

Overview of magnetic structures (Irreps vs MSG and spinSG) – Part 1

Andrew S. Wills

Duke University (19–24 July 2026)



Department of Chemistry
Faculty of Mathematical and Physical Sciences



Magnetic structures – What they are, and how that changed

Andrew S. Wills

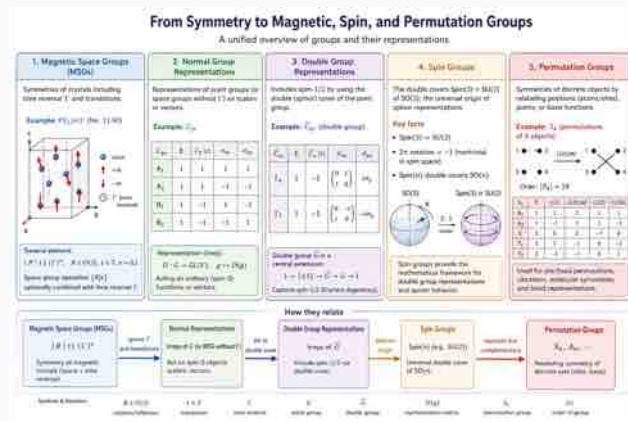
Duke University (19–24 July 2026)



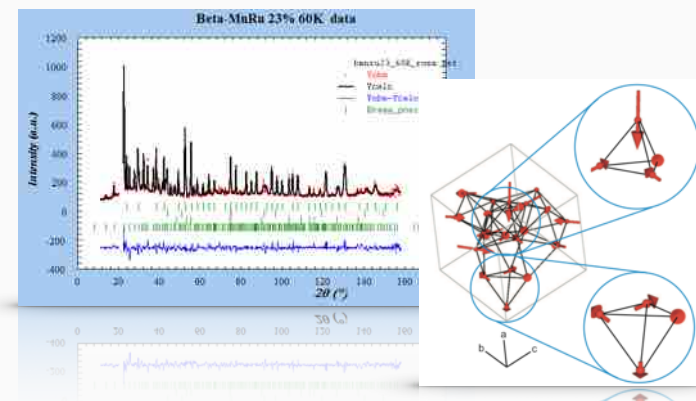
Department of Chemistry
Faculty of Mathematical and Physical Sciences



Magnetic space groups, normal group representations, double group representations, spin groups and permutation groups



Complex incommensurate magnetic ordering, e.g. $\text{B-Mn}_{1-x}\text{Ru}_x$ ($x=0.12$)



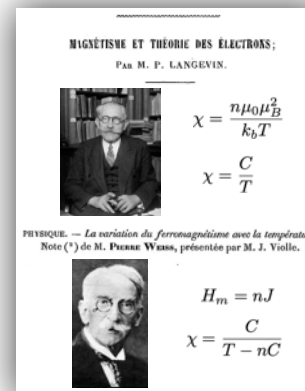
Some background theories and some of the people



There is a lot of history. It can create confusion and inconsistencies...

1927 Wigner, Heisenberg, Hunds, Heitler – **Quantum mechanics exchange coupling**
 1930 Heesch – **Antisymmetry**
 1931 Wigner – **Antiuunitary symmetry** (quantum theory)
 1937 Landau, Dzyaloshinski – **Phase transitions**
 1953, 55, 57. – Shubnikov, Zamorzaev Belov – **B+W groups**
 1958, Dzyaloshinski, 1960 Moriya – **Antisymmetric exchange**
 1959 Villain and Kaplan – **Eigenvectors, eigenvalues** – minimum energy spin arrangement
 1959 Yoshimori – **Incommensurate magnetic structures** (theory)
 1959 Wigner – **Antiuunitary theory** – corepresentations
 1962 Bertaut – **Exchange interactions and Hamiltonians**
 1964 Kovalev – **Representation theory**
 1963 Dimmock – **Group theory of phase transitions**
 1966 Brinkman and Elliot **Spin space groups**
 1968 Bertaut – **Representation theory**
 1979 Izyumov – **Exchange multiplets**
 1981 Jaric; 1984 Stokes and Hatch – **Isotropy subgroups**
 2001 Sikora – **Quadrupoles in magnetic structures**
 1980 Janner and Janssen – **Magnetic superspace groups** (1-D modulation)
 2022 Šmejkal, Sinova, Jungwirth – **Altermagnetism**

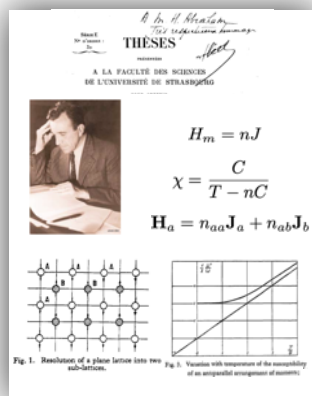
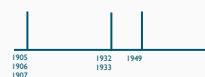
Diamagnetism, Paramagnetism, Ferromagnetism



P. Langevin, Ann. de Chim. et de Phys. 5, 70 (1905)
 Electronic theory of diamagnetism
 Kinetic theory of paramagnetism, explaining Curie law

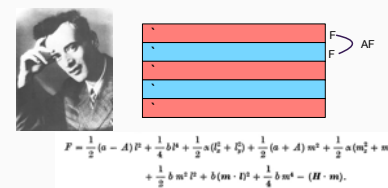
P. Weiss, C. R. Ac. Sc. 143 1137 (1906); J. Phys. 6, 666 (1907)
 Interactions between moments
 'Molecular field' (fictitious, uniform)
 Spontaneous magnetisation
 Ferromagnets
 Curie-Weiss law

Negative molecular field



L. Néel, Ann. de Phys. 17, 5 (1932). C.R. Acad. Sci. Paris, 203, 304 (1936)
 Negative local molecular field
 ➡ Antiparallel arrangement of sublattices
 ➡ Transition temperature T_N
Magneto-crystalline coupling
 – Moments have preferred directions
 'Imperfect antiferromagnetism'

Negative molecular field



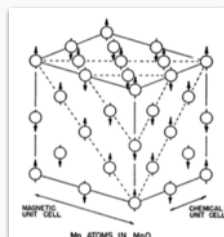
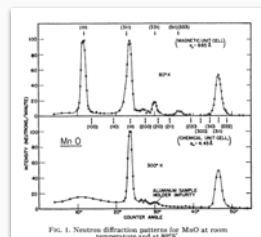
L.D. Landau, Phys. Z. Sowjet 4, 675 (1933).
 Layered material
 Positive interactions within layer, negative between

Anatole Abragam on Landau

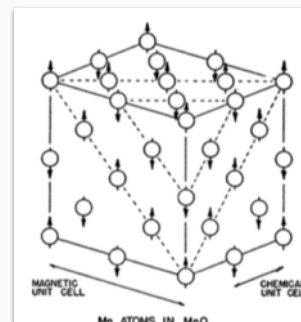
Landau did think of a model for anti ferromagnetism but rejected it because he found that it disagreed with the requirements of quantum mechanics. Neel, who did not care much about the requirements of quantum mechanics - which he probably did not even know - went ahead and published his model, and extrapolated the consequences. Some compromises with the requirements of quantum mechanics were later found, having turned out to be a little less inflexible than was thought. It is a danger to be too learned, or 'Sancta Simplicitas'.

Magnetic structure determination and analysis – *Theory and Software*

Challenges – how do we describe magnetic structures, and how do we determine them?



Foundations – pillars



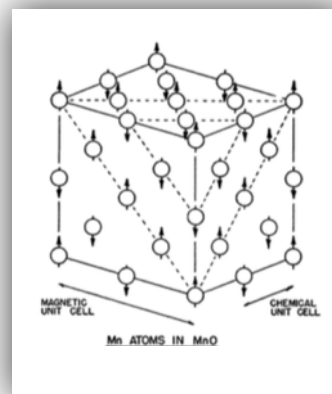
1927 Wigner, Heisenberg, Hunds, Heitler – Quantum mechanics
exchange coupling
 1930 Heesch – **Antisymmetry**
 1931 Wigner – **Antiunitary symmetry** (quantum theory)
 1937 Landau, Dzyaloshinski – **Phase transitions**
 1953, 55, 57, – Shubnikov, Zamorzaev Belov – **B+W groups**
 1958, Dzyaloshinski, 1960 Moriya – **Antisymmetric exchange**
 1959 Villain and Kaplan – **Eigenvectors, eigenvalues** – minimum energy spin arrangement
 1959 Yoshimori – **Incommensurate magnetic structures** (theory)
 1959 Wigner – **Antiunitary theory** – corepresentations
 1962 Bertaut – **Exchange interactions and Hamiltonians**
 1964 Kovalev – **Representation theory**
 1963 Dimmock – **Group theory of phase transitions**
 1966 Brinkman and Elliot **Spin space groups**
 1968 Bertaut – **Representation theory**
 1979 Izyumov – **Exchange multiplets**
 1981 Jaric; 1984 Stokes and Hatch – **Isotropy subgroups**
 2001 Sikora – **Quadrupoles in magnetic structures**
 1980 Janner and Janssen – **Magnetic superspace groups** (1-D modulation)
 2022 Šmejkal, Sinova, Jungwirth – **Altermagnetism**

Foundations – pillars



1927 Wigner, Heisenberg, Hunds, Heitler – Quantum mechanics
exchange coupling
 1930 Heesch – **Antisymmetry**
 1931 Wigner – **Antiunitary symmetry** (quantum theory)
 1937 Landau, Dzyaloshinski – **Phase transitions**
 1953, 55, 57, – Shubnikov, Zamorzaev Belov – **B+W groups**
 1958, Dzyaloshinski, 1960 Moriya – **Antisymmetric exchange**
 1959 Villain and Kaplan – **Eigenvectors, eigenvalues** – minimum energy spin arrangement
 1959 Yoshimori – **Incommensurate magnetic structures** (theory)
 1959 Wigner – **Antiunitary theory** – corepresentations
 1962 Bertaut – **Exchange interactions and Hamiltonians**
 1964 Kovalev – **Representation theory**
 1963 Dimmock – **Group theory of phase transitions**
 1966 Brinkman and Elliot **Spin space groups**
 1968 Bertaut – **Representation theory**
 1979 Izyumov – **Exchange multiplets**
 1981 Jaric; 1984 Stokes and Hatch – **Isotropy subgroups**
 2001 Sikora – **Quadrupoles in magnetic structures**
 1980 Janner and Janssen – **Magnetic superspace groups** (1-D modulation)
 2022 Šmejkal, Sinova, Jungwirth – **Altermagnetism**

The first challenge



How to describe a magnetic structure?

- Its symmetry
- Its translation properties
- Its physical properties
- Its Hamiltonian

Extensions to symmetry



- H. Heesch**, Z. Kristallogr. 73, 325 (1930)
Multidimensional generalisation of classical groups with **antisymmetry**
32 → 122 (dichromatic point groups)
- A. V. Shubnikov**, *Symmetry and antisymmetry of finite figures* (in Russian). Moscow: (1951)
Reintroduces antisymmetry, 4D groups
Describes and illustrates the dichromatic point groups.
Explains uses
- A. M. Zamorzaev**, Ph.D. (1953); Kristallografiya, 2, 15. (1957);
Sov. Phys. Crystallogr. 2, 10 (1957)
Derives the 1651 dichromatic space groups
Listed by Belov, Neronova and Smirnova (1955)

Extensions to symmetry



'A mathematician constructs the science of symmetry without use of a figure. A crystallographer thinks this approach to be either useless or even senseless.'

