Representational analysis of magnetic structures

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New Trends in Magnetic Structure Determination
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Applications of Representation Analysis

Molecular vibrations
Hybridized and molecular orbitals
Crystal-field splitting
Electronic-transition selection rules
Crystal band structure
Landau theory of phase transitions
Parameterize crystal distortions

magnetic

displacive

occupational

lattice strain
Group representations

Discovered by Ferdinand Frobenius (Germany, 1897).

Representations map group elements onto matrices that obey the same multiplication table as the group.

\[ 2_x 2_y = 2_z \quad \rightarrow \quad \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \]
Irreducible representations (irreps)

\[ R1: \quad 1 \rightarrow (1) \quad 2_x \rightarrow (\overline{1}) \quad 2_y \rightarrow (1) \quad 2_z \rightarrow (\overline{1}) \]

\[ R2: \quad 1 \rightarrow (1) \quad 2_x \rightarrow (1) \quad 2_y \rightarrow (\overline{1}) \quad 2_z \rightarrow (\overline{1}) \]

\[ R3: \quad 1 \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad 2_x \rightarrow \begin{pmatrix} \overline{1} \\ 0 \end{pmatrix} \quad 2_y \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad 2_z \rightarrow \begin{pmatrix} \overline{1} \\ 0 \end{pmatrix} \]

*Reducible representation:*  
\[ R3 = R1 \oplus R2 = \begin{pmatrix} R1 & 0 \\ 0 & R2 \end{pmatrix} \]

*Irreducible* representations can’t be separated into smaller pieces!

Irreps are **recipes for symmetry breaking**!
Irreps provide a symmetry-based coordinate system (parameter set) for describing deviations from symmetry.

Orthogonality and completeness relations (1904-07)

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2_x</th>
<th>2_y</th>
<th>2_z</th>
</tr>
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<tbody>
<tr>
<td>( \Gamma_1 )</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \Gamma_2 )</td>
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<td>( \Gamma_3 )</td>
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<td>( \Gamma_4 )</td>
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Irrep basis function

Irrep mode

Order parameter component

Symmetry-adapted basis function

Symmetry mode

Distortion modes (too vague)

Normal modes (superposition of modes of same irrep)
Familiar symmetry modes

Action of point group = 222 on \( p_y \) orbital

Under the group operations, a \( p_y \) orbital transforms like which irrep?

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</table>

\( p_z \) \( p_x \) \( p_y \)
Familiar symmetry modes

Action of point group = 222 on \(d_{yz}\) orbital

Under the group operations, a \(d_{yz}\) orbital transforms like which irrep?

<table>
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<tr>
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| \(d_{x^2-y^2}, d_{z^2}\) |
|\(p_z, d_{xy}\) |
|\(p_x, d_{yz}\) |
|\(p_y, d_{xz}\) |
Irreps of the symmetry group of a sphere: O(3)

Irreps of the translational group of a periodic signal

Spherical harmonics!

Familiar symmetry modes

\[ l = 0 \]
\[ l = 1 \]
\[ l = 2 \]
\[ l = 3 \]
Multiply the matrix of an unprimed operator by \(-1\) to obtain the matrix of the corresponding primed operator.
Irrep $mM_5$ of $P4mm1'$

2D magnetic irrep

$4_z^-$ is a $90^\circ$ CW rotation

$$4_z^- = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad mM_5(4_z^-) = \begin{pmatrix} 0 & \bar{1} \\ 1 & 0 \end{pmatrix}$$

In 3D real space:

$$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} y \\ \bar{x} \\ z \end{pmatrix}$$

In 2D carrier space:

$$\begin{pmatrix} 0 & \bar{1} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \bar{B} \\ A \end{pmatrix}$$
$\text{Irrep } mM_5 \text{ of } P4mm1'$

2D magnetic irrep

$$
\begin{align*}
1' \\
2'_z \\
t_z \\
m_{xy} \\
m'_{xy} \\
m_{\bar{x}y} \\
m_{x} \\
m_{y} \\
m_{4^+_z} \\
m_{4^-_z} \\
m'_{4^+_z} \\
m'_{4^-_z} \\
m_{x} \\
m_{y}'
\end{align*}
$$

$\begin{align*}
\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & \bar{1} \end{pmatrix} & \begin{pmatrix} \bar{1} & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ \bar{1} & 0 \end{pmatrix} & \begin{pmatrix} 0 & \bar{1} \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \bar{1} \\ \bar{1} & 0 \end{pmatrix}
\end{align*}$
Distortion space

For a given subgroup symmetry and cell size, the collection of all variable structural parameters spans a vector space that contains all possible distortions.

