Dynamic generation of scalar chirality and topological Hall effect in spiral magnets

Igor Mazin *(t)*

Nirmal Ghimire *(e)*

Department of Physics and Quantum Materials Center, George Mason University

also Lekh Poudel, Rebecca Dally, Markus Bleuel, and Jeff Lynn (NIST), N. Thapa Magar and M. Afshar (GMU), Michael A. McGuire (ORNL), J. Samuel Jiang and John Mitchell (ANL)

Useful discussions with Huibo Cao (ORNL), Predrag Nicolic (GMU) and Rafael Fernandes (UMN)

Outline

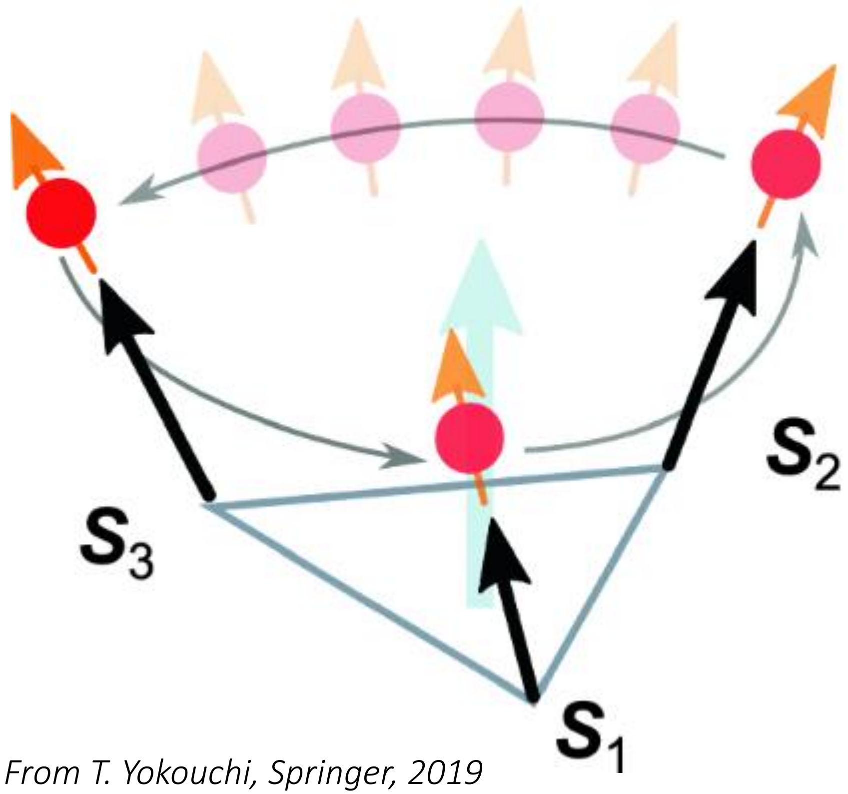
- Topological HE and Scalar Spin Chirality
  - Special role of Transverse Conical Spirals
- The case of YMn_6Sn_6
  - Introducing the material
  - Introducing the ground state magnetic spiral
  - Magnetometry and neutron scattering
  - (H,T) phase diagram
  - Decomposition of the Hall effect; topological Hall effect (THE)
  - Density functional calculations (magnetism)
  - Mean field theory at T=0; revealing the nature of the 4 major phases
- Finite-temperature fluctuations: a phenomenological theory of fluctuation-induced ("nematic") THE
- Other examples: Fe_3Ga_4, $LaMn_2Ge_2$, ScFeGe.

Hall effect: Ordinary, Anomalous and Topological

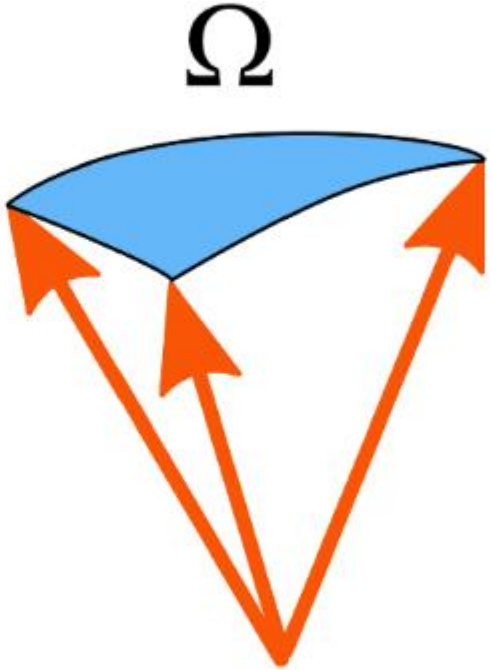
- Ordinary Hall effect (Lorenz force) $\rho_{yx} = R_0 B$
- Anomalous Hall effect (internal exchange field+SOC)
- Topological Hall effect (scalar spin chirality)

$$R_0 = -{}^{1}/_{ne}$$
$$B = \mu_0 H$$

$$\rho_{yx} = R_0 B + \underbrace{\rho_{yx}^{A}}_{R_S \mu_0 M}$$



From T. Yokouchi, Springer, 2019



Two points to note:

- While people usually invoke double-exchange, Kohn-Sham electrons always follow the local magnetization
- **S_1-S_2-S_3-S_1** must form a closed loop.

Scalar chirality and spin spirals

Continuous approximation:

$$b_\alpha = \varepsilon^{\alpha\beta\gamma}\, \mathbf{M} \cdot (\partial_\beta \mathbf{M} \times \partial_\gamma \mathbf{M}).$$

(***b*** = topological field)

- Single helical spiral: coplanar, ***b*** =0
- Two helical spirals $\boldsymbol{M} = \boldsymbol{M}_1 + \boldsymbol{M}_2$,

  $$\partial_z \boldsymbol{M}_1 = \omega_1 \boldsymbol{M}_1 \times \hat{\boldsymbol{z}};\, \partial_y \boldsymbol{M}_2 = \omega_2 \boldsymbol{M}_2 \times \hat{\boldsymbol{y}}$$

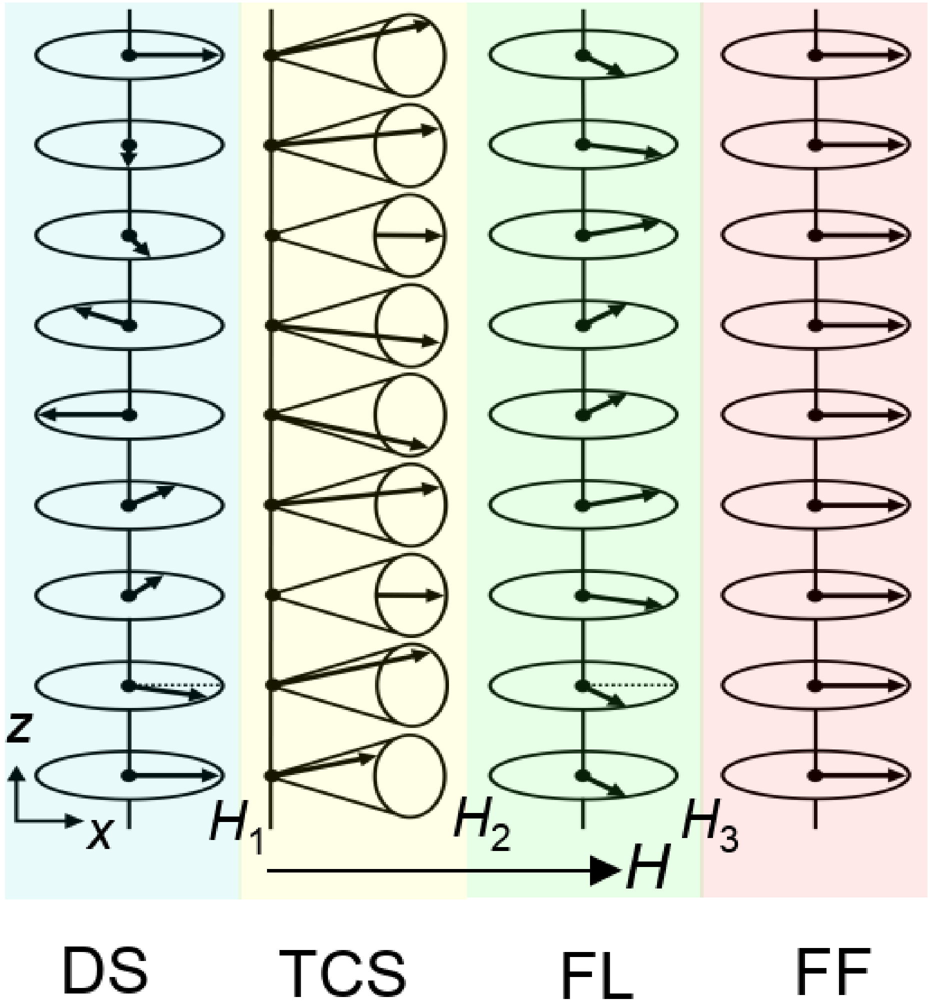
  $$b_x = \boldsymbol{M} \cdot \partial_z \boldsymbol{M}_1 \times \partial_y \boldsymbol{M}_2$$

  $$\propto (\boldsymbol{M}_1 + \boldsymbol{M}_2) \cdot (\boldsymbol{M}_1 \times \hat{\boldsymbol{z}})(\boldsymbol{M}_2 \times \hat{\boldsymbol{y}}) = \boldsymbol{0}$$
- Three helical spirals (x,y,z): ***b***≠0
- Single transverse conical spiral: ***b***=0

  $$\mathbf{M} = \mathbf{M}_x + \mathbf{m}$$

  $$\mathbf{M}_x = const$$

  $$\frac{\partial \mathbf{M}}{\partial z} = \frac{\partial \mathbf{m}}{\partial z} = \mathbf{m} \times \mathbf{x}$$



Scalar chirality and spin spirals

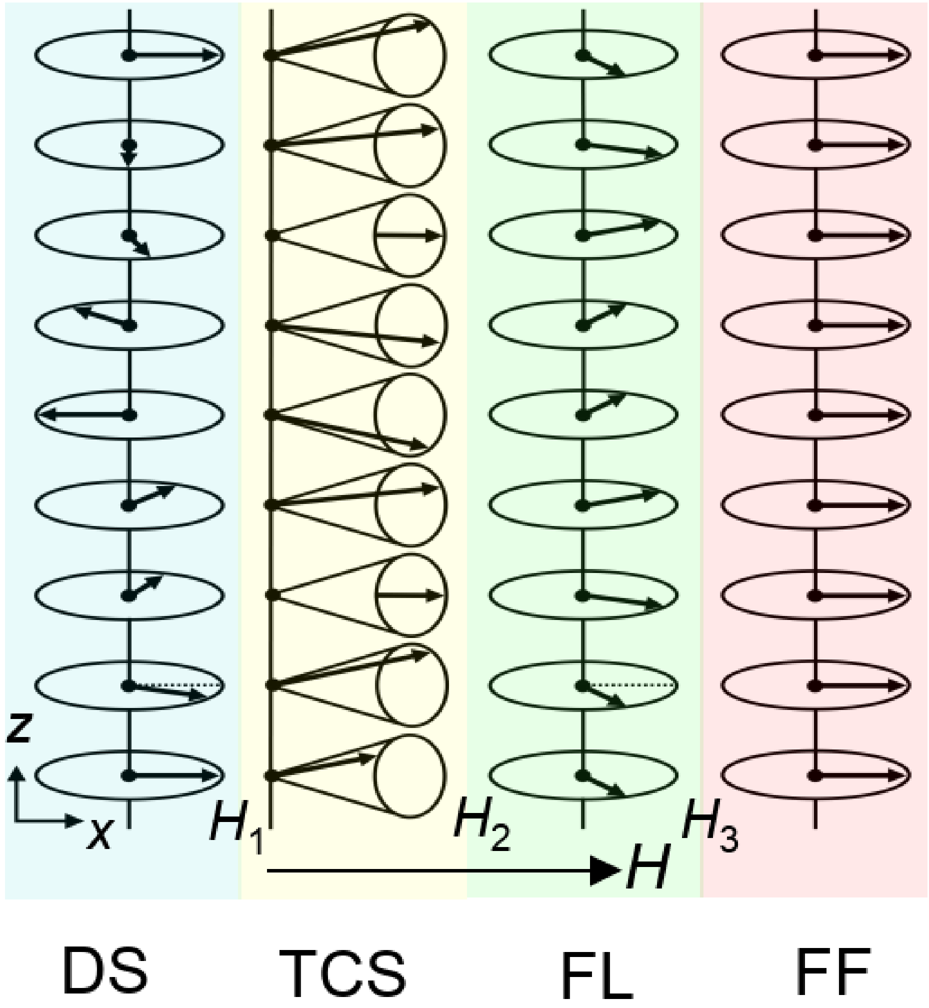
$$b_\alpha = \varepsilon^{\alpha\beta\gamma}\, \mathbf{M}\cdot(\partial_\beta \mathbf{M} \times \partial_\gamma \mathbf{M}).$$

- Single transverse conical spiral (z) + single helical spiral (y)

$$\mathbf{M} = M_x \hat{\mathbf{x}} + \mathbf{m} + \boldsymbol{\mu}$$

$$\frac{\partial \mathrm{M}}{\partial z} = \frac{\partial \mathbf{m}}{\partial z} = \mathbf{m}\times\hat{\mathbf{x}}$$

$$\frac{\partial \mathrm{M}}{\partial y} = \frac{\partial \boldsymbol{\mu}}{\partial y} = \boldsymbol{\mu}\times\boldsymbol{\omega}$$

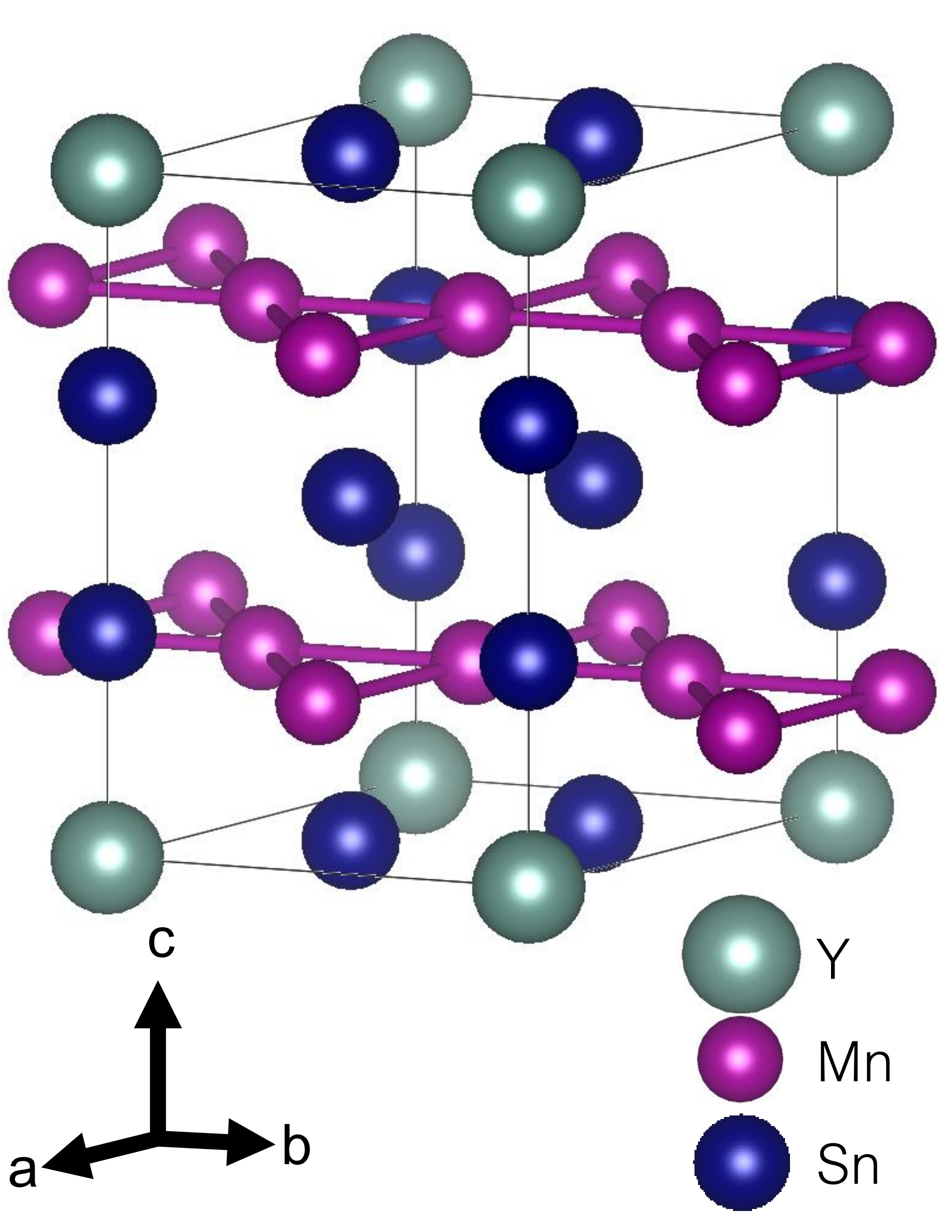


$$b_x = (\boldsymbol{\mu}\cdot\mathbf{m})[\boldsymbol{\mu}\cdot\hat{y}] - (\boldsymbol{\mu}\cdot\hat{\mathbf{x}})[\boldsymbol{\mu}\cdot(\boldsymbol{\omega}\times\mathbf{m})] = k_y m_z \mu^2$$

