Representational Analysis of the space group I m m m with the propagation vector $\mathbf{k}$=(.5, 0, .5).

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1 Cut and Paste LaTeX summary for Kovalev's IRs

Representational analysis[1, 2, 3, 4, 5, 6] allows the determination of the symmetry-allowed magnetic structures that can result from a second-order magnetic phase transition, given the crystal structure before the transition and the propagation vector of the magnetic ordering. These calculations were carried out using version 2K of the program SARA*h*-Representational Analysis.[7] They involve first the determination of the space group symmetry elements, g, that leave the propagation vector $\mathbf{k}$ invariant: these form the little group $G_{\mathbf{k}}$. The magnetic representation of a crystallographic site can then be decomposed in terms of the irreducible representations (IRs) of $G_{\mathbf{k}}$:

$$\Gamma_{Mag} = \sum_{\nu} n_{\nu} \Gamma_{\nu}^{\mu} \tag{1}$$

where n_{ν} is the number of times that the IR Γ_{ν} of order μ appears in the magnetic representation Γ_{Mag} for the chosen crystallographic site.

In our case, the crystal structure of *insert composition formula/name* before the phase transition is described in the space group I m m m (#71). This space group involves 2 centring operations and 8 symmetry operations (Appendix A). Of these symmetry operations 4 leave the propagation $\mathbf{k}$ invariant or transform it into an equivalent vector (Appendix B).

The decomposition of the magnetic representation Γ_{Mag} in terms of the non-zero IRs of $G_{\mathbf{k}}$ for each crystallographic site examined, and their associated basis vectors, $\boldsymbol{\psi}_n$, are given in Tables 1 and 2. The labeling of the propagation vector and the IRs follows the scheme used by Kovalev[8].

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IR	BV	Atom	BV components					
			$m_{\parallel a}$	$m_{\parallel b}$	$m_{\parallel c}$	$im_{\parallel a}$	$im_{\parallel b}$	$im_{\parallel c}$
Γ_1	$\boldsymbol{\psi}_1$	1	0	2	0	0	0	0
		2	0	2	0	0	0	0
Γ_2	$\boldsymbol{\psi}_2$	1	2	0	0	0	0	0
		2	-2	0	0	0	0	0
	$\boldsymbol{\psi}_3$	1	0	0	2	0	0	0
		2	0	0	-2	0	0	0
Γ_3	$\boldsymbol{\psi}_4$	1	2	0	0	0	0	0
		2	2	0	0	0	0	0
	$\boldsymbol{\psi}_5$	1	0	0	2	0	0	0
		2	0	0	2	0	0	0
Γ_4	$\boldsymbol{\psi}_6$	1	0	2	0	0	0	0
		2	0	-2	0	0	0	0

Table 1: Basis vectors for the space group I m m m with $\mathbf{k}_{14} = (.5,\ 0,\ .5)$.The decomposition of the magnetic representation for the Ho site $(.5,\ 0,\ .2025)$ is $\Gamma_{Mag} = 1\Gamma_1^1 + 2\Gamma_2^1 + 2\Gamma_3^1 + 1\Gamma_4^1$. The atoms of the nonprimitive basis are defined according to 1: $(.5,\ 0,\ .2025)$, 2: $(.5,\ 0,\ .7975)$.

IR	BV	Atom	BV components					
			$m_{\parallel a}$	$m_{\parallel b}$	$m_{\parallel c}$	$im_{\parallel a}$	$im_{\parallel b}$	$im_{\parallel c}$
Γ_1	$\boldsymbol{\psi}_1$	1	0	4	0	0	0	0
Γ_3	$\boldsymbol{\psi}_2$	1	4	0	0	0	0	0
	$\boldsymbol{\psi}_3$	1	0	0	4	0	0	0

Table 2: Basis vectors for the space group I m m m with $\mathbf{k}_{14} = (.5,\ 0,\ .5)$.The decomposition of the magnetic representation for the Ni site $(0,\ 0,\ 0)$ is $\Gamma_{Mag} = 1\Gamma_1^1 + 0\Gamma_2^1 + 2\Gamma_3^1 + 0\Gamma_4^1$. The atom of the primitive basis is defined according to 1: $(0,\ 0,\ 0)$.

IR	BV	Point Group	Shubnikov Group
Γ_1	$\boldsymbol{\psi}_1$	2/m	N/A
Γ_2	$\boldsymbol{\psi}_2$	2/m	N/A
	$\boldsymbol{\psi}_3$	2	N/A
Γ_3	$\boldsymbol{\psi}_4$	2/m	N/A
	$\boldsymbol{\psi}_5$	2	N/A
Γ_4	$\boldsymbol{\psi}_6$	2/m	N/A

Table 3: The point symmetry and Shubnikov space group for the space group I m m m with $\mathbf{k}_{14} = (.5,\ 0,\ .5)$.The decomposition of the magnetic representation for the Ho site $(.5,\ 0,\ .2025)$ is $\Gamma_{Mag} = 1\Gamma_1^1 + 2\Gamma_2^1 + 2\Gamma_3^1 + 1\Gamma_4^1$.

