lattice → 230 space groups (SG) ← 32 point groups

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

⇒

R(♖) = ♜
R(☺)= ☹
R(↑) = ↓

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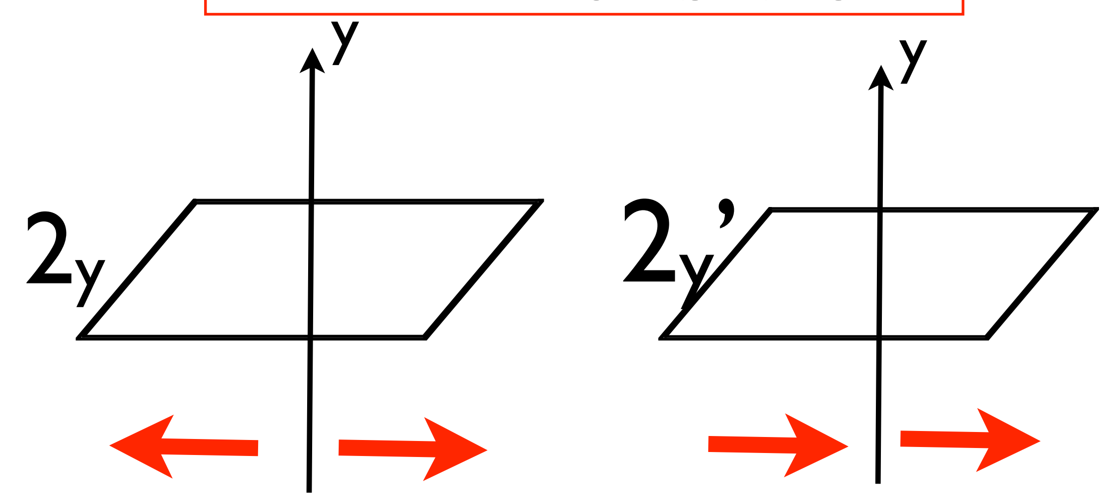

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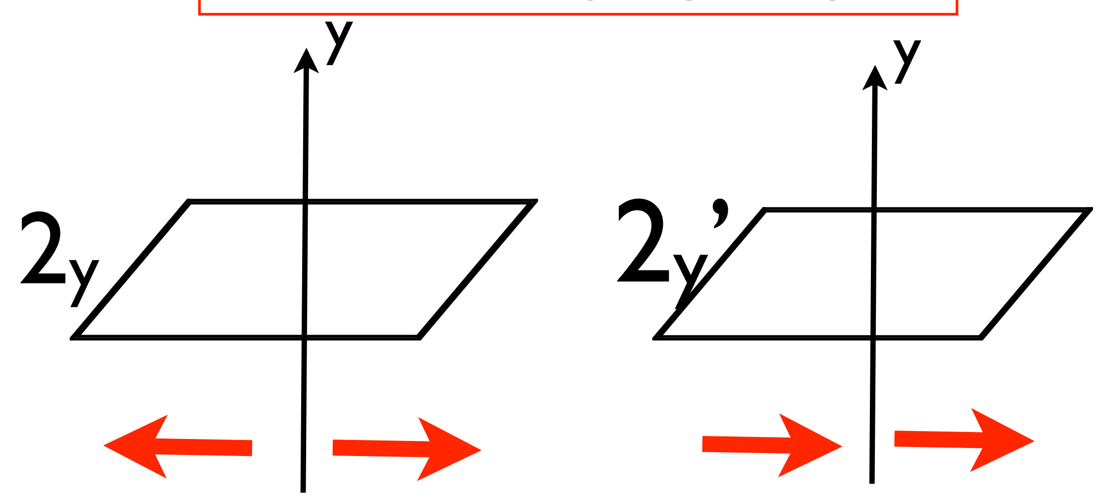
Magnetic Groups = (subgroup of) space group $G \otimes$ R-group

additional elements:
'anti-elements' g'=($g \cdot R$), $g \in G$



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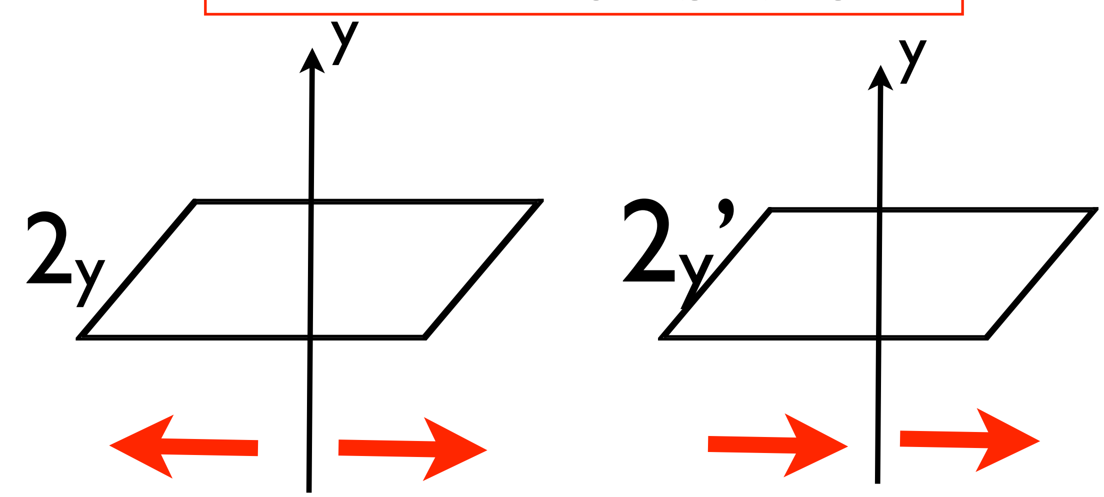
230 (gray) paramagnetic groups Sh_p
<u>1,1' ∈ Sh_p</u> ⇒ **S**=0 , e.g. *Pnma1'*



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

230 Single-color magnetic groups
<u>no antielements</u>

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

antisymmetry: Heesch (1929), Shubnikov (1945).
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Examples of Magnetic Space Groups (MSG)◆

59	$Pmmn$
	$Pm'mn$
	$Pmmn'$
	$*Pm'm'n$
	$*Pmm'n'$
	$Pm'm'n'$
	$P_{2c}mmn$
	$P_{2c}m'mn$
	$P_{2c}m'm'n$

62	$Pnma$
	$Pn'ma$
	$Pnm'a$
	$Pnma'$
	$*Pn'm'a$
	$*Pnm'a'$
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	$Pn'm'a'$

◆ Two setting are possible OG and BNS

Examples of Magnetic Space Groups (MSG)♦

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Ferromagnetic groups: point symmetry allows FM orientation of spins
Only 275 FM groups out of 1651…(~17%, 1/6th)

♦ Two setting are possible OG and BNS

Examples of Magnetic Space Groups (MSG)◆

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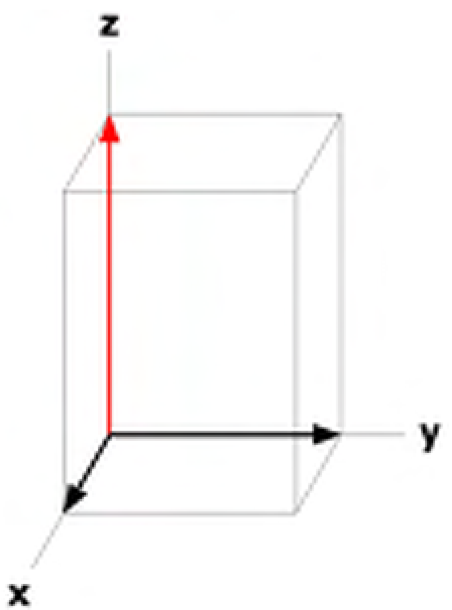
recap:
for ‘anti-elements’ g’=($g\cdot R$), $g \in G$
g can be a pure translation *t*, so *t’* gives centering/doubling



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

◆ Two setting are possible OG and BNS

Magnetic Space Groups MSG and propagation vector

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

- commensurate (C) : |**k**|=m/n, m,n: integers. For large (m,n) **k** should be considered incommensurate (IC)
- incommensurate IC |**k**|≠ m/n

MSG: only 3D-crystallographic symmetry elements, e.g. no arbitrary rotation angles, only 60, 90, 120, 180 degrees

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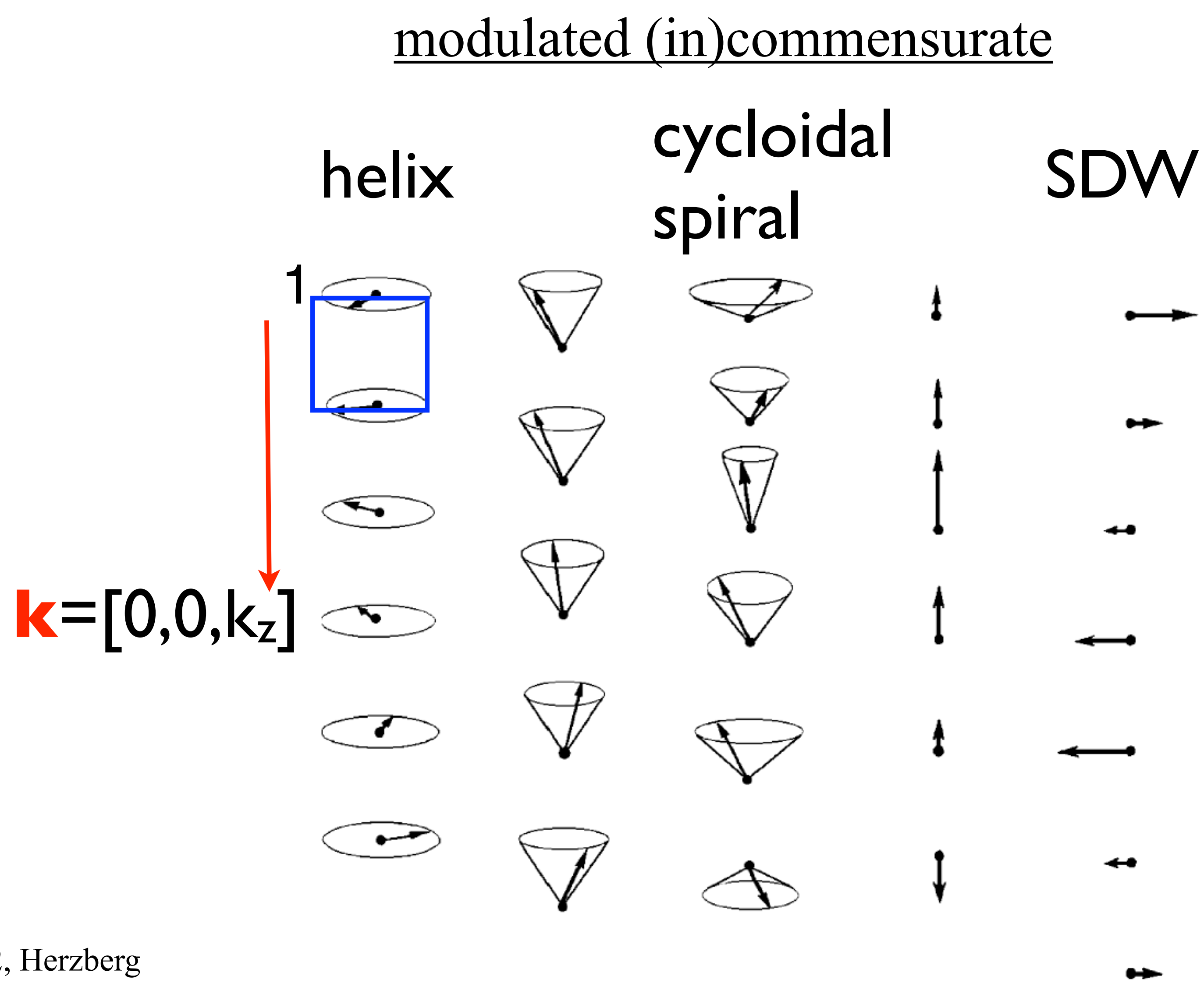
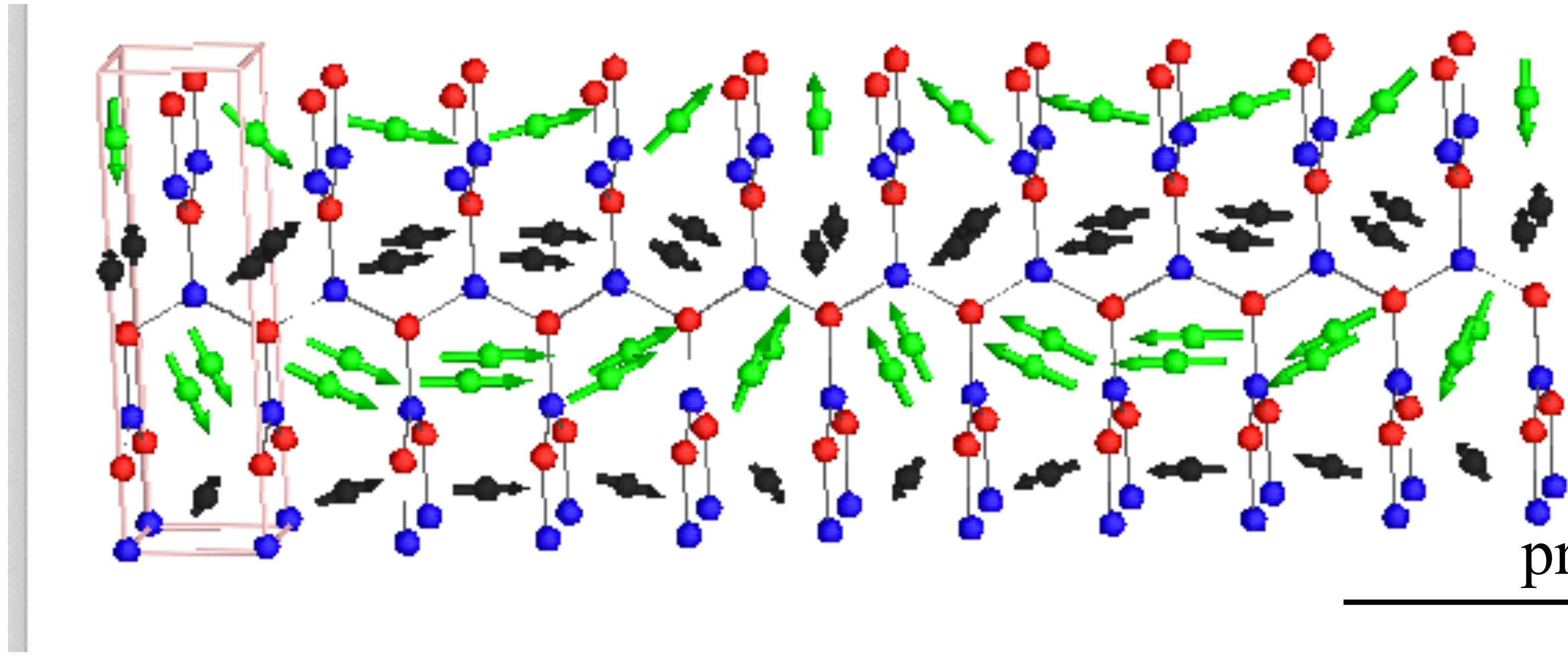
MSG: only 3D-crystallographic symmetry elements, e.g. no arbitrary rotation angles, only 60, 90, 120, 180 degrees



Superspace group concept



propagation vector **k**


J. Phys.: Condens. Matter **24** (2012) 163201

position $\boldsymbol{r}_{l\mu} = \boldsymbol{l} + \boldsymbol{r}_{\mu}$ ($\boldsymbol{l}$ being a lattice translation of the basic structure) is given by the value of the function $A_{\mu}(x_4)$ at $x_4 = \boldsymbol{k} \cdot \boldsymbol{r}_{l\mu}$:

$$A_{l\mu} = A_{\mu}(x_4 = \boldsymbol{k} \cdot \boldsymbol{r}_{l\mu}). \qquad (1)$$

These atomic modulation functions can be expressed by a Fourier series of the type

$$A_{\mu}(x_4) = A_{\mu,0} + \sum_{n=1,\ldots} [A_{\mu,ns} \sin(2\pi n x_4) + A_{\mu,nc} \cos(2\pi n x_4)]. \qquad (2)$$

x1 - x

x2 - y

x3 - z

x4 - internal coordinate is "just" a 2π normalised phase

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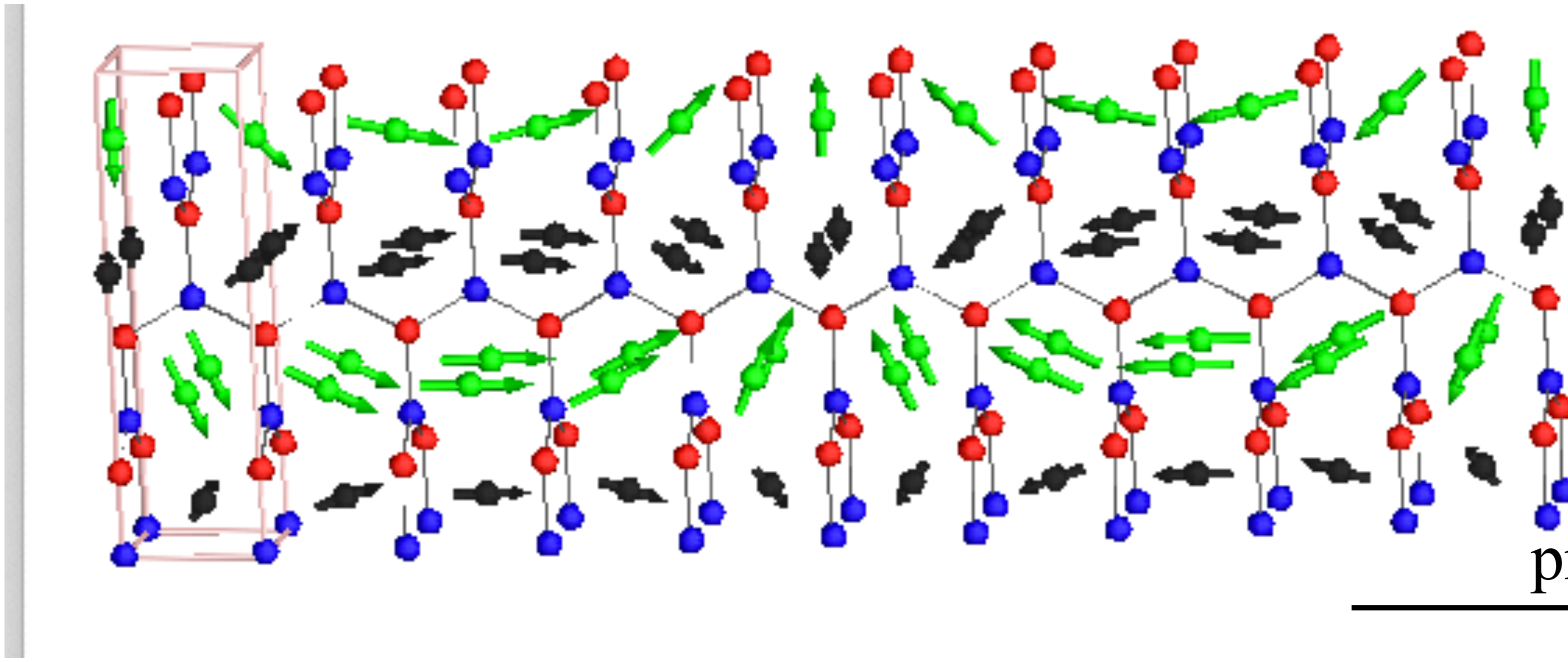

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Example of MSSGs

Table 1. Representative operations of the centrosymmetric superspace group $P\bar{1}1'(\alpha\beta\gamma)0s$ described by using generalized Seitz-type symbols (left column) and symmetry cards

$\{1\|0000\}$	x_1	x_2	x_3	x_4	$+m$
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	$+m$
$\{1'\|000\frac{1}{2}\}$	x_1	x_2	x_3	$x_4+\frac{1}{2}$	$-m$
$\{\bar{1}'\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4+\frac{1}{2}$	$-m$

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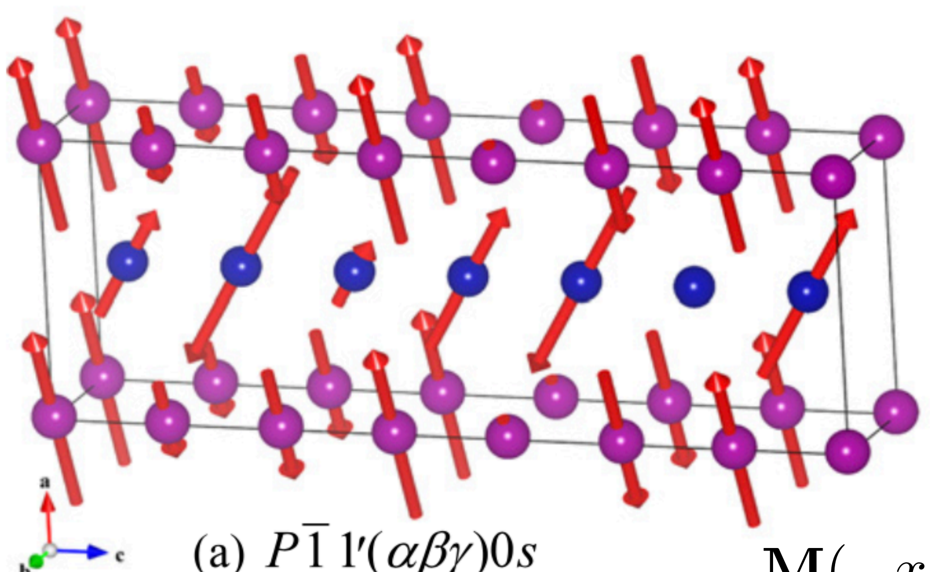
Some simple, maybe unexpected, exemplary consequences



(a) $P\bar{1}1'(\alpha\beta\gamma)0s$

This MSSG restrict all atoms located in special positions to be in phase and only AM is allowed for them.

$$\mathbf{M}(-x_4)=\mathbf{M}(x_4) \quad \rightarrow \mathbf{M}\sim\mathbf{m}\cdot\cos(2\pi x_4)$$

1	*h*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$
1	*g*	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$
1	*f*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$
1	*e*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$
1	*d*	$\bar{1}$	$\frac{1}{2},0,0$
1	*c*	$\bar{1}$	$0,\frac{1}{2},0$
1	*b*	$\bar{1}$	$0,0,\frac{1}{2}$
1	*a*	$\bar{1}$	$0,0,0$

Combined RA and MSG description of magnetic structures

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MSG Examples:

Shubnikov 3D		3D+1 superspace
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87.4.736	I4/m'	I41'(0,0,g)ss
87.5.737	I4'/m'	I41'(0,0,g)0s
87.6.738	I_P4/m	

3D+2 superspace

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irrep Example:

I4/m, k=0 has 8 1D irreps τ_1,... τ_8.

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

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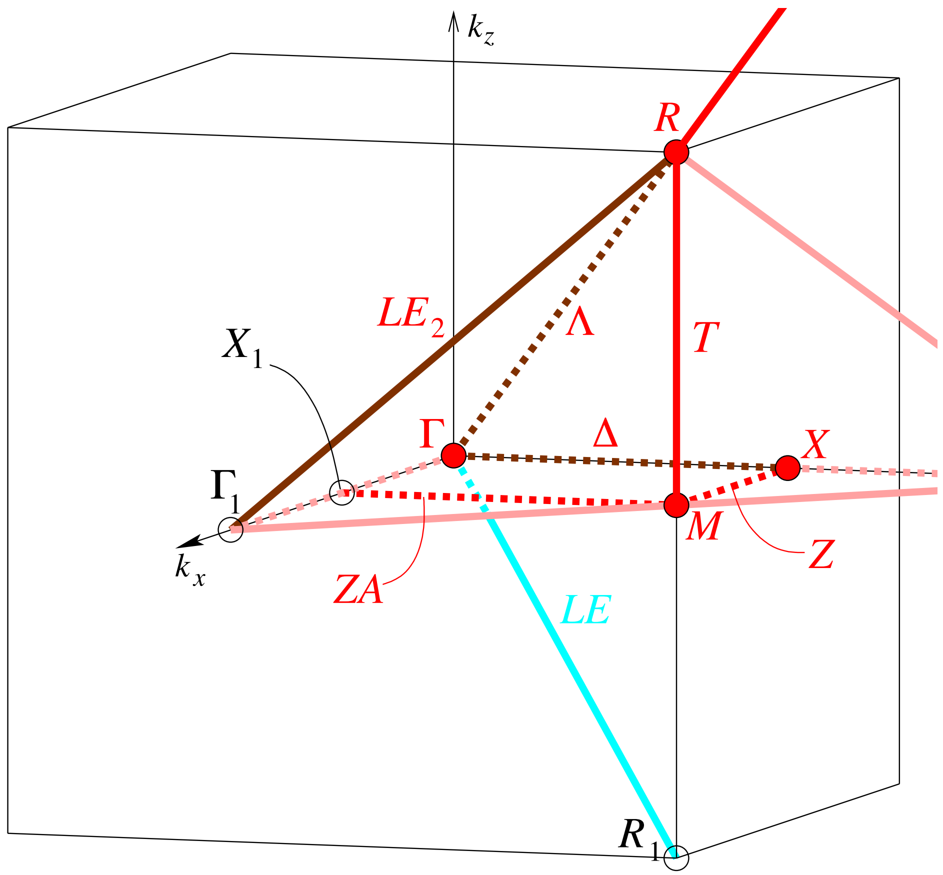
Nomenclature of propagation (or wavevectors) vectors k and irreps

The determination, classification, labelling and tabulation of irreducible representations (irreps) of space groups are based on the use of propagation wavevectors **k**. CMDL notation for **k**.◆

propagation vector = a point on/inside BZ

Brillouine zone (BZ) of space group P2_13 (198)



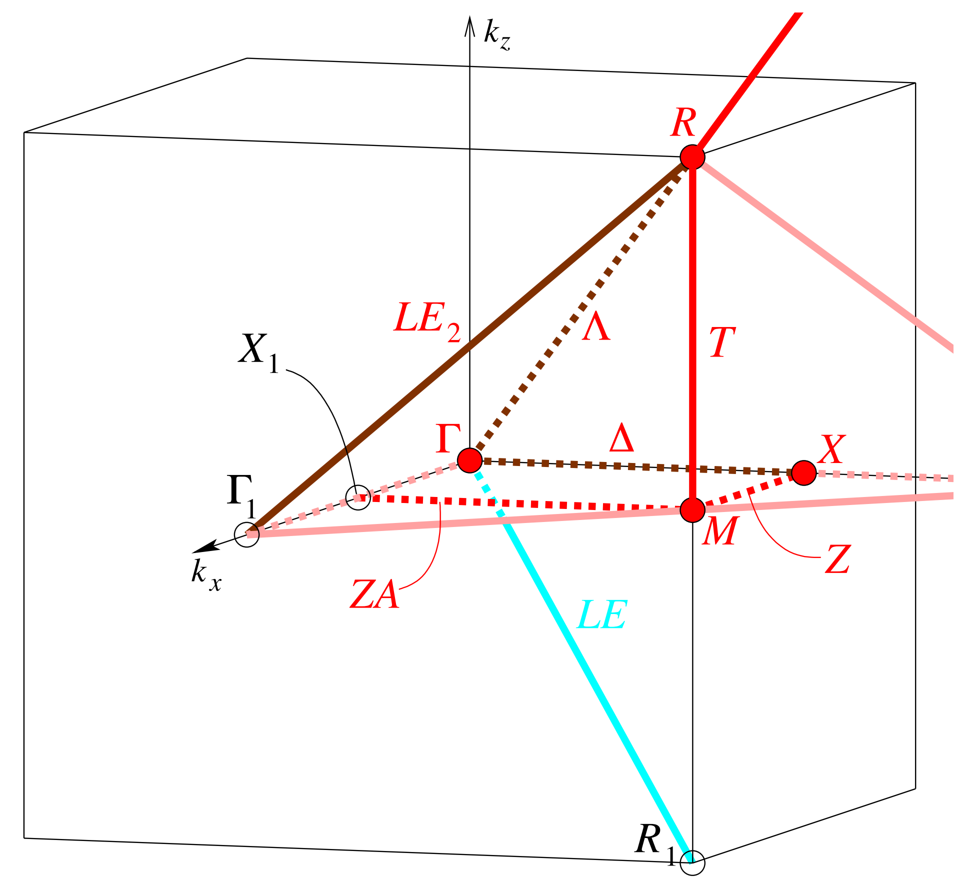
P2_13 is famous because of topological MnSi, MnGe, …

"Brillouin-zone database on the Bilbao Crystallographic Server"
Mois I. Aroyo et al, Acta Cryst. (2014). **A70**, 126–137

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

Symmetry types of propagation vectors k

Brillouine zone (BZ) of cubic P2_13



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http://www.cryst.ehu.es

propagation vector = a point on/inside BZ

k-vector description		ITA des
		Wyckoff
k-vector label	Conventional basis	Multiplicity
GM	0,0,0	1
R	1/2,1/2,1/2	1
M	1/2,1/2,0	3
X	0,1/2,0	3
LD (LE)	u,u,u	4
DT	0,u,0	6
ZA	1/2,u,0	6
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T	1/2,1/2,u	6
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-k is NOT in LD, but in LE u,u,-u

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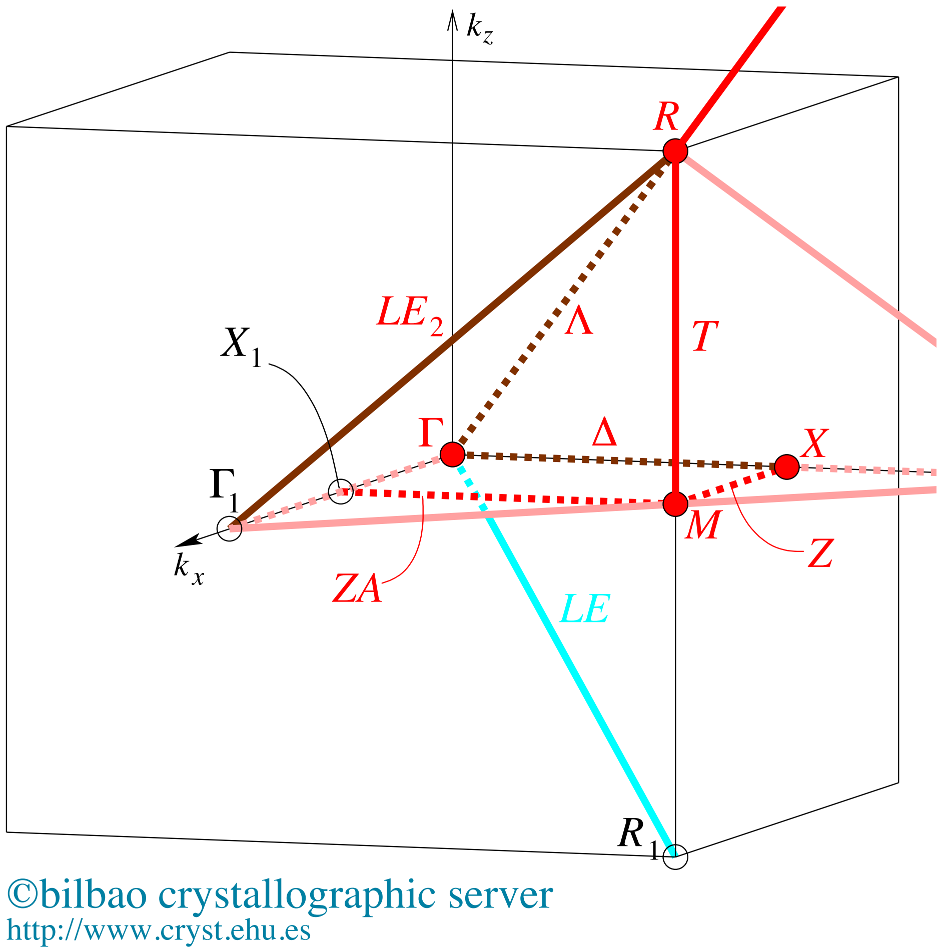

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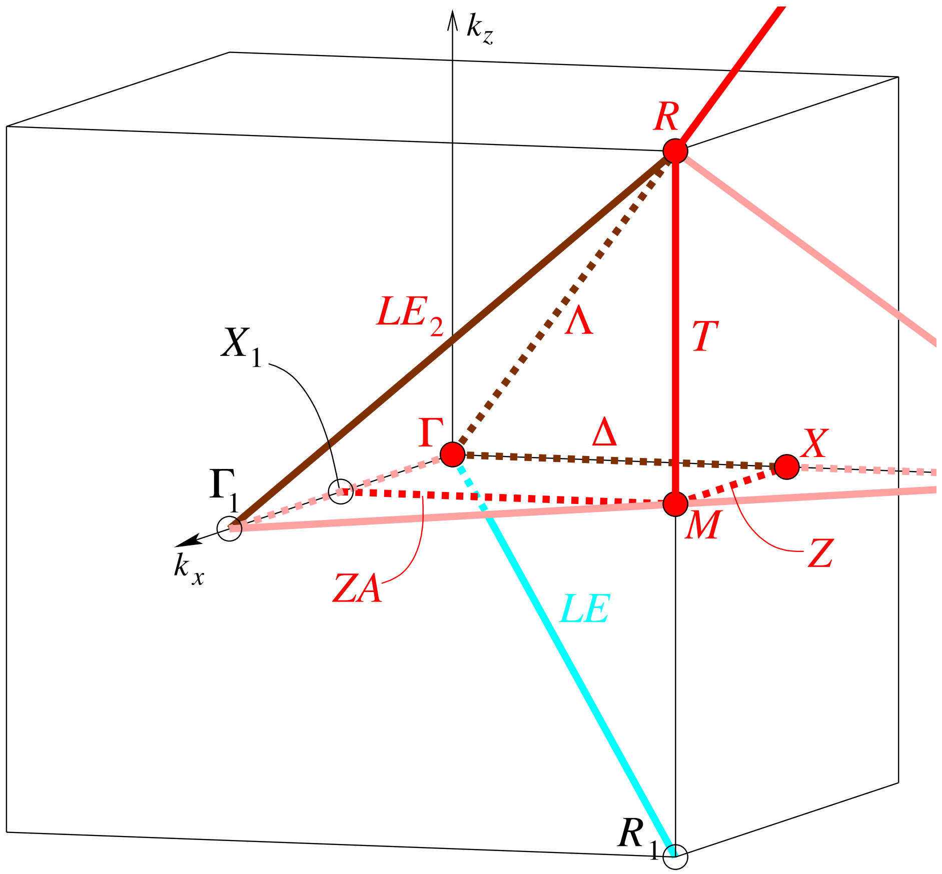

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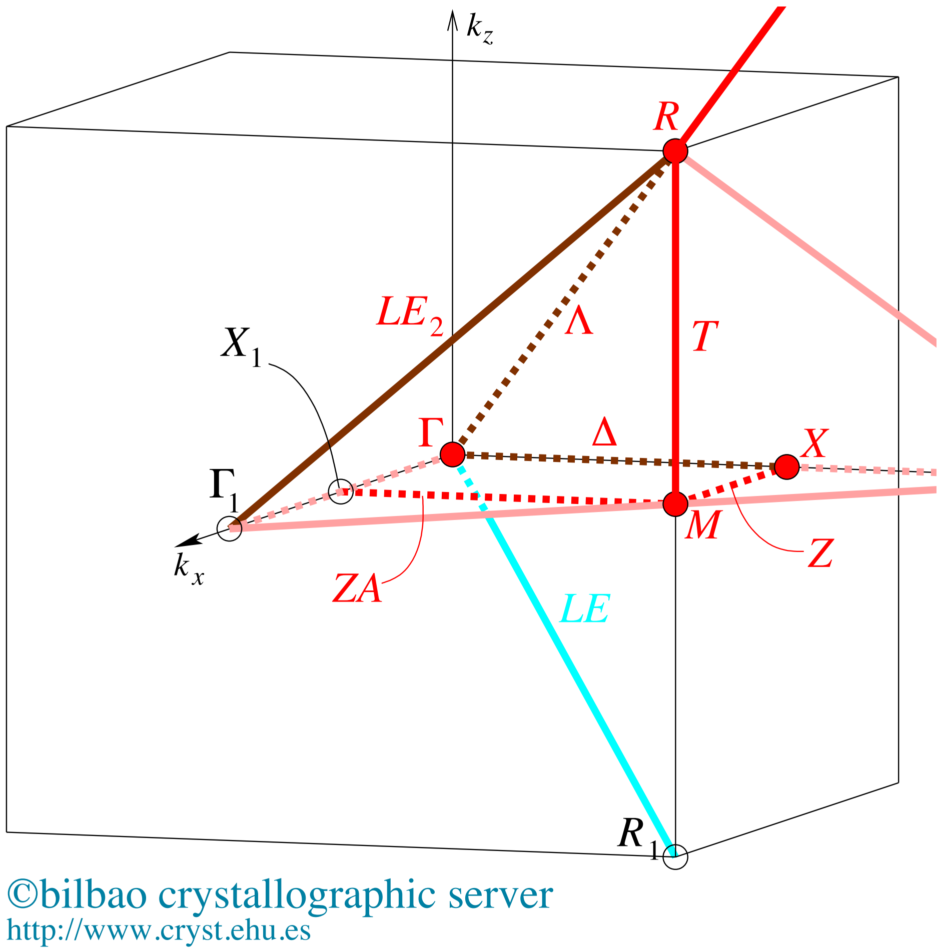

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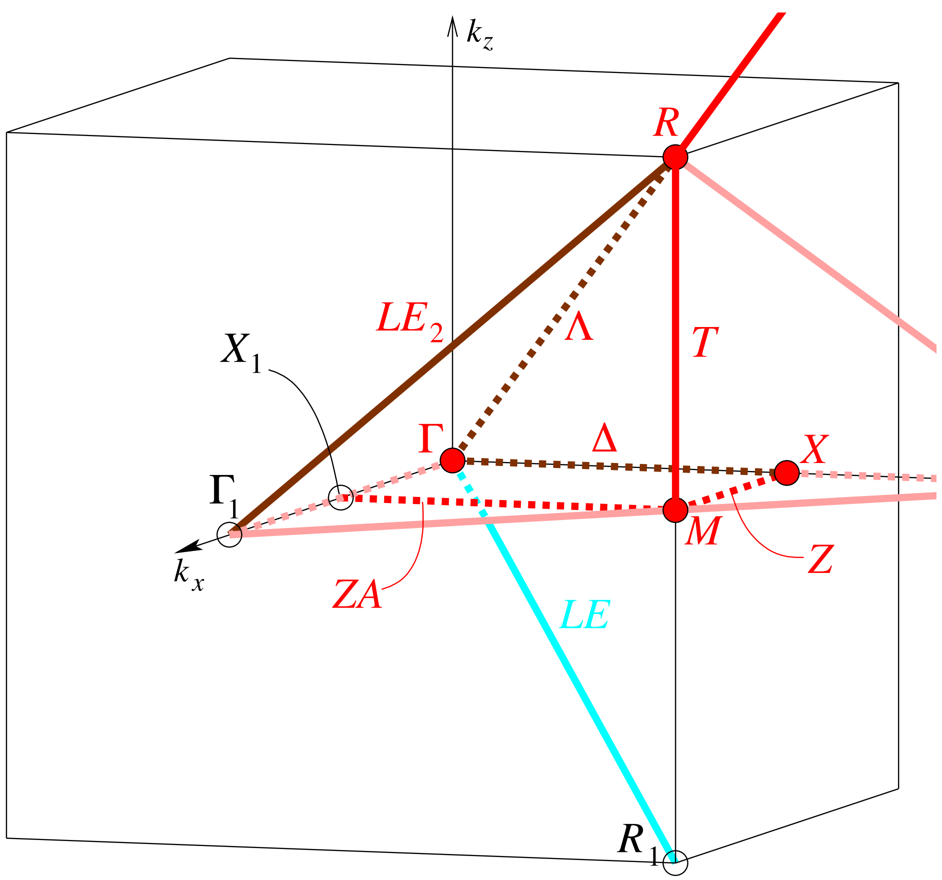

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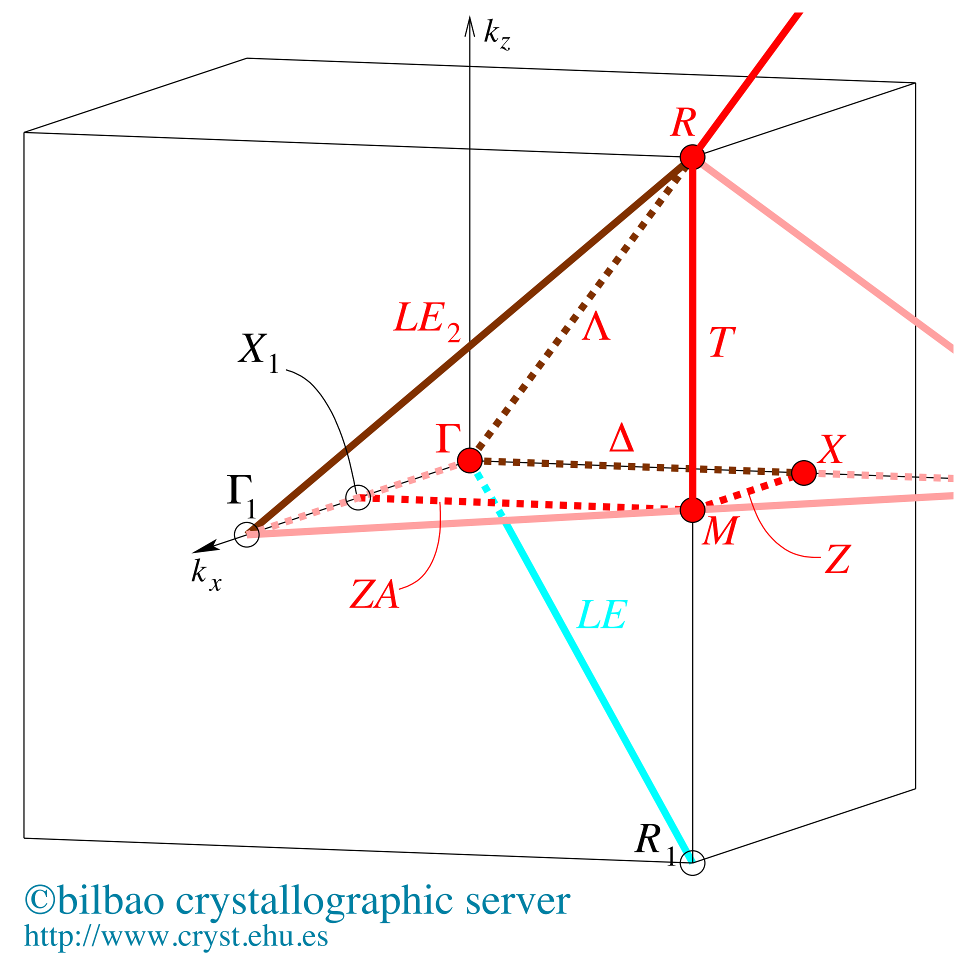
- incommensurate IC |**k**|≠ m/n
  - special IC-vectors also possible, e.g. [0,u,0] in cubic or tetragonal SG.