The case of YMn_6Sn_6

- Introducing the material
- Introducing the ground state magnetic spiral
- Magnetometry and neutron scattering
- (*H*,*T*) phase diagram
- Decomposition of the Hall effect; topological Hall effect (THE)
- Density functional calculations (magnetism)
- Mean field theory at *T*=0; revealing the nature of the 4 major phases

Introducing the material



Stacking sequence:

(Y, Sn) – Mn – (Sn)– Mn – (Y, Sn)

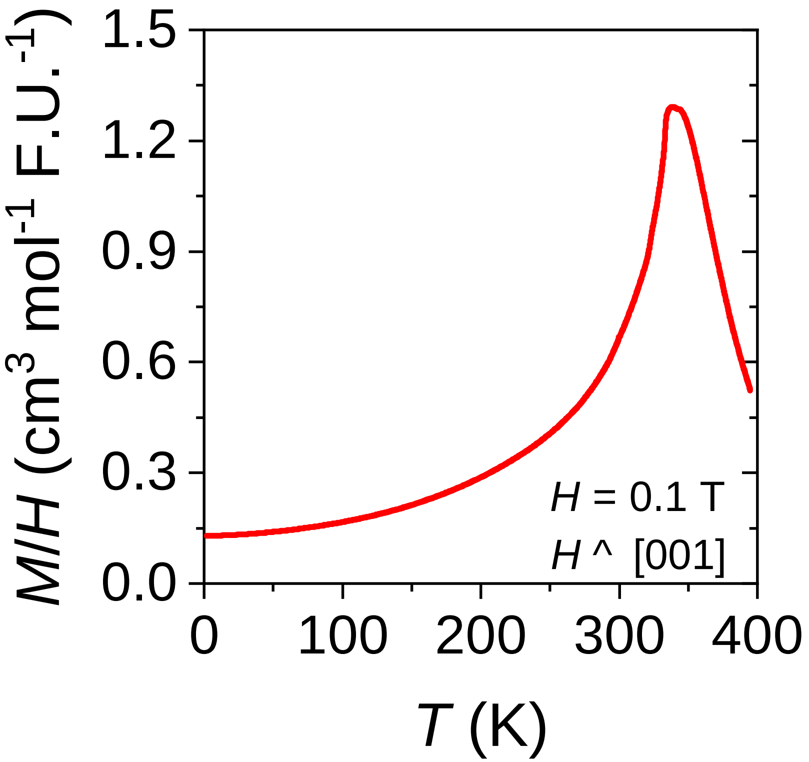
A good metal

Intralayer interaction: strongly FM

Interlayer interaction:

mixed, long-range

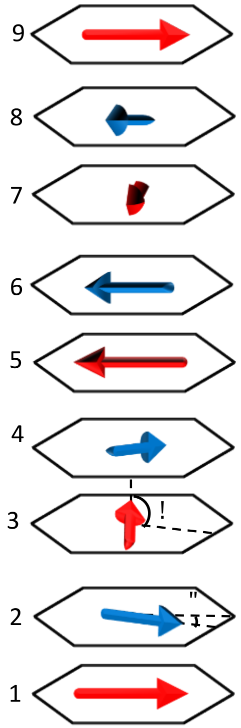
Individual Mn layers: Kagome (irrelevant)



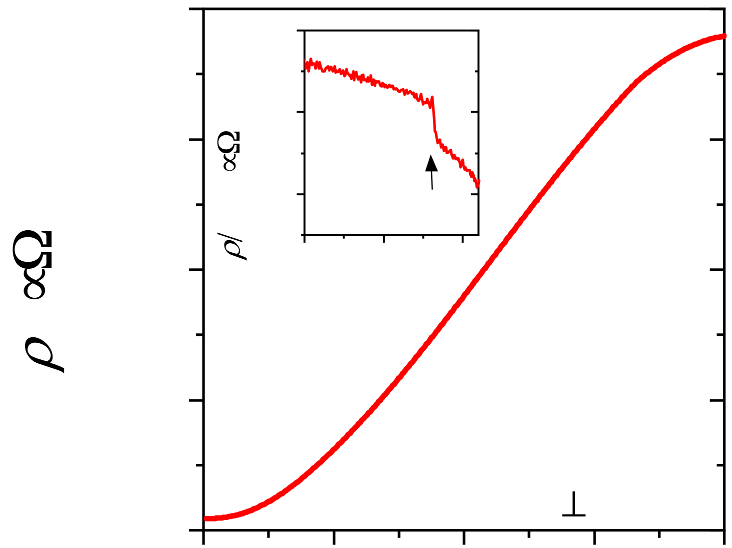
Antiferromagnetic ordering below 345 K

Venturini *et al.*,J. Alloy. Comp. 236, 102 (1996)

Rosenfeld *et al.*,J. Physica B 403, 1898 (2008)

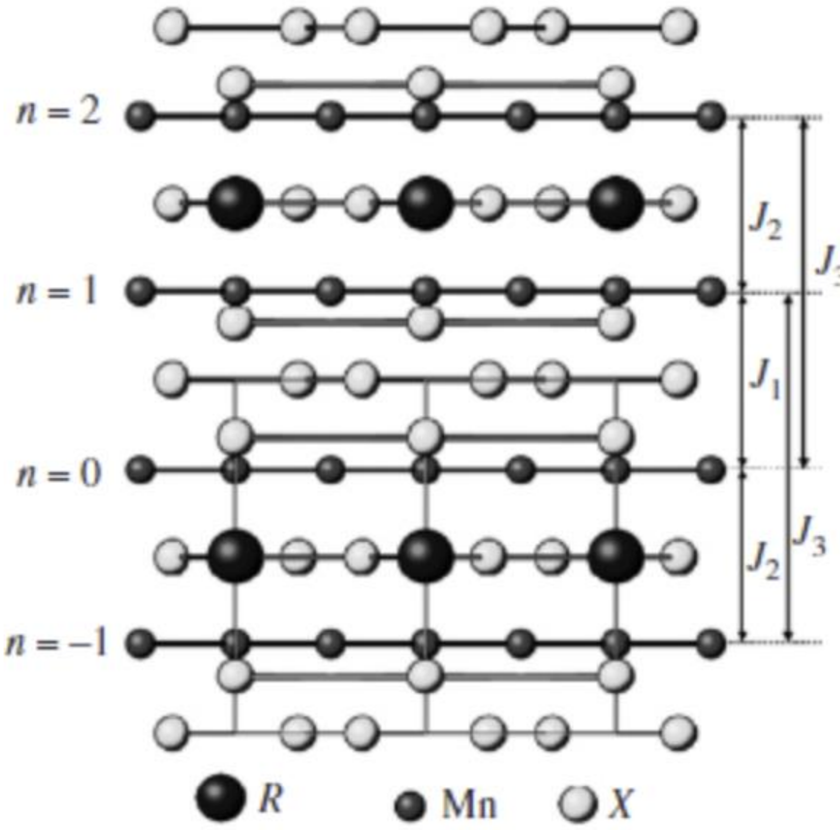


Staggered spiral at low temperature



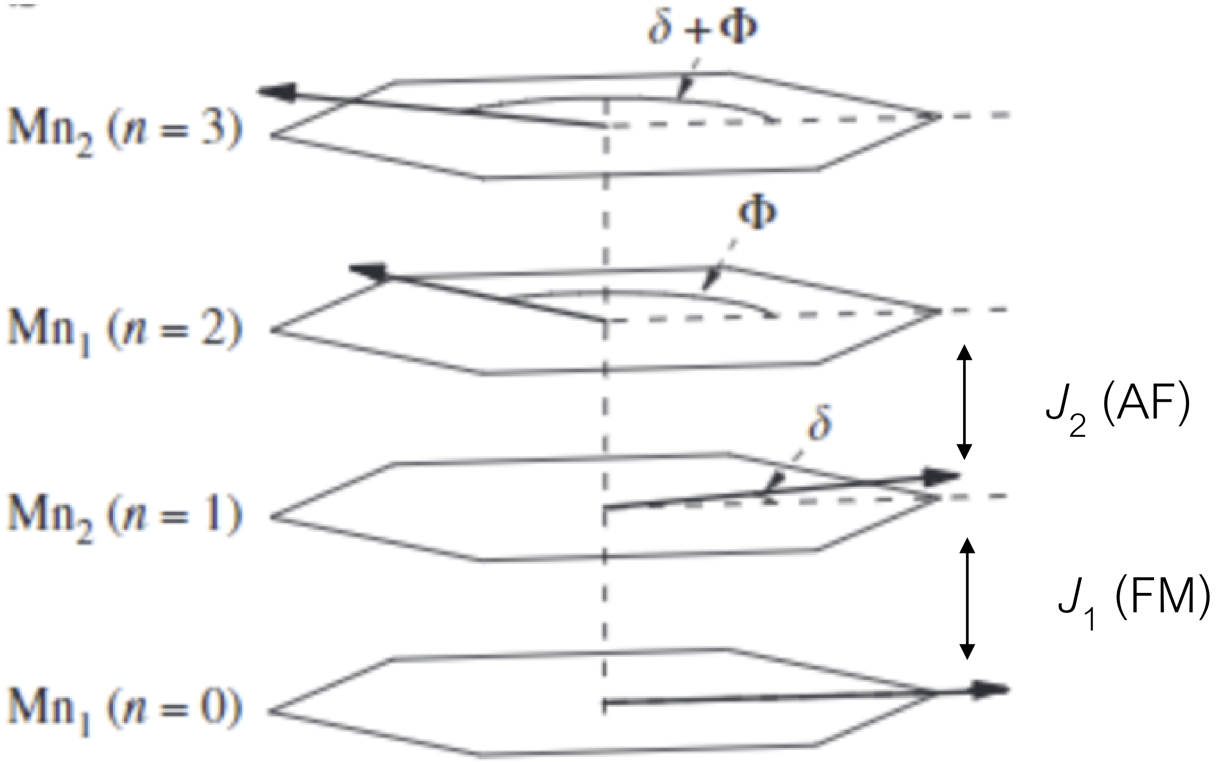
A good metal

Introducing the ground state magnetic spiral



R = Y, X = Sn

Stacking sequence:

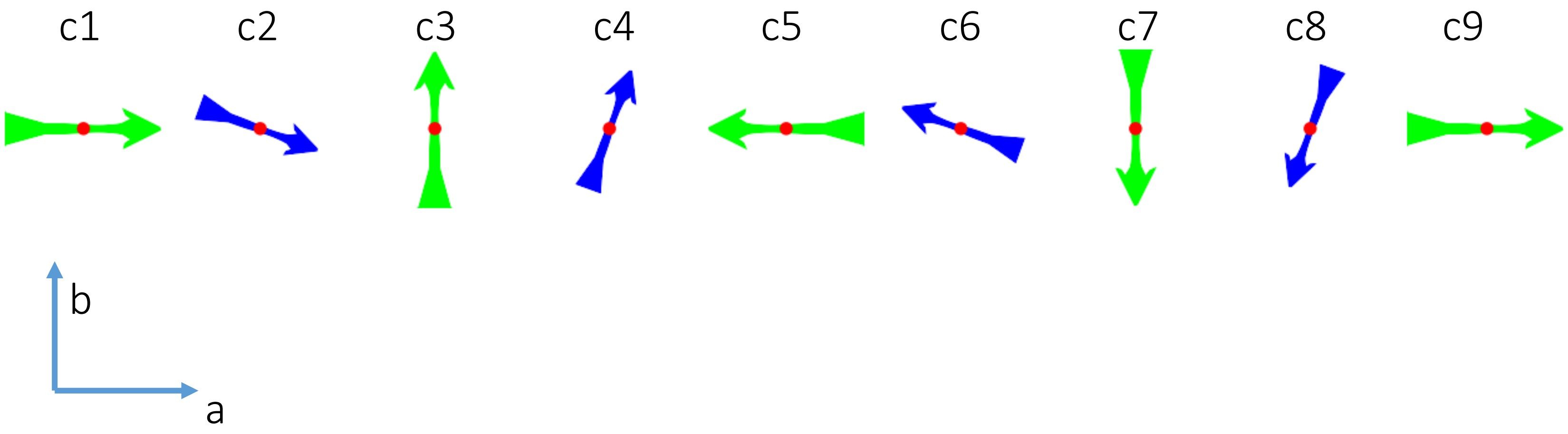


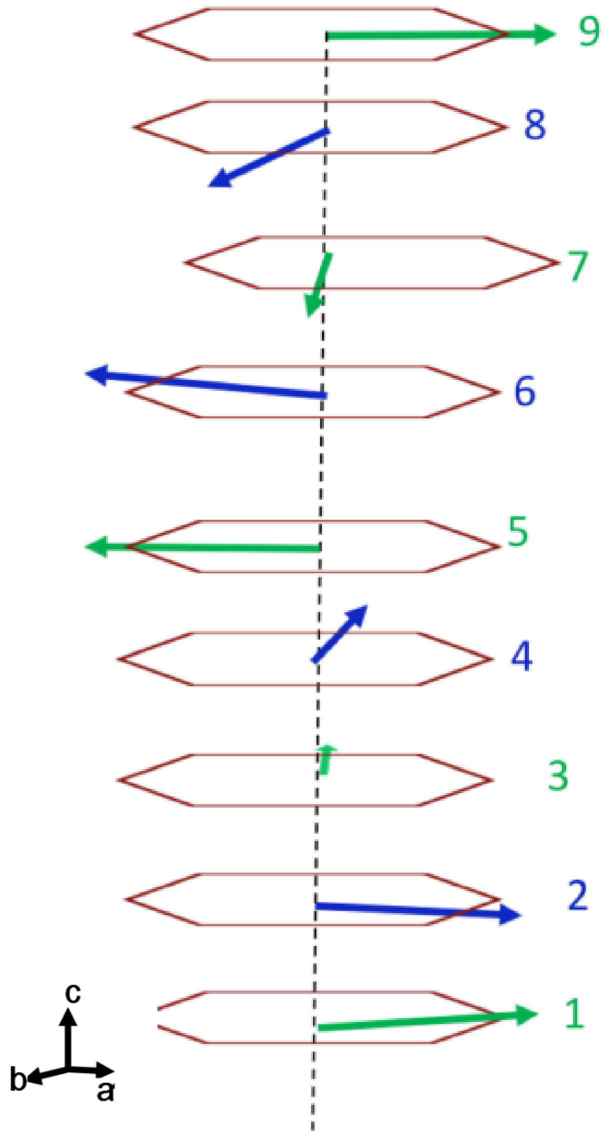
E.V. Rosenfeld & N.V. Mushnikov. *Physica B*, **403**, 1898–1906 (2008).

