Hubbard models for non-relativistic odd-parity spin-splitting

Daniel F. Agterberg
University of Wisconsin – Milwaukee

DOE DE-SC0021971 NSF DMREF-2323857

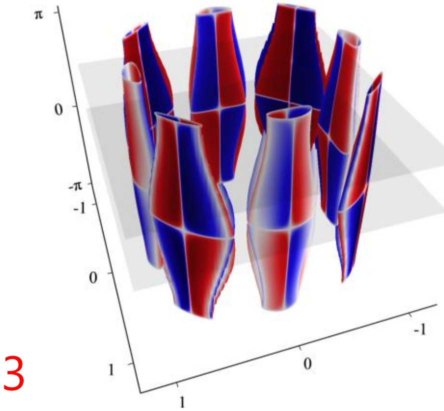
1- Non-relativistic spin-splittings.
2- Sublattice Hubbard models (and briefly altermagnetism).
3- Odd-parity spin-splitting (and other ferroic orders) from lattice doubling antiferromagnetism.

PRB **110**, 144412 (2024), PRL **76**, 046701 (2025), arXiv:2508.21673 (2025).

Mercè Roig

PRB **110**, 144412 (2024)

Morten Christensen



Yue Yu

PRL **76**, 046701 (2025)

arXiv: 2508.21673

Reuel Dsouza

h-wave spin texture in $LaFeAs_{1-x}P_x$

Magnus Lyngby

Mats Barkman

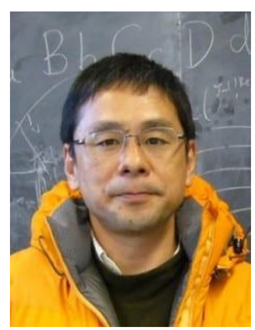
Rune Ekman

Jannik Gondolf

Christian Rasmussen

Brian Andersen

Andreas Kreisel



Tatsuya Shishidou

Mike Weinert

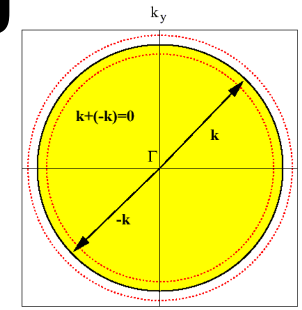
You

2 postdocs available:

agterber@uwm.edu

TI symmetry and spin-splitting

Non-magnetic state: time-reversal (T), inversion (I).
Both I and T take ***k*** to –***k***.

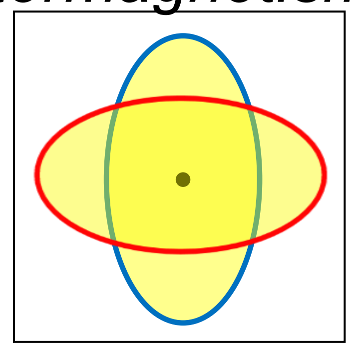


2-fold spin-like degeneracy from (TI)^2=-1 at each ***k*.** Need to break TI symmetry to split spins.

Breaking T and preserving I will give *altermagnetism* (AM)

$$H_{spin} = (\cos k_x - \cos k_y)\,\sigma_z$$

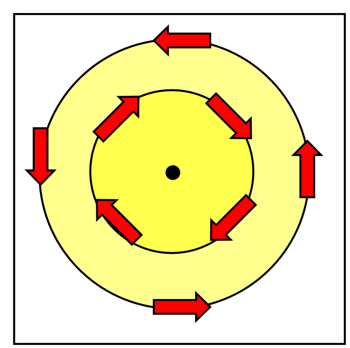
Smejkal et al, PRX (2022)



Breaking I and preserving T will give *odd-parity magnetism*

$$H_{spin} = \sin(k_x)\sigma_y - \sin(k_y)\sigma_x$$

Rashba SOC

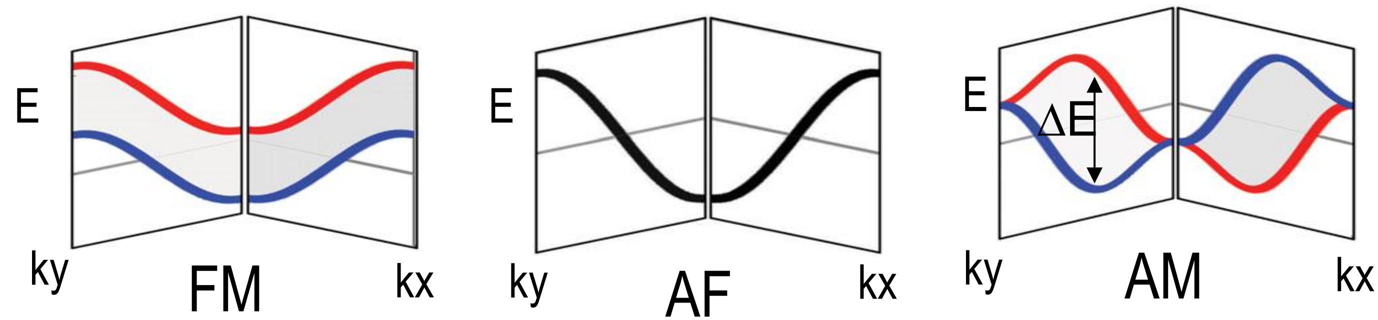


Non-Relativistic Spin-Splittings

When spin and spatial transformations decoupled:

$$[R_{spin}||R_{space}] = [C_2||C_4]$$

Find three *collinear* magnetic states: FM, AF, AM



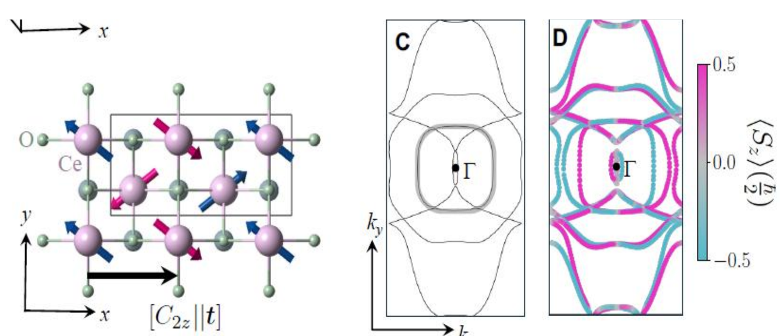
Smejkal et al, PRX (2022).

d-wave

k_x^2-k_y^2

ΔE (Spin-Splitting) not due to SOC and *can be large (100 meV)*

Large spin-splittings also possible in *noncollinear* states:

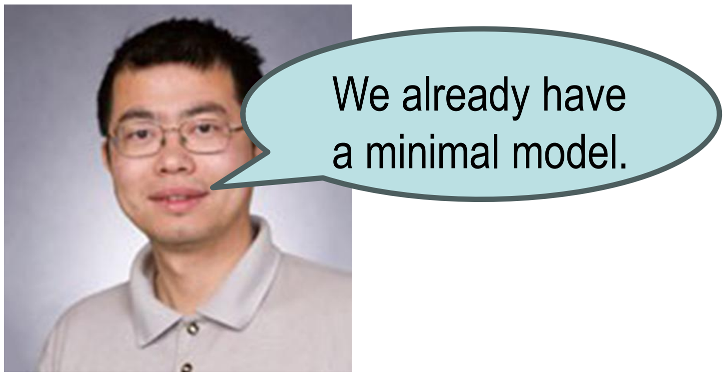


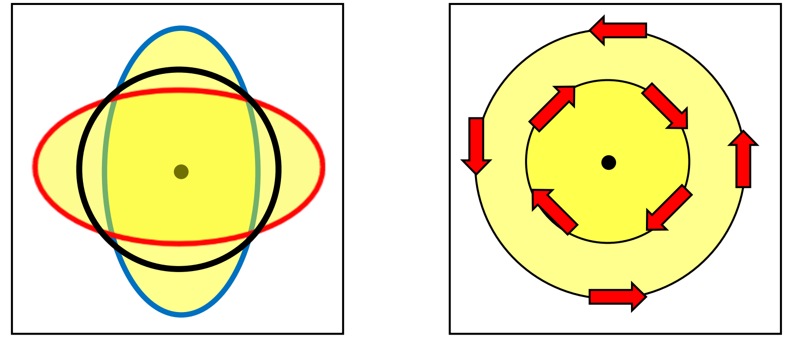
Example: p-wave magnetism *coplanar* CeNiAsO
Hellenes et al, arXiv:2309.01607

Allowed spin-splittings classified in PRXs 2024 – More than 100000 spin-space groups (Xiao et al, Chen et al, Jiang et al)

Goal here is minimal Hubbard-like models for such spin-textures.

Prior Minimal Models





Gorkov and Sokal (1992), Wu, Sun, Fradkin, Zhang, PRB (2007),

Single band theory: Pomeranchuck instability of the Fermi surface in spin-channel (Stoner instability is example)

Can deform Fermi surface into altermagnetic spin-splittings or odd-parity spin-splittings. These are interaction-driven *non-relativistic spin-splittings*.

Here spin-splitting is the primary order parameter.