Brillouine zone (BZ) of cubic P2_13



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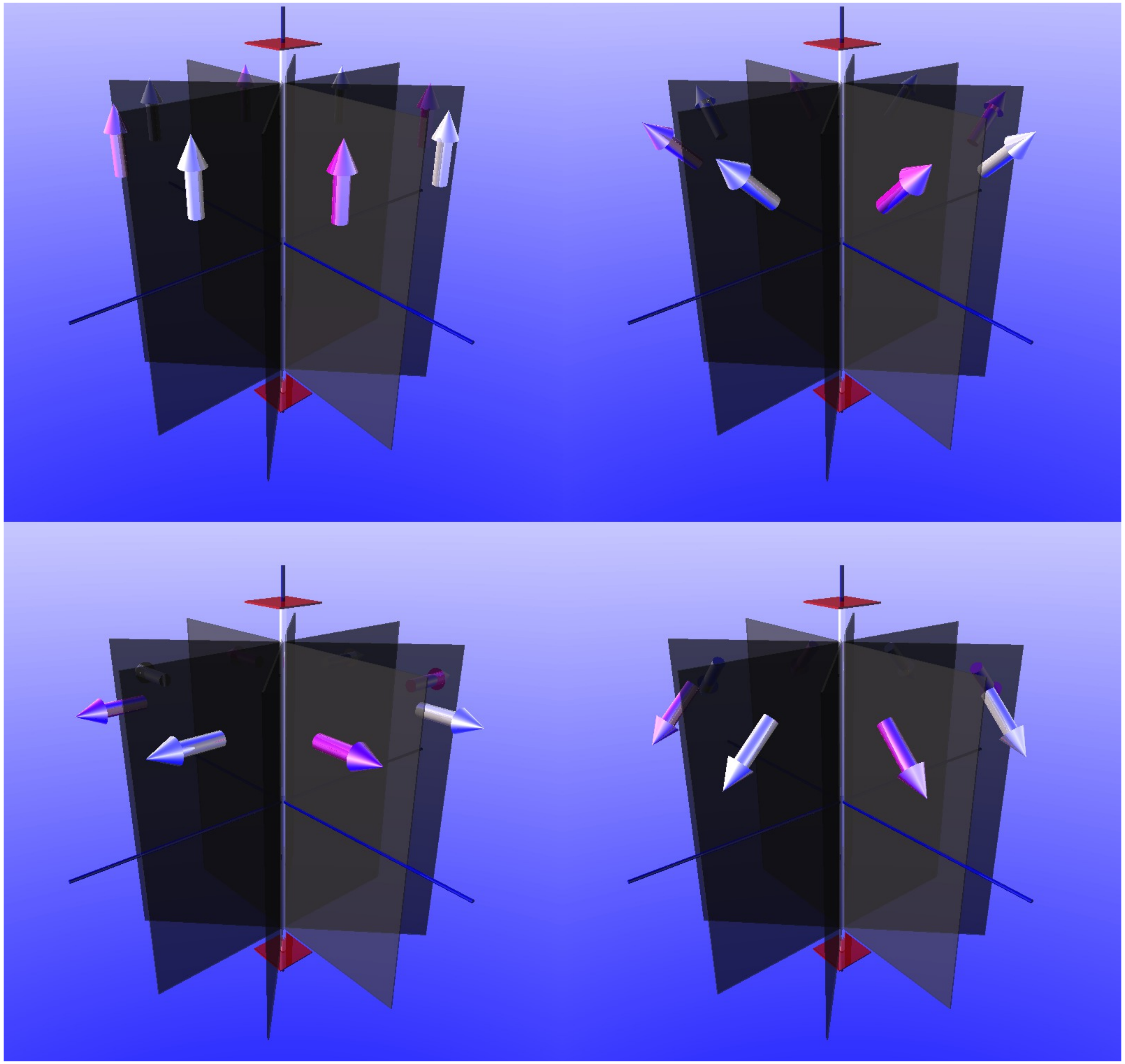
Propagation vector star and arms from point group

The k-vector stars of space group $I4_1md$ (109)



https://mpg.web.cmu.edu

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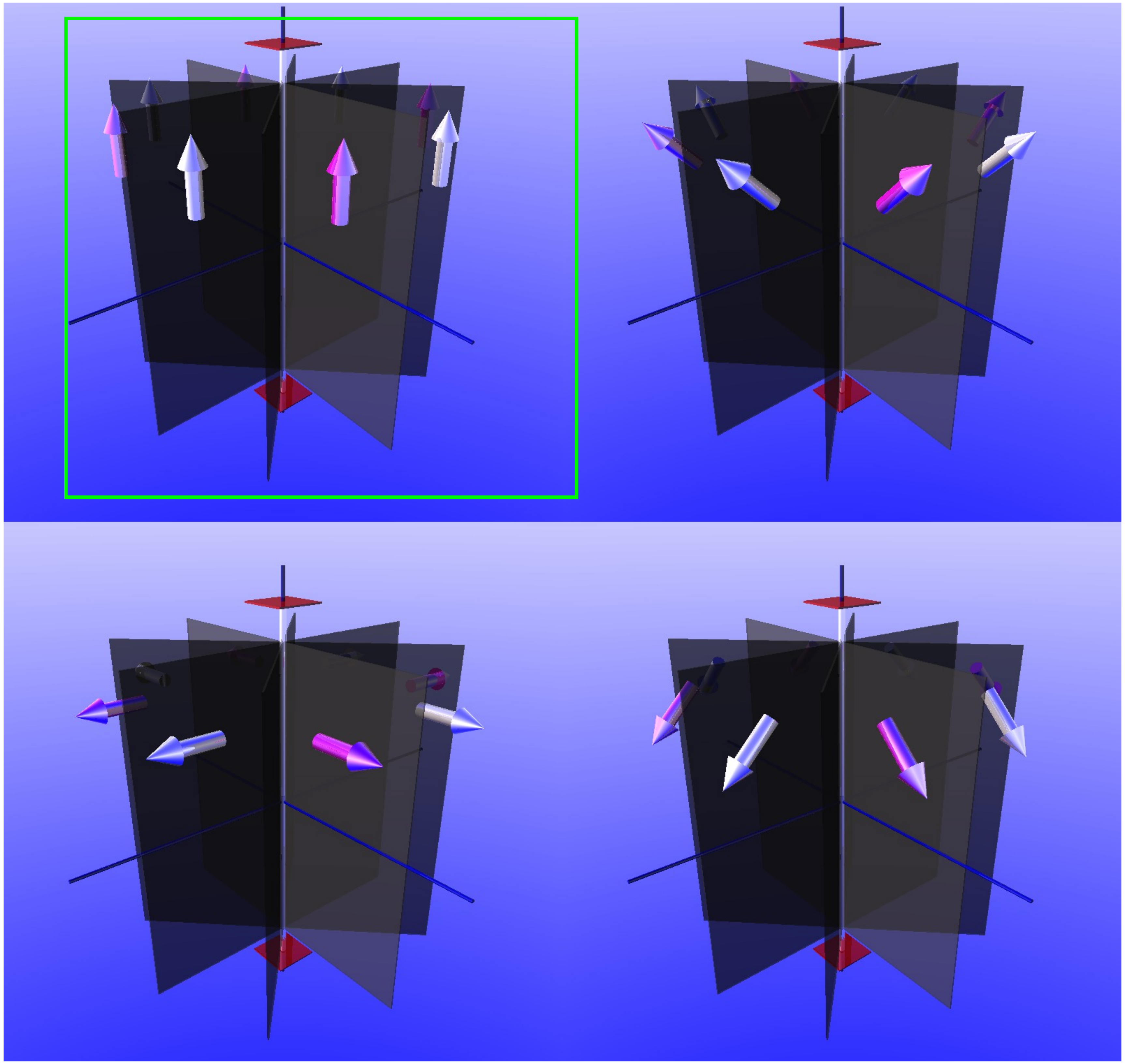

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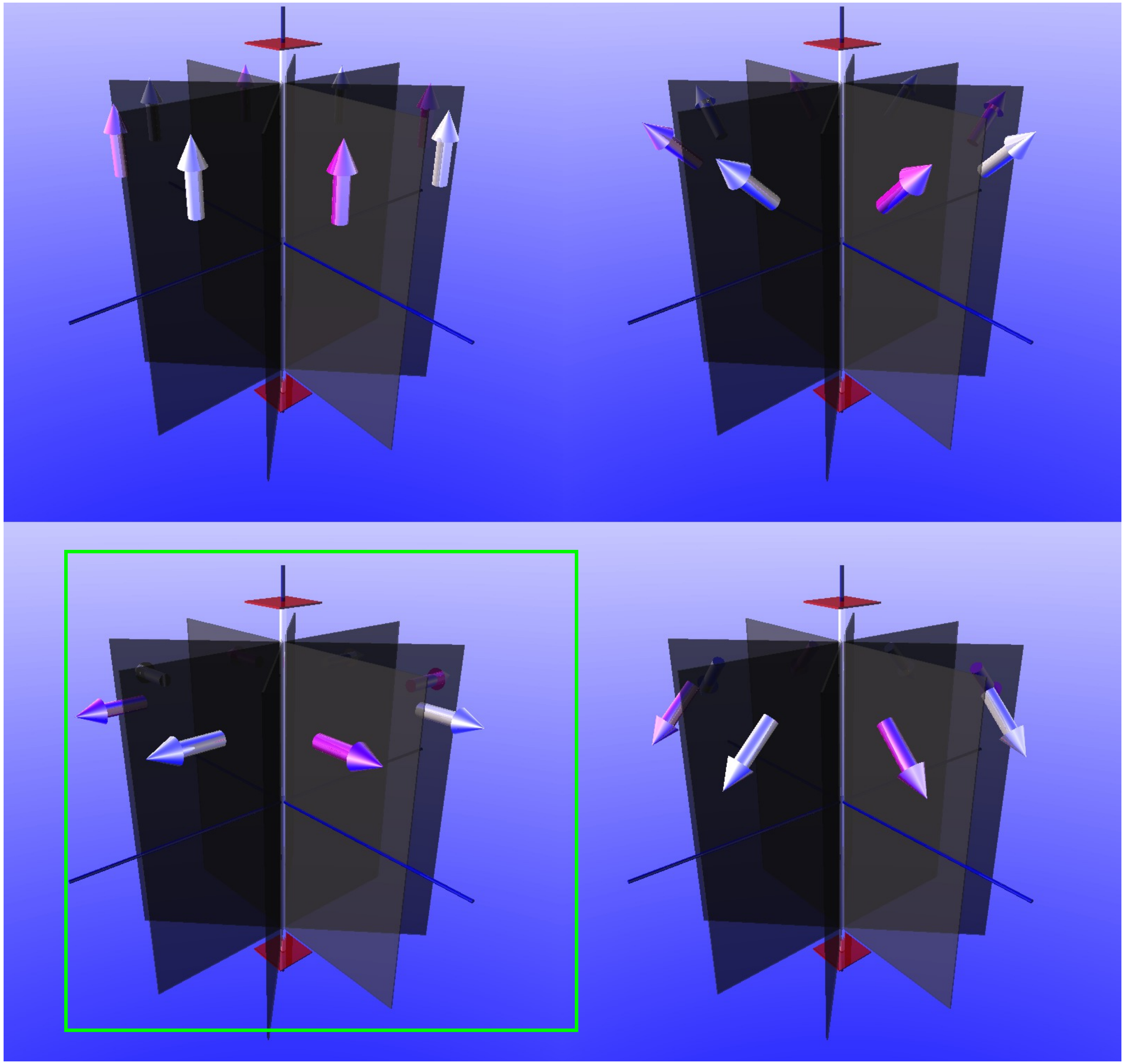

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Multi-arm structures. Little group.

$I4_1md$ k1= $[g, 0, 0]$ SM point of BZ

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $4^{+}(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$ (4) $4^{-}(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) m $x,0,z$ (6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$ (7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$ (8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},x,z$

symmetry operators

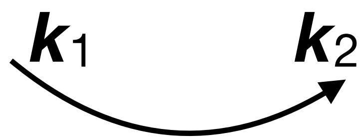
(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
(5) $x,\bar{y},z$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$ (7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{1}{4}$ (8) $y+\frac{1}{2},x,z+\frac{3}{4}$

Multi-arm structures. Little group.

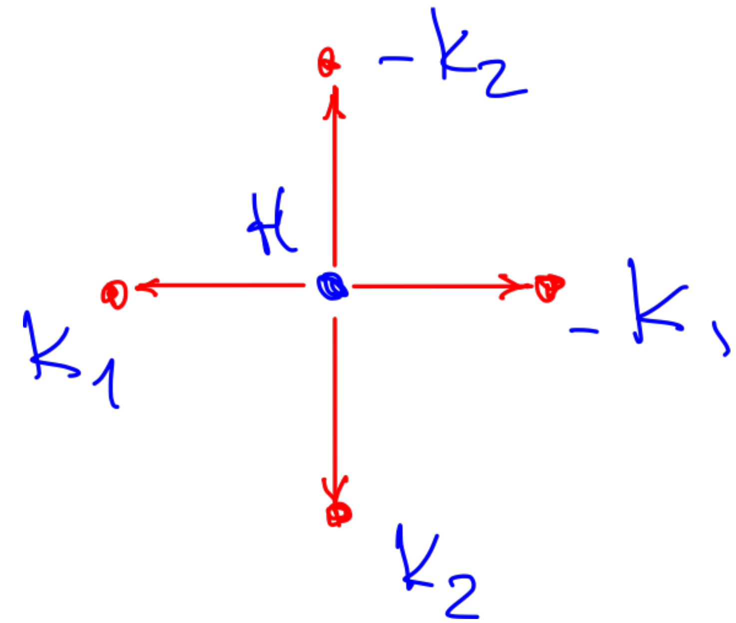
I4$_1$md k1= $[g, 0, 0]$ SM point of BZ

Propagation vector star has four arms

$$\{[g,0,0],[0,g,0]\}$$



$$\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$$



(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^{-}(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) m $x,0,z$	(6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},x,z$

symmetry operators

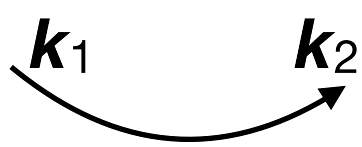
(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
(5) $x,\bar{y},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{1}{4}$	(8) $y+\frac{1}{2},x,z+\frac{3}{4}$

Multi-arm structures. Little group.

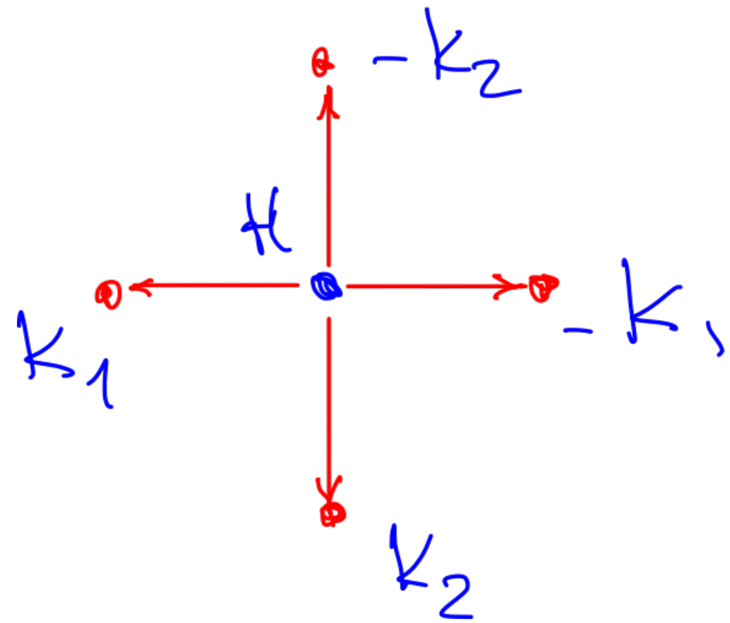
I4$_1$md k1= $[g, 0, 0]$ SM point of BZ

Propagation vector star has four arms

$$\{[g, 0, 0], [0, g, 0]\}$$



$$\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$$



(1) 1 (5) m $x,0,z$

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

(3) $4^{+}(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$ (7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$

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symmetry operators

k1 (little group G_k):
(1) x,y,z
(5) $x,\bar{y},z$

-k1:
(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$
(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

k2:
(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$
(7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{1}{4}$

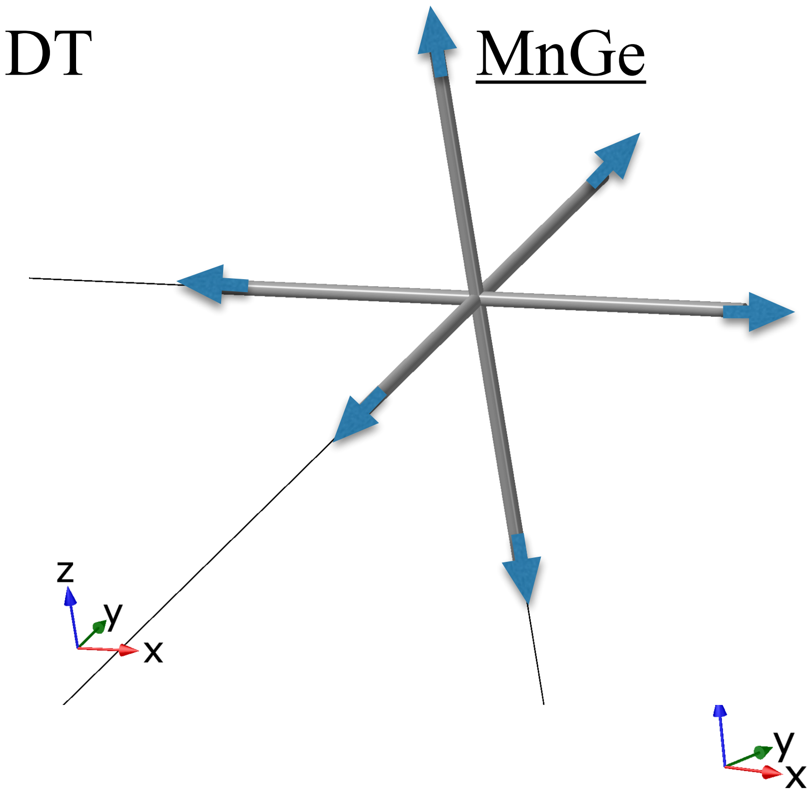
(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$

k2:
(8) $y+\frac{1}{2},x,z+\frac{3}{4}$

Examples of propagation vector stars

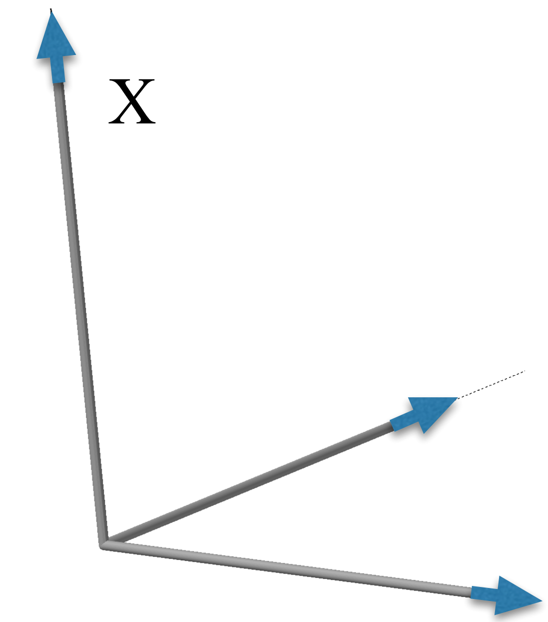
P2_13: 8 symops, three 2-fold and there 3-fold rotations

DT MnGe



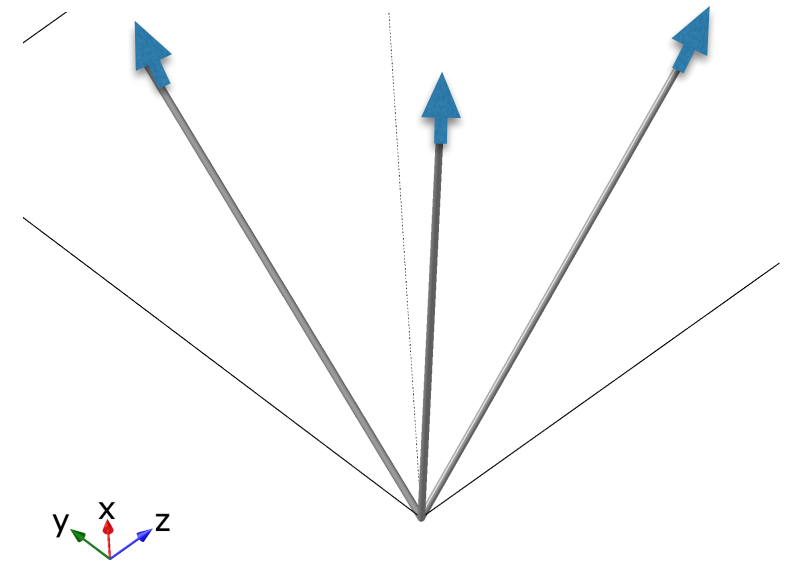
6-arms 0b0

X



3-arms 0½0

M



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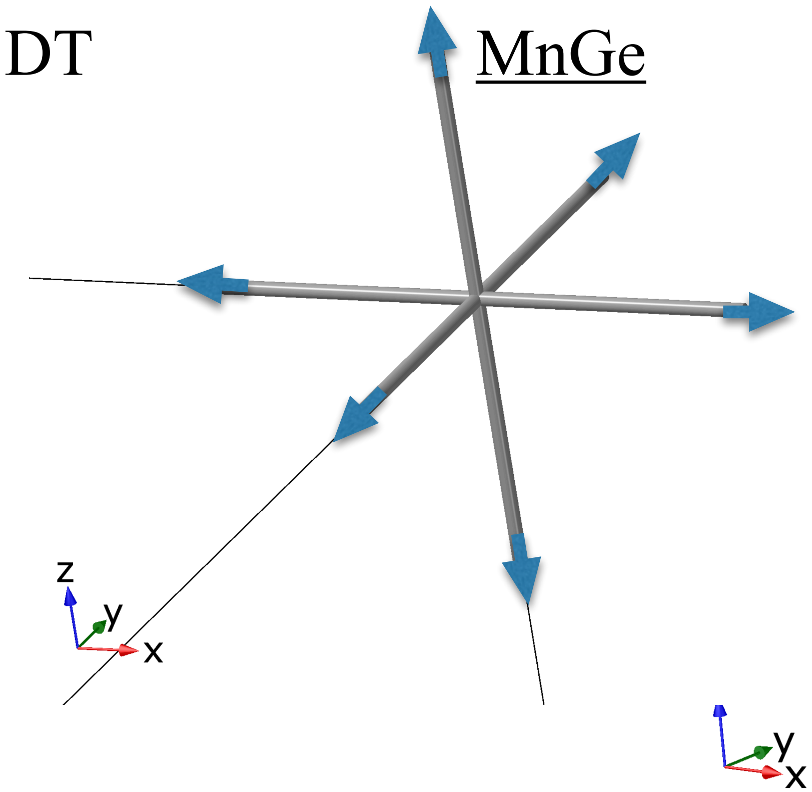
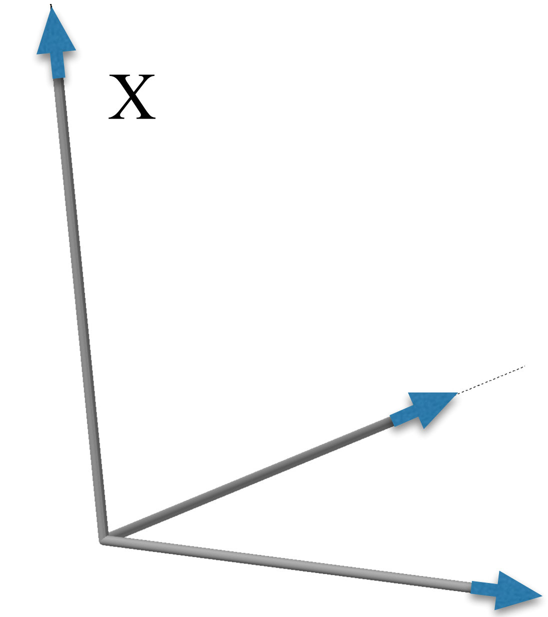


6-arms 0b0

X



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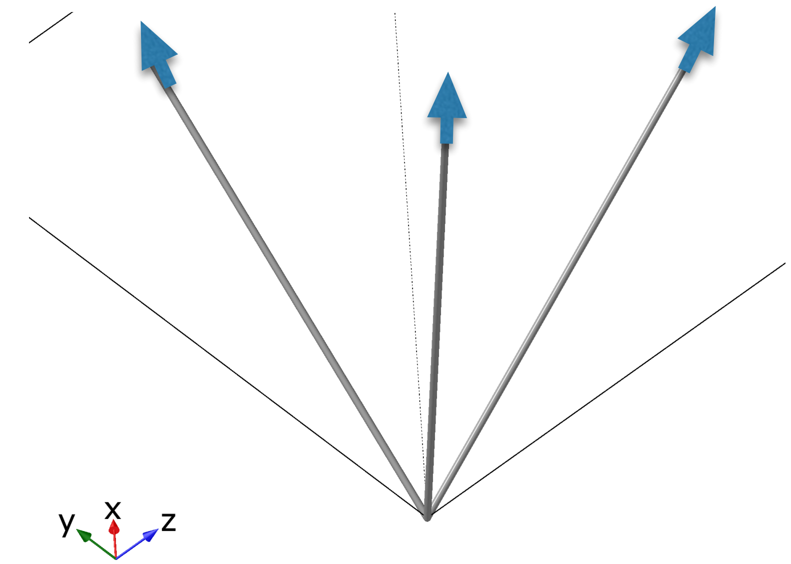
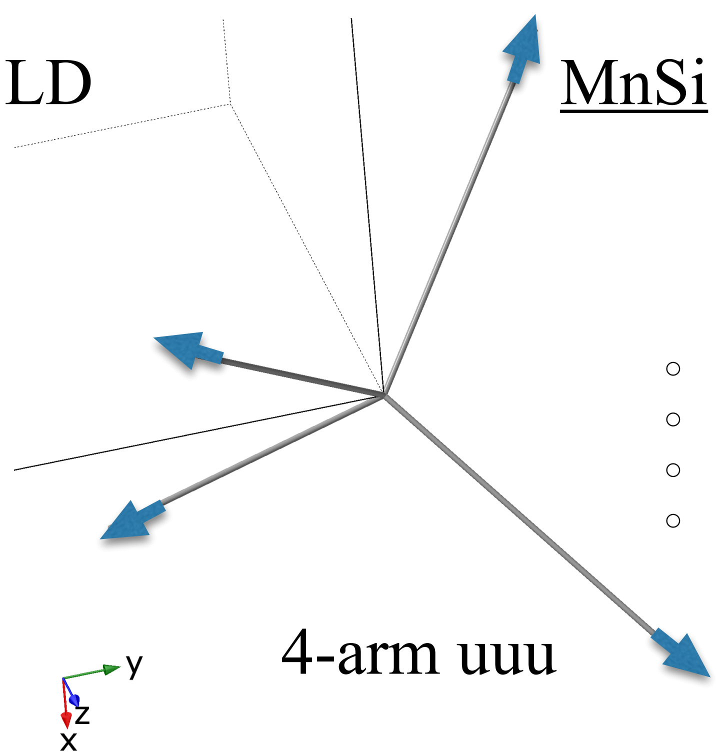


3-arms ½½0

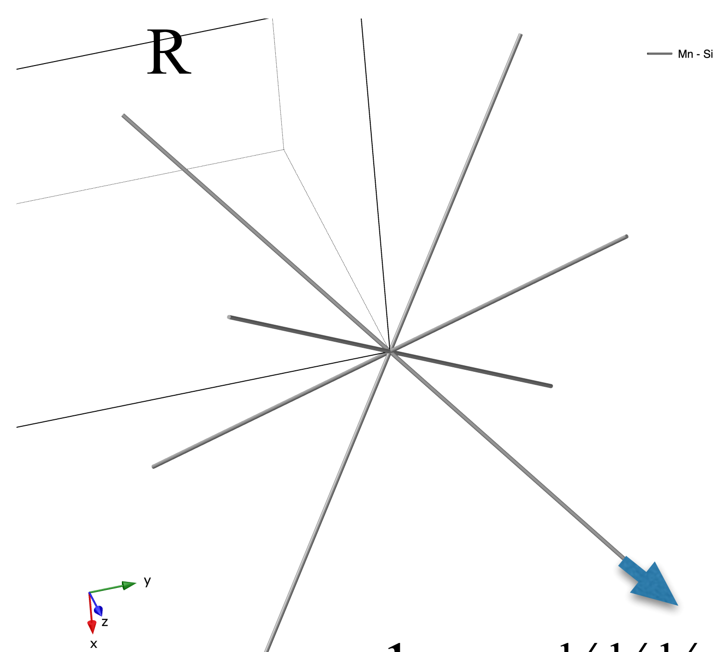
LD MnSi



- u u u
- -u -u u
- -u u -u
- u -u -u

4-arm uuu

R



1-arm ½½½

Nomenclature of space group irreps using an example

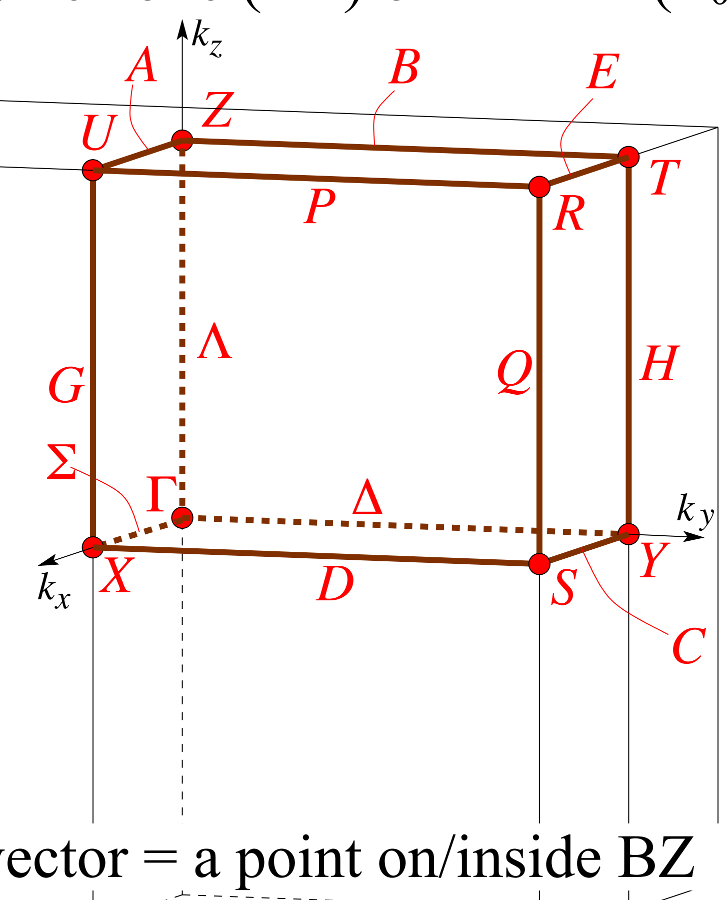
SG *Pnma* at X-point k=[1/2,0,0] of BZ, two 2D-irreps, e.g. mX1

g: Group elements, d^{kv}: matrices or irreducible representation *irrep* or *IR*

g = 1 2_x 2_y 2_z -1 n m a

Brillouine zone (BZ) 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 H=0
...	T	0,1/2,1/2	1	g	mmm
...	R	1/2,1/2,1/2	1	h	mmm



propagation vector = a point on/inside BZ

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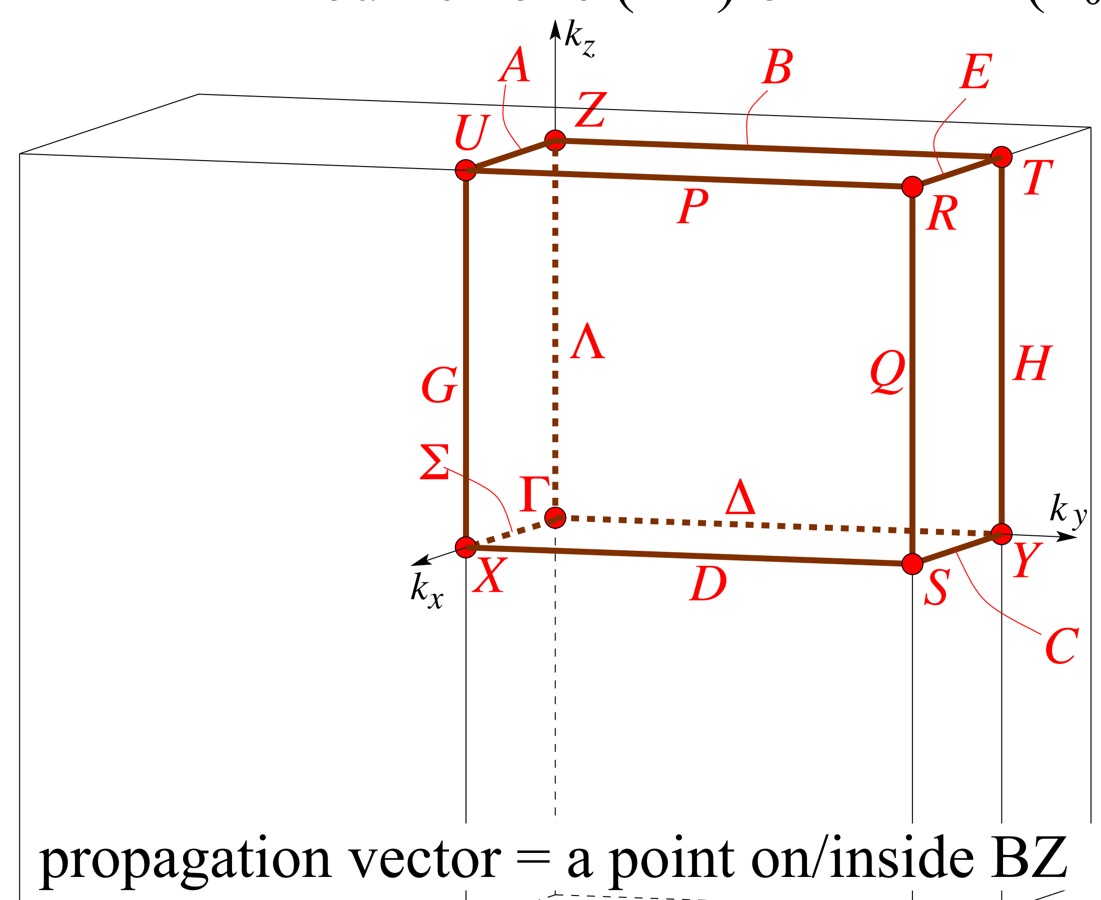
$$g = \quad 1 \quad 2_x \quad 2_y \quad 2_z \quad -1 \quad n \quad m \quad a$$

$$d^{X1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

Dimension_total=D_of_PIR × arms

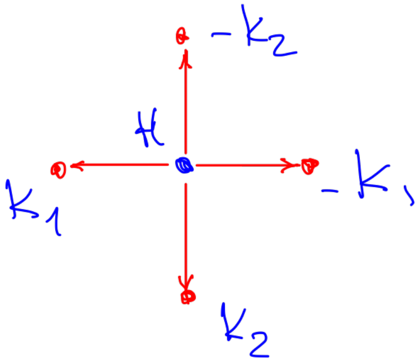
Brillouine zone (BZ) of Pmmm (Γ_0)



propagation vector = a point on/inside BZ multi-dimensional irrep naturally appear for the multi-arm structures

Dimension of irrep of the propagation vector star

CeAlGe, $I4_1md$, no. 109 k1=[u,0,0] irreps SM1 & 2



one k1, irrep of little group G_k

	SM1	SM2
$\{1\|t_1,t_2,t_3\}$	$e^{i2\pi t_1 u}$	$e^{i2\pi t_1 u}$
$\{m_{010}\|0,0,0\}$	1	-1

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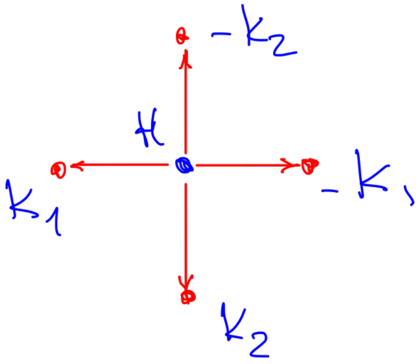

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k1 & -k1 irrep

$\{2_{001}\|0,0,0\}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$\{m_{010}\|0,0,0\}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
$\{m_{100}\|0,0,0\}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

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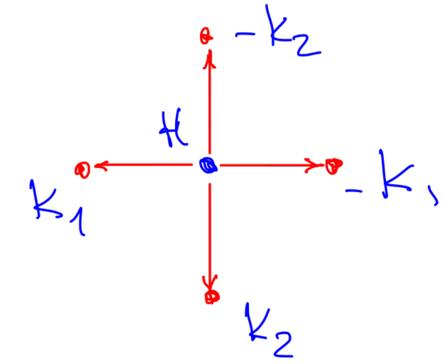

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all vectors k1 , -k1 & k2 , -k2. The IRREP to be used together with symmetry

$\{2_{001}\|0,0,0\}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$
$\{4^+_{001}\|0,1/2,1/4\}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ \mathrm{Cos}(\pi u) & \mathrm{Sin}(\pi u) & 0 & 0 \\ -\mathrm{Sin}(\pi u) & \mathrm{Cos}(\pi u) & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ \mathrm{Cos}(\pi u) & \mathrm{Sin}(\pi u) & 0 & 0 \\ -\mathrm{Sin}(\pi u) & \mathrm{Cos}(\pi u) & 0 & 0 \end{pmatrix}$
$\{4^-_{001}\|0,1/2,1/4\}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \mathrm{Cos}(\pi u) & -\mathrm{Sin}(\pi u) & 0 & 0 \\ -\mathrm{Sin}(\pi u) & -\mathrm{Cos}(\pi u) & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \mathrm{Cos}(\pi u) & -\mathrm{Sin}(\pi u) & 0 & 0 \\ -\mathrm{Sin}(\pi u) & -\mathrm{Cos}(\pi u) & 0 & 0 \end{pmatrix}$
$\{m_{010}\|0,0,0\}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

Multidimensional irreps result in several magnetic modes S_0 in RA★

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1. multi-dimentional (nD) irreducible representation generates *nD* magnetic modes $\boldsymbol{S}_0{}^1$, $\boldsymbol{S}_0{}^2$, $\boldsymbol{S}_0{}^3$… $\boldsymbol{S}_0{}^{nD}$

$$\mathbf{S}(0) \sim \sum_{l=1}^{nD} C_l \mathbf{S}_0^l$$

any relations between mixing coefficients

C_l ?

