Magnetic Refinement (Symmetry)

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Magnetic symmetry

- Axioms of group theory and the crystallographic point groups
- Magnetic point groups
- Magnetic space groups (commensurate structures)
- Irreducible representations

We will not consider incommensurate structures and superspace groups (not enough time!)

Axioms of group theory

Axiom #1: Closure by composition

- A group has a well defined binary operation known as composition, which is denoted by the symbol $\circ$
- For the matrix representation of symmetry operators, composition is matrix multiplication
- If two symmetry operators, say *f* and *g,* are in a group, their composition generates another operator of the group, *h,* and hence the group is closed by composition
- Composition is not necessarily commutative

Axioms of group theory

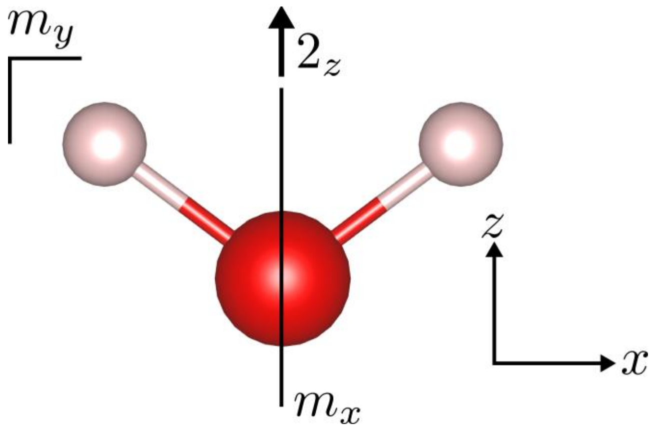
Axiom #1: Closure by composition

Example: $\{1, 2_z, m_x, m_y\}$

$$2_z \circ m_x = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \circ \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = m_y$$

$$m_x \circ m_y = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \circ \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = 2_z$$

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



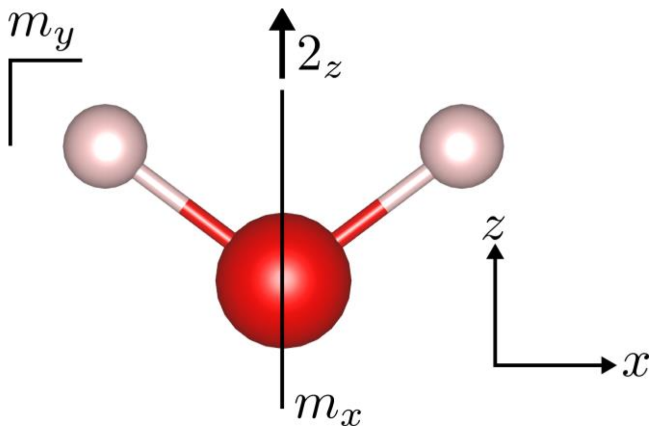
Axioms of group theory

Axiom #1: Closure by composition

Example: {1, 2_z, m_x, m_y}

Closure by composition summarised by a **group multiplication table**

	1	2_z	m_x	m_y
1	1	2_z	m_x	m_y
2_z	2_z	1	m_y	m_x
m_x	m_x	m_y	1	2_z
m_y	m_y	m_x	2_z	1



Axioms of group theory

Axiom #2: Associativity

Composition **is associative**. If f, g, and h belong to the same group

$$(f \circ g) \circ h = f \circ (g \circ h)$$

Axiom #3: The identity operator

Every group must contain the identity operator, 1 (sometimes labelled 'E')

$$g \circ 1 = 1 \circ g = g$$

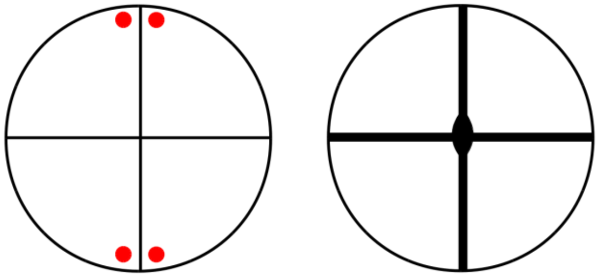
Axiom #4: Inverse operators

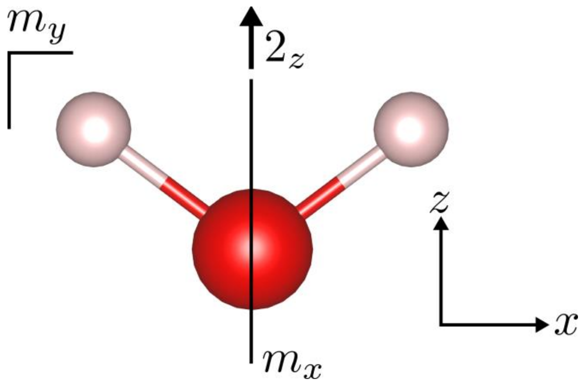
It follows from axiom 1 and axiom 3 that it must be possible to compose any operator, say f, with another operator, say g, and obtain 1

$$g = f^{-1}$$

Crystallographic point groups

- 'Crystallographic': dealing with symmetry operators for which Bravais lattices are invariant
- 'Point': dealing with symmetry operators that together leave at least one point in space invariant
- 'Groups': Sets of symmetry operators that satisfy the axioms of group theory
- There exists finite number of sets of rotation and rotoinversion operators with n = 1,2,3,4, or 6 that satisfy the axioms of a group. These are the 32 crystallographic point groups
- Example: Point group *mm2* = $\{1, 2_z, m_x, m_y\}$





Subgroups

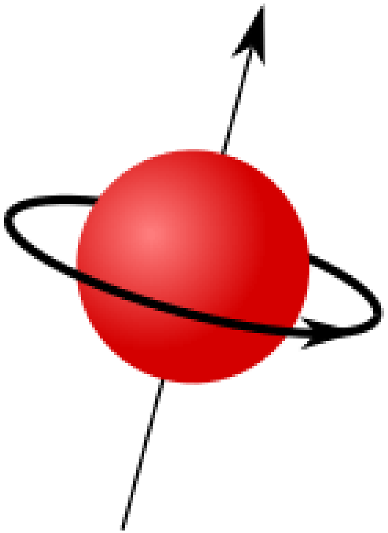
$$H \leq G$$

- A set of symmetry operators of a group that is also a group
- For example: {1}, {1, 2_z}, {1, m_x}, {1, m_y}, {1, 2_z, m_x, m_y} are subgroups of {1, 2_z, m_x, m_y}
- N.B. A group is counted as a subgroup of itself!

