Symmetry in the spin-orbit free limit: spin groups & representation theory



Quantum Geometry and Transport of Collective Excitations in (Non-)Magnetic Insulators



Overview

- Intro to spin groups •
- Co-representation theory of spin point • groups
- Do we need spin group theory? •
- Landau theories for collinear altermagnets

Collaborators

My advisor!





Judit Romhányi UC Irvine



Paul McClarty Université Paris-Saclay



Jeff Rau University of Windsor



University of Windsor





Intro to spin groups

Hana Schiff Thursday, May 8th, 2025

Quantum Geometry and Transport of Collective Excitations in (Non-)Magnetic Insulators







An operation \hat{O} that transforms the state $|\psi\rangle$ such that

 $\hat{O} | \psi \rangle = | \psi \rangle$

 $|\psi\rangle$ transforms as a scalar, "invariant" under \hat{O}



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Magnetic order





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...of a Hamiltonian

An operation \hat{O} that transforms the Hamiltonian \mathcal{H}

Shared eigenspaces





An operation \hat{O} that transforms the state $|\psi\rangle$ such that

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 $|\psi\rangle$ transforms as a scalar, "invariant" under \hat{O}







Crystallographic point groups



Symmetries of finite figures compatible with a 3D lattice

32 groups



Crystallographic point groups



Moritz L. Frankenheim



1826

Johann F. C. Hessel



1830

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Crystallographic space groups



230 groups



Symmetries of finite figures compatible with a 3D lattice

32 groups





Curie

Ralph W.G. Wyckoff









1891







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Symmetries of finite figures compatible with a 3D lattice

32 groups





Curie

Ralph W.G. Wyckoff

6/*mmm*

Evgraf Fedorov 1891

Arthur M. **Schoenflies**





1651 groups



William **Barlow**



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Crystallographic space groups



230 groups



Symmetries of finite figures compatible with a 3D lattice

32 groups





Pierre Curie

Ralph W.G. Wyckoff





Alexander M Zamorzaev



Ben Zion Tavger

Magnetic groups

V. Zaitsev E. I. Sokolov J. O. Dimmock R. G. Wheeler





6/*mmm*



Arthur M. **Schoenflies**



Magnetic point groups 122 groups Magnetic space groups

1651 groups

Shubnikov

1951

Erwin-Félix





Spin Orbit Coupling (SOC)



- Spins are "locked" to the lattice
- Transformation applied to both lattice and spins
- Spins are axial, time-reversal (TR) odd vectors





Spin Orbit Coupling (SOC)



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Magnetic symmetry & spin-orbit coupling **1830** Point groups **1890** Space groups **1960** Magnetic groups **2020** Spin groups Negligible or No SOC Spins (and Hilbert) space) decoupled from lattice Ex: Heisenberg $\mathscr{H} = \sum J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$ Spin-space elements from $\mathbf{O}^{s}(3) \equiv \mathbf{SO}(3) + \tau \mathbf{SO}(3)$ 8







Magnetic symmetry & spin-orbit coupling **1830** Point groups **1890** Space groups **1960** Magnetic groups **2020** ---->

Spin groups





Magnetic symmetry & spin-orbit coupling **1960** Magnetic groups **2020**

Spin groups



Magnetic symmetry & spin-orbit coupling **1830** Point groups **1890** Space groups **1960** Magnetic groups **2020** Spin groups Real materials have SOC! Why is this useful? **Topological magnons** Z. Xiao, J. Zhao, Y. Li, R. Shindou, Z.D. 164.5 Song Phys. Rev. X 14, 031037 (2024) ີ∂ 164.0 **Topological electronic** E 163.5 (and magnetic) states Chirality splitting 163.0 А wavevecto Exotic nodal-line and X. Chen, Y. Liu, P. Liu, Y. A. Corticelli, R. Moessner, Yui, J. Ren, J, Li, A. P. McClarty Phys. Rev. B Zhang, Q. Liu, Nature -point semimetals 105, 064430 (2022) 640, 349-354 (2025) Exotic otherwise forbidden TIs





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Magnetic symmetry & spin-orbit coupling **1830** Point groups **1890** Space groups 1960 Magnetic groups 2020 Spin groups Real materials have SOC! Why is this useful? **Topological magnons** Altermagnets Z. Xiao, J. Zhao, Y. Li, R. Shindou, Z.D. Song Phys. Rev. X 14, 031037 (2024) 164. ≥164.0 Topological electronic (and magnetic) states E 163.5 Chirality splitting 163.0 Α wavevecto Exotic nodal-line and X. Chen, Y. Liu, P. Liu, Y. L. Šmejkal, J. Sinova A. Corticelli, R. Moessner, Yui, J. Ren, J, Li, A. P. McClarty Phys. Rev. B and T. Jungiwirth, Phys. Zhang, Q. Liu, Nature -point semimetals 105,064430 (2022) Rev. X 12, 040501 (2022) 2412.18025 640, 349-354 (2025) Exotic otherwise **Precise when SOC is negligible, and dictates** forbidden TIs salient features of systems with weak SOC.







1830 Point groups **1890** Space groups















Spin operation [S||E]Only spins transform $|S||E| M^{\alpha}(\mathbf{r}) = S_{\alpha\beta} M^{\beta}(\mathbf{r})$

All [S||R] leaving magnetic order invariant: spin group X $\underline{X} < O^{s}(3) \times E(3)$

Spin group transformations



Generically different operations on spins and lattice

Many more possible groups!