Introducing the ground state magnetic spiral

Antiferromagnetic ordering at T ~ 340 K

Ground state (T~0):
An incommensurate helical spiral with moments in the ab-plane, $q \sim (0,0,0.25)$
Period: approximately 8 Mn layers





Magnetometry

1. H||c

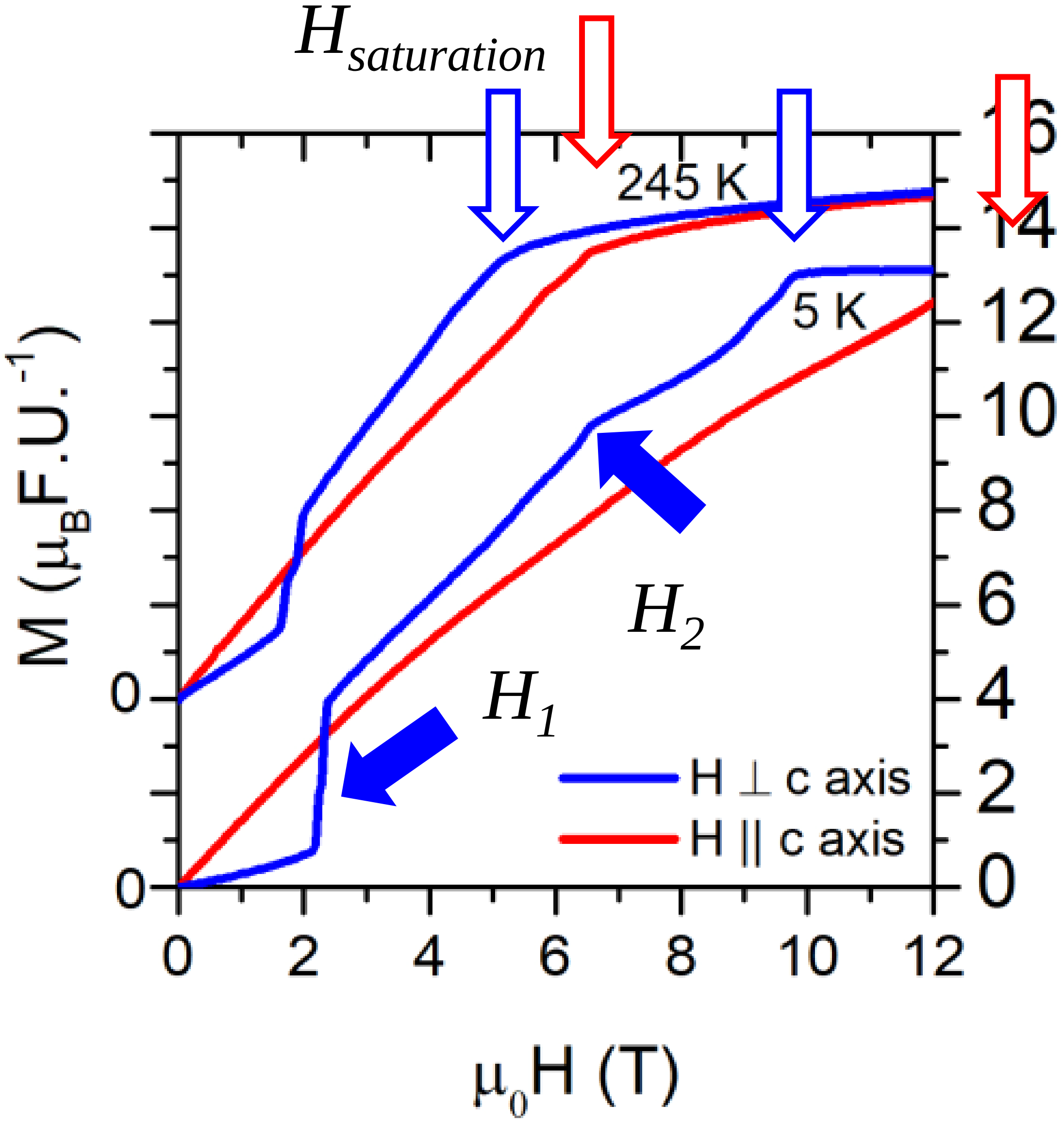
No phase transitions, quasilinear behavior

2. H||ab

Two transitions at T=0, at least one first order

Spin flops?

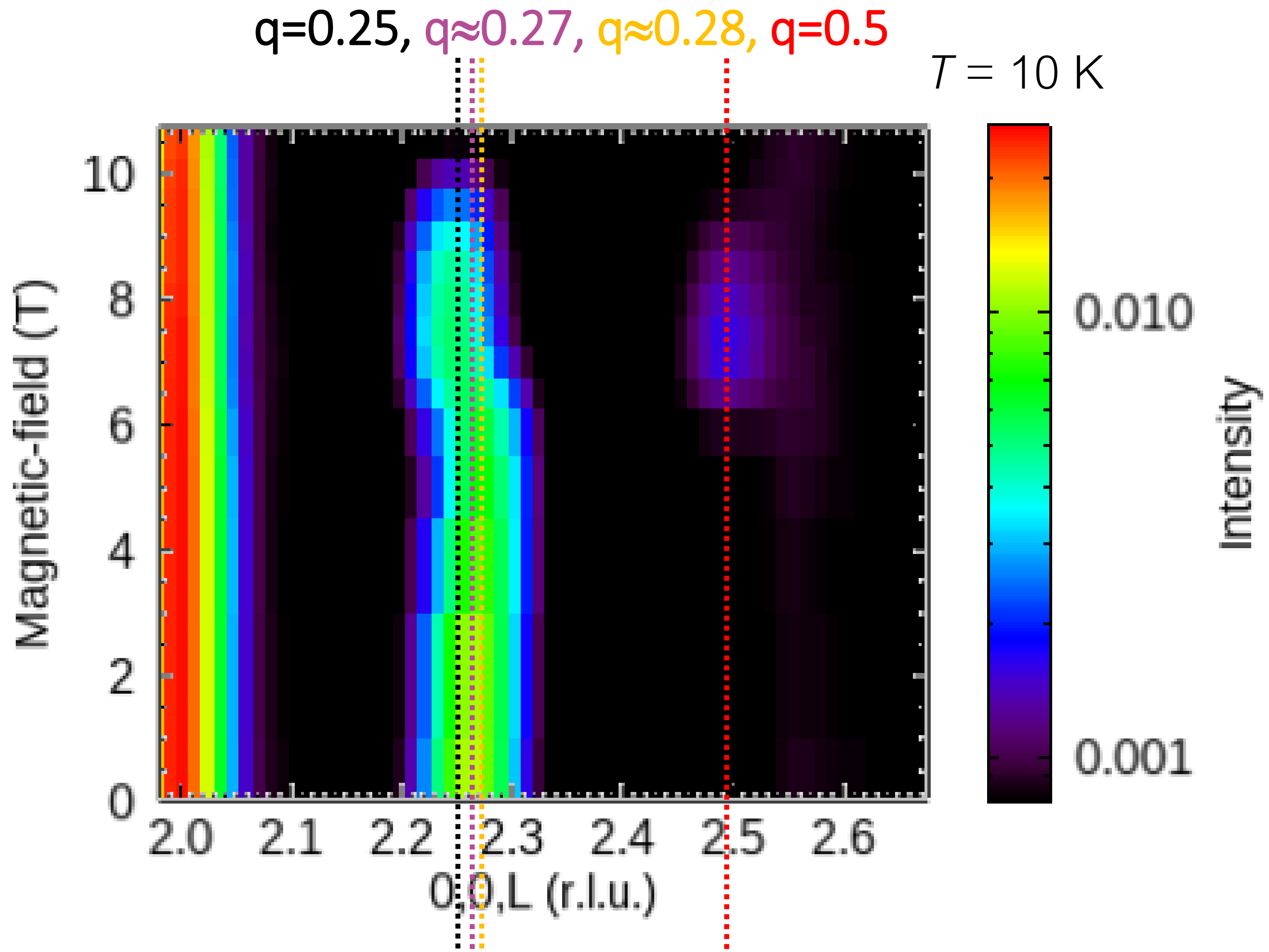
Why two?



Neutron scattering

1. $H=H_1$: q shifts by a few %%, intensity drops by a factor of two

2. $H=H_2$: q discontinuously jumps to exactly q=0.25, and a satellite appears at q=0.5

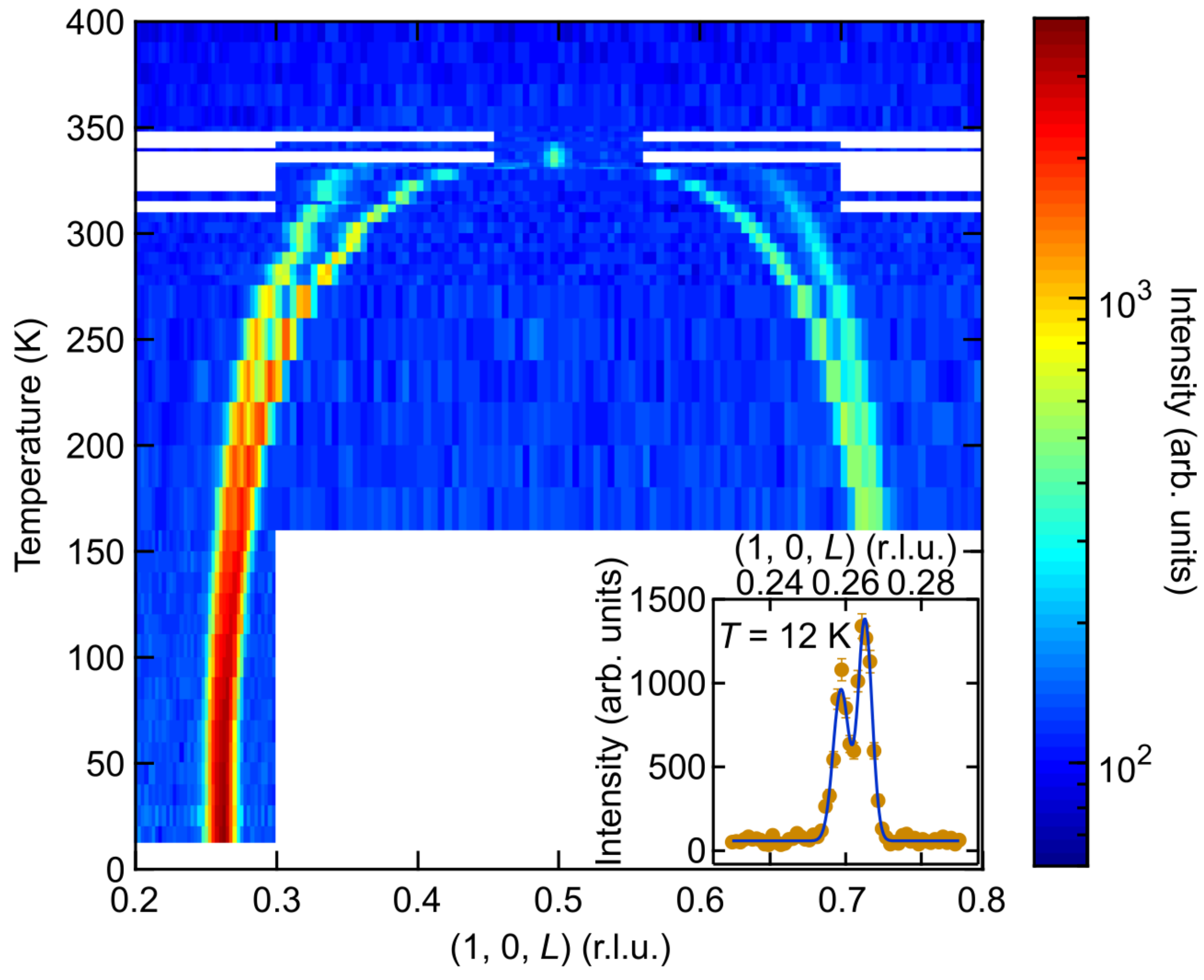


Neutron scattering

1. $H=H_1$: q shifts by a few %%, intensity drops by a factor of two

2. H_2: q discontinuously jumps to exactly q=0.25, and a satellite appears at q=0.5

3. With temperature, the $H=0$ spiral splits into two (is modulated) and the periodicity continuously reduces from ~4 cells to exactly 2 (AF collinear?)

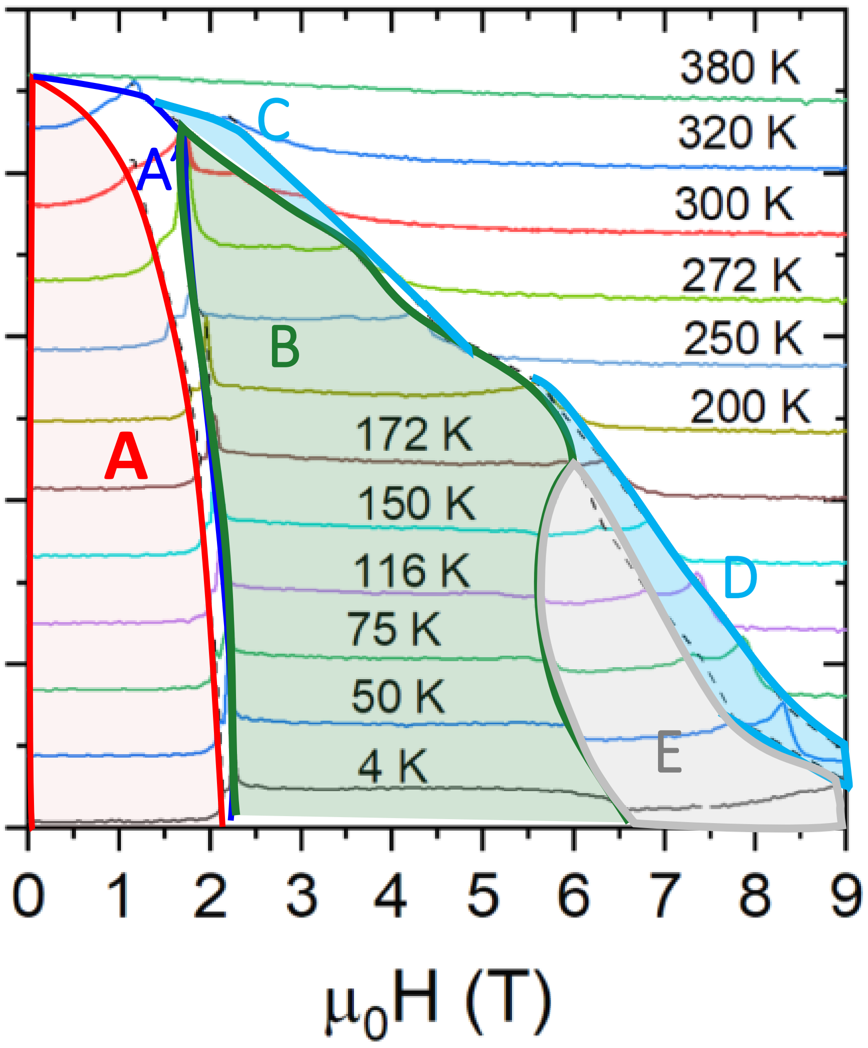


(H,T) phase diagram

From magnetometry, neutrons and differential susceptibility:

Phase A: low field.
Phase A': reflects splitting of the spirals
Phase B appears after the first flop
Phase C and D exist in near vicinity of the Neel T (Mermin-Wagner?)
Phase E appears after the second flop

I will argue that we fully understand the underlined phases and that the phase B (and only it) is topologically nontrivial



Density functional calculations (magnetism)

$$H = \boxed{\sum_{i,j} J_n \mathbf{n}_i \cdot \mathbf{n}_j} + \boxed{\sum_{i,j} J_p \mathbf{n}_i \cdot \mathbf{n}_j} + \boxed{K \sum_i (n_i^z)^2} + \boxed{\sum_i J^z n_i^z \cdot n_{i+1}^z} + \boxed{\sum_i \mathbf{n}_i \cdot \mathbf{H}}$$

Full Hamiltonian

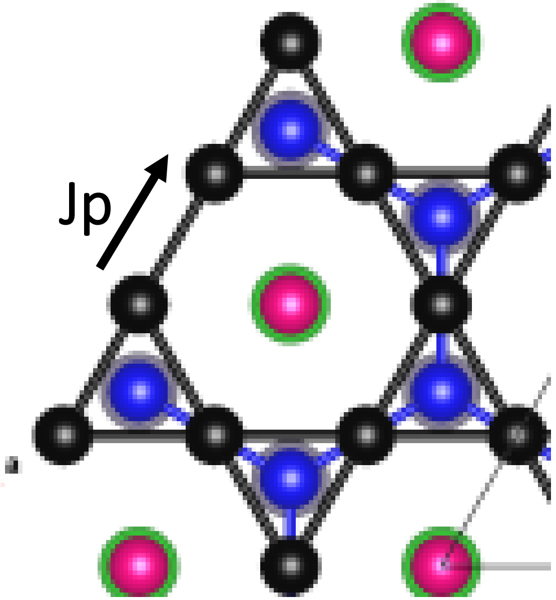
Interplanar exchange

Intraplanar exchange

Single-site anisotropy

Ising exchange

Zeeman interaction



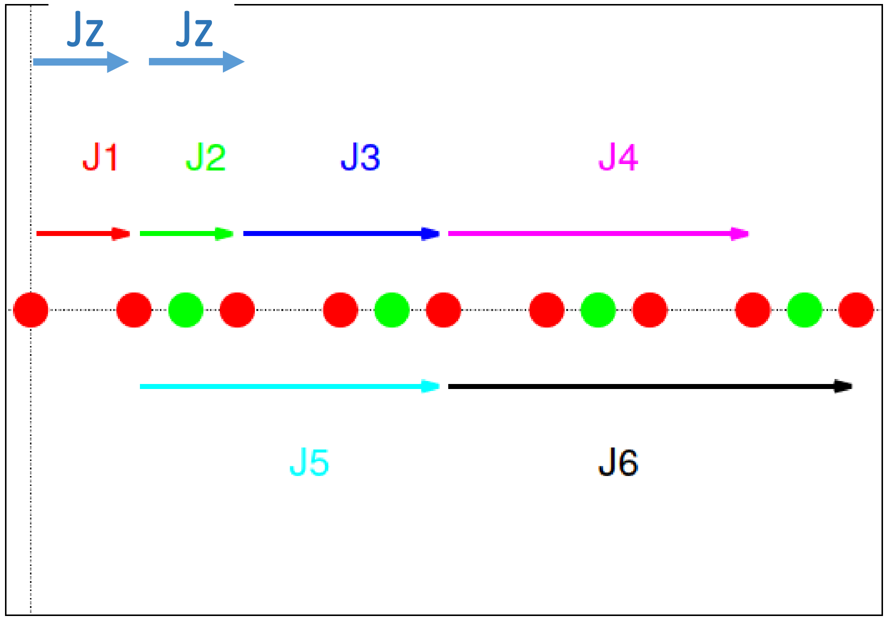


FIG. 2. First 6 exchange interactions between Mn layers. Red: Mn layer; green: spacer layer including Y