$P4mm1'$

parent

$2 \times 2$ supercell

4 unique atoms in supercell $\rightarrow$ 8 structural parameters in the $xy$ plane
Symmetry modes yield an orthogonal basis for distortion space.

$k = (0,0,0)\quad m\Gamma_5(a,b)\quad P2'$

$k = (1/2,0,0)\quad mM_5(a,b)\quad P_{a2}$

$k = (1/2,0,0)\quad mX_3(a,b)\quad P_{cmm2}$

$k = (1/2,0,0)\quad mX_4(a,b)\quad P_{cba2}$

Symmetry modes yield an orthogonal basis for distortion space.
Symmetry modes yield an orthogonal basis for distortion space.

\( k = (0,0,0) \)
\( m\Gamma_5(a,b) \)
\( P2' \)

\( k = (1/2, 1/2, 0) \)
\( mM_5(a,b) \)
\( Pa2 \)

\( k = (1/2, 0, 0) \)
\( mX_3(a,b) \)
\( Pcm2 \)

\( k = (1/2, 0, 0) \)
\( mX_4(a,b) \)
\( Pcba2 \)

Symmetry modes yield an orthogonal basis for distortion space.
La$_2$CoRuO$_6$

Displacive
\[ [1/2, 1/2, 0]M_3^+ \]
\[ [1/2, 0, 0]X_5^+ \]
\[ [1/4, 1/4, 1/4]R_4^+ \]

Site order (Co/Ru)
\[ [1/2, 1/2, 1/2]R_4^+ \]

Magnetic (Co)
\[ [1/4, 1/4, 1/4]mA_3 \]

Non-magnetic case: WO$_3$

Symmetry relationships

Phase transitions

Irreps/OPDs

Describe the structures of each of the phases with a common parameter set. Demonstrates generality.
• One mode can affect many symmetry-distinct atoms. One atom can be affected by many modes.

• Symmetry-modes span the same configurational space as traditional coordinates if all relevant \( k \)-points, irreps, and OPD components are considered simultaneously. Number of free variables is conserved!

• The relationship between traditional and symmetry-mode coordinate systems is linear! Related by a square numerical invertible matrix derived from group representation theory.

• Symmetry modes often provide the more natural/efficient basis. Even complicated magnetic structures are often described by the modes of a single irrep!
A recipe for symmetry breaking

Example: $mM_5$ irrep of $P4mm1'$

\[
\begin{pmatrix}
1 \\
2'_z \\
t_z \\
m_{xy'} \\
m_{\bar{xy}}' \\
m_{xy} \\
\bar{m}_{xy} \\
t_x, t_y \\
m_{x'} \\
m_y' \\
4^+_z \\
4^-_z \\
4^+_z \\
m_x \\
m_y \\
\end{pmatrix}
\]

\[
G = \begin{pmatrix}
1 & 0 \\
0 & 1 \\
0 & 0 \\
1 & 0 \\
0 & 1 \\
0 & 1 \\
0 & 0 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
\end{pmatrix}
\]

Find the group elements whose matrices leave some vector invariant.

\[
\begin{pmatrix}
a \\
b \\
\end{pmatrix} \Rightarrow \{g_1, g_2\} \quad \begin{pmatrix}
a \\
0 \\
\end{pmatrix} \Rightarrow \{g_1, g_5\} \quad \begin{pmatrix}
a \\
b \\
\end{pmatrix} \Rightarrow \{g_1\}
\]

$P_cma2$  $C_\alpha mm2$  $P_\alpha 2$

The vector used is called the order parameter direction or OPD. The resulting symmetry is called an isotropy subgroup of the parent.
A recipe for symmetry breaking

