

Part 3: Finger food

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Phase transitions in crystalline solids - Introductions to Landau and SARAh

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I. Landau theory - second-order phase transitions

- The minimum in free energy defines the equilibrium state

$$\left(\frac{\partial G}{\partial Q}\right)_{Q_0} = 0, \left(\frac{\partial^2 G}{\partial Q^2}\right)_{Q_0} > 0$$

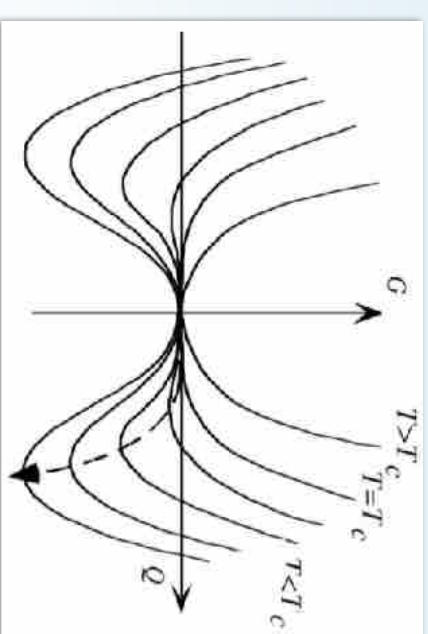
- Free energy varies **continuously** as a function of temperature
 - Symmetry change is not continuous
- Assume that the free energy can be expanded as a function of an **order parameter** with temperature-dependent coefficients
 - Order parameter could be polarisation, strain, mixing coefficients
 - The minima also change as a function of temperature

$$G = G_0 + \frac{1}{2}rQ^2 + dQ^3 + uQ^4$$

Landau (1937), Landau and Lifshitz (1950):

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Landau theory



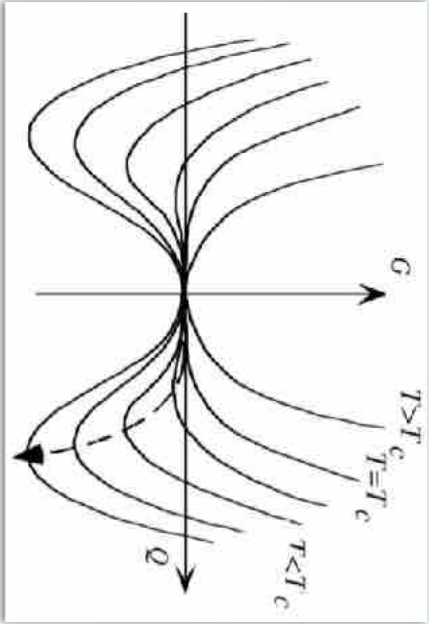
For $T > T_c$,
 $r(T) > 0$

For $T < T_c$,
 $r(T) < 0$

- The condition $G(-Q) = G(Q)$ requires that the power series only has even powers of **Q**
 - We will truncate the power series as soon as practically possible
- $$G = G_0 + \frac{1}{2}rQ^2 + dQ^3 + uQ^4$$

4

Landau theory



For $T > T_c$,
 $r(T) > 0$

For $T < T_c$,
 $r(T) < 0$

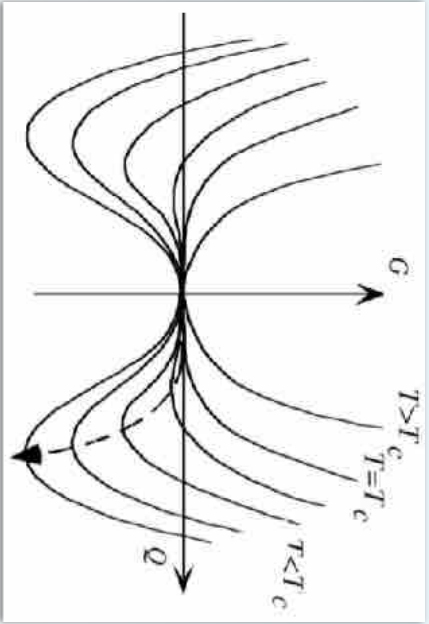
Assuming r is linear in $T \rightarrow$ Use $r(T - T_c)$,

where T_c is the critical temperature

$$G = G_0 + \frac{1}{2}rQ^2 + dQ^3 + uQ^4$$

and take the other coefficients as temperature independent.

Landau theory



For $T > T_c$,
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Assuming r is linear in $T \rightarrow$ Use $r(T - T_c)$,

where T_c is the critical temperature

$$G = G_0 + \frac{1}{2}r(T - T_c)Q^2 + uQ^4$$

and take the other coefficients as temperature independent.

Landau theory - some specifics for us

- The reference structure is the space group **G₀** before the magnetic order
- The Hamiltonian needs to be invariant under **G₀**
- The resulting **symmetry group** of the structure is a subgroup of **G₀**. Symmetry group means that we are considering **real moments** or **real energy terms** under symmetry operations
- Order parameters characterise the transition : its strength (modulus) and the symmetry that remains in the phase **after the ordering**
- The mixing coefficients are the refined parameters of a magnetic structure

- **They are also valid order parameters for Landau theory**

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

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

Landau (1937), Landau and Lifshitz (1950):

Landau theory

- Rewrite the free energy in terms of **polynomial of degree n** that is invariant under **G₀**, so

$$G = G_0 + \frac{1}{2}rQ^2 + dQ^3 + uQ^4$$

becomes

$$G = \sum_n P_n \{ \vec{\eta}_\lambda \}$$

e.g. where

or

etc

$$\vec{\eta} = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} \quad \vec{\eta} = \begin{pmatrix} C_1 \\ 0 \end{pmatrix}$$

Landau (1937), Landau and Lifshitz (1950):

Landau theory

- In **IR space** we need to be able to describe the action of the symmetry operations on, e.g.

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

- This is done by considering the action of the IR matrix of a given symmetry operation g, define this as

$$g\vec{\eta} = D_{\nu}(g)\vec{\eta}$$

- Simplify things by looking at the unique matrices of an IR, these form the image of the IR.
- Look at which operates leave **η** invariant and which change it to symmetry related vectors (**compare this with making the star of k**)
- Use this set of {**η**} to calculate the polynomial of invariants, as F must be invariant under these operations. The result has to be consistent (invariant) under all these operations simultaneously, e.g.

$$F = r(\eta_1^2 + \eta_2^2 + \eta_3^2) + v\eta_1\eta_2\eta_3 + u_1(\eta_1^4 + \eta_2^4 + \eta_3^4) + u_2(\eta_1^2\eta_2^2 + \eta_1^2\eta_3^2 + \eta_2^2\eta_3^2) \quad 8$$

Landau (1937), Landau and Lifshitz (1950):

Landau theory - back to our magnetic structures

- As we know **η**, for a given IR of G_k we can use make a list of which symmetry operations leave it invariant or reverse it. These form the MPGs or the MSGs of the relevant basis vector combination

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

- The unique collection of MPGs or MSGs within an IR define a set of important {**η**}
- If two representations contain the some of the same image matrices, then the same MPGs and MSGs can occur in the different IRs. (The same symmetry group may span IRs), even if the degrees of freedom are orthogonal!
- If this happens, coupling can occur between them. One IR may drive the transition (primary) and another may be induced by it through coupling. This is a secondary order parameter. They are not expected to have the same temperature dependence, but will have the same critical temperature