Density functional calculations (magnetism)

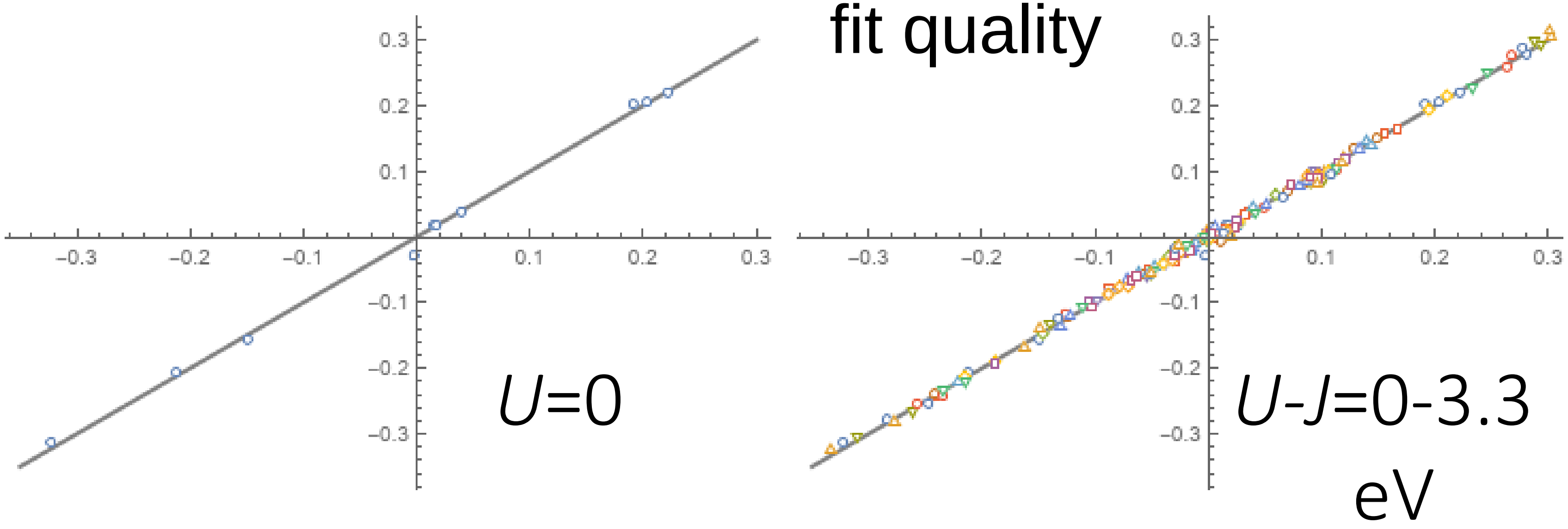
Full Hamiltonian

Eleven collinear magnetic patterns in 1x1x4 supercell (8 Mn layers): udddddddu, udddddud, uddddudd, uddduuud, uddduuud, ududdudu, udududdu, udududud, uudduudd, uuduuudd, uuuuuuuu

Energies fitted to (n≤6)

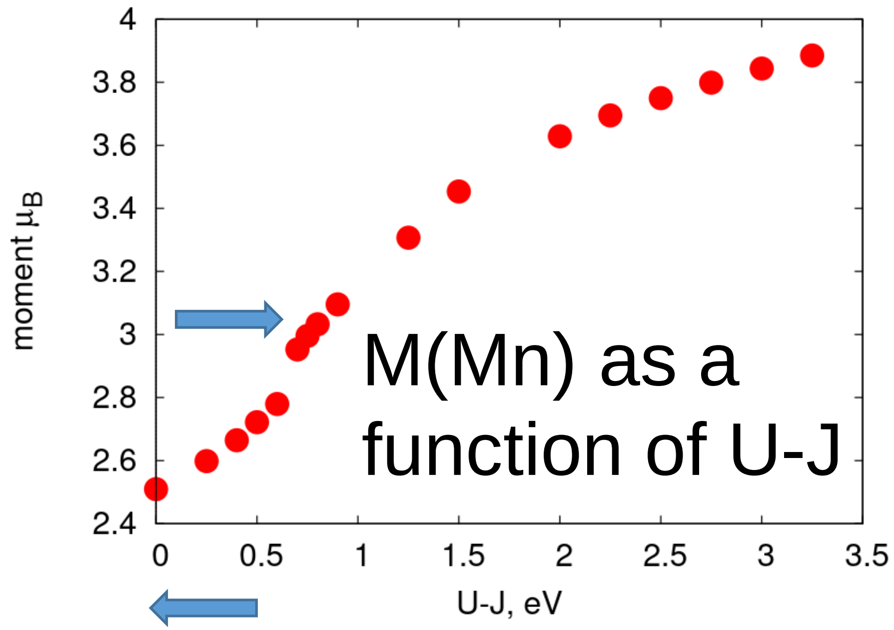
$$\boxed{\sum_{i,j} J_n \mathbf{n}_i \cdot \mathbf{n}_j}$$

fit quality

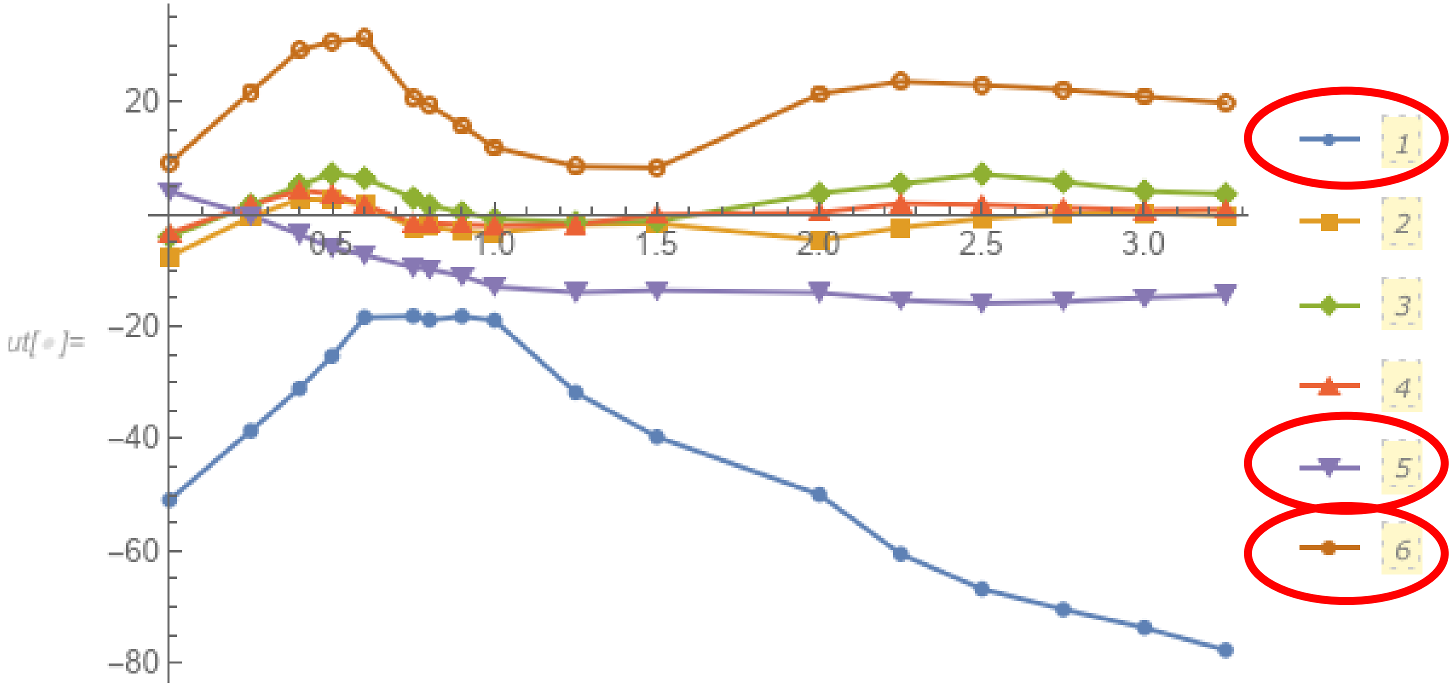


J_p is fitted to planar FM and AF calculations (with SOC). K and J^z are fitted to udududud and uuuuuuuu for the magnetization directions (001) and (100)

Density functional calculations (magnetism)



Very fluctuating!



Long-range (RKKY?)

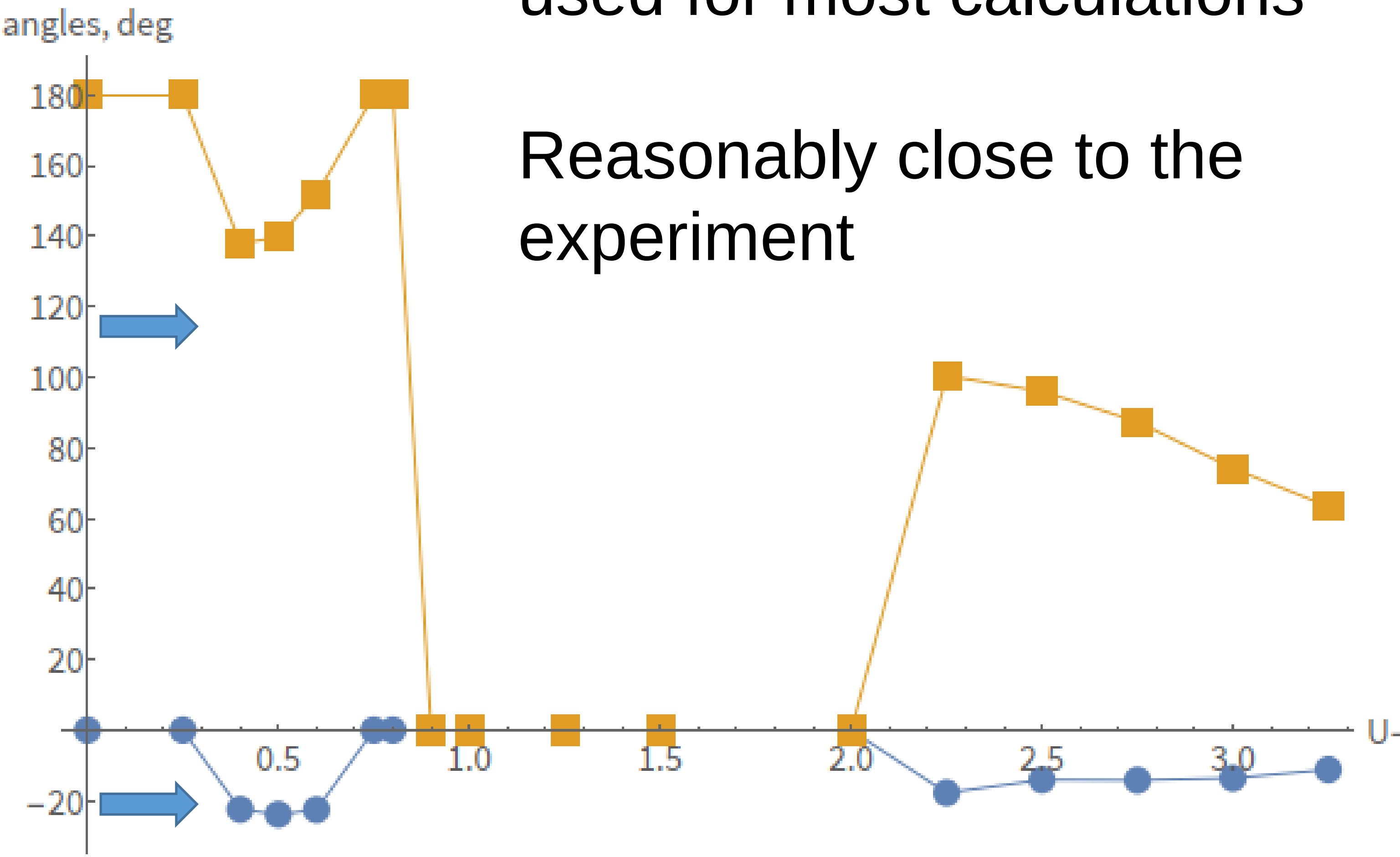
FIG. 4. Fitted values of the exchange constants J_1–J_6 as a function of $U-J$.

Density functional calculations (magnetism)

	Full	Reduced	Minimal
J1	-12.9	-12.9	-12.9
J2	7.3	4.7	4.7
J3	-0.1	-2.2	-2.2
J4	0.1	n/a	n/a
J5	-0.2	n/a	n/a
J6	-0.5	n/a	n/a
Jp	-53	-53	-53
K	-0.3	-0.3	0.2
Jz	0.5	0.5	n/a

U-J ~ 0.5 eV
used for most calculations

Reasonably close to the experiment



Density functional calculations (magnetism)

RAMIFICATIONS:

1. Strongly Mermin-Wagner system
   - $T_N \sim J_p/(const + log\frac{J_p}{J_1})$ ~30 meV
   - $H_{sat} \sim J_1 \ll T_N$ ~0.7 meV
2. Strong parametric frustration -> spirals
3. Strong fluctuations, especially near T_N

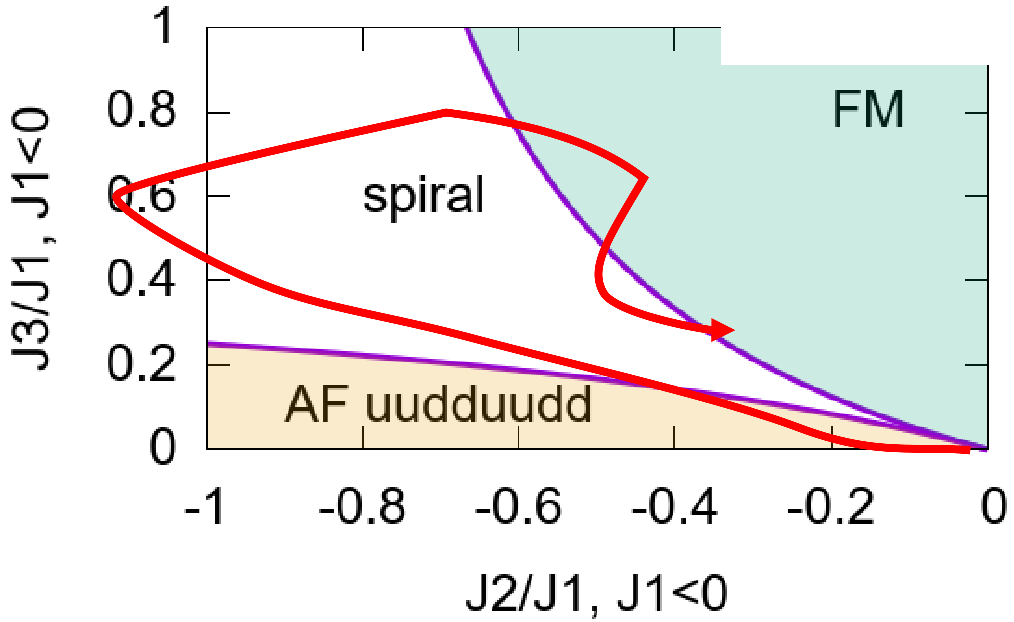
Mean field theory at T=0, H=0: minimal model

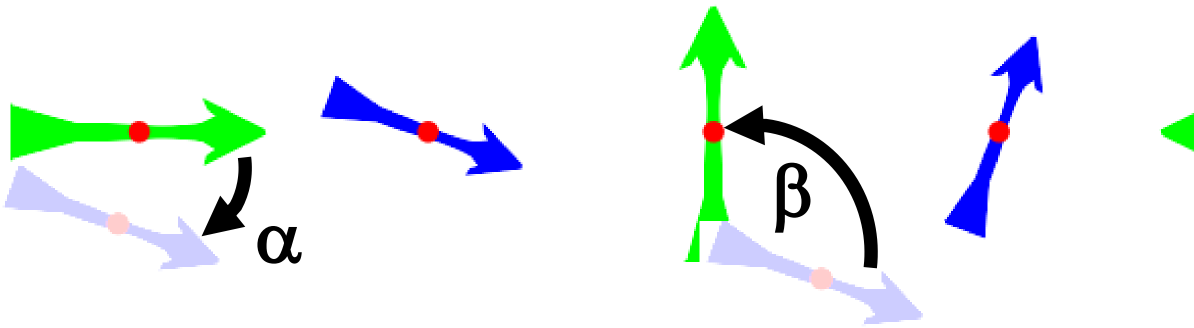
$$H = \sum_{i,j} J_{1,2,3}\, \mathbf{n}_i \cdot \mathbf{n}_j + \sum_{i,j} \cancel{J_x\, \mathbf{n}_i} \cdot \mathbf{n}_j + K \sum_i (n_i^z)^2 + \sum_i \cancel{J^z n_i^z} \cdot n_{i+1}^z + \sum_i \mathbf{n}_i \cdot \mathbf{H}$$