Shubnikov

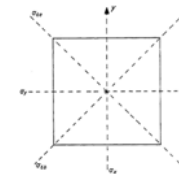
- H. Heesch**, Z. Kristallogr. 73, 325 (1930)
Multidimensional generalisation of classical groups with **antisymmetry**
32 → 122 (dichromatic point groups)
- A. V. Shubnikov**, *Symmetry and antisymmetry of finite figures* (in Russian). Moscow: (1951)
Reintroduces antisymmetry, 4D groups
Describes and illustrates the dichromatic point groups.
Explains uses
- A. M. Zamorzaev**, Ph.D. (1953); Kristallografiya, 2, 15. (1957);
Sov. Phys. Crystallogr. 2, 10 (1957)
Derives the 1651 dichromatic space groups
Listed by Belov, Neronova and Smirnova (1955)

Extensions to symmetry



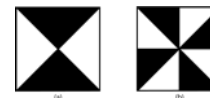
- H. Heesch**, Z. Kristallogr. 73, 325 (1930)
Multidimensional generalisation of classical groups with **antisymmetry**
32 → 122 (dichromatic point groups)
- A. V. Shubnikov**, *Symmetry and antisymmetry of finite figures* (in Russian). Moscow: (1951)
Reintroduces antisymmetry, 4D groups
Describes and illustrates the dichromatic point groups.
Explains uses
- A. M. Zamorzaev**, Ph.D. (1953); Kristallografiya, 2, 15. (1957);
Sov. Phys. Crystallogr. 2, 10 (1957)
Derives the 1651 dichromatic space groups
Listed by Belov, Neronova and Smirnova (1955)

Antiferromagnetic order



Symmetry operations of a square (4mm, C4v)

$$4mm = E, C_{4z}^+, C_{4z}^-, C_{2z}, \sigma_x, \sigma_y, \sigma_{da}, \sigma_{db}$$



Black and white squares to illustrate (a) 4'mm' and (b) 4m'm'

$$4'mm' = E, \theta C_{4z}^+, \theta C_{4z}^-, C_{2z}, \sigma_x, \sigma_y, \theta \sigma_{da}, \theta \sigma_{db}$$

$$4m'm' = E, C_{4z}^+, C_{4z}^-, C_{2z}, \theta \sigma_x, \theta \sigma_y, \theta \sigma_{da}, \theta \sigma_{db}$$

Antisymmetry operator, θ

Create compound symmetry operation, $\theta \{R|t\}$

(Type 1) - Colourless

Ordinary point group or space group (Type 1)

(Type 2) - Grey (paramagnetic)

Add θ to all symmetry operations in point group or space group

(Type 3) - Black and white

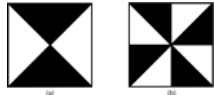
Replace half of the elements of ordinary point group or space group by their product with θ

The 58 black and white or magnetic point groups
The 1191 black and white space groups

Constructing B+W groups

	E	C_{2z}	C_{4z}	σ_x	σ_{yz}
		C_{4z}	σ_x	σ_{yz}	
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

Construction from character table for $4mm$, add to all operations of 1D real irreps with character -1



Black and white squares to illustrate (a) $4'mm'$ and (b) $4m'm'$
 $4'mm' = E, \theta C_{4z}^+, \theta C_{4z}^-, C_{2z}, \sigma_x, \sigma_y, \theta \sigma_{da}, \theta \sigma_{db}$
 $4m'm' = E, C_{4z}^+, C_{4z}^-, C_{2z}, \theta \sigma_x, \theta \sigma_y, \theta \sigma_{da}, \theta \sigma_{db}$

Antisymmetry operator, θ

Create compound symmetry operation, $\theta \{R|t\}$

(Type 1) - Colourless

Ordinary point group or space group (Type 1)

(Type 2) - Grey (paramagnetic)

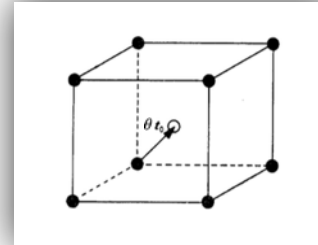
Add θ to all symmetry operations in point group or space group

(Type 3) - Black and white

Replace half of the elements of ordinary point group or space group by their product with θ
 The 58 black and white or magnetic point groups
 The 1191 black and white space groups



Constructing B+W groups



Antisymmetry operator, θ

Create compound symmetry operation, $\theta \{R|t\}$

(Type 1) - Colourless

Ordinary point group or space group (Type 1)

(Type 2) - Grey (paramagnetic)

Add θ to all symmetry operations in point group or space group

(Type 3) - Black and white

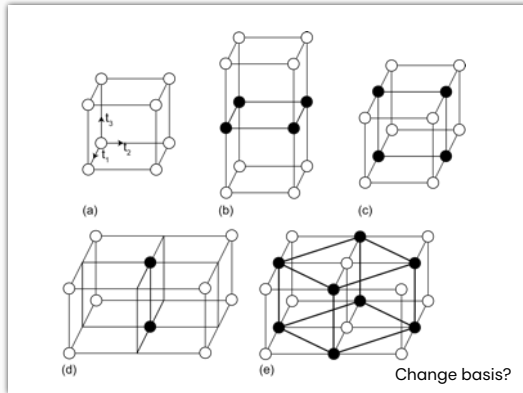
Replace half of the elements of ordinary point group or space group by their product with θ
 The 58 black and white or magnetic point groups
 The 1191 black and white space groups

(Type 3, 4) - Black and white

All operations of the space group
 All operations of the space group combined with and anti translation



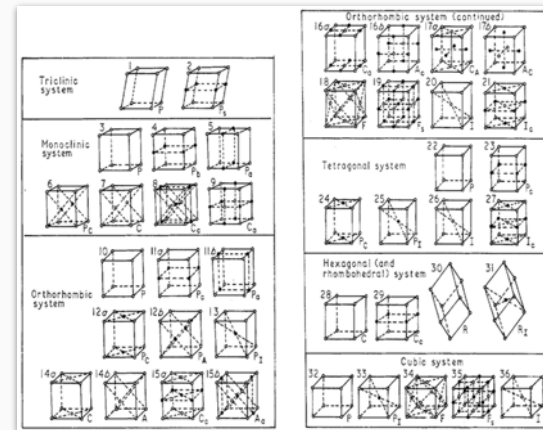
Applying antisymmetry to the Bravais lattices, examples



Change basis?



Extended Bravais lattices



Bravais lattices:

- 14 (ordinary)
- 22 (B+W)
- » 36

Space groups:

- 230 (Type 1)
- 230 (Type 2)
- 674 (Type 3)
- 517 (Type 4)
- » 1651



From the abstract to the applied...

Application of Shubnikov groups to magnetic structures – 'Magnetic Space Groups'

- The Shubnikov dichromatic (black and white) point and (Zamorzaev's 1953) space groups are general (abstract) constructs with an additional operation of colour change, such as to describe ferroelectricity
- The recent confirmation of antiparallel moments in magnetic structures (1949) caused rapid take-up
- Considering magnetic symmetry and introducing **time-reversal as a symmetry operation that reverses moment vectors (linear operator)** led Tavger and Zaitsev (1956) to derive point groups for magnetic order
- In 1962 Dimmock and Wheeler applied the group structure (half not primed / half primed) to the time / **time-reversal operation developed by Wigner (1931) – an antilinear operation**
 - ➡ Defining the primed operations as time-reversed formed the 'magnetic space groups' also called the 'space – time' groups, **M**

$$\mathbf{M} = \mathbf{H} + A\mathbf{H} \text{ where } A \text{ is time-reversal}^*$$

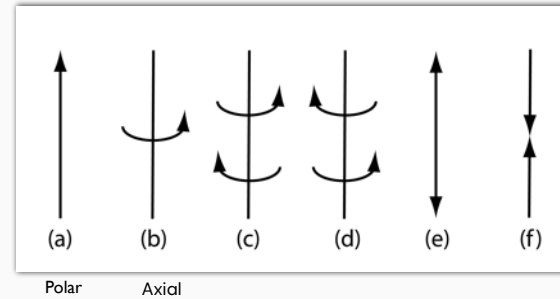
Eugene Wigner

$$\begin{aligned} H|\psi\rangle &= E|\psi\rangle \\ H(T|\psi\rangle) &= E(T|\psi\rangle) \\ T^2 &= -1 \\ \langle\psi|T|\psi\rangle &= 0 \\ T|\psi\rangle &= |\psi\rangle^* \end{aligned}$$



* time-reversal is a linear operation or an antilinear operation is important
B. A. Tavger and V. M. Zaitsev, Soviet Physics JETP 3, 430 (1956)

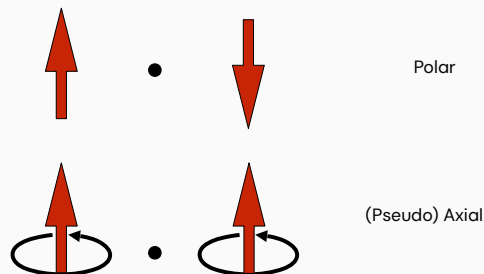
Magnetic structures also need the symmetry of magnetic moments



Polar vectors are reversed **by inversion operation**, axial vectors are not.



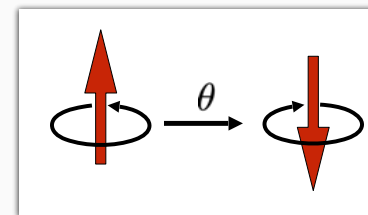
Symmetry of magnetic moments and polar vectors under improper rotations



Polar vectors are reversed **by inversion operation**, axial vectors are not.



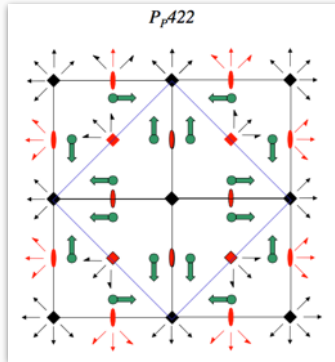
Landau, time reversal (θ), and quantum mechanics



- Time-reversal reverses moment directions.
 - Classical picture (Bohr-like electric currents)
 - Quantum mechanics?
 - Which antisymmetry operator should we use?
 - ➡ Complex conjugation



Magnetic space groups



Propagate
trial moment
orientations



Pictures for 1651 magnetic space groups
for the Wyckoff sites:

Daniel Litvin,
Acta Cryst. A57 729 (2001)
<http://www.bk.psu.edu/faculty/litvin/>

Extending groups – from 2 to 3 colours

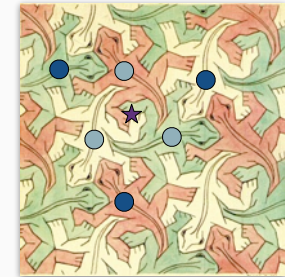
M.C. Escher

Lizard (No. 104) (1959)

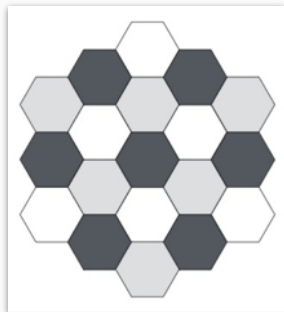
*Study of Regular Division of the Plane
with Reptiles (1939)*



- B-W change → 'time-reversal'
- Colour cycling – phase change



Polychromatic space groups, P-type



Extension 1) add more colours, e.g. 3-colour groups

- Now introduce a group of colour permutations
- Cyclic colour-change was added as an operation to some of the normal symmetry operations to form compound operations
- Colour-changing operation causes a cycling through a series of p-colours (p>2)



Belov, N. V. and Tarkhova, T.N. (1956). "Groups of colored symmetry." (In Russian.)
Kristallografiya, 1, 4–13.