Landau (1937), Landau and Lifshitz (1950):

Landau theory

- The symmetry group of the magnetic structure should a subgroup of the space group before the transition
- A transition should involve a single IR, that of the G₀
- When there are more than one arms to the star, the symmetry operations are divided amongst the arms (cosets)
- Bringing together these symmetry-related operations recovers those of G₀
- So, the rotationally related IRs of G_k{**k**} come together, they define a collection of matrices that involve all the operations of G₀.
- Explore which IR of G₀ has non-zero overlap with this set of IRs.
- It is this IR that Landau says guides the transition, it could couple IRs within different little groups G_k that have different k-vectors
- Bertaut broke away from this G₀-based description to focus on G_k. A single IR of G_k is a good starting point, but there may be coupling from IRs with isotropy groups with the same MSG/MPG or when viewed from G₀**

Landau (1937), Landau and Lifshitz (1950):

Landau Theory- When it doesn't work it might still be useful :-)

- Irreducible representations still classify symmetry types
- The observation of several IRs involved in a magnetic transition (structure) gives you information about the energy drives
- The difference between weakly and strongly first order

$$\hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4$$

Landau (1937), Landau and Lifshitz (1950):

Order Parameter ('Isotropy') groups

- Linking IRs to Magnetic Groups

Order Parameter ('Isotropy') groups

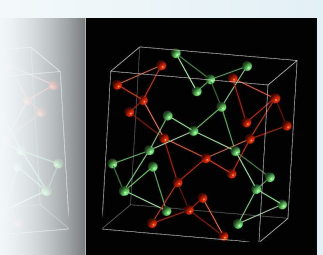
Linking IRs to Magnetic Groups

$P-6mm2$
 $D_{3h} \times 1$
 $K_{IT} = \{(-1, 0, 0)$
 $(0, 1, 0)$
 $(0, 0, 1)\}$

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8	Γ_9	Γ_{10}	Γ_{11}	Γ_{12}	Γ_{13}	Γ_{14}	Γ_{15}	Γ_{16}	Γ_{17}	Γ_{18}	Γ_{19}	Γ_{20}	Γ_{21}	Γ_{22}	Γ_{23}	Γ_{24}	Γ_{25}	Γ_{26}	Γ_{27}	Γ_{28}	Γ_{29}	Γ_{30}	Γ_{31}	Γ_{32}	Γ_{33}	Γ_{34}	Γ_{35}	Γ_{36}	Γ_{37}	Γ_{38}	Γ_{39}	Γ_{40}	Γ_{41}	Γ_{42}	Γ_{43}	Γ_{44}	Γ_{45}	Γ_{46}	Γ_{47}	Γ_{48}	Γ_{49}	Γ_{50}	Γ_{51}	Γ_{52}	Γ_{53}	Γ_{54}	Γ_{55}	Γ_{56}	Γ_{57}	Γ_{58}	Γ_{59}	Γ_{60}	Γ_{61}	Γ_{62}	Γ_{63}	Γ_{64}	Γ_{65}	Γ_{66}	Γ_{67}	Γ_{68}	Γ_{69}	Γ_{70}	Γ_{71}	Γ_{72}	Γ_{73}	Γ_{74}	Γ_{75}	Γ_{76}	Γ_{77}	Γ_{78}	Γ_{79}	Γ_{80}	Γ_{81}	Γ_{82}	Γ_{83}	Γ_{84}	Γ_{85}	Γ_{86}	Γ_{87}	Γ_{88}	Γ_{89}	Γ_{90}	Γ_{91}	Γ_{92}	Γ_{93}	Γ_{94}	Γ_{95}	Γ_{96}	Γ_{97}	Γ_{98}	Γ_{99}	Γ_{100}	Γ_{101}	Γ_{102}	Γ_{103}	Γ_{104}	Γ_{105}	Γ_{106}	Γ_{107}	Γ_{108}	Γ_{109}	Γ_{110}	Γ_{111}	Γ_{112}	Γ_{113}	Γ_{114}	Γ_{115}	Γ_{116}	Γ_{117}	Γ_{118}	Γ_{119}	Γ_{120}	Γ_{121}	Γ_{122}	Γ_{123}	Γ_{124}	Γ_{125}	Γ_{126}	Γ_{127}	Γ_{128}	Γ_{129}	Γ_{130}	Γ_{131}	Γ_{132}	Γ_{133}	Γ_{134}	Γ_{135}	Γ_{136}	Γ_{137}	Γ_{138}	Γ_{139}	Γ_{140}	Γ_{141}	Γ_{142}	Γ_{143}	Γ_{144}	Γ_{145}	Γ_{146}	Γ_{147}	Γ_{148}	Γ_{149}	Γ_{150}	Γ_{151}	Γ_{152}	Γ_{153}	Γ_{154}	Γ_{155}	Γ_{156}	Γ_{157}	Γ_{158}	Γ_{159}	Γ_{160}	Γ_{161}	Γ_{162}	Γ_{163}	Γ_{164}	Γ_{165}	Γ_{166}	Γ_{167}	Γ_{168}	Γ_{169}	Γ_{170}	Γ_{171}	Γ_{172}	Γ_{173}	Γ_{174}	Γ_{175}	Γ_{176}	Γ_{177}	Γ_{178}	Γ_{179}	Γ_{180}	Γ_{181}	Γ_{182}	Γ_{183}	Γ_{184}	Γ_{185}	Γ_{186}	Γ_{187}	Γ_{188}	Γ_{189}	Γ_{190}	Γ_{191}	Γ_{192}	Γ_{193}	Γ_{194}	Γ_{195}	Γ_{196}	Γ_{197}	Γ_{198}	Γ_{199}	Γ_{200}
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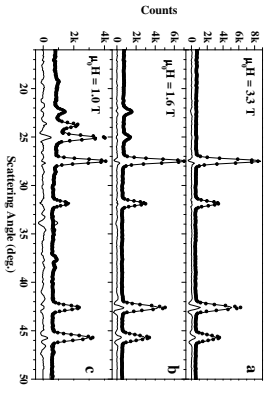
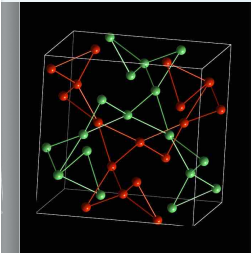
Γ_1 Γ_2 Γ_3 Γ_4 Γ_5 Γ_6 Γ_7 Γ_8 Γ_9 Γ_{10} Γ_{11} Γ_{12} Γ_{13} Γ_{14} Γ_{15} Γ_{16} Γ_{17} Γ_{18} Γ_{19} Γ_{20} Γ_{21} Γ_{22} Γ_{23} Γ_{24} Γ_{25} Γ_{26} Γ_{27} Γ_{28} Γ_{29} Γ_{30} Γ_{31} Γ_{32} Γ_{33} Γ_{34} Γ_{35} Γ_{36} Γ_{37} Γ_{38} Γ_{39} Γ_{40} Γ_{41} Γ_{42} Γ_{43} Γ_{44} Γ_{45} Γ_{46} Γ_{47} Γ_{48} Γ_{49} Γ_{50} Γ_{51} Γ_{52} Γ_{53} Γ_{54} Γ_{55} Γ_{56} Γ_{57} Γ_{58} Γ_{59} Γ_{60} Γ_{61} Γ_{62} Γ_{63} Γ_{64} Γ_{65} Γ_{66} Γ_{67} Γ_{68} Γ_{69} Γ_{70} Γ_{71} Γ_{72} Γ_{73} Γ_{74} Γ_{75} Γ_{76} Γ_{77} Γ_{78} Γ_{79} Γ_{80} Γ_{81} Γ_{82} Γ_{83} Γ_{84} Γ_{85} Γ_{86} Γ_{87} Γ_{88} Γ_{89} Γ_{90} Γ_{91} Γ_{92} Γ_{93} Γ_{94} Γ_{95} Γ_{96} Γ_{97} Γ_{98} Γ_{99} Γ_{100} Γ_{101} Γ_{102} Γ_{103} Γ_{104} <