Hubbard Models: Altermagnets

- Minimal two-Wyckoff model: sublattice τ_i, spin σ_i

$$H = \varepsilon_{0,k} + t_{x,k}\tau_x + t_{z,k}\tau_z + \tau_z \vec{J}\cdot\vec{\sigma}$$

Self-consistent RPA Neel order is ***Primary order***

Hopping between magnetic ions

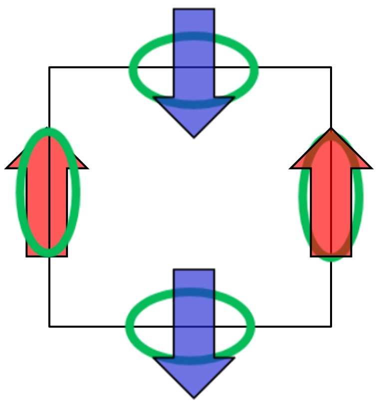
$$\vec{N} \in \Gamma_N \otimes \Gamma_A^S$$

Spatial symmetry

Spin vector

Asymmetric crystal hopping - τ_z and $t_{z,k}$ have symmetry Γ_N

e.g. Γ_N is B_{1g} x^2-y^2



SG 123,
Wyckoff 2f

$$E_{\pm,\pm} = \varepsilon_{0,k} \pm \sqrt{t_{x,k}^2 + (|\vec{J}| \pm t_{z,k})^2}$$

Nodes in ΔE when $t_{z,k}=0$ $\quad \Delta E \propto \sqrt{|t_{z,k}|J}$

$$t_{x,k} = t\cos\frac{k_x}{2}\cos\frac{k_y}{2}$$

$$t_{z,k} = t(\cos k_x - \cos k_y)$$

Lieb Lattice model

Spin-splitting is a "secondary" order parameter:
Asymmetric crystal hopping (t_{zk}) determines spin-splitting

*Spin splitting: **Ferroic** magnetic octupole order (McClarty, Rau PRL 2024)*

Minimal Hubbard Models

a) Find space groups with Wyckoff position of multiplicity 2 (2 atom sublattice)

b) Require the *Wyckoff site symmetry contains inversion* (*for altermagnets*)

c) Include on-site Hubbard and all tight-binding terms allowed by symmetry

d) Study within RPA

- Gives altermagnetic spin-splitting as a secondary order parameter (d-wave, g-wave, i-wave). 40 space group/Wyckoff symmetry pairs.
- Understand when altermagnetism is stable - band degeneracies help.
- Understand spin-orbit coupling and origin of AHE and ferromagnetism in AM
- Understand the appearance of Weyl lines in electronic spectrum
- Generalizable to theories of non-relativistic odd-parity spin-splittings – *include Wyckoff pairs related by inversion symmetry*.

Phys. Rev. B **110**, 144412 (2024)
Nature Communications **16**, 2950 (2025)
Phys. Rev. B **111**, 174436 (2025)
Phys. Rev. Lett., (2025)
Phys. Rev. Lett., (2025)
arXiv:2509.03247 (2025)
arXiv:2508.21073 (2025)

See Also:
Brekke et al, PRB 108, 224421 (2023).
Antonenko et al, PRL 134 096703 (2025)

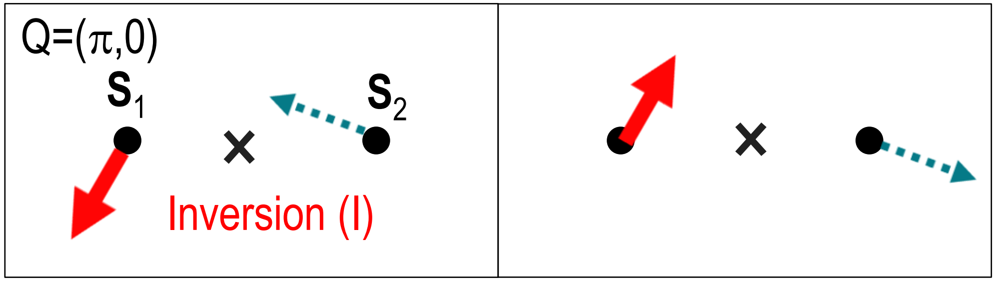
See Brian's talk for more applications to altermagnetism.