Spin space groups (a.k.a. spin groups)



Kitz (1965),

Brinkman and Elliott (1966)

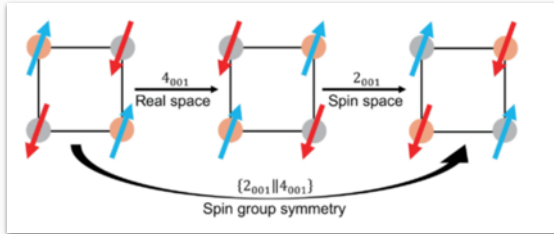
Opechowski and Dreyfus (1971)

Extension 2) separate spin and geometric operations
Spin space groups

- Symmetry operations are separated into ones that act on
 - the atomic positions (geometric space)
 - magnetic moments
- The group acting on magnetic moments can contain operations that are **not** in the group applied to atomic positions
 - Suited to **isotropic spins (low spin-orbit coupling limit)**
- **P-Type groups** are more restrictive as the colour change is tied to the space operation
 - Presence of spin-orbit coupling



Spin space groups / (spin groups)



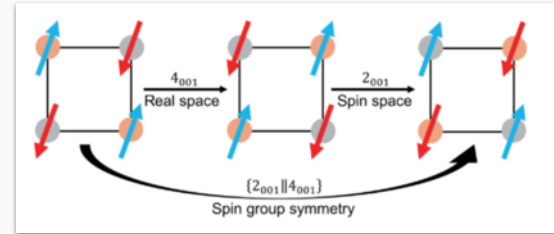
Schematic of a spin space group symmetry of an antiferromagnetic structure

- a fourfold rotation (4_{001}) in real space followed by
- a twofold rotation (2_{001}) in spin space returns the magnetic structure back to the initial configuration
- constituting a spin group symmetry $\{2_{001} || 4_{001}\}$

X. Chen, J. Ren et al, PhysRevX.14.031038 (2024)



Spin space groups / (spin groups)



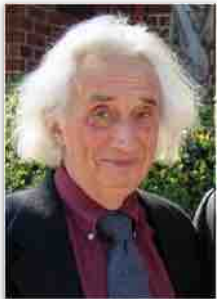
Schematic of a spin space group symmetry of an antiferromagnetic structure

- a fourfold rotation (4_{001}) in real space followed by
- a twofold rotation (2_{001}) in spin space returns the magnetic structure back to the initial configuration
- constituting a spin point group symmetry $\{2_{001} || 4_{001}\}$

X. Chen, J. Ren et al, Phys Rev X 14 031038 (2024)



Representation theory and magnetic structures



I. Dzyaloshinskii

- Ph.D. student of Landau.
- Major successes were the explanation of weak ferromagnetism in antiferromagnets and helical structures. Generalised by Tôru Moriya
- Pioneered the use of basis vectors from representation theory for the description of magnetic structures.
- Used irreducible representations of the **magnetic point groups/ magnetic class** to find the eigenfunctions and basis vectors of a phenomenological Hamiltonian, i.e. the magnetic structure.

I.E. Dzyaloshinskii (1957) Zh.Eksp. Teor. Fiz. **32**, 1547 (1957)
I.E. Dzyaloshinskii (1964) Zh.Eksp. Teor. Fiz. **46**, 1420 (1964)



“Representation analysis of magnetic structures” – the method of Bertaut



Acta Cryst. (1968), A24, 217

Representation Analysis of Magnetic Structures

By E. F. BERTAUT

Laboratoire d'Electronique et de Physique de Minéral C.N.R.S., B.P. 319 et
Laboratoire de Diffraction Neutronique, C.E.N.G., B.P. 205, Grenoble 38, France

Table 4. Representations and magnetic groups in $Pham$ ($k=0$)

Representations	Characters of the generators			Elements and anti-elements		Magnetic groups
	2_{1x}	2_{1y}	T	2_{1x}	2_{1y}	
Γ_1	1	1	1	2_{1x}	T	$Pham$
Γ_2	1	-1	1	2_{1y}	T	$Pha'm'$
Γ_3	-1	1	1	2_{1x}	T	$Ph'am'$
Γ_4	-1	-1	1	2_{1y}	T	$Ph'a'm'$
Γ_5	1	1	-1	2_{1x}	T	$Ph'am$
Γ_6	1	-1	-1	2_{1y}	T	$Ph'a'm$
Γ_7	-1	1	-1	2_{1x}	T	$Ph'a'm$
Γ_8	-1	-1	-1	2_{1y}	T	$Pham'$

E.F. Bertaut, Acta. Cryst. A24, 217 (1968)

- Applied k-vector (**focus**)
- Showed magnetic space groups could be constructed from character tables of the irreducible representations (of G_k)
- Used projection method to generate basis functions
- Fourier series

$$\vec{\psi}_{j,\nu}^k = \vec{\psi}_{i,\nu}^k e^{-2\pi i \vec{k} \cdot \vec{r}_{ij}}$$

$$\vec{m}_j = \sum_{\nu, \vec{k}} C_{\nu}^k \vec{\psi}_{i,\nu}^k e^{-2\pi i \vec{k} \cdot \vec{r}_{ij}}$$



“Representation analysis” of magnetic structures – commensurate and incommensurate

$$G_0 \xrightarrow{\vec{k}} G_{\vec{k}}$$

C_{4v}	E	C_{2v}	C_{2v}	σ_v	σ_v'	σ_v''
E	E	C_{2v}	C_{2v}	σ_v	σ_v'	σ_v''
C_{2v}	C_{2v}	E	σ_v	σ_v'	σ_v''	σ_v
C_{2v}	C_{2v}	E	σ_v	σ_v'	σ_v''	σ_v
σ_v	σ_v	σ_v''	σ_v'	E	C_{2v}	C_{2v}
σ_v'	σ_v'	σ_v	σ_v''	C_{2v}	E	C_{2v}
σ_v''	σ_v''	σ_v	σ_v'	C_{2v}	C_{2v}	E

“A set of matrices, each corresponding to a single operation in a group, that can be combined amongst themselves in a manner parallel to the group elements.” (Cotton, Chemical applications of group theory)

Refine using the mixing coefficients

$$\vec{m}_j = \sum_{\nu, \vec{k}} C_{\nu}^{\vec{k}} \vec{\psi}_{\nu, \vec{k}} e^{-2\pi i \vec{k} \cdot \vec{r}_j}$$

Projection of symmetry modes (basis vectors) associated with the Irreducible Representations (IRs)

Table 1
Irreducible representations of $R3c-C_{3h}$, $k = 0$ and $R3m-C_{3h}$, $k = 0$ and $k = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$

Symmetry operations	1	2	3	4	5	6
Representations	1	2	3	4	5	6
Γ_1	A_1	A_2	A_3	A_4	A_5	A_6
Γ_2	A_1	A_2	A_3	A_4	A_5	A_6
Γ_3	A_1	A_2	A_3	A_4	A_5	A_6

BASIS VECTOR COMPONENTS FOR EACH SITE OBTAINED BY CLASSICAL PROJECTION:
(NOTE THAT THESE ARE WITH RESPECT TO SPACE GROUP AXES)

IR # 1, BASIS VECTOR # 1 (ABSOLUTE NUMBER: 1)	1
ATOM 1	1
ATOM 2	1
ATOM 3	1
IR # 2, BASIS VECTOR # 1 (ABSOLUTE NUMBER: 2)	2
ATOM 1	2
ATOM 2	2
ATOM 3	2
IR # 3, BASIS VECTOR # 1 (ABSOLUTE NUMBER: 3)	3
ATOM 1	3
ATOM 2	3
ATOM 3	3
IR # 4, BASIS VECTOR # 1 (ABSOLUTE NUMBER: 4)	4
ATOM 1	4
ATOM 2	4
ATOM 3	4
IR # 5, BASIS VECTOR # 1 (ABSOLUTE NUMBER: 5)	5
ATOM 1	5
ATOM 2	5
ATOM 3	5
IR # 6, BASIS VECTOR # 1 (ABSOLUTE NUMBER: 6)	6
ATOM 1	6
ATOM 2	6
ATOM 3	6

Developments in representational analysis...

- Aside from Bertaut, general development of the representation theory of crystal and magnetic structures, including
 - Bradley, Cracknell, Altmann
 - Dimmock, Wheeler
 - Birman
 - Koster
 - Toledano
- Magnetism focussed
 - Kovalev
 - Best known for Irreducible Representations of the Space groups (1961, 1987, 1993)
 - A source of representations, corepresentations, induced representations and complete ‘full group’ irreducible representations
 - Pioneered and developed the application of space group representation and corepresentations to the symmetry of magnetic crystals, magnetic order and phase transitions, induced properties. (1964, 1965, 1970, 1975)
 - Izyumov
 - Exchange multiplets (1980) – invariance of the exchange Hamiltonian under the rotation of all spins
 - Links spin space groups and representational analysis
 - Basis vectors (1979)
 - Strong links with neutron scattering
 - Stokes, Hatch and Campbell
 - Merged representational theory basis vectors into Isotropy groups and MSGs

O.V. Kovalev, Sov. J. Low Temp. Phys. **1**, 749–750 (1975)

O.V. Kovalev and A.G. Gorbanyuk, J. Phys. Chem. Solids **31**, 149–161 (1970)

O.V. Kovalev, Sov. Physics – Solid State **5**, 2309 (1964)

O.V. Kovalev, Sov. Physics – Crystallography **9**, 665 (1965)

Yu. A. Izyumov, Journal of Magnetism and Magnetic Materials **15–18**, 497–498 (1980)

Yu. A. Izyumov and V.E. Naish, Journal of Magnetism and Magnetic Materials **12**, 239–248 (1979)

Yu. A. Izyumov, V.E. Naish and S. B. Petrov, Journal of Magnetism and Magnetic Materials **13**, 267–274 (1979)



Altermagnetism

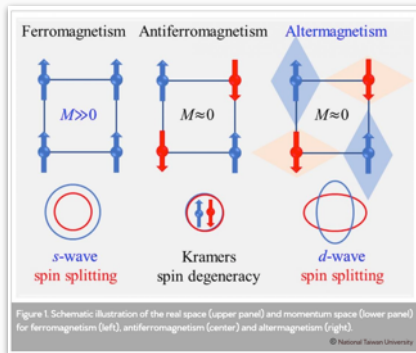


Figure 1 Schematic illustration of the real space (upper panel) and momentum space (lower panel) for ferromagnetism (left), antiferromagnetism (center) and altermagnetism (right).
© National Taiwan University

L. Šmejkal, J. Sinova, and T. Jungwirth Phys. Rev. X **12**, 031042 (2022)
L. Šmejkal, J. Sinova, and T. Jungwirth Phys. Rev. X **12**, 040501 (2022)
C.-T. Liao, Y.-C. Wang, et al. Phys. Rev. Lett. **133**, 056701 (2024)

Initial model

- **Collinear**, fully compensated magnetic order ($M = 0$ by symmetry, like an AFM)
- **Opposite-spin** sublattices related by a rotation (proper or improper) – not by inversion or translation
- **This breaks the combined PT or Tt symmetry** that normally forces $\epsilon(\uparrow, \mathbf{k}) = \epsilon(\downarrow, \mathbf{k})$ at every $\mathbf{k}$
- Result: **spin-up and spin-down bands are non-degenerate** at generic $\mathbf{k}$, degenerate only on nodal planes/lines – giving momentum-space spin splitting with even-parity symmetry (d-, g-, i-wave)
- Requires **decoupling spin and spatial symmetry operations**
 - Spin space groups, not conventional magnetic space groups
 - Are seeing coloured point groups tensors, and representation theory

Paolo Radaelli, Phys Rev B **110** 214428 (2024)

S. Hayami, Y. Yanagi, and H. Kusunose, Phys. Rev. B **102**, 144441 (2020).



Representation analysis vs. magnetic space groups vs spin space groups

Group theory

- The study of a set of symmetry operations that leave some mathematics or physical objects invariant
- Provide labels to characterise symmetry
- **Magnetic space groups are types of groups**
 - Magnetic space groups (Tavger and Zaitsev, Landau) used linear time-reversal (reversing moment vectors)
 - Magnetic space groups (Dimmock and Wheeler) used antiunitary time-reversal (e.g. complex conjugation)
- **Spin space groups are symmetry groups have different rules, provide different labels**
 - Zero spin orbit coupling may be contained within Izyumov’s exchange multiplets
 - Are there other symmetries to look at? Could space time groups provide the explanations?