Angular momentum

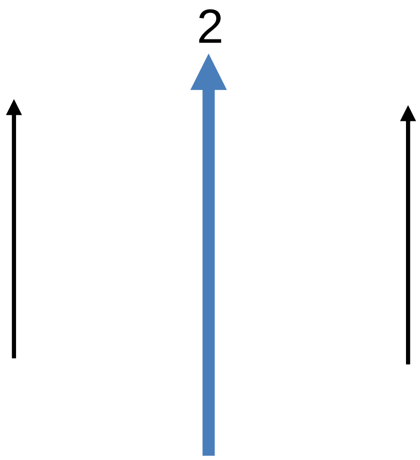
$$\boldsymbol{\mu}_{\boldsymbol{S}} = -g_S \frac{\mu_{\mathrm{B}}}{\hbar} \boldsymbol{S} \qquad \boldsymbol{\mu}_{\boldsymbol{L}} = -g_L \frac{\mu_{\mathrm{B}}}{\hbar} \boldsymbol{L}$$

Angular momentum transforms as a
time-odd axial vector

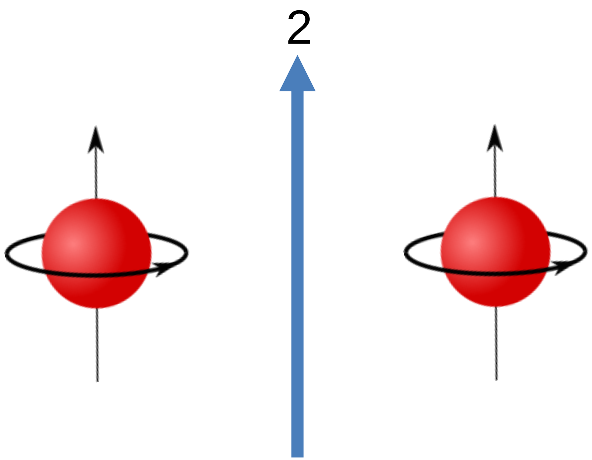


Angular momentum: rotation

Polar vector

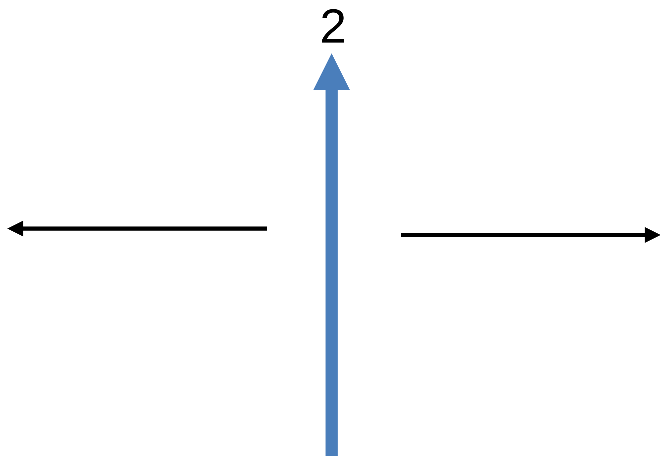


Time odd axial vector

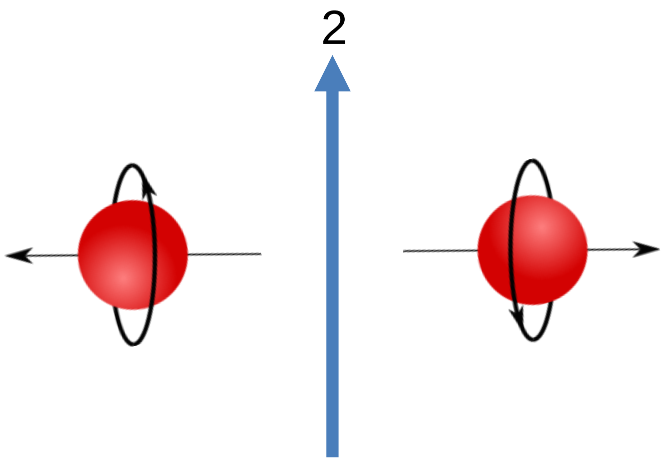


Angular momentum: rotation

Polar vector



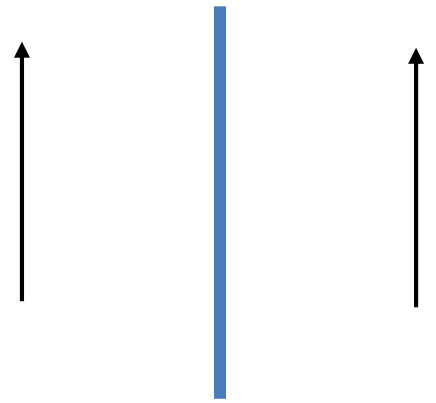
Time odd axial vector



Angular momentum: mirror

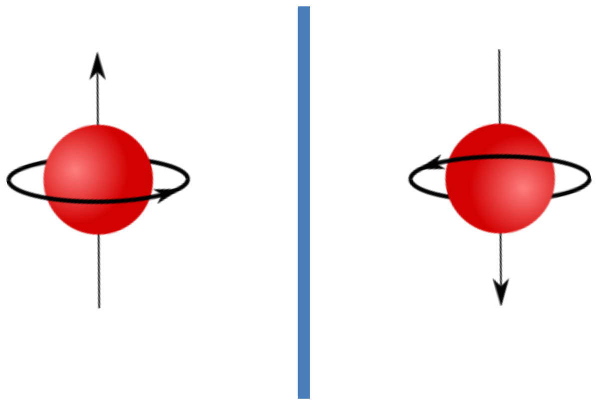
Polar vector

m



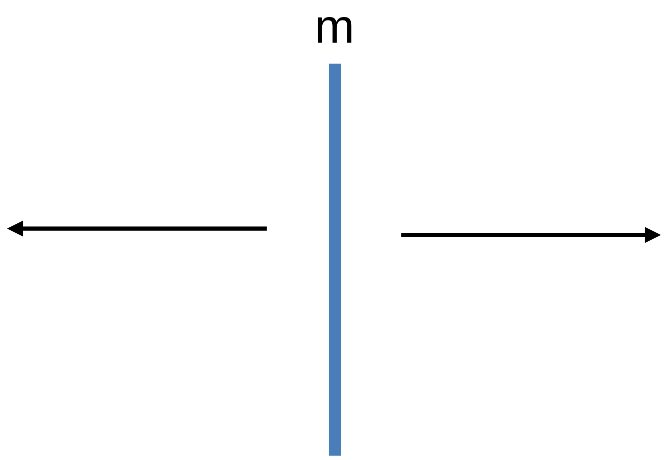
Time odd axial vector

m

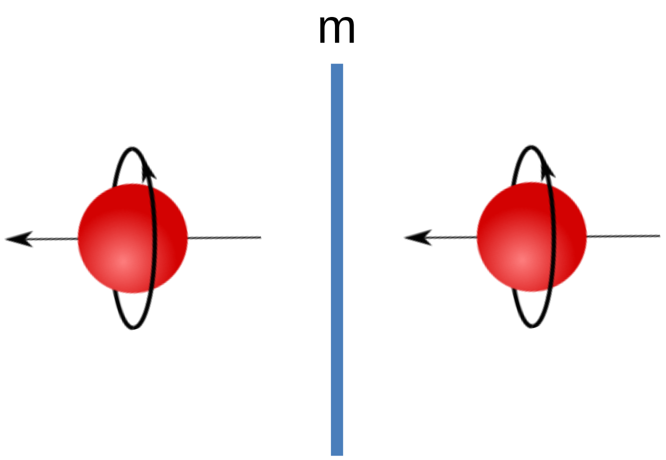


Angular momentum: mirror

Polar vector



Time odd axial vector



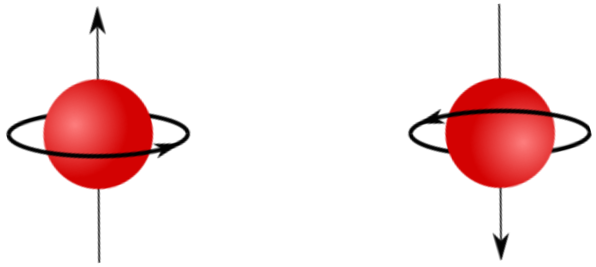
Angular momentum: time reversal

Polar vector

1’