 $\left[S\|R\right]M^{\alpha}(\mathbf{r}) = S_{\alpha\beta}M^{\beta}(R^{-1}\mathbf{r})$



Spin operation [S||E]Only spins transform $|S||E| M^{\alpha}(\mathbf{r}) = S_{\alpha\beta} M^{\beta}(\mathbf{r})$







All elements [S||E]form a normal subgroup, the **spin-only group** $\mathbf{b} = \{ [S||E] \in \mathbf{X} \}$



 $\left[S\|R\right]M^{\alpha}(\mathbf{r}) = S_{\alpha\beta}M^{\beta}(R^{-1}\mathbf{r})$



Spin operation

[S||E]

Only spins transform



$\underline{\mathbf{X}} = \underline{\mathbf{b}} \times \underline{\mathbf{S}}$

The non-trivial (NT) spin group S only contains [S||R] where $R \neq E$

All elements [S||E] form a normal subgroup, the **spin-only group**

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depends on mutual spin orientations

D.B. Litvin, W. Opechowski, Physica Vol. 76, Iss. 3, (1974)

Spin groups \underline{X} $\mathbf{X} = \mathbf{b} \times \mathbf{S}$ Spin-only group $\underline{\mathbf{b}} = \{ [S || E] \in \underline{\mathbf{X}} \}$ Non-trivial spin group [S||R] with $R \neq E$





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Coplanar $\mathbf{b}^{\mathbb{Z}_2} \cong \{E, \tau 2_+\}$ $2_{\perp}: \ \pi \ \text{rotation about} \\ \text{axis } \perp \ \text{to normal}$ $\tau 2_{\perp}$ is a mirror in the plane of the spins

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 $\mathbf{X} = \mathbf{b} \times \mathbf{S}$ **Spin-only group** $\underline{\mathbf{b}} = \{ [S || E] \in \underline{\mathbf{X}} \}$ Non-trivial spin group [S||R] with $R \neq E$ $\begin{bmatrix} S \| R \end{bmatrix} M^{\alpha}(\mathbf{r}) = S_{\alpha\beta} M^{\beta}(R^{-1}\mathbf{r})$





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Group derivation algorithm

Find all NT spin groups











For each ordinary parent group G :









For each ordinary parent group G : ← List all normal subgroups $g \triangleleft G$









For each ordinary parent group G : + List all normal subgroups $g \triangleleft \underline{G}$ + Determine quotient groups $\underline{B} \cong \underline{G}/g$









- For each ordinary parent group G:
- + List all normal subgroups $g \triangleleft \underline{G}$
- + Determine quotient groups $\underline{\mathbf{B}} \cong \underline{\mathbf{G}}/\mathbf{g}$
 - Option 1: determine explicit isomorphism between \underline{B} and \underline{G}/g









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 representation of <u>G</u> with kernel g











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15

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 - Option 2: generate O(3) representation of <u>G</u> with kernel g
- + Form $\underline{\mathbf{S}} = \underline{\mathbf{g}} + [B_2 || G_2] \underline{\mathbf{g}} + [B_3 || G_3] \underline{\mathbf{g}} + \dots$



















Wladyslaw Opechowski







Afonso Guerreiro + HS

Paul McClarty

Judit Romhányi





◆ 598 non-trivial SPGs • 90 are B&W groups.

Wladyslaw Opechowski







Afonso Guerreiro + HS

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Yutong Yu Ao Zhang Jiayu Li,

Qihang Liu Caiheng Li





- ◆ 598 non-trivial SPGs
 - 90 are B&W groups.
- + 90 collinear SPGs
 - 32 ferromagnetic, when $\mathbf{B} = \{E\}$
 - 58 antiferromagnetic when **B** = {*E*, τ }

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Recall: $\underline{B} \cong \underline{G}/g$, and $\underline{\mathbf{B}} = \{B \mid [B \| G] \in \underline{\mathbf{X}}\} \text{ is the group}$ of elements acting on spins

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- ◆ 252 coplanar SPGs
 - When $\mathbf{B} = \mathbf{C}_n$ or \mathbf{D}_n

Recall: $\underline{B} \cong \underline{G}/g$, and $\underline{\mathbf{B}} = \{B \mid [B \| G] \in \underline{\mathbf{X}}\} \text{ is the group}$ of elements acting on spins

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Wladyslaw Opechowski



Original Litvin table

1	¹ 4 ¹ 2 ¹ 2	
2	$1_4^2 2_2^2 2_2$	
m.	¹ 4 ^m 2 ^m 2	
ī	¹ 4 ¹ 2 ¹ 2	
2	² 4 ¹ 2 ² 2	
ш	^m 4 ¹ 2 ^m 2	
ī	1 ₄ 1 ₂ 1 ₂	
222	$2_{x_4}^{2}_{y_2}^{2}_{z_2}^{2}$	
mm 2	² z4 ^m x2 ^m y2	
	m _{x4} ² z2 ^{my} 2	
2/m	² 4 ¹ 2 ^m 2	
	1 ₄ 22 ^m 2	
	m4 ¹ 2 ² 2	
422	4 ₂₄ 2 ₂₂ 2xy2	422
4 mm	⁴ z4 ^m x2 ^m xym	42'2'
42m	$\overline{4}_{z_4}^2 x_2^m x_2^y$	4'22'