Representational theory

- Application of how the symmetry operations act on physical ops mathematical objects.
- It is a branch of group theory
- The mechanics of magnetic phase transitions, the ordering process, properties, selection rules, topological band structure properties, basis vectors (symmetry adapted modes), site tensors (e.g. atomic orbitals, multipoles), isotropy groups, Landau’s theory of phase transitions
- Staged structure allows decoration (from scalar to magnetic moments) to degenerate and show couplings

Different languages and tools

- Provide different perspectives, such as in crystallography and physics, e.g. $M = H + AH$ where A is time-reversal*
- Have different tools. They allow different questions, answers and insight,



Representation analysis vs. magnetic space groups vs spin space groups

- **Group theory**
 - The study of a set of symmetry operations that leave some mathematics or physical objects invariant
 - Provide labels to characterise symmetry
 - **Magnetic space groups are types of groups**
 - Magnetic space groups (Tavger and Zaitsev, Landau) used linear time-reversal (reversing moment vectors)
 - Magnetic space groups (Dimmock and Wheeler) used antiunitary time-reversal (e.g. complex conjugation)
- **Spin space groups are symmetry groups have different rules, provide different labels**
 - Zero spin orbit coupling may be contained within Izumov's exchange multiplets
 - Are there other symmetries to look at? Could space time groups provide the explanations?
- **Representational theory**
 - Application of how the symmetry operations act on physical ops mathematical objects.
 - It is a branch of group theory
 - The mechanics of magnetic phase transitions, the ordering process, properties, selection rules, topological band structure properties, basis vectors (symmetry adapted modes), site tensors (e.g. atomic orbitals, multipoles), isotropy groups, Landau's theory of phase transitions
 - Staged structure allows decoration (from scalar to magnetic moments) to degenerate and show couplings
- **Different languages and tools**
 - Provide different perspectives, such as in crystallography and physics, e.g $M = H + AH$ where A is time-reversal*
 - Have different tools. They allow different questions, answers and insight,



Representation analysis vs. magnetic space groups vs spin space groups

- **Group theory**
 - The study of a set of symmetry operations that leave some mathematics or physical objects invariant
 - Provide labels to characterise symmetry
 - **Magnetic space groups are types of groups**
 - Magnetic space groups (Tavger and Zaitsev, Landau) used linear time-reversal (reversing moment vectors)
 - Magnetic space groups (Dimmock and Wheeler) used antiunitary time-reversal (e.g. complex conjugation)
- **Spin space groups are symmetry groups have different rules, provide different labels**
 - Zero spin orbit coupling may be contained within Izumov's exchange multiplets
 - Are there other symmetries to look at? Could space time groups provide the explanations?
- **Representational theory**
 - Application of how the symmetry operations act on physical ops mathematical objects.
 - It is a branch of group theory
 - The mechanics of magnetic phase transitions, the ordering process, properties, selection rules, topological band structure properties, basis vectors (symmetry adapted modes), site tensors (e.g. atomic orbitals, multipoles), isotropy groups, Landau's theory of phase transitions
 - Staged structure allows decoration (from scalar to magnetic moments) to degenerate and show couplings
- **Different languages and tools**
 - Provide different perspectives, such as in crystallography and physics, e.g $M = H + AH$ where A is time-reversal*
 - Have different tools. They allow different questions, answers and insight,

Tools and frameworks



1927 Wigner, Heisenberg, Hunds, Heitler – Quantum mechanics exchange coupling
 1930 Heesch – Antisymmetry
 1931 Wigner – Antiunitary symmetry (quantum theory)
 1937 Landau, Dzyaloshinski – Phase transitions
 1953, 55, 57, – Shubnikov, Zamorzaev Belov – B+W groups
 1958, Dzyaloshinski, 1960 Moriya – Antisymmetric exchange
 1959 Villain and Kaplan – Eigenvectors, eigenvalues – minimum energy spin arrangement
 1959 Yoshimori – Incommensurate magnetic structures (theory)
 1959 Wigner – Antiunitary theory – corepresentations
 1962 Bertaut – Exchange interactions and Hamiltonians
 1964 Kovalev – Representation theory
 1963 Dimmock – Group theory of phase transitions
 1966 Brinkman and Elliot Spin space groups
 1968 Bertaut – Representation theory
 1979 Izumov – Exchange multiplets
 1981 Jaric; 1984 Stokes and Hatch – Isotropy subgroups
 2001 Sikora – Quadrupoles in magnetic structures
 1980 Janner and Janssen – Magnetic superspace groups (1-D modulation)
 2022 Šmejkal, Sinova, Jungwirth – Altermagnetism

Tools and frameworks



There is a lot of history. It can create confusion and inconsistencies...

1927 Wigner, Heisenberg, Hunds, Heitler – Quantum mechanics exchange coupling
 1930 Heesch – Antisymmetry
 1931 Wigner – Antiunitary symmetry (quantum theory)
 1937 Landau, Dzyaloshinski – Phase transitions
 1953, 55, 57, – Shubnikov, Zamorzaev Belov – B+W groups
 1958, Dzyaloshinski, 1960 Moriya – Antisymmetric exchange
 1959 Villain and Kaplan – Eigenvectors, eigenvalues – minimum energy spin arrangement
 1959 Yoshimori – Incommensurate magnetic structures (theory)
 1959 Wigner – Antiunitary theory – corepresentations
 1962 Bertaut – Exchange interactions and Hamiltonians
 1964 Kovalev – Representation theory
 1963 Dimmock – Group theory of phase transitions
 1966 Brinkman and Elliot Spin space groups
 1968 Bertaut – Representation theory
 1979 Izumov – Exchange multiplets
 1981 Jaric; 1984 Stokes and Hatch – Isotropy subgroups
 2001 Sikora – Quadrupoles in magnetic structures
 1980 Janner and Janssen – Magnetic superspace groups (1-D modulation)
 2022 Šmejkal, Sinova, Jungwirth – Altermagnetism

Symmetry tools



Frameworks, puzzle pieces, blocks to build with and try to understand a QM phenomena.



Overview of magnetic structures (Irreps vs MSGs and spinSGs) – Part 2

Andrew S. Wills

Duke University (19–24 July 2026)



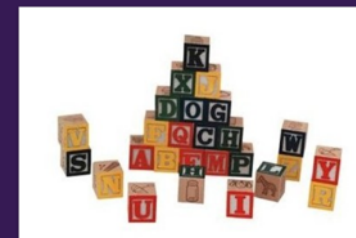
Department of Chemistry
Faculty of Mathematical and Physical Sciences



Magnetic structures – Deeper into the application of Representational Analysis

Andrew S. Wills

Duke University (19–24 July 2026)



Department of Chemistry
Faculty of Mathematical and Physical Sciences

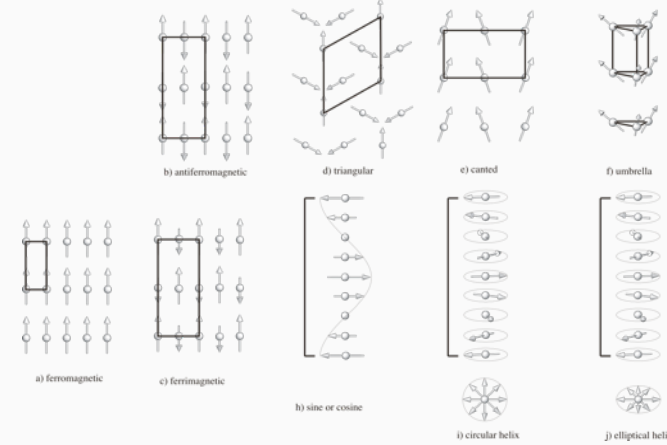


Why should an experimentalist use symmetry?

- Magnetic structures are complex
- Information is destroyed in many ways
 - The magnetic form factor: $J(\mathbf{Q})$
 - The magnetic structure factor: $F_{M\perp}(\mathbf{Q})$
 - Powder averaging (S, k - domains)
 - Domain averaging (powder, single crystal)
- ➔ Under-defined problems



Atomic moments in a crystalline environment



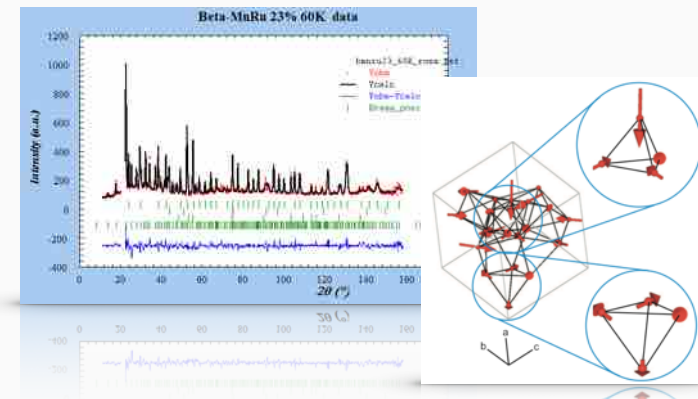
Atomic moments in a crystalline environment

Point group symmetry of spin chains	Point group		
	No lattice	Cubic lattice	Hexagonal lattice
Collinear longitudinal	$\infty/m\bar{1}$	$4/m\bar{3}m$	$6/m\bar{3}m$
Collinear transversal	$m\bar{1}$	$m\bar{1}$	$m\bar{1}$
Collinear transversal oblique	$12/m\bar{1}$	$12/m\bar{1}$	$12/m\bar{1}$
Proper screw	$\infty 2$	422	622
Conical screw	$\infty 2$	422	622
Cycloid	$2m\bar{1}$	$2m\bar{1}$	$2m\bar{1}$
Elliptical cycloid	$2m\bar{1}$	$2m\bar{1}$	$2m\bar{1}$
Transverse cone	$2mm$	$2mm$	$2mm$
Elliptical oblique cycloid	$1m\bar{1}$	$1m\bar{1}$	$1m\bar{1}$



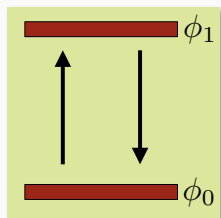
J. Manuel Perez-Mato RAMS 5

Complex incommensurate magnetic ordering, e.g. $B-Mn_{1-x}Ru_x$ ($x=0.12$)



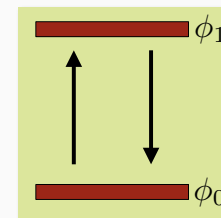
Group theory/ representation theory uses

- Selection rules for transitions
 - From a initial state
 - To a final state
 - Transition characterised by transition operator
- Overlap integrals
 - Couple terms of the same symmetry
- Coupling integrals
 - Couple terms of different symmetries
- The integrand must be invariant under application of all symmetry operations



Group theory/ representation theory uses

- ground state, ϕ_0
- excited state, ϕ_1
- transition operator, $\hat{O}$
- transition integral $\int \phi_1^* \hat{O} \phi_0 d\tau = \langle \phi_1 | \hat{O} | \phi_0 \rangle$
- if ϕ_1 and $\hat{O}\phi_0$ have different symmetries, the integral is zero (use $\hat{O} = \hat{\mu}$ for IR, $\hat{O} = \hat{\alpha}$ for Raman, etc)