Time odd axial vector

1’



Magnetic point groups

The time reversal group $I = \{1, 1'\}$

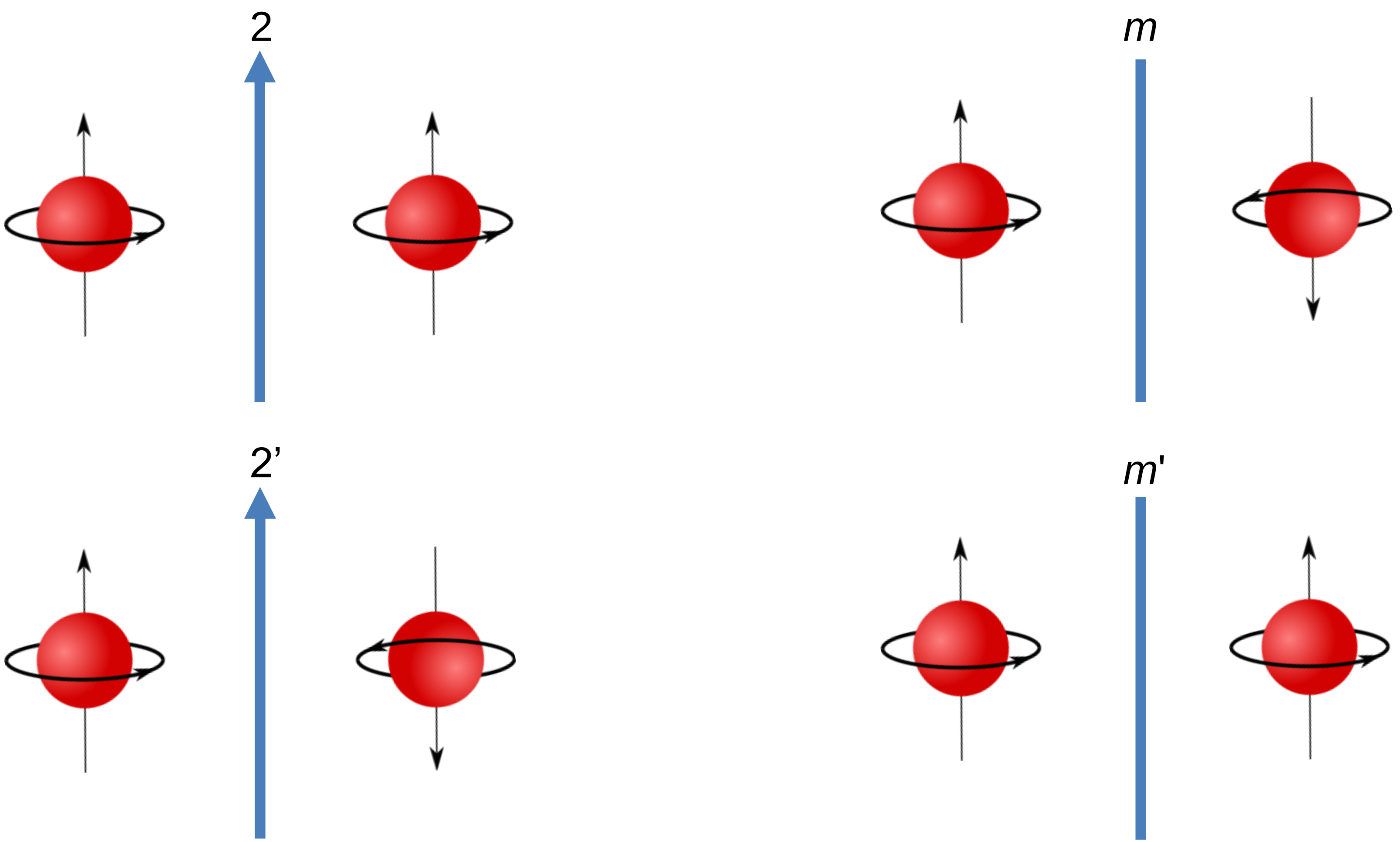
The magnetic point groups, *M*, are subgroups of the direct product of the crystallographic point groups, *G*, with the time reversal group, *I*.

$$M \leq G \times I$$

Lets take $G = \frac{2}{m} = \{1, 2, \bar{1}, m\}$

$$G \times I = \{1, 2, \bar{1}, m, 1', 2', \bar{1}', m'\}$$

Magnetic point groups



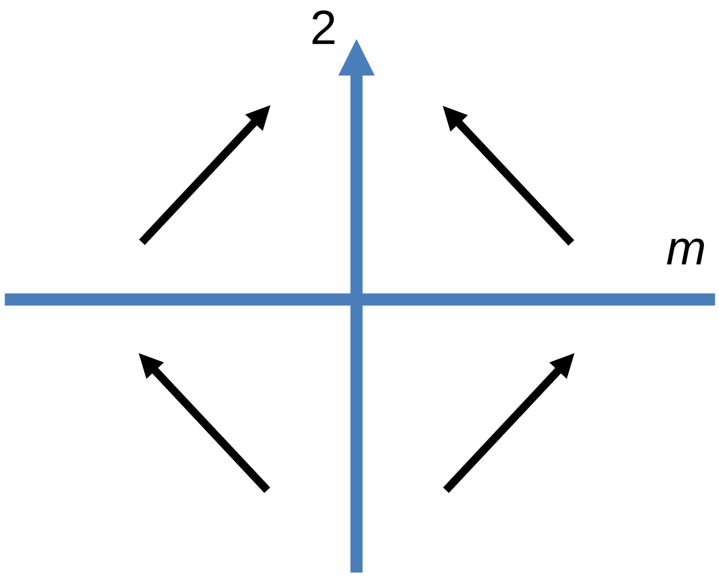
Magnetic point groups

$$G \times I = \{1, 2, \bar{1}, m, 1', 2', \bar{1}', m'\}$$

Consider the magnetic point group $M = G$

$$M = \{1, 2, \bar{1}, m\}$$

$$\frac{2}{m}$$



- Same symmetry as *G*
- Allows magnetic order
- Called a **Type I** magnetic point group

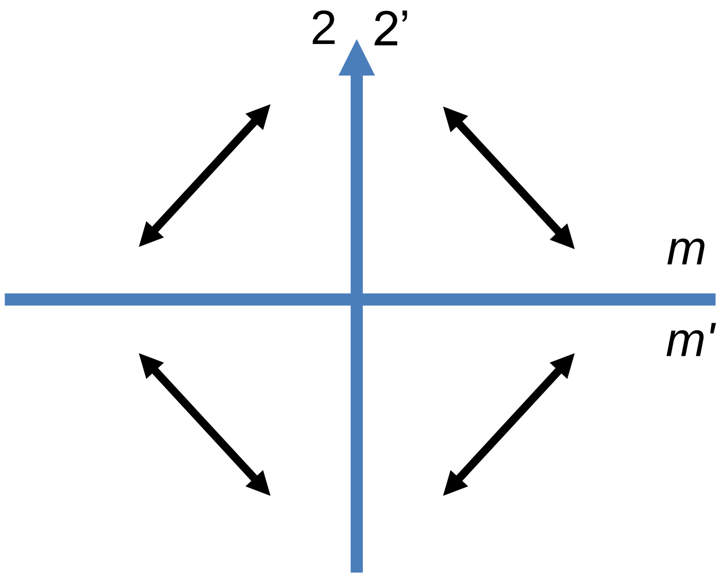
Magnetic point groups

$$G \times I = \{1, 2, \bar{1}, m, 1', 2', \bar{1}', m'\}$$

Consider the magnetic point group $M = G \times I$

$$M = \{1, 2, \bar{1}, m, 1', 2', \bar{1}', m'\}$$

$$\frac{2}{m}1'$$



- This is the paramagnetic group or ‘grey’ group
- Does not allow magnetic order
- Called a **Type II** magnetic point group