Example: \( m\Gamma_5 \) irrep of \( P4mm1' \)

\[
\begin{bmatrix}
1 \\
2' \\
t_x, t_y, t_z \\
m_x' \\
m_y \\
m_y' \\
m_x \\
m_x' \\
1' \\
m_{xy}' \\
m_{xy} \\
m_{xy}' \\
4^+ \\
4^- \\
4^+ ' \\
4^- \\
m_{xy} \\
m_{xy}' \\
g_1 \\
g_2 \\
g_3 \\
g_4 \\
g_5 \\
g_6 \\
g_7 \\
g_8
\end{bmatrix}
\]

\[
G = \begin{pmatrix}
1 & 0 \\
0 & 1 \\
\bar{1} & 0 \\
0 & \bar{1} \\
\bar{1} & 0 \\
0 & \bar{1} \\
1 & 0 \\
\bar{1} & 0
\end{pmatrix}
\]

Find the group elements whose matrices leave some vector invariant.

\[
\begin{pmatrix}
a \\
0
\end{pmatrix} \Rightarrow \{ g_1, g_2 \} \\
\begin{pmatrix}
2'
\end{pmatrix} \Rightarrow \{ g_1, g_5 \} \\
\begin{pmatrix}
a \\
b
\end{pmatrix} \Rightarrow \{ g_1 \} \\
Pm'm2' \\
Cm'm2' \\
P2'
\]

The vector used is called the order parameter direction or OPD.
The resulting symmetry is called an isotropy subgroup of the parent.
$m \Gamma_4^+$ irrep of $Pm\bar{3}m1'$

Order Parameter Directions

- $Pm\bar{3}m1'$
- $(a,0,0)$
- $(a,a,0)$
- $(a,a,a)$
- $(a,b,0)$
- $(a,a,b)$

5 epikernels

kernal = $(a,b,c)$
Each SG irrep defined at a specific $k$ vector

Cell doubling along $a$ axis: $\rightarrow (\frac{1}{2},0,0)$

Distinct $k$ in the Brillouin zone have distinct irreps (matrices depend on $k$). But two distinct $k$ separated by a reciprocal-lattice vector are equivalent (have identical irreps). Just consider 1$\text{st}$ Brillouin zone.
k-vector labels (Miller & Love)

- Primitive Cubic
- Face-Centered Cubic
- Body-Centered Cubic
- Primitive Tetragonal
- Face-Centered Ortho
- Rhombohedral
Miller & Love vs Kovalev symbols

primitive cubic

\[ \begin{align*}
\text{GM, } k12 & \ (0,0,0) \\
R, \ k13 & \ (1/2,1/2,1/2) \\
X, \ k10 & \ (0,1/2,0) \\
M, \ k11 & \ (1/2,1/2,0)
\end{align*} \]
The star of a $k$-vector

Full set of inequivalent $k$ vectors related by symmetry

\[
\begin{align*}
(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) & \quad (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \\
(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) & \quad (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \\
(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) & \quad (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \\
(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) & \quad (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})
\end{align*}
\]

\[
\begin{align*}
(1,0,0) & \quad (\bar{1}, 0, 0) \\
(0,1,0) & \quad (0, \bar{1}, 0) \\
(0,0,1) & \quad (0,0, \bar{1})
\end{align*}
\]

$[1\bar{1}0]_{fcc}$
The star of a $k$-vector

Full set of inequivalent $k$ vectors related by symmetry

\[
\begin{align*}
(1/2, 1/2, 1/2) \\
(1/2, -1/2, 1/2) \\
(1/2, 1/2, 1/2) \\
(-1/2, 1/2, 1/2)
\end{align*}
\]

\[
(1/2, 1/2, 1/2) - (1/2, 1/2, 1/2) = (1,1,1)_{\text{fcc}}
\]

\[
\begin{align*}
(1,0,0) \\
(0,1,0) \\
(0,0,1)
\end{align*}
\]

\[
(1,0,0) - (-1,0,0) = (2,0,0)_{\text{fcc}}
\]

$[110]_{\text{fcc}}$
Complete (full-star) space-group irreps

$mX_4(a, b)$ \hspace{2cm} \mathbf{k} = (\frac{1}{2}, 0, 0), (0, \frac{1}{2}, 0) \hspace{2cm} P_Cba2$