Used in molecular orbital theory - LCAO

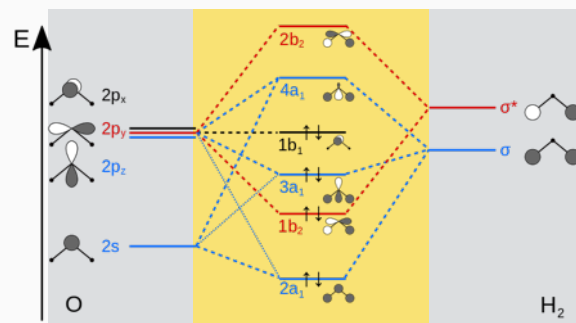
Huckel theory : molecular orbitals are linear combinations of atomic orbitals

$$\Psi = \sum_i C_i \phi_i$$

If the molecule has symmetry, group theory predicts which atomic orbitals can contribute to each molecular orbital

Symmetry-adapted LCAOs (SALCs)

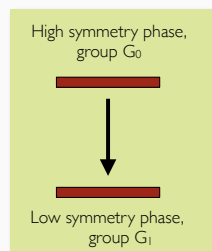
Molecular orbitals - interactions between AOs with same symmetry



Orbitals of central atom

SALCs of H atoms

Phase transitions in solids



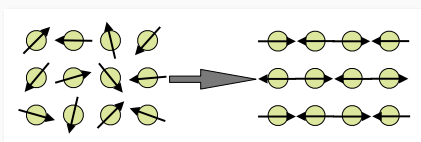
Symmetry operations are lost, e.g. "time-reversal", the symmetry under $t \rightarrow -t$ for an electric current (Bohr model) or in the Schrödinger equation

Phase transitions often involve going between phases with different symmetry
Transitions are classified as either 1st order (inhomogeneous) or 2nd order (homogeneous/ continuous)

2nd order transitions follow Landau theory

A simple example:

Paramagnetic $\rightarrow$ Antiferromagnetic



Symmetry operations in solids

Symmetry operation	Symmetry element	Symbol
Identity (do nothing)		E
Rotation by $360^\circ/n$ (a 'proper' rotation)	n -fold axis	C_n
Reflection	mirror plane	σ_v, σ_h or σ_d
Inversion	Centre of Inversion	i
Rotation by $360^\circ/n$ followed by inversion (an 'improper' rotation)	n -fold axis + a centre of inversion	S_n

TABLE I. Symmetry operations in point groups (isolated molecules).

Rotation + translation	Screw axis	N_j
Reflection + translation	Glide plane	a, b, c, n, d

TABLE II. Additional symmetry operations present in extended solids (crystals).



Groups – putting these operations together makes the crystallographic point groups and space groups

G_0

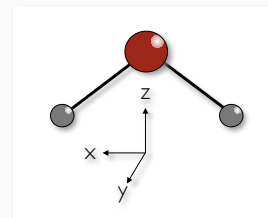
- a set of elements $A, B, C, \dots$
- the product of 2 elements is a member of the group $AB \in G$
- the product is associative $A(BC) = (AB)C$
- there exists a unique identity (E)
- every element has a unique inverse

$$AA^{-1} = A^{-1}A = E$$

The order of a group, h is the number of elements in a group



Applying operations in sequence – the multiplication table



C_{2v}	E	$C_2(Z)$	σ_{xz}	σ_{yz}
E	E	$C_2(Z)$	σ_{xz}	σ_{yz}
$C_2(Z)$	$C_2(Z)$	E	σ_{yz}	σ_{xz}
σ_{xz}	σ_{xz}	σ_{yz}	E	$C_2(Z)$
σ_{yz}	σ_{yz}	σ_{xz}	$C_2(Z)$	E

Labels and matrices

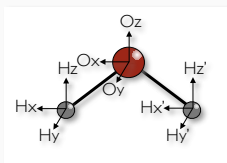
4 different operations

C_{2v} E $C_2(Z)$ σ_{xz} σ_{yz}



Block-diagonal matrices – Simplifying matrix representatives

Change to block structure. Blocks are multiplied separately



$$\sigma(xz) \times C_2(z) = \sigma(yz)$$

$$\begin{pmatrix} \square & 0 \\ 0 & \square \end{pmatrix} \times \begin{pmatrix} \square & 0 \\ 0 & \square \end{pmatrix} = \begin{pmatrix} \square & 0 \\ 0 & \square \end{pmatrix} \leftarrow U D(g) U^{-1}$$

$$\begin{pmatrix} \square & 0 \\ 0 & \square \end{pmatrix} \times \begin{pmatrix} \square & 0 \\ 0 & \square \end{pmatrix} = \begin{pmatrix} \square & 0 \\ 0 & \square \end{pmatrix}$$



Irreducible representations (IRs, irreps)



In matrix terms:

- A **representation is reducible** if there is a similarity transformation (change of basis) that sends all the matrices $d(g)$ to the same block-diagonal form
- The smallest blocks for the irreducible representations (irreps, IRs)
- All other representatives can be written in terms of these IRs

A finite group has a limited number of these IRs

$$\begin{pmatrix} \square \end{pmatrix} \times \begin{pmatrix} \square \end{pmatrix} = \begin{pmatrix} \square \end{pmatrix}$$

$$\begin{pmatrix} \square \end{pmatrix} \times \begin{pmatrix} \square \end{pmatrix} = \begin{pmatrix} \square \end{pmatrix}$$



IRs and the Great Orthogonality Theorem



If D is a reducible representation.

The number of times that a representation i appears in a decomposition of D is

$$n_i = \frac{1}{h} \sum_{g \in G} \chi_i(g)^* \chi(g)$$



	C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1	1
A_2	1	1	-1	-1
E	2	-1	0	0
D	3	0	1	1

$$n_{A_1} = 1/6(1 \times 3 + 2 \times [1 \times 0] + 3 \times [1 \times 1]) = 1$$

$$n_{A_2} = 1/6(1 \times 3 + 2 \times [1 \times 0] + 3 \times [-1 \times 1]) = 0$$

$$n_E = 1/6(2 \times 3 + 2 \times [-1 \times 0] + 3 \times [0 \times 1]) = 1$$



IRs- point groups and space groups

Irreducible representations

- "a set of matrices, each corresponding to a single operation of the group, that can be combined amongst themselves in a manner parallel to the group elements"
- Irreducible- these are building blocks of symmetries
- In point groups irreducible representations are order 1 (A,B), 2 (E), 3 (T), e.g. T_{2g} , E_g
- In space groups the rotational-translational operations lead to IRs of order up to 6
- **Marked increase in the complexity of possible structures**



Irreducible Representations of Space Groups

Table 1
Irreducible representations of $R3c-C_{3v}^1, k=0$ and $R3m-C_{3v}^2, k=0$ and $k=\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$

Symmetry operations	I	J	J^2	C or m	CJ or mJ	CJ^2 or mJ^2
Representations						
Γ_1 A_1 r_1	1	1	1	1	1	1
Γ_2 A_2 r_2	1	1	1	-1	-1	-1
Γ_3 E r_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon^2 \end{pmatrix}$	$\begin{pmatrix} \epsilon^2 & 0 \\ 0 & \epsilon \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon^2 \end{pmatrix}$	$\begin{pmatrix} \epsilon^2 & 0 \\ 0 & \epsilon \end{pmatrix}$
Magnetic moment transformations						
example 1	S_{1x}	S_{1x}	S_{1y}	$-S_{1y}$	$-S_{1x}$	$-S_{1z}$
example 2	S_{1x}	S_{1x}	S_{2y}	$-S_{2y}$	$-S_{2y}$	$-S_{2z}$
	S_{1y}	S_{2x}	S_{2z}	$-S_{2x}$	$-S_{1z}$	$-S_{3y}$
	S_{1z}	S_{3y}	S_{2x}	$-S_{2z}$	$-S_{1y}$	$-S_{3x}$

Projection

Projecting a vector of the vector space into the space of the IR gives the symmetry adapted basis vectors/modes

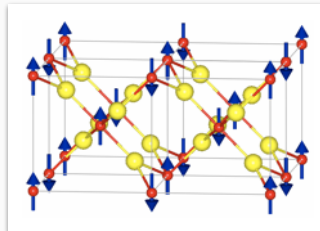
$$\hat{P}_\nu^\lambda = \sum_{g \in G} d_\nu^\lambda(g)^* \hat{g}$$

For example,

- spherical harmonics → atomic orbitals
- polar vectors → displacements and electric dipoles
- axial vectors → magnetic moments

Crystalline materials: a starting point for symmetries

1. Translational symmetry
 - Propagation vector, $\mathbf{k}$
2. Space groups/ point groups
 - parent symmetry
 - compatibility with $\mathbf{k}$
 - compatibility with the magnetic order
3. Atom position
4. Magnetic moment
5. The Hamiltonian



Definition of magnetic structures, phonons, electronic orbitals

A linear combination of plane waves (basis vectors, Fourier components)

Bloch waves – Eigenfunctions of a periodic Hamiltonian can be constructed from Fourier components

$$\vec{\psi}_{j,\nu}^{\vec{k}} = \vec{\psi}_{i,\nu}^{\vec{k}} e^{-2\pi i \vec{k} \cdot \vec{r}_{ij}}$$

$$\vec{m}_j = \sum_{\nu, \vec{k}} C_\nu^{\vec{k}} \vec{\psi}_{i,\nu}^{\vec{k}} e^{-2\pi i \vec{k} \cdot \vec{r}_{ij}}$$

- Once the moments in the primitive unit cell are defined, the $\mathbf{k}$ vector defines every other spin in the structure

Definition of magnetic structures, phonons, electronic orbitals

A linear combination of plane waves (basis vectors, Fourier components)

Bloch waves – Eigenfunctions of a periodic Hamiltonian can be constructed from Fourier components

$$\psi_{j,\nu}^k = \psi_{i,\nu}^k e^{-2\pi i \mathbf{k} \cdot \mathbf{t}_{ij}}$$

$$m_j = \sum_{\nu, \mathbf{k}} C_{\nu}^k \psi_{i,\nu}^k e^{-2\pi i \mathbf{k} \cdot \mathbf{t}_{ij}}$$

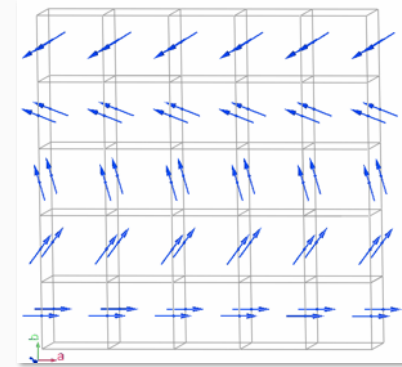
- Once the moments in the primitive unit cell are defined, the $\mathbf{k}$ vector defines every other spin in the structure



The formalism of the propagation vector, $\mathbf{k}$

$$\vec{m}_j = \sum_{\nu, \vec{k}} C_{\nu}^{\vec{k}} \vec{\psi}_{i,\nu}^{\vec{k}} e^{-2\pi i \vec{k} \cdot \vec{t}_{ij}}$$

- Example – single moment in the asymmetric unit (the primitive unit cell)
- Once $\mathbf{k}$ is defined, total degrees of freedom = 3
 - Don't need to increase unit cell or change basis



$\mathbf{k}$ -vector reduces space group symmetry : $G_0 \rightarrow G_k$

Constructing G_k (the space group of the propagation vector)

- Need only consider the rotational part (h) of symmetry operation (g):

$$g = \{h | \vec{\tau}\}$$

- a subset of space group G_0 elements $A, B, C, \dots$ that leave the $\mathbf{k}$ -vector invariant $G_k \in G_0$

$$\text{i.e. } \vec{k}' = \vec{k}h \pm \vec{\tau} \quad \leftarrow \text{Reciprocal lattice vector}$$

- i.e. defines those that are compatible with the translational symmetry of $\mathbf{k}$

$$G_k \subseteq G_0$$



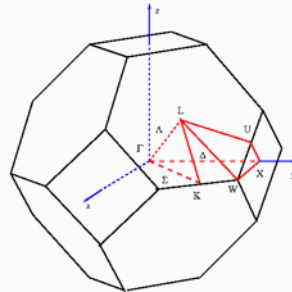
Space group G_0 , $\mathbf{k}$ -vector, G_k

#227	$\mathbf{k}=(0\ 0\ 0)$ (Γ)	48 elements
	$\mathbf{k}=(0.5\ 0\ 0)$ (K)	8
	$\mathbf{k}=(0.5\ 0.5\ 0.5)$ (L)	12

- Different points, lines, planes correspond to different symmetries. They will have different G_k .