Magnetic point groups

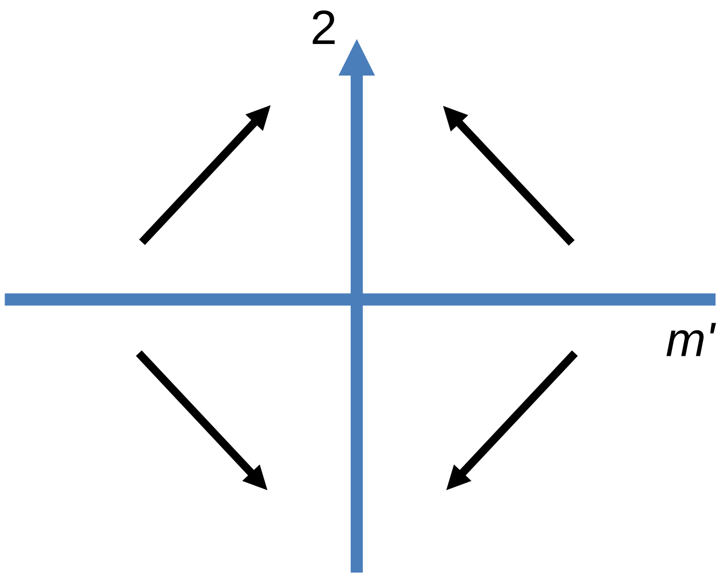
$$G \times I = \{1, 2, \bar{1}, m, 1', 2', \bar{1}', m'\}$$

Consider the magnetic point group $M = H + (G - H)1'$
where *H* is a subgroup of *G* of order 2

$$H = \{1, 2\}$$

$$M = \{1, 2, \bar{1}', m'\}$$

$$\frac{2}{m'}$$



- Allows magnetic order
- Called a **Type III** magnetic point group

Magnetic point groups

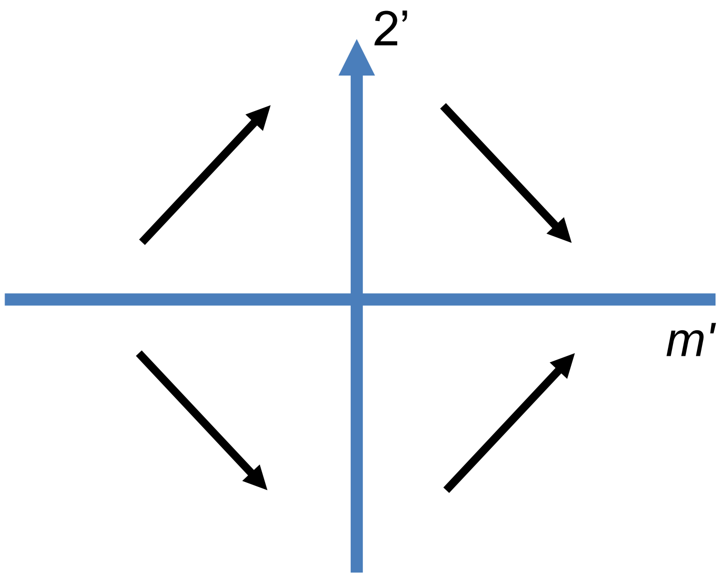
$$G \times I = \{1, 2, \bar{1}, m, 1', 2', \bar{1}', m'\}$$

Consider the magnetic point group $M = H + (G - H)1'$
where *H* is a subgroup of *G* of order 2

$$H = \{1, \bar{1}\}$$

$$M = \{1, 2', \bar{1}, m'\}$$

$$\frac{2'}{m'}$$



- Allows magnetic order
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Magnetic point groups

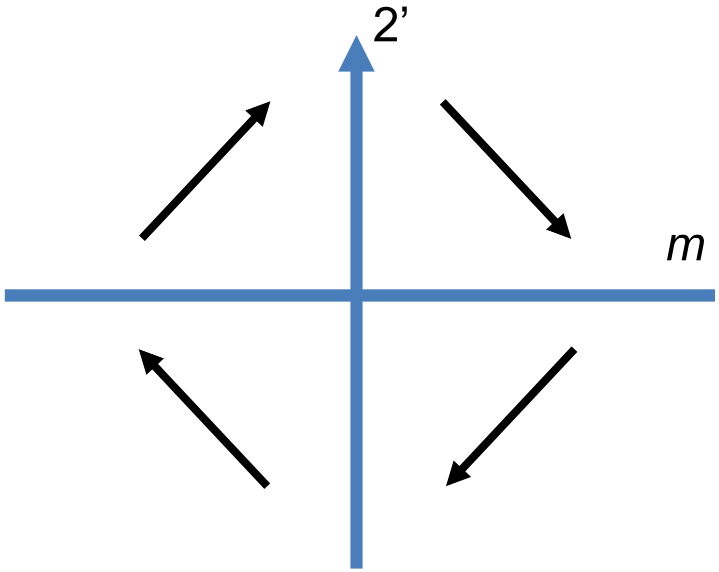
$$G \times I = \{1, 2, \bar{1}, m, 1', 2', \bar{1}', m'\}$$

Consider the magnetic point group $M = H + (G - H)1'$
where *H* is a subgroup of *G* of order 2

$$H = \{1, m\}$$

$$M = \{1, 2', \bar{1}', m\}$$

$$\frac{2'}{m}$$

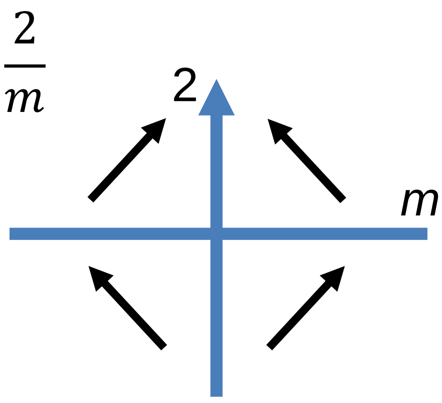


- Allows magnetic order
- Called a **Type III** magnetic point group

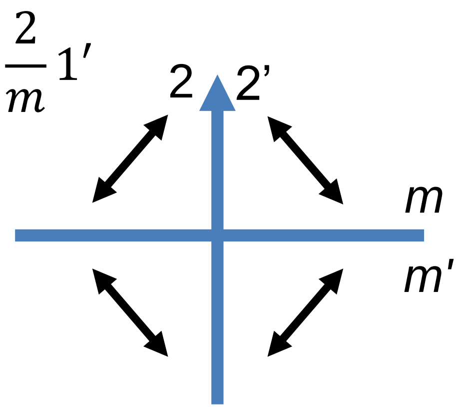
Magnetic point groups

$$G \times I = \{1, 2, \bar{1}, m, 1', 2', \bar{1}', m'\} \qquad M \leq G \times I$$