IR	BV	Point Group	Shubnikov Group
Γ_1	$\boldsymbol{\psi}_1$	2/m	N/A
Γ_3	$\boldsymbol{\psi}_2$	2/m	N/A
	$\boldsymbol{\psi}_3$	-1	N/A

Table 4: The point symmetry and Shubnikov space group for the space group I m m m with $\mathbf{k}_{14} = (.5,\ 0,\ .5)$.The decomposition of the magnetic representation for the Ni site $(0,\ 0,\ 0)$ is $\Gamma_{Mag} = 1\Gamma_1^1 + 0\Gamma_2^1 + 2\Gamma_3^1 + 0\Gamma_4^1$.

2 Application of the Landau Theory

For a second-order transition a powerful simplification to the number of possible structures arises as a consequence of the Landau theory: the ordering transition can involve *only* one IR becoming critical. Accordingly, the basis vectors[1] involved in the resulting structure are limited to those associated with a single IR and the number of "symmetry-allowed" magnetic structures possible for a particular crystallographic site is simply the number of nonzero IRs in the decomposition of its magnetic representation. The number of degrees of freedom to be refined at any one time is then simply the number of basis vectors associated with the IR under study.

Remark: the application to Landau Theory to a given system will depend on the number of crystallographic sites and the the number of phase transitions involved. The reader is encouraged to read the account given in Ref. [9] for further information.

3 Acknowledgments and copyright

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[10] While the *Jones faithful representations* conventionally correspond to the vector formed from the operation of the rotation part of the element, R, on the site coordinates $(x,\ y,\ z)$, here we use it to demonstrate the effect of the complete symmetry operator, g.

A Elements in the group $\mathbf{G}_0$

Element g_n	Rotation matrix R	IT notation $g_n = \{R \mid \boldsymbol{\tau}\ \}$	Kovalev notation $g_n = \{h_n \mid \boldsymbol{\tau}\ \}$	Jones symbol
g_1	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\{E\mid 0\ 0\ 0\}$	$\{h_1 \mid\ 0\ 0\ 0\}$	x, y, z
g_2	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\{C_{2z}\mid 0\ 0\ 0\}$	$\{h_4 \mid\ 0\ 0\ 0\}$	$-x, -y, z$
g_3	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\{C_{2y}\mid 0\ 0\ 0\}$	$\{h_3 \mid\ 0\ 0\ 0\}$	$-x, y, -z$
g_4	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\{C_{2x}\mid 0\ 0\ 0\}$	$\{h_2 \mid\ 0\ 0\ 0\}$	$x, -y, -z$
g_5	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\{I\mid 0\ 0\ 0\}$	$\{h_{25} \mid\ 0\ 0\ 0\}$	$-x, -y, -z$
g_6	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\{\sigma_z\mid 0\ 0\ 0\}$	$\{h_{28} \mid\ 0\ 0\ 0\}$	$x, y, -z$
g_7	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\{\sigma_y\mid 0\ 0\ 0\}$	$\{h_{27} \mid\ 0\ 0\ 0\}$	$x, -y, z$
g_8	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\{\sigma_x\mid 0\ 0\ 0\}$	$\{h_{26} \mid\ 0\ 0\ 0\}$	$-x, y, z$

Table 5: Symmetry operators of the space group I m m m. The notations used are of the International Tables, where the elements are separated into rotation[3] and translation components, and the *Jones faithful representations*[10].

B Elements in the group $\mathbf{G}_k$

Element g_n	Rotation matrix R	IT notation $g_n = \{R \mid \boldsymbol{\tau}\ \}$	Kovalev notation $g_n = \{h_n \mid \boldsymbol{\tau}\ \}$	Jones symbol
g_1	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\{E\mid 0\ 0\ 0\}$	$\{h_1 \mid\ 0\ 0\ 0\}$	x, y, z
g_3	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\{C_{2y}\mid 0\ 0\ 0\}$	$\{h_3 \mid\ 0\ 0\ 0\}$	$-x, y, -z$
g_5	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\{I\mid 0\ 0\ 0\}$	$\{h_{25} \mid\ 0\ 0\ 0\}$	$-x, -y, -z$
g_7	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\{\sigma_y\mid 0\ 0\ 0\}$	$\{h_{27} \mid\ 0\ 0\ 0\}$	$x, -y, z$

Table 6: Symmetry elements of the little group $G_{\mathbf{k}}$. The notations used are of the International Tables, where the elements are separated into rotation[3] and translation components, and the *Jones faithful representations*[10].