Minimal models for odd-parity magnetism are similar

Odd-parity spin-splitting: Ginzburg Landau

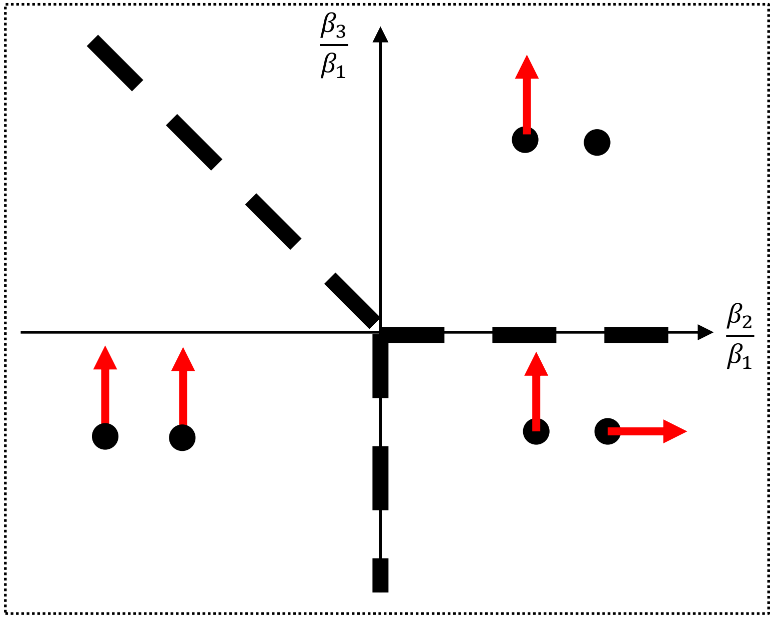
Sublattice Hubbard models: also find Q=(π,π) or Q=(π,0) instabilities.

Why does CeNiAsO, an antiferromagnet with Q=(π,0) have p-wave magnetism? Hellenes et al, arXiv:2309.01607.



Assume global spin-rotational invariance:

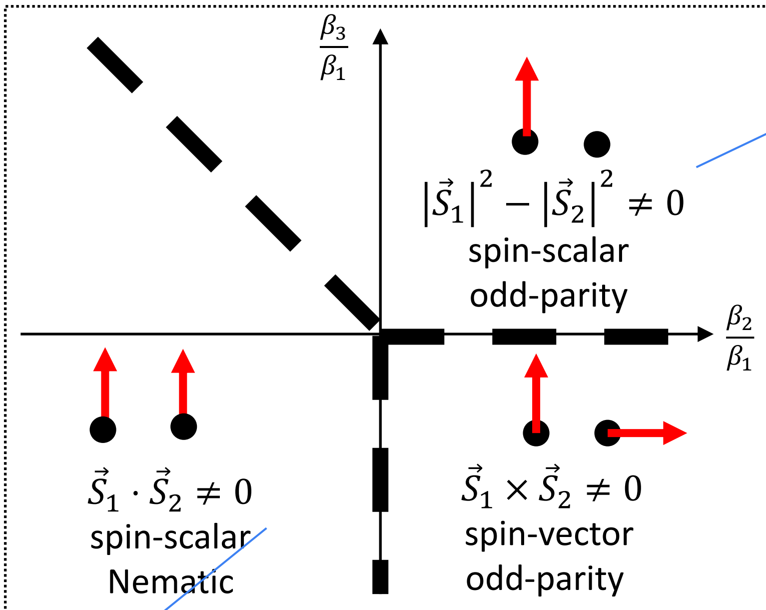
$$F_{GL} = \alpha \left(\sum_i \vec{S_i} \cdot \vec{S_i} \right) + \beta_1 \left(\sum_i \vec{S_i} \cdot \vec{S_i} \right)^2 + \beta_2 \left(\vec{S_1} \cdot \vec{S_2} \right)^2 + \beta_3 \left(\vec{S_1} \cdot \vec{S_1} \right) \left(\vec{S_2} \cdot \vec{S_2} \right)$$

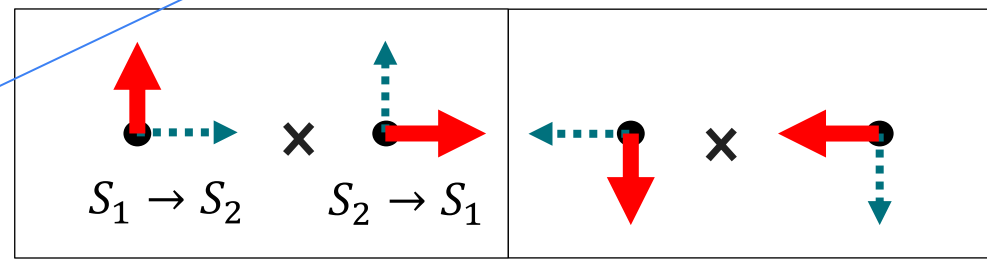


Induced ferroic orders

Each state has a translation invariant or ferroic order:

This phase subject of Watanabe, Arita PRL **134**, 266703 (2025)



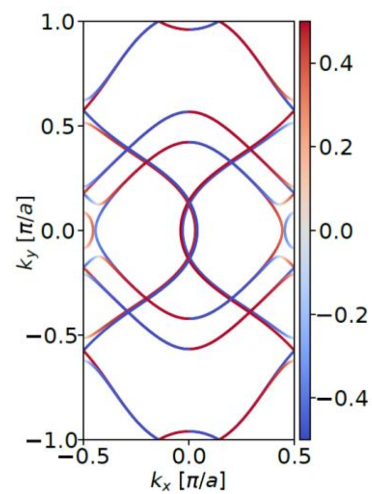


$$\overrightarrow{S_1} \times \overrightarrow{S_2} \xrightarrow{\mathrm{I}} -\overrightarrow{S_1} \times \overrightarrow{S_2}$$

$\overrightarrow{S_1} \times \overrightarrow{S_2}$ is translation/time-reversal invariant and odd-parity

Nematic order in Fe-based materials.