★Representation Analysis

what if several magnetic modes S_0^1, S_0^2, S_0^3... are possible in RA?

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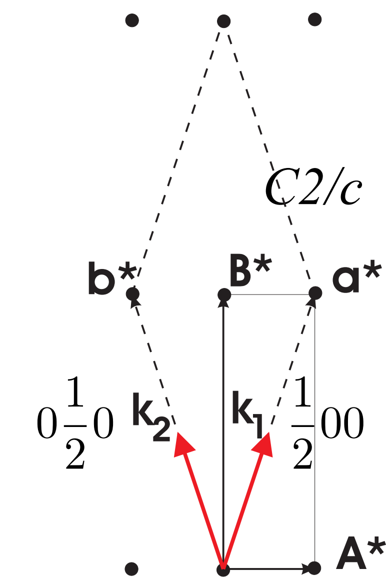
2. multi-*Arm*/multi-**k** structure (non-equivalent $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_m$….) *nA* magnetic modes $\boldsymbol{S}_0{}^1$, $\boldsymbol{S}_0{}^2$, $\boldsymbol{S}_0{}^3$... $\boldsymbol{S}_0{}^{nA}$

RA: widespread unfavourable paradigm that one-**k** is enough…



Example of mutiarm, full star {$\mathbf{k}_1$,$\mathbf{k}_2$}: J. Phys.: Condens. Matter **26** 496002

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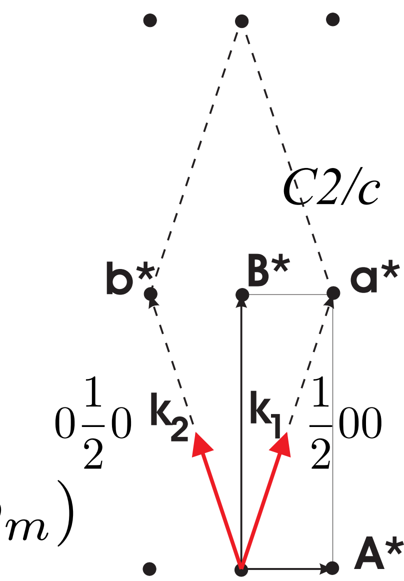

Example of mutiarm, full star {$\mathbf{k}_1$,$\mathbf{k}_2$}: J. Phys.: Condens. Matter **26** 496002

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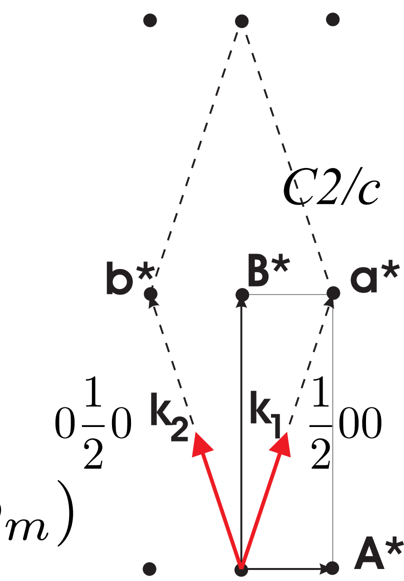

Example of mutiarm, full star {$\mathbf{k}_1$,$\mathbf{k}_2$}: J. Phys.: Condens. Matter **26** 496002

any relations between mixing coefficients C_l *or* C'_m ?

No from RA alone…

Yes from magnetic symmetry!

An essence of using RA and MSG
or
A recipe for finding the ISOTROPY magnetic subgroup of the parent

The general scheme of RA and MSG

Parent grey space group

↓

choice of star of k vector

↓

choice of irrep of the k-star

↓

order parameter direction OPD for the k-star irrep

↓

isotropy (OPD is inv.) magnetic subgroup

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Find symmetry breaking for *Pnma1'* at X-point [1/2,0,0] of BZ for irrep mX1

g: Group elements, *G*: matrices or irreducible representation *irrep*, 1': time inversion

g = 1 2_x 2_y 2_z -1 n m a

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

$g' = g \cdot 1'$

$G' = G \cdot (-1)$

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g =	1	2_x	2_y	2_z	-1	n	m	a	
G =	$\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}0&-1\\1&0\end{bmatrix}$	$\begin{bmatrix}-1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}0&-1\\-1&0\end{bmatrix}$	$\begin{bmatrix}-1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}0&-1\\-1&0\end{bmatrix}$	$\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}0&-1\\1&0\end{bmatrix}$	$\begin{pmatrix}a\\b\end{pmatrix}$

g’ = *g* · 1’

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resulting symmetry → Isotropy subgroup

OP= $\begin{pmatrix}a\\a\end{pmatrix}$

g = 1 m

g’ = 2_z’ n’

Isotropy subgroup → P_bmn2_1

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g: Group elements, *G*: matrices or irreducible representation *irrep*, 1': time inversion

g = 1, 2_x, 2_y, 2_z, -1, n, m, a

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

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g = 1, m → P_bmn2_1

g' = $2_z'$, n'

OP= $\begin{pmatrix}a\\0\end{pmatrix}$

g = 1, m → $P_a1\ 2_1/m\ 1$

g' = $2_x'$, -1'

OP= $\begin{pmatrix}a\\b\end{pmatrix}$

g = 1, m → $P_a1\ m\ 1$

"Usual" Representation Analysis RA in case of multidimensional irreps and/or multi-arm

Some consequences of usual practice of RA

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1. Only general direction of order parameter OPD (kernel) in representation carrier space is considered. For example for 3D irrep OPD=(a,b,c): no special (a,0,0), (a,a,0), (a,a,a) … ⇒ symmetry lost
   Solutions that are considered do not have maximal possible symmetry

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Multi-k or multi-arm structures

case 1.

no apparent relations between several $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$, … vectors - no extra symmetry relations between modes S($\mathbf{k}_1$), S($\mathbf{k}_2$), S($\mathbf{k}_3$)… and no advantage of using symmetry arguments

case 2.

the **k** vectors are *arms* of k-vector *star* - S($\mathbf{k}_1$), S($\mathbf{k}_2$), S($\mathbf{k}_3$)… might be symmetry related

- **k** and -**k** are NOT always arms…

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case 1a.

…, **BUT** there is a primary irrep **P** that breaks the symmetry so that allows secondary irrep **S** in the MSG generated by irrep **P**.

case 2.

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- **k** and -**k** are NOT always arms…

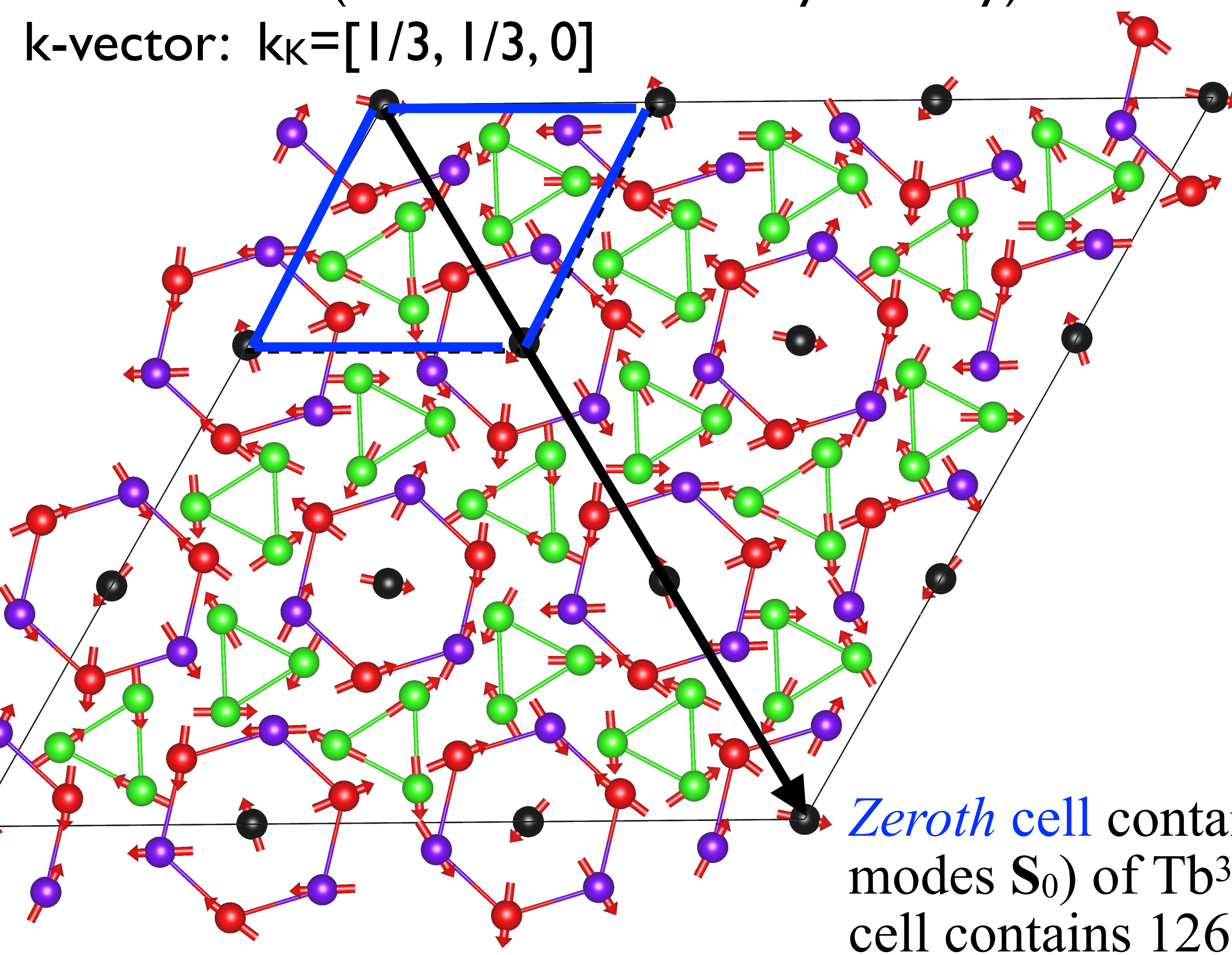
2k magnetic structure was missed using RA

Antiferromagnetic (à la cycloidal spiral) three sub-lattice ordering in $Tb_{14}Ag_{51}$

P6/m → Pm' (lowest monoclinic symmetry)

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

PHYSICAL REVIEW B 72, 134413 (2005)



Zeroth cell contains 13 spins (and 5+5+3 =13 modes S_0) of Tb^{3+}. Conventional magnetic unit cell contains 126 spins of Tb^{3+}!!

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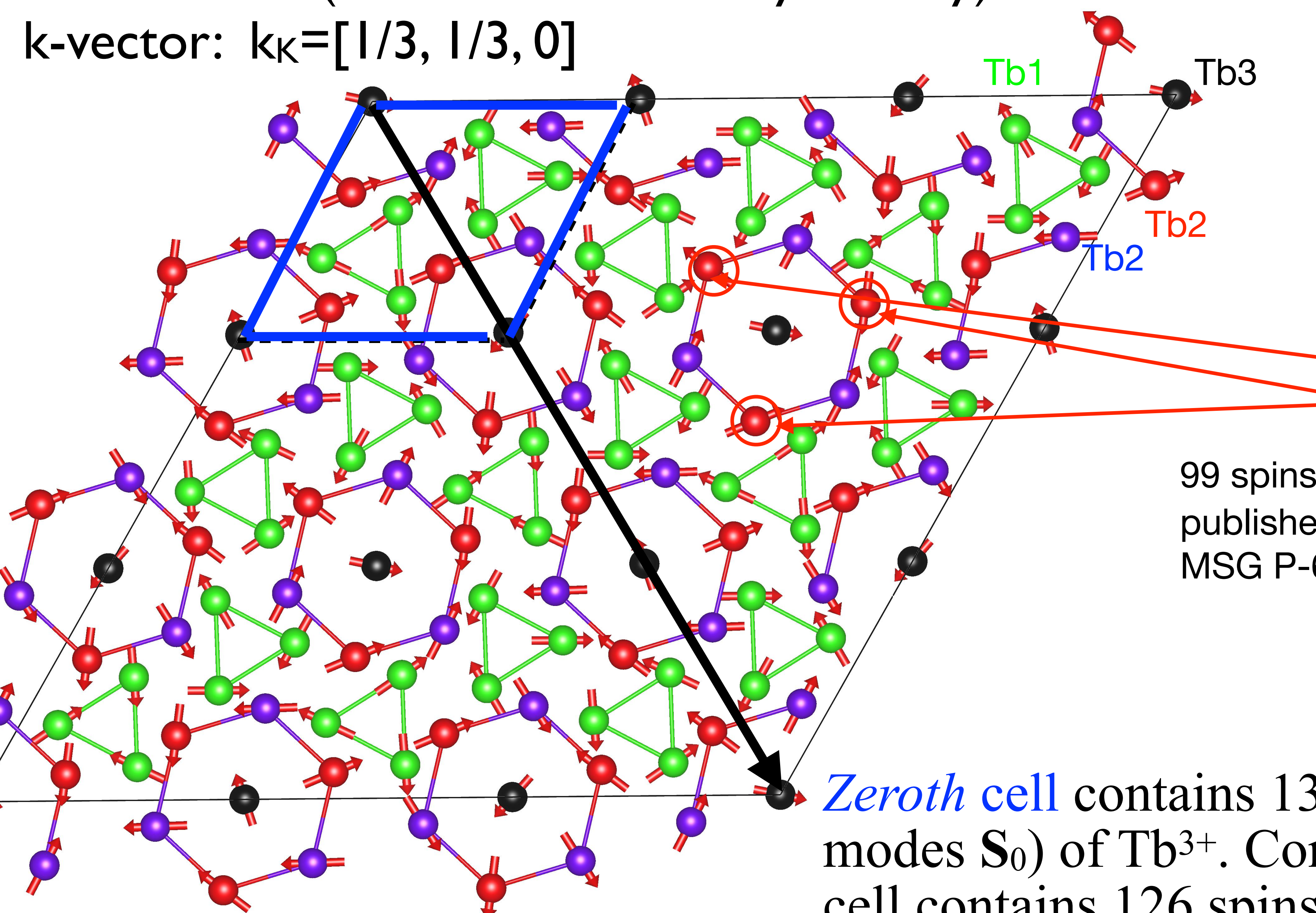

Manu Perez Mato

Only three of 13 independent sites are "wrong" => Pm'

99 spins in the 3 x 3 x 1 cell of the published model comply with the MSG P-6', while 27 do not.

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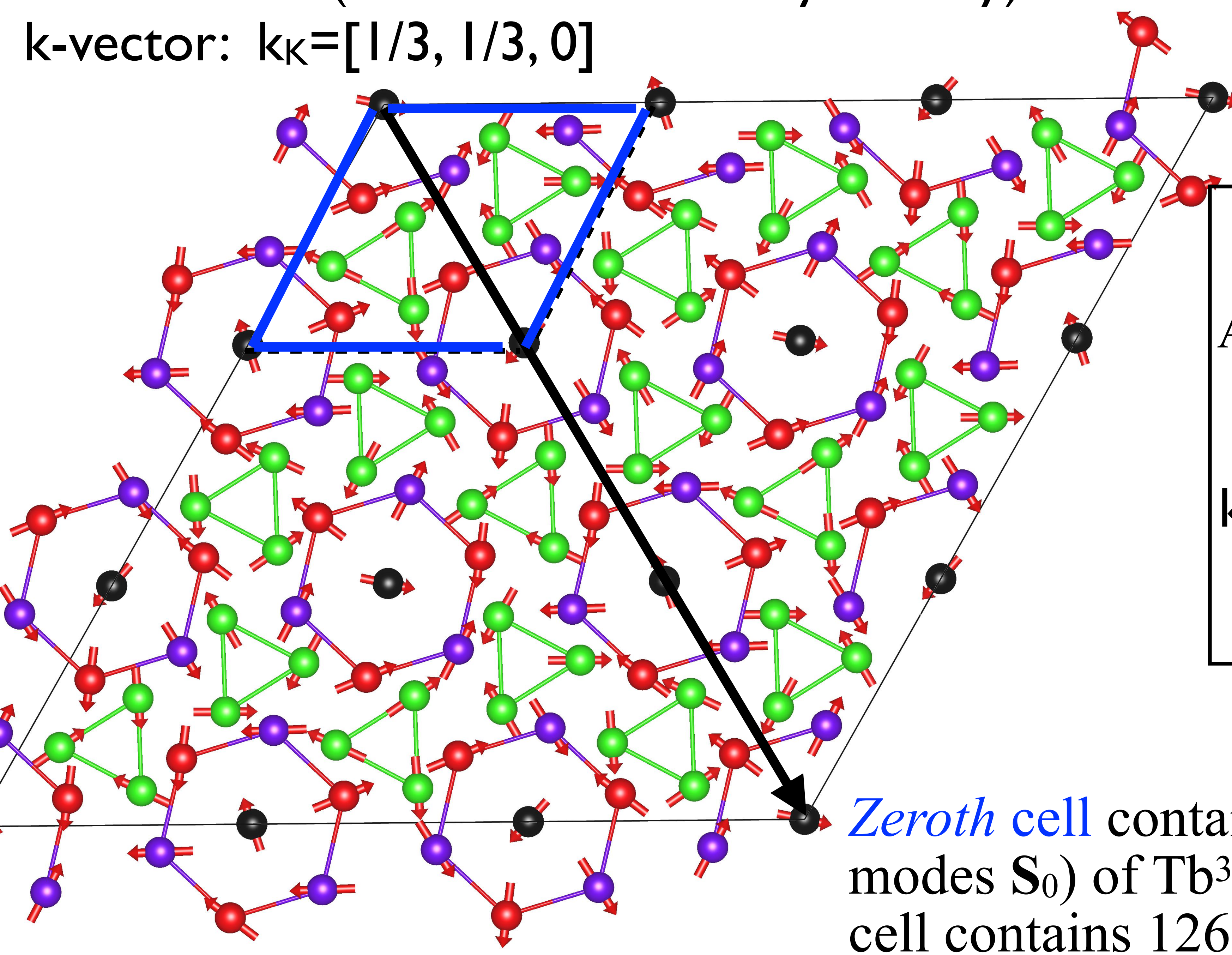

maximal possible symmetry for 4D irrep

Acta Cryst. (2022). B**78**, 172-178

P6/m → P-6'

k-vectors: k_K=[1/3, 1/3, 0] and $3k_K$=[0,0,0]

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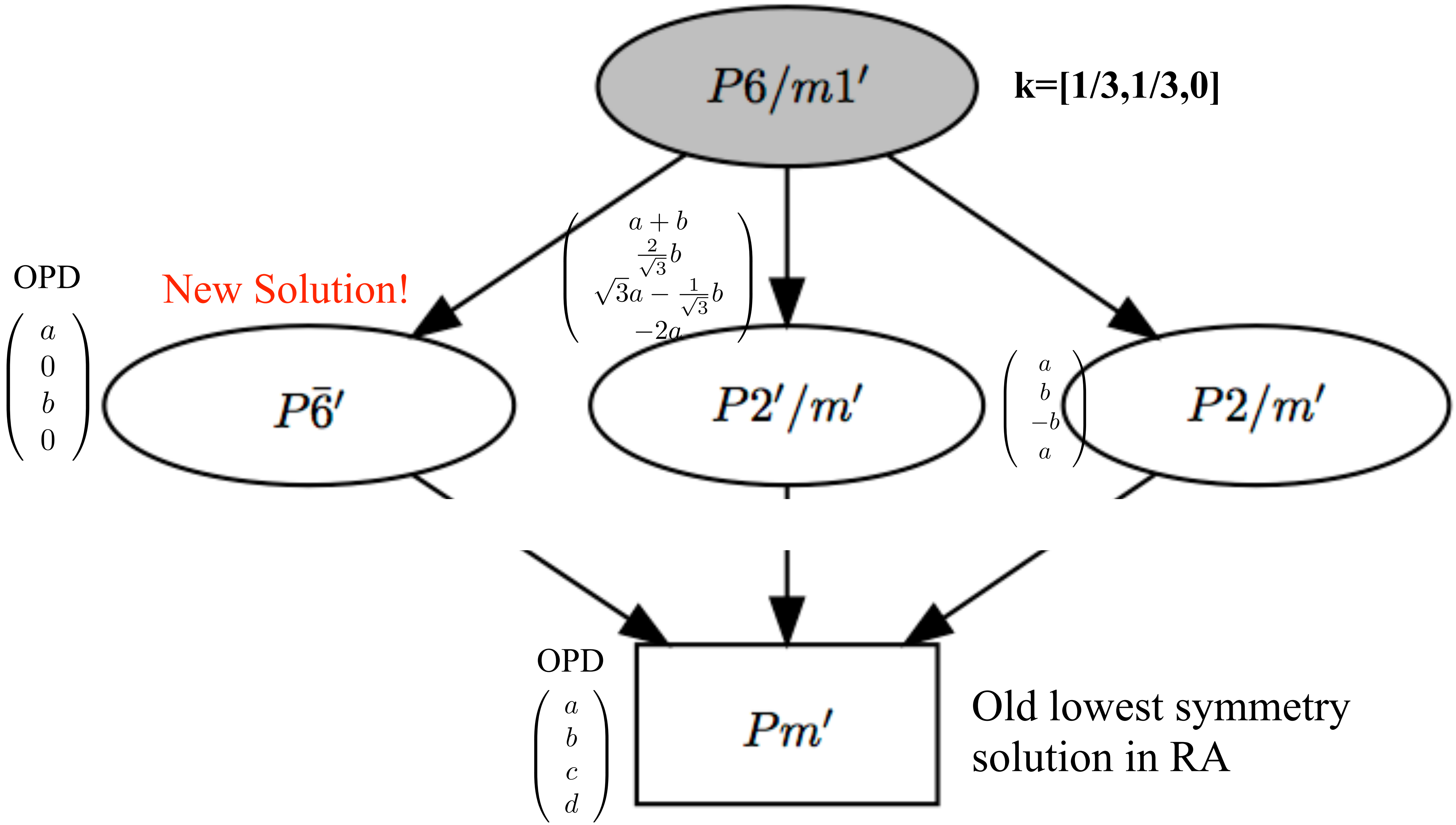
Possible alternative magnetic symmetries if the spin arrangement transforms according to the four-dimensional physically irreducible representation mK4K6.



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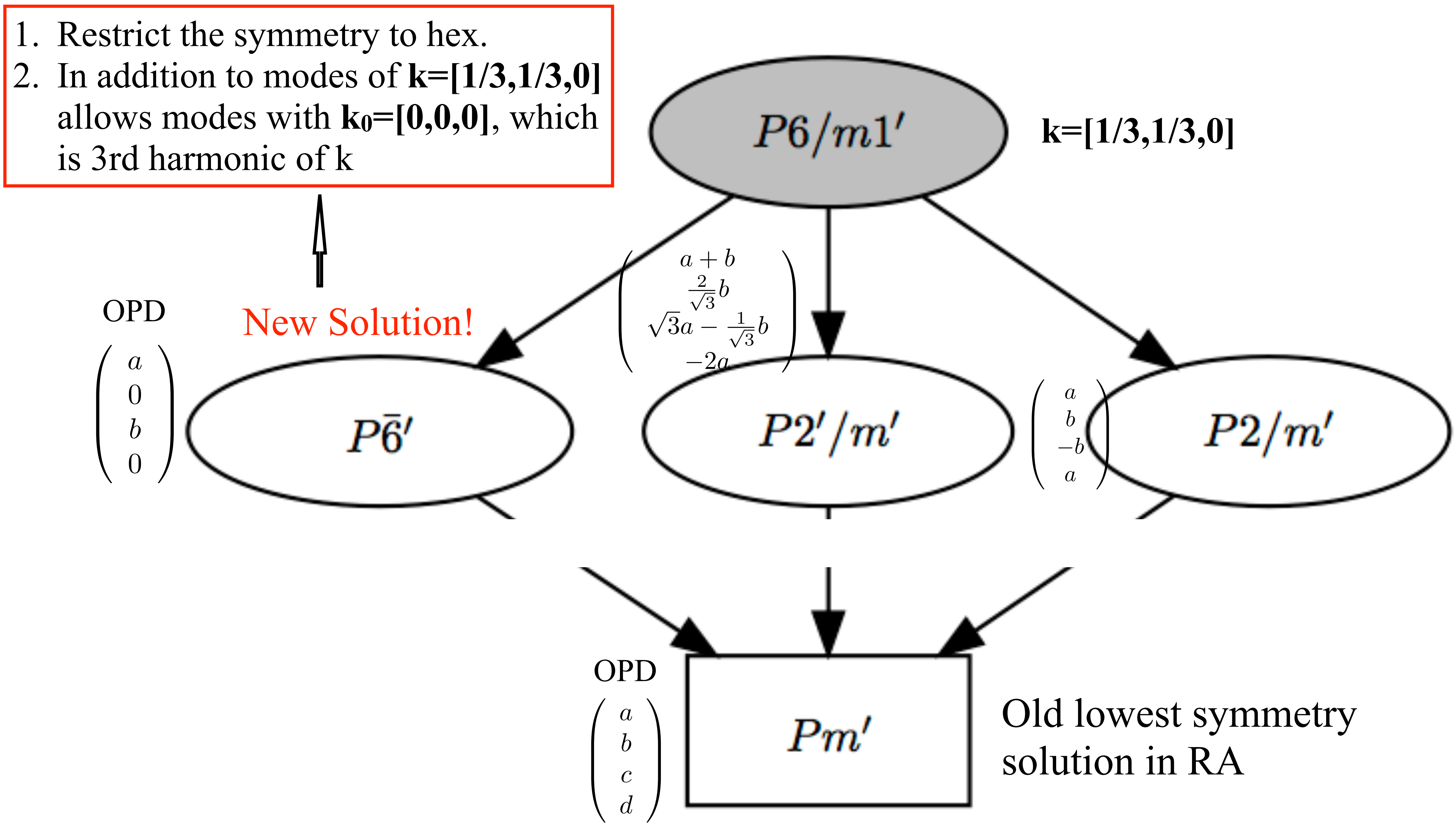
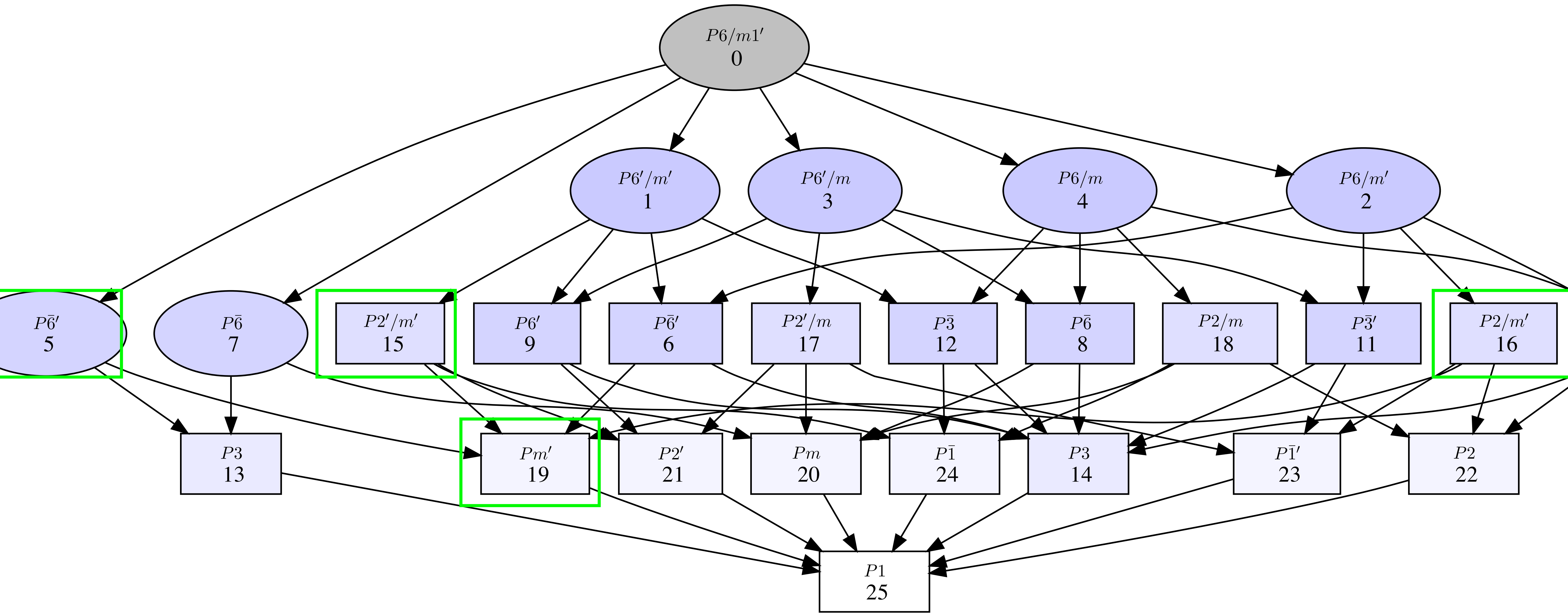


A Note: If we use only magnetic symmetry without irreps

too many subgroups to consider and we loose the concept of single irrep active at the transition

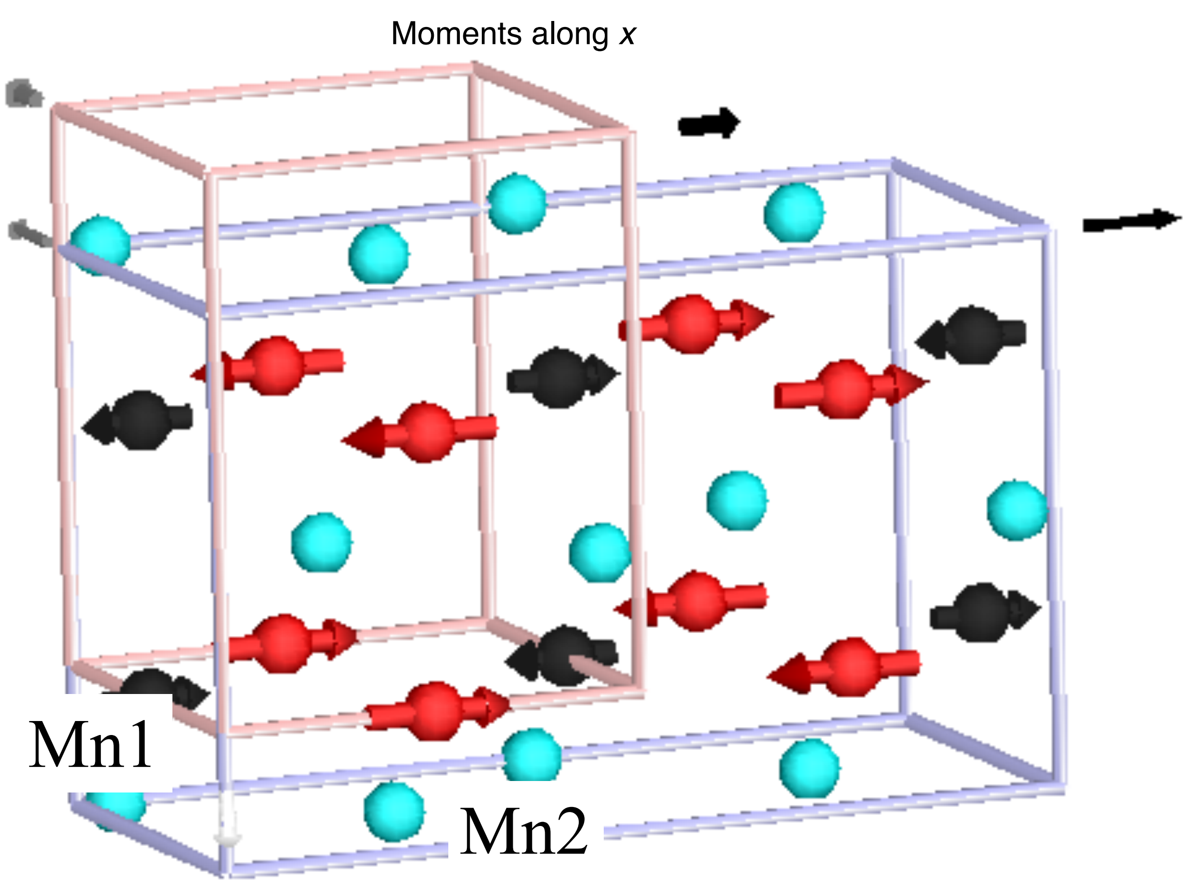


Two examples of the power of the RA & symmetry for magnetic structures

multiferroic $TmMnO_3$

one-arm two dimensional irrep **k**=[1/2,0,0].

Ferro-electric phase polar magnetic group P_bmn2_1



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

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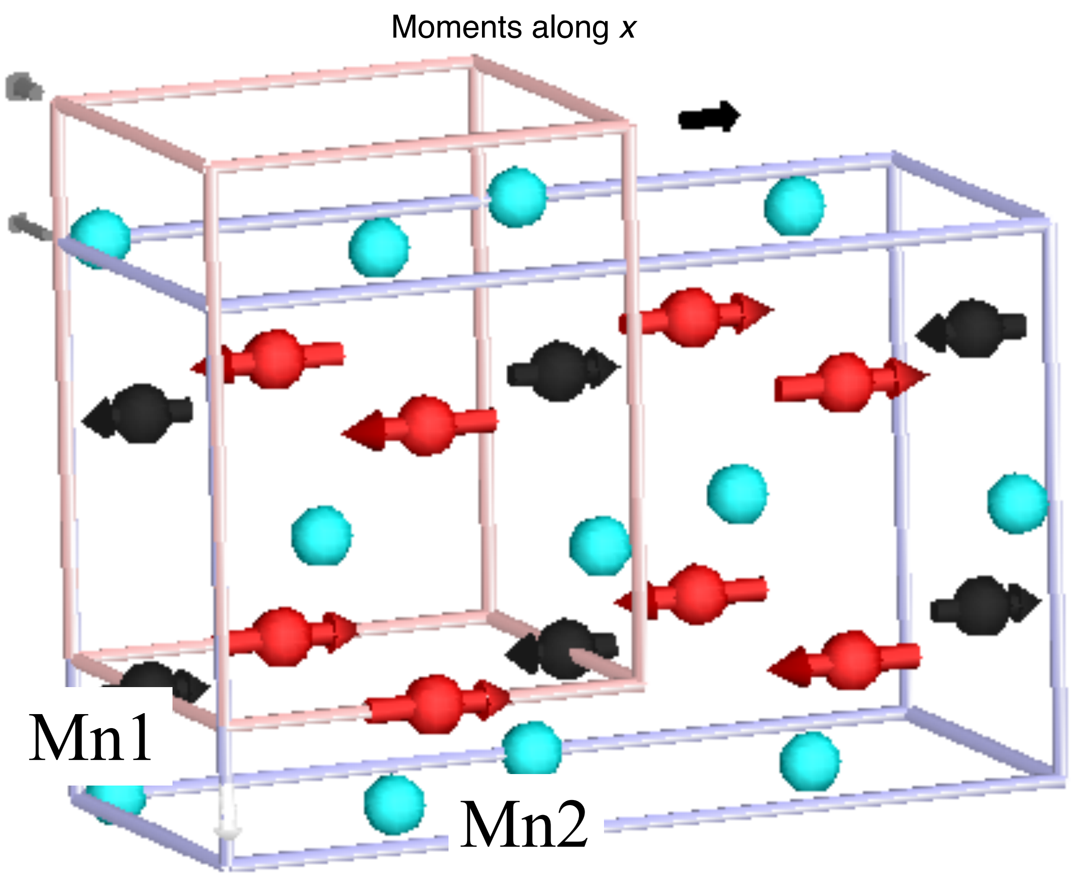

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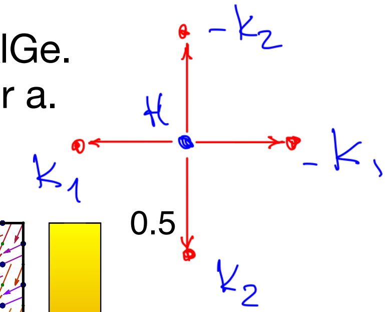
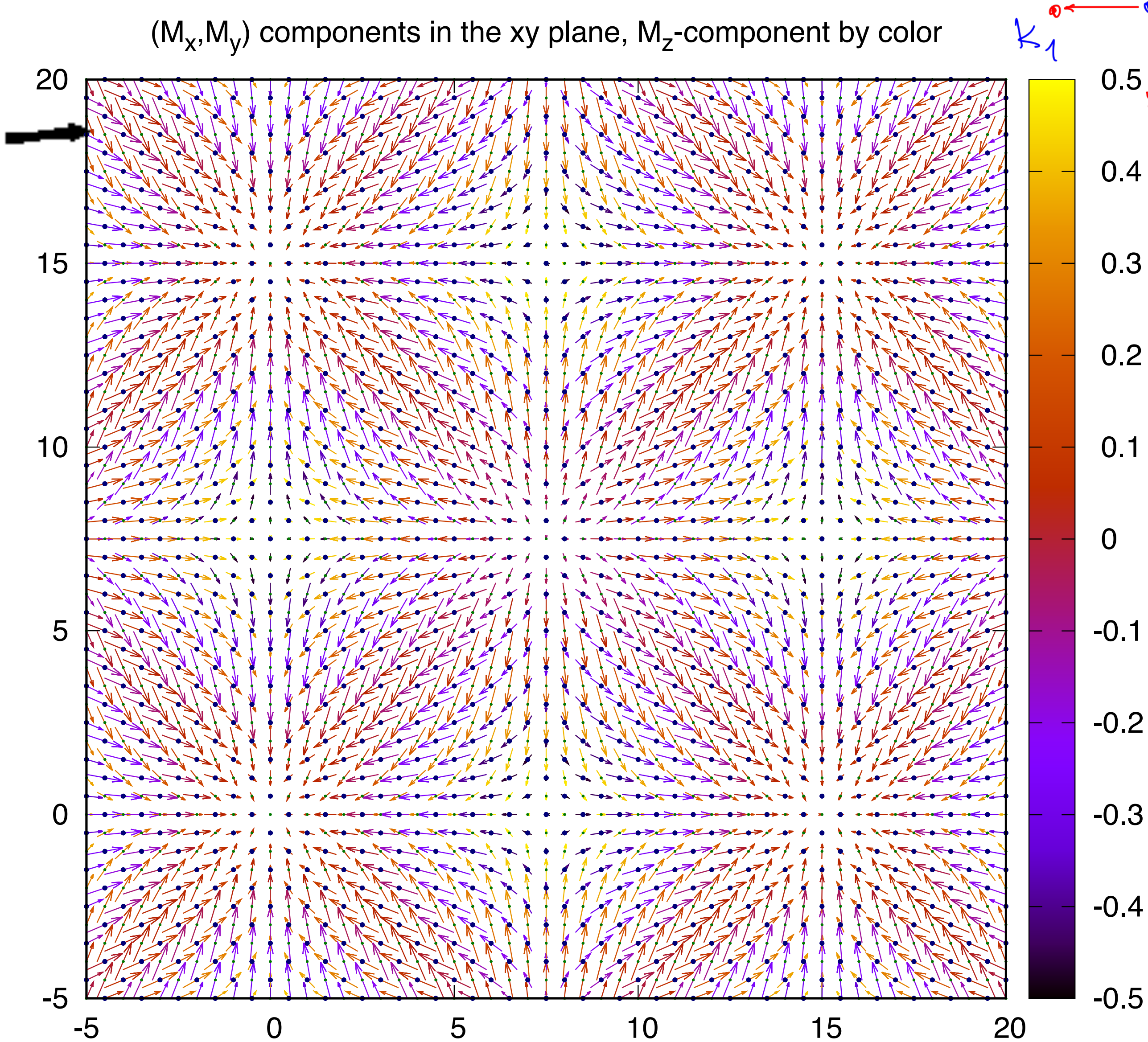
magnetic Weyl semimetal CeAlGe

Topologically nontrivial magnetisation textures in real-space ==> topological Hall effect (THE). Full star superspace 3D+2 group I4_1md1'(a00)000s(0a0)0s0s

View along the z-(c-)axis of the magnetic structure of CeAlGe. The x- and y-axes are in units of in-plane lattice parameter a.





