Interplay of transport and domain walls in nodal semimetals

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MRS Spring mtg, Phoenix, 4/18

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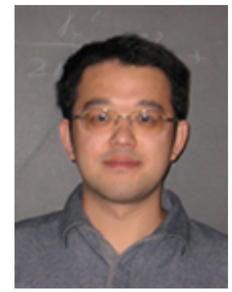