Analytical solution

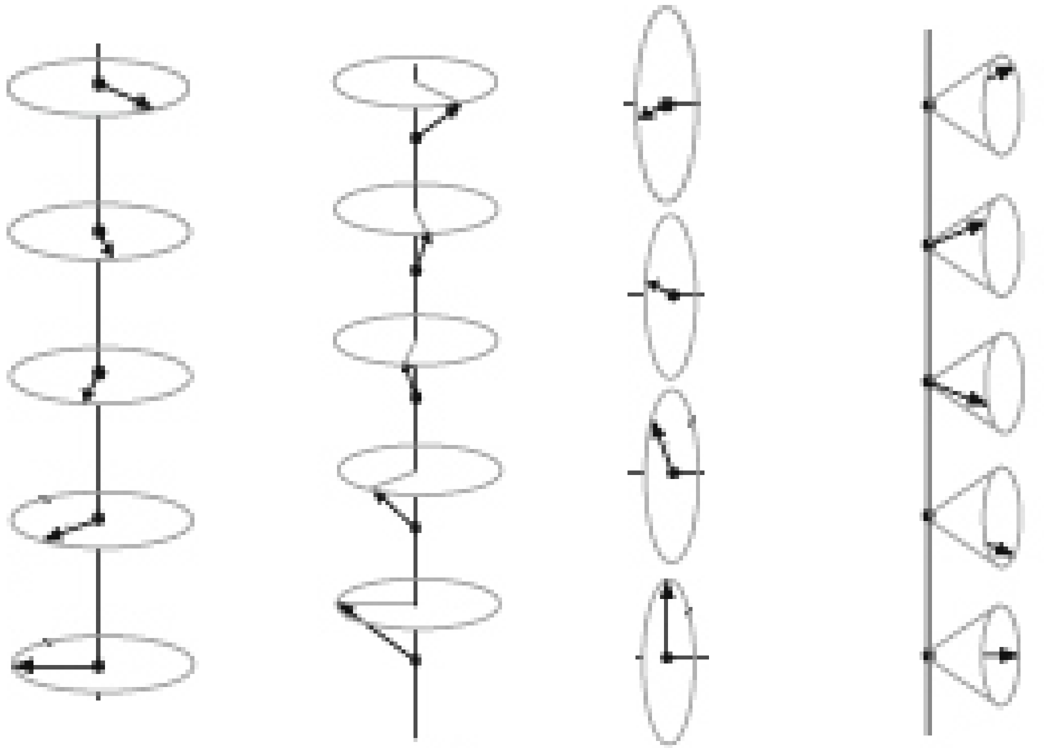
$$\alpha = -sign(J_1 J_3) \cos^{-1}\left(\frac{J_2 J_3}{J_1^2} - \frac{J_3}{J_2} - \frac{J_2}{4J_3}\right)$$

$$\beta = \cos^{-1}\left(\frac{J_3 J_1}{J_2^2} - \frac{J_1}{4J_3} - \frac{J_3}{J_1}\right),$$





Mean field theory at T=0, H=0: minimal model



H=0 helix

$H_z>0$ longitudinal conical

K<0 doesn't exist

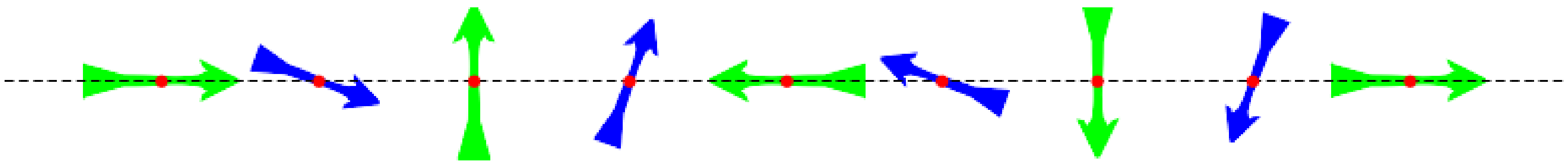
$H_x>H_1$ transverse conical

$$H_1 \sim \sqrt{JK} \sim 3.5 \text{ T}$$

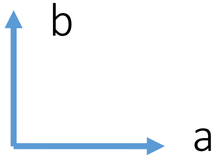
However, the model has another spin-flop!

Mean field theory at T=0, H>0: minimal model

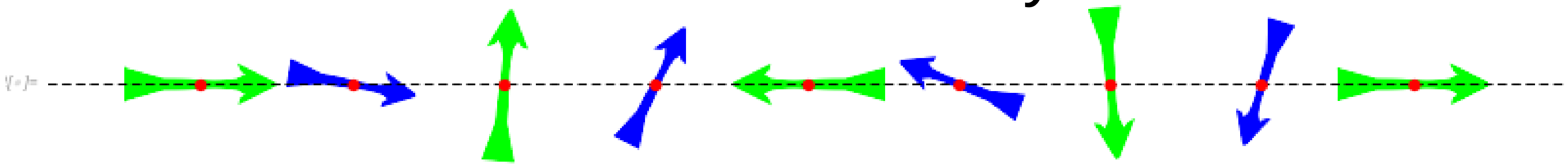
Two different *coplanar* solutions!



1) Flat spiral (helix),

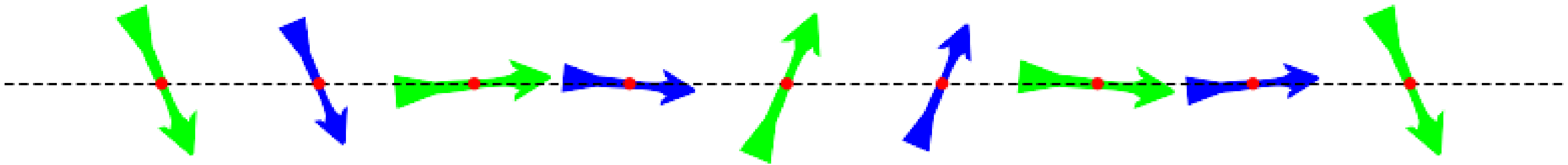


distorted by the field



Important: the second structure has perio-dicity of 1x1x4 for M_y, but of 1x1x2 for M_x

2) Commensurate 8-layers structure



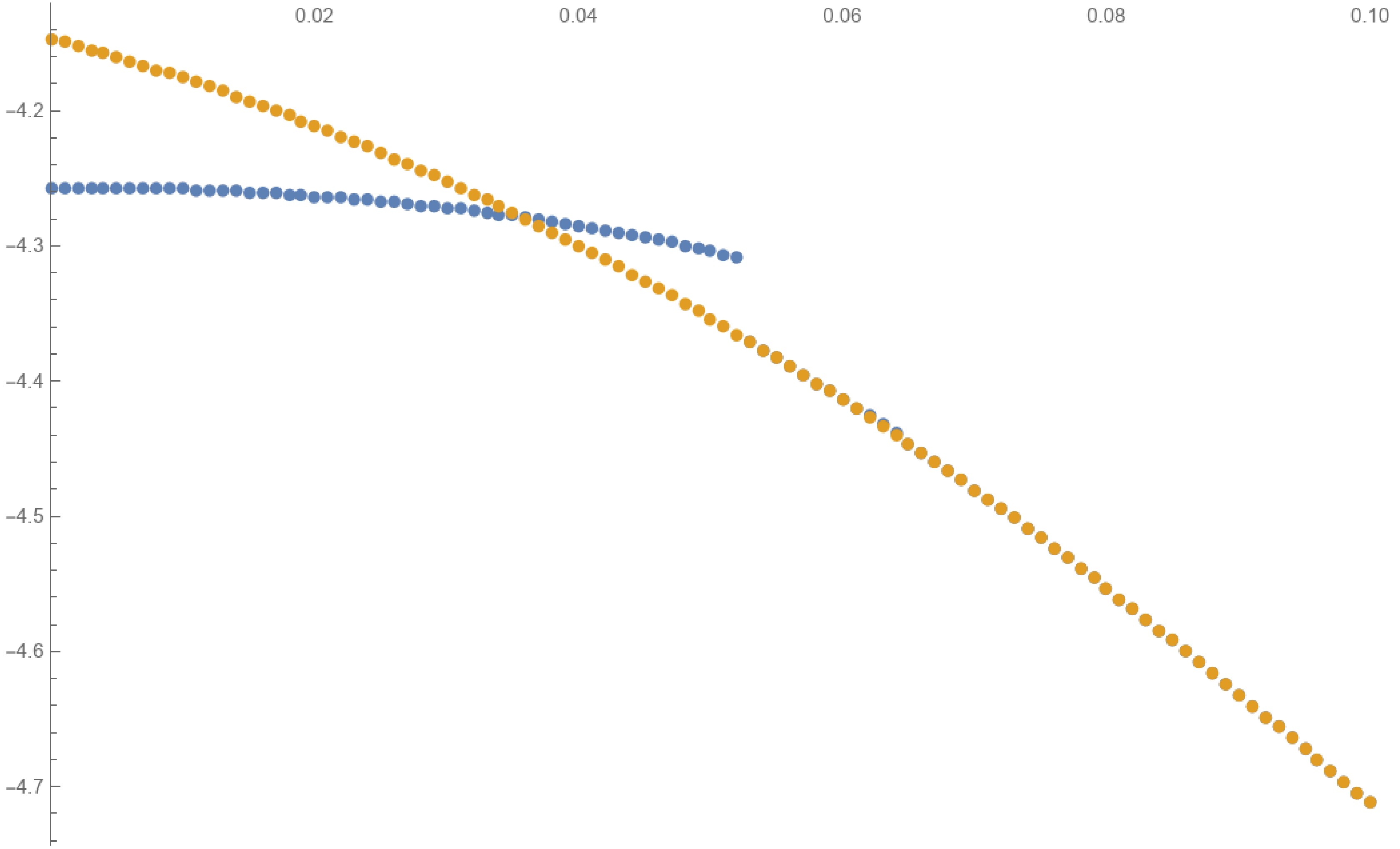
Mean field theory at T=0, H>0: minimal model

1) Distorted helix

2) Commensurate 8-layers structure

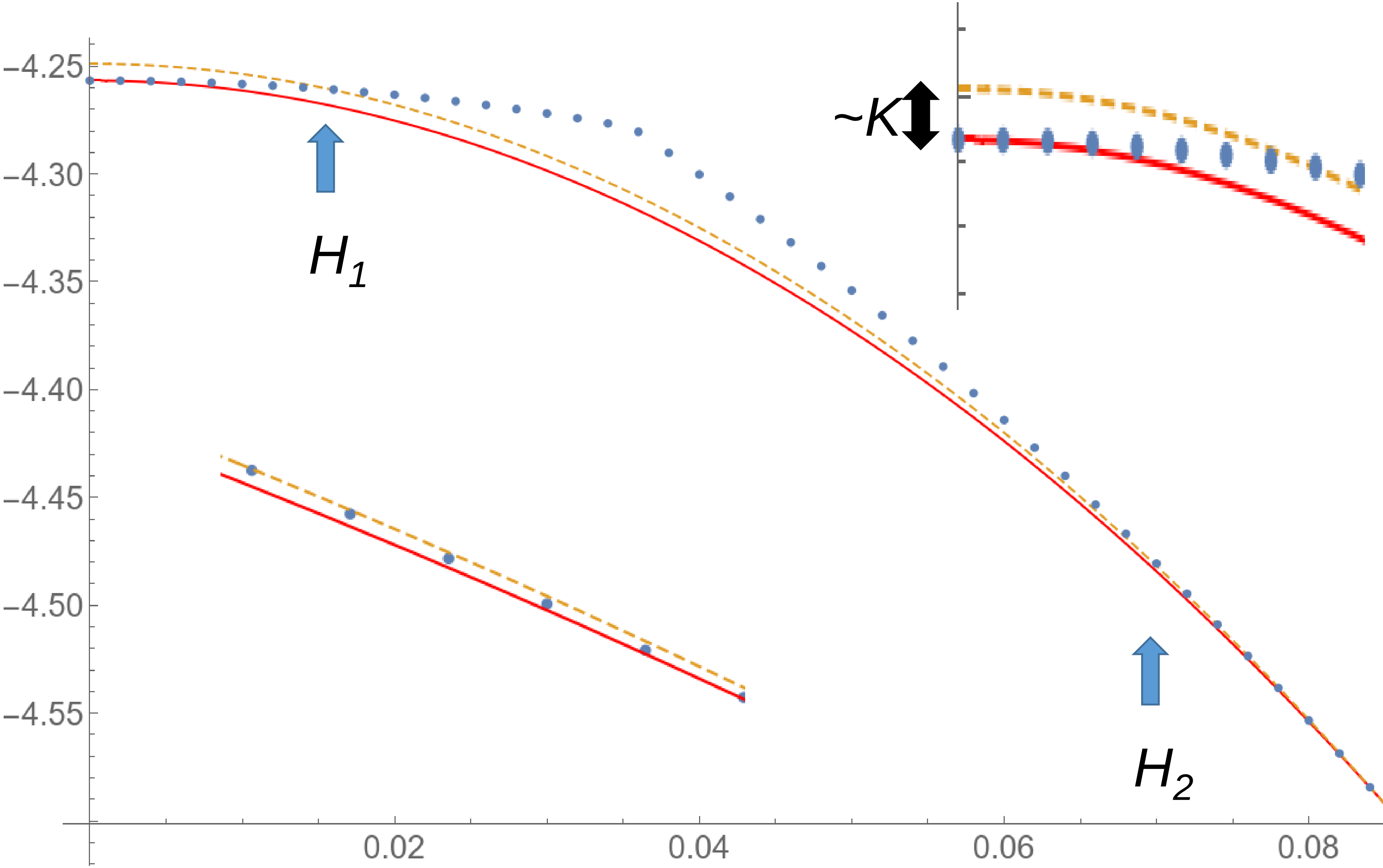
These are the only coplanar solutions!

Now let's add the third dimension



Mean field theory at T=0, H>0: minimal model

1. Longitudinal conical (no K)
2. Coplanar (two different phases)
3. Transverse conical (with K)



Mean field theory at T=0, H=0: minimal model

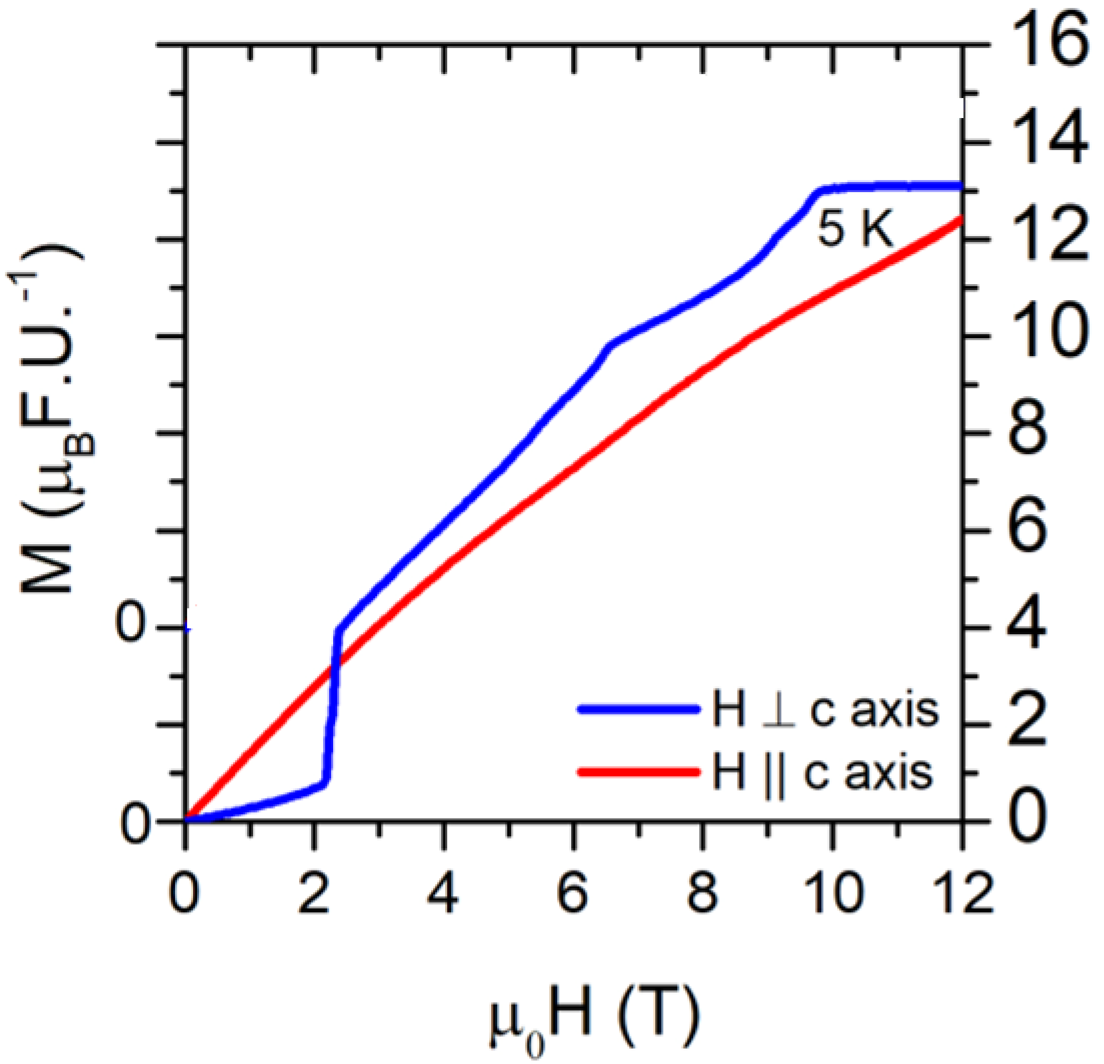
$$H=\sum_{i,j} J_{ij}\,\mathbf{n}_i\cdot\mathbf{n}_j+\sum_{i,j}\cancel{J_{x}\,\mathbf{n}_i}\cdot\mathbf{n}_j+K\sum_i (n_i^z)^2+\sum_i \cancel{J^z n_i^z}\cdot n_{i+1}^z+\sum_i \mathbf{n}_i\cdot\mathbf{H}$$