P. Puphal, et al, Physical Review Letters, 124, 017202 (2020)

Superspace magnetic structure in Weyl semimetal CeAlGe. Multi arm antiferromagnetic order.

BULK SINGLE-CRYSTAL GROWTH OF THE … PHYSICAL REVIEW MATERIALS 3, 024204 (2019)

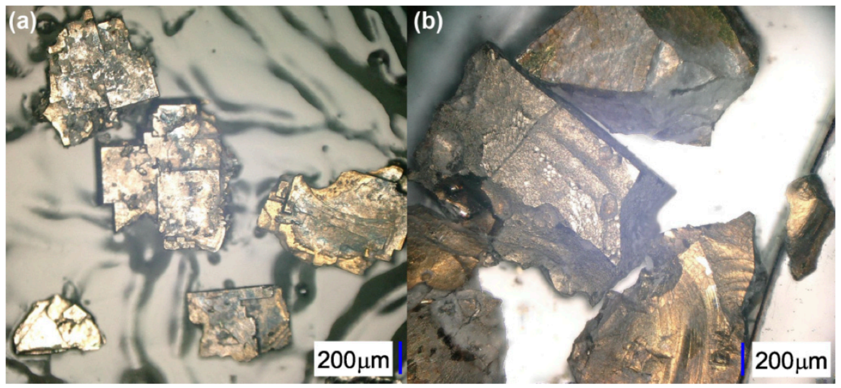


FIG. 2. Pictures of the flux-grown crystals of (a) CeAlGe and (b) PrAlGe right after flux removal using NaOH-H_2O, and before subsequent annealing.

FIG. 3. Photos of (a) the cast CeAlGe rod, and the floating-zone-grown crystals of (b) CeAlGe and (c) PrAlGe.

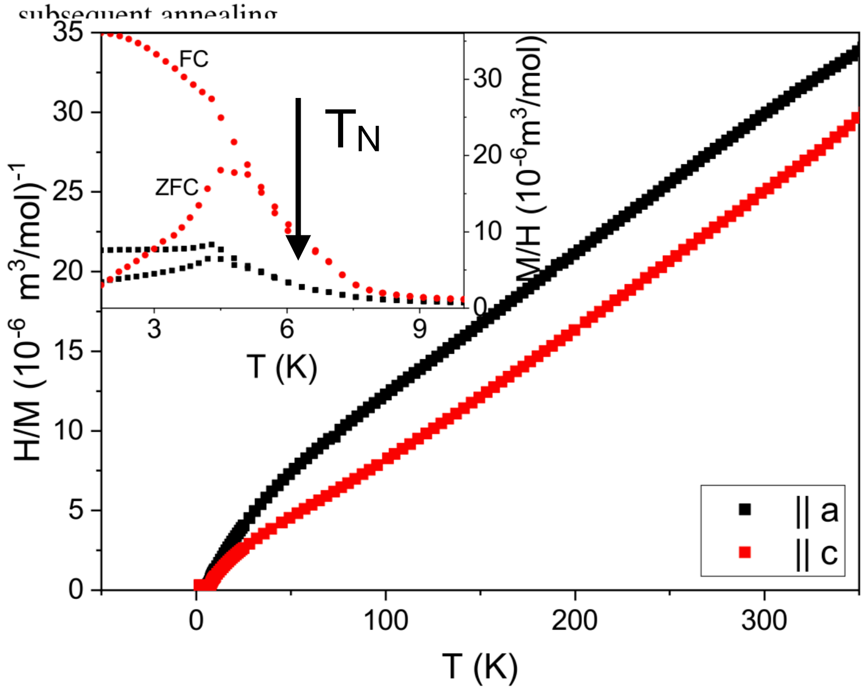
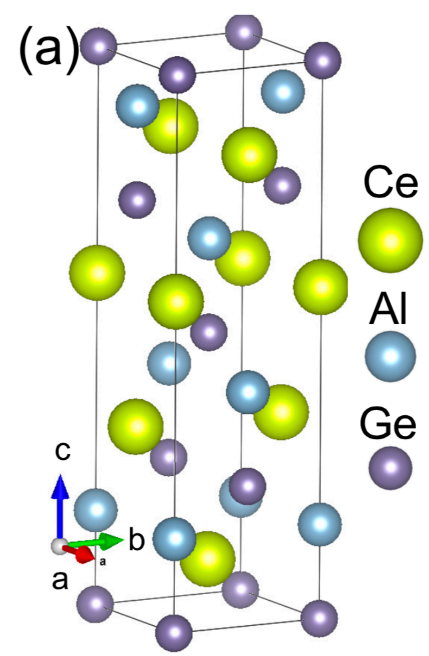


FIG. 8. Magnetic data obtained on a floating-zone-grown CeAlGe single crystal with a mass of 125.4 mg. The magnetic



Space Group: 109 I4_1md C4v-11
non-centrosymmetric
Lattice parameters:
a=4.25717, c=14.64520

Ce1 4a (0,0,z), z=-0.41000 single magnetic Ce site

Neutron diffraction experiments: HRPT and DMC, SANS at PSI Switzerland, D33, at ILL France
Resistivity: Topologicall Hall Effect in University of Tokyo

Samples: both powder and single crystals of CeAlGe grown at PSI in Solid State Chemistry group

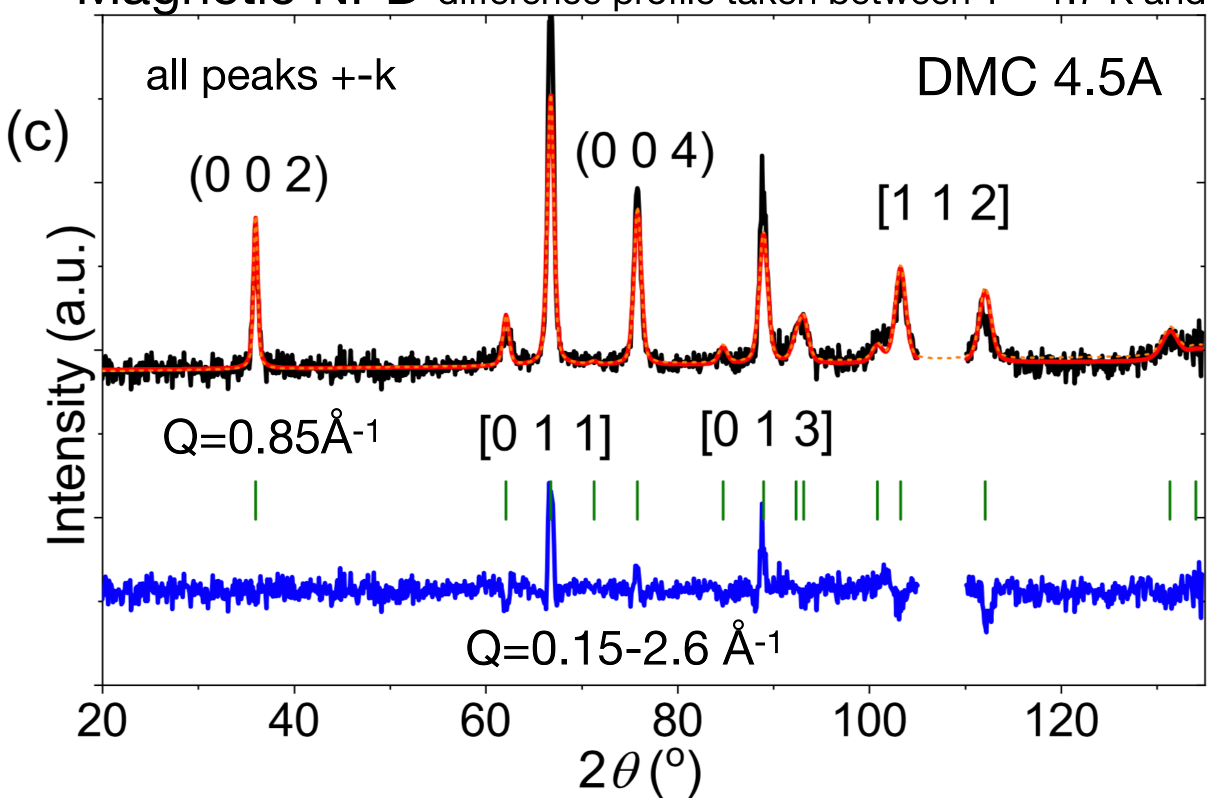
P. Puphal, et al, Physical Review Letters, 124, 017202 (2020)

Magnetic peaks are well seen from both powder and s.c. neutron diffraction

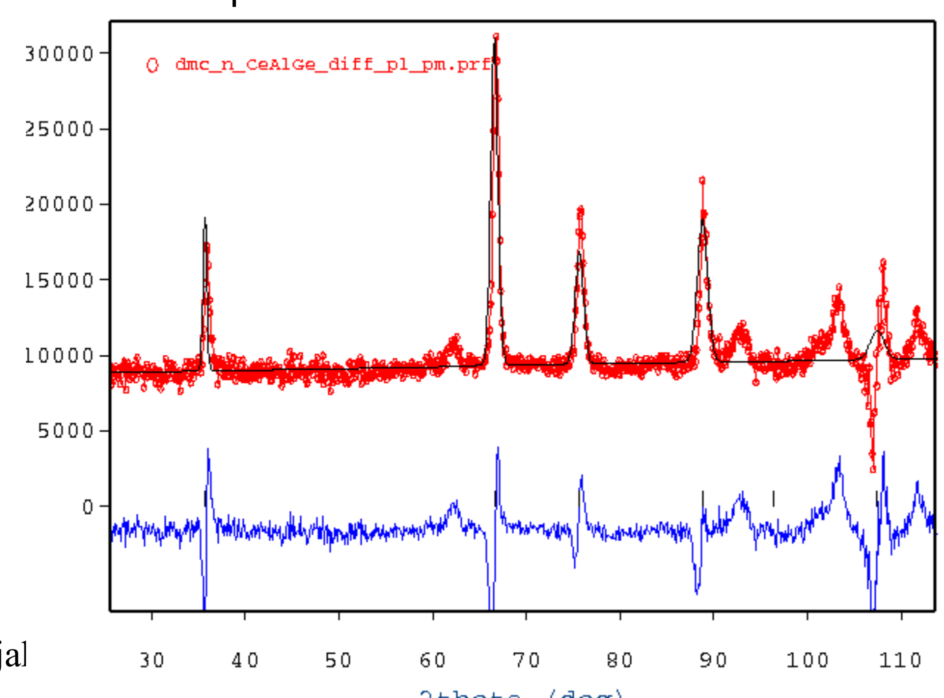
CeAlGe

k1=[g,0,0], SM point of BZ, g=0.06503(22) ~65Å

Magnetic NPD difference profile taken between T = 1.7 K and 10 K



Gamma point k=0 does not fit NPD



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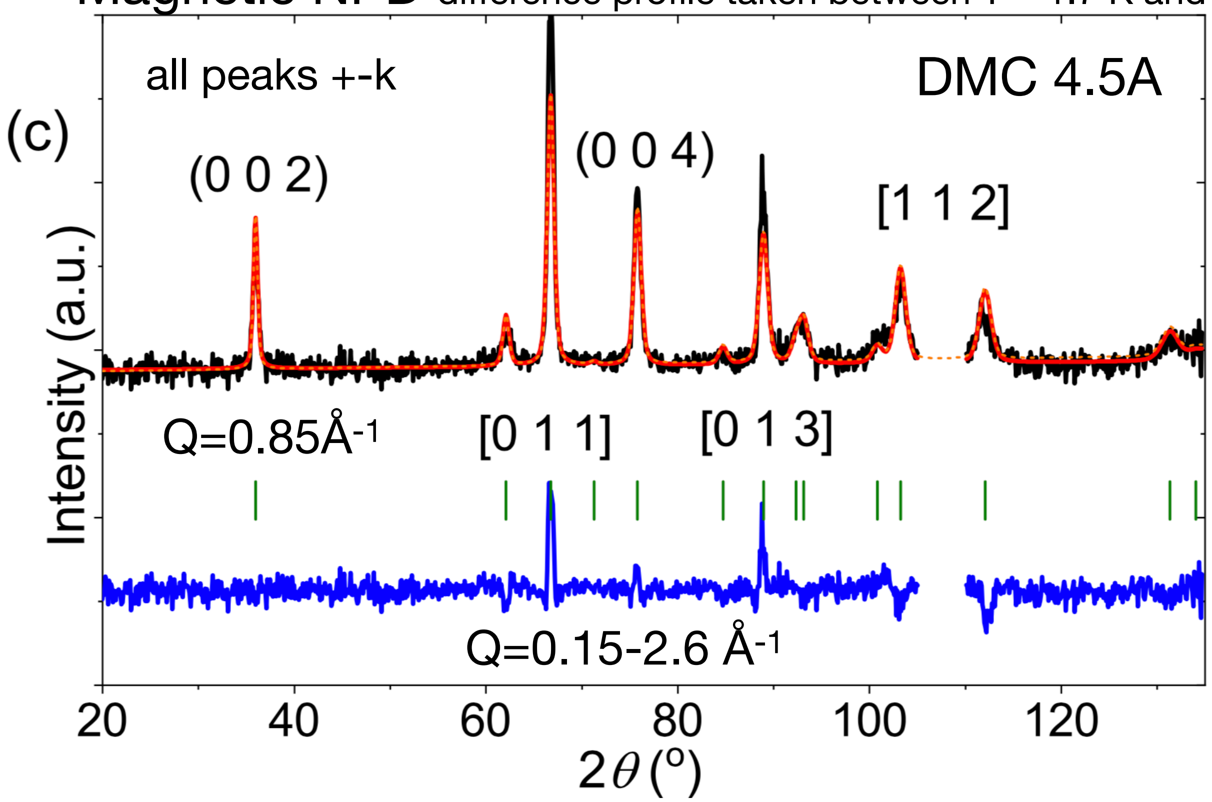

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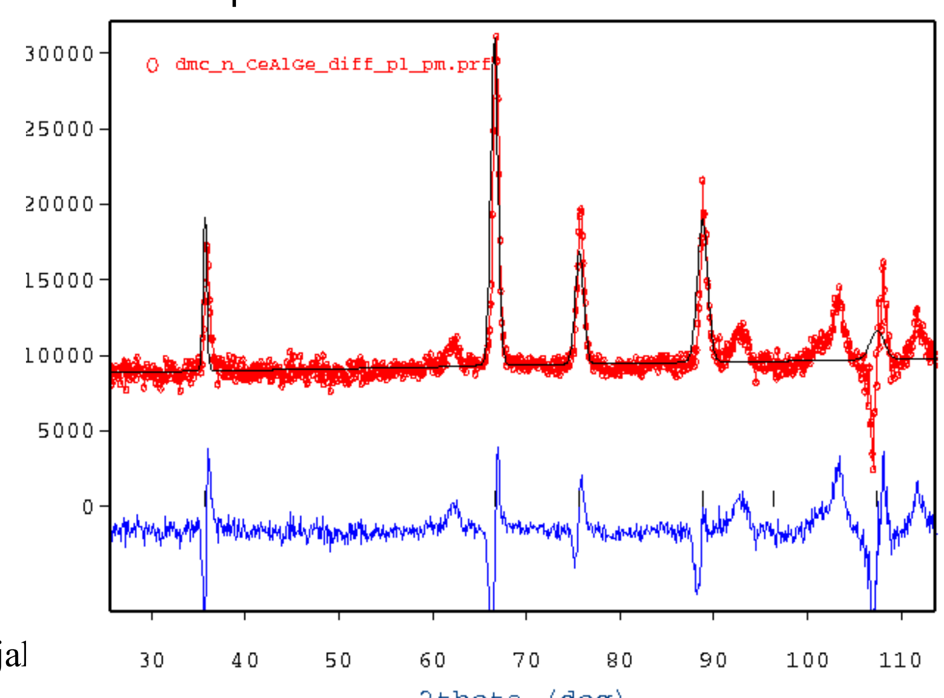
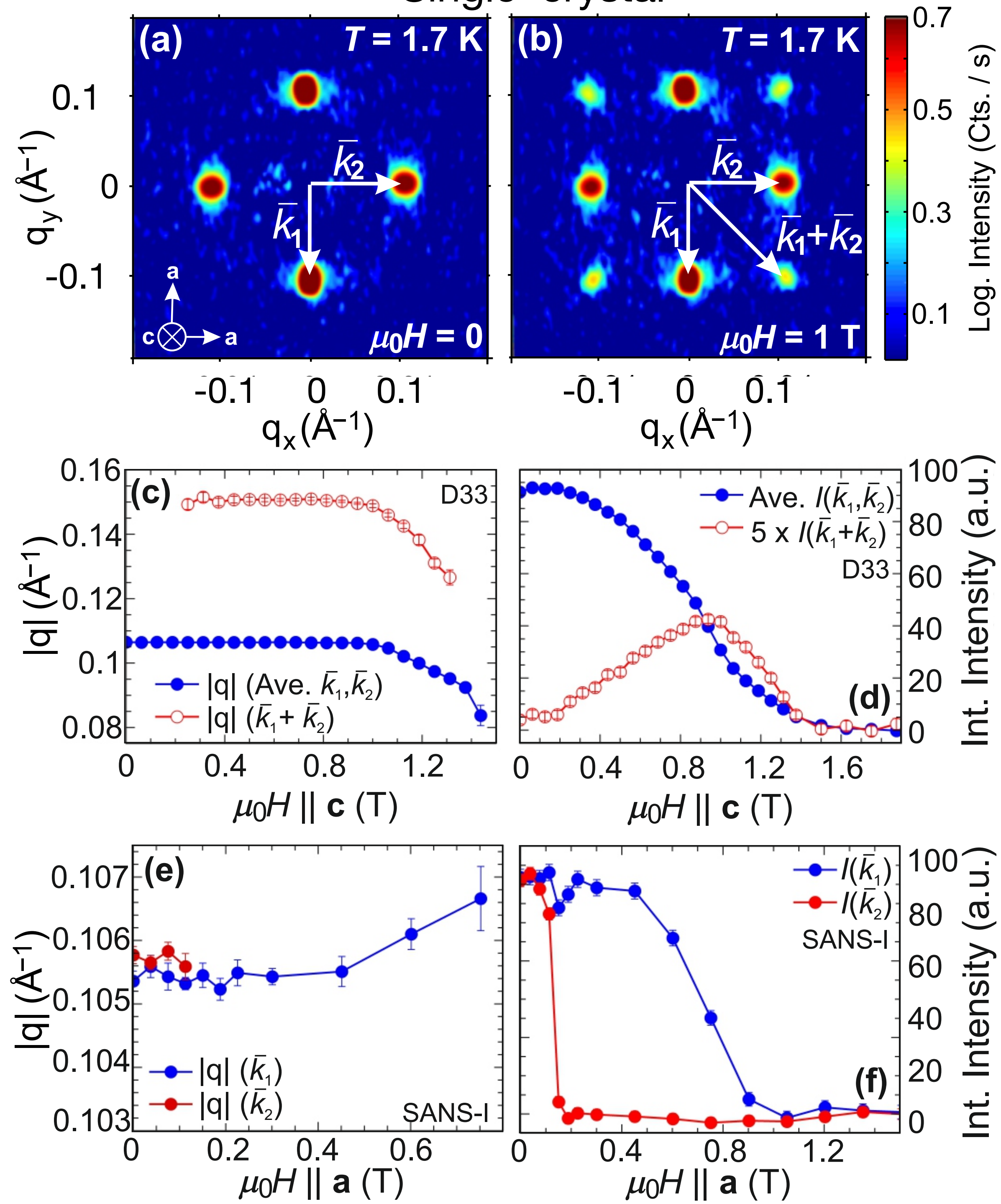


k1=[g,0,0], k2=[0,g,0]

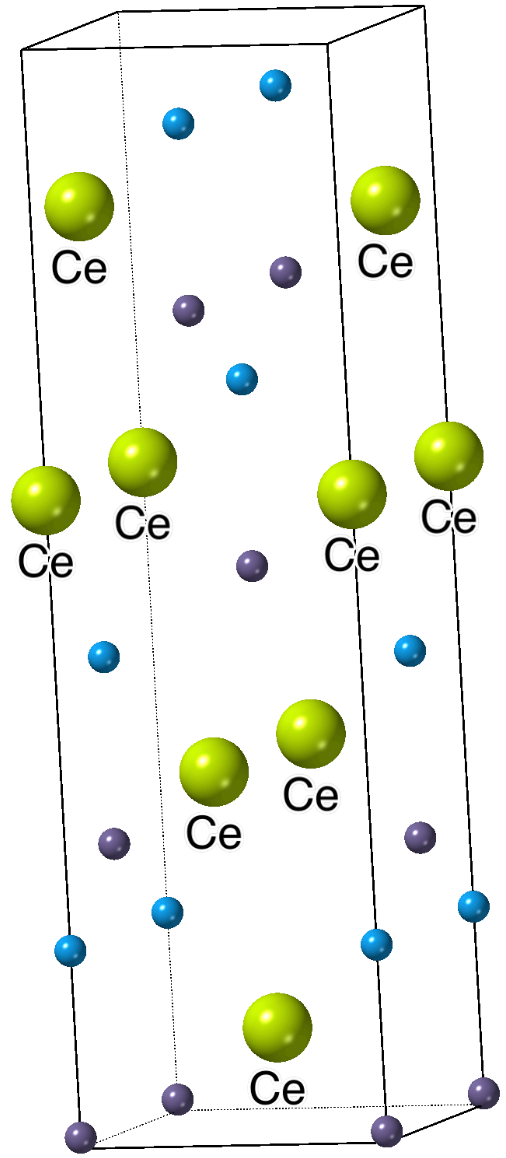
Single crystal



P. Puphal, et al, Physical Review Letters, 124, 017202 (2020)

One k-case, standard representation analysis without magnetic group symmetry arguments.

Space group $I4_1md$:
8 symops & I-centering,
Ce 4a (0,0,z) single
magnetic Ce site: 4
atoms per cell



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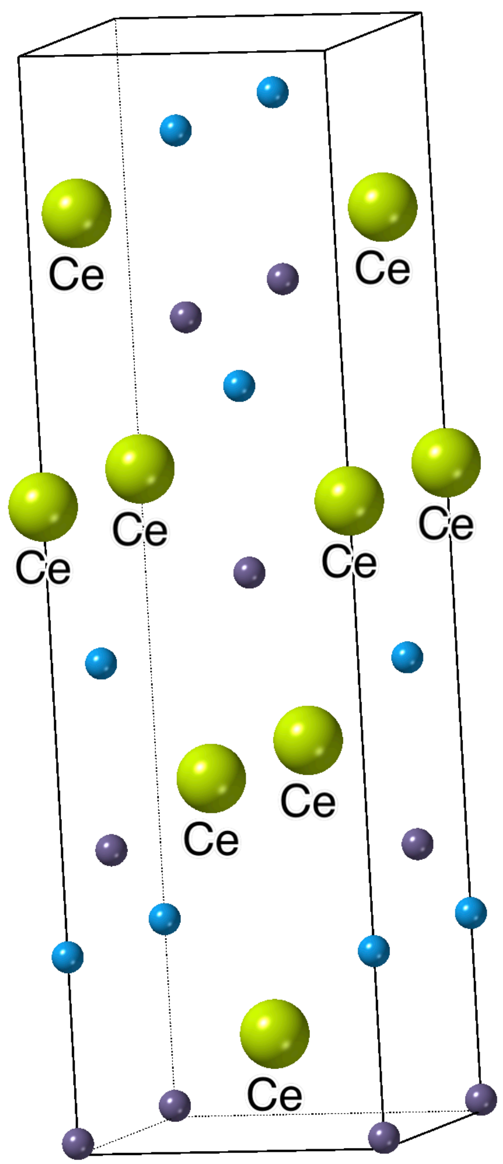
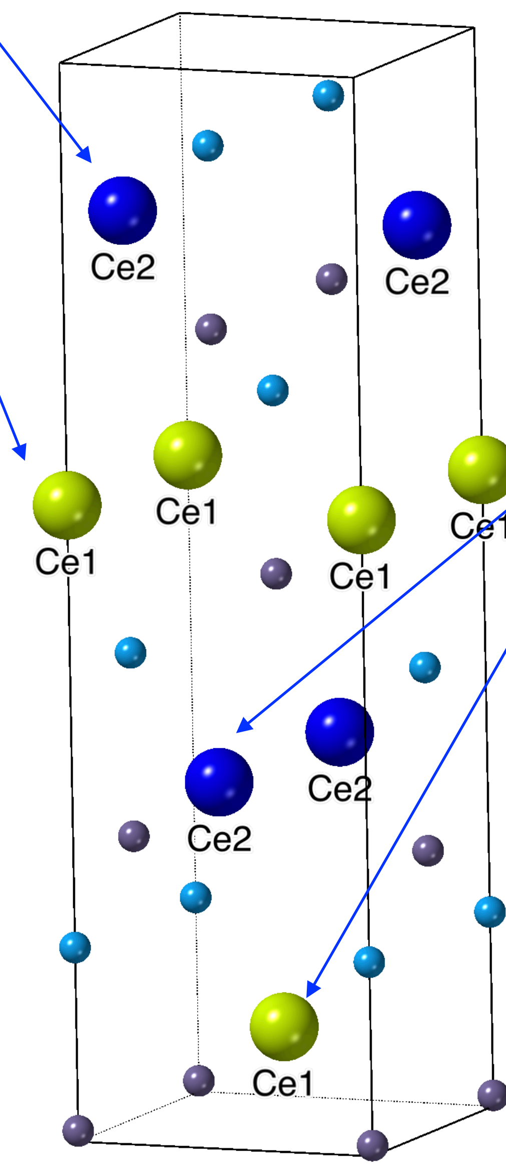
4(a) $Ce1(0,0,z)$

$Ce2(0,\frac{1}{2},z+\frac{1}{4})$

$\bar{y},x+\frac{1}{2},z+\frac{1}{4}$

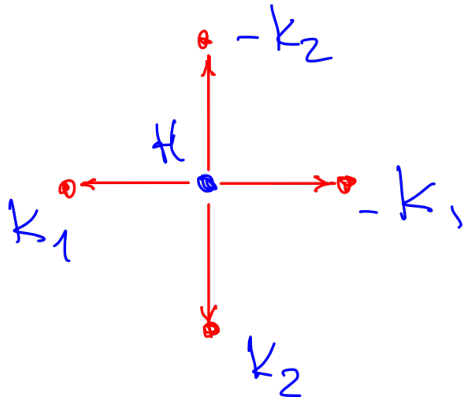


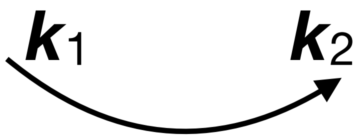


Two other Ce's are generated by I-centering translations (½, ½, ½)+

One k-case, standard representation analysis without magnetic group symmetry arguments: Space group $I4_1md$, Ce 4a (0,0,z) - maybe move this to above

Propagation vector star $\{[g,0,0],[0,g,0]\}$





$$\bar{y}, x+\frac{1}{2}, z+\frac{1}{4}$$

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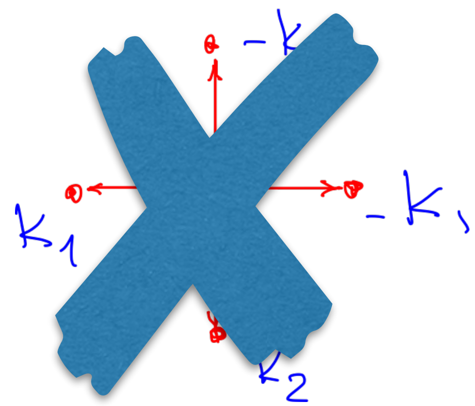

$\boldsymbol{k}_1 \rightarrow \boldsymbol{k}_2$

$$\bar{y}, x+\frac{1}{2}, z+\frac{1}{4}$$

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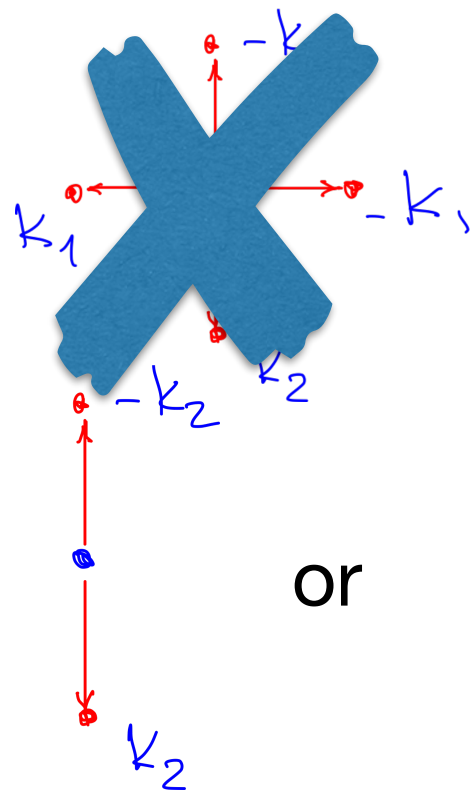
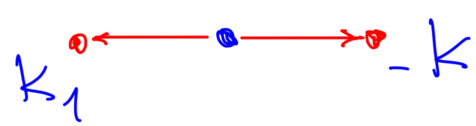


or



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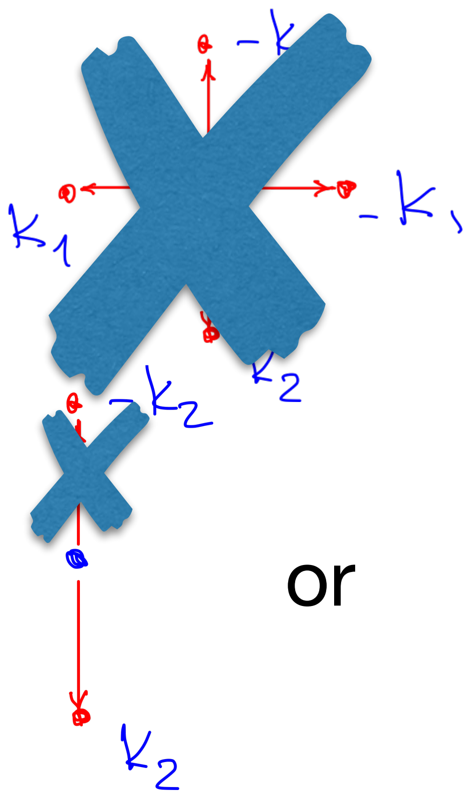
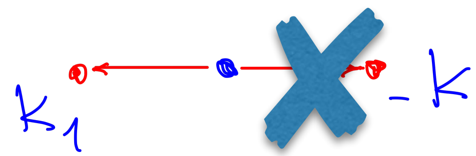


$\boldsymbol{k}_1 \curvearrowright \boldsymbol{k}_2$

$$\bar{y}, x+\frac{1}{2}, z+\frac{1}{4}$$

or

Group G_k has x,y,z
only 2 symops $x,\bar{y},z$ out of 8!

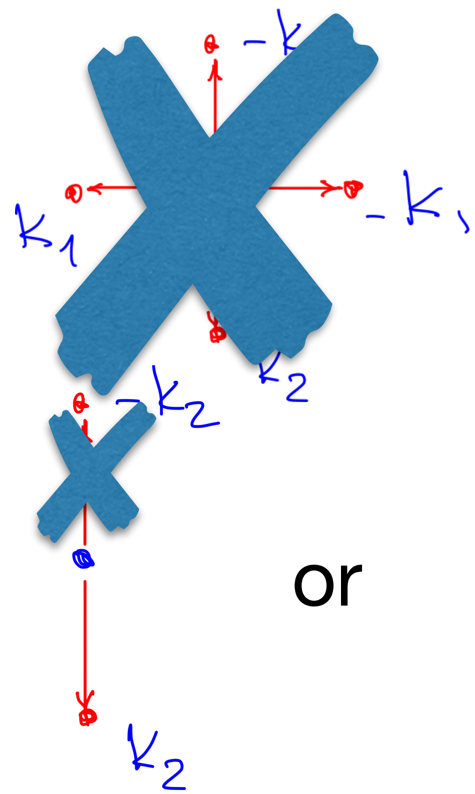


$\mathrm{Ce1}(0,0,z)$
$\mathrm{Ce2}(0,\frac{1}{2},z+\frac{1}{4})$

Two independent sites.
No symmetry relations between Ce1 and Ce2

One k-case, standard representation analysis without magnetic group symmetry arguments: Space group $I4_1md$, Ce 4a (0,0,z) - maybe move this to above

Propagation vector star $\{[g,0,0],[0,g,0]\}$

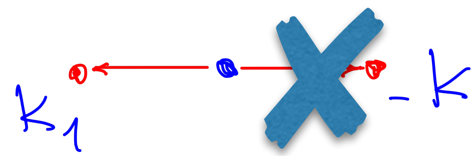


or

$\boldsymbol{k}_1 \rightarrow \boldsymbol{k}_2$

$\bar{y}, x+\frac{1}{2}, z+\frac{1}{4}$

Group G_k has only 2 symops x,y,z $x,\bar{y},z$ out of 8!