Example: GGG, complex magnetic ordering



- Highly frustrated lattice with the gamet structure
- 24 magnetic Gd ions per unit cell, divided into two interpenetrating sublattices
- Difference neutron powder diffraction profiles for in an applied field of (a) 3.3 T, (b) 1.6 T and (c) 1.0 T at T = 80 mK
- Peaks cannot be indexed on commensurate magnetic cell
- Neutron powder diffraction data
 - Conventional wisdom: take the positions of the observed reflections, compare with positions predicted by trial-and-error/random search
 - Too many possibilities, not a prayer...

Example: GGG, complex magnetic ordering

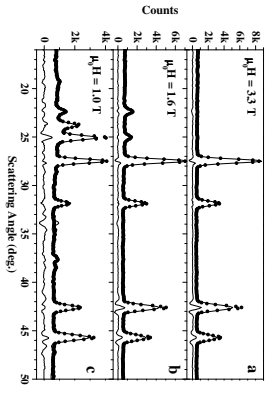
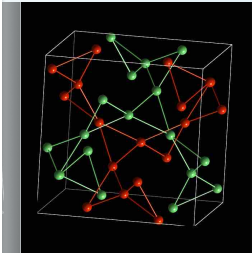


J.R. Stewart et al, J. Phys. Condens. Matter 18,L37 (2006)

15

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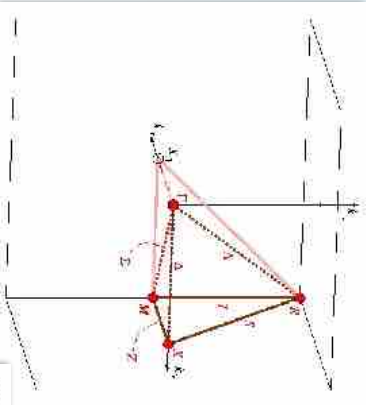
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Field, T	$k_1 = (000)$	$k_2 = (001)$	$k_3 = (0, 0, 0.724)$
1.0	•	•	•
1.6	•	•	•
3.3	•	•	•