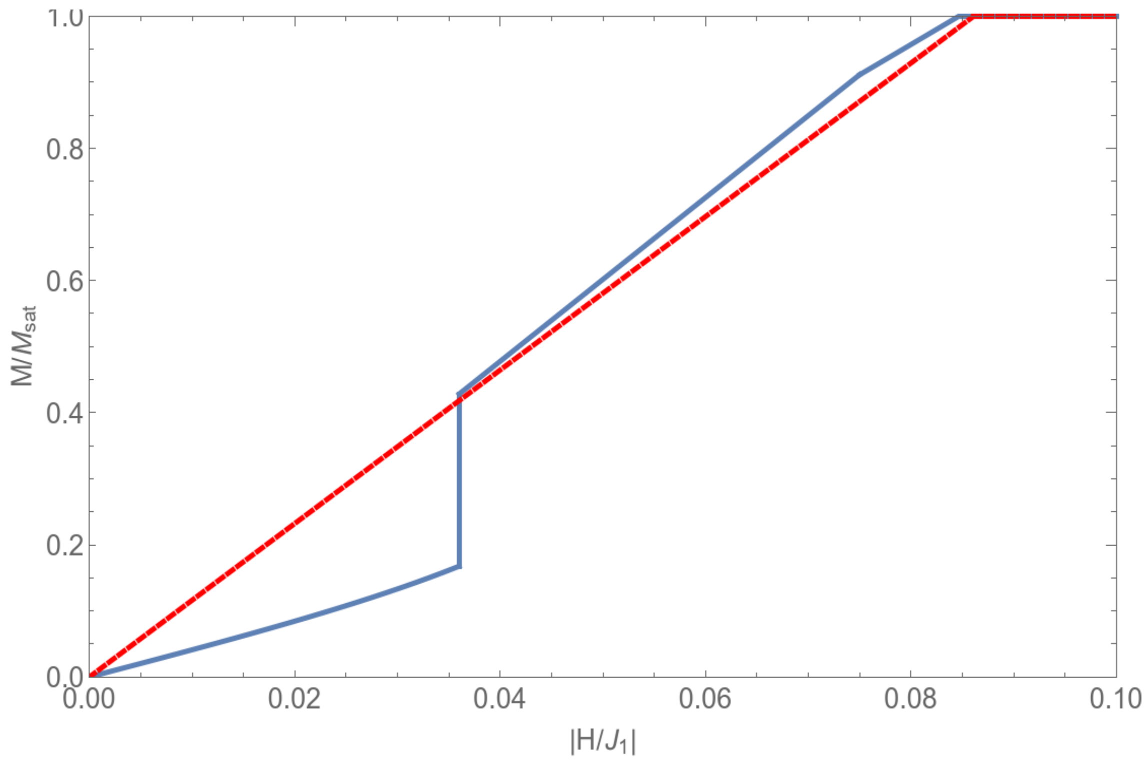
1,2,3

$J_{1,2} \rightarrow J_{1,2}+J^z$; $|J_1| \rightarrow |J_1|-J^z$; $J_2 \rightarrow |J_2|+J^z$

$q \rightarrow q+\delta q$; $\delta q/q \sim |J^z/J| \sim +1\%$

Mean field theory: comparison with the experiment





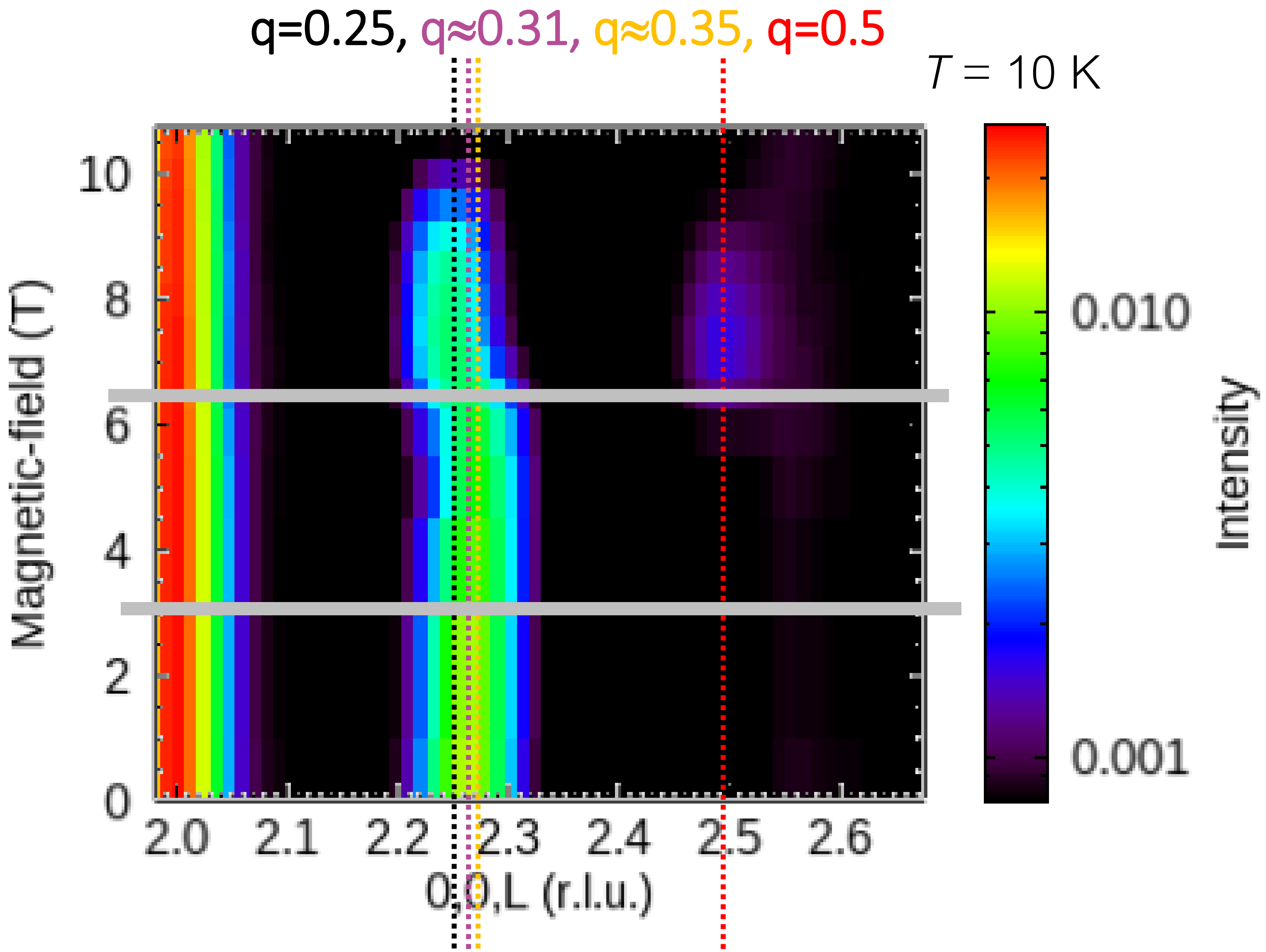
Good qualitative agreement

Mean field theory: comparison with neutrons

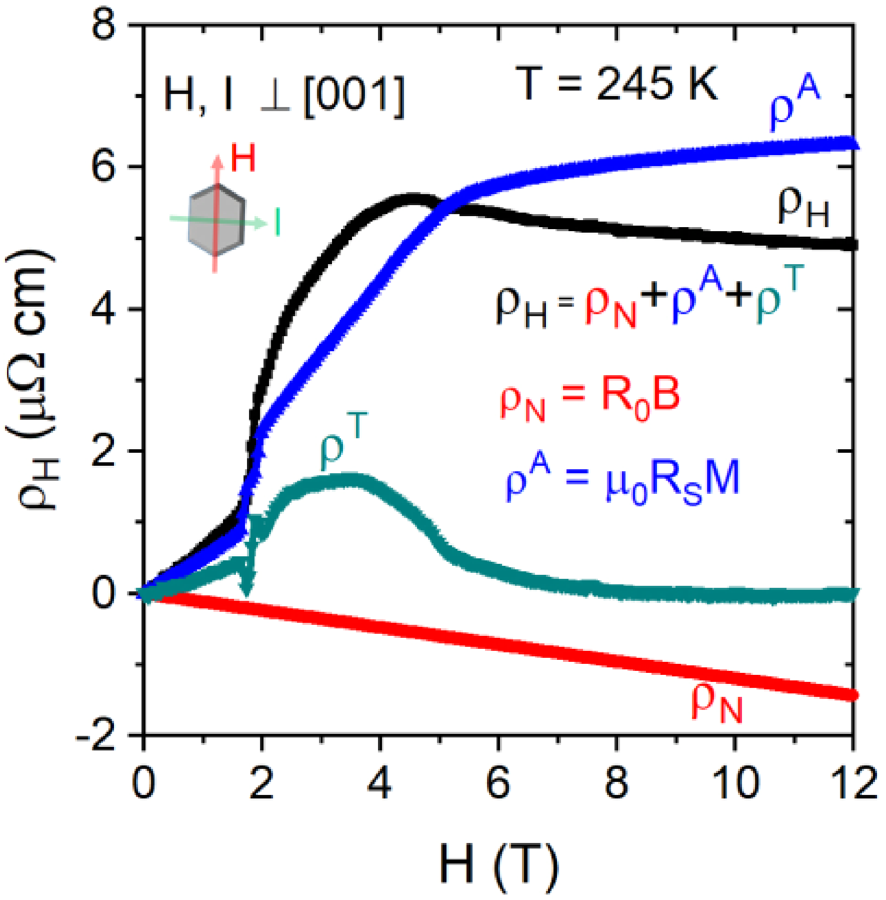
1. $H=H_1$: q shifts by a few %%, intensity drops by a factor of two

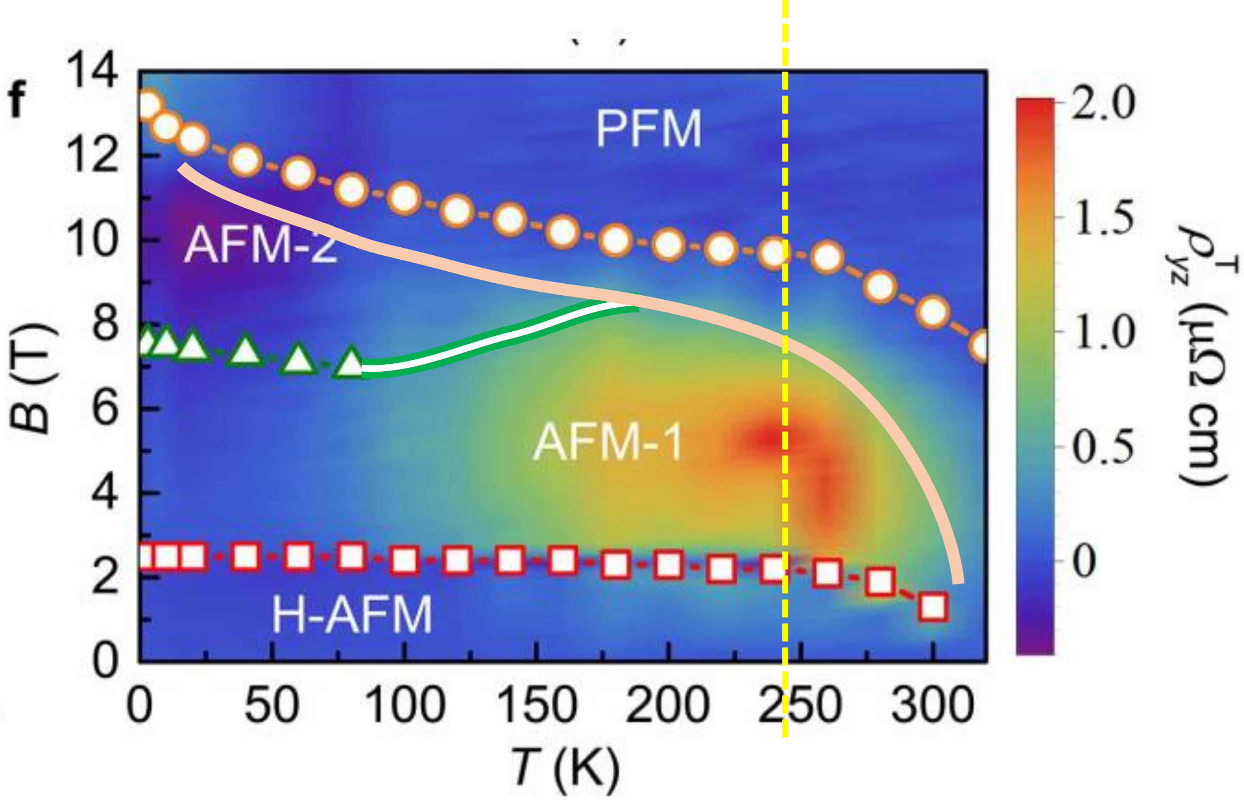
2. H_2: q discontinuously jumps to exactly q=0.25, and a satellite appears at q=0.5