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Two independent sites. No symmetry relations between Ce1 and Ce2

Group G_k has two 1D irreps

	τ1	τ2
x,y,z	1	1
$x,\bar{y},z$	1	-1

One k-case, standard representation analysis without magnetic group symmetry arguments: Space group $I4_1md$, Ce 4a (0,0,z)

Solution: SM2 irreducible representation

- **Cycloid in ac-plane for k1=[g,0,0]**, in bc=lane for k2=[0,g,0]
- two magnetic domains (twins)

Lowest monoclinic MSSG
8.1.4.2.m33.2 Bm.1'(a,b,0)ss

$k=|\boldsymbol{k}_1|=|\boldsymbol{k}_2|=g$

$$\mathbf{M}_{Ce(i)} = m_{ix}\sin(2\pi kx)\mathbf{e}_{\boldsymbol{x}} + m_{iz}\sin(2\pi kx+\varphi_i)\mathbf{e}_{\boldsymbol{z}}, \quad i=1,2$$

Experimental values (μ_B) :
Ce1: m_{1x}= -0.64(1), m_{1z} =-0.30(6)
Ce2: m_{2x}= -1.50(2), m2z = 0.46(8)

$\varphi_1=\varphi_2\approx 90°$

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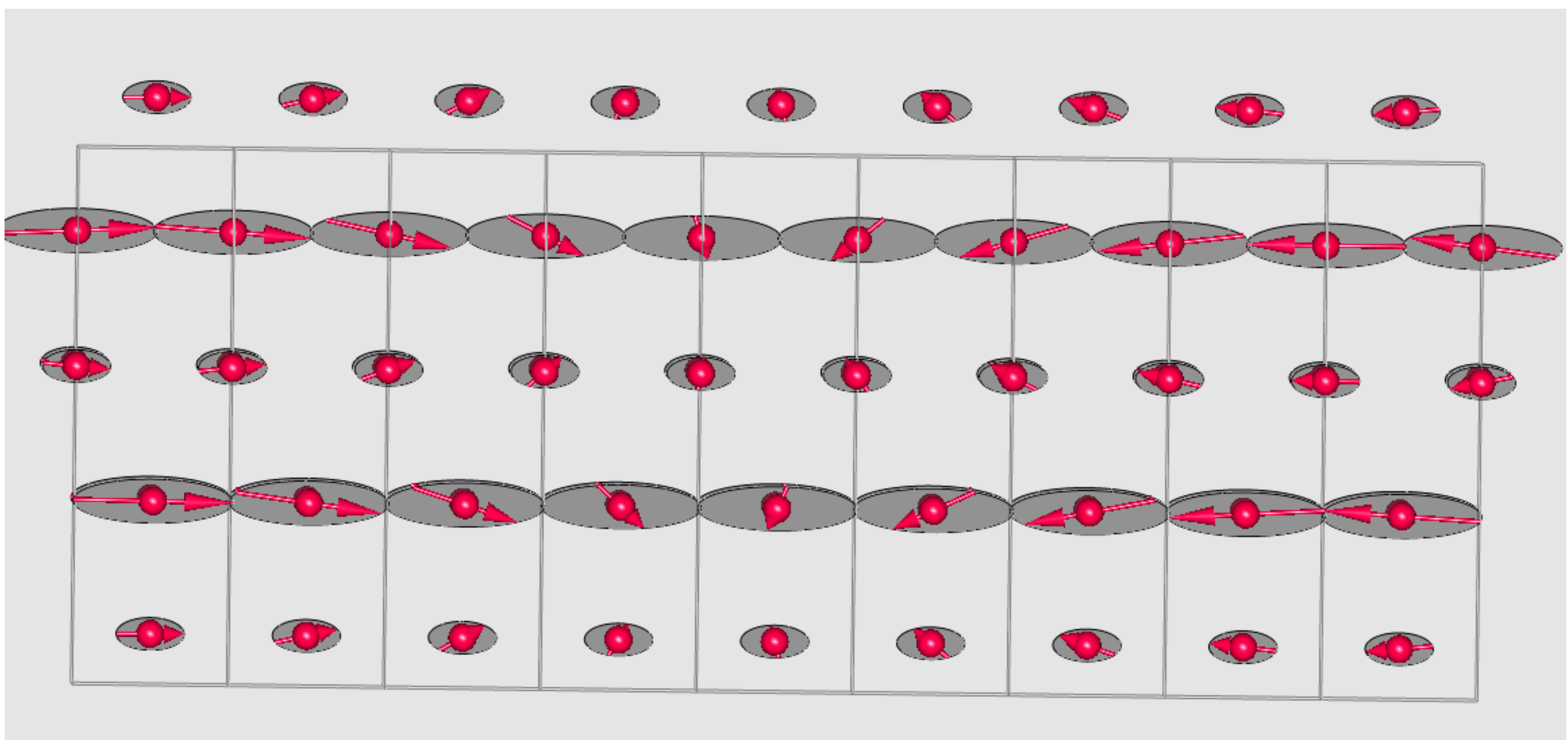

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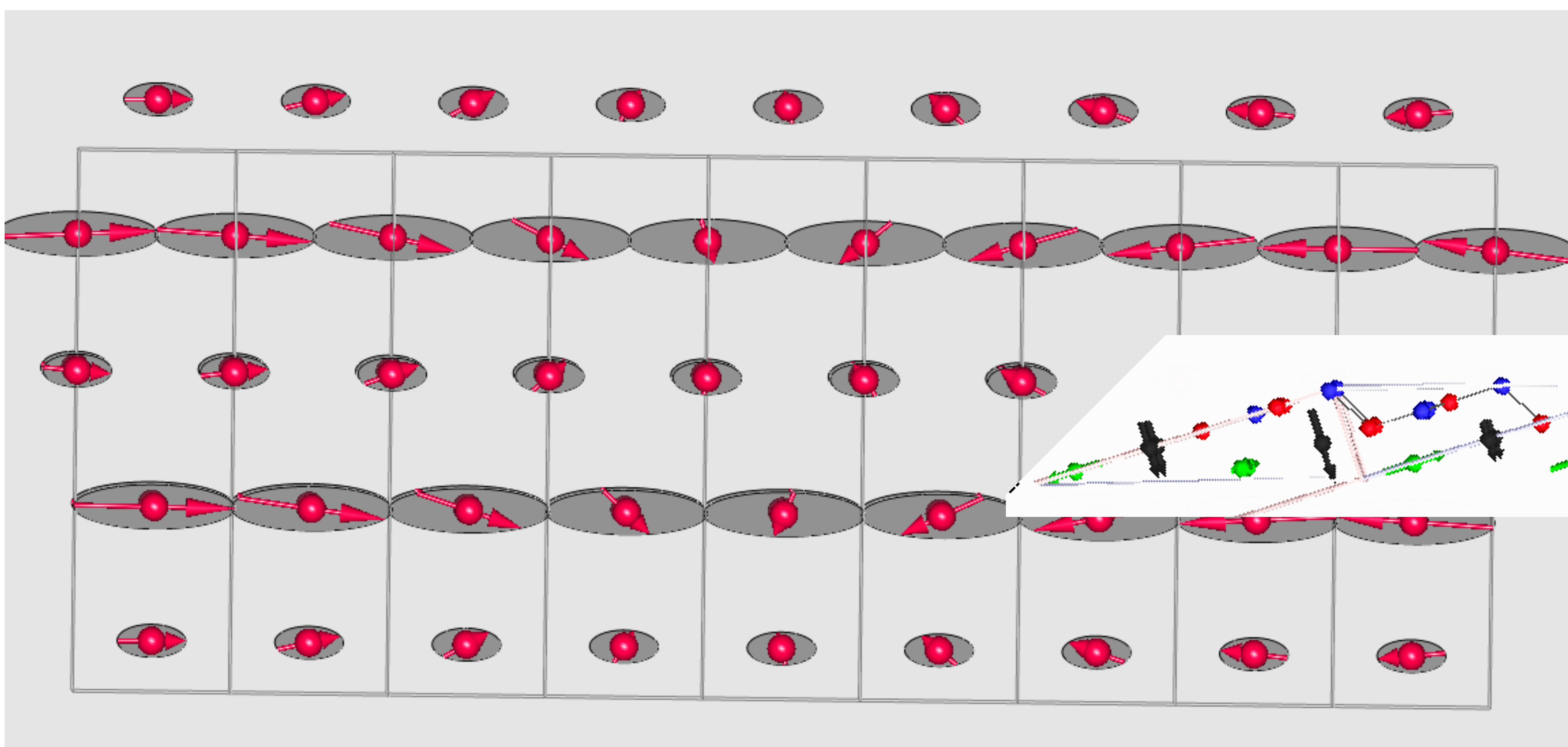
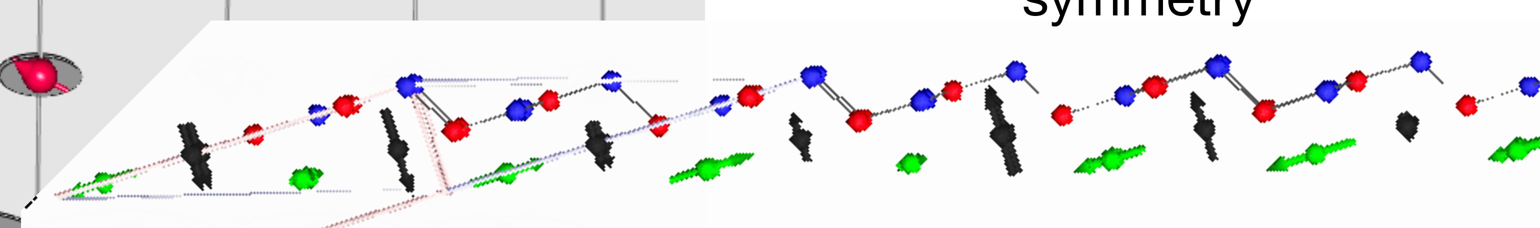
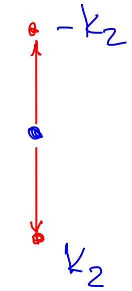
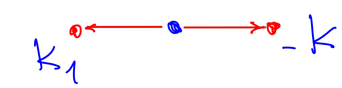


Note: if $\varphi_1=\varphi_2=0$ → amplitude modulation, different symmetry



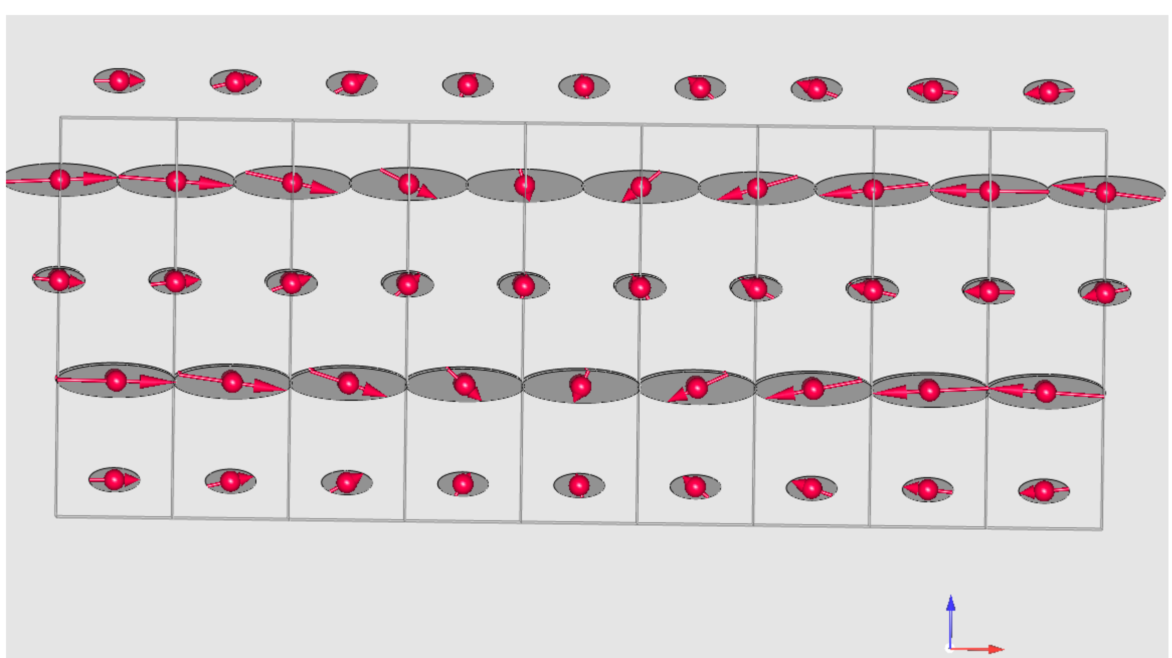
Symmetry of cycloid. 3D+1 superspace group for SM2 irrep

I4$_1$md1' Advantage of magnetic symmetry when keeping {+**k**,-**k**} 

or 

I2mm1'(0,0,g)0s0s

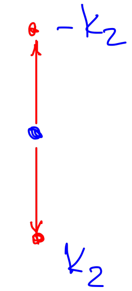
$$\mathbf{M}_{Ce(i)} = m_{ix}\sin(2\pi kx)\mathbf{e}_{\boldsymbol{x}} + m_{iz}\cos(2\pi kx)\mathbf{e}_{\boldsymbol{z}}, \quad i = 1, 2$$



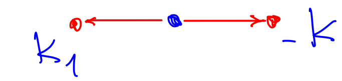
Experimental values:
Ce1: m_{1x}= -0.64(1), m_{1z} =-0.30(6)
Ce2: m_{2x}= -1.50(2), m2z = 0.46(8)

Symmetry of cycloid. 3D+1 superspace group for SM2 irrep

$I4_1md1'$ Advantage of magnetic symmetry when keeping {+**k**,-**k**}



or



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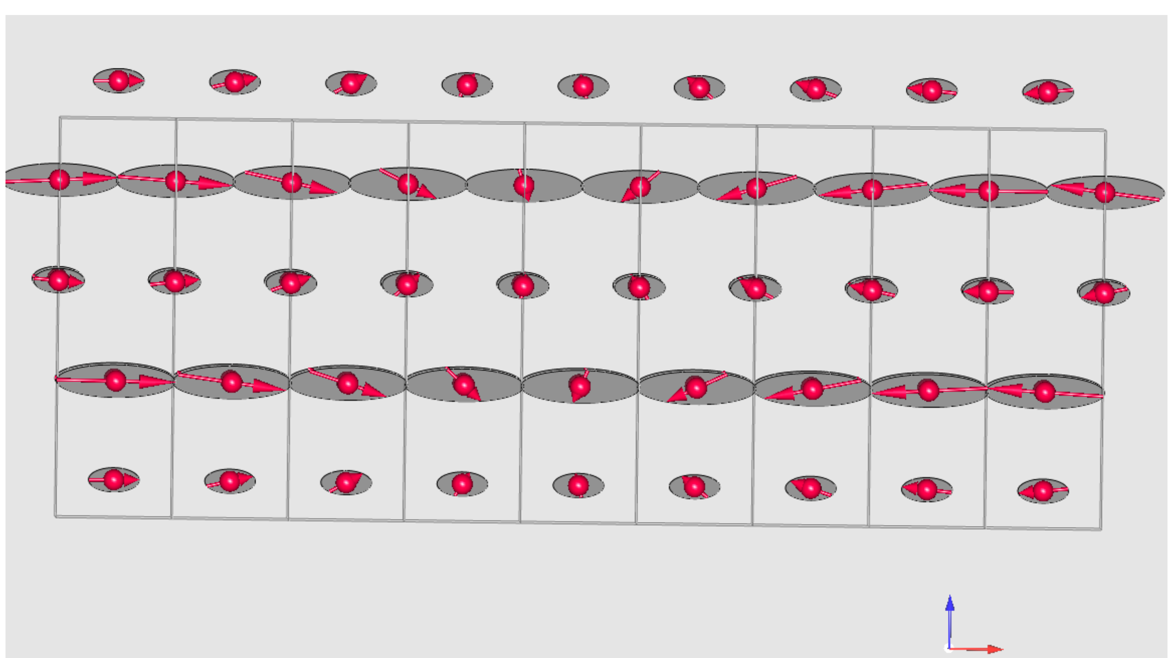
$$\mathbf{M}_{Ce(i)} = m_{ix}\sin(2\pi kx)\mathbf{e}_{\boldsymbol{x}} + m_{iz}\cos(2\pi kx)\mathbf{e}_{\boldsymbol{z}}, \quad i = 1, 2$$

phase shift 90 degrees between x and y-components is fixed by symmetry!



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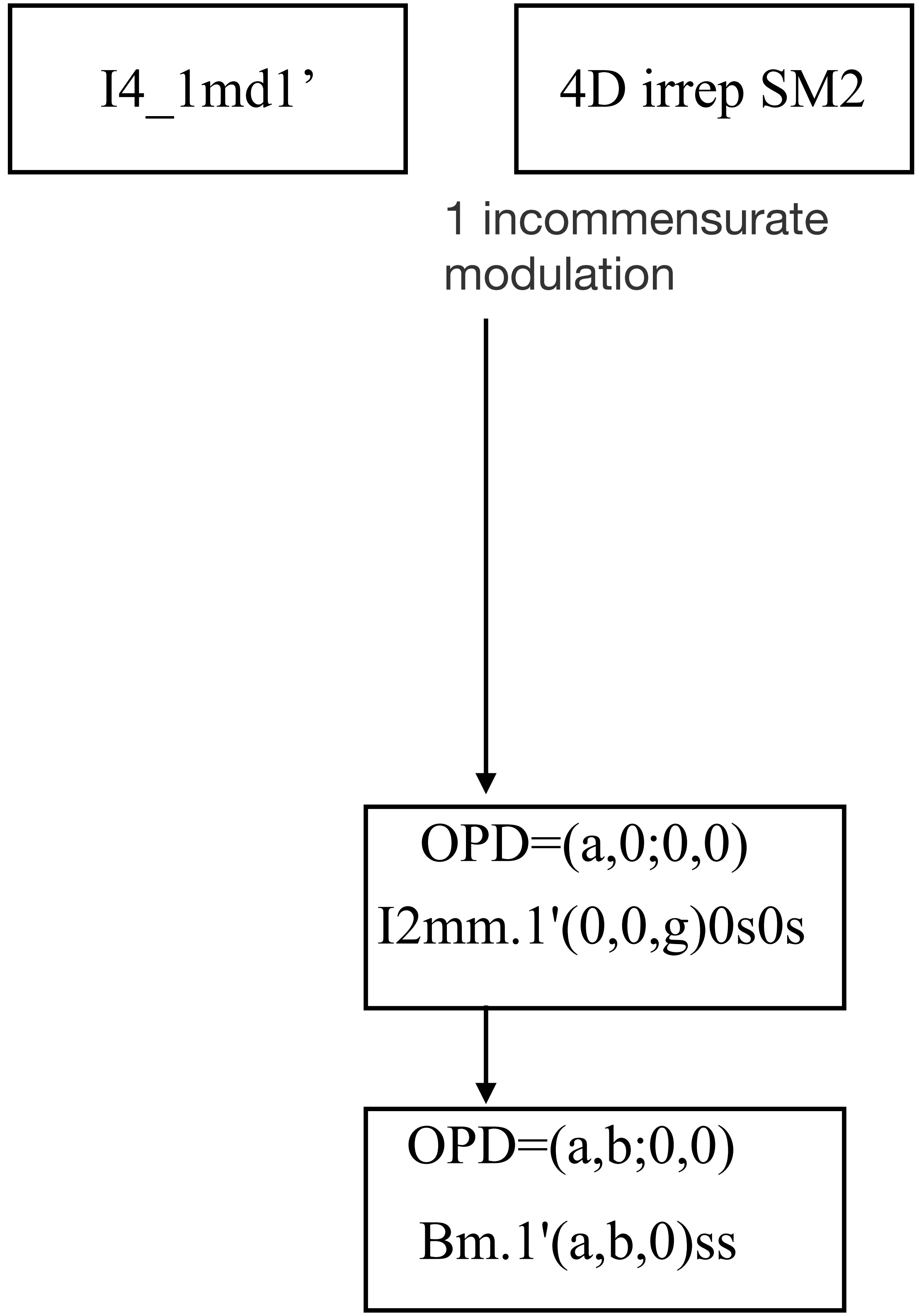
subgroup tree for I4_1md [u,0,0]+[0,u,0]



irrep OPD

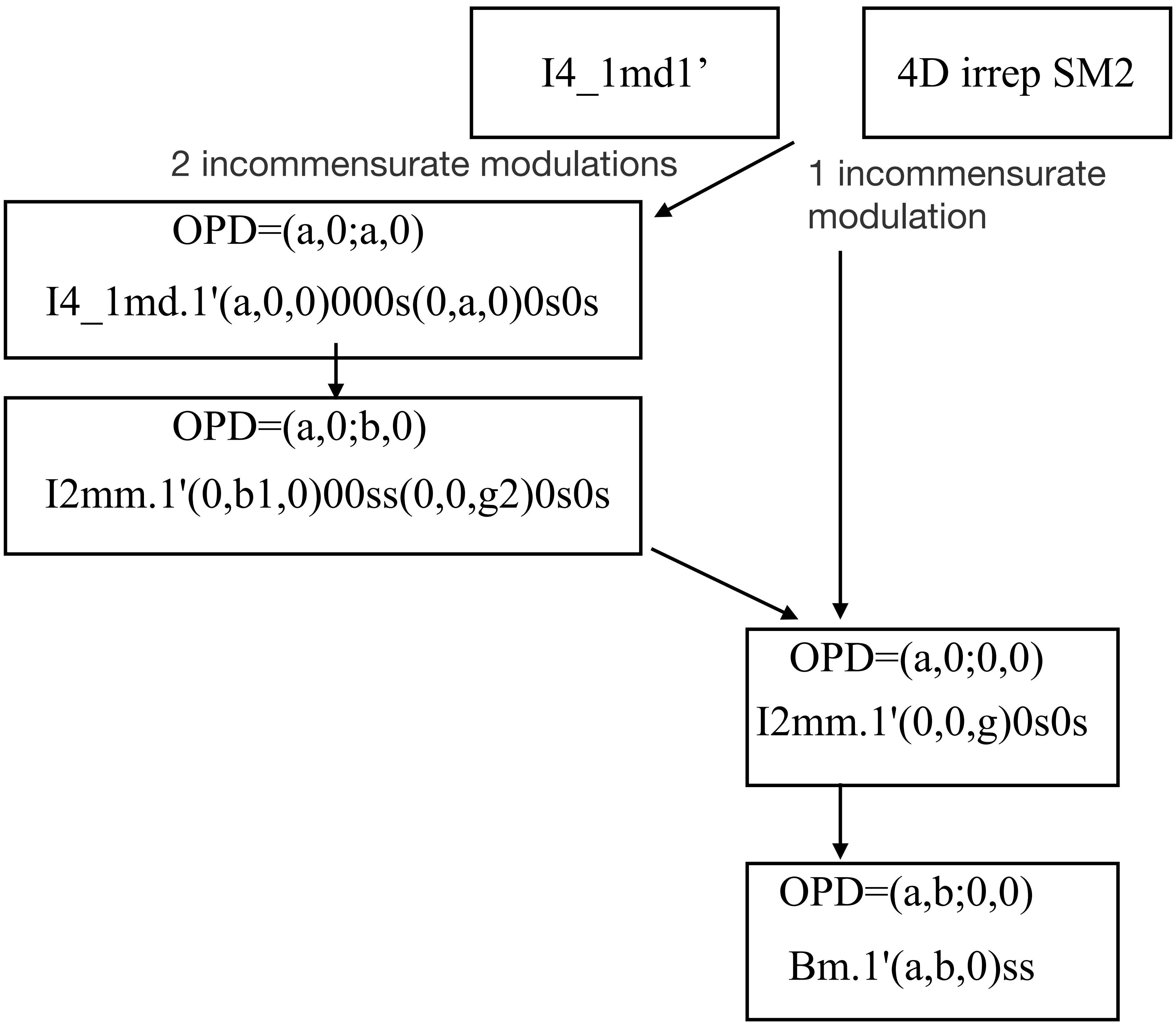
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ \mathrm{Cos}(\pi u) & \mathrm{Sin}(\pi u) & 0 & 0 \\ \mathrm{Sin}(\pi u) & \mathrm{Cos}(\pi u) & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \mathrm{Cos}(\pi u) & -\mathrm{Sin}(\pi u) & 0 & 0 \\ \mathrm{Sin}(\pi u) & -\mathrm{Cos}(\pi u) & 0 & 0 \end{pmatrix}$$

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

subgroup tree for I4_1md [u,0,0]+[0,u,0]



irrep OPD

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$$\begin{matrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ \mathrm{Cos}(\pi u) & \mathrm{Sin}(\pi u) & 0 & 0 \\ \mathrm{Sin}(\pi u) & \mathrm{Cos}(\pi u) & 0 & 0 \end{matrix} \Bigg)$$

$$\begin{matrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \mathrm{Cos}(\pi u) & -\mathrm{Sin}(\pi u) & 0 & 0 \\ \mathrm{Sin}(\pi u) & -\mathrm{Cos}(\pi u) & 0 & 0 \end{matrix} \Bigg)$$

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

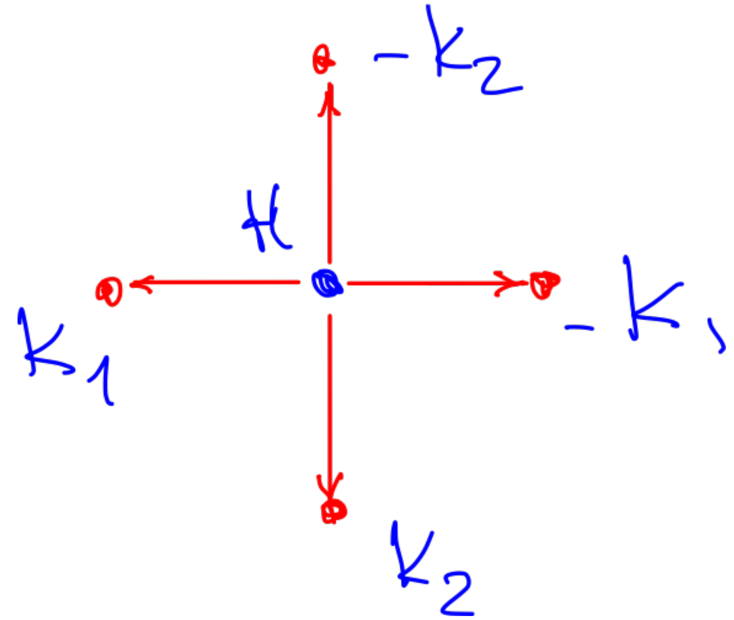
CeAlGe: Maximal symmetry full star superspace 3D+2 magnetic group I4_1md1'(a00)000s(0a0)0s0s

$I4_1md1'$ IR: mSM2 , k-active= (g,0,0),(0,g,0)

↓

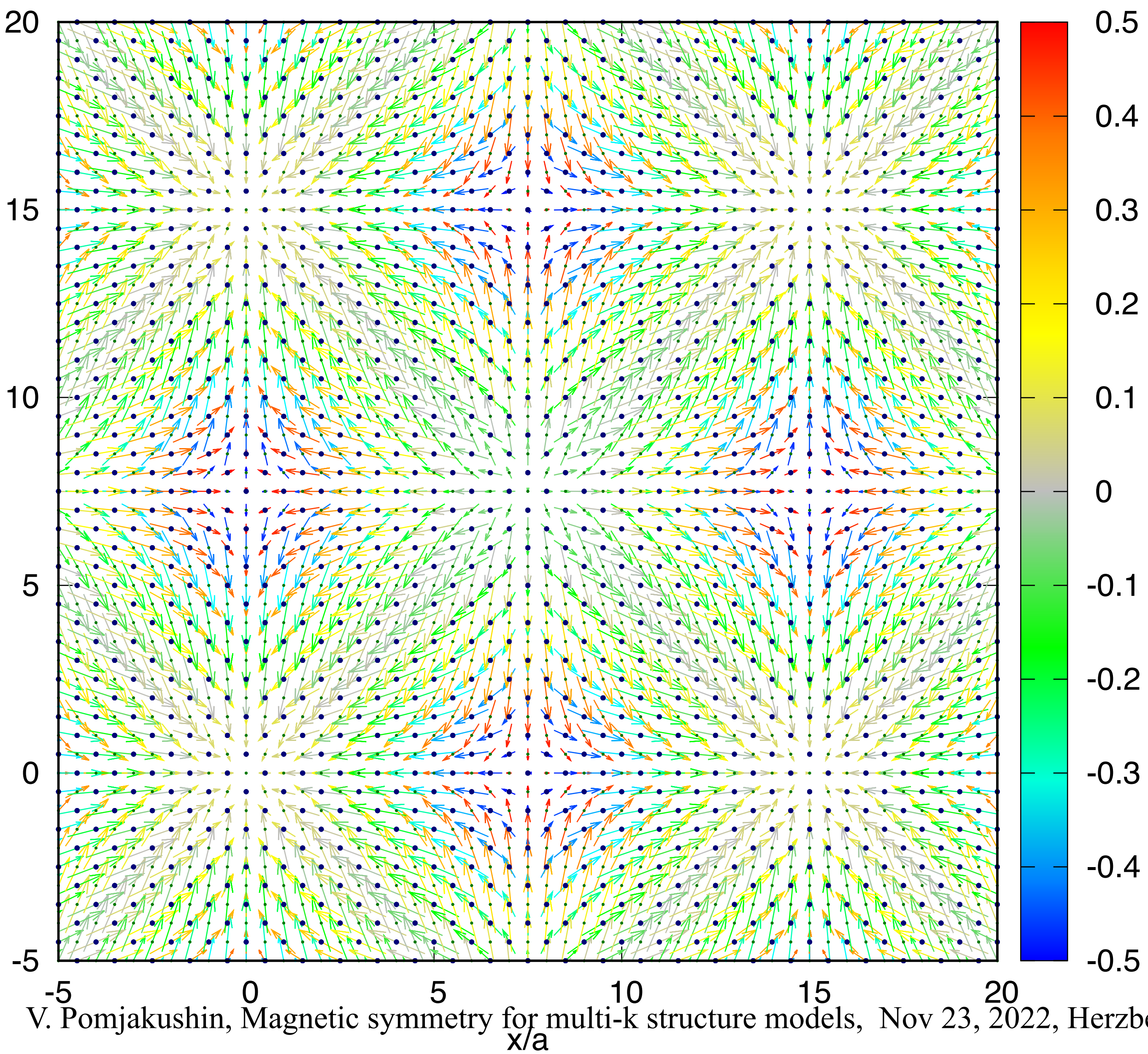
I4_1md1'(a,0,0)000s(0,a,0)0s0s
single Ce site: Ce1 and Ce2 equivalent

k1=[g,0,0], SM point of BZ,
g=0.06503(22): four arms



View along the z-(c-)axis of the magnetic structure of CeAlGe.
The x- and y-axes are in units of in-plane lattice parameter a.

(M_x,M_y) components in the xy plane, M_z-component by color



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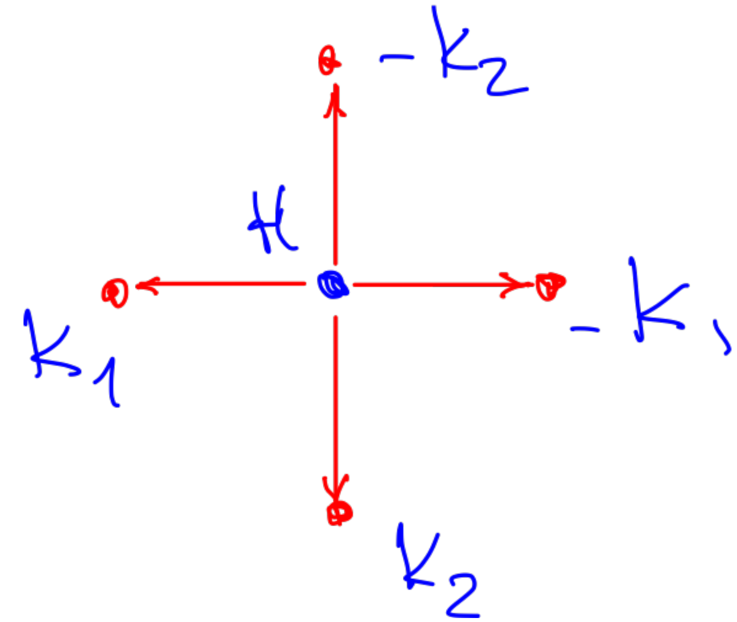

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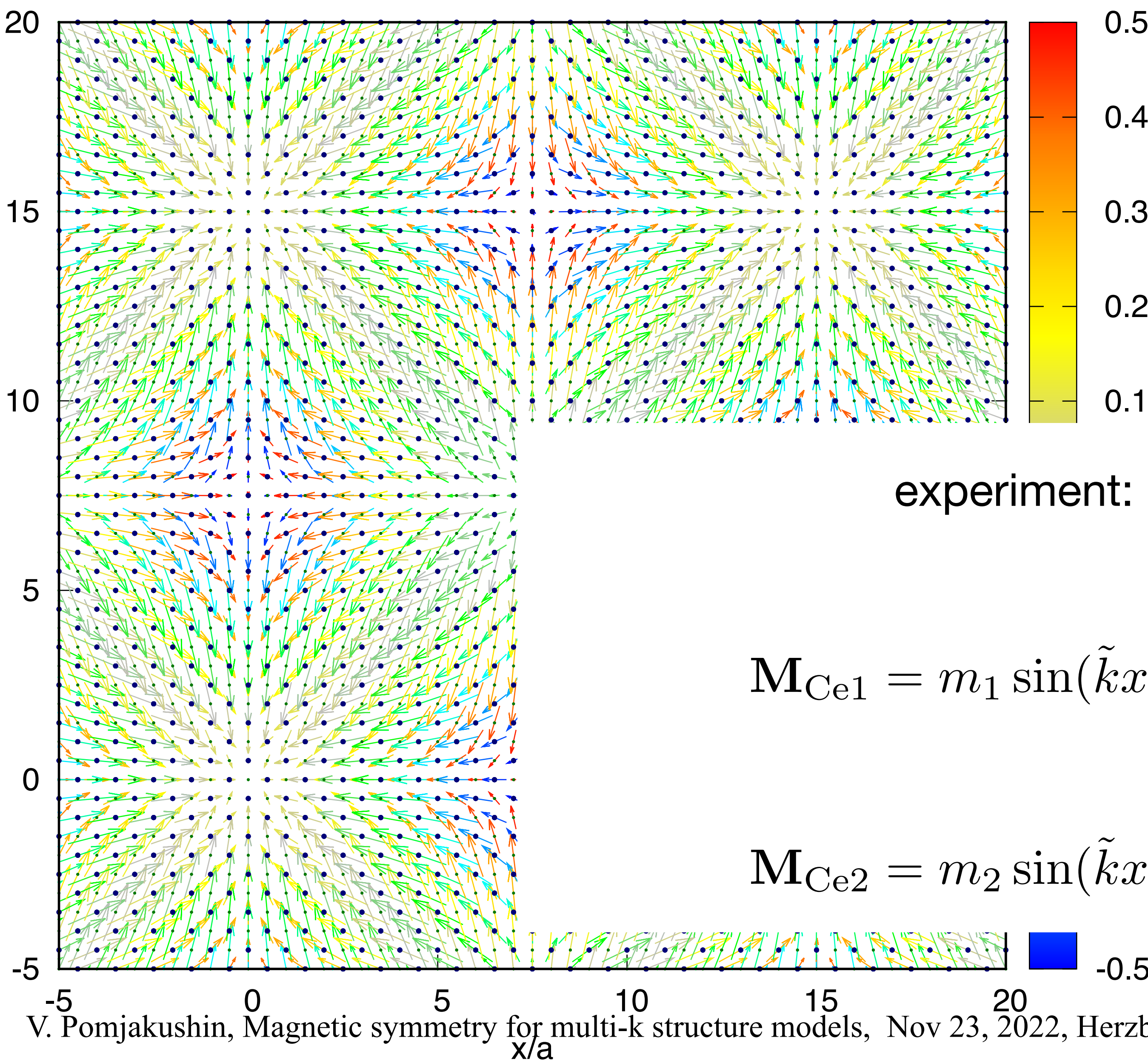

All Ce are equivalent and their moments are given symmetrically by 4 parameters

experiment: (m1,m2,m3,m4) = (0.44(1), 1.02(1), –0.21(5), 0.29(7)) μ_B.

$\tilde{k}=2\pi|\mathbf{k}_1|=2\pi|\mathbf{k}_2|=2\pi g$

$$\mathbf{M}_{\mathrm{Ce1}} = m_1 \sin(\tilde{k}x)\mathbf{e}_{\boldsymbol{x}} + m_2 \sin(\tilde{k}y)\mathbf{e}_{\boldsymbol{y}} + \Big(m_3 \cos(\tilde{k}x) + m_4 \cos(\tilde{k}y)\Big)\,\mathbf{e}_{\boldsymbol{z}}$$

$$\mathbf{M}_{\mathrm{Ce2}} = m_2 \sin(\tilde{k}x)\mathbf{e}_{\boldsymbol{x}} + m_1 \sin(\tilde{k}y)\mathbf{e}_{\boldsymbol{y}} + \Big(m_4 \cos(\tilde{k}x) + m_3 \cos(\tilde{k}y)\Big)\,\mathbf{e}_{\boldsymbol{z}}$$

CeAlGe: Maximal symmetry full star superspace 3D+2 magnetic group I4_1md1'(a00)000s(0a0)0s0s

$I4_1md1'$ IR: mSM2 , k-active= (g,0,0),(0,g,0)

↓

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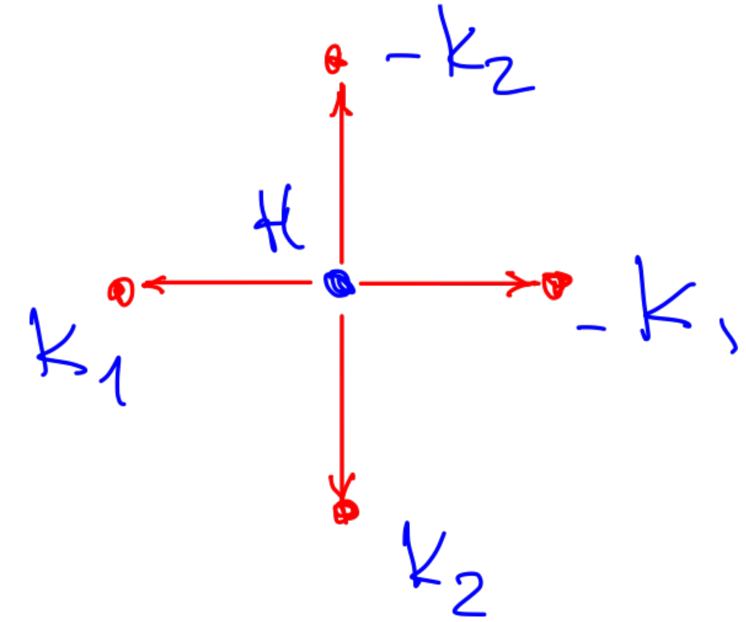

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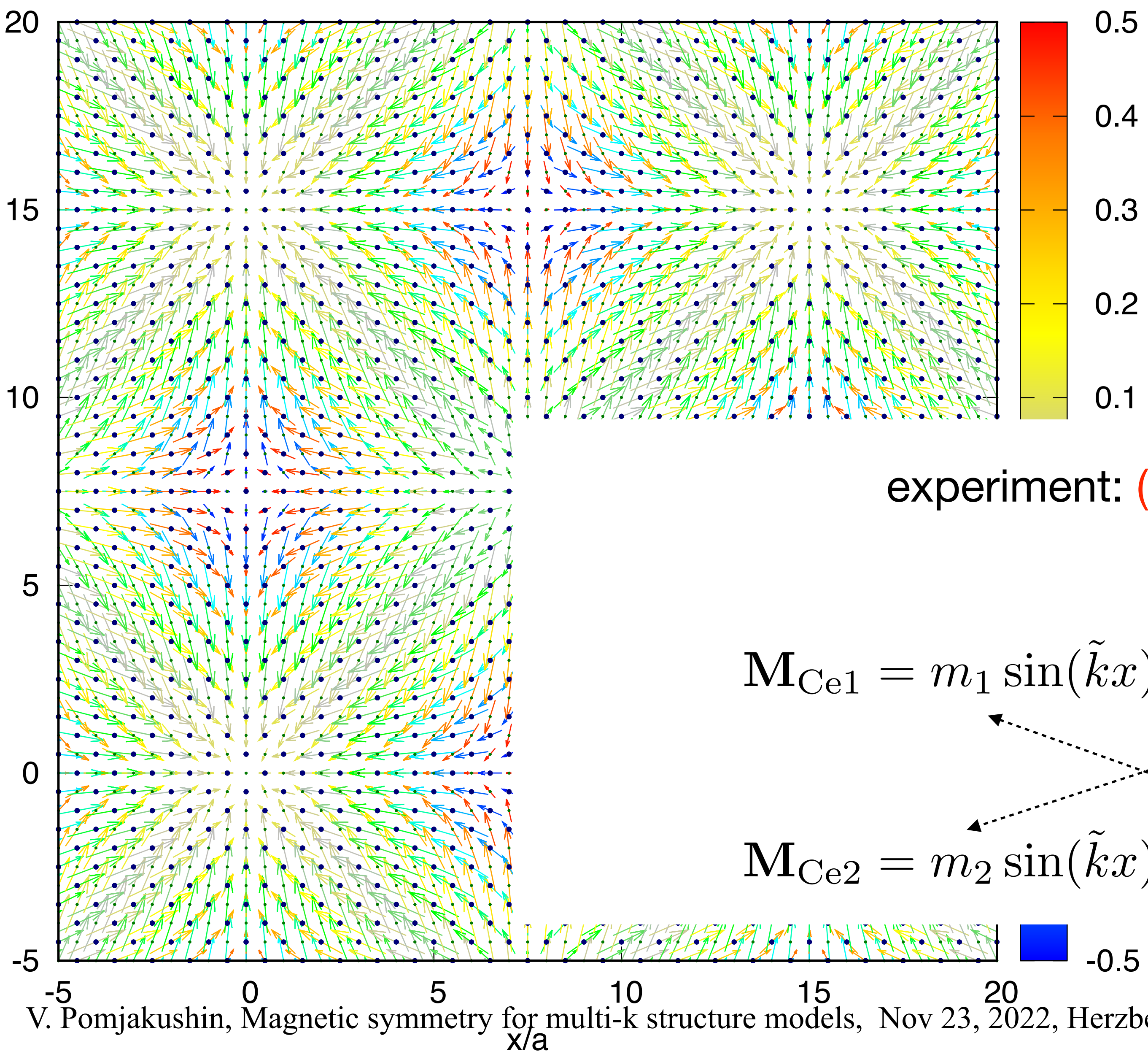