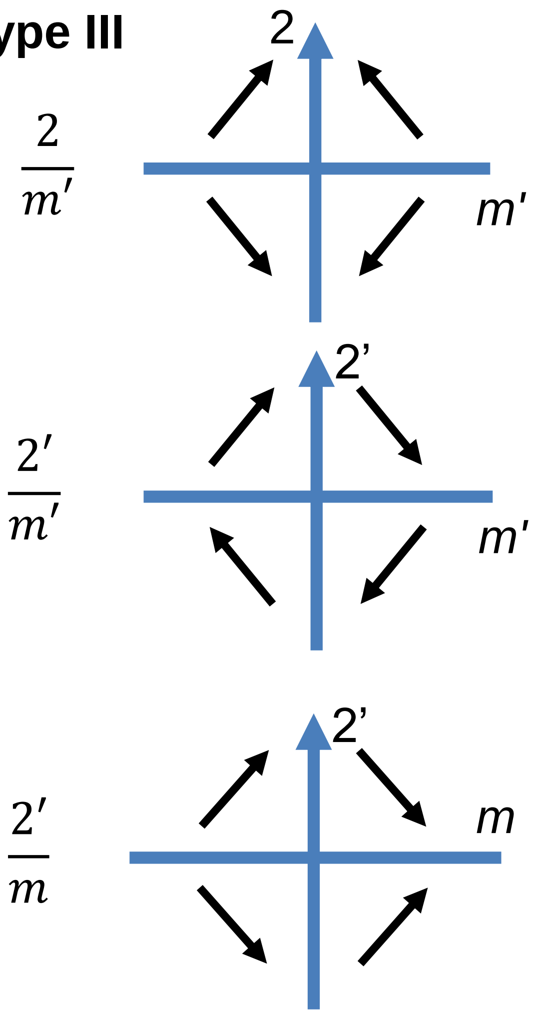
Type I



Type II



Type III



Magnetic point groups

32 **Type I** + 32 **Type II** + 58 **Type III** =
122 ‘magnetic’ point groups

Cyan: ferromagnetic
Red: ferroelectric
Purple: both

Crystallographic point groups	Grey point groups	Magnetic point groups				
1	1'					
$\bar{1}$	$\bar{1}1'$	$\bar{1}'$				
2	21'	2'				
m	m1'	m'				
2/m	2/m1'	2'/m'	2/m'	2'/m		
222	2221'	2'2'2				
mm2	mm21'	m'm'2	2'm'm			
mmm	mmm1'	mm'm'	m'm'm'	mmm'		
4	41'	4'				
$\bar{4}$	$\bar{4}1'$	$\bar{4}'$				
4/m	4/m1'	4'/m	4/m'	4'/m'		
422	4221'	4'22'	42'2'			
4mm	4mm1'	4'mm'	4m'm'			
$\bar{4}2m$	$\bar{4}2m1'$	$\bar{4}'2m'$	$\bar{4}'m2'$	$\bar{4}2'm'$		
4/mmm	4/mmm1'	4'/mmm'	4/mm'm'	4/m'm'm'	4/m'mm	4'/m'm'm
3	31'					
$\bar{3}$	$\bar{3}1'$	$\bar{3}'$				
32	321'	32'				
3m	3m1'	3m'				
$\bar{3}m$	$\bar{3}m1'$	$\bar{3}m'$	$\bar{3}'m'$	$\bar{3}'m$		
6	61'	6'				
$\bar{6}$	$\bar{6}1'$	$\bar{6}'$				
6/m	6/m1'	6'/m'	6/m'	6'/m		
622	6221'	6'22'	62'2'			
6mm	6mm1'	6'mm'	6m'm'			
$\bar{6}m2$	$\bar{6}m21'$	$\bar{6}'2m'$	$\bar{6}'m2'$	$\bar{6}m'2'$		
6/mmm	6/mmm1'	6'/m'mm'	6/mm'm'	6/m'm'm'	6/m'mm	6'/mmm'
23	231'					
$m\bar{3}$	$m\bar{3}1'$	$m'\bar{3}'$				
432	4321'	4'32'				
43m	43m1'	4'3m'				
$m\bar{3}m$	$m\bar{3}m1'$	$m\bar{3}m'$	$m'\bar{3}'m'$	$m'\bar{3}'m$		

Magnetic space groups

$$M \leq G \times I$$

Lets take $G = P\frac{2}{m} = \{1, 2, \bar{1}, m\} \times T_G$

$$M = G = P\frac{2}{m}.1$$

- This is the 'colourless' group
- Allows magnetic order
- Called a **Type I** magnetic space group

$$M = G \times I = P\frac{2}{m}.1'$$

- This is the paramagnetic group or 'grey' group
- Does not allow magnetic order
- Called a **Type II** magnetic space group

Magnetic space groups

$$M \leq G \times I$$

$M = H + (G - H)1'$, where *H* is a subgroup of *G* of order 2

Case 1: *H* is a *Translationenglieiche* subgroup of *G* (one in which all translation symmetry is retained *i.e.* $T_H = T_G$) and hence the order of point group P_H is lower than that of P_G

- This is a black and white group with an ordinary Bravais lattice
- Allows magnetic order
- Called a **Type III** magnetic space group