D. B. Litvin, Acta Crystallographica A 33 (2), 279 (1977)





+ HS

Paul McClarty

Judit Romhányi

	I	, ,	, ,
422	130	$^{1}4^{1}2^{1}2$	422
	131	$^{1}4^{2}2^{2}2$	422
	132	$^{1}4^{m}2^{m}2$	42′2′
	133	$^{1}4^{\overline{1}}2^{\overline{1}}2$	42′2′
	134	$^{2}4^{2}2^{1}2$	422
	135	${}^{m}4{}^{m}2{}^{1}2$	4′2′2
	136	$\overline{1}4\overline{1}2^{1}2$	4′2′2
	137	$2_x 4^{2_z} 2^{2_y} 2^{2_y}$	422
	138	$2_{z}4^{m_{x}}2^{m_{y}}2$	42′2′
	139	$m_x 4^{2_z} 2^{m_y} 2$	4′2′2
	140	$^{2}4^{\overline{1}}2^{m}2$	42′2′
	141	$1^{\overline{1}}4^{2}2^{m}2$	4′2′2
	142	$^{m}4^{\overline{1}}2^{2}2$	4′2′2
	143	$4_{z}4^{2_{x}}2^{2_{xy}}2^{2_{xy}}2^{2_{xy}}$	422
	144	$4_{z}4^{m_{x}}2^{m_{xy}}m$	42′2′
	145	$\overline{4z}4^{2_{x}}2^{m_{xy}}2$	4'2'2



Jun Ren Yutong Yu Ao Zhang Jiavu Li.

Qihang Liu

HS, A. Corticelli, A. Guerreiro, J. Romhányi, P. McClarty, SciPost Phys. 18, 109 (2025)







Spin space groups Depends on unit cell enlargement

Supercells up to order 8

230 1191

 $G^{S} = 1$

100612 SSGs

- ◆ 1421 collinear
- ◆ 16383 coplanar
- ◆ 87308 non-coplanar

67475 SSGs

- ◆ 1421 collinear
- ◆ 9542 coplanar
- ◆ 56512 non-coplanar

Identify the spin group from .cif, .mcif or .txt

1191 15192

n, *n*2, *n*22 (except 1, 2)

Noncoplanar SSG (87 308)

Others Polyhedra

86 951 357

FINDSPINGROUP: Identify Spin Group and Related Properties

Online Program: FINDSPINGROUP [1]



Manual: International notation of Spin Space Group and How to use FINDSPINGROUP

International Symbol of G_{NS} Symbols of L_0 , G_0 , i_t , i_k , G^s output Standard Magnetic Cell Operations of G_{SS} , etc





Qihang Liu

Xiaobing Chen Jun Ren Yanzhou Zhu Yutong Yu Ao Zhāng Pengfei Liu, Jiayū Li, Yuntian Liu Caiheng Li



Zhi-Da Song

Zhenyu Xiao Jianzhou Zhao Yanqi Li Ryuichi Shindou



Yi Jiang Ziyin Song Zhong Fang Hongming Weng Jian Yang

Chen Fang

Families ~ mod. symmetry of the propagation vector

$\triangle \hat{\mathcal{P}}$ -invariant $\diamond \hat{\mathcal{T}}$ -invariant • Generic points - Action of $\hat{\mathcal{P}}\hat{\mathcal{T}}$

Supercells up to order 12

183498 SSGs

- ◆ 1421 collinear
- ◆ 24788 coplanar
- ◆ 157289 non-coplanar

Groups & group elements for SSGs:

Types of SSG Make selection 🔶		Welcome to the Spin Space Group Database							
Spacegroup number	eg. 230.1.1	1 or 230.1.1.1.L			× All possib	le SSG 🗢	Search		
Select -	Fou	Found 1746 entries, showing 1746				3 4	> »		
H Spacegroup number	SSG number 🇊	dimension (Group number of pure lattice symmetry	Point group of Q	Point group of spin part	supercell 🕽	Action		
$L_{h} = T \cdot T_{u} $	132.1.1.1	3	132	1	1	[1]	Details		

Search based on parent group, list elements, etc... Spin Space Group

Database





(Co-)representation Theory

Hana Schiff Thursday, May 8th, 2025

Quantum Geometry and Transport of Collective Excitations in (Non-)Magnetic Insulators



Ordinary representation theory $\mathbf{G} = \{E, g_1, g_2, g_3, \dots\}$ $D(\underline{\mathbf{G}}) =$





Irreducible representation "building blocks"





Time-reversal (TR) **must** be represented by an **antiunitary** operator.



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Antiunitary elements τg : composition of unitary operation g with TR τ



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Any group containing antiunitary elements: $\underline{\mathbf{G}} = \underline{\mathbf{H}} + a\underline{\mathbf{H}}$

Where **<u>H</u>** is unitary, half size of <u>**G**</u>, and $a = \tau g$





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Antiunitary elements τg : composition of unitary operation g with TR τ

Representations not homomorphisms onto matrices anymore!

If $a = \tau g$ and h is unitary:

D(h)D(a) = D(ha) $D(a)D^{\star}(h) = D(ah)$

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— Can derive a set of irreducible matrices satisfying these properties from the irreps of $\underline{\mathbf{H}}$





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Let $d^{(\mu)}(\mathbf{H})$ be an irrep of H. Depending on transformation under conjugation by a (and \star): **(a)** (b) (C) $d^{(\mu)}(a^2) d^{(\mu)\star a}$ $d^{(\mu)}$ $d^{(\mu)}$ $Zd^{(\mu)}$ $d^{(\mu)}$ $Zd^{(\mu)}$ $d^{(\mu)}$ $d^{(\mu)\star a}$ $-Zd^{(\mu)}$ $d^{(\mu)}$ H $a\mathbf{H}$ H aH $a\mathbf{H}$ H







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Let $d^{(\mu)}(\underline{\mathbf{H}})$ be an irrep of $\underline{\mathbf{H}}$. Depending on transformation under conjugation by a (and \star):

Dimmock indicator:

$$\frac{1}{|\underline{\mathbf{H}}|} \sum_{h \in \underline{\mathbf{H}}} \chi^{(\mu)} \left((ah)^2 \right) = \begin{cases} +1 & (\mathbf{a}) & \text{No} \\ -1 & (\mathbf{b}) & \text{doubling} \\ 0 & (\mathbf{c}) & \text{Doubling} \end{cases}$$







Time-reversal (TR) **must** be represented by an **antiunitary** operator.