The Brillouin zone and different G_k , e.g. FCC

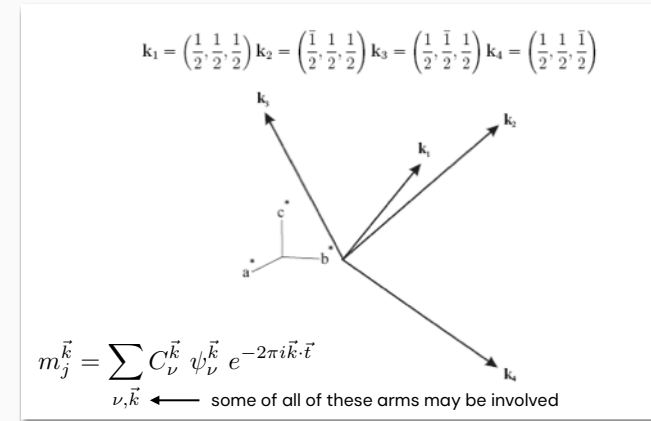


$$\vec{k}' = \vec{k}h \pm \vec{\tau}$$

- The symmetry types of the different points in reciprocal space
- Different points, lines and planes have different compatible symmetry operations; different G_k
- (Care with axis system)
- Several notations exist, Kovalev, Miller and Love, etc



The star of the propagation vector e.g. $k=(0.5\ 0.5\ 0.5)$ in space group $Fd\bar{3}m$,



Back to the space group G_0

G_0 is the space group of the crystal structure a set of elements A,B,C...

–Group structure of symmetry operations

- the product of 2 elements is a member of the group $A \in BG$
- the product is associative $A(BC)=(AB)C$
- there exists a unique identity (E)
- every element has a unique inverse
- $AA^{-1}=A^{-1}A=E$

–Groups have irreducible representations

– G_k is also a space group ...



Irreducible Representations of Space Groups

Constructed from the little space group G_k

Character tables are not enough

Source is important– calculated or tabulated

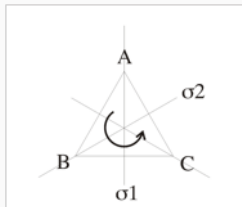
Table 1
Irreducible representations of $R3c-C_{3v}^4$, $k=0$ and $R3m-C_{3v}^4$, $k=0$ and $k=(\frac{1}{2}\frac{1}{2}\frac{1}{2})$

Symmetry operations	I	J	J^2	c or m	cJ or mJ	cJ^2 or mJ^2
Representations						
Γ_1 A_1 r_1	1	1	1	1	1	1
Γ_2 A_2 r_2	1	1	1	-1	-1	-1
Γ_3 E r_3	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} \epsilon & \\ & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} \epsilon^* & \\ & \epsilon \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} \epsilon & \\ & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} \epsilon^* & \\ & \epsilon \end{pmatrix}$
Magnetic moment transformations						
example 1	S_{1x}	S_{1z}	S_{1y}	$-S_{2y}$	$-S_{2x}$	$-S_{2z}$
example 2	S_{1x}	S_{3z}	S_{2y}	$-S_{2y}$	$-S_{2y}$	$-S_{3z}$
	S_{1y}	S_{3x}	S_{2z}	$-S_{2x}$	$-S_{1z}$	$-S_{3y}$
	S_{1z}	S_{3y}	S_{2x}	$-S_{2z}$	$-S_{1y}$	$-S_{3x}$



The permutation representation Γ_{perm}

Recap- a crystal structure is invariant under the symmetry operations of its point/space group. However, equivalent positions can be interchanged, permuted

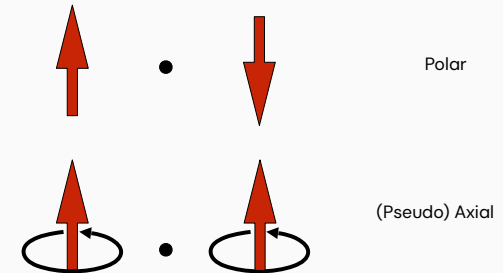


$$\begin{array}{lll}
 A \rightarrow A & A \rightarrow C & A \rightarrow B \\
 \sigma 1: B \rightarrow C & \sigma 2: B \rightarrow B & 3^+: B \rightarrow C \\
 C \rightarrow B & C \rightarrow A & C \rightarrow A \\
 \chi(\sigma 1) = 1 & \chi(\sigma 2) = 1 & \chi(3^+) = 0
 \end{array}$$

Γ_{perm} describes how all the atoms are permuted



Symmetry of magnetic moments and polar vectors under improper rotations



Polar vectors are reversed **by inversion operation**, axial vectors are not.



Symmetry of magnetic moments and displacement vectors under improper rotations

$$\text{Polar} \\
 R(I)\vec{M} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} -m_x \\ -m_y \\ -m_z \end{pmatrix}$$

$$\text{Axial} \\
 R(I)\vec{M} = \det(h) \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} \quad \det(I) = -1$$

Polar vectors are reversed by inversion operation, axial vectors are not. Mathematically, we can deal with this by multiplying by the determinant



Putting it all together- the magnetic (displacement) representation

The permutation representation and the axial vector representation are independent

$$\Gamma_{\text{mag}} = \Gamma_{\text{permutation}} \times \Gamma_{\text{axial}}$$

- The magnetic representation can be decomposed into IRs of G_k

$$\Gamma_{\text{mag}} = \sum_{\nu} n_{\nu} \Gamma_{\nu}$$

- The number of times IR Γ_{ν} appears is given by

$$n_{\nu} = \frac{1}{n(G_k)} \sum_{g \in G_k} \chi_{\Gamma_{\text{mag}}}(g) \chi_{\Gamma_{\nu}}(g)^*$$



Putting it all together- the magnetic (displacement) representation

The number of times IR Γ_ν appears is given by

$$n_\nu = \frac{1}{n(G_k)} \sum_{g \in G_k} \chi_{\Gamma_{mag}}(g) \chi_{\Gamma_\nu}(g)^*$$

This depends on the atomic site and may look like

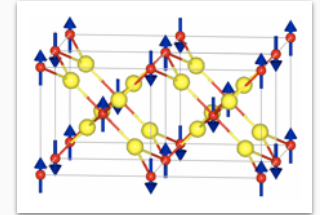
or $\Gamma_{mag,2a} = 1\Gamma_1^{(1)} \oplus 1\Gamma_2^{(1)} \oplus 0\Gamma_3^{(2)}$

$$\Gamma_{mag,6c} = 2\Gamma_1^{(1)} \oplus 0\Gamma_2^{(1)} \oplus 2\Gamma_3^{(2)}$$



Basis functions

The symmetry space of the basis vectors of an IR is unique.



Calculated using the projection operator

$$\psi_\nu^{i\lambda} = \sum_{g \in G_k} d_\nu^\lambda(g)^* \delta_{i,gi} e^{-2\pi i \mathbf{k} \cdot (\mathbf{r}_{gi} - \mathbf{r}_i)} \det(h) R^h \phi_\beta$$

and a series of test functions, e.g.

$$\vec{\phi}_1 = (1 \ 0 \ 0), \vec{\phi}_2 = (0 \ 1 \ 0), \vec{\phi}_3 = (0 \ 0 \ 1)$$



Basis vector spaces

IR	BV	Basis vector components					
		m_{1a}	m_{1b}	m_{1c}	m_{2a}	m_{2b}	m_{2c}
Γ_1	ψ_1	0	0	1	0	0	-1
Γ_3	ψ_2	1	0	0	1	0	0
	ψ_3	0	1	0	0	-1	0
Γ_5	ψ_4	1	0	0	-1	0	0
	ψ_5	0	1	0	0	1	0
Γ_7	ψ_6	0	0	1	0	0	1

Space group Pnnm, $\mathbf{k}=(000)$, $\mathbf{m}_1=(0 \ 0 \ 0)$ and $\mathbf{m}_2=(.5 \ .5 \ .5)$



Basis vectors

Define a degree of freedom

- Follows the symmetry of the associated IR
- Can be used to classify symmetry

Does not decrease number of degrees of freedom

- i.e. 3 moment degrees of freedom per atom
- n atoms will have $3n$ basis vectors
- Simplicity from dealing with the categories separately (MSGs do this too)

Define symmetry as a linear combination, refine in terms of mixing (weighting) coefficients

$$\vec{m} = \sum_i C_i \vec{\psi}_i$$



When working with complex BVs

$$\vec{m} = \sum_i C_i \vec{\psi}_i$$

A purely imaginary basis vector is as real as a purely real one...

$$\vec{\psi}_1 = (1, 0, 0); \vec{\psi}_2 = (i, 0, 0)$$

$$\vec{\psi}_2 = -i \cdot \vec{\psi}_1$$

– They are equivalent

The linear combination of basis vectors can be sophisticated

$$\vec{\psi}_1 + \vec{\psi}_1^* = 2\text{Re}(\vec{\psi}_1)$$

$$(-i \times \vec{\psi}_1) + (i \times \vec{\psi}_1^*) = 2\text{Im}(\vec{\psi}_1)$$



Making magnetic structures with basis vectors

Expanding the exponential

- The eigenfunctions of an electrons with a periodic Hamiltonian are Bloch waves. with the form:

$$\vec{m}_j = \sum_{\nu, \vec{k}} C_{\nu}^{\vec{k}} \vec{\psi}_{i, \nu}^{\vec{k}} e^{-2\pi i \vec{k} \cdot \vec{t}_{ij}}$$

- Magnetic structures are eigenfunctions of the spin-dependent electronic Hamiltonian and have the same form
- If we expand the exponential, we see that it is made up of a **Real** cosine part and an **Imaginary** sine part

$$\vec{m}_j = \sum_{\nu, \vec{k}} C_{\nu}^{\vec{k}} \vec{\psi}_{i, \nu}^{\vec{k}} \left[\cos(-2\pi \vec{k} \cdot \vec{t}) + i \sin(-2\pi \vec{k} \cdot \vec{t}) \right]$$

- This formalism very general and we will see that it can describe simple and exotic structures, such as sinusoidal and helical structures



Basis vectors and k-vectors

- Ψ is real and $\mathbf{k}$ is such that the sine component is non-zero
 - Leads to $\mathbf{m}_j$ being complex, so need to make it real
 - The moment vector for an atom in the n th cell related to that in the zeroth cell by translation $\mathbf{t}_i$ is given by

$$\mathbf{m}_j = C_{\nu}^k \psi_{i, \nu}^k e^{-2\pi i k \cdot \mathbf{t}_{ij}} + C_{\nu}^k \psi_{i, \nu}^{-k} e^{-2\pi i (-k) \cdot \mathbf{t}_{ij}}$$

$$\mathbf{m}_j = C_{\nu}^k \psi_{i, \nu}^k e^{-2\pi i k \cdot \mathbf{t}_{ij}} + C_{\nu}^k (\psi_{i, \nu}^k)^* e^{-2\pi i (-k) \cdot \mathbf{t}_{ij}}$$