R.M. Fernandes, P. P. Orth, and J Schmalian, ARCMP (2019)



CeNiAsO

$\overrightarrow{S_1} \times \overrightarrow{S_2}$ can generate fermionic spin-splitting $\sigma_z f(k)$

$f(k)=-f(-k)$ (reminiscent of Rashba SOC)

When is F_{GL} valid?

- In F_{GL}, $\overrightarrow{S_1} \cdot \overrightarrow{S_2}$ typically appears. This forbids $\overrightarrow{S_1} \times \overrightarrow{S_2} \neq 0$ and $|\vec{S}_1|^2 - |\vec{S}_2|^2 \neq 0$ states.

- $\overrightarrow{S_1} \cdot \overrightarrow{S_2}$ *term vanishes in non-symmorphic space groups with Q at the Brillouin zone boundary (allows mixed parity representations).*

- Classify space groups, wavevectors, and representation of symmetries for which F_{GL} is correct (421 theories).

- This determines form of f(k) in in spin-splitting from coplanar state

- Find: p, f, and h-wave spin-splittings

P	Spin-splitting	Space group & Wavevector
C_{2h}	k_z	$11(C_1^*, D_1^*, E_1^*, Z_1^*), 14(C_1^*, Z_1^*), 63(R_1), 176(L_1)$
C_{4h}	k_z	$84(A_1, Z_1), 85(A_1, M_1), 86(M_1, Z_1), 88(M_1)$
C_{6h}	k_z	$176(A_1)$
D_{2h}	$k_{z,y,x}$	$48(S_{1,2}, T_{1,2}, U_{1,2}, X_{1,2}, Y_{1,2}, Z_{1,2}), 49(R_{1,2}, T_{1,2}, U_{1,2}, Z_{1,2}), 50(R_{1,2}, S_{1,2}, T_{1,2}, U_{1,2}, X_{1,2}, Y_{1,2}),$ $51(R_{1,2}, S_{1,2}, U_{1,2}, X_{1,2}), 52(R_{1,2}, U_{1,2}, X_{1,2}, Y_{1,2}, Z_{1,2}), 53(S_{1,2}, T_{1,2}, X_{1,2}, Z_{1,2}),$ $54(S_{1,2}, T_{1,2}, X_{1,2}, Z_{1,2}), 55(T_{1,2}, U_{1,2}, X_{1,2}, Y_{1,2}), 56(X_{1,2}, Y_{1,2}, Z_{1,2}), 57(S_{1,2}, U_{1,2}, Y_{1,2}, Z_{1,2}),$ $58(X_{1,2}, Y_{1,2}, Z_{1,2}), 59(T_{1,2}, U_{1,2}, X_{1,2}, Y_{1,2}), 60(X_{1,2}, Y_{1,2}, Z_{1,2}), 61(X_{1,2}, Y_{1,2}, Z_{1,2}),$ $62(X_{1,2}, Y_{1,2}, Z_{1,2}), 63(T_{1,2}, Z_{1,2}), 64(T_{1,2}, Z_{1,2}), 66(T_{1,2}, Z_{1,2}), 68(T_{1,2}, Z_{1,2}), 70(T_{1,2}, Y_{1,2}, Z_{1,2}),$ $124(R_{1,2}), 125(R_{1,2}, X_{1,2}), 126(R_{1,2}, X_{1,2}), 127(R_{1,2}, X_{1,2}), 128(X_{1,2}), 129(R_{1,2}, X_{1,2}), 130(X_{1,2}),$ $132(R_{1,2}), 133(R_{1,2}, X_{1,2}), 134(R_{1,2}, X_{1,2}), 135(R_{1,2}, X_{1,2}), 136(X_{1,2}), 137(R_{1,2}, X_{1,2}), 138(X_{1,2}),$