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Theorem: non-trivial spin groups S are isomorphic to their parent group G.





Non-trivial SPGs: X = S



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If S is unitary:

 $S \cong G$ implies that S has the same irreps as ordinary PG G.

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Non-trivial SPGs: X = S

If S is unitary:

 $\mathbf{S} \cong \mathbf{G}$ implies that \mathbf{S} has the same irreps as ordinary PG G.

If S is antiunitary: $S = S^* + aS^*$

 S^* has the same irreps as a PG G^* , and so S has the same co-irreps as B&W PG $\mathbf{G}^{\star} + \tau a_o \mathbf{\underline{G}}^{\star}$. $a = [a_s \| a_o]$

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 S^{\star} has the same irreps as a PG G^{\star} , and so S has the same co-irreps as B&W PG $\underline{\mathbf{G}}^{\star} + \tau a_o \underline{\mathbf{G}}^{\star}$. $a = [a_s \| a_o]$



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Non-trivial SPGs: X = S

If S is unitary:

 $S \cong G$ implies that S has the same irreps as ordinary PG G.

If S is antiunitary: $S = S^* + aS^*$

 S^* has the same irreps as a PG G^* , and so S has the same co-irreps as B&W PG $\underline{\mathbf{G}}^{\star} + \tau a_o \underline{\mathbf{G}}^{\star}$. $a = [a_s \| a_o]$



Theorem: non-trivial spin groups \mathbf{S} are isomorphic to their parent group \mathbf{G} .

Non-trivial SPGs: X = S

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$\mathbf{S} = \mathbf{S}^{\star} + a\mathbf{S}^{\star}$ If S is antiunitary:

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Unitary S:

All elements of **S** are $[E||g]: \underline{\mathbf{S}} = \underline{\mathbf{G}}$

$\underline{\mathbf{X}} \cong \mathbf{SO}(2) \times \underline{\mathbf{G}} + [\tau 2_{\perp} || E] \mathbf{SO}(2) \times \underline{\mathbf{G}}$





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 $\mathbf{X} \cong \mathbf{SO}(2) \times \mathbf{G} + [\tau 2 \mid ||E] \mathbf{SO}(2) \times \mathbf{G}$

Irreps of $SO(2) \times G$ are $e^{i\mu\varphi} \Delta^{(\nu)}$ where $\mu \in \mathbb{Z}$ and $\Delta^{(\nu)}$ is an irrep of **G**.





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Indicators of $e^{i\mu\varphi}\Delta^{(\nu)}$ given by $\Delta^{(\nu)}$ in grey PG $\mathbf{G} + \tau \mathbf{G}$ (i.e. reality)

$b^{\infty} \times {}^{1}3$	$\{R_{\varphi},E\}$	$\{\mathbf{R}_{\varphi}, \mathbf{E}\} \qquad \left\{\mathbf{R}_{\varphi}, \mathbf{C}_{3z}\right\}$		$\left\{ \tau 2_{\perp} \mathbf{R}_{\varphi} , \mathbf{C}_{3z} \right\}$	
Γ1	e ^{iσφ}	€ ^{iσφ}	e ^{iσφ}	e ^{iσφ}	
Γ2	$\begin{pmatrix} e^{\mathbf{i}\sigma\varphi} & 0 \\ 0 & e^{\mathbf{i}\sigma\varphi} \end{pmatrix}$	$\begin{pmatrix} e^{\frac{2i\pi}{3}+i\sigma\varphi} & 0\\ 0 & e^{-\frac{2i\pi}{3}+i\sigma\varphi} \end{pmatrix}$	$\begin{pmatrix} 0 & \mathbf{e}^{\mathbf{i} \sigma \varphi} \\ \mathbf{e}^{\mathbf{i} \sigma \varphi} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \mathbf{e}^{\frac{2\mathbf{i}\pi}{3} + \mathbf{i}\sigma\varphi} \\ \mathbf{e}^{-\frac{2\mathbf{i}\pi}{3} + \mathbf{i}\sigma\varphi} & 0 \end{pmatrix}$	





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Antinitary S:

$\underline{\mathbf{S}} = \underline{\mathbf{S}}^{\star} + a\underline{\mathbf{S}}^{\star} \quad \text{Let } a = [\tau || a_o]$ $\underline{\mathbf{X}} = \underline{\mathbf{X}}_{1/2} + [\tau 2_{\perp} || E] \underline{\mathbf{X}}_{1/2} \quad \text{with}$ $\underline{\mathbf{X}}_{1/2} = \mathbf{SO}(2) \times \underline{\mathbf{S}}^{\star} + [2_{\perp} || a_o] \, \mathbf{SO}(2) \times \underline{\mathbf{S}}^{\star}$



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Irreps of $\underline{\mathbf{X}}_{1/2}$ a priori unknown & new!

Co-irreps are not trivially found from knowledge of irreps $\Delta^{(\nu)}$ of **G**.