$$P\frac{2'}{m} \qquad P\frac{2}{m'} \qquad P\frac{2'}{m'}$$

Magnetic space groups

$$M \leq G \times I$$

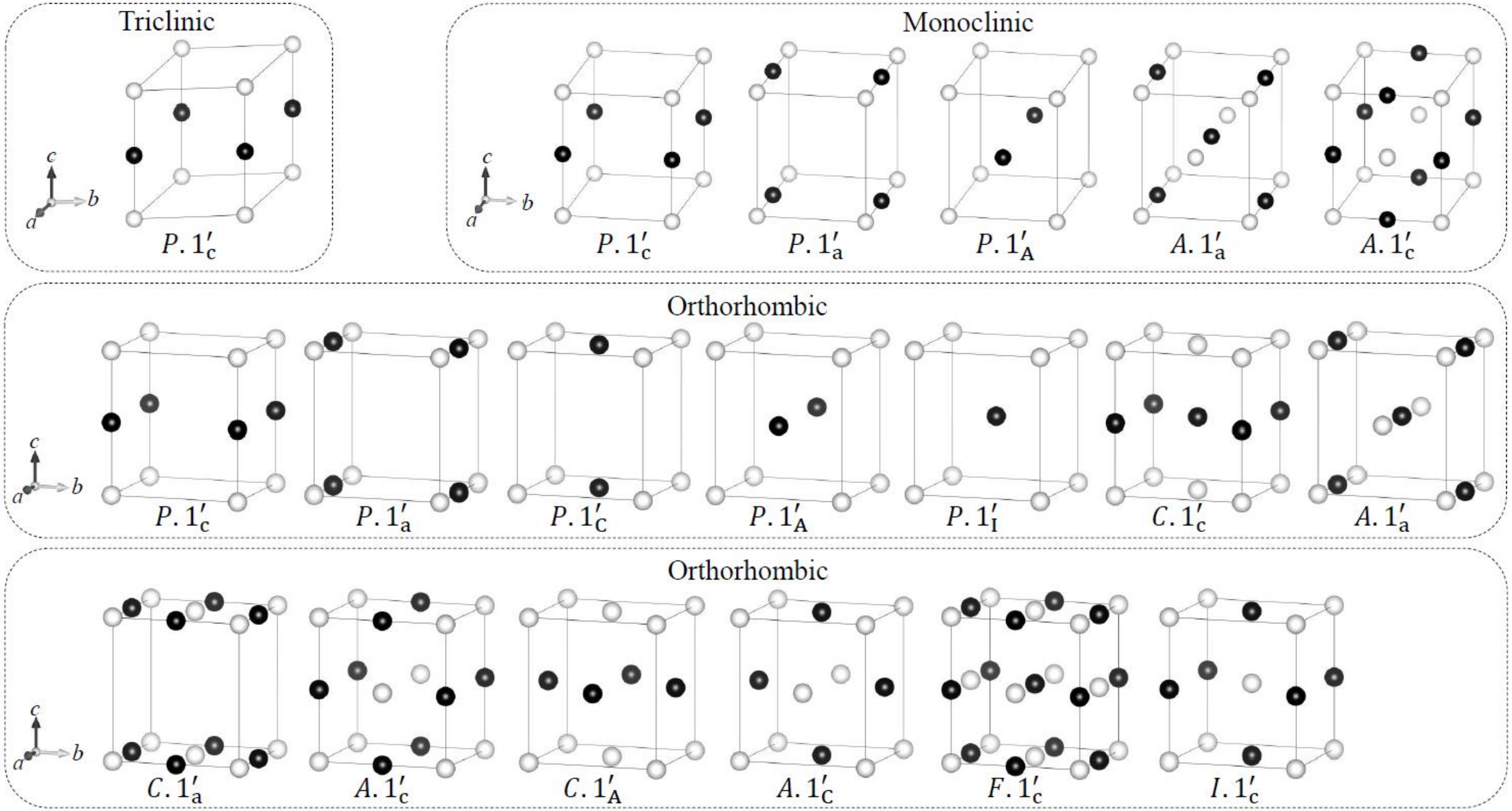
$M = H + (G - H)1'$, where *H* is a subgroup of *G* of order 2

Case 2: *H* is a *Klassenglieiche* subgroup of *G* (one in which translation symmetry is lowered *i.e.* $T_H < T_G$) and hence the order of point group P_H is the same as that of P_G

- This is a black and white group with a black and white Bravais lattice
- Allows magnetic order
- Called a **Type IV** magnetic space group

$$P\frac{2}{m}.1'_a \qquad P\frac{2}{m}.1'_b \qquad P\frac{2}{m}.1'_C$$

Magnetic space groups



Magnetic space groups

230 **Type I** + 230 **Type II** + 674 **Type III** + 517 **Type IV** = 1651 ‘magnetic’ space groups

IUCr / Daniel B. Litvin: https://www.iucr.org/publ/978-0-9553602-2-0

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

Landau theory

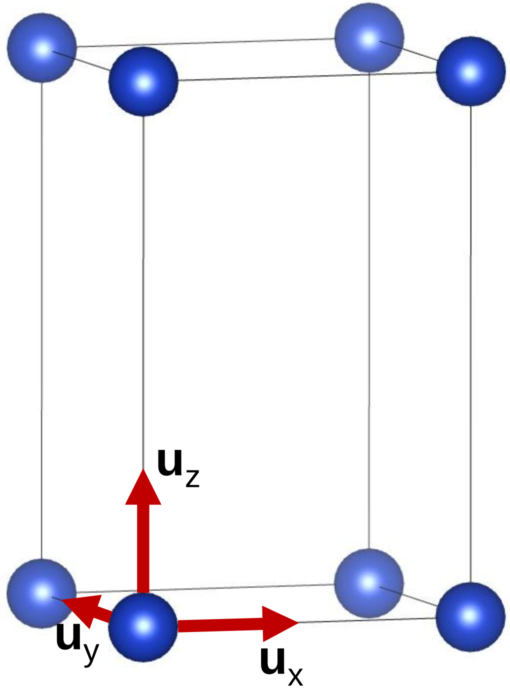
- The vast majority of paramagnetic to (anti)ferromagnetic phase transitions are second order (continuous)

- The Landau theory of second order phase transitions requires the primary magnetic order parameter to transform by a single **irreducible representation**…

- … only condensation of a single normal mode can lead to a *continuous* change of the system.

Representations

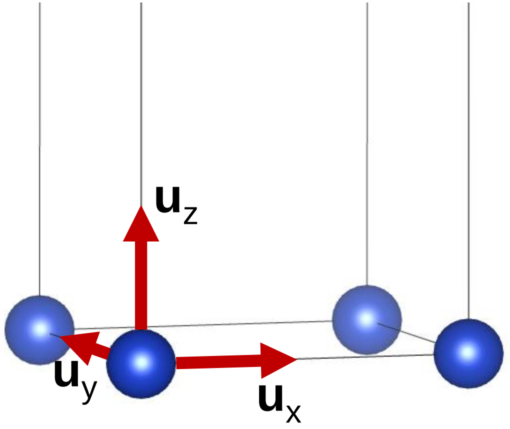
- Take a vector space $V_p=(\mathbf{u}_x,\mathbf{u}_y,\mathbf{u}_z)$, where $\mathbf{u}_i$ describe **polar** distortions
- Assume displacements same in every unit cell (the following can be extended to $k\neq0$)
- We will take space group *P4/m* as an example



Representations

The set of matrices M(g) is a **representation** of the group *P4/m* on the vector space V_p

1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&-1\end{pmatrix}$



Irreducible representations

Can we divide up the vector space V into smaller **irreducible** subspaces?

1	2_{001}	4^{+}_{001}	4^{-}_{001}	$\bar{1}$	m_{001}	$\bar{4}^{+}_{001}$	$\bar{4}^{-}_{001}$
$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&-1\end{pmatrix}$

Irreducible representations

Can we divide up the vector space V into smaller **irreducible** subspaces?

1	2_{001}	4^{+}_{001}	4^{-}_{001}	$\bar{1}$	m_{001}	$\bar{4}^{+}_{001}$	$\bar{4}^{-}_{001}$
$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&-1\end{pmatrix}$

$$B = P^{-1}AP, \qquad P = \begin{pmatrix}1&i&0\\i&1&0\\0&0&1\end{pmatrix}$$

1	2_{001}	4^{+}_{001}	4^{-}_{001}	$\bar{1}$	m_{001}	$\bar{4}^{+}_{001}$	$\bar{4}^{-}_{001}$
$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-i&0&0\\0&i&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}i&0&0\\0&-i&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}i&0&0\\0&-i&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}-i&0&0\\0&i&0\\0&0&-1\end{pmatrix}$

Irreducible representations: Characters

Can we divide up the vector space V into smaller **irreducible** subspaces?