Microscopic theory

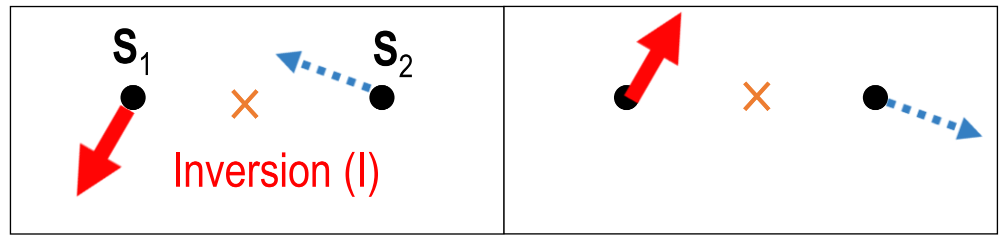
Usual mean-field theory for SDW:

$$H = \begin{pmatrix} \varepsilon_k & \overrightarrow{J_q} \cdot \vec{\sigma} \\ \overrightarrow{J_q} \cdot \vec{\sigma} & \varepsilon_{k+q} \end{pmatrix}$$

$\varepsilon_k = -\varepsilon_{k+q}$

Nesting - is good for SDW (cuprates)

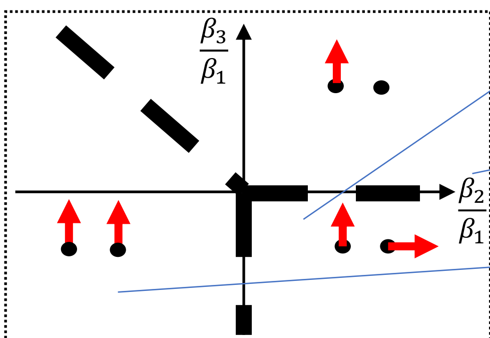
How does this change with a sublattice?



Here, simple 1D problem, Q=π:

$$H = \begin{pmatrix} \varepsilon_k + t\cos\frac{k_x}{2}\tau_x & M_q \\ M_q & \varepsilon_{k+q} - t\sin\frac{k_x}{2}\tau_y \end{pmatrix}$$

$$M_q = J[\tau_0(\sigma_x + \sigma_y) + \tau_z(\sigma_x - \sigma_y)]$$



$\overrightarrow{S_1} \times \overrightarrow{S_2}$ find a large spin splitting ~$(Jt)^{1/2} \sin k_x\, \sigma_z$.

$\vec{S}_1^2 - \vec{S}_2^2$ find SOC free Berry curvature dipole.

$\overrightarrow{S_1} \cdot \overrightarrow{S_2}$ find (generalized) electronic nematic order also ~$(Jt)^{1/2}$

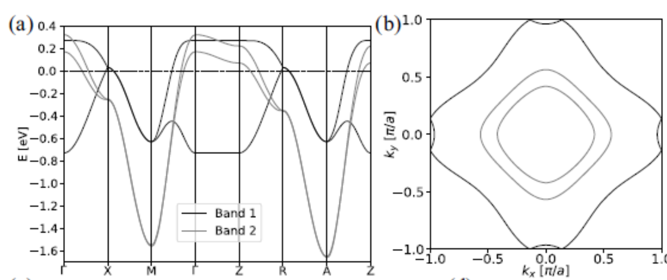
Nematic order in Fe-based materials.

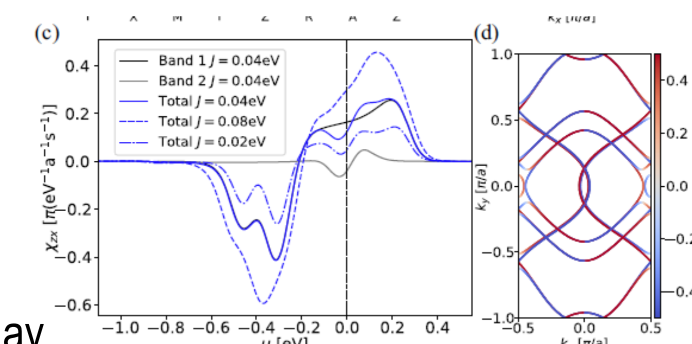
R.M. Fernandes, P. P. Orth, and J Schmalian, ARCMP (2019)