Indexing complex magnetic ordering with SARAh



A.S. Willis, Z. Kristallogr. Suppl. 30 (2009) 39-44

Point [16]	Point [17]	Coordinates	Point [16]	Point [17]	Coordinates
k_1	A	$(1, 0, 0)$	k_2	A	$(1, 0, 0)$
k_3	B	$(0, 1, 0)$	k_4	X	$(0, 0, 1)$
k_5	C	$(0, 0, 1)$	k_6	Y	$(1, 1, 0)$
k_7	D	$(1, 1, 0)$	k_8	Z	$(1, 0, 1)$
k_9	E	$(1, 0, 1)$	k_{10}	F	$(0, 1, 1)$
k_{11}	G	$(1, 1, 1)$	k_{12}	H	$(1, 0, 0)$
k_{13}	I	$(0, 1, 0)$	k_{14}	J	$(1, 0, 1)$
k_{15}	K	$(0, 1, 1)$	k_{16}	L	$(1, 1, 0)$
k_{17}	M	$(1, 0, 1)$	k_{18}	N	$(0, 1, 1)$
k_{19}	O	$(1, 1, 1)$	k_{20}	P	$(1, 0, 0)$
k_{21}	Q	$(0, 1, 0)$	k_{22}	R	$(1, 0, 1)$
k_{23}	S	$(0, 1, 1)$	k_{24}	T	$(1, 1, 0)$
k_{25}	U	$(1, 0, 1)$	k_{26}	V	$(0, 1, 1)$
k_{27}	W	$(1, 1, 1)$	k_{28}	X	$(1, 0, 0)$
k_{29}	Y	$(0, 1, 0)$	k_{30}	Z	$(1, 0, 1)$
k_{31}	A	$(1, 0, 0)$	k_{32}	B	$(0, 1, 0)$
k_{33}	C	$(0, 0, 1)$	k_{34}	D	$(1, 1, 0)$
k_{35}	E	$(1, 0, 1)$	k_{36}	F	$(0, 1, 1)$
k_{37}	G	$(1, 1, 1)$	k_{38}	H	$(1, 0, 0)$
k_{39}	I	$(0, 1, 0)$	k_{40}	J	$(1, 0, 1)$
k_{41}	K	$(0, 1, 1)$	k_{42}	L	$(1, 1, 0)$
k_{43}	M	$(1, 0, 1)$	k_{44}	N	$(0, 1, 1)$
k_{45}	O	$(1, 1, 1)$	k_{46}	P	$(1, 0, 0)$
k_{47}	Q	$(0, 1, 0)$	k_{48}	R	$(1, 0, 1)$
k_{49}	S	$(0, 1, 1)$	k_{50}	T	$(1, 1, 0)$
k_{51}	U	$(1, 0, 1)$	k_{52}	V	$(0, 1, 1)$
k_{53}	W	$(1, 1, 1)$	k_{54}	X	$(1, 0, 0)$
k_{55}	Y	$(0, 1, 0)$	k_{56}	Z	$(1, 0, 1)$
k_{57}	A	$(1, 0, 0)$	k_{58}	B	$(0, 1, 0)$
k_{59}	C	$(0, 0, 1)$	k_{60}	D	$(1, 1, 0)$
k_{61}	E	$(1, 0, 1)$	k_{62}	F	$(0, 1, 1)$
k_{63}	G	$(1, 1, 1)$	k_{64}	H	$(1, 0, 0)$
k_{65}	I	$(0, 1, 0)$	k_{66}	J	$(1, 0, 1)$
k_{67}	K	$(0, 1, 1)$	k_{68}	L	$(1, 1, 0)$
k_{69}	M	$(1, 0, 1)$	k_{70}	N	$(0, 1, 1)$
k_{71}	O	$(1, 1, 1)$	k_{72}	P	$(1, 0, 0)$
k_{73}	Q	$(0, 1, 0)$	k_{74}	R	$(1, 0, 1)$
k_{75}	S	$(0, 1, 1)$	k_{76}	T	$(1, 1, 0)$
k_{77}	U	$(1, 0, 1)$	k_{78}	V	$(0, 1, 1)$
k_{79}	W	$(1, 1, 1)$	k_{80}	X	$(1, 0, 0)$
k_{81}	Y	$(0, 1, 0)$	k_{82}	Z	$(1, 0, 1)$
k_{83}	A	$(1, 0, 0)$	k_{84}	B	$(0, 1, 0)$
k_{85}	C	$(0, 0, 1)$	k_{86}	D	$(1, 1, 0)$
k_{87}	E	$(1, 0, 1)$	k_{88}	F	$(0, 1, 1)$
k_{89}	G	$(1, 1, 1)$	k_{90}	H	$(1, 0, 0)$
k_{91}	I	$(0, 1, 0)$	k_{92}	J	$(1, 0, 1)$
k_{93}	K	$(0, 1, 1)$	k_{94}	L	$(1, 1, 0)$
k_{95}	M	$(1, 0, 1)$	k_{96}	N	$(0, 1, 1)$
k_{97}	O	$(1, 1, 1)$	k_{98}	P	$(1, 0, 0)$
k_{99}	Q	$(0, 1, 0)$	k_{100}	R	$(1, 0, 1)$
k_{101}	S	$(0, 1, 1)$	k_{102}	T	$(1, 1, 0)$
k_{103}	U	$(1, 0, 1)$	k_{104}	V	$(0, 1, 1)$
k_{105}	W	$(1, 1, 1)$	k_{106}	X	$(1, 0, 0)$
k_{107}	Y	$(0, 1, 0)$	k_{108}	Z	$(1, 0, 1)$
k_{109}	A	$(1, 0, 0)$	k_{110}	B	$(0, 1, 0)$
k_{111}	C	$(0, 0, 1)$	k_{112}	D	$(1, 1, 0)$
k_{113}	E	$(1, 0, 1)$	k_{114}	F	$(0, 1, 1)$
k_{115}	G	$(1, 1, 1)$	k_{116}	H	$(1, 0, 0)$
k_{117}	I	$(0, 1, 0)$	k_{118}	J	$(1, 0, 1)$
k_{119}	K	$(0, 1, 1)$	k_{120}	L	$(1, 1, 0)$
k_{121}	M	$(1, 0, 1)$	k_{122}	N	$(0, 1, 1)$
k_{123}	O	$(1, 1, 1)$	k_{124}	P	$(1, 0, 0)$
k_{125}	Q	$(0, 1, 0)$	k_{126}	R	$(1, 0, 1)$
k_{127}	S	$(0, 1, 1)$	k_{128}	T	$(1, 1, 0)$
k_{129}	U	$(1, 0, 1)$	k_{130}	V	$(0, 1, 1)$
k_{131}	W	$(1, 1, 1)$	k_{132}	X	$(1, 0, 0)$
k_{133}	Y	$(0, 1, 0)$	k_{134}	Z	$(1, 0, 1)$
k_{135}	A	$(1, 0, 0)$	k_{136}	B	$(0, 1, 0)$
k_{137}	C	$(0, 0, 1)$	k_{138}	D	$(1, 1, 0)$
k_{139}	E	$(1, 0, 1)$	k_{140}	F	$(0, 1, 1)$
k_{141}	G	$(1, 1, 1)$	k_{142}	H	$(1, 0, 0)$
k_{143}	I	$(0, 1, 0)$	k_{144}	J	$(1, 0, 1)$
k_{145}	K	$(0, 1, 1)$	k_{146}	L	$(1, 1, 0)$
k_{147}	M	$(1, 0, 1)$	k_{148}	N	$(0, 1, 1)$
k_{149}	O	$(1, 1, 1)$	k_{150}	P	$(1, 0, 0)$
k_{151}	Q	$(0, 1, 0)$	k_{152}	R	$(1, 0, 1)$
k_{153}	S	$(0, 1, 1)$	k_{154}	T	$(1, 1, 0)$
k_{155}	U	$(1, 0, 1)$	k_{156}	V	$(0, 1, 1)$
k_{157}	W	$(1, 1, 1)$	k_{158}	X	$(1, 0, 0)$
k_{159}	Y	$(0, 1, 0)$	k_{160}	Z	$(1, 0, 1)$
k_{161}	A	$(1, 0, 0)$	k_{162}	B	$(0, 1, 0)$
k_{163}	C	$(0, 0, 1)$	k_{164}	D	$(1, 1, 0)$
k_{165}	E	$(1, 0, 1)$	k_{166}	F	$(0, 1, 1)$
k_{167}	G	$(1, 1, 1)$	k_{168}	H	$(1, 0, 0)$
k_{169}	I	$(0, 1, 0)$	k_{170}	J	$(1, 0, 1)$
k_{171}	K	$(0, 1, 1)$	k_{172}	L	$(1, 1, 0)$
k_{173}	M	$(1, 0, 1)$	k_{174}	N	$(0, 1, 1)$
k_{175}	O	$(1, 1, 1)$	k_{176}	P	$(1, 0, 0)$
k_{177}	Q	$(0, 1, 0)$	k_{178}	R	$(1, 0, 1)$
k_{179}	S	$(0, 1, 1)$	k_{180}	T	$(1, 1, 0)$
k_{181}	U	$(1, 0, 1)$	k_{182}	V	$(0, 1, 1)$
k_{183}	W	$(1, 1, 1)$	k_{184}	X	$(1, 0, 0)$
k_{185}	Y	$(0, 1, 0)$	k_{186}	Z	$(1, 0, 1)$
k_{187}	A	$(1, 0, 0)$	k_{188}	B	$(0, 1, 0)$
k_{189}	C	$(0, 0, 1)$	k_{190}	D	$(1, 1, 0)$
k_{191}	E	$(1, 0, 1)$	k_{192}	F	$(0, 1, 1)$
k_{193}	G	$(1, 1, 1)$	k_{194}	H	$(1, 0, 0)$
k_{195}	I	$(0, 1, 0)$	k_{196}	J	$(1, 0, 1)$
k_{197}	K	$(0, 1, 1)$	k_{198}	L	$(1, 1, 0)$
k_{199}	M	$(1, 0, 1)$	k_{200}	N	$(0, 1, 1)$

2. An introduction to SARAh and SARAh Refine

Overview

- **SARAh**
 - Why I started on this road
 - What it does
 - Why it does what it does
 - Why it's different
 - How it does it
 - Why I like it...

SARAh- what it does

- SARAh = **S**imulated **A**nnealing and **R**epresentational **A**nalysis
 - Perform symmetry analysis of possible magnetic structures using Representational (and Corepresentational Theory)
 - Information for analysing data and understanding phase transitions
 - Clip-on front-end to facilitate reverse Monte Carlo refinement of structures in GSAS using basis vectors and mixing coefficients
 - *Symmetry-free simulated annealing is not normally enough*
 - Clip-on front-end for FullProf using basis vectors and mixing coefficients

SARAh- Why it does what it does

- History (back in the 90s...)
 - Magnetic structures are largely misunderstood
 - K-vector often unknown
 - Few people knew how to do representational theory.
 - Only a handful of examples in the literature
 - Irreducible representation sources :
 - Books
 - Karep
 - Kovalev (little understood)
 - Basis functions
 - calculated by hand
 - CS
 - Mody
- » Generally there was much confusion!