1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&-1\end{pmatrix}$

1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
Γ_{V_p}							
3	-1	1	1	-3	1	-1	-1
$\Gamma_3^- \oplus \Gamma_4^-$							
2	-2	0	0	-2	2	0	0
Γ_1^-							
1	1	1	1	-1	-1	-1	-1

Irreducible representations: Character table

	1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
Γ_1^+	1	1	1	1	1	1	1	1
Γ_1^-	1	1	1	1	-1	-1	-1	-1
Γ_2^+	1	1	-1	-1	1	1	-1	-1
Γ_2^-	1	1	-1	-1	-1	-1	1	1
$\Gamma_3^+ \oplus \Gamma_4^+$	2	-2	0	0	2	-2	0	0
$\Gamma_3^- \oplus \Gamma_4^-$	2	-2	0	0	-2	2	0	0

$$\Gamma_{V_p} = \Gamma_1^- + (\Gamma_3^- \oplus \Gamma_4^-)$$

Irreducible representations: Decomposition theorem

$$\Gamma_{V_p} = \sum_{ij} a_i^j \Gamma_i^j \qquad a_i^j = \frac{1}{h}\sum_g \chi_{\Gamma_{V_p}}(g)\chi_{\Gamma_i^j}(g)$$

	1	**2_{001}**	**4^+_{001}**	**4^-_{001}**	**$\bar{1}$**	**m_{001}**	**$\bar{4}^+_{001}$**	**$\bar{4}^-_{001}$**
Γ_{V_p}	3	-1	1	1	-3	1	-1	-1
Γ_1^+	1	1	1	1	1	1	1	1
Γ_1^-	1	1	1	1	-1	-1	-1	-1
Γ_2^+	1	1	-1	-1	1	1	-1	-1
Γ_2^-	1	1	-1	-1	-1	-1	1	1
$\Gamma_3^+ \oplus \Gamma_4^+$	2	-2	0	0	2	-2	0	0
$\Gamma_3^- \oplus \Gamma_4^-$	2	-2	0	0	-2	2	0	0

Irreducible representations: Decomposition theorem

$$\Gamma_{V_p} = \sum_{ij} a_i^j \Gamma_i^j \qquad a_i^j = \frac{1}{h}\sum_g \chi_{\Gamma_{V_p}}(g)\chi_{\Gamma_i^j}(g) \qquad a_1^+ = \frac{1}{8}(3-1+1+1-3+1-1-1) = 0$$

	1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
Γ_{V_p}	3	-1	1	1	-3	1	-1	-1
Γ_1^+	1	1	1	1	1	1	1	1
Γ_1^-	1	1	1	1	-1	-1	-1	-1
Γ_2^+	1	1	-1	-1	1	1	-1	-1
Γ_2^-	1	1	-1	-1	-1	-1	1	1
$\Gamma_3^+ \oplus \Gamma_4^+$	2	-2	0	0	2	-2	0	0
$\Gamma_3^- \oplus \Gamma_4^-$	2	-2	0	0	-2	2	0	0

Irreducible representations: Decomposition theorem

$$\Gamma_{V_p} = \sum_{ij} a_i^j \Gamma_i^j \qquad a_i^j = \frac{1}{h}\sum_g \chi_{\Gamma_{V_p}}(g)\chi_{\Gamma_i^j}(g) \qquad a_1^- = \frac{1}{8}(3-1+1+1+3-1+1+1) = 1$$

	1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
Γ_{V_p}	3	-1	1	1	-3	1	-1	-1
Γ_1^+	1	1	1	1	1	1	1	1
Γ_1^-	1	1	1	1	-1	-1	-1	-1
Γ_2^+	1	1	-1	-1	1	1	-1	-1
Γ_2^-	1	1	-1	-1	-1	-1	1	1
$\Gamma_3^+ \oplus \Gamma_4^+$	2	-2	0	0	2	-2	0	0
$\Gamma_3^- \oplus \Gamma_4^-$	2	-2	0	0	-2	2	0	0

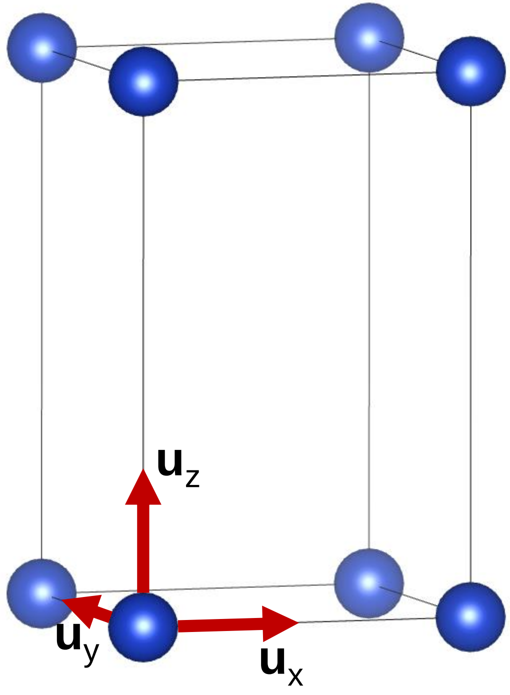
Representations

- Take a vector space $V_m=(\mathbf{u}_x,\mathbf{u}_y,\mathbf{u}_z)$, where $\mathbf{u}_i$ describe **axial** distortions

- Assume displacements same in every unit cell (the following can be extended to $k\neq0$)

- We will take space group *P4*/*m* as an example

- This is a **model for ferromagnetism**



Representations

The set of matrices M(g) is a **representation** of the group *P4/m* on the vector space V_m

1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}$

1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
$m\Gamma_3^+ \oplus m\Gamma_4^+$							
2	-2	0	0	2	-2	0	0
$m\Gamma_1^+$							
1	1	1	1	1	1	1	1

Irreducible representations (character table)

	1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
$m\Gamma_1^+$	1	1	1	1	1	1	1	1
$m\Gamma_1^-$	1	1	1	1	-1	-1	-1	-1
$m\Gamma_2^+$	1	1	-1	-1	1	1	-1	-1
$m\Gamma_2^-$	1	1	-1	-1	-1	-1	1	1
$m\Gamma_3^+ \oplus m\Gamma_4^+$	2	-2	0	0	2	-2	0	0
$m\Gamma_3^- \oplus m\Gamma_4^-$	2	-2	0	0	-2	2	0	0

$$\Gamma_{V_m} = \Gamma_1^+ + (\Gamma_3^+ \oplus \Gamma_4^+)$$

Irreducible representations (character table)

	1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$	
$m\Gamma_1^+$	1	1	1	1	1	1	1	1	*P4/m*
$m\Gamma_1^-$	1	1	1	1	-1	-1	-1	-1	*P4/m'*
$m\Gamma_2^+$	1	1	-1	-1	1	1	-1	-1	*P4'/m*
$m\Gamma_2^-$	1	1	-1	-1	-1	-1	1	1	*P4'/m'*
$m\Gamma_3^+ \oplus m\Gamma_4^+$	2	-2	0	0	2	-2	0	0	*P2'/m'*
$m\Gamma_3^- \oplus m\Gamma_4^-$	2	-2	0	0	-2	2	0	0	*P2'/m*

The number of **Type I** and **Type III** magnetic space groups derived from space group G are equal to the number of distinct 1-D IR's (Bertaut. Acta Cryst. A24, 217 (1968))

Irreducible representations (character table)

	1	2_{001}	4^{+}_{001}	4^{-}_{001}	$^{-}_{001}$	
$m\Gamma_1^+$	1	1	1	1	1	*P4/m*
$m\Gamma_1^-$	1	1	1	1	-1	*P4/m'*
$m\Gamma_2^+$	1	1	-1	-1	-1	*P4'/m*
$m\Gamma_2^-$	1		-1	-1	1	*P4'/m'*
$m\Gamma_3^+ \oplus m\Gamma_4^+$	2	-2	0	0	0	*P2'/m'*
$m\Gamma_3^- \oplus m\Gamma_4^-$	2	-2	0	0	0	*P2'/m*