67 Candidate Materials from Magndata

Spin odd-parity **Odd-parity magnet**	$DyMn_2O_5$(55X,1.324), $Tm_5Pt_2In_4$(55T,1.790*), $CoNb_2O_6$(60Y,1.224),
	$La_{3/8}Ca_{5/8}MnO_3$(62Z,1.173), $La_{1/3}Ca_{2/3}MnO_3$(62Z,1.174),
	$La_{1/3}Ca_{2/3}MnO_3$(62X,1.175), Gd_2BaCuO_5(62Z,1.443), Er_2Pt(62X,1.444),
	CeNiAsO(129X,1.272*), Sr_2FeO_3Cl(129M,1.380,1.382*), Sr_2FeO_3Br(129M,1.381,1.383*),
	Sr_2FeO_3F(129M,1.385,1.386,1.387*), $NiCr_2O_4$(141M,1.688), $Dy_2Co_3Al_9$(63Z,1.267)
Scalar odd-parity	Na_2MnF_5(14Z,1.55*), Lu_2MnCoO_6(14A,1.32*), $YbLuCoMnO_6$(14B,1.329*),
	Lu_2CoMnO_6(14B,1.330*), Yb_2CoMnO_6(14B,1.328*), $SmMn_2O_5$(55X,1.192),
	$DyMn_2O_5$ (55X,1.599,1.76), $PrMn_2O_5$(55X,1.325), $Sr_2Fe_3Se_2O_3$(55U,1.463,1.626),
	$Tb_5Pd_2In_4$(55Y,1.697*), $FeNb_2O_6$(60Y,1.655), $BaCdVO(PO_4)_2$(61Y,1.298),
	$LuMnO_3$(62X,1.101), $HoMnO_3$(62X,1.20), $PrNiO_3$(62T,1.43), $NdNiO_3$(62T,1.45),
	$TmMnO_3$(62X,1.341), $SmNiO_3$(62T,1.353), $EuNiO_3$(62T,1.354), HoNiGe(62T,1.374),
	$Na_2CuSO_4Cl_2$(62X,1.682), $NiCr_2O_4$(141M,1.685), $Na_2Ni_2TeO_6$(193L,1.646*), MnS_2(205X,1.18)
Scalar and/or spin odd-parity	$PrMn_2O_5$(55X,1.19), $GdMn_2O_5$(55X,1.54,1.299,1.300), $BiMn_2O_5$(55U,1.74,1.75),
	$Tm_5Ni_2In_4$(55T,1.170*), $NdNiO_3$(62T,1.44), Cs_2CoCl_4(62T,1.51),$LuMnO_3$(62X,1.340)
Nematic	$Fe(ND_3)_2PO_4$ (14B,1.66), $NaMnGe_2O_6$(15A,1.260), $PrFe_2Al_8$(55U,1.681), VOCl(59R,1.37),
	MnV_2O_6(60Z,1.196), $NiNb_2O_6$(60Y,1.654), $CoNb_2O_6$(60Z,1.656), $BaNd_2O_4$(62T,1.95),
	ErNiGe(62Y,1.379), Y_2BaCuO_5(62T,1.445), $SrNd_2O_4$(62T,1.577), $DyBaCuO_5$(62Y,1.650),
	Dy_2TiO_5(62Y,1.698), PrPdSn(62T,1.744) , Ho_2BaCuO_5(62Y,1.651), DyGe(63Y,1.361)
	Li_2VOSiO_4(129M,1.9), Sr_2CoO_3Cl(129M,1.389), $Fe_{1.05}Te$(129R,1.434),
	$NdNiMg_{15}$ (129M,1.457), HoSbTe(129X,1.749), $Dy_3Ru_4Al_12$ (194L,1.115)