$b^{\infty} \times \overline{1}2$	$\{R_{\varphi},E\}$	$\left\{ 2_{\perp} \; \mathbf{R}_{\varphi} , \; \mathbf{C}_{2\mathbf{z}} \right\}$	$\{\tau 2_{\perp} \mathbf{R}_{\varphi}, \mathbf{E}\}$	$\left\{ \tau \mathbf{R}_{\varphi}, \mathbf{C}_{2z} \right\}$	
Γ1	1	1	1	1	
Γ2	1	-1	1	-1	
Γ ₃	$ \left(\begin{array}{ccc} \mathbb{e}^{\mathbf{i}\mathbf{v}\boldsymbol{\varphi}} & 0 \\ 0 & \mathbb{e}^{-\mathbf{i}\mathbf{v}\boldsymbol{\varphi}} \end{array}\right) $	$ \left(\begin{array}{ccc} 0 & \mathbf{e}^{-\mathbf{i}\mathbf{v}\boldsymbol{\varphi}} \\ \mathbf{e}^{\mathbf{i}\mathbf{v}\boldsymbol{\varphi}} & 0 \end{array}\right) $	$ \left(\begin{array}{ccc} \mathbf{e}^{\mathbf{i}\mathbf{v}\boldsymbol{\varphi}} & 0 \\ 0 & \mathbf{e}^{-\mathbf{i}\mathbf{v}\boldsymbol{\varphi}} \end{array}\right) $	$ \left(\begin{array}{ccc} 0 & \mathbf{e}^{-\mathbf{i}\mathbf{v}\varphi} \\ \mathbf{e}^{\mathbf{i}\mathbf{v}\varphi} & 0 \end{array}\right) $	

HS, A. Corticelli, A. Guerreiro, J. Romhányi, P. McClarty, SciPost Phys. 18, 109 (2025)





Non-trivial SPGs

Irreps of parent PG <u>**G**</u>, or co-irreps of B&W PG <u>**G**</u> + τa_o <u>**G**</u>

 $a = [a_s || a_o]$



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Irreps of parent PG $\underline{\mathbf{G}}$, or co-irreps of B&W PG $\underline{\mathbf{G}} + \tau a_o \underline{\mathbf{G}}$ $a = [a_s || a_o]$

Coplanar SPGs

Co-irreps of grey $PGG + \tau G$





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Coplanar SPGs

Co-irreps of grey PG $\underline{\mathbf{G}} + \tau \underline{\mathbf{G}}$



Collinear SPGs

Unitary <u>S</u>:

Co-irreps induced from $SO(2) \times \underline{G}$, based on reality of $\Delta^{(\nu)}(\underline{G})$

Antiunitary \underline{S} :

Co-irreps induced from $\underline{\mathbf{X}}_{1/2}$, are **new** and non-trivial!





Do we need the spin groups?

Hana Schiff Thursday, May 8th, 2025

Quantum Geometry and Transport of Collective Excitations in (Non-)Magnetic Insulators



Do we need the spin groups? Usually yes, sometimes no!

Hana Schiff Thursday, May 8th, 2025

Quantum Geometry and Transport of Collective Excitations in (Non-)Magnetic Insulators







HS, A. Corticelli, A. Guerreiro, J. Romhányi, P. McClarty, SciPost Phys. 18, 109 (2025)

L. Šmejkal, J. Sinova and T. Jungiwirth, Phys. Rev. X 12, 040501 (2022)

Unconventional magnons

X Chen Y Liu P Liu, Y. Yui, J. Ren J, Li, A. Zhang, Q Liu, <u>Nature 640,</u> 349-354 (2025)









Landau theory for collinear altermagnets

Equivalent formulation for collinear systems without spin groups



Salient physics from the SO-free limit even for real materials with some SOC











Ideal Altermagnets



Litvin, Opechowski, Ph Volume 76, Issue 3 (1

Decoupled spin orbital space

Spins and lattic can transform independently

Spin groups

Šmejkal, Sinova, Jungwirth, Phys. Rev. X 12, 031042 (2022)

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Ideal Altermagnets



Alternating spin-splitting



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Where to place magnetic ions?





Ideal Altermagnets Spin-orbit free $\mathbf{N} = \mathbf{S}_A - \mathbf{S}_B$ Compensated Alternating spin-splitting

Decoupled spin & orbital space

Spins and lattice can transform independently

Spin groups



Translation & inversion don't connect \uparrow / \downarrow

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Translation & inversion don't connect \uparrow / \downarrow

Where to place magnetic ions?

Under space group operations

Preserves \uparrow and \downarrow $N \rightarrow N$



Swaps \uparrow and \downarrow $N \rightarrow -N$



We focus on case where translations act trivially!







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Altermagnetic if:

N transforms as a 1D, \mathbb{R} inversion even irrep of the crystal point group: Γ_{N}









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For all Wyckoff positions:

Form permutation representation, check if it contains 1D, \mathbb{R} inversion even irrep of crystal point group













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Translation & inversion don't connect \uparrow / \downarrow

Where to place magnetic ions?