SARAh- Why it does what it does

- Refining a magnetic structure from NPD
 - GSAS uses Red/Black symmetry (restricted, difficult, leads to confusion- 'magnetic unit cell'), used only by the few...
 - FullProf had many different ways of defining structures
 - e.g. rotation matrices, separate definition for helices
 - Complicated, so users built libraries of pcrs
 - Users were typically very confused

SARAh- Why it does what it does

- Make the refinement more physical :
 - **Use a symmetry framework**
 - » **Restrict models to being physically reasonable**
 - » **Create link between magnetic structures and the underlying physics**
- Enable researchers to refine directly in terms of symmetry output
 - Use mixing coefficients as refinement variables
 - Use basis vectors and k-vectors to define symmetry relationships
 - » **Create a general refinement system**
 - *Do not reinvent the wheel (i.e. let users use GSAS, FullProf)*
 - » **SARAh as a suite of programs**
 - Symmetry calculations
 - Refinement assistant
 - *Help* unspecialised users as much as possible
 - k -search with FullProf
 - » **Generate better understanding, better analyses**

SARAh- How it does it

- **GSAS implementation**
 - SARAh controls all aspects of symmetry and the moment orientations, the rest is normal GSAS
 - P1 phase in GSAS (avoid red/ black, allow complex symmetries), Full magnetic cell
 - Lock down non-magnetic variables
 - Set GSAS for 2-3 LS cycles (i.e. converge), normal user control
 - SARAh edits .exp file to insert all atom positions
 - User selects symmetry type (representation, basis vectors)
 - SARAh matches atoms being refined, replaces moments, launches GENLES
 - RMC/Simulated Annealing refinement

SARAh- How it does it

- **Fullprof implementation**
 - External front end to prepare and edit the pcr file, write fst file
 - Not command line, simplest user choices. Buttons, scroll bars, etc
 - Help user as much as possible*****
 - Simplicity, simplicity, simplicity*****
 - Unique k-search engine
 - Main technical difficulties are with:
 - Format in FullProf, its ongoing development !! Complex basis vectors but real or imaginary mixing coefficients...
 - Definition of the magnetic structure- Fullprof over-defines the structure, better to generate each moment l time

OK, I have data where do I go from here?

- **Do we know the k vector**
 - We hope
 - Do we know that there is more than one? Maybe...
- **Carry out representational analysis calculations**
- **Do we know which IR is primary?**
 - No, so cycle through IRs until you find it
 - At this point freely explore coefficients
- **Do we know the order parameter direction?**
 - Now we have the IR, search through mixing coefficient combinations
 - Add basis vectors if fit is improved
- **Add secondary IR if the fit is improved**
 - Search through mixing coefficient combinations
- **Add another k vector if there are peaks that do not line up**
 - » Repeat as needed

Things to keep in mind

- **k-vectors in centred cells need to be handled with care, e.g. k=(100) in BCC**
 - When in doubt, convert to primitive and transform to centred setting
- **Representational analysis calculations do not get rid of degrees-of-freedom**
 - Symmetry is about classifying them
 - Deal with only a few variables at a time. More models, each with fewer variables
 - Order parameter directions mean even fewer at a time (only a couple may be active)
- **Basis vectors can be complex**
 - Enjoy what this can make as a structure
 - The space that they define shows you what is possible within your unknown Hamiltonian. Think of the physics you are looking for
- **Relate your analysis to other information**
 - Don't use diffraction in isolation

Things to keep in mind

- **If you need to couple IRs**
 - Do it consciously - think about it (Does this make sense? How does it work with Landau theory? What can cause it?)
- **Are there things that you cannot see?**
 - e.g. multi k structures. Very cool and we know little about them (because we rarely think about them)
- **Multiple phase transitions and 1st order transitions**
 - Typically high temperature one is 2nd order; the low temp one is 1st order (often involving another IR coming in)
 - 1st order does not follow Landau theory, but might (mostly). A sliding scale
 - Treat the 'single IR law' as a reference. Look for where it is broken and think about what this means within the IR of G₀!
- **Building up magnetic structures**
 - The Fourier sum can build any magnetic structure. Just keep adding what you need.

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

Add what you need, when you need it ...

- Building-up the magnetic structure

- **Ockham's razor**

- **pluralitas non est ponenda sine necessitate**

(“plurality should not be posited without necessity”)

my version

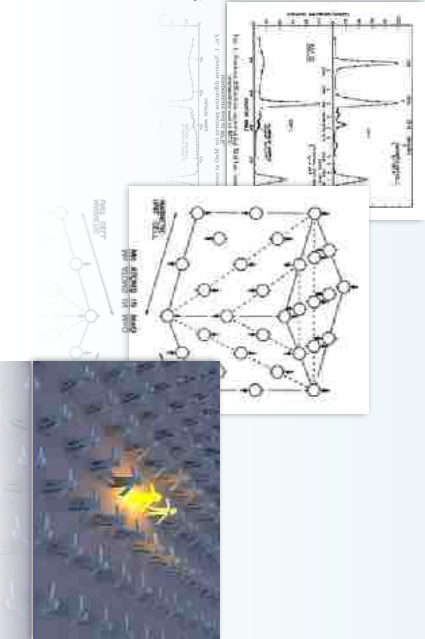
don't introduce unnecessary variables, use symmetry and physics to reduce them

- Work out what the necessity is
 - Think about why!
 - There lies the fun...
- There lies the physics

Refining magnetic structures using representational theory and SARAh - learning from simplicity and *Serendipity*

Andrew S. Wills

UCL Chemistry
Associate Dean for Research
Mathematical and Physical Sciences



Refining magnetic structures and symmetry analysis
Start with ‘what are they?’

- ‘Original’ SARAh - Representational Analysis (1999)
 - **History** - refinements using manually defined magnetic space groups (GSAS, FullProf) or one of several structure definitions (FullProf), e.g. helical structure. Quite specialist. Lots of mistakes, particularly over what a k-vector is..
 - **Performed calculations of representational analysis** (Bertaut’s method) using the tables of Kovalev to give irreducible representations (IRs) and basis vectors (BVs)
 - **SARAh-Refine** was a front-end (meta-program) that took the BVs from SARAh, substituted related moments into the **GSAS** exp file, ran GENLES, read the results and carried out **simulated annealing** (**reverse-Monte Carlo**). Moved refinement from moment components to basis vectors and mixing coefficients - **direct basis vector refinement**

$$\{m_a, m_b, m_c\} \rightarrow \vec{m}_j = \sum_{\nu,k} C_{\nu}^k \vec{\psi}_{k,\nu}^h, \quad e^{-2\pi i k \cdot t_{i,j}}$$

- **SARAh** = Simulated Annealing and Representational Analysis (works for commensurate and single-k incommensurate structures)
- FullProf then introduced mixing coefficient refinement and **SARAh-Refine** was extended to work with **FullProf** and **TOPAS** by making template for the magnetic phases and editing the refinement files.