Here, the two irrep dimensions correspond to the k-vectors of the star.
Selecting an isotropy subgroup

parent space-group symmetry

\[ k \text{-star} \]
finite number of types (e.g. \( \Gamma, \Delta, X \)), but \( \infty \) number of points

\[ \text{irrep} \]
finite number for each \( k \)-star (e.g. \( X_1^+, X_3^+, X_5^- \))

order-parameter direction (OPD)
finite number for each irrep; special points/lines/planes in abstract carrier space

isotropy subgroup
[1] space-group or superspace-group type
[2] supercell basis (relative to parent)
[3] origin of supercell (relative to parent).
Same SG type but different bases

Importance of basis is common knowledge.
Two distinct cases with same basis = \{(2,0,0),(0,2,0),(0,0,1)\}

Different supercell origins often result in entirely different isotropy subgroups -- not common knowledge!

origin: \((0,0,0)\)
origin: \((\frac{1}{2},0,0)\)
The k-SUBGROUPSMAG program of the Bilbao Crystallographic Server calculates the kernel and the epikernels of an irrep and presents them in graphical format. The k-maximal subgroups correspond to the simple OPDs (i.e. OPDs with a single variable). The lower epikernels correspond to more complicated OPDs that are superpositions of simple OPDs.

The kernel arises from the most general OPD, and includes all of the freedoms of all of the simple OPDs.

Subgroup listing from k-SUBGROUPSMAG

Subgroup listing from ISODISTORT (includes OPD, group number, basis, and origin):

- P1 (a,0,0) 123.345 P4/mm/m', basis={0,1,0),(0,0,1),(1,0,0)}, origin=(0,0,0), s=1, i=6, k-active= (0,0,0)
- P2 (a,a,0) 65.486 Cmm/m', basis={{1,1,0},(-1,1,0),(0,0,1)}, origin=(0,0,0), s=1, i=12, k-active= (0,0,0)
- P3 (a,a,a) 166.101 R-3m', basis={(-1,0,1),(0,1,-1),(1,-1,-1)}, origin=(0,0,0), s=1, i=8, k-active= (0,0,0)
- C1 (a,b,0) 10.46 P2'/m', basis={(-1,0,0),(0,0,1),(0,1,0)}, origin=(0,0,0), s=1, i=24, k-active= (0,0,0)
- C2 (a,a,b) 12.62 C2'/m', basis={{1,1,0},(-1,1,0),(0,0,1)}, origin=(0,0,0), s=1, i=24, k-active= (0,0,0)
- S1 (a,b,c) 2.4 P-1, basis={{0,0,1),(0,1,0),(-1,0,0)}, origin=(0,0,0), s=1, i=48, k-active= (0,0,0)
Complete space-group irreps
(at any commensurate \( k \) point)
ISO-IR, Stokes & Campbell (2014)
Tabulated – not real-time

Complete space-group irreps
(any commensurate or incommensurate \( k \))
real-time calculations

Analogy: integers \( \rightarrow \) rational numbers \( \rightarrow \) real numbers

Little-\( k \) group irreps
Faddeyev; Kovalev; Zak, Casher, Glück & Gur; Bradley, Cracknell, Davies, Miller, Love (1964-1979)

Complete space-group irreps
at special-\( k \) points
Simultaneous action of entire \( k \) star.
8 cases worked \textit{manually} (1968-1984).

all 4777 space groups irreps at special \( k \);
15239 isotropy subgroups [green book].

Space-group irrep calculations

reciprocal space
(0 0 1)

(\( \frac{1}{2} \frac{1}{2} 0 \))

(\( \frac{1}{4} \frac{3}{4} 0 \))

(1 0 0)

(\( \alpha 0 0 \))

Analogy:
integers \( \rightarrow \) rational numbers \( \rightarrow \) real numbers
Cycloidal magnetic structure. The transverse $m\Sigma_2$ and longitudinal $m\Sigma_3$ order parameters are superposed 90° out of phase.

This combination breaks the inversion symmetry and can therefore couple to ferroelectric $\Gamma_4^+$ irrep, making it a multi-ferroic material.