3. All features predicted by the theory!



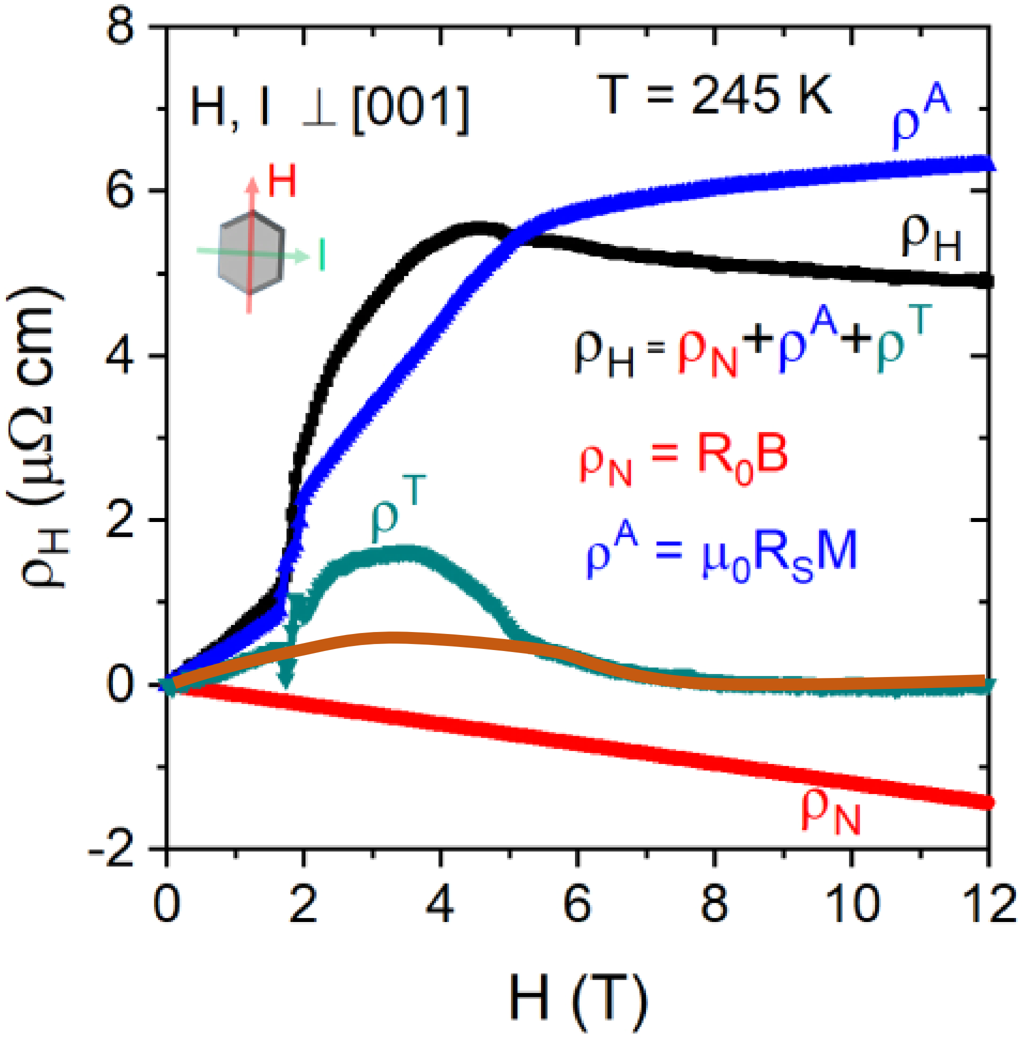
Decomposition of the Hall effect

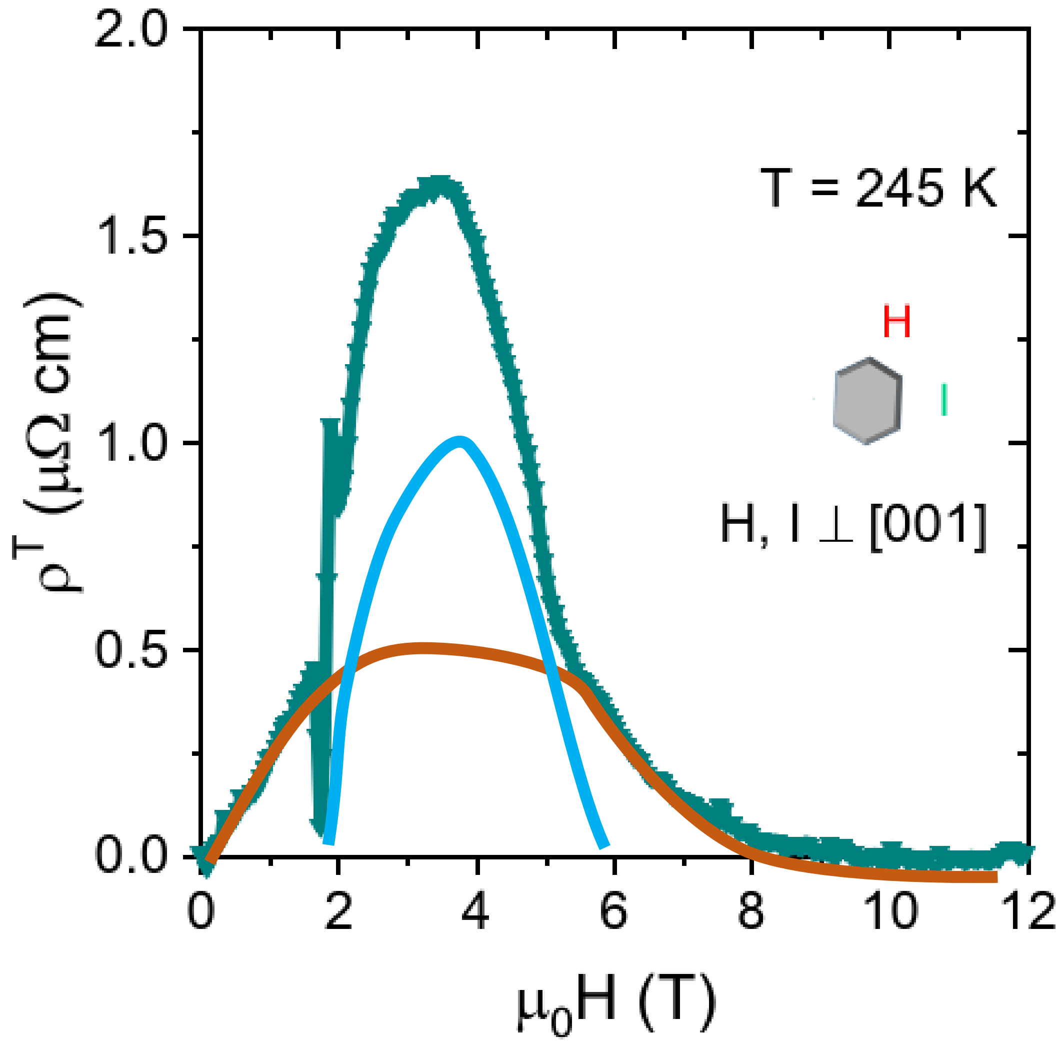




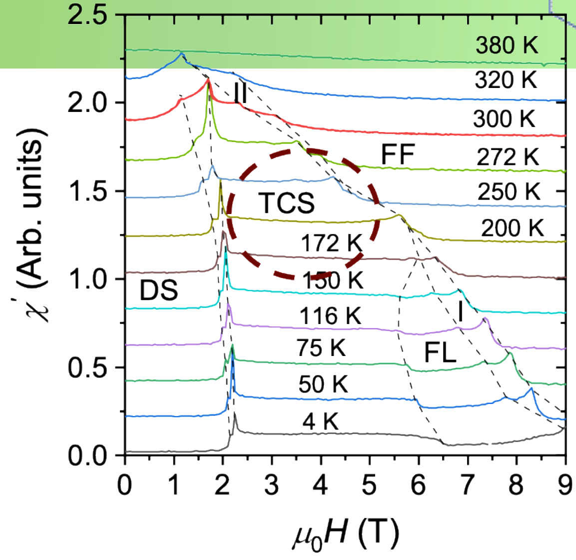
Phys. Rev. B 103, 014416 (2021)

Topological Hall effect



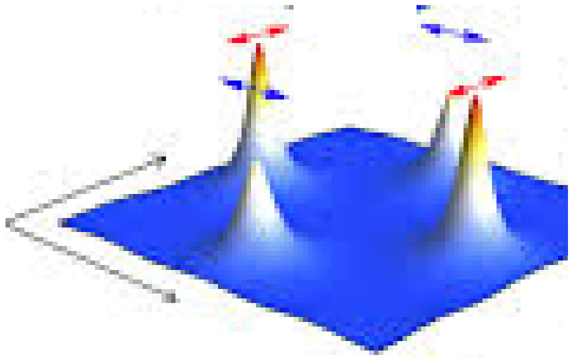


New mechanism of topological Hall effect: Nematic spin chirality

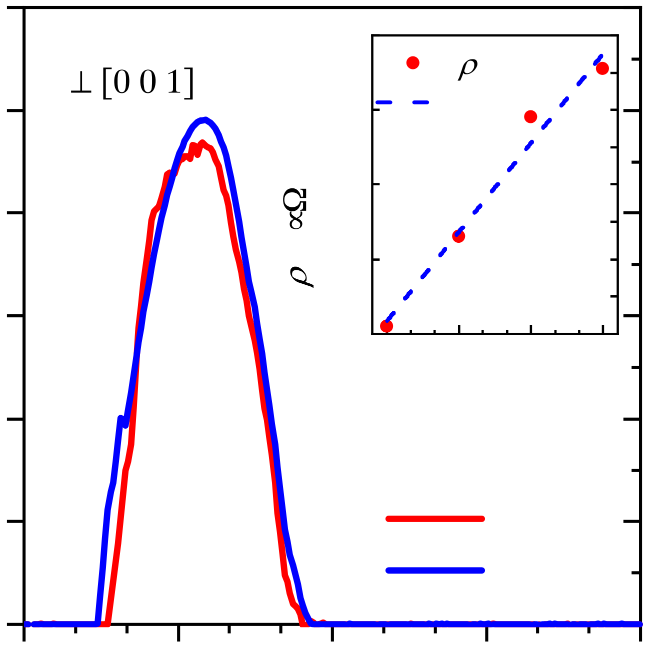


Nematic susceptibility in $BaFe_2As_2$: fluctuations of one kind grow at the expense of the others.

$$b_x = -k_y m_z \mu^2$$



$$\langle b_x \rangle = \frac{\int B k_y e^{-A k_y^2 J/T}\left(e^{C H_x k_y/T} - e^{-C H_x k_y/T}\right) dk_y}{\int e^{-A k_y^2 J/T}\left(e^{C H_x k_y/T} + e^{-C H_x k_y/T}\right) dk_y}$$



$$\langle b_x \rangle = const \cdot T M_z^2 H_x = const \cdot (1 - M^2/M_s^2) T H_x.$$

Ghimire et al., Science Advances 2020; 6 : eabe2680 (2020)

Summary: observations explained

- 1. Continuous variation of magnetization with the field in H||c
- 2. Numerically small value of H_{sat} ($M_{sat}H_{sat}$ ~0.35 meV) compared to the Neel temperature (k_BT_N~30 meV)
- 3. Three separate magnetic phases at T=0, with the critical fields $0 < H_1 < H_2 < H_{sat}$
- 4. Strong change of the differential spin susceptibility, accompanied by a small increase in the magnetic ordering vector, but no discernable change in transport, at $H = H_1$
- 5. Discontinuous change in the neutron scattering intensity at $H = H_1$, by approximately a factor of two
- 6. Discontinuous commensuration of the magnetic ordering vector from q~0.27 to q =1/4 at $H = H_2$, with a simultaneous appearance of a weaker peak at the double vector (q =1/2)
- 7. Topological Hall effect appearing solely for $H_1 < H < H_2$, and only at elevated temperatures.

Summary: observations NOT explained

1. Nature of the exchange coupling along *c*

1. Quasi-2D in spin-majority -> strong RKKY

2. Continuous variation of magnetic ordering vector with T from ~0.25 to ½

2. Do fluctuation decrease J_3/J_1?

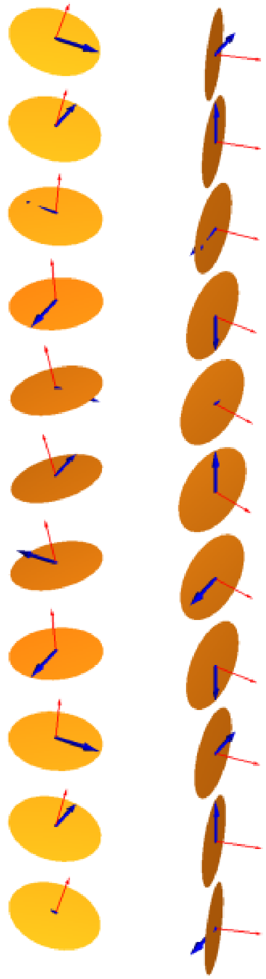
3. Splitting of the spiral into two, increasing with temperature

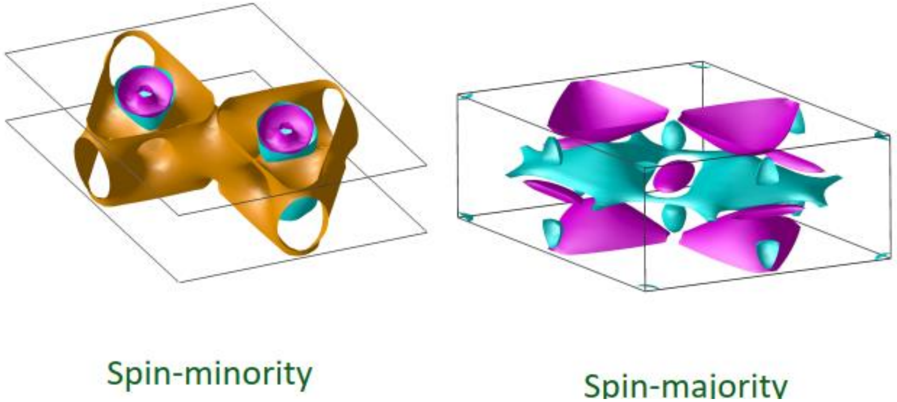
3. Beats?

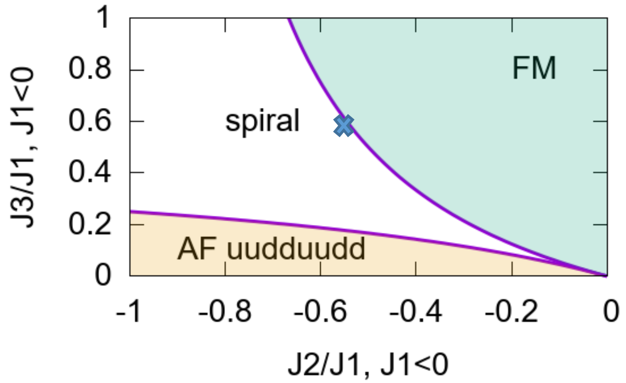
3. Competition of phase space and anisotropy?

4. Nature of two narrow phase regions near T_N

4. Not in mean field







Clearly fluctuations play a key role!

Aftermath

Referee: “Your mechanism is so simple, transparent and seemingly universal, why has it not been observed before?”

Our answer: “First, I’ve never borrowed your lawnmower, second, it was already broken”

First, it is not that universal: It needs to be (i) a decent metal (ii) have a TCS as a ground state in the relevant field and temperature range and (iii) the spiral has to couple strongly with the conduction electrons, i.e., be itinerant (f-electron RAUS!)

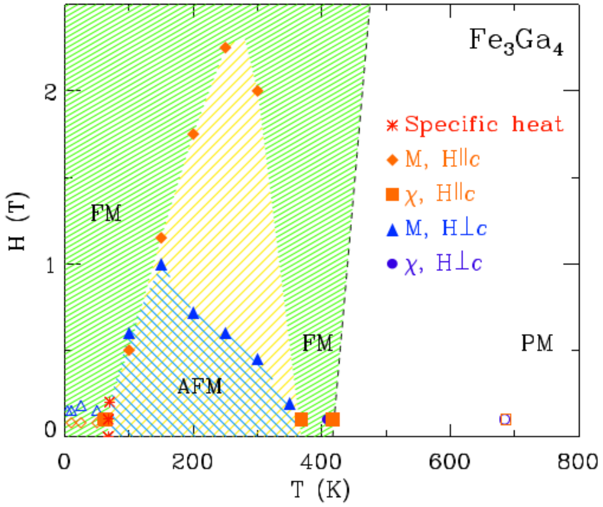
Second, it has been observed.

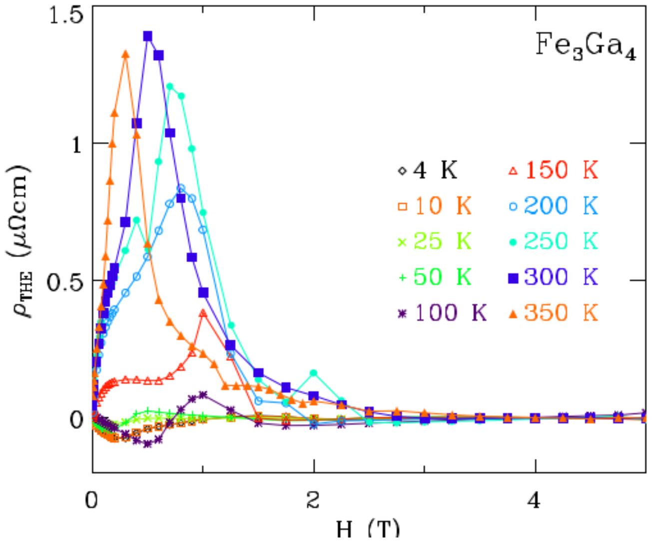
Case of Fe_3Ga_4

PHYSICAL REVIEW B **91**, 144409 (2015)

Competing magnetic states, disorder, and the magnetic character of Fe_3Ga_4

J. H. Mendez,[1] C. E. Ekuma,[1,2] Y. Wu,[1] B. W. Fulfer,[3] J. C. Prestigiacomo,[1] W. A. Shelton,[2,4] M. Jarrell,[1,2] J. Moreno,[1,2] D. P. Young,[1] P. W. Adams.[1] A. Karki.[1] R. Jin.[1] Julia Y. Chan,[5] and J. F. DiTusa[1,*]

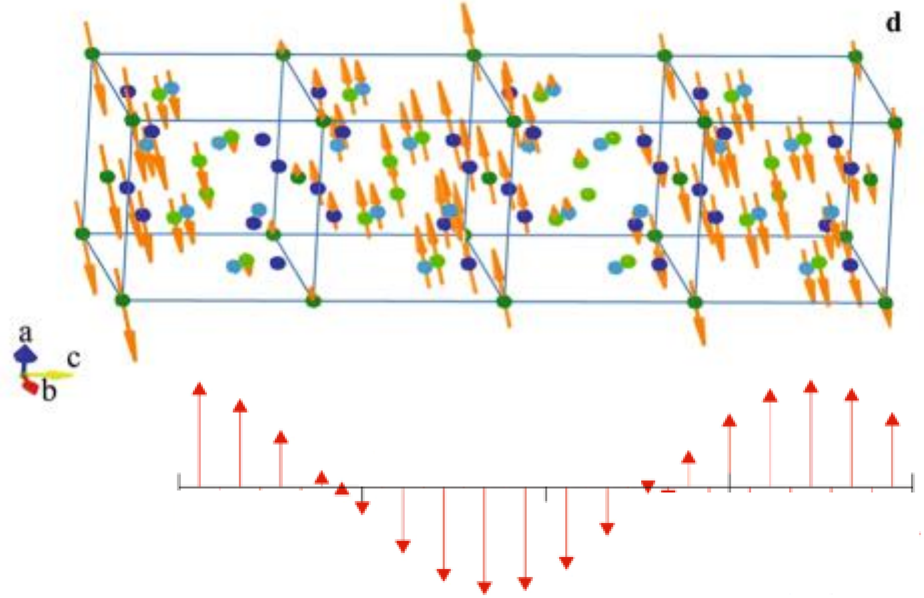




…we assert that there is likely a noncoplanar magnetic moment at low fields in Fe_3Ga_4 so that an AHE stemming from a topolo-gical contribution to the Hall effect… Since there are no reliable data determining the character of the magnetic order in Fe_3Ga_4 we are not able to completely resolve this issue at this time.