PG	SG	WP	$\Gamma_{\mathbf{N}}$		PG	SG	WP	$\Gamma_{\mathbf{N}}$
422	94	$\{8g, 4d, 4c\}$	$\{B_1, A_2, B_2\}$		$\overline{4}$ m2	115	$\{8l\}$	$\{B_1, B_2, A$
		$\{4f, 4e, 2b, 2a\}$	$\{B_2\}$				$\{4i,4h\}$	$\{A_2\}$
	95	$\{8d\}$	$\{B_1, A_2, B_2\}$				$\{4k,4j,2g,2f,2e\}$	$\{B_1\}$
		$\{4b, 4a\}$	$\{B_1\}$			116	$\{8j,4i,4h,4g\}$	$\{B_1,B_2,A$
		$\{4c\}$	$\{B_2\}$				$\{4f, 4e, 2b, 2a\}$	$\{A_2\}$
	96	$\{8b\}$	$\{B_1, A_2, B_2\}$				$\{2d, 2c\}$	$\{B_2\}$
		$\{4a\}$	$\{B_2\}$			117	$\{8i,4f,4e\}$	$\{B_1,B_2,A$
	97	$\{16k, 8j, 8i, 8f, 4e, 4d\}$	$\{B_1, A_2, B_2\}$				$\{4h,4g,2d,2c\}$	$\{A_2\}$
		$\{8h, 4c\}$	$\{B_1\}$				$\{2b, 2a\}$	$\{B_2\}$
		$\{8g, 2b\}$	$\{B_2\}$			118	$\{8i,4h,4e\}$	$\{B_1, B_2, A$
	98	$\{16g, 8f, 8c\}$	$\{B_1, A_2, B_2\}$	210/2	230		$\{4g,4f,2d,2c\}$	$\{A_2\}$
		$\{8e, 8d, 4b, 4a\}$	$\{B_2\}$	snac			$\{2b, 2a\}$	$\{B_2\}$
$4 \mathrm{mm}$	99	$\{8g\}$	$\{B_1, B_2, A_2\}$	spuc		119	$\{16j, 8i, 8h, 4f, 4e, 2d, 2c\}$	$\{B_1,B_2,Z_1\}$
		$\{4f, 4e, 2c\}$	$\{B_1\}$	grou	ps		$\{8g, 2b\}$	$\{A_2\}$
		$\{4d\}$	$\{B_2\}$			120	$\{16i, 8g, 8f, 8e, 4c, 4a\}$	$\{B_1,B_2,Z$
	100	$\{8d\}$	$\{B_1, B_2, A_2\}$	1107/1	721		$\{8h, 4d\}$	$\{A_2\}$
		$\{2a\}$	$\{A_2\}$		/51		$\{4b\}$	$\{B_2\}$
		$\{4c, 2b\}$	$\{B_2\}$	Wyck	off	121	$\{16j,8h,8g,4d\}$	$\{B_1,B_2,A$
	101	$\{8e, 4c\}$	$\{B_1, B_2, A_2\}$	positio	ons		$\{8f, 4c\}$	$\{B_1\}$
		$\{4d, 2b, 2a\}$	$\{B_2\}$	positi			$\{8i, 4e, 2b\}$	$\{B_2\}$
	102	$\{8d, 4b\}$	$\{B_1, B_2, A_2\}$			122	$\{16e, 8d, 8c, 4b\}$	$\{B_1,B_2,Z$
		$\{4c, 2a\}$	$\{B_2\}$				$\{4a\}$	$\{A_2\}$
	103	$\{8d, 4c\}$	$\{B_1, B_2, A_2\}$		4/mmm	123	$\{16u, 8q, 8p\}$	$\{B_{1g}, A_{2g},$
		$\{2b, 2a\}$	$\{A_2\}$				$\{8t, 8s, 4o, 4n, 4m, 4l, 4i, 2f, 2e\}$	$\{B_{1g}\}$
	104	$\{8c, 4b\}$	$\{B_1, B_2, A_2\}$				$\{8r, 4k, 4j\}$	$\{B_{2g}\}$
		$\{2a\}$	$\{A_2\}$			124	$\{16n, 8m, 8i, 4e\}$	$\{B_{1g}, A_{2g},$
	105	$\{8f\}$	$\{B_1, B_2, A_2\}$				$\{4h, 4g, 2d, 2b\}$	$\{A_{2g}\}$
		$\{4e, 4d, 2c, 2b, 2a\}$	$\{B_1\}$				$\{8l, 8k, 4f\}$	$\{B_{1g}\}$
	106	$\{8c, 4b, 4a\}$	$\{B_1, B_2, A_2\}$				$\{8j\}$	$\{B_{2g}\}$
	107	$\{16e, 8d, 4b\}$	$\{B_1, B_2, A_2\}$			125	$\{16n\}$	$\{B_{1g}, A_{2g},$
HS	S. Mo	Clarty, Ray, Roj	mhánvi.					
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even irrep of crystal point group




Evading spin groups

High symmetry phase



Spin group

If crystalline & magnetic unit cells coincide:

only need collinear spin point groups









What is the correspondence between point group irreps and (non-trivial) spin point groups, that allows us to avoid using the spin groups entirely?

Non-trivial Spin Point Group



Trivial Irrep: f composed with spin-only τ or 2₁ represented by +1

Each 1D, \mathbb{R} , inversion-even irrep of a point group corresponds to one of the possible altermagnetic (non-trivial) spin point groups.

Point Group



Non-trivial Irrep: f represented by -1



McClarty, Rau, Phys. Rev. Lett. 132, 176702 (2024)



Ideal Altermagnets

Spin-orbit free & compensated





Order parameter: $\mathbf{N} = \mathbf{S}_A - \mathbf{S}_B$ (transforms as Γ_{N} in crystal point group)

Multipolar pseudo-primary order parameter

r [r. **Γ** μ₁ $\mu_n \mathbf{J} \longrightarrow \mathbf{I}$

Transforms as $[V^n]$ in crystal point group

McClarty, Rau, Phys. Rev. Lett. 132, 176702 (2024)

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McClarty, Rau, Phys. Rev. Lett. 132, 176702 (2024)

Multipole $d^3r xy \mathbf{m}(\mathbf{r})$



Condition for linear multipole and N:

33



Hayami, Yanagi, Kusunose J. Phys. Soc. Jpn. 88, 123702 (2019)

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Multipole $d^3r xy \mathbf{m}(\mathbf{r})$



Lowest order multipole determines spin splitting

Condition for linear multipole and N:

 $F \sim \Gamma$

Spin splitting



Coupling to N

coupling between $\Gamma_{\mathbf{N}} \in [V^n]$

$$\mathbf{N} \cdot \left[d^3 r x y \mathbf{m}(\mathbf{r}) \right]$$

Allowed term in the free energy

Classify

Multipoles fully specify the the SOfree Landau theory

For each 1D, \mathbb{R} irrep of a crystal point group (i.e. for each Γ_N) find lowest order *n* multipole