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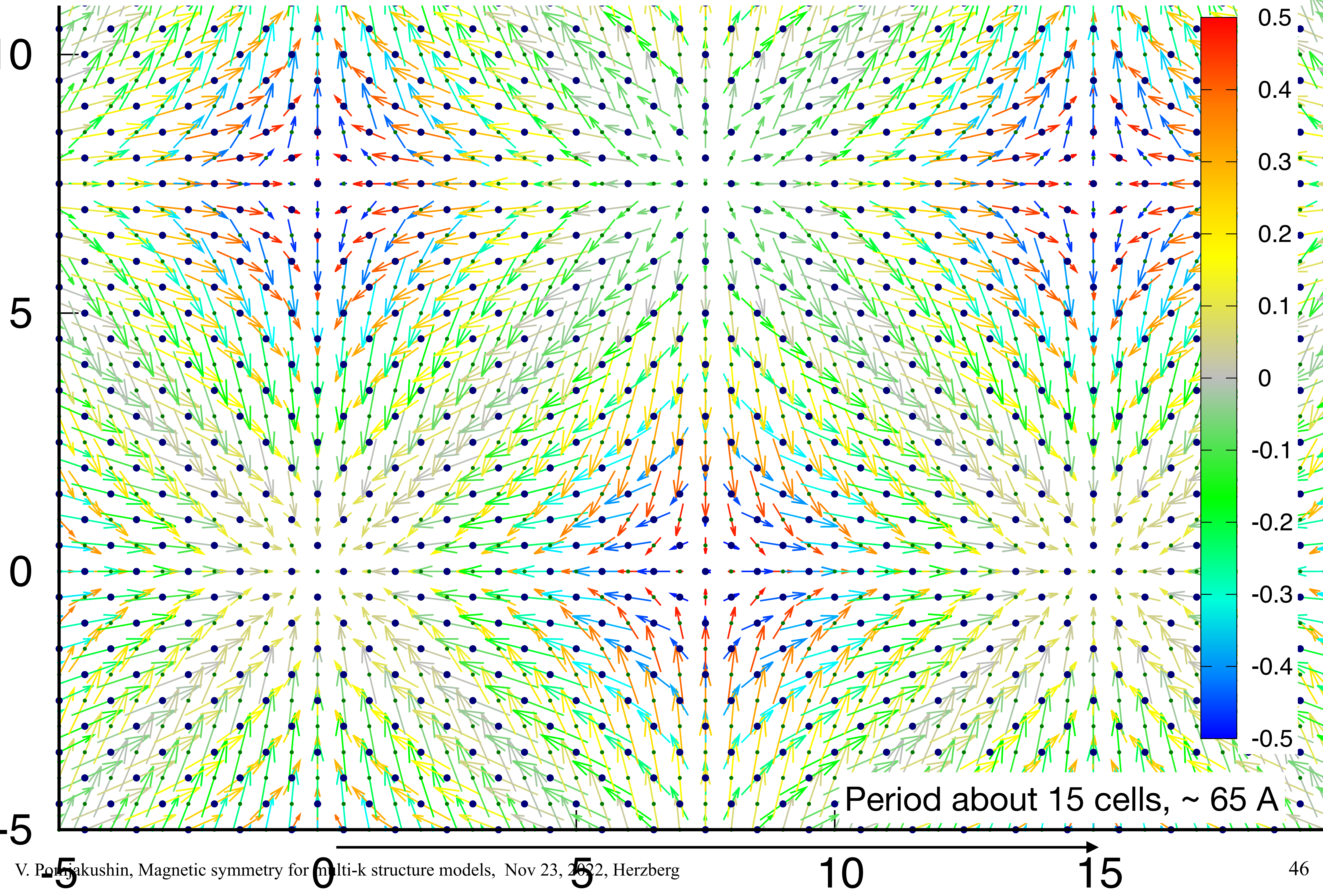
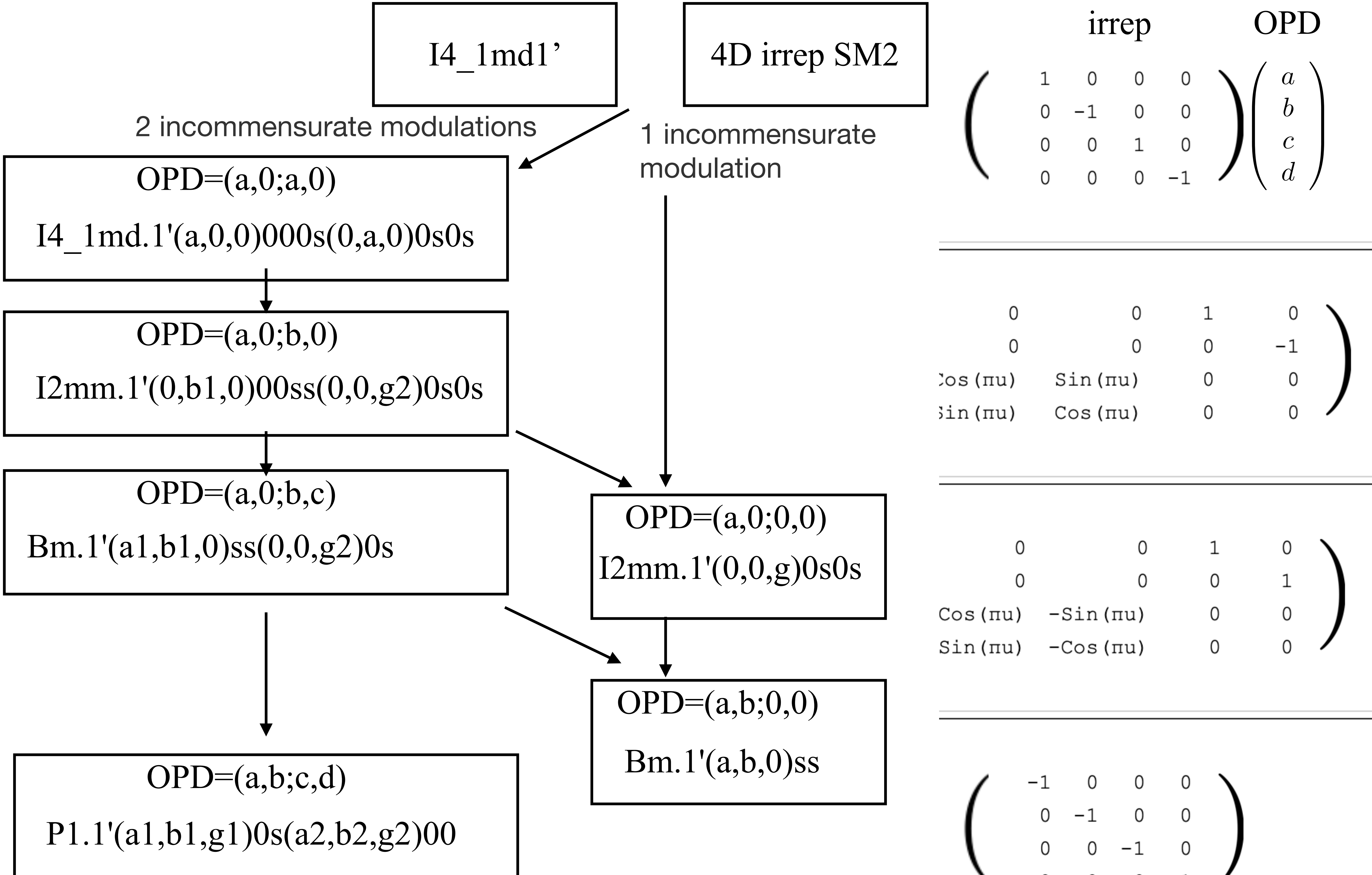
$$\mathbf{M}_{\mathrm{Ce1}} = m_1 \sin(\tilde{k}x)\mathbf{e}_{\boldsymbol{x}} + m_2 \sin(\tilde{k}y)\mathbf{e}_{\boldsymbol{y}} + \left(m_3 \cos(\tilde{k}x) + m_4 \cos(\tilde{k}y)\right)\mathbf{e}_{\boldsymbol{z}}$$

$$\mathbf{M}_{\mathrm{Ce2}} = m_2 \sin(\tilde{k}x)\mathbf{e}_{\boldsymbol{x}} + m_1 \sin(\tilde{k}y)\mathbf{e}_{\boldsymbol{y}} + \left(m_4 \cos(\tilde{k}x) + m_3 \cos(\tilde{k}y)\right)\mathbf{e}_{\boldsymbol{z}}$$

CeAlGe: Maximal symmetry full star superspace 3D+2 magnetic group
I4_1md1'(a00)000s(0a0)0s0s



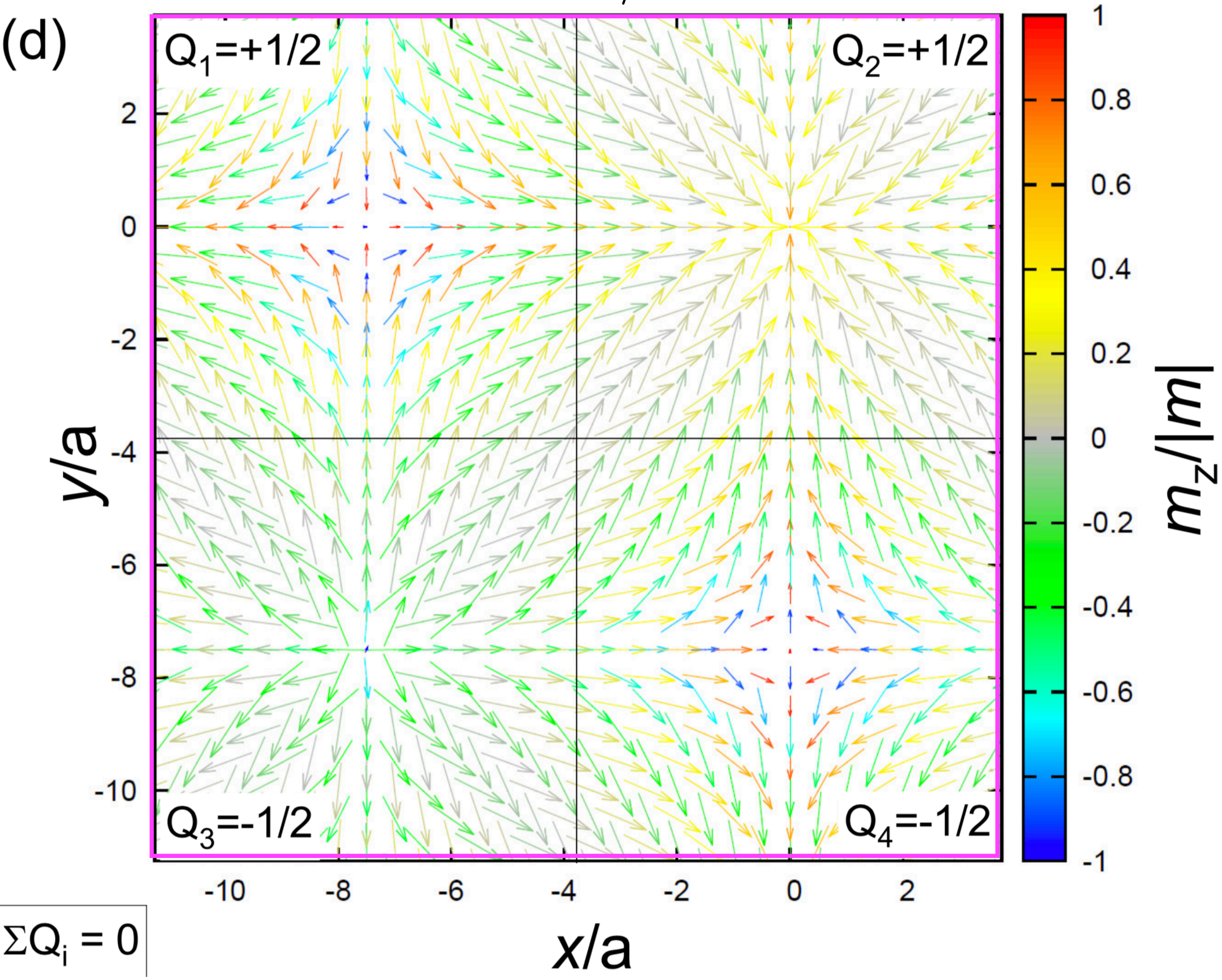
subgroup tree for I4_1md [u,0,0]+[0,u,0]



Topological density and charge. H=0

experiment: (m1,m2,m3,m4) = (0.44(1), 1.02(1), −0.21(5), 0.29(7)) μB.

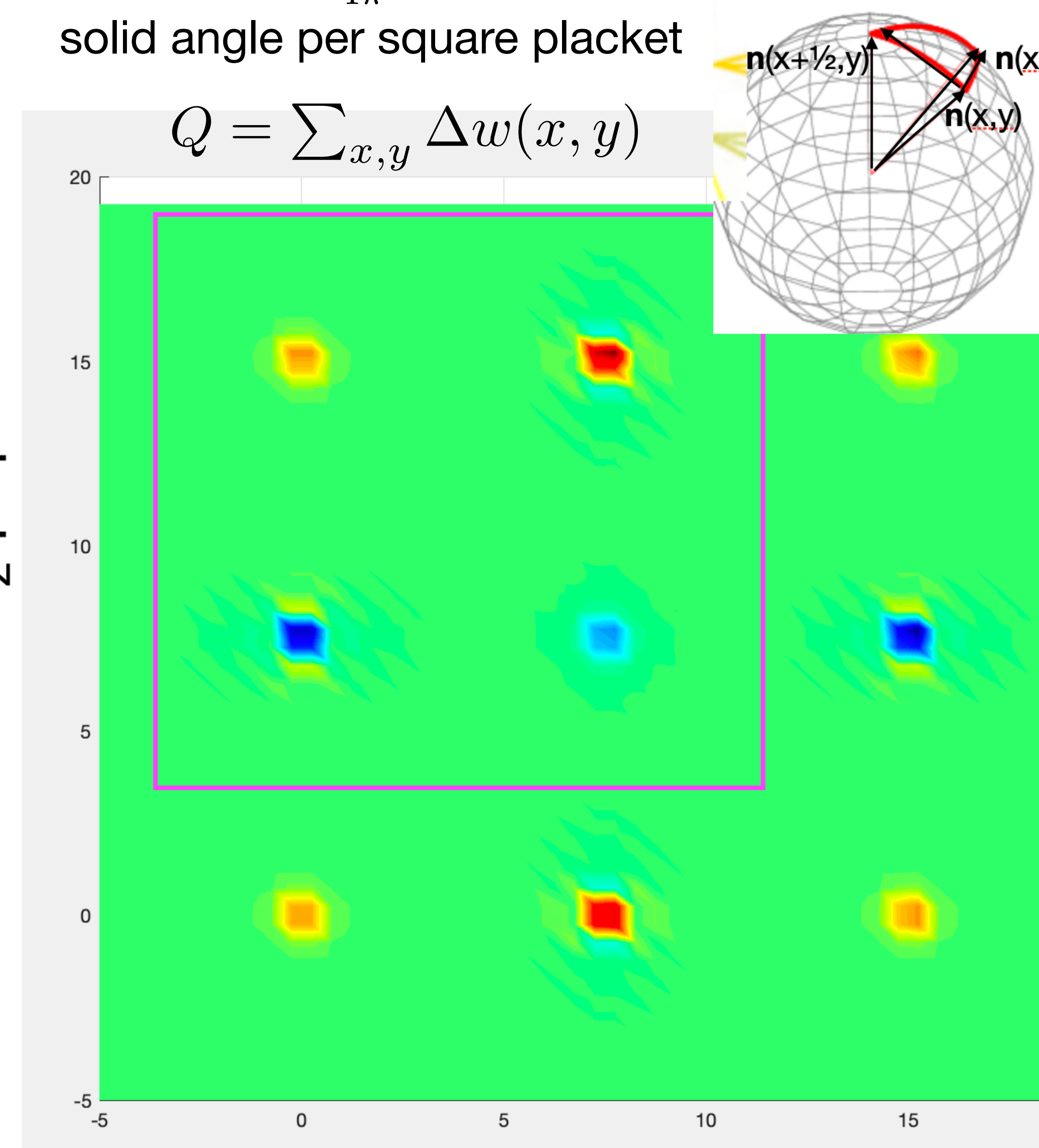
$$\mathbf{n} = \mathbf{M}/M$$



$$\Delta w(x,y) = \frac{1}{4\pi}\left(\mathbf{n}\cdot[\Delta\mathbf{n}_x \times \Delta\mathbf{n}_y]\right)$$

solid angle per square placket

$$Q = \sum_{x,y} \Delta w(x,y)$$

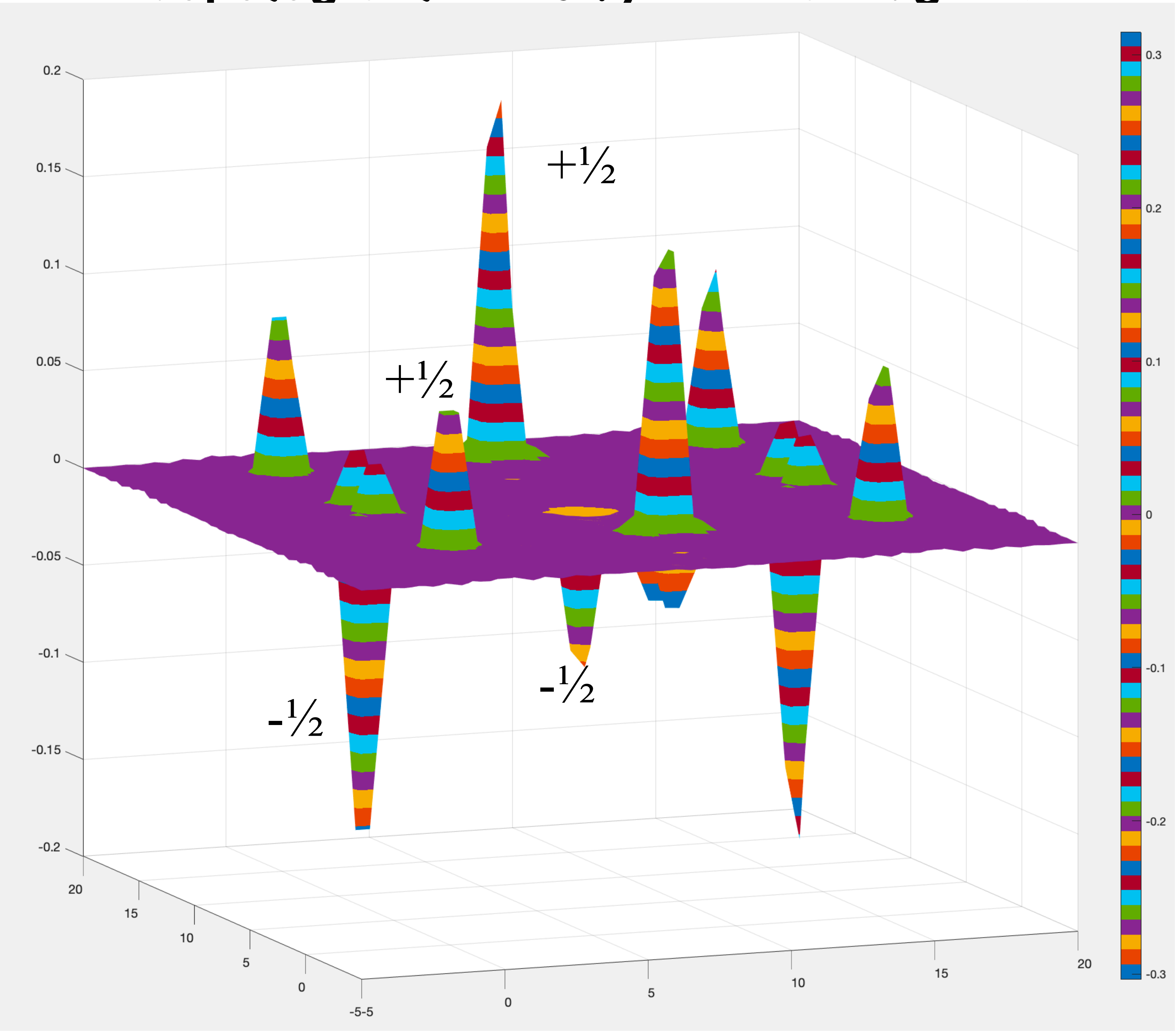


$$\mathbf{M}_{\mathrm{Ce2}} = m_2 \sin(\tilde{k}x)\mathbf{e_x} + m_1 \sin(\tilde{k}y)\mathbf{e_y} + \left(m_4 \cos(\tilde{k}x) + m_3 \cos(\tilde{k}y)\right)\mathbf{e_z}$$

$$\mathbf{M}_{\mathrm{Ce1}} = m_1 \sin(\tilde{k}x)\mathbf{e_x} + m_2 \sin(\tilde{k}y)\mathbf{e_y} + \left(m_3 \cos(\tilde{k}x) + m_4 \cos(\tilde{k}y)\right)\mathbf{e_z}$$

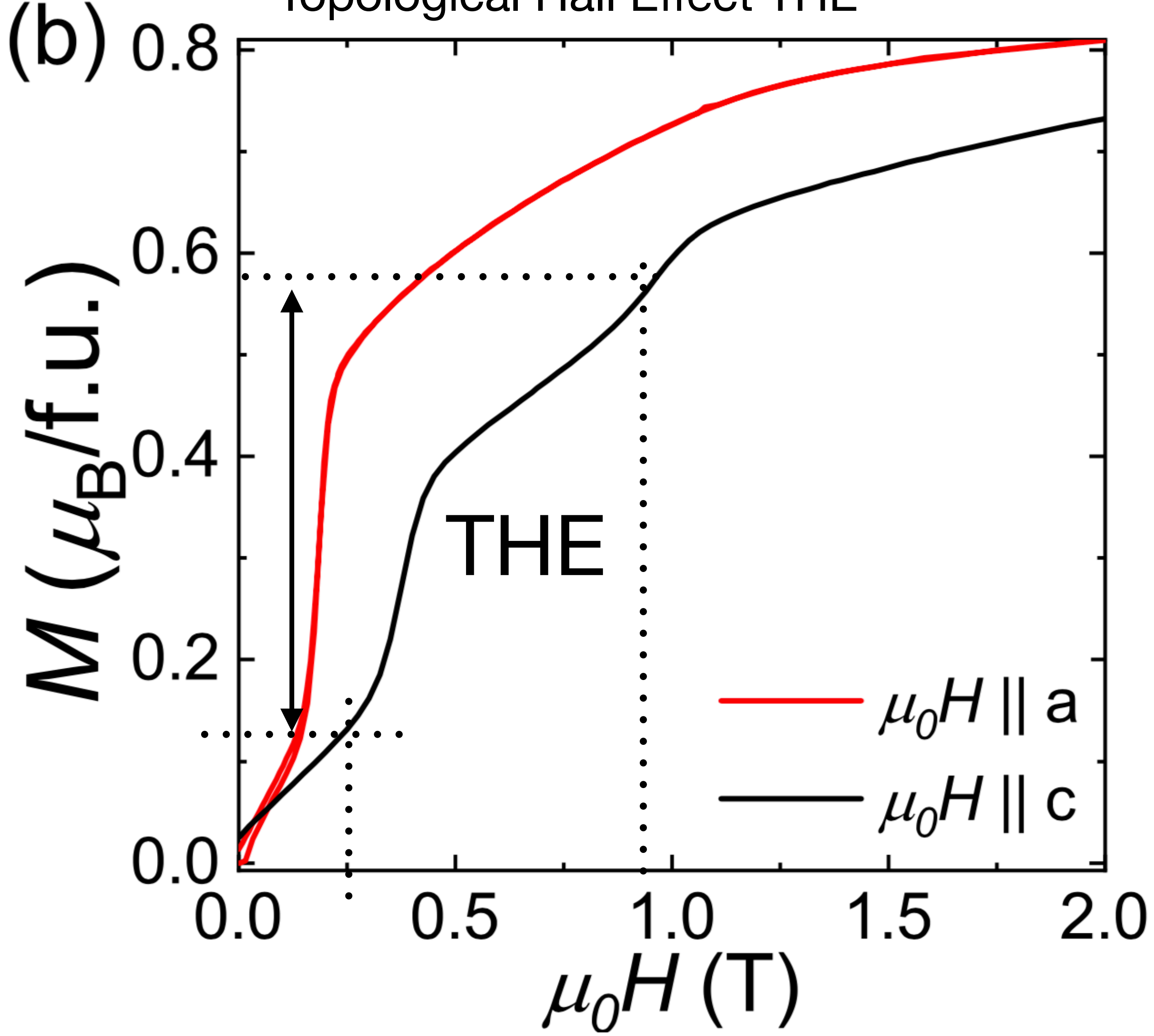
$\tilde{k} = 2\pi|\boldsymbol{k}_1| = 2\pi|\boldsymbol{k}_2| = 2\pi g$

Topological density and charge. H=0

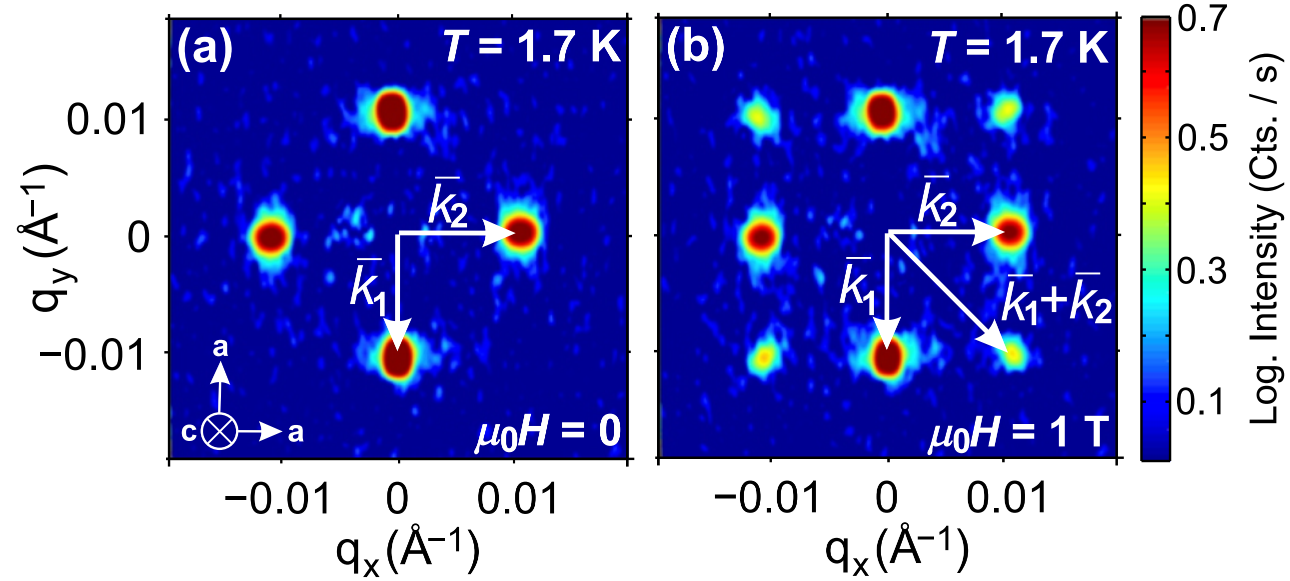


Experimental proof comes from behaviour in external field

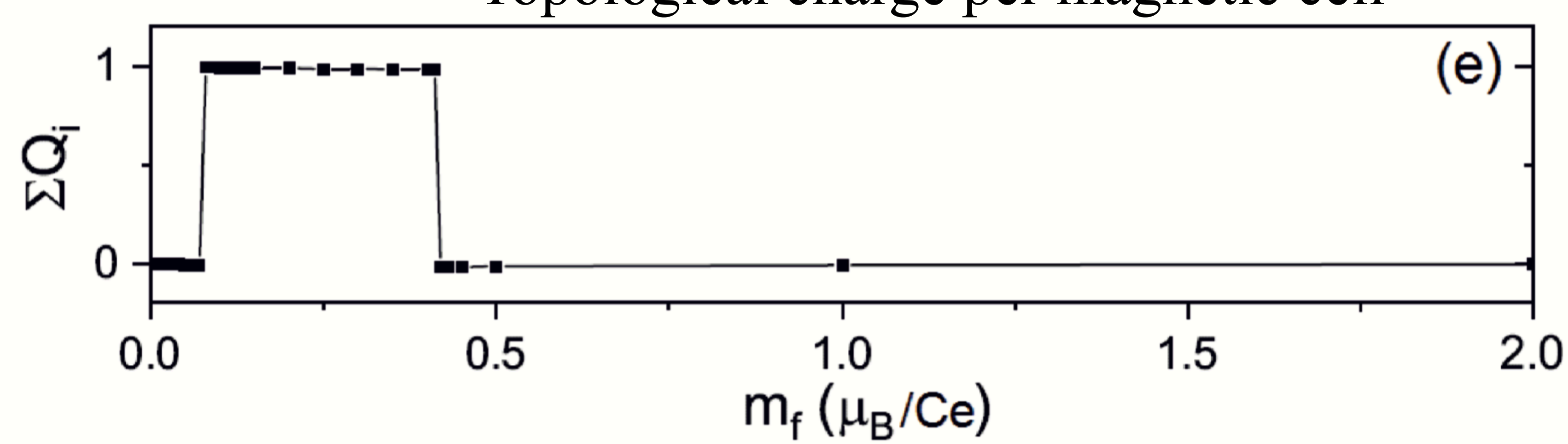
Topological Hall Effect THE



SANS diffraction: k1+k2+0 is 3rd order harmonics in external field



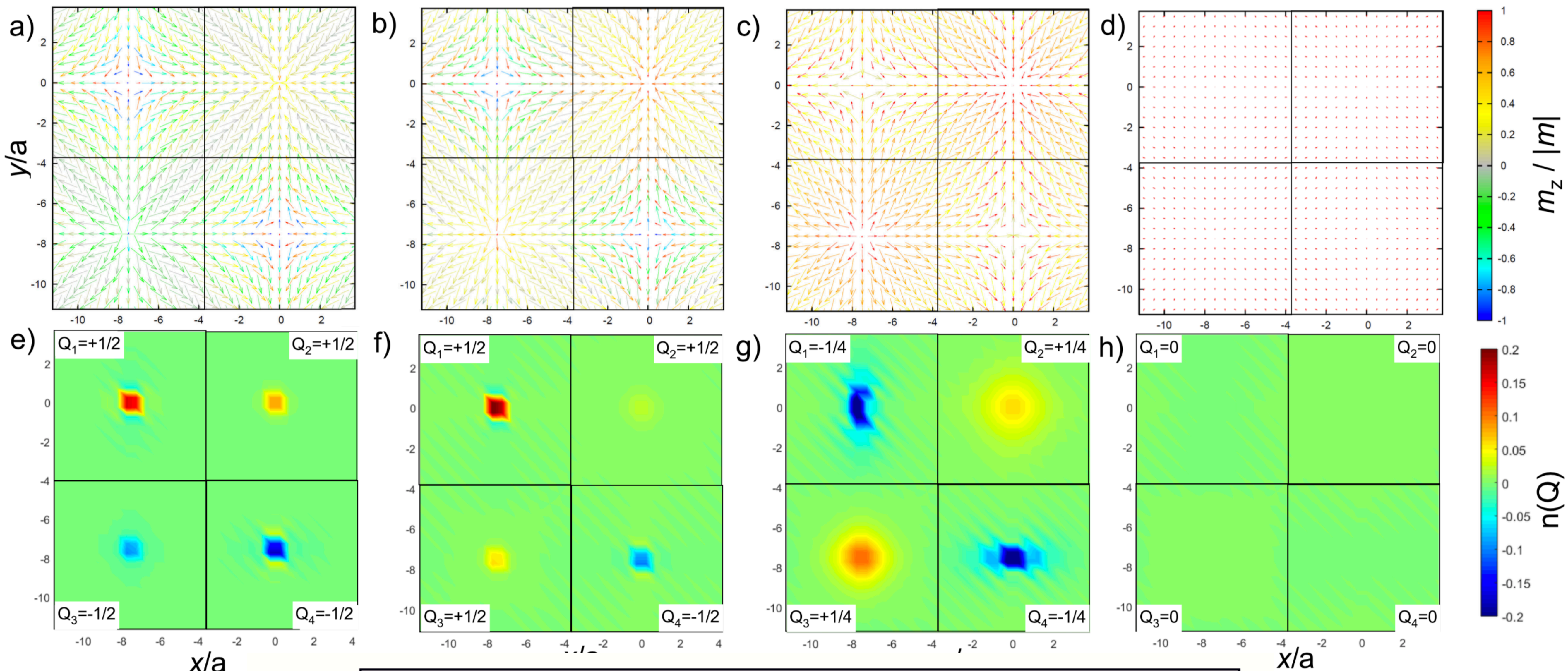
Topological charge per magnetic cell



Simulation of external field ~ FM component along z-axis

experiment: (m1,m2,m3,m4) = (0.44(1), 1.02(1), −0.21(5), 0.29(7)) μ_B.

mf = 0 μB mf = 0.3 μB mf = 0.5 μB



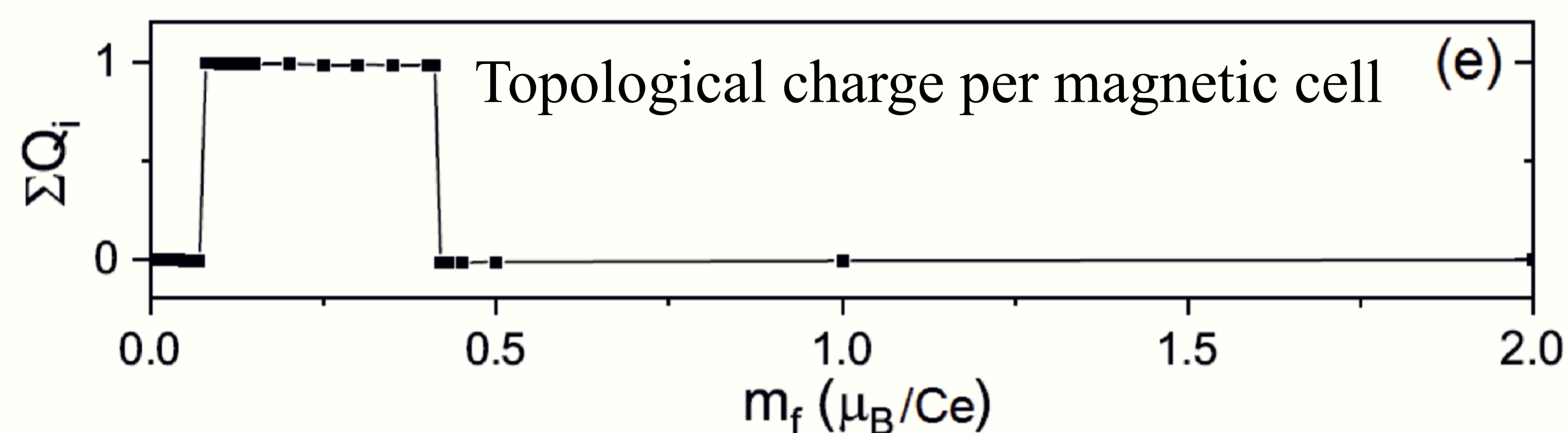


Figure 10. Compari ... canting fields along th

-direction out of th ... μ_B. a-d) The first row

mages shows the vi ... $m_f = 0.2\,\mu_B$ (b) are th

same ones shown in ... lane lattice parameter

Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

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

magnetic symmetry AND representation

only representation

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Construction of basis functions (normal modes)

Constraints on the mixing coefficients of basis function for >1D *irrep* and/or multi-arm star of **k**,

Magnetic structure made from linear combination of normal modes.

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magnetic symmetry AND representation

is *irrep* real and 1D, and single arm {**k**}-star?

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

only representation

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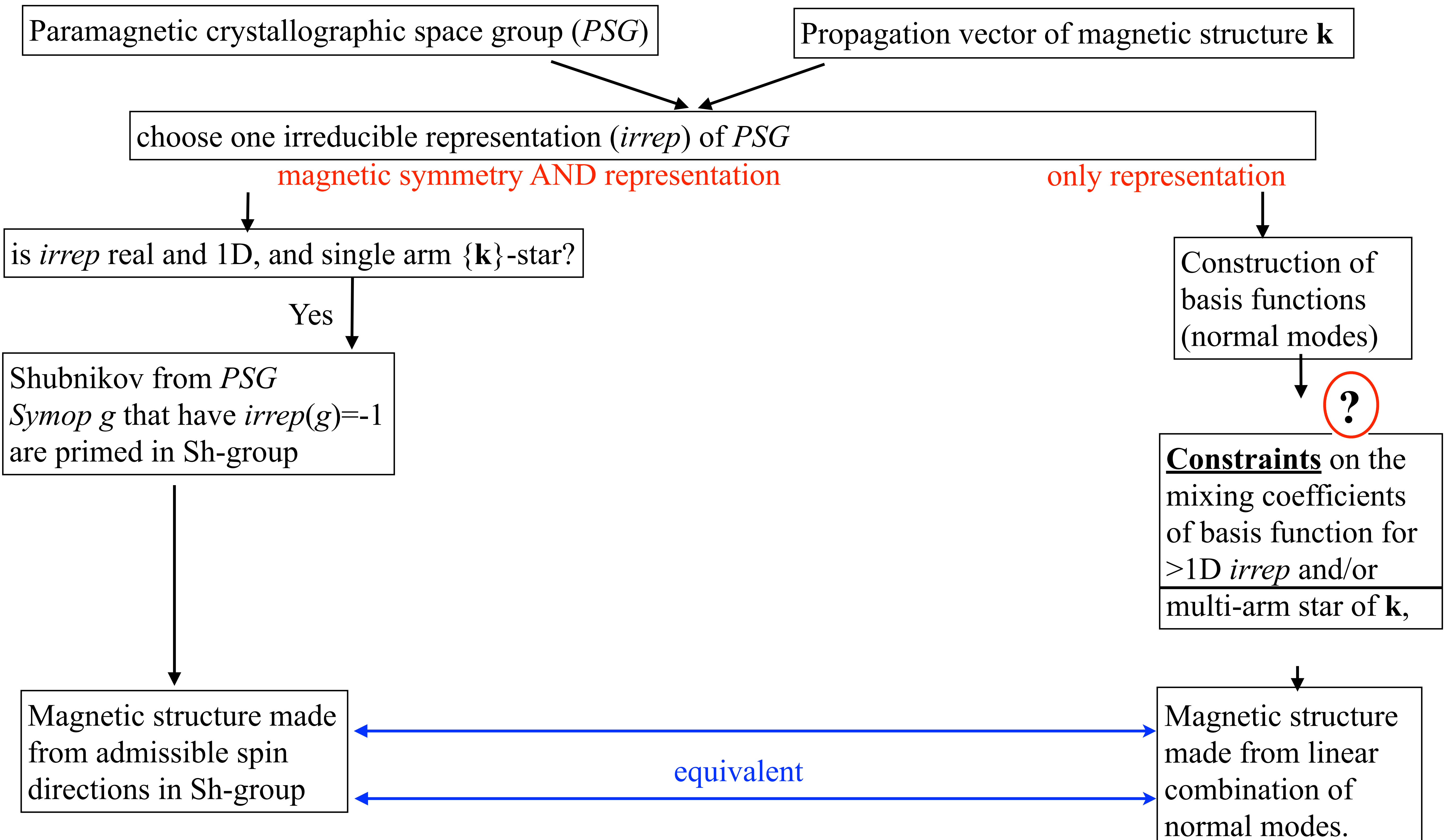

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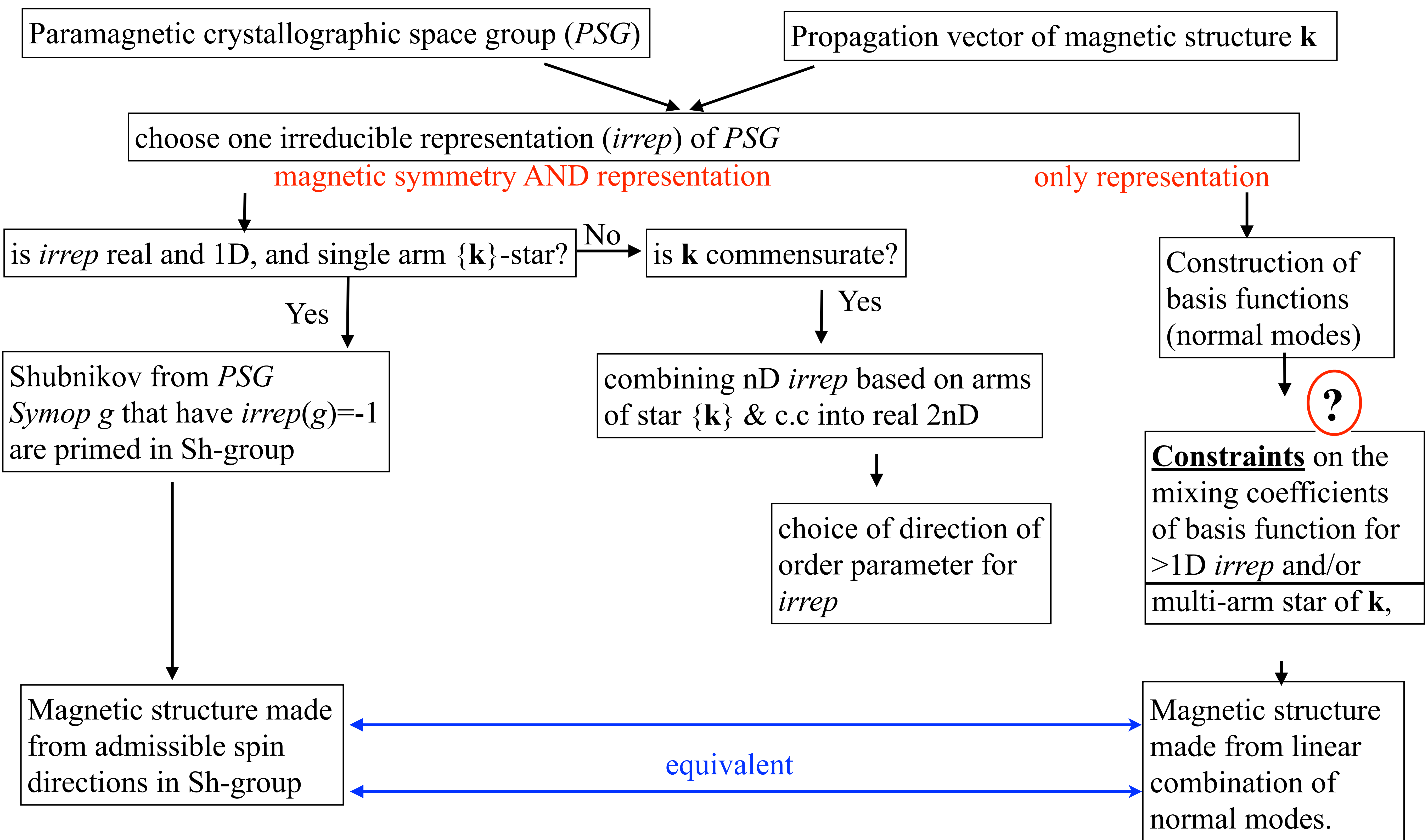