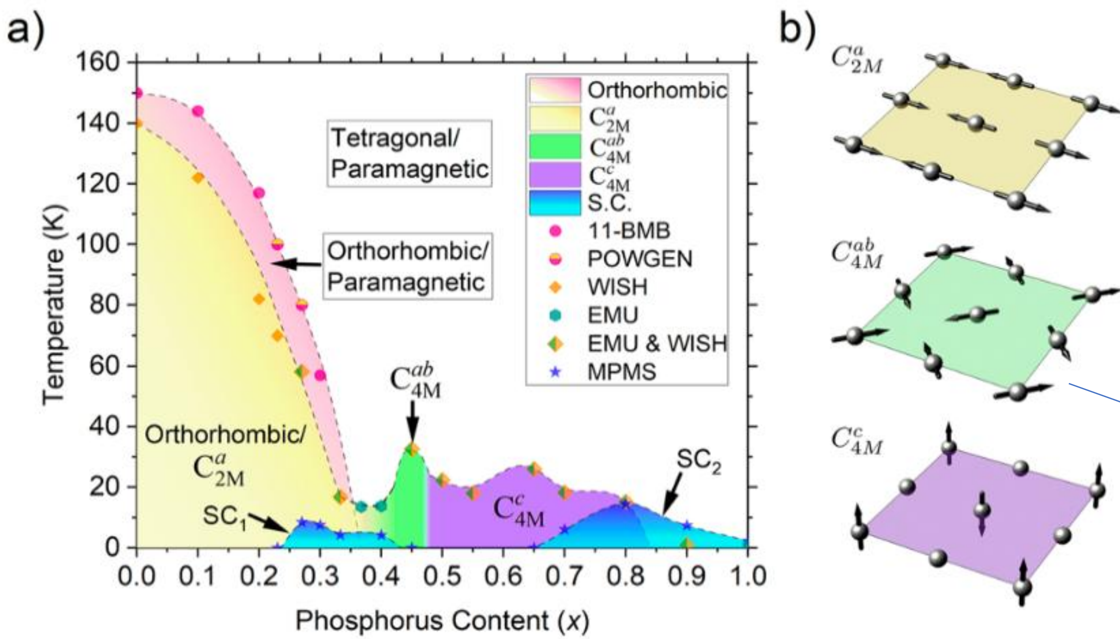
CeNiAsO





Also find SOC-free Edelstein effect – Chakraborty talk later today

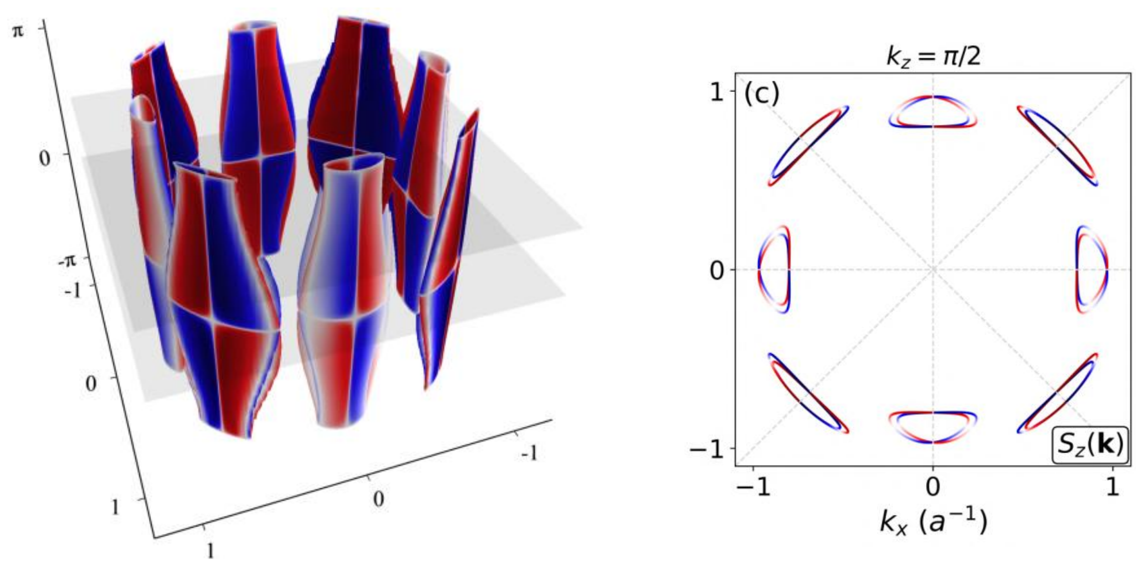
H-wave magnetism in $LaFeAs_{1-x}P_x$



Stadel et al., Communications Physics (2022): $LaFeAs_{1-x}P_x$

Space group P4/nmm (129)
$Q=(\pi,\pi)$

h-wave: $k_x k_y k_z (k_x^2 - k_y^2)\sigma_z$



See poster by Andreas Kreisel, where SOC is also included (with interesting consequences)

Conclusions

Sublattice-based tight-binding Hubbard models for magnetism

Applies to monoclinic, orthorhombic, tetragonal, hexagonal materials. Yields d-wave, g-wave, and i-wave altermagnets.

AFM non-symmorphic lattices also allow odd-parity spin-splitting based on co-planar magnetism – many materials examples.

Odd-parity magnetism competes with nematic and multiferroic states.

Odd-parity spin-splittings are large, h-wave spin splitting is predicted for $LaFeAs_{1-x}P_x$

Nematic generalizations of Fe-based materials and spin-scalar odd-parity states are competing states – and are also of interest.

Quasi-symmetry

- Why do our minimal models predict spin FM moment ~λ^2_{soc} for some altermagnetic states and ~ λ_{soc} for others?

- Answer is quasi-symmetry: an approximate higher symmetry that emerges when only a single SOC component is included.
- Example $(\lambda_{x,k},\lambda_{y,k},\lambda_{z,k})=(0,0,\lambda_{z,k})$, spin-rotations around the z-axis

- Consider point group D_{4h} with a B_{2g} altermagnet:

- GL coupling term is $m_x J_y + m_y J_x \xrightarrow{4-\text{fold}}$ -($m_x J_y + m_y J_x$), so forbidden.
- Note that $m_x J_y - m_y J_x$ is the only bilinear that is allowed. It is this that gives all the non-zero terms in the theory.

- This argument is very general (only requires that AM is purely exchange driven).