Refining magnetic structures, symmetry analysis of magnetic structures

- **web SARAh** (2018)
 - Move from Windows-based codes to web code with calculations carried out in **Wolfram Mathematica**. Functionality independent of operating system, users do not need licences.
 - Performs the same calculations as original SARAh - Representational Analysis (following Bertaut's method) to give Irreducible Representations (IRs) and basis vectors (BVs)
 - Extended to include (amongst other things)
 - **Stationary vectors** (analogous to 'isotropy groups', of Jovic and the Isotropy suite) but using the **Black+White point groups** rather than magnetic space groups
 - These define high-symmetry structures within the space of an IR
 - Treat commensurate and incommensurate structures as the same
 - **Exchange Multiplets** (Izyumov) to connect IRs with isotropic spin and exchange symmetry
- **webSARAh Refine** (2022)
 - Works with FullProf: Makes magnetic phases, edits .pcr file directly for easy selection and refinement of BVs (using B+W stationary groups and exchange multiplets)

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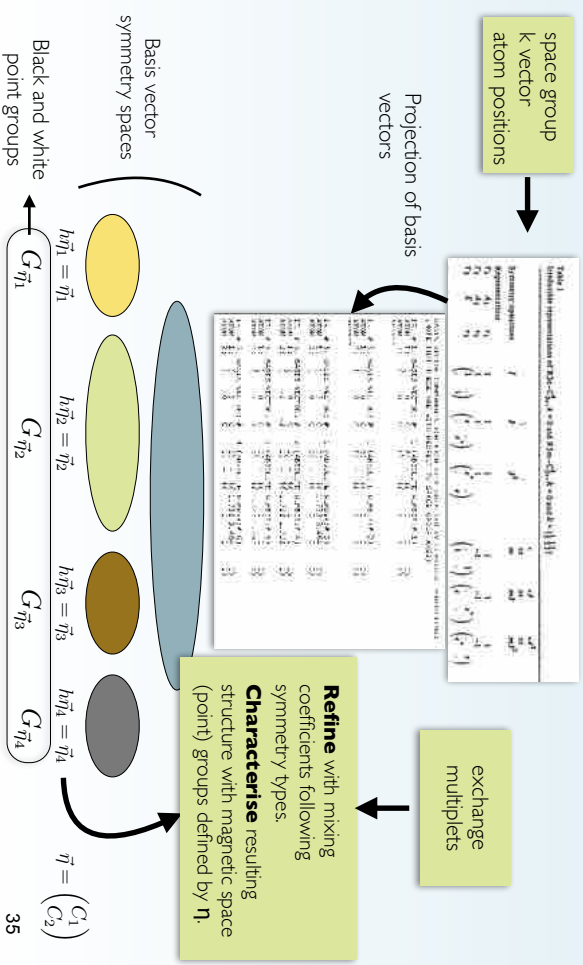
Symmetry analysis and refining magnetic structures

Now move to ‘why this one?’

- **Current developments** - moving beyond the mechanics of describing magnetic structures and helping create understanding of the physical reasons for a magnetic structure to form. See this as key to control or properties and intelligent design)
 - Introduce **anti-unitary symmetry** (Wigner) which brings in complex conjugation and time-reversal in a complete way
 - Calculations of **invariant polynomials** to enable better understanding of energy drives for a given magnetic structure, also to reduce confusion over Landau theory...
 - **Quadrupoles** - **tensor analysis** and useful for **orbital ordering**
 - ‘**Serapsis**’ - another view of the relationships between representation theory and magnetic space groups and spin groups
 - *Making coherent use of the various theories to maximise the information that we have and use when we analyse magnetic structures - a philosophy and an educational-piece*

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SARAh- Refine Flow chart



Broadening the foundations SARAh



- 1927 Wigner; Heisenberg, Hunds, Heitler -exchange coupling
- **1936 Wigner - Antiunitary symmetry**
- **1937 Landau, Dzyaloshinski - Phase transitions**
- **1953, 55, 57, - Shubnikov, Zanozraev**
Belov - B+W groups
- 1958, Dzyaloshinski, 1960 Moriya,
- 1959 Villain and Kaplan eigenvectors and positive eigenvalues - minimum energy spin arrangement
- 1962 Bertaut - Exchange interactions and Hamiltonians
- **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**

History can make confusions and be daunting...

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Broadening the foundations SARah



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- **1936 Wigner - Anticommutary symmetry**
1937 Landau, Dzyaloshinski - Phase transitions
- **1953, 55, 57, - Shubnikov, Zanozraev**
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- **1981 Jaric; 1984 Stokes and Hatch**
Isotropy subgroups
- **2001 Sikora - Quadrupoles**

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Try to make an easier path...

Add what you need, when you need it ...

- My building-up principle for magnetic structures

Ockham's razor

- **pluralitas non est ponenda sine necessitate**
 - ▶ ("plurality should not be posited without necessity")
 - ▶ ("don't use variables unless you need to")
 - ▶ ("don't make your refinement any harder than you need to")

Theories help you work out what the necessity is

- Think about why!
- There lies the fun...
- There lies the physics

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Symmetry analysis and refining magnetic structures

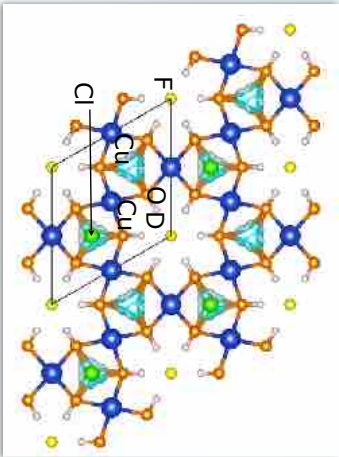
Epilogue

- Landau was not entirely wrong in his view that antiferromagnetic states were unstable with respect to quantum fluctuations.
- This notion was continued by the Nobel prize winning physics Phil Anderson in 1973. He was exploring how Neel order could be destabilised by quantum fluctuations. This was a route to a new type of magnetic ground state called the **Resonating Valence Bond (RVB)** state, that was defined by fluctuations and topology rather than static order and local symmetry.
- Anderson proposed that the RVB could be favoured by frustration and would underlie the transition to high temperature superconductivity in the cuprates.
- Landau's ideas would later point to an entirely new direction in condensed matter science and a new class of electronic state called **quantum spin liquids** and started the search for example materials. Most notably studies of **S=1/2 kagome antiferromagnets** ...

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S = 1/2 kagome antiferromagnets

Madeleine Georgopoulou (UCL, ILL) and Björn Fåk (ILL)

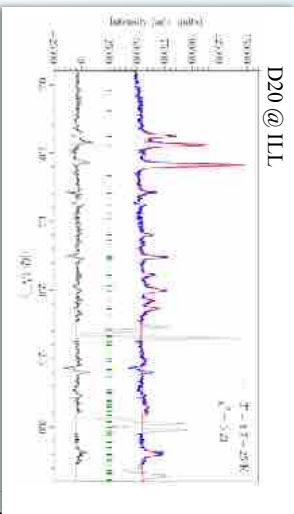


Claringbullite: Cu₄(OD)₆FCI

- AA stacking of kagome planes
- P6₃/mmc at high temperature
- Pnma at low temperature
- **µSR**: antiste disorder is an order of magnitude lower than in herbertsmithite
- Magnetic order T<17 K
- Goal - use exchange interactions to understand the Hamiltonian of the Zn-doped material, ZnCu₃(OD)₆FCI which we believe to be an candidate quantum spin liquid

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Cu₄(OD)₆FCI: Magnetic structure from neutron diffraction and exchange model

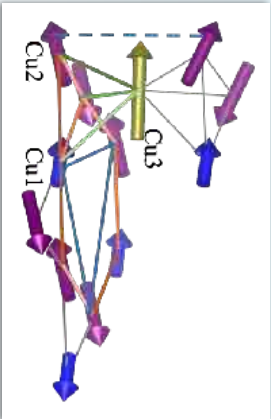


- Magnetic space group: *Pn'm'a*
- **k = 0**, Irrep Γ_7 (Kovalev's notation)
- 3 Cu sites with different sized ordered moments. **Complex canting!**