Spin density wave instability in a ferromagnet (2018)

Yan Wu[1], Zhenhua Ning[1], Huibo Cao[2], Guixin Cao[1], Katherine A. Benavides[3], S. Karna[1], Gregory T. McCandless[3], R. Jin[1], Julia Y. Chan[3], W. A. Shelton[4] & J. F. DiTusa[1]



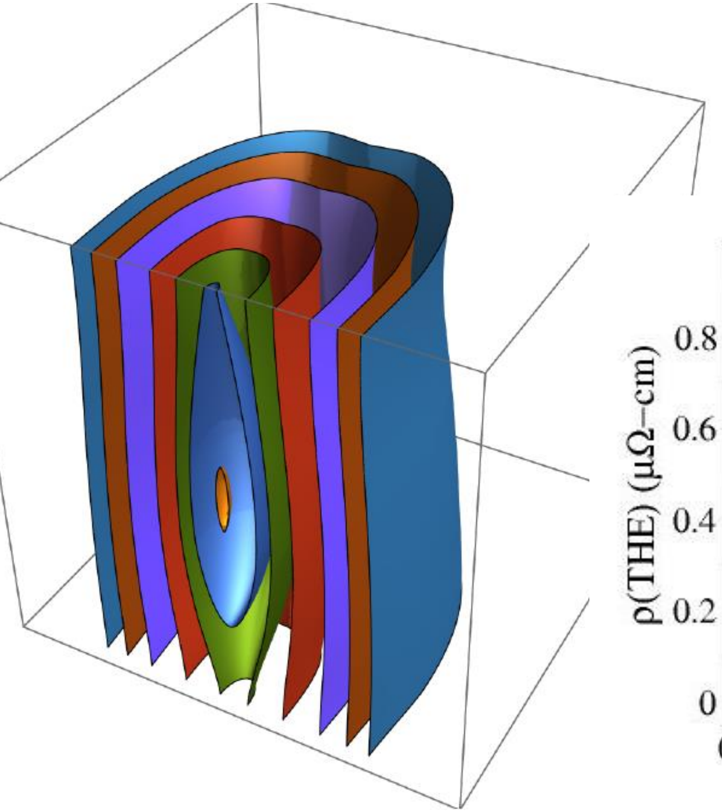
Case of Fe_3Ga_4

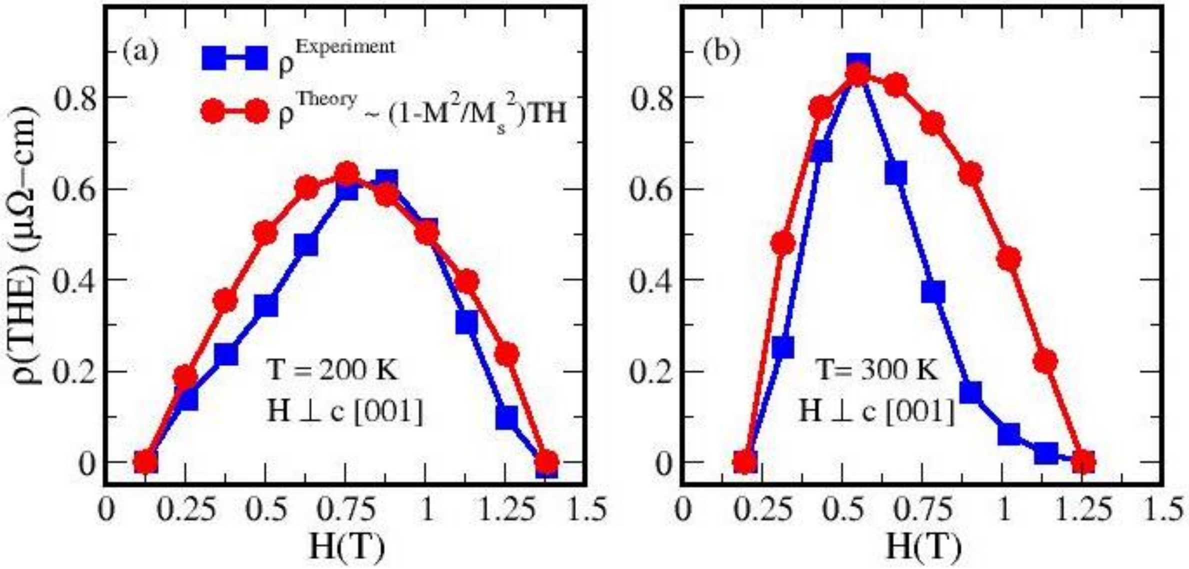
we searched for a helical magnetic … A model magnetic structure was found with magnetic moments rotating in the ab-plane having an R=13.2, comparable to that of the ISDW model.

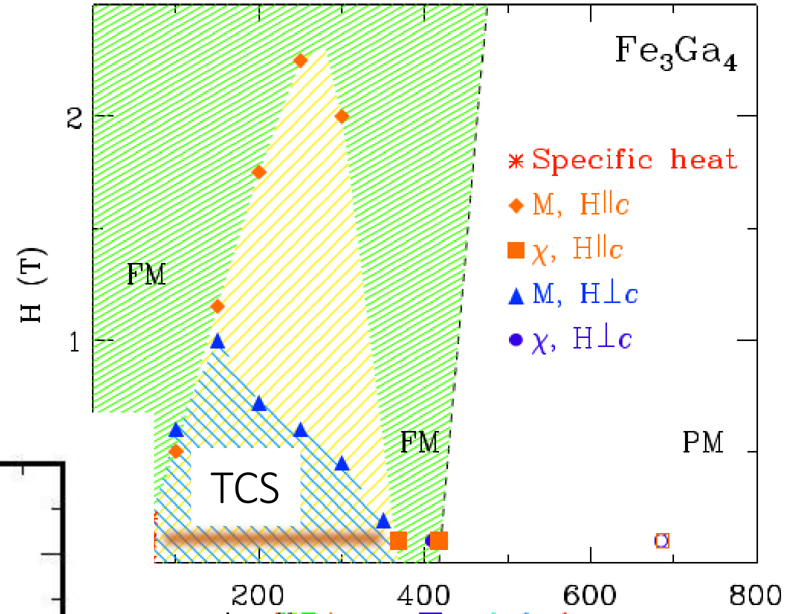
$$q = (0\ 0\ 0.29)$$

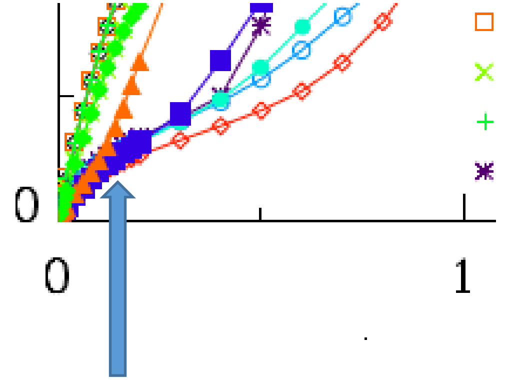
Our calculations: $\boldsymbol{q} = (0,0,0.22)$

An amplitude wave **absolutely** unstable

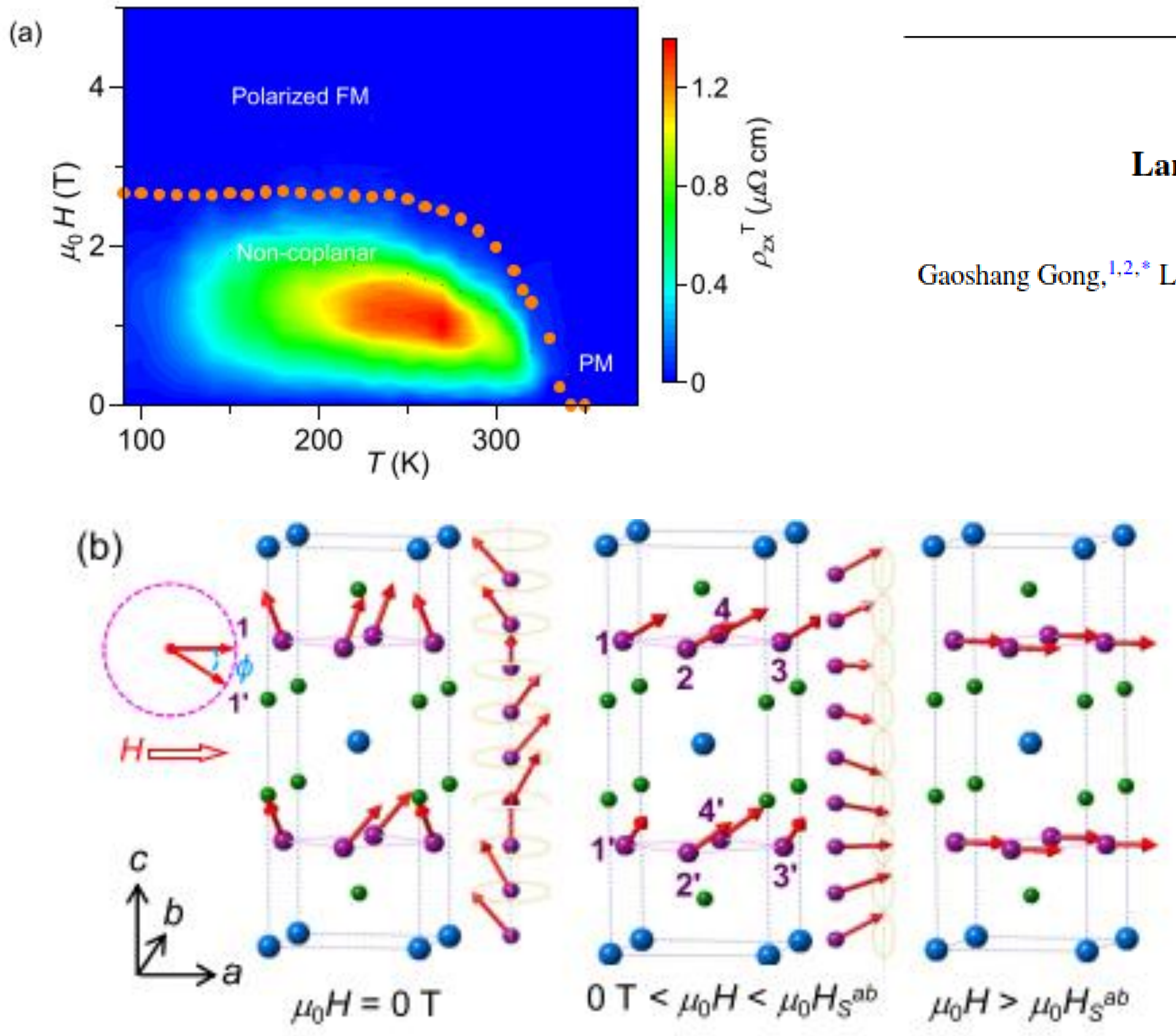








Case of $LaMn_2Ga_2$



PHYSICAL REVIEW MATERIALS **5**, 034405 (2021)

Large topological Hall effect near room temperature in noncollinear ferromagnet $LaMn_2Ge_2$ single crystal

Gaoshang Gong,[1,2,*] Longmeng Xu,[1,*] Yuming Bai,[1] Yongqiang Wang,[2] Songliu Yuan,[1] Yong Liu,[3] and Zhaoming Tian

…due to the presence of tilted angles between adjacent Mn layers in the projected ab plane [see the left side of Fig. 6(b)], nonzero chiral spin configurations will be formed, producing an emergent magnetic field (B_{eff})

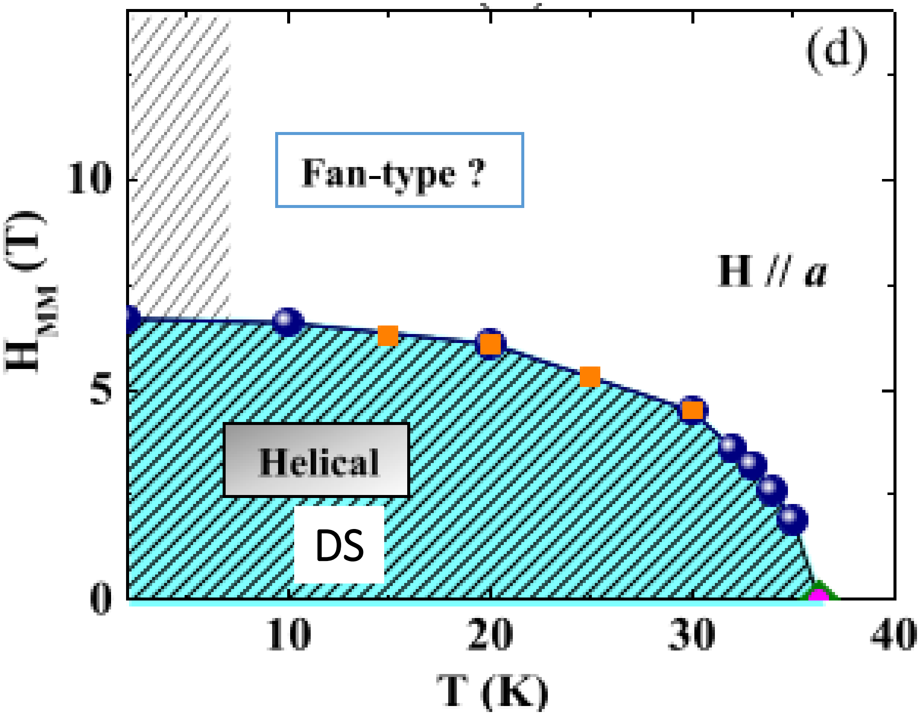
…it will not!
But a fluctuation-driven “nematic” B_{eff} **WILL!**

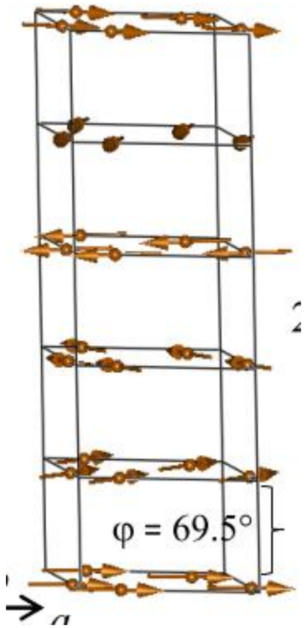
Case of ScFeGe

PHYSICAL REVIEW B **103**, 014443 (2021)

Helical magnetic order and Fermi surface nesting in noncentrosymmetric ScFeGe

Sunil K. Karna,[1,2,*] D. Tristant,[3] J. K. Hebert,[1,†] G. Cao,[1,4] R. Chapai,[1] W. A. Phelan,[1,†] Q. Zhang,[1,5] Y. Wu,[1,5] C. Dhital, Y. Li,[1] H. B. Cao,[5] W. Tian,[5] C. R. Dela Cruz,[5] A. A. Aczel,[5] O. Zaharko,[7] A. Khasanov,[8] M. A. McGuire,[9] A. Roy,[10] W. Xie,[11,‡] D. A. Browne,[1] I. Vekhter,[1] V. Meunier,[12] W. A. Shelton,[3] P. W. Adams,[1] P. T. Sprunger,[1,10] D. P. Young,[1] R. Jin,[1] and J. F. DiTusa[1,§]





…For unknown reason, the structure NEVER FLOPS INTO TCS!

Our theory predicts no THE!

… and none is observed… (J. diTusa, private communication)

Now.
Powered by Northrop Grumman

The intersection of technology, innovation & creativity.

RELATED ARTICLES

SCIENCE

Doug Bonderud

Hiding in Plain Sight? The Argument for Invisible Aliens

Are invisible aliens living among us in shadow biospheres? Is extraterrestrial life hiding in

DOUG BONDERUD
Apr 6th 2020

Hiding in Plain Sight? The Argument for Invisible Aliens