– As

$$\psi_{i, \nu}^{-k} = \psi_{i, \nu}^{k*}$$

- Substitution and expansion of the exponential leads to

$$\vec{m}_j = 2\text{Re}(\vec{\psi}_{i, \nu}^k) \left[\cos(-2\pi \vec{k} \cdot \vec{t}_{ij}) \right] + 2\text{Im}(\vec{\psi}_{i, \nu}^k) \left[\sin(-2\pi \vec{k} \cdot \vec{t}_{ij}) \right]$$

- Where the second term is zero as Ψ is real $\rightarrow$ Amplitude modulated sine structure (spin density wave)

(*Note BVs know if the atom is on an inversion centre)



Basis vectors and k-vectors

- Ψ is real and $\mathbf{k}$ is such that the sine component is non-zero
 - Leads to $\mathbf{m}_j$ being complex, so need to make it real
 - The moment vector for an atom in the n th cell related to that in the zeroth cell by translation $\mathbf{t}_i$ is given by

$$\mathbf{m}_j = C_{\nu}^k \psi_{i, \nu}^k e^{-2\pi i k \cdot \mathbf{t}_{ij}} + C_{\nu}^k \psi_{i, \nu}^{-k} e^{-2\pi i (-k) \cdot \mathbf{t}_{ij}}$$

$$\mathbf{m}_j = C_{\nu}^k \psi_{i, \nu}^k e^{-2\pi i k \cdot \mathbf{t}_{ij}} + C_{\nu}^k (\psi_{i, \nu}^k)^* e^{-2\pi i (-k) \cdot \mathbf{t}_{ij}}$$

– As

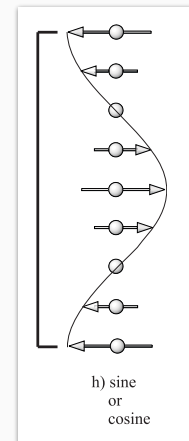
$$\psi_{i, \nu}^{-k} = \psi_{i, \nu}^{k*}$$

- Substitution and expansion of the exponential leads to

$$\vec{m}_j = 2\text{Re}(\vec{\psi}_{i, \nu}^k) \left[\cos(-2\pi \vec{k} \cdot \vec{t}_{ij}) \right] + 2\text{Im}(\vec{\psi}_{i, \nu}^k) \left[\sin(-2\pi \vec{k} \cdot \vec{t}_{ij}) \right]$$

- Where the second term is zero as Ψ is real $\rightarrow$ Amplitude modulated sine structure (spin density wave)

(*Note BVs know if the atom is on an inversion centre)



Basis vectors and k-vectors

- Ψ is complex and $\mathbf{k}$ is incommensurate

- Leads to $\mathbf{m}$ being complex, so need to make real moments
- The atomic vector for an atom in the n th cell related to that in the zeroth cell by translation $\mathbf{t}$ is given by

$$\mathbf{m}_j = C_{\nu}^k \psi_{i,\nu}^k e^{-2\pi i \mathbf{k} \cdot \mathbf{t}_{ij}} + C_{\nu}^k (\psi_{i,\nu}^k)^* e^{-2\pi i (-\mathbf{k}) \cdot \mathbf{t}_{ij}}$$

- Substitution and expansion of the exponential leads to

$$\vec{m}_j = 2\text{Re}(\vec{\psi}_{i,\nu}^k) [\cos(-2\pi \vec{k} \cdot \vec{t}_{ij})] + 2\text{Im}(\vec{\psi}_{i,\nu}^k) [\sin(-2\pi \vec{k} \cdot \vec{t}_{ij})]$$

- Where the second term is non-zero.
- If the real and imaginary parts are not parallel $\rightarrow$ circular or elliptical helix

(*Note SARAH, works with atoms in the zeroth unit cell)



Basis vectors and k-vectors

- Ψ is complex and $\mathbf{k}$ is incommensurate

- Leads to $\mathbf{m}$ being complex, so need to make real moments
- The atomic vector for an atom in the n th cell related to that in the zeroth cell by translation $\mathbf{t}$ is given by

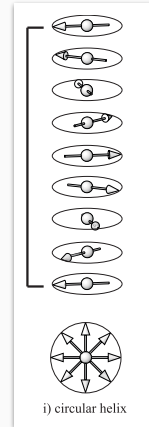
$$\mathbf{m}_j = C_{\nu}^k \psi_{i,\nu}^k e^{-2\pi i \mathbf{k} \cdot \mathbf{t}_{ij}} + C_{\nu}^k (\psi_{i,\nu}^k)^* e^{-2\pi i (-\mathbf{k}) \cdot \mathbf{t}_{ij}}$$

- Substitution and expansion of the exponential leads to

$$\vec{m}_j = 2\text{Re}(\vec{\psi}_{i,\nu}^k) [\cos(-2\pi \vec{k} \cdot \vec{t}_{ij})] + 2\text{Im}(\vec{\psi}_{i,\nu}^k) [\sin(-2\pi \vec{k} \cdot \vec{t}_{ij})]$$

- Where the second term is non-zero.
- If the real and imaginary parts are not parallel $\rightarrow$ circular or elliptical helix

(*Note SARAH, works with atoms in the zeroth unit cell)



Basis vectors and k-vectors

- Ψ is complex and $\mathbf{k}$ is incommensurate

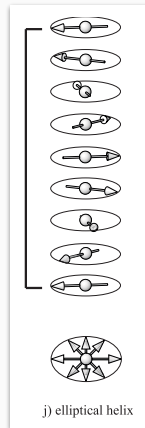
- Leads to $\mathbf{m}$ being complex, so need to make real moments
- The atomic vector for an atom in the n th cell related to that in the zeroth cell by translation $\mathbf{t}$ is given by

$$\mathbf{m}_j = C_{\nu}^k \psi_{i,\nu}^k e^{-2\pi i \mathbf{k} \cdot \mathbf{t}_{ij}} + C_{\nu}^k (\psi_{i,\nu}^k)^* e^{-2\pi i (-\mathbf{k}) \cdot \mathbf{t}_{ij}}$$

- Substitution and expansion of the exponential leads to

$$\vec{m}_j = 2\text{Re}(\vec{\psi}_{i,\nu}^k) [\cos(-2\pi \vec{k} \cdot \vec{t}_{ij})] + 2\text{Im}(\vec{\psi}_{i,\nu}^k) [\sin(-2\pi \vec{k} \cdot \vec{t}_{ij})]$$

- Where the second term is non-zero.
- If the real and imaginary parts are not parallel $\rightarrow$ circular or elliptical helix



(*Note SARAH, works with atoms in the zeroth unit cell)



Building structures : basis vectors and k-vectors

- **A sine structure helix**
 - $\mathbf{k}$ incommensurate
 - Ψ has is real, in a plane that contains (longitudinal) or does not contain (transverse) $\mathbf{k}$
- **A circular helix**
 - $\mathbf{k}$ incommensurate
 - Ψ has is complex, and has non-collinear real and imaginary components (equal magnitude) in a plane that does not contain $\mathbf{k}$
- **A conical structure**
 - $\mathbf{k}$ incommensurate
 - Ψ has is complex, and has non-collinear real and imaginary components (equal magnitude) in a plane that does not contain $\mathbf{k}$
 - $\mathbf{k}=(000)$
 - Ψ is ferromagnetic and is perpendicular to the helix
- **A cycloid**
 - $\mathbf{k}$ incommensurate
 - Ψ has is complex, and has non-collinear real and imaginary components (equal magnitude) in a plane that contains $\mathbf{k}$



Reading structures by basis vectors or MSGs

Point group symmetry of spin chains

	No lattice	Cubic lattice	Hexagonal lattice
Collinear longitudinal	$\infty/mn1'$	$4/mmm1'$	$6/mmm1'$
Collinear transversal	$mnm1'$	$mnm1'$	$mnm1'$
Collinear transversal oblique	$12/m11'$	$12/m11'$	$12/m11'$
Proper screw	$\infty 21'$	$4221'$	$6221'$
Conical screw	$\infty 2'$	$42'2'$	$62'2'$
Cycloid	$2mm1'$	$2mm1'$	$2mm1'$
Elliptical cycloid	$2mm1'$	$2mm1'$	$2mm1'$
Transverse cone	$2mm'$	$2mm'$	$2mm'$
Elliptical oblique cycloid	$1m11'$	$1m11'$	$1m11'$

J. Manuel Perez-Mato RAMS 5



Linking IRs and MSGs – Symmetry of basis vector combinations

Table 4. Representations and magnetic groups in $Pbam$ ($\mathbf{k}=0$)

Representations	Characters of the generators			Elements and antielements			Magnetic groups
	2_{1z}	2_{1y}	$\bar{1}$				
Γ_1	1	1	1	2_x	2_y	$\bar{1}$	$Pbam$
Γ_2	1	-1	1	2_x	$2_y'$	$\bar{1}$	$Pba'm'$
Γ_3	-1	1	1	$2_x'$	$2_y'$	$\bar{1}$	$Pb'am'$
Γ_4	-1	-1	1	$2_x'$	$2_y'$	$\bar{1}$	$Pb'a'm'$
Γ_5	1	1	-1	2_x	2_y	$\bar{1}'$	$Pb'am$
Γ_6	1	-1	-1	2_x	$2_y'$	$\bar{1}'$	$Pba'm$
Γ_7	-1	1	-1	$2_x'$	2_y	$\bar{1}'$	$Pb'a'm$
Γ_8	-1	-1	-1	$2_x'$	$2_y'$	$\bar{1}'$	$Pbam'$

Within a 1D IR all basis vectors have the same MSG

E.F. Acta Cryst. **A24**, 217 (1968).

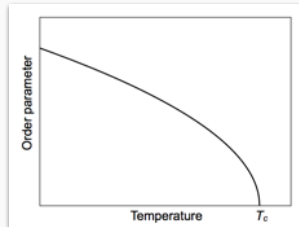


Linking IRs and MSGs – Symmetry of basis vector combinations

$$m_j^{\vec{k}} = \sum_{\nu, \vec{k}} C_{\nu}^{\vec{k}} \psi_{\nu}^{\vec{k}} e^{-2\pi i \vec{k} \cdot \vec{r}}$$

The basis vector space of an IR can define MSGs through an order parameter, $\vec{\eta} = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$

- Symmetry groups based on the mixing coefficients can be defined according to which symmetry operations have IR matrices that leave a vector in IR space invariant (the isotropy group), or reverse it:
- Unprimed operations correspond to $d(h)\vec{\eta} = \vec{\eta}$ primed operations correspond to $d(h)\vec{\eta} = -\vec{\eta}$



- During the transition, symmetry breaks. The symmetry group changes from G to a subgroup H

$$G \rightarrow H$$

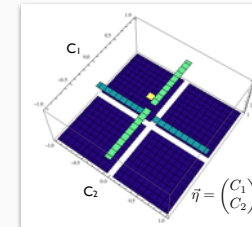


Linking IRs and MSGs – Symmetry of basis vector combinations

$$m_j^{\vec{k}} = \sum_{\nu, \vec{k}} C_{\nu}^{\vec{k}} \psi_{\nu}^{\vec{k}} e^{-2\pi i \vec{k} \cdot \vec{r}}$$

The basis vector space of an IR can define MSGs through an order parameter, $\vec{\eta} = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$

- Symmetry groups based on the mixing coefficients can be defined according to which symmetry operations have IR matrices that leave a vector in IR space invariant (the isotropy group), or reverse it:
- Unprimed operations correspond to $d(h)\vec{\eta} = \vec{\eta}$ primed operations correspond to $d(h)\vec{\eta} = -\vec{\eta}$



- During the transition, symmetry breaks. The symmetry group changes from G to a subgroup H

$$G \rightarrow H$$



Order Parameter ('Isotropy') groups

- Linking IRs to Magnetic Groups

Der Parameter ('Isotropy') groups

Linking IRs to Magnetic Groups

P - 6 m 2
D 3h 1

kIT: $\left\{ \begin{matrix} - \\ -4, \quad 0, \quad 0 \end{matrix} \right\}$

IR

	h1	h10	h16	h19
IR i1	(1)	(1)	(1)	(1)
IR i2	(1)	(1)	(-1)	(-1)
IR i3	(-1)	(-1)	(1)	(-1)
IR i4	(-1)	(-1)	(-1)	(1)