M. Georgopoulou, *et al.*, Phys. Rev. B 107, 024416 (2023).
K. Tustain, *et al.*, Chem. Mater. 33, 9638 (2021).

Cu site	Claringbullite Γ_7		
	Moment size (μ_B)	AFM out-of-plane canting	FM in-plane canting
Cu1	0.3	0	0
Cu2	0.4	18	0
Cu3	0.5	0	17

Cu₄(OD)₆FCI: Magnetic structure from neutron diffraction and exchange model



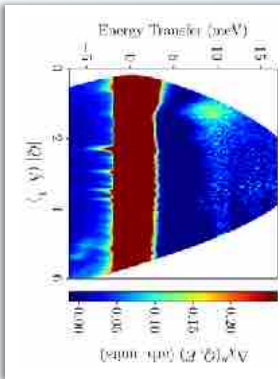
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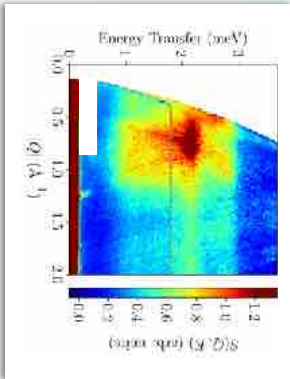
M. Georgopoulou, *et al.*, Phys. Rev. B 107, 024416 (2023).
K. Tustain, *et al.*, Chem. Mater. 33, 9638 (2021).

Cu₄(OD)₆FCI: Spin waves using data from PANTHER and IN5 @ ILL

$T=1.8 - 100$ K
 $E_f = 19.2$ meV
 $Q=1.25 \text{ \AA}^{-1}$, Bandwidth = 8.3 meV,



$T=1.6$ K, $E_f = 3.55$ & 5.11 meV
 $Q=0.73 \text{ \AA}^{-1}$, Bandwidth = 2.77 meV,
Zero-energy gap = 0.45 meV.

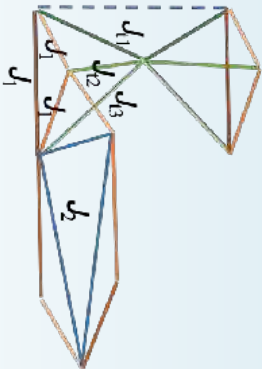


- Two magnetic responses gapped from each other
- Gapless excitations

M. Georgopoulou, B. Fåk, D. Boldrin and A.S. Willis, (2021), [doi:10.5291/ILL-DATA.INTER.516](https://doi.org/10.5291/ILL-DATA.INTER.516)
M. Georgopoulou, B. Fåk, D. Boldrin, J. Olivier and A.S. Willis, (2021), [doi:10.5291/ILL-DATA.INTER.519](https://doi.org/10.5291/ILL-DATA.INTER.519)

Cu₄(OD)₆FCI: Modelling spin waves in SpinW Results

- Starting point: DFT and tenth-order high-temperature series expansion!
 - 4 exchanges: did not stabilise the experimental magnetic structure (no go in SpinW)
- Claringbullite, this work
 - ‘‘Serendipity’’: new protocol for determining exchanges that stabilise observed magnetic structure?
- Antiferromagnetic lagome + interplanar exchanges
- Ferromagnetic ‘tripod’ exchanges
- $DM = 10\% J_{ij}$
- $\theta_w = -95$ K (exp. = -136 K)



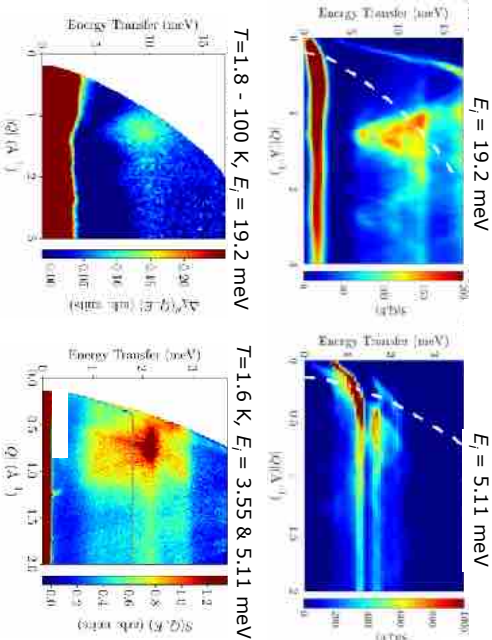
J_i	Value (meV)
J_1	14
J_{11}	-6.5
J_{12}	-3.5
J_{13}	-6
J_c	4
J_2	0.2

¹ H. O. Jeschke, *et al.*, Phys. Rev. B 92, 094417 (2015).
² A. S. Willis, Serendipity, *unpublished*.

Cu₄(OD)₆FCI: Modelling spin waves in SpinW

Model versus experiment

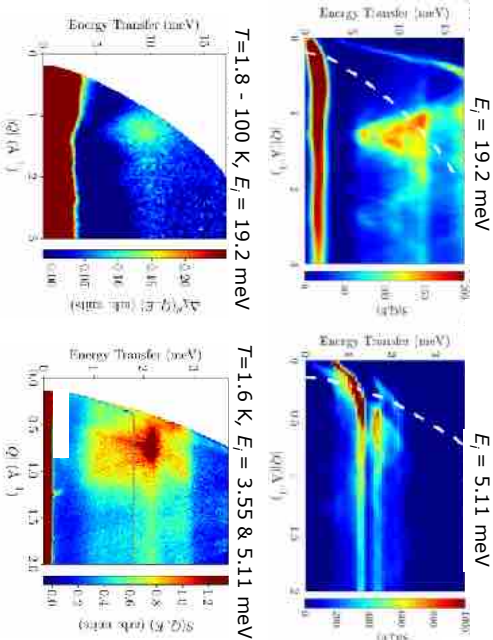
- 2 magnetic responses with appropriate gap sizes.
- 10 meV excitation: good agreement in Q and bandwidth.
- 2 meV excitation: two excitation bands but less good agreement.
- (not necessarily the end, but a very good start)



M. Georgopoulou, *et al.*, Phys. Rev. B 107, 024416 (2023).

Cu₄(OD)₆FCI: Modelling spin waves in SpinW

J _i	Value (meV)
J ₁	14
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J ₁₂	-3.5
J ₁₃	-6
J _c	4
J ₂	0.2



M. Georgopoulou, *et al.*, Phys. Rev. B 107, 024416 (2023).

And now the ‘how’...

Cu₄(OD)₆FCI: Modelling spin waves in SpinW Analysis technique?

- The 4 exchange parameters from literature did not give a stable magnetic structure in SpinW and could not be used to model the spin wave spectra
- Need something that can handle 8 exchange interactions
- What to do?
 - Use eigenvectors?
 - Use Monte Carlo?