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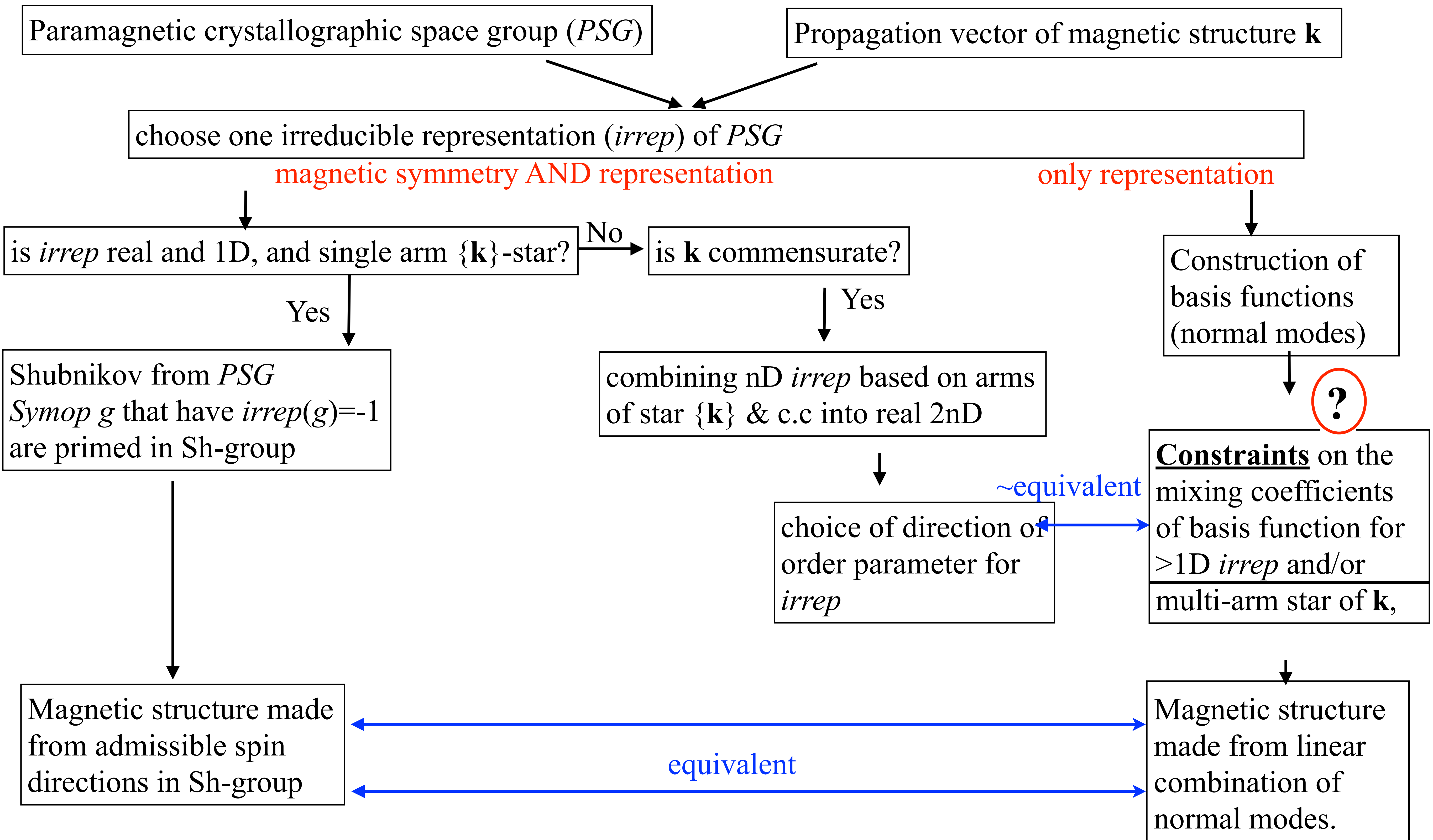

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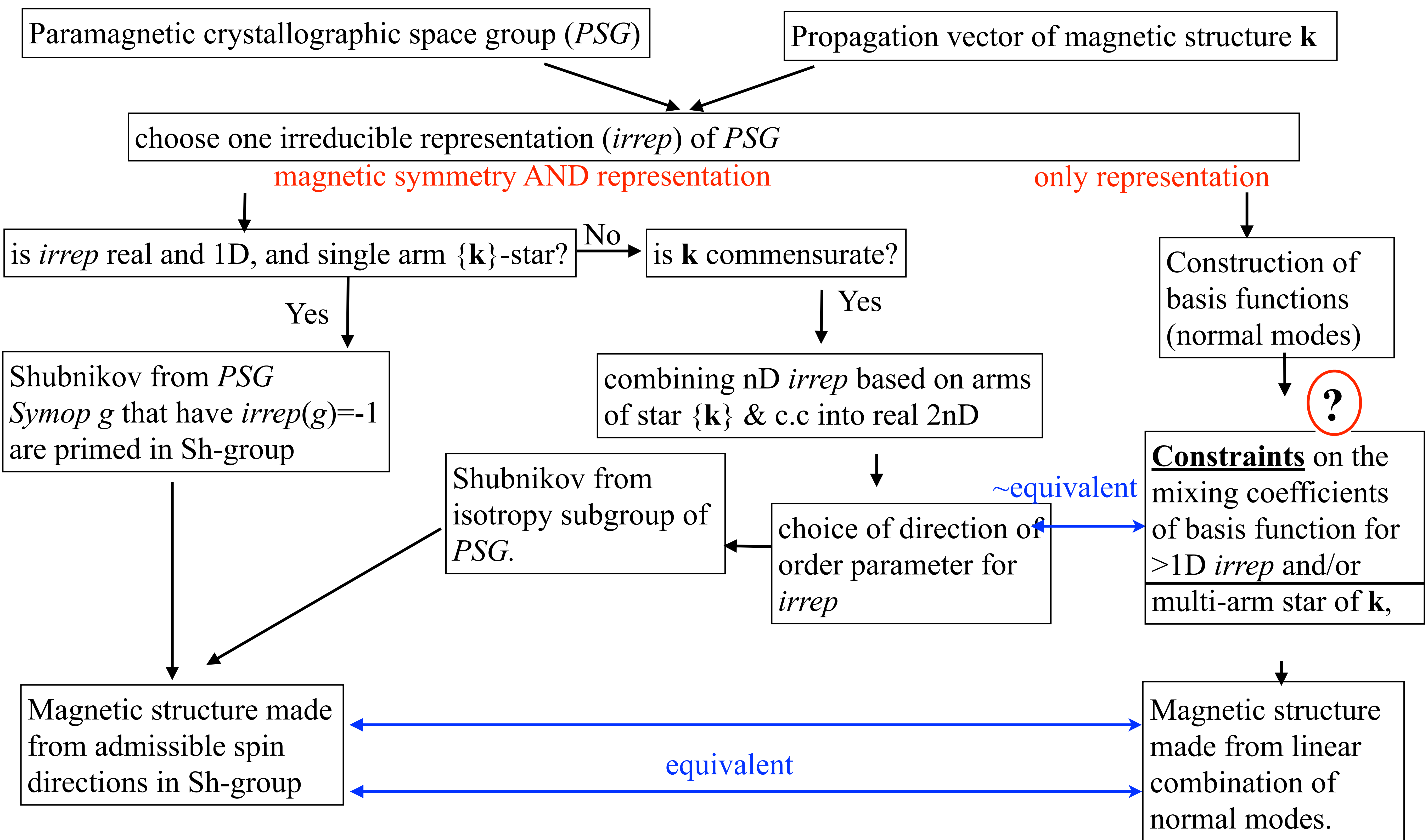

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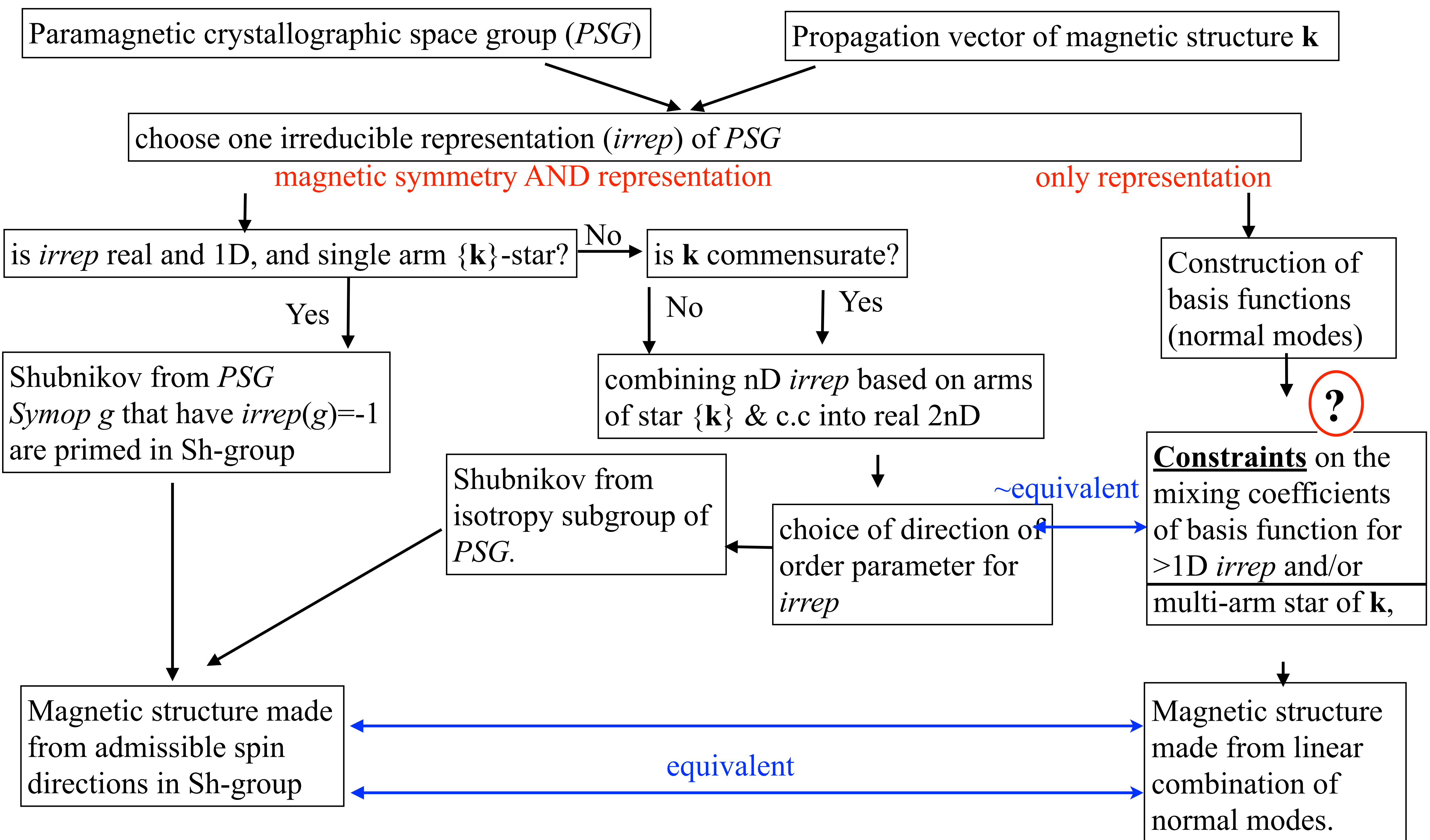

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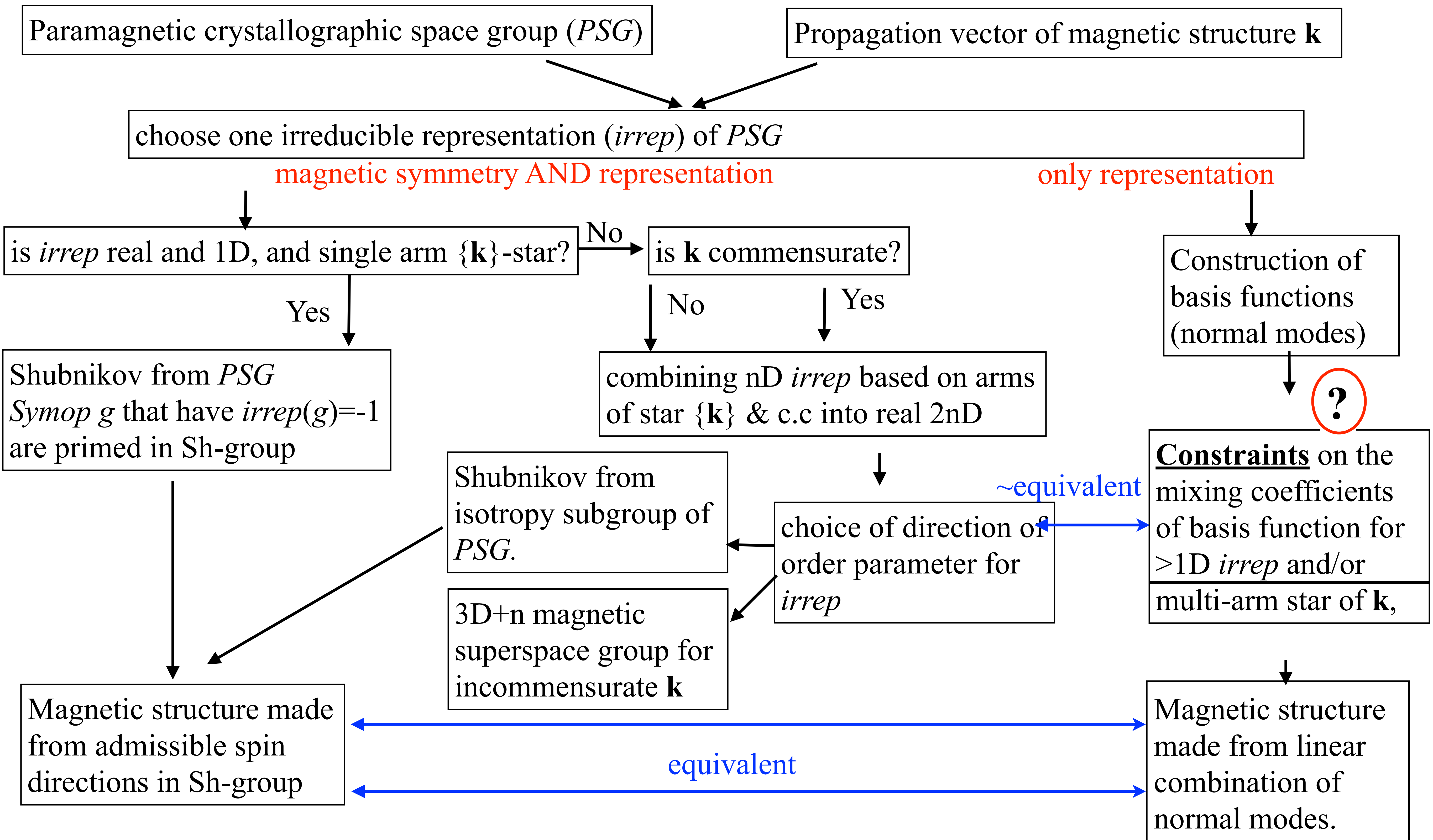

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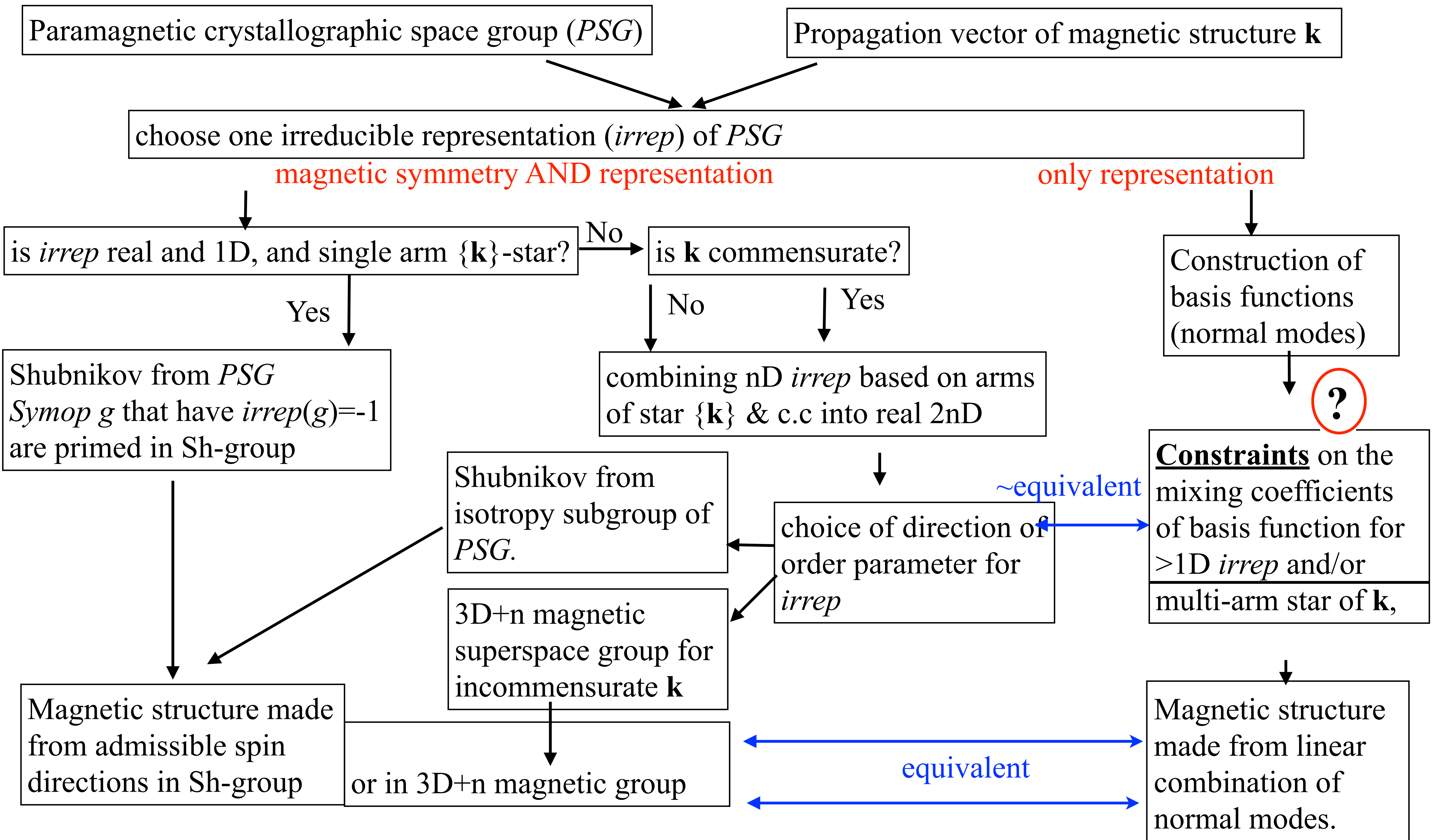

Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

The disadvantage of using only RA:

In general: there are no rules to make **constraints**, (except ones based on physical grounds)

but the **constraints** appear in a natural way from magnetic group symmetry arguments

The disadvantage of using only magnetic subgroups:

We ***loose the concept of single irrep*** active at the transition - too many “unphysical” subgroups

Shubnikov from isotropy subgroup of *PSG*.

3D+n magnetic superspace group for incommensurate **k**

choice of direction of order parameter for *irrep*

~equivalent

mixing coefficients of basis function for >1D *irrep* and/or

multi-arm star of **k**,

Magnetic structure made from admissible spin directions in Sh-group

or in 3D+n magnetic group

equivalent

Magnetic structure made from linear combination of normal modes.

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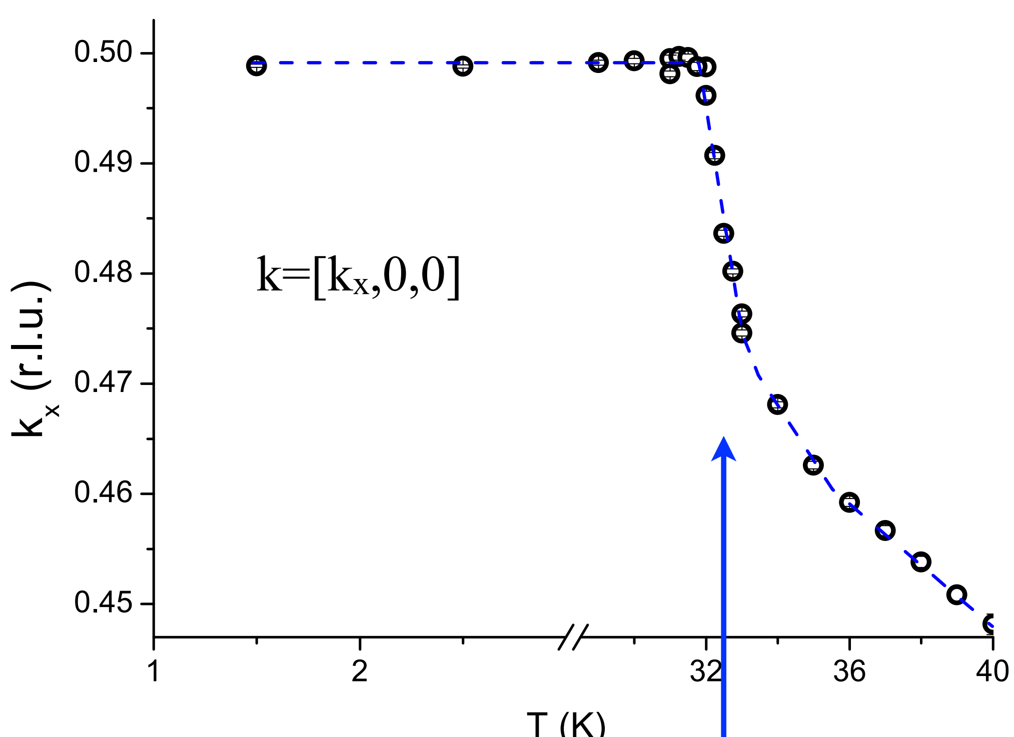
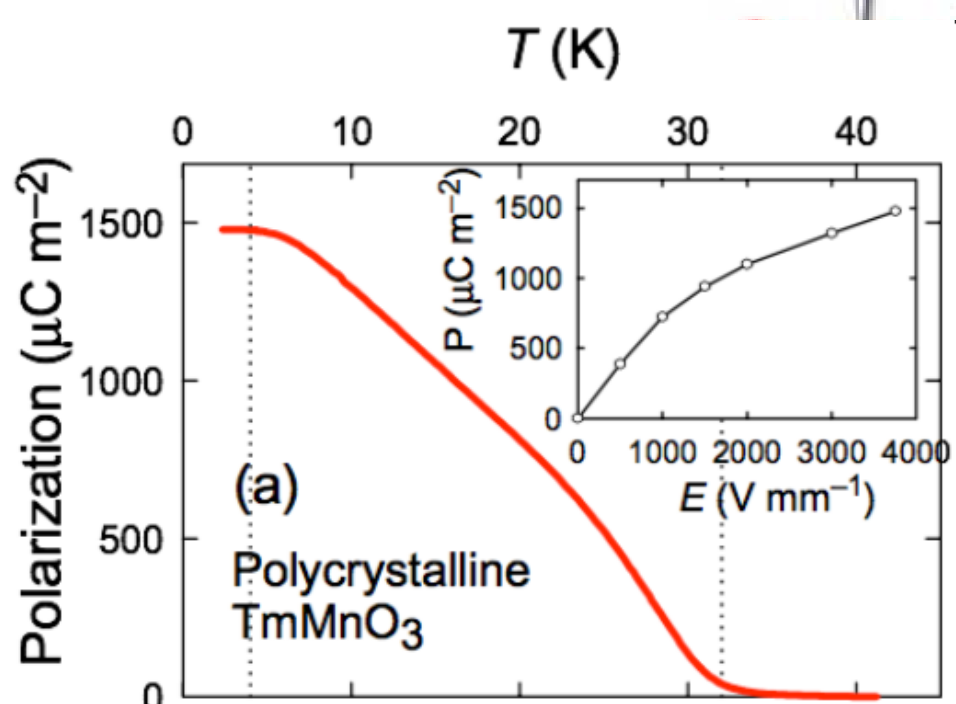
The End

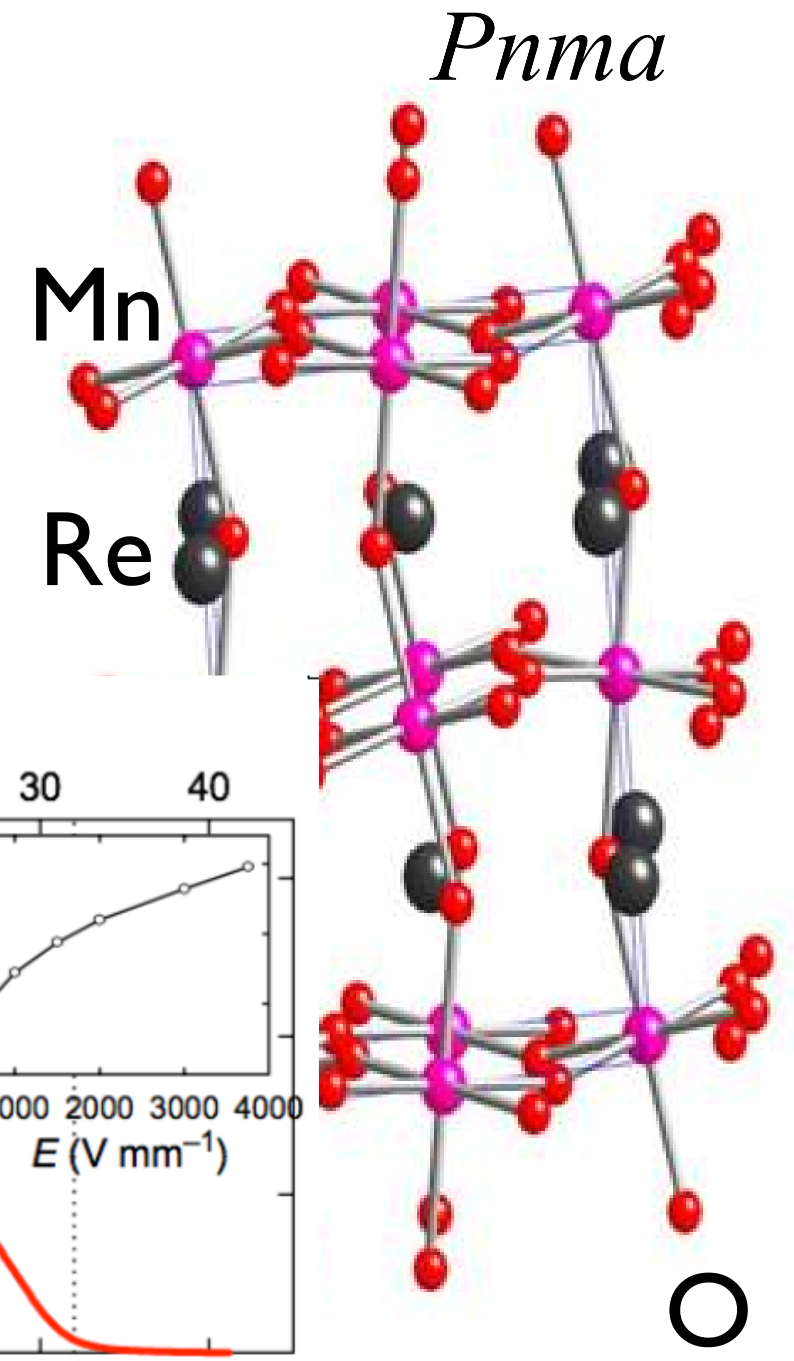
Thank you!

Antiferromagnetic order in orthorhombic multiferroic $TmMnO_3$

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







magnetic $T_{Néel}$ & electric: T_C

New Journal of Physics 11, 043019 (2009)

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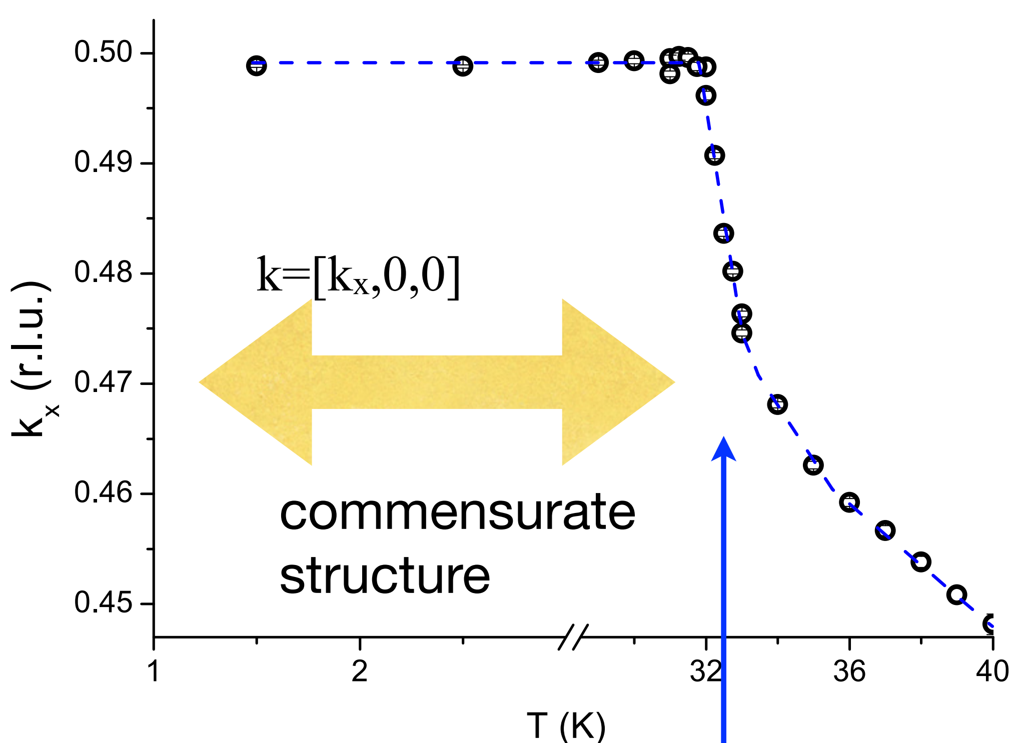
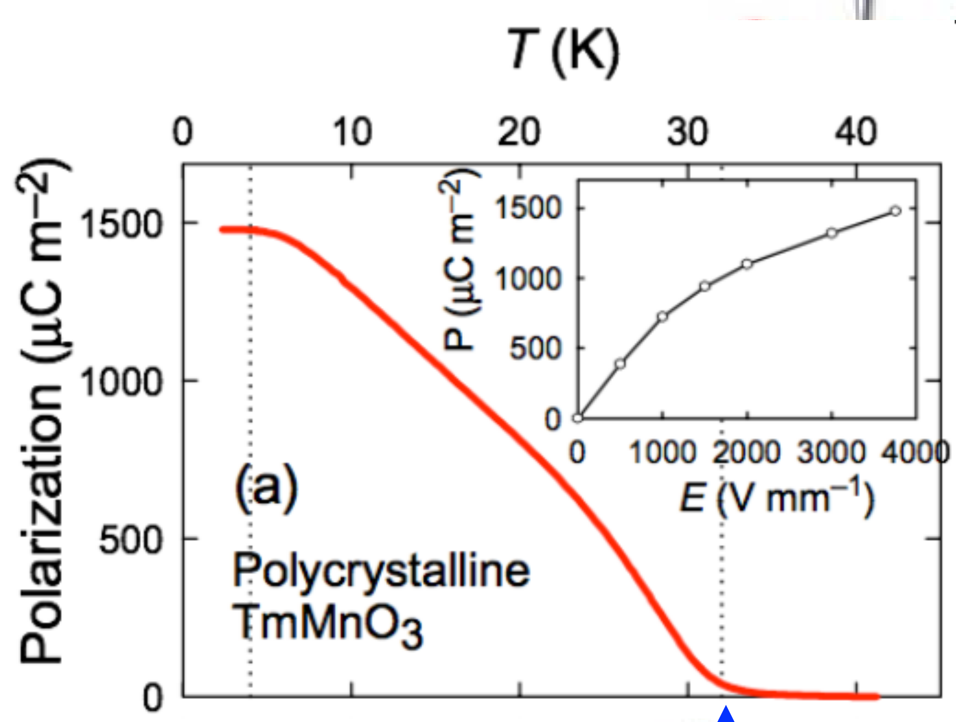
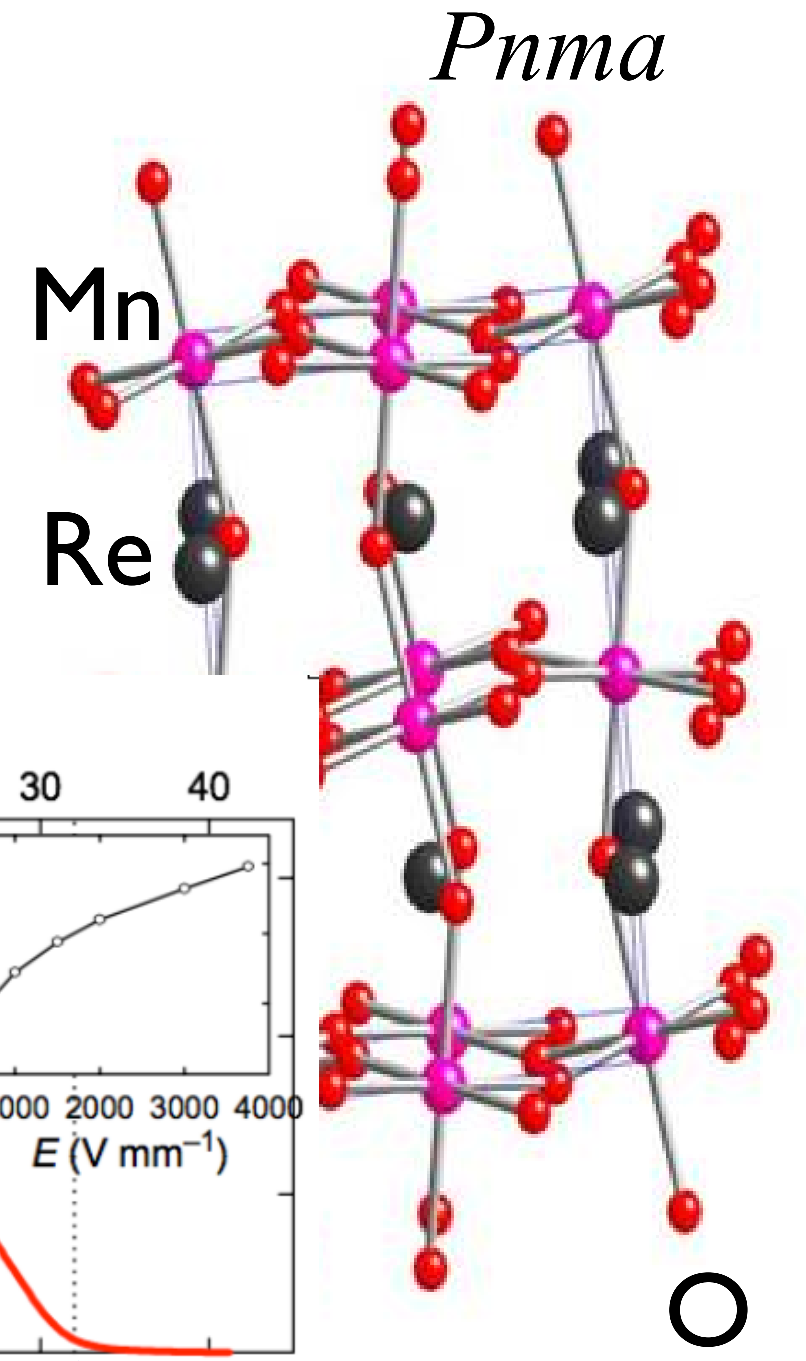
2. Constraints on basis functions vs. superspace for the incommensurate two arm **k**=[1/2±δ,0,0]. {**k**}={-**k**,+**k**}. Para-electric phase (3D+1) superspace magnetic group *Pmcn1’(00g)000s [Pnma, bca]*





magnetic $T_{Néel}$ & electric: T_C

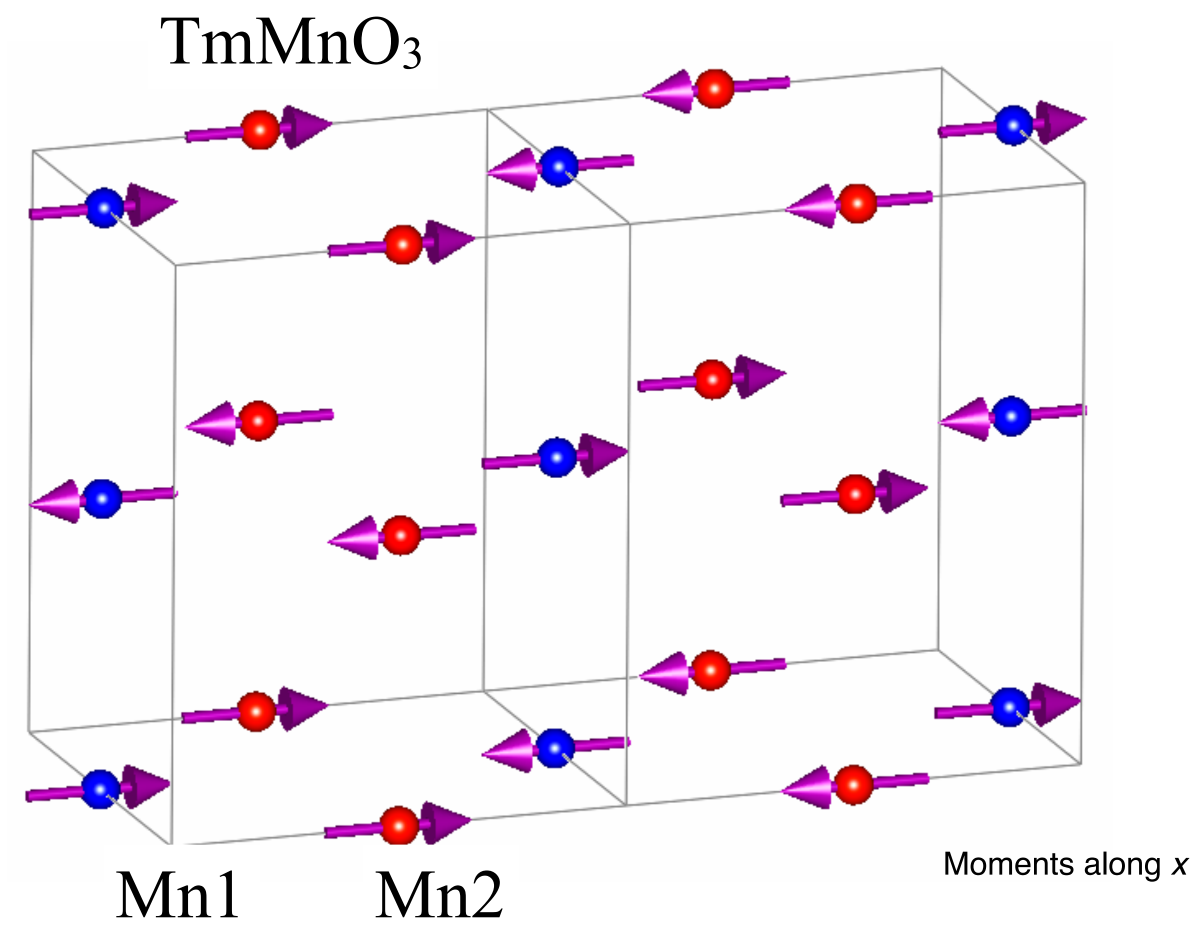


New Journal of Physics 11, 043019 (2009)