K: $\left\{ \begin{matrix} [-1/4, 0, 0] \\ (0, 1/4, 0) \\ (1/4, 0, -1/4) \end{matrix} \right\}$

	h1	h3	h5	h8	h10	h12	h14	h16	h18	h19	h21	h23
CIR i1	1 0 0	0 0 1	0 1 0	0 0 1	1 0 0	0 1 0	0 1 0	1 0 0	0 0 1	1 0 0	0 1 0	0 0 1
	1 1 0	0 1 0	0 0 1	0 1 0	0 0 1	1 0 0	0 0 1	0 1 0	0 0 1	0 1 0	1 0 0	0 1 0
	0 0 1	0 1 0	1 0 0	1 0 0	0 1 0	0 0 1	1 0 0	0 0 1	0 1 0	0 1 0	0 0 1	1 0 0
CIR i2	1 0 0	0 0 1	0 1 0	0 0 1	1 0 0	0 1 0	0 -1 0	-1 0 0	0 0 -1	-1 0 0	0 -1 0	0 -1 0
	1 1 0	1 0 0	0 0 1	0 1 0	0 0 1	1 0 0	0 0 -1	0 -1 0	-1 0 0	0 0 -1	-1 0 0	0 -1 0
	0 0 1	0 1 0	1 0 0	1 0 0	0 0 1	0 0 1	0 0 -1	0 0 -1	0 0 -1	0 0 -1	0 0 -1	-1 0 0
CIR i3	1 0 0	0 0 1	0 1 0	0 -1 0	-1 0 0	0 -1 0	0 1 0	1 0 0	0 0 1	-1 0 0	0 -1 0	0 -1 0
	1 1 0	1 0 0	0 0 1	0 -1 0	0 0 -1	-1 0 0	0 0 1	0 1 0	1 0 0	0 0 -1	-1 0 0	0 -1 0
	0 0 1	0 1 0	1 0 0	-1 0 0	0 -1 0	0 0 -1	1 0 0	0 0 1	0 1 0	0 -1 0	0 -1 0	-1 0 0
CIR i4	1 0 0	0 0 1	0 1 0	0 -1 0	-1 0 0	0 -1 0	0 -1 0	-1 0 0	0 0 -1	1 0 0	0 1 0	0 0 1
	1 1 0	1 0 0	0 0 1	0 -1 0	0 0 -1	-1 0 0	0 0 -1	0 -1 0	0 -1 0	0 1 0	0 1 0	0 1 0
	0 0 1	0 1 0	1 0 0	-1 0 0	0 -1 0	0 0 -1	-1 0 0	0 0 -1	0 -1 0	0 1 0	0 0 1	1 0 0

IR

	h1	h3	h5	h8	h10	h12	h14	h16	h18	h19	h21	h23
CIR i1	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i2	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i3	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i4	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)

IR

	h1	h3	h5	h8	h10	h12	h14	h16	h18	h19	h21	h23
CIR i1	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i2	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i3	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i4	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)

IR

	h1	h3	h5	h8	h10	h12	h14	h16	h18	h19	h21	h23
CIR i1	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i2	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i3	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)
CIR i4	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)

IR

	h1	h3	h5	h8	h10	h12	h14
--	----	----	----	----	-----	-----	-----

IR Dimension 2+ analysis with Fourier series

[illegible]

- Their symmetry space may not correspond to a magnetic space group
- different symmetry spaces within an IR
- Where symmetries are common across IRs there is likely to be coupling

Refine with mixing coefficients following symmetry types.

Characterise resulting structure with magnetic space (point) groups defined by η .

Projection of basis vectors

Basis vector

Magnetic space
point groups

$$\begin{aligned} d(h)\vec{\eta} &= \vec{\eta} \\ d(h)\vec{\eta} &= -\vec{\eta} \end{aligned}$$

$$\vec{\eta} = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$$

Linking IRs and Spin Space Groups - Exchange multiplets

Izyumov

Exchange group G_{ex} has a high symmetry than the space group G

- Invariance to global rotation of spins, $G_{\text{ex}} = G_a \otimes G_s$, where G_a is the space group acting only on the atomic positions and G_s is the group of rotations in spin space
- In a parallel manner, the magnetic representation Γ_{mag} has a spatial part (the permutation representation, Γ_{perm}) in direct product with the axial vector representation V
 - Γ_{perm} can be decomposed over IRs Γ^k
 - Under a given Γ^k in Γ_{perm} , the set of crystal magnetic states with fixed wave vector k having the same exchange energy form exchange multiplets
 - Scalars do not know about directions in space, so the scalar representation holds only information on relative orientations

Anisotropy breaks the degeneracy of the exchange multiplet, causing the common result of order under a subset of IRs.

	Γ_{O_h}						
Exchange multiplets	(CuI)	Γ^1	Γ^2	Γ^3	Γ^4	Γ^5	Γ^6
$\Gamma^1 \otimes \hat{\Psi}$	0	0	1	0	1	0	
$\Gamma^2 \otimes \hat{\Psi}$	0	0	0	1	0	1	
$\Gamma^3 \otimes \hat{\Psi}$	1	0	0	0	1	0	
$\Gamma^4 \otimes \hat{\Psi}$	0	1	0	0	0	1	
$\Gamma^5 \otimes \hat{\Psi}$	1	0	1	0	2	0	
$\Gamma^6 \otimes \hat{\Psi}$	0	1	0	1	0	2	

Linking Spin Space Groups and IRs – Exchange multiplets

MSGs, IRs and spin space groups. Action of a symmetry operation

- MSGs have a 1:1 mapping of the operation and its effect on a magnetic moments:
 - Rotate (and translate) or rotate (and translate) and reverse.
- $D = 1$ IRs have the same 1:1 mapping. They are functionally identical to a MSG
- $D > 1$ can have more mappings - we project different BVs from each row.
 - This makes a symmetry space that can have more than 1 effect for a given symmetry operation
 - Spin space groups and exchange multiplets expand mapping further
- Combining basis vectors from different IRs because they share the same symmetry group
 - Joins subsets of the basis vector spaces from the different IRs
 - Izumov's reasoning is that this can happen because of a shared structure of scalar permutations and eigenvalues - and so a shared exchange energy.
- The IR matrices can hold a more sophisticated relationship between spatial symmetry operations and the orientations of the magnetic moments. Spin space groups, exchange multiplets (and coreps) take this even further.

Anti-linear time-reversal

- Time reversal doubles the group. We have the (normal) unitary operations (g), but also a set of antiunitary operations (a) made from normal operations have been combined with time-reversal, θ

- As time-reversed $\mathbf{k}$ corresponds to $-\mathbf{k}$, this creates $G(\mathbf{k}, -\mathbf{k})$
- 3 types of **corepresentations** form under time-reversal
 - Type A.** Time reversal doubles the group in an often 'trivial' manner.
 - Type B.** Time-reversal doubles the degeneracy of an IR
 - Type C.** Time-reversal joins 2 IRs that are related by complex conjugation.
 - These may be within $G_{\mathbf{k}}$ (and so correspond to the same $\mathbf{k}$ vector)
 - Or may combine operations related to $G_{\mathbf{k}}$ and $G_{-\mathbf{k}}$.
- Combining $\mathbf{k}$ and $-\mathbf{k}$ basis vectors can make a real space

C. Herring Phys. Rev. **52**, 361(1937)

E. P. Wigner, Group Theory and its Application to Quantum Mechanics of Atomic Spectra. London: Academic Press (1959).

Variation I. When $-\mathbf{k}$ is not a member of $\{\mathbf{k}\}$

$$M(\mathbf{k}) = G + \theta G$$

$$D(g) = \begin{pmatrix} \Delta(g) & 0 \\ 0 & \Delta(g)^* \end{pmatrix} D(a) = \begin{pmatrix} 0 & \kappa \Delta(g) \\ \Delta(g)^* & 0 \end{pmatrix}$$

Variation II. When $-\mathbf{k}$ is a member of $\{\mathbf{k}\}$

$$M(\mathbf{k}) = G(\mathbf{k}, a_0) = G(\mathbf{k}) + a_0 G(\mathbf{k})$$

Type a. These contain only one irreducible representation, Δ .

$$D(g) = \Delta(g), D(a) = \Delta(aa_0^{-1})\beta,$$

where β satisfies $\beta\beta^* = \Delta(a_0^2)$ and $\beta\bar{\Delta}(g) = \Delta(g)\beta$.

Type b. This involves the same irreducible representation of the unitary subgroup, Δ , twice:

$$D(g) = \begin{pmatrix} \Delta(g) & 0 \\ 0 & \Delta(g) \end{pmatrix}, D(a) = \begin{pmatrix} 0 & \Delta(aa_0^{-1})\beta \\ -\Delta(aa_0^{-1})\beta & 0 \end{pmatrix}$$

with $\beta\beta^* = -\Delta(a_0^2)$ and $\beta\bar{\Delta}(g) = \Delta(g)\beta$.

Type c. Here two irreducible representations, Δ and $\bar{\Delta}$, that are not equivalent combine to form an irreducible corepresentation.

$$D(g) = \begin{pmatrix} \Delta(g) & 0 \\ 0 & \bar{\Delta}(g) \end{pmatrix}, D(a) = \begin{pmatrix} 0 & \Delta(aa_0^{-1}) \\ \Delta(aa_0^{-1})^* & 0 \end{pmatrix},$$

Today - Monday

Ideas under some current tools

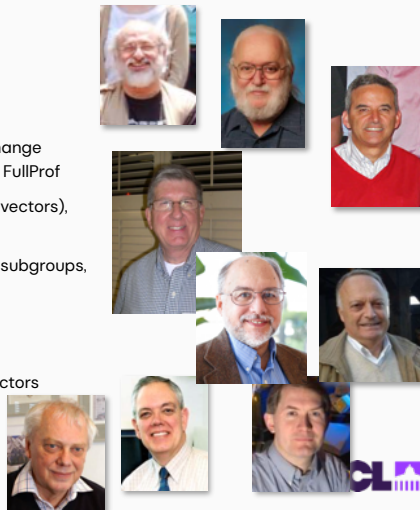
- SARAh** - Representation theory (basis vectors), exchange multiplets, couplings, invariants, maximal subgroups, FullProf
- Isotropy** - MSG, MSSG, representation theory (basis vectors), couplings, invariants
- BCS** - MSG, MSSG, tables (e.g IRs), tensors, maximal subgroups, spin (space) groups
- FullProf** - Full basis vector, MSG, MSSG refinement (commensurate / incommensurate)
- MAG2POL** - MSG, MSSG, calculated IRs and basis vectors
- GSAS II** - MSG, MSSG refinement



Today - Monday

Ideas under some current tools

- SARAh** - Representation theory (basis vectors), exchange multiplets, couplings, invariants, maximal subgroups, FullProf
- Isotropy** - MSG, MSSG, representation theory (basis vectors), couplings, invariants
- BCS** - MSG, MSSG, tables (e.g IRs), tensors, maximal subgroups, spin (space) groups
- FullProf** - Full basis vector, MSG, MSSG refinement (commensurate / incommensurate)
- MAG2POL** - MSG, MSSG, calculated IRs and basis vectors
- GSAS II** - MSG, MSSG refinement



Tomorrow - Tuesday

SARAh -

- Current web apps
 - FullProf
 - WebRepresentational Analysis
 - Coupling IRs
 - Shared symmetry (MPGs)
 - Exchange multiplets
 - Landau theory
 - Maximal subgroups
- Some developments
 - Serendipity
 - Altermagnetism in real and reciprocal space