Early ideas - Villain, Lyons and Kaplan,

- The problem is that this gives a global phase
- Not much information for non-collinear structures where the the angles between the moments are not simple

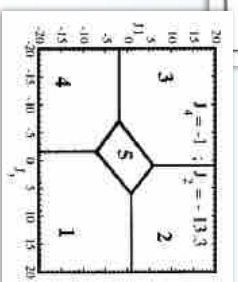
$$\xi_{ij}(\mathbf{k}) = -\sum_{\mathbf{r}_p} J_{ij}(\mathbf{R}_p) e^{2\pi i \mathbf{k} \cdot \mathbf{R}_p}$$

Structure	M_{11}	M_{12}	M_{21}	M_{22}	M_{31}	M_{32}
1. $\mathbf{k}=(1,0,0)$	+	-	-	+	-	+
2. $\mathbf{k}=(0,1,0)$	+	+	+	+	+	+
3. $\mathbf{k}=(0,0,1)$	+	+	+	+	+	+
4. $\mathbf{k}=(1,0,0)$	+	+	+	+	+	+
5. $\mathbf{k}=(0,1,0)$	+	+	+	+	+	+

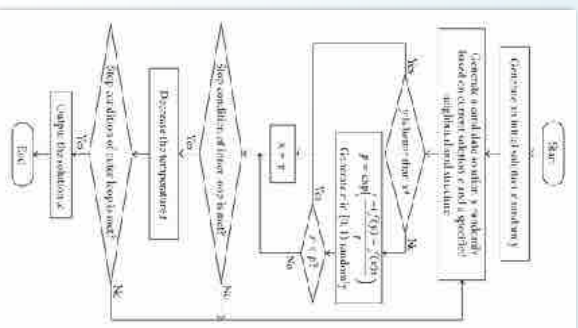
Case of disordered or incommensurate structures

- Tends to be used to make high-level phase diagrams
- This cannot be used algebraically for complex matrices as the eigenvectors will involve complex roots. Use grid search

This technique isn't heavily used to understand the orderings of magnetic structures



Early ideas - Monte Carlo



1. Follow Bertand - set up an exchange matrix. Include Dzyaloshinski and Moriya vectors
2. Go beyond Bertand's theory and use the exchange matrix to perform symmetry analysis of the related isotropic exchange Hamiltonian
3. Monte Carlo- conventional thought may be to
 1. Make a large unit cell/set boundary conditions
 2. Take a set of exchange values (vector in the space of exchange interactions)
 3. determine stable magnetic structure by MC protocol - make changes to spin structure,
 4. Repeat to validate solution
4. Problem - **computationally very expensive**. I started from needing to go beyond the literature models, and the next step looked like an **8 exchange values**. Taking 10 trial values for each **exchange energy gives > 10⁸ sets of SA runs**. With 1 hour per run this direction of study effectively fails... Need another way...

Cu₄(OD)₆FCI: Modelling spin waves in SpinW

- The 4 exchange parameters from literature did not give a stable magnetic structure in SpinW and could not be used to model the spin wave spectra
- Need something that can handle 8 exchange interactions
- What to do?
 - Use eigenvectors? Not enough 'angular resolution'
 - Use Monte Carlo? Too expensive/slow for this problem
- Something more creative? ... Literally focusing on the problem - **what stabilises the experimental structure...**

Cu₄(OD)₆FCI: Modelling spin waves in SpinW

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Foundations of Serendipity

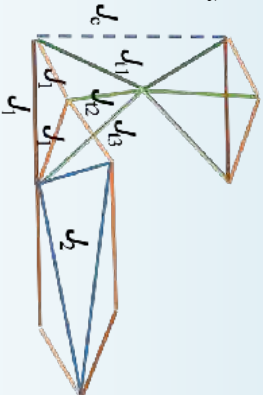
Some background theories



- 1906 Weiss
 - 1937 Landau, Dzyaloshinski - Phase transitions
 - 1936 Wigner - Antunitary symmetry
 - 1946 Luttinger-Tisza - minimum energy spin arrangement. 1958, Dzyaloshinski, 1960 Moriya,
 - 1959, 60s Vlain and Kaplan eigenvectors and positive eigenvalues - minimum energy spin arrangement
 - 1962 Bertaut - Exchange interactions and Hamiltonians
 - 1968 Bertaut - Representation theory
 - 1979 Izyumov - Exchange multiplets
 - 1981 Jaric; 1984 Stokes and Hatch Isotropy subgroups
 - Serapis is likely to be helpful with possible tie in with Landau theory
- A. S. Wills, Serendipity, unpublished.

Cu₄(OD)₆FCI: Modelling spin waves in SpinW

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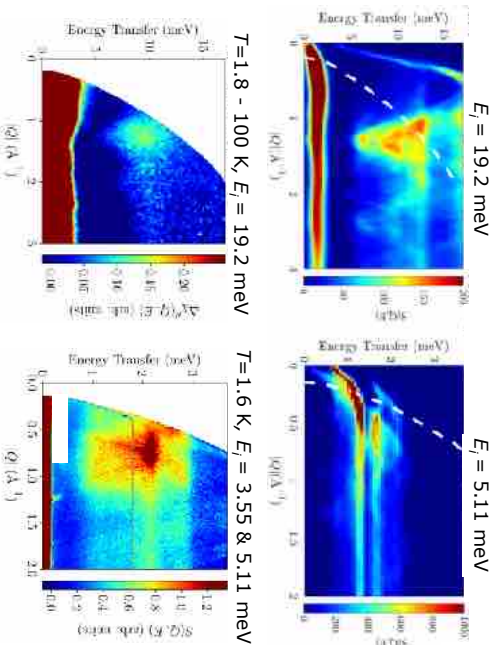
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Need more test systems!

M. Georgopoulou, *et al.*, Phys. Rev. B 107, 024416 (2023).
A. S. Wills, Serendipity, unpublished.

Cu₄(OD)₆FCI: Modelling spin waves in SpinW

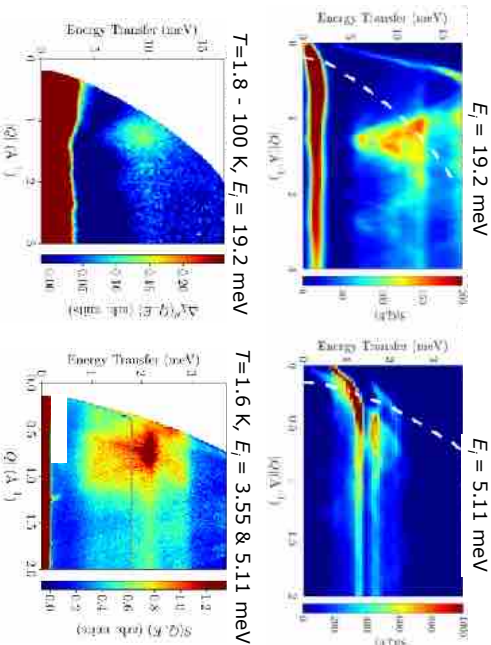
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M. Georgopoulou, *et al.*, Phys. Rev. B 107, 024416 (2023).

Symmetry analysis, refining magnetic structures, stability conditions, spin wave analysis

- **My current developments** - moving beyond the mechanics of describing magnetic structures and focussing on creating understanding of the physical reasons for a magnetic structure to form
- **A personal view**
 - Software needs to be based on physical principles (AI development now moves towards physics-encoded AI)
 - History often makes inconsistencies and confusion
 - **webSARAh, webSARAh-Refine** have a development track to make a clear path through historical theories and refine the analysis technique of direct basis vector refinement.
 - **Serendipity** is a new way to study magnetic stabilities (and help spin wave studies). It was built for Claringbullite (a rather hard problem). I am very happy to discuss ideas and learn more from people that actually understand spin waves
 - **SERAPSIS** is (I hope) going to connect symmetry ideas and make clarity