Symmetry analysis using both RA and magnetic subgroups

Pnma k=[1/2,0,0], *irrep*: **2D** mX1(τ_1)

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



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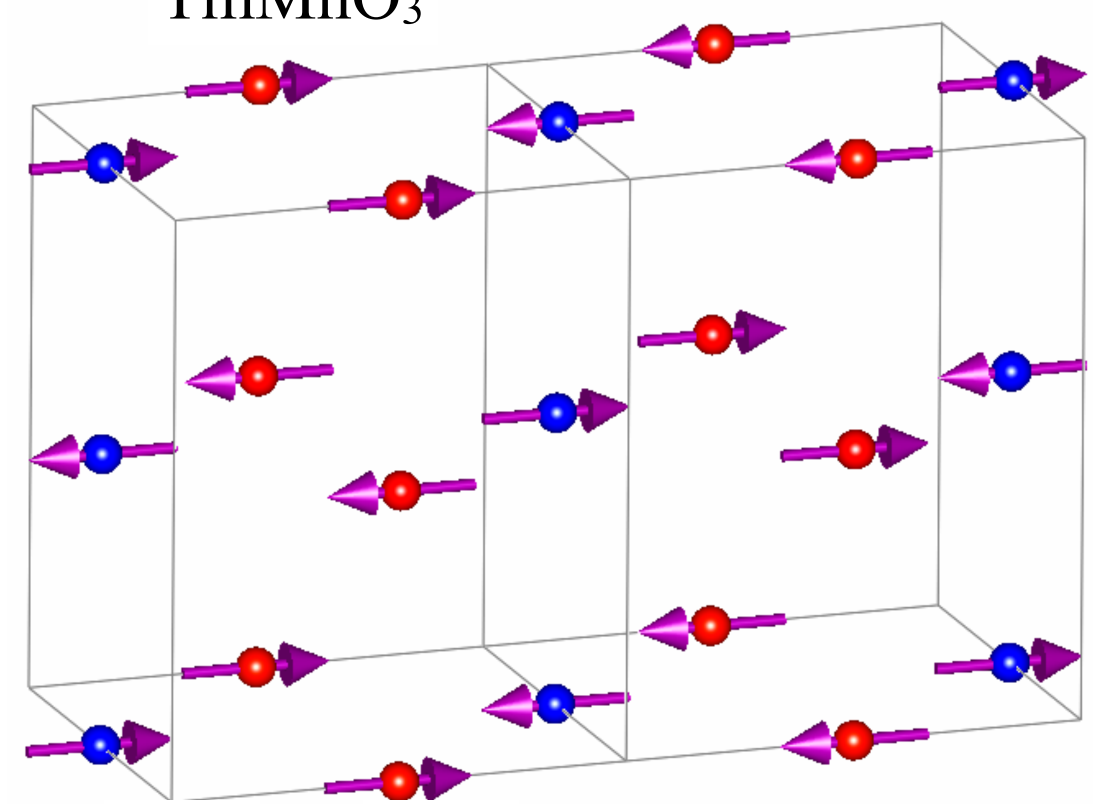
P3 (a,a) 31.129 P_bmn2_1, basis={(0,1,0),(2,0,0),(0,0,-1)}, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)
C1 (a,b) 6.21 P_am, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

Order parameter direction

Magnetic Shubnikov Space group

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

$TmMnO_3$



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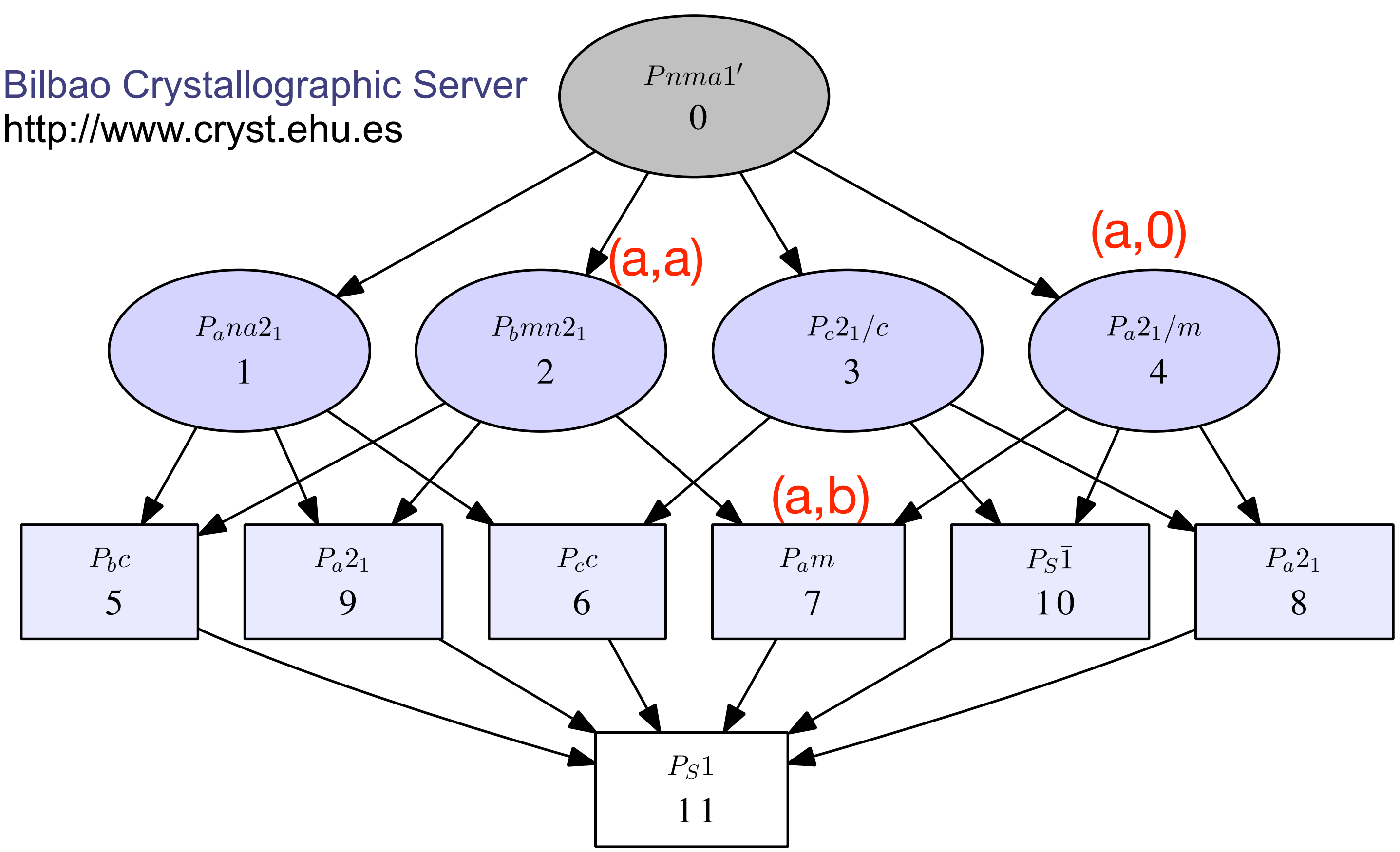

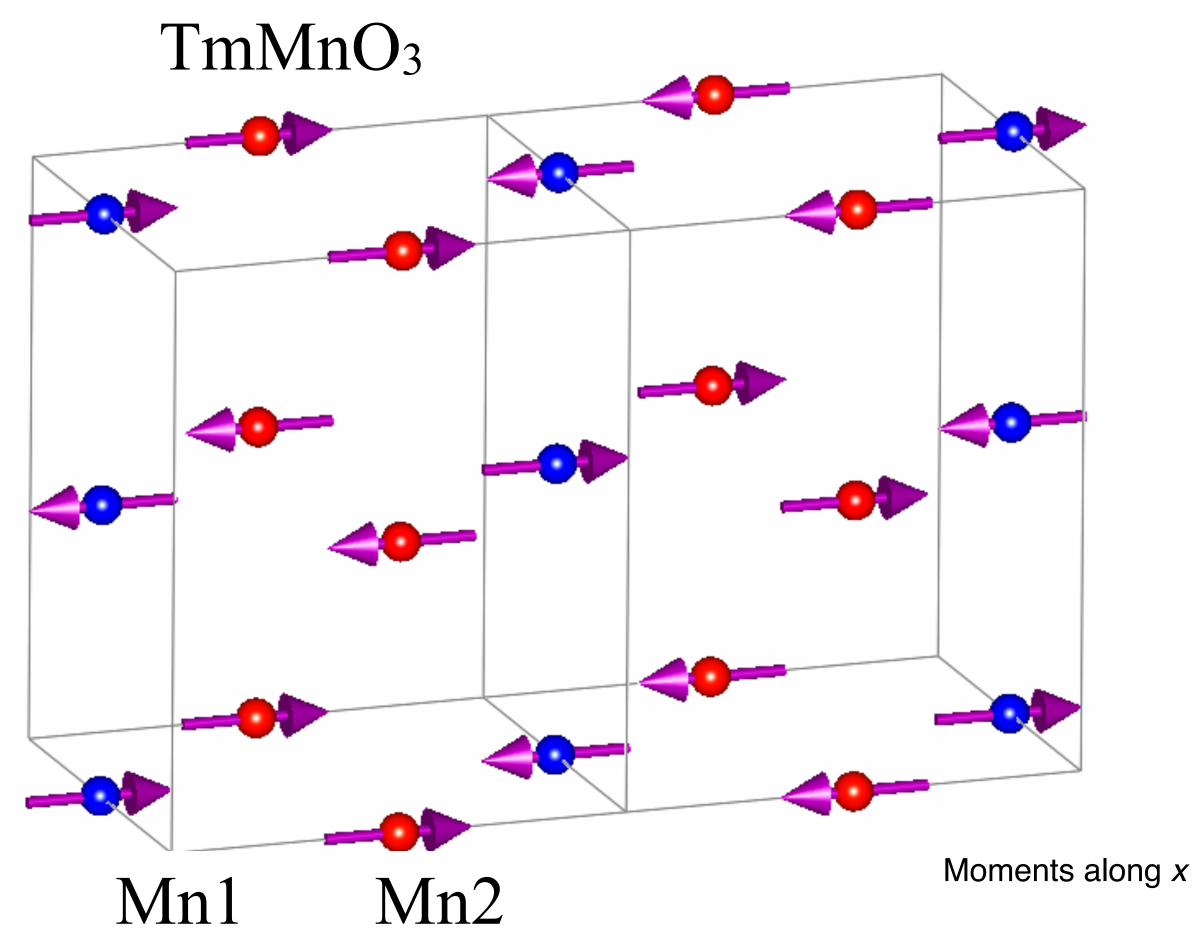

Case 1: magnetic mode E1 -> most symmetric maximal subgroup of Pnma1'

Pnma k=[1/2,0,0], *irrep*: **2D** mX1(τ_1)

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

ISODISTORT

Version 6.1.8, November 2014

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Order parameter direction ↓ | Magnetic Shubnikov Space group ↓

P1 (a,0) 11.55 P_a2_1/m, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,0,0)

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

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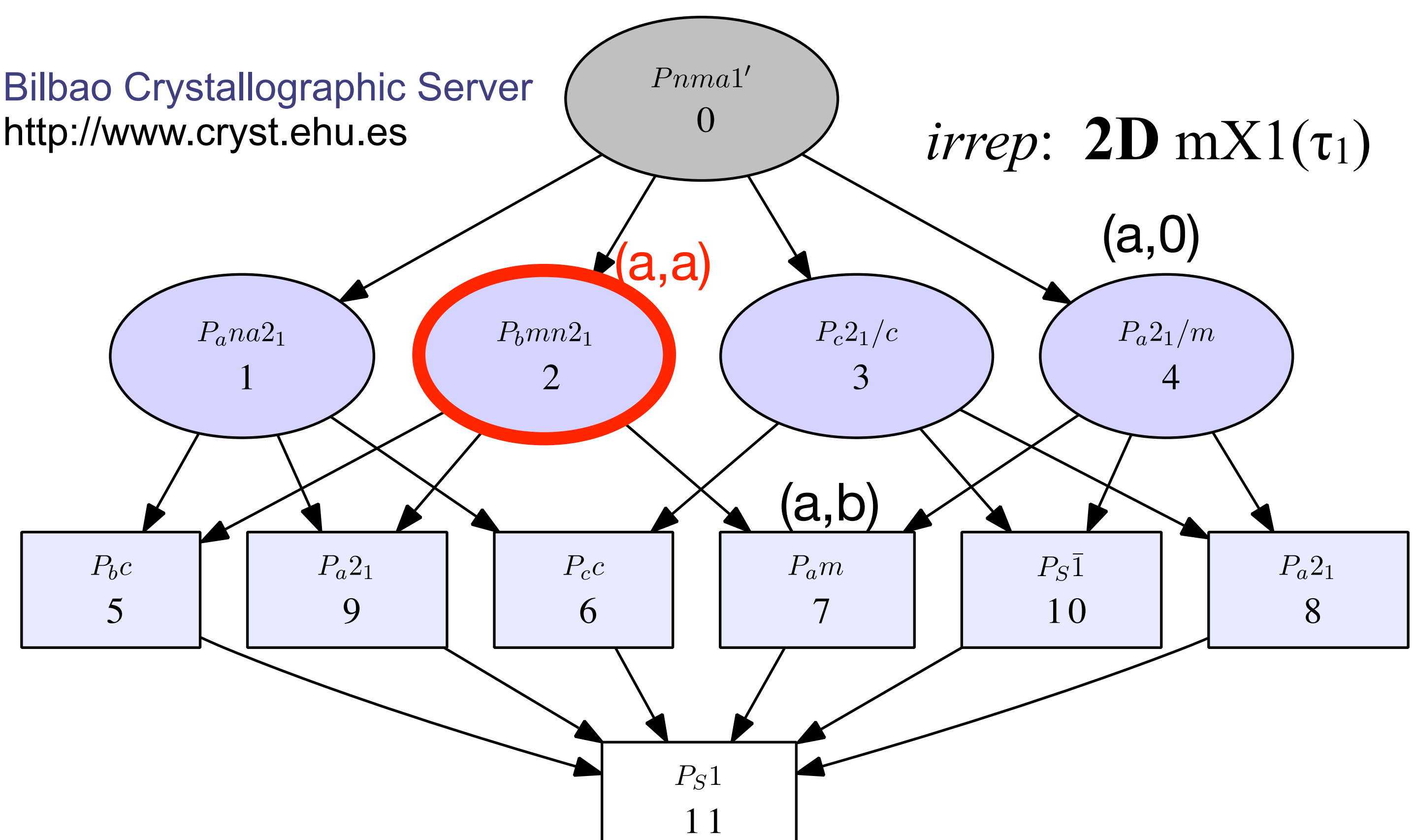
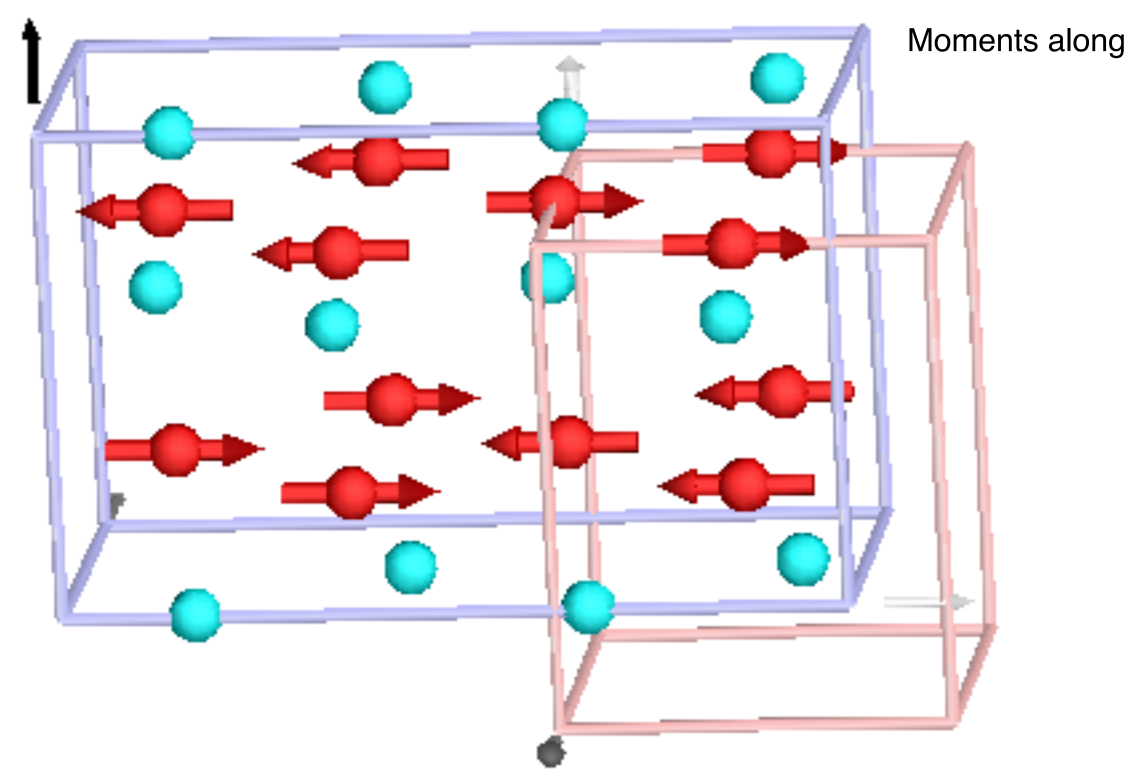


$TmMnO_3$



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Order parameter direction ↓

Magnetic Shubnikov Space group ↓

Solution!

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orthorhombic *Pmn2$_1$*

(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) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$

(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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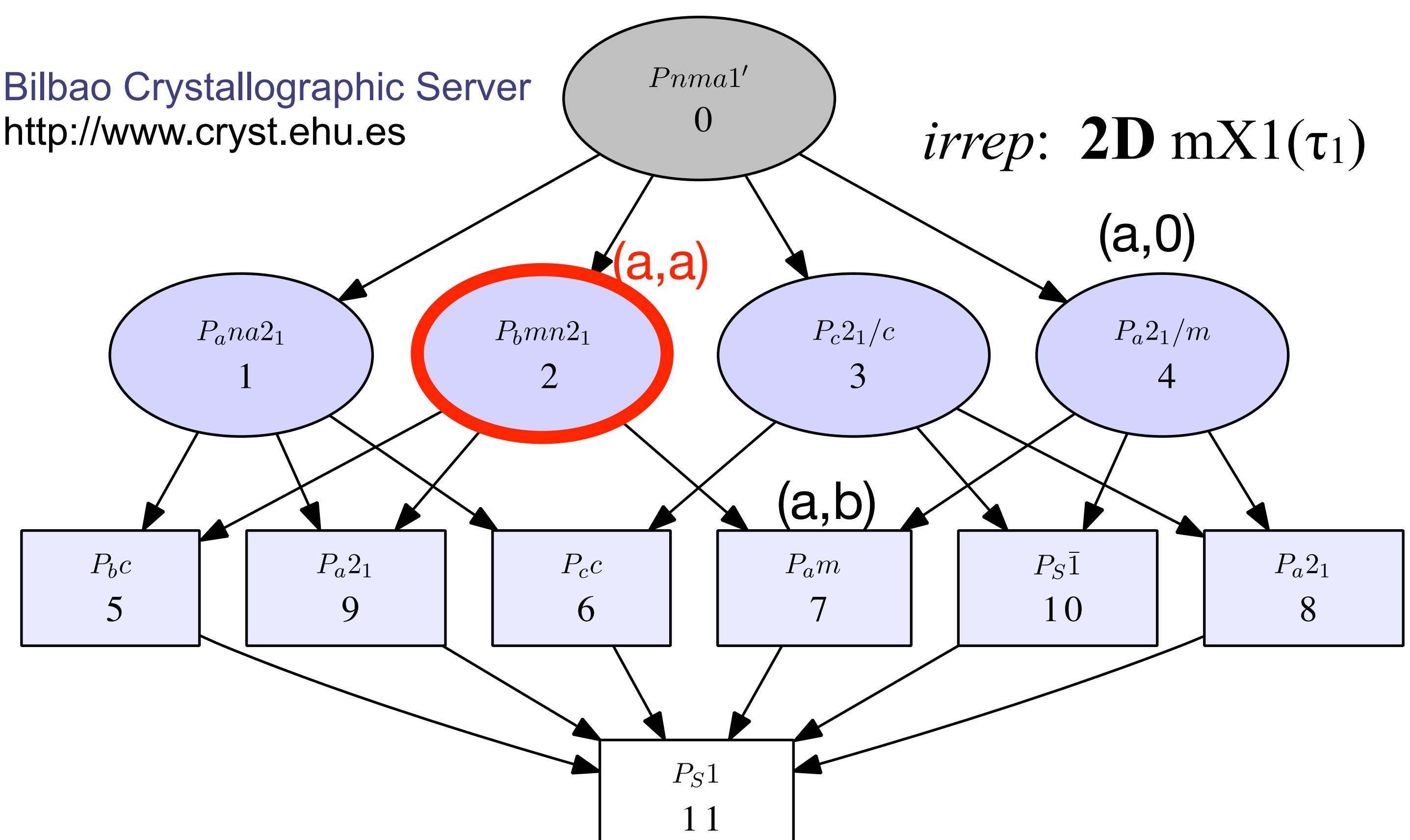
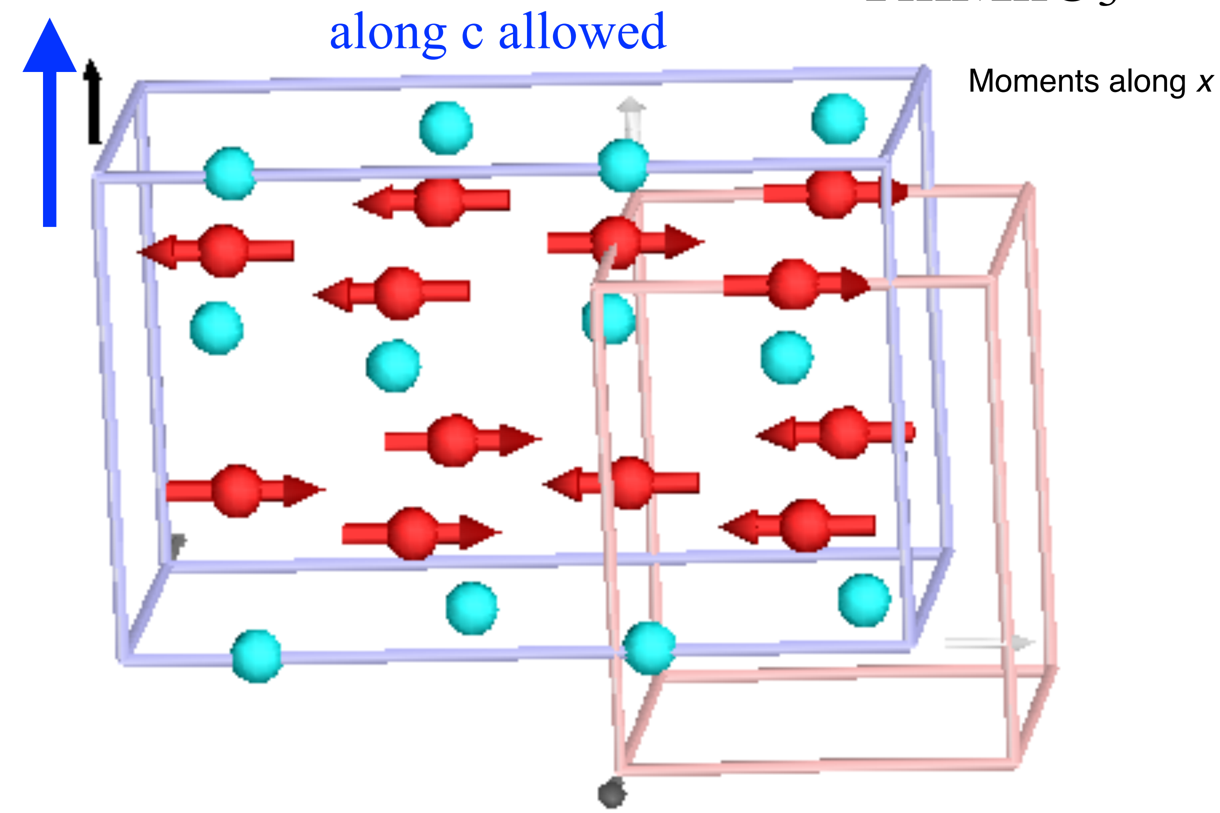


irrep: **2D** mX1(τ_1)

Electric polarisation along c allowed

$TmMnO_3$



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

Order parameter direction ↓

Magnetic Shubnikov Space group ↓

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P3 (a,a) 31.129 P_bmn2_1, basis={(0,1,0),(2,0,0),(0,0,-1)}, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)

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

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

monoclinic Pm

(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) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$

(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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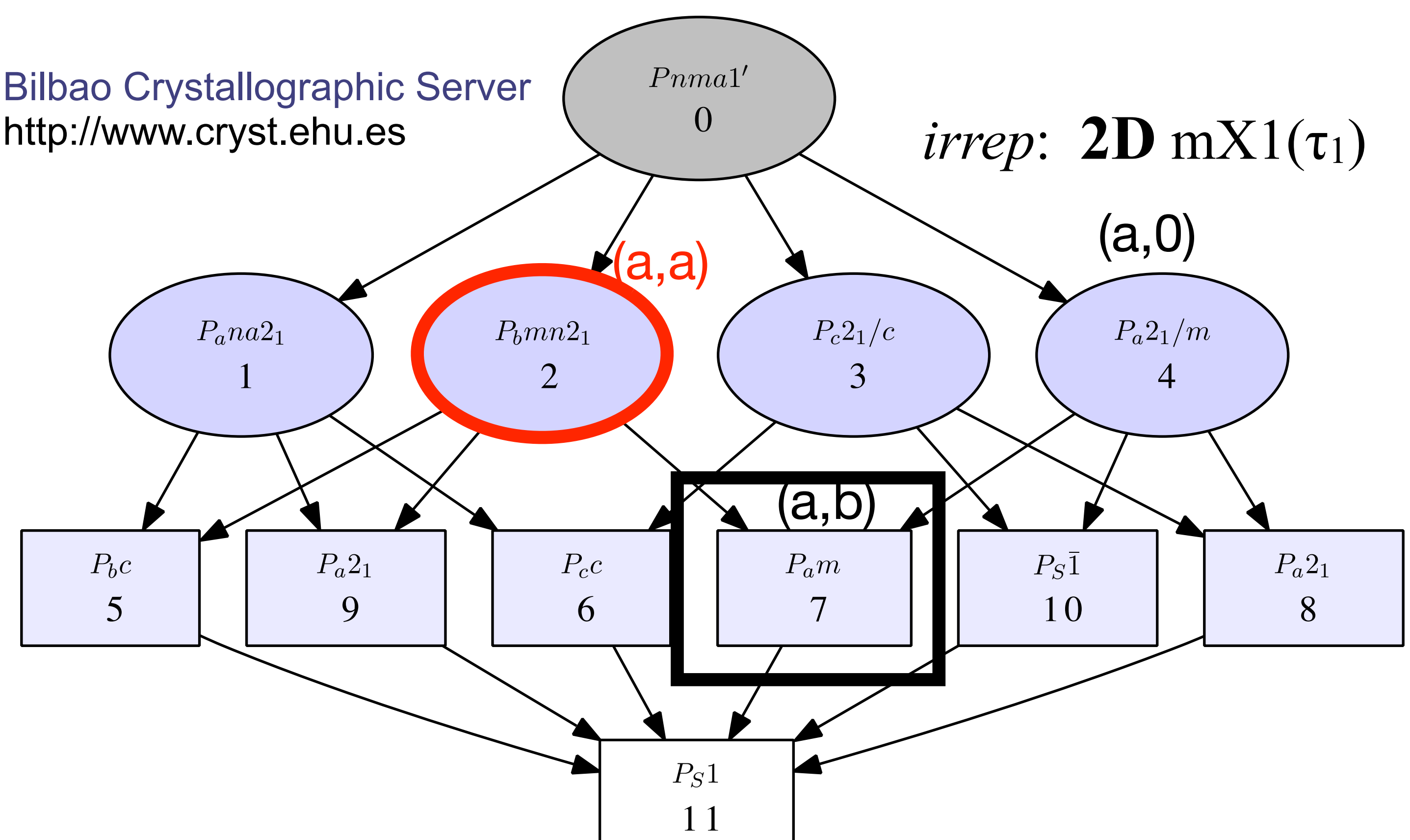
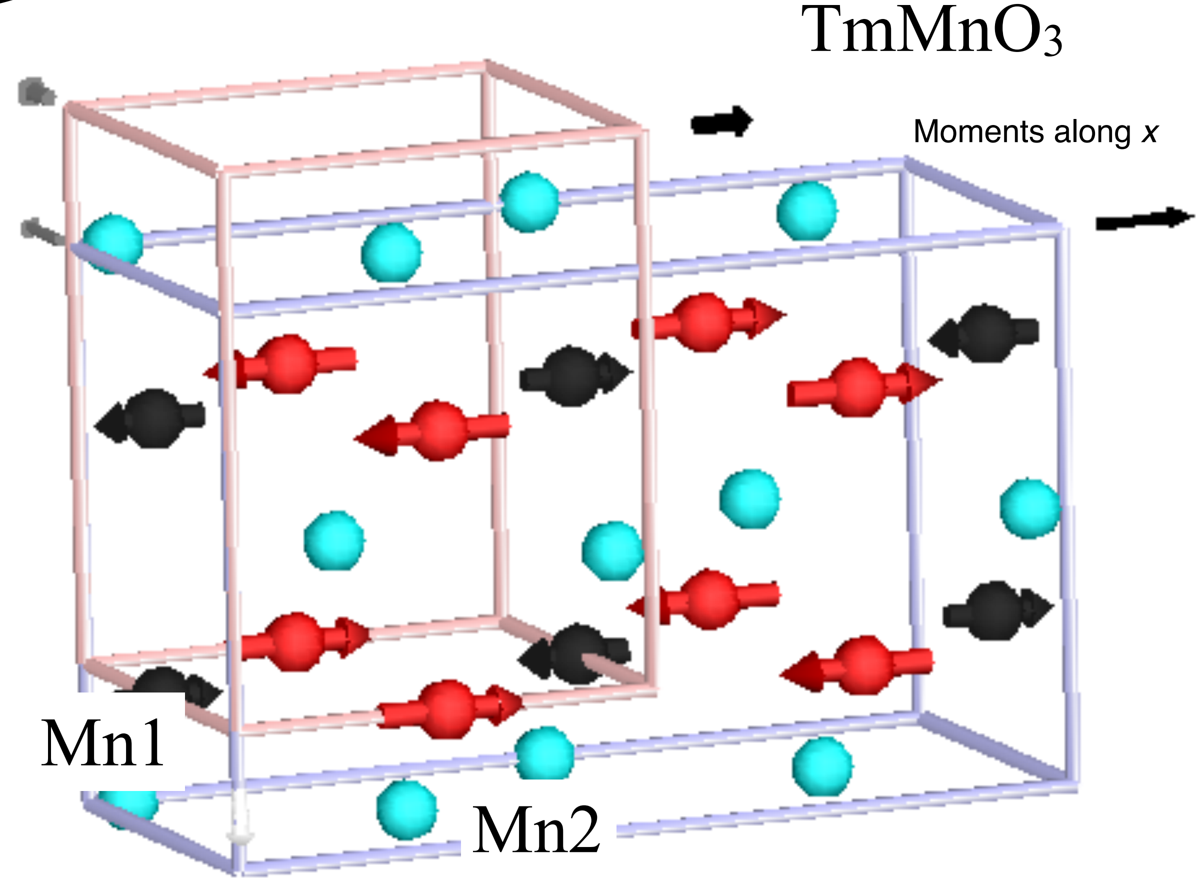
irrep: **2D** mX1(τ_1)

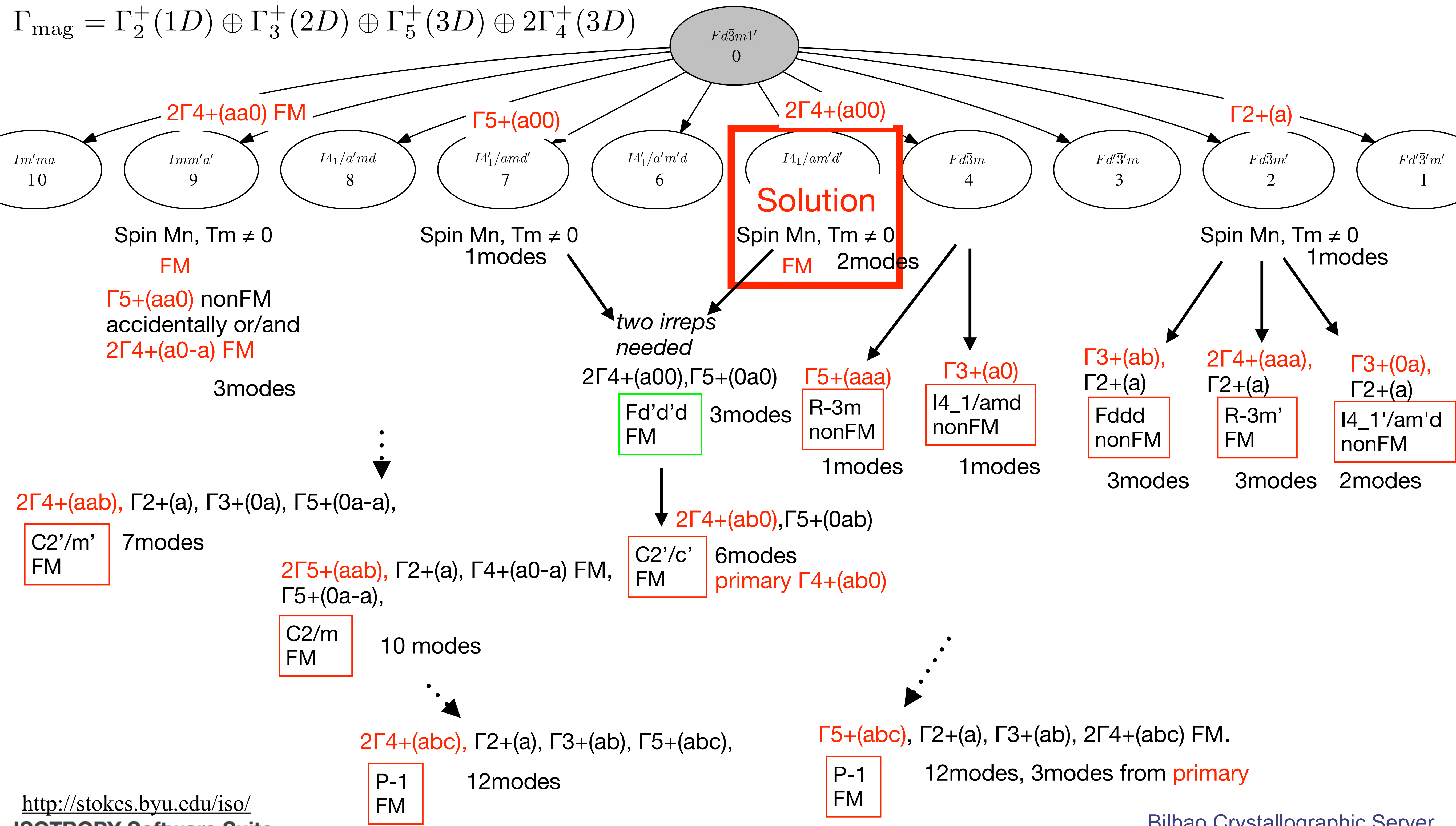




Magnetic structure of Pyrochlore $Tm_2Mn_2O_7$ at Γ-point k=0

Maximal and non-maximal MG for the parent SG 227 (*Fd-3m*) at gamma point k = (0, 0, 0) generated by *one irrep* for 16d (1/2,1/2,1/2), 16c (0,0,0) position

$$\Gamma_{\text{mag}} = \Gamma_2^+(1D) \oplus \Gamma_3^+(2D) \oplus \Gamma_5^+(3D) \oplus 2\Gamma_4^+(3D)$$



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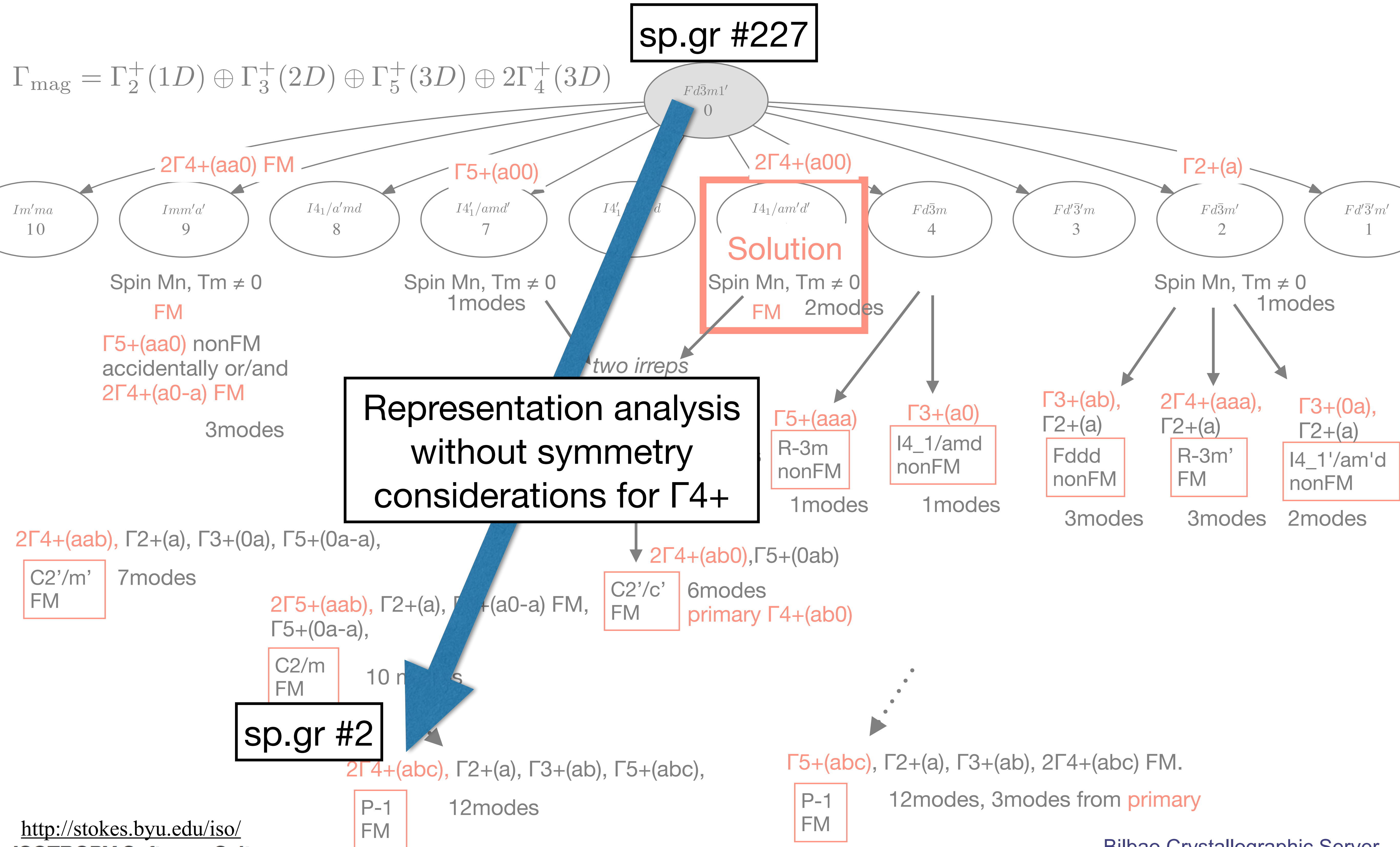

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