Cyan: ferromagnetic
Red: ferroelectric
Purple: both

Crystallographic point groups	Grey point groups	Magnetic point groups				
1	1'					
$\bar{1}$	$\bar{1}$1'	$\bar{1}$'				
2	21'	2'				
m	m1'	m'				
2/m	2/m1'	2'/m'	2/m'	2'/m		
222	2221'	2'2'2				
mm2	mm21'	m'm'2	2'm'm			
mmm	mmm1'	mm'm'	m'm'm'	mmm'		
4	41'	4'				
$\bar{4}$	$\bar{4}$1'	$\bar{4}$'				
4/m	4/m1'	4'/m	4/m'	4'/m'		
422	4221'	4'22'	42'2'			
4mm	4mm1'	4'mm'	4m'm'			
$\bar{4}$2m	$\bar{4}$2m1'	$\bar{4}$'2m'	$\bar{4}$'m2'	$\bar{4}$2'm'		
4/mmm	4/mmm1'	4'/mmm'	4/mm'm'	4/m'm'm'	4/m'mm	4'/m'm'm
3	31'					
$\bar{3}$	$\bar{3}$1'	$\bar{3}$'				
32	321'	32'				
3m	3m1'	3m'				
$\bar{3}$m	$\bar{3}$m1'	$\bar{3}$m'	$\bar{3}$'m'	$\bar{3}$'m		
6	61'	6'				
$\bar{6}$	$\bar{6}$1'	$\bar{6}$'				
6/m	6/m1'	6'/m'	6/m'	6'/m		
622	6221'	6'22'	62'2'			
6mm	6mm1'	6'mm'	6m'm'			
$\bar{6}$m2	$\bar{6}$m21'	$\bar{6}$'2m'	$\bar{6}$'m2'	$\bar{6}$m'2'		
6/mmm	6/mmm1'	6'/m'mm'	6/mm'm'	6/m'm'm'	6/m'mm	6'/mmm'
23	231'					
m$\bar{3}$	m$\bar{3}$1'	m'$\bar{3}$'				
432	4321'	4'32'				
43m	43m1'	4'3m'				
m$\bar{3}$m	m$\bar{3}$m1'	m$\bar{3}$m'	m'$\bar{3}$'m'	m'$\bar{3}$'m		

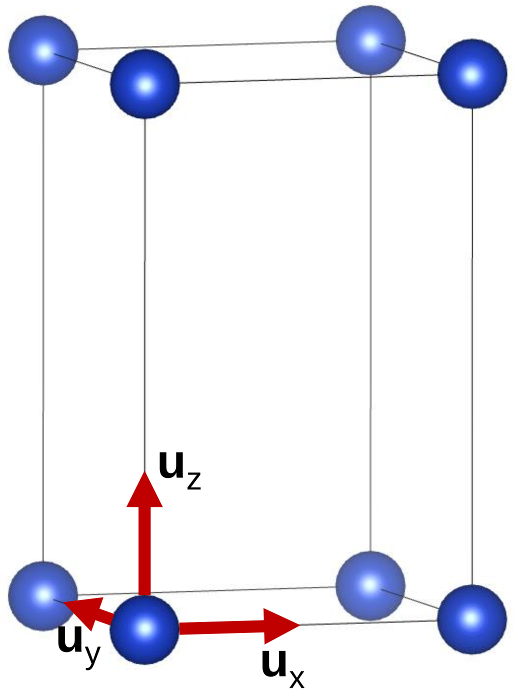
The number of **Type I** and **Type III** magnetic ... ce group
G are equal to the number of distinct 1-D IR' ... (1968))

Symmetry adapted modes

We began with the decomposition of the *P4/m* representation in the basis of ferromagnetic modes and found

$$\Gamma_{V_m} = m\Gamma_1^+ + (m\Gamma_3^+ \oplus m\Gamma_4^+)$$

In general, symmetry adapted modes can be obtained from the representations using the projection operator



Symmetry adapted modes

$m\Gamma_1^+$

$$P_j = \frac{d_j}{h}\sum_i \chi_j(g_i)g_i(V) \qquad \phi = P_jV$$

$$\frac{1}{8}\Bigg(\chi_{m\Gamma_1^+}(1)\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}+\chi_{m\Gamma_1^+}(2_{001})\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}+\chi_{m\Gamma_1^+}(4_{001}^+)\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}+\chi_{m\Gamma_1^+}(4_{001}^-)\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}$$
$$+\chi_{m\Gamma_1^+}(\bar{1})\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}+\chi_{m\Gamma_1^+}(m_{001})\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}+\chi_{m\Gamma_1^+}(\bar{4}_{001}^+)\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}+\chi_{m\Gamma_1^+}(\bar{4}_{001}^-)\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}\Bigg)$$

$$=\begin{pmatrix}0&0&0\\0&0&0\\0&0&1\end{pmatrix} \qquad P_jV_m=\begin{pmatrix}0&0&0\\0&0&0\\0&0&1\end{pmatrix}\begin{pmatrix}\boldsymbol{u}_x\\\boldsymbol{u}_y\\\boldsymbol{u}_z\end{pmatrix}\propto\begin{pmatrix}0\\0\\\boldsymbol{u}_z\end{pmatrix}$$

Symmetry adapted modes

$m\Gamma_3^+ \oplus m\Gamma_4^+$

$$P_j = \frac{d_j}{h}\sum_i \chi_j(g_i) g_i(V) \qquad \phi = P_j V$$

$$\frac{2}{8}\Bigg(\chi_{m\Gamma_3^+\oplus m\Gamma_4^+}(1)\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix} + \chi_{m\Gamma_3^+\oplus m\Gamma_4^+}(2_{001})\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix} + \chi_{m\Gamma_3^+\oplus m\Gamma_4^+}(4^+_{001})\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$$
$$+ \chi_{m\Gamma_3^+\oplus m\Gamma_4^+}(4^-_{001})\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix} + \chi_{m\Gamma_3^+\oplus m\Gamma_4^+}(\bar{1})\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix} + \chi_{m\Gamma_3^+\oplus m\Gamma_4^+}(m_{001})\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$$
$$+ \chi_{m\Gamma_3^+\oplus m\Gamma_4^+}(\bar{4}^+_{001})\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix} + \chi_{m\Gamma_3^+\oplus m\Gamma_4^+}(\bar{4}^-_{001})\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}\Bigg)$$

$$= 2\begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix} \qquad P_j V_m = \begin{pmatrix}2&0&0\\0&2&0\\0&0&0\end{pmatrix}\begin{pmatrix}\boldsymbol{u}_x\\\boldsymbol{u}_y\\\boldsymbol{u}_z\end{pmatrix} \propto \begin{pmatrix}\boldsymbol{u}_x\\\boldsymbol{u}_y\\0\end{pmatrix}$$

Irreducible representations

- The Landau theory of second order phase transitions requires the primary magnetic order parameter to transform by a single **irreducible representation**

- An irreducible representation of a group is a set of matrices on a vector space, defined in a basis with no reducible vector subspaces

- Irreducible representation ⇔ symmetry adapted modes ⇔ magnetic space group

- The irreducible representations of the space groups, symmetry adapted modes, order parameters, and magnetic space groups have all been calculated for you!

E.g. Bilbao Crystallographic Server or ISODISTORT