Find n = 1, 2, 3, 4, 6

Find explicit multipole component(s) (by finding invariant polynomial of order n)

Just 54 possible SO-free Landau theories for collinear altermagnets (whose chemical and magnetic unit cells coincide)





Real Altermagnets



Order parameter: $\mathbf{N} = \mathbf{S}_A - \mathbf{S}_B$ (transforms as $\Gamma_{\mathbf{N}} \otimes aeV$)

Multipolar pseudo-primary order parameter

$$\int d^3r \left[r_{\mu_1} \dots r_{\mu_n}\right] \mathbf{m}(\mathbf{r})$$

Transforms as $[V^n] \otimes aeV$

Locked spin & orbital space

Spins transform with lattice

Magnetic groups

SOC < Splitting

Dominant features from SO-free limit

Presence of SOC changes symmetry



Real Altermagnets



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Physical property tensors

 ξ : tensor for physical property of interest (e.g. Hall conductivity, magnetoresistance...



SOC paramagnetic group rep. (point group + time-reversal)





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Coupling to N

Requires that



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SOC paramagnetic group rep. (point group + time-reversal)



Coupling to N

Requires that $\Gamma_{\mathbf{N}} \otimes aeV \in \Gamma_{\mathcal{E}}$

When is this guaranteed?



Real Altermagnets



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Transforms as $[V^n] \otimes aeV$

Locked spin & orbital space

Spins transform with lattice

Magnetic groups

SOC < Splitting

Dominant features from SO-free limit

Presence of SOC changes symmetry

Physical property tensors

 ξ : tensor for physical property of interest (e.g. Hall conductivity, magnetoresistance...



SOC paramagnetic group rep. (point group + time-reversal)



Coupling to N

Requires that $\Gamma_{\mathbf{N}}$ \in When is this guaranteed?





Real Altermagnets



Order parameter: $N = S_A - S_B$ (transforms as $\Gamma_{\mathbf{N}} \otimes aeV$)

Multipolar pseudo-primary order parameter

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Coupling classes

Just 4 classes of observable properties ξ according to n

Multipole rank (n)	Representation
1	aV, aeV^2
2	aeV
3	aeV^2
4, 6	$aeV[V^2]$

Inherently altermagnetic! (Can distinguish AFM from AM)

HS, McClarty, Rau, Romhányi, <u>arXiv:2412.18025</u>, (2024)



Γ_{ξ}	n	Quantity (ξ)	Defining equation	Tensor part	operty tensors
aV	1	Polar Toroidal Moment ${\cal T}_i$	-	Full	Posponso To
	_	Pyrotoroidic tensor r_i	$T_i = r_i \Delta T$	Full	perty of interest
		Magnetization M_i	-	Full	gnetoresistance)
		Electric conductivity σ_{ij}	$J_i = \sigma_{ij} E_j$	$\sigma^A_{lpha} = rac{1}{2} arepsilon_{lpha i j} \sigma^A_{i j}$	
		Soret thermodiffusion tensor s_{ij}	$J_i = s_{ij} (\nabla T)_j$	$s^A_{\alpha} = \frac{1}{2} \varepsilon_{\alpha i j} s^A_{i j}$	hetic group rep.
aeV	2	Thermal conductivity κ_{ij}	$q_i = \kappa_{ij} (\nabla T)_j$	$\kappa^A_{\alpha} = \frac{1}{2} \varepsilon_{\alpha i j} \kappa^A_{i j}$	- time-reversal) ^{\$\sigma_A\$=\$}
		Peltier tensor π_{ij}	$q_i = \pi_{ij} J_j$	$\tilde{S}_{\alpha} = \frac{1}{2} \varepsilon_{\alpha i i} (\pi^A + \beta^A)$	
		Seebeck tensor β_{ij}	$E_i = \beta_{ij} (\nabla T)_j$	$\sim \alpha \qquad 2^{\circ \alpha i j (n_{ij} + \rho_{ij})}$	
		Spontaneous Faraday effect F_{ij}	-	$F_{\alpha} = \frac{1}{2} \varepsilon_{\alpha i j} F_{i j}$	
aeV^2	1 & 3	Magnetoelectric tensor α_{ij}	$M_i = \alpha_{ij} E_j$	Full	Coupling class
	4 & 6	Piezomagnetic tensor Λ_{ijk}	$M_i = \Lambda_{ijk} \Sigma_{jk}$	Full	
		Second order magnetoelectric tensor α_{ijk}	$M_i = \alpha_{ijk} E_j E_k$	Full	Just 4 classes of
		Magneto-optic Kerr effect z_{ijk}^S	$\varepsilon_{ij} = i z_{ijl}^S H_l$	Full	
		Quadratic magneto-optic Kerr effect iC^A_{ijkl}	$\varepsilon_{ij} = C^A_{ijkl} H_k H_l$	$C_{\alpha kl} = \frac{1}{2} \varepsilon_{\alpha ij} C^A_{ijkl}$	observable properti
$aeV[V^2]$		Magnetoresistance R_{ijk}	$E_i = R_{ijk} J_j H_k$	$R_{ijk}^S = \frac{1}{2}(R_{ijk} + R_{jik})$	according to n
		Righi-Leduc magnetor hermal tensor Q_{ijk}	$q_i = Q_{ijk} (\nabla T)_j H_k$	$Q_{ijk}^S = \frac{1}{2}(Q_{ijk} + Q_{jik})$	
		Ettinghausen tensor M_{ijk}	$q_i = M_{ijk} J_j H_k$	$S_{\cdots i} = \frac{1}{2} (M^S_{\cdot} + N^S_{\cdot})$	$- \qquad \qquad \text{Multipole rank } (n) \qquad \qquad \text{Representat}$
		Nernst tensor N_{ijk}	$E_i = N_{ijk} (\nabla T)_j H_k$	$\mathcal{L}_{ijk} = 2 (\mathcal{L}_{ijk} + \mathcal{L}_{ijk})$	$1 \qquad aV, ae$
		Magnetic resistance tensor T_{ijkl}	$E_i = T_{ijkl} J_j H_k H_l$	$T^A_{\alpha kl} = \frac{1}{2} \varepsilon_{\alpha ij} T^A_{ijkl}$	2 aeV
		Magneto-heat-conductivity tensor \mathcal{S}_{ijkl}	$q_i = \mathcal{S}_{ijkl} (\nabla T)_j H_k H_l$	$\mathcal{S}^{A}_{\alpha k l} = \frac{1}{2} \varepsilon_{\alpha i j} \mathcal{S}^{A}_{i j k l}$	4.6
		Piezoresistivity tensor Π_{ijkl}	$\Delta \rho_{ij} = \Pi_{ijkl} \Sigma_{kl}$	$\Pi^A_{\alpha kl} = \frac{1}{2} \varepsilon_{\alpha ij} \Pi^A_{ijkl}$	
		Magneto–Seebek tensor α_{ijkl}	$E_i = \alpha_{ijkl} (\nabla T)_j H_k H_l$	$\tilde{A} = \frac{1}{2} \epsilon \cdots (\alpha^A = P^A)$	Inherently altermaane
		Magneto-Peltier tensor P_{ijkl}	$q_i = P_{ijkl} H_k H_l H_j$	$\Lambda = 4^{c\alpha i j (\alpha_{ijkl} - 1_{ijkl})}$	(Can distinguish AFM from
			1410		