Major historical controversy unnecessary. Just consider the whole $k$-star ($\pm k$) to get the symmetry and physical properties right!
Incommensurate example: Skyrmion lattice

In this image, we used $\alpha \approx 0.11$

The lattice of clockwise magnetic whirlpools.

$$m\Lambda_1(a, 0, a, 0, a, 0)$$

of $P6mm1'$

$$k_1 = (2\alpha, -\alpha, 0)$$

$$k_2 = (-\alpha, 2\alpha, 0)$$

$$k_3 = (-\alpha, -\alpha, 0)$$

$$k_3 = -(k_1 + k_2)$$
Irreps vs Pirreps

\[ \Gamma(g) \eta = \eta \quad \Gamma(g) = a + ib \quad \eta = \eta_R + i\eta_I \]

\[ \Gamma_P(g) = \begin{pmatrix} \Gamma(g) & 0 \\ 0 & \Gamma^*(g) \end{pmatrix} \]

\[ \eta_P = \begin{pmatrix} \eta \\ \eta^* \end{pmatrix} \]

\[ \Gamma_P(g) \eta_P = \begin{pmatrix} \Gamma(g) & 0 \\ 0 & \Gamma^*(g) \end{pmatrix} \begin{pmatrix} \eta \\ \eta^* \end{pmatrix} = \begin{pmatrix} \Gamma(g) \eta \\ \Gamma(g)^* \eta^* \end{pmatrix} = \begin{pmatrix} \eta \\ \eta^* \end{pmatrix} = \eta_P \]

Bring to real form via similarity transform with \( S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \)

\[ \Gamma_P'(g) = S \Gamma_P(g) S^{-1} = \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \quad \eta_P' = S \eta_P = \sqrt{2} \begin{pmatrix} \eta_R \\ \eta_I \end{pmatrix} \]

\[ \Gamma_P'(g) \eta_P' = \eta_P' \]

A physically-irreducible representation (pirrep) can always be brought to real form, and has order parameters equivalent to those of complex irrep.
Complex irrep dimension = \( d e n_k \)

Pirrep dimension = \( d e n_k t \)

\( de = \) number of arms in the star of \( k \)

\( d = \) number of arm-pairs in the star of \( \{k, -k\} \)

\( e = \frac{(de)}{d} = 1 \) or \( 2 \)

\( n_k = \) dimension of the little group of \( k \)

\( t = 1 \) (real: type 1) or \( 2 \) (complex: type 2 or 3)
Irrep analysis depends on parent origin

Example: cubic perovskite ($Pm\bar{3}m$)

Mn at $a(0,0,0)$

Mn at $b(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

origin shift
Magnetic modes (single-\(k\) point)

MODY (W. Sikora, F. Bialas, L. Pytlik, 1992)
- Treats scalar, vector, axial vector and higher-order tensor OPs.

SARAh (A. Wills)
- Interfaced to GSAS and Fullprof for magnetic modes (2001).
- Global-search algorithm explores all modes of all irreps at one \(k\) vector.

BASIREPS (J. Rodriguez-Carvajal, 2003)
- Integrated within Fullprof for magnetic & displacive refinements.

Applications were primarily for magnetic cases because many magnetic structures can be described with a single sinusoidal magnetic wave. This proved not to be the case with other types of order parameters.
General OP types, full $k$ star, multi-$k$

ISOTROPY (Stokes, Hatch, 1998)
- Project strain, displacive, or magnetic symmetry modes
- Full $k$ star at special and non-special commensurate $k$ points

ISODISTORT (Stokes, Campbell, Hatch, 2005)
- Simultaneous mode parameterization of an entire structure
- General full-$k$-star, multi-$k$, multi-irrep, multi-OP distortions
- Filtered search, interactive visualization, crystallographic I/O
- Automated mode decomposition (2006)
- Full use of space-group symmetry (or superspace symmetry 2014)

REPRES/AMPLIMODES (Bilbao Cryst. Server team, 2006/2009)
- Full-$k$-star, multi-$k$, multi-irrep displacive decompositions

JANA (V. Petricek, M. Dusek, L. Palatinus, 2011)
- Integrated calculation of displacive and magnetic modes.
- Allows refinements involving entire $k$ star.
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Juan Rodriguez-Carvajal (FULLPROF)
Institut Laue-Langevin, France