34

HS, McClarty, Rau, Romhányi, <u>arXiv:2412.18025</u>, (2024)







FIG. 2. The crystal structure of MnTe with space group symmetry $P6_3/mmc$. Magnetic Mn ions (red and blue denote magnetic sublattices) reside on the 2a Wyckoff positions, at $\{0, 0, 0\}$ and $\{0, 0, \frac{1}{2}\}$ within the unit cell. The Te ions (gray) occupy the Wyckoff positios 4e, at $\{\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\}$, and $\{\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\}$.

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Krempasky et al. Nature volume 626, pages 517–522 (2024)

Structure



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Lowest order multipole: $\int d^3r [r_{\mu_1} \dots r_{\mu_n}] \mathbf{m}(\mathbf{r})$

SO-free Landau Theory



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SO-free L Lowest o $\int d^3r [r_{\mu}]$

 $V = A_{1u} \bigoplus E_{2u}$ $[V^2] = 2A_{1g} \bigoplus A_{2g} \bigoplus E_{2g} \bigoplus 2E_{1g}$ $[V^3] = 3A_{1u} \bigoplus 4A_{2u} \bigoplus B_{2u} \bigoplus B_{1u}$ $\bigoplus 3E_{2u} \bigoplus 6E_{1u}$

$$\begin{array}{c} \text{andau Theor} \\ \text{order multipole:} \\ \\ \mu_1 \cdots r_{\mu_n} \mathbf{m}(\mathbf{r}) \\ \\ F_{2u} \\ \\ \mathbf{A}_{2g} \oplus E_{2g} \oplus 2E_{1g} \end{array}$$

X



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andau Theory order multipole:

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TABLE IV. Transformation properties of the order parameter \mathbf{N} in MnTe and the part of the magnetoresistance that is symmetric in the first two indices.

Irrep.	Order	Magnetoresistance componen	
	parameter		
B_{1g}	N_z	$2R_{xyx}^S + R_{xxy}^S - R_{yyy}^S$	
E_{2g}	$\binom{N_x}{N_y}$	$\begin{pmatrix} 2R_{xyz}^S \\ R_{xxz}^S - R_{yyz}^S \end{pmatrix} \\ \begin{pmatrix} R_{yzx}^S + R_{xzy}^S \\ R_{xzx}^S - R_{yzy}^S \end{pmatrix}$	





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andau Theory

 $r_{\mu_1} \dots r_{\mu_n}$] **m(r)**

 E_{2u} $A_{2g} \oplus E_{2g} \oplus 2E_{1g}$ $4A_{2u} \oplus B_{2u} \oplus B_{1u}$ $4A_{2u} \oplus 6E_{1u}$ $9A_{2g} \oplus 4B_{2g} \oplus 4B_{1g}$ $2g \oplus 16E_{1g}$ 4 $x^{2}) \mathbf{m}(\mathbf{r})$

SOC Landau Theory

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Néel components transform as

$$\left\{N_x, N_y\right\} \sim E_{2g}$$

 $N_z \sim B_{1g}$

Observed experimentally!











Derive all SO-free Landau theories

- All structures (space groups WP)
 compatible with AM
- + All irreps characterizing AM N
- All minimal multipoles coupling to AM N





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Guaranteed (allowed) effects with SOC **determined** by SO-free multipoles





inherited from ideal SO-free limit

Bridge SO-free & SOC limits

- SO-free multipole gives insight into symmetry with SOC
 FX TABLES!
- Classify response tensors by symmetry type & multipole order

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Conclusions

Hana Schiff Thursday, May 8th, 2025

Quantum Geometry and Transport of Collective Excitations in (Non-)Magnetic Insulators





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[S||R]

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For collinear systems especially, we can avoid directly using spin groups, taking advantage of an equivalent approach via non-trivial irreps of the paramagnetic group.





Thanks. hschiff@uci.edu ArXiv 2412.18025 SciPostPhys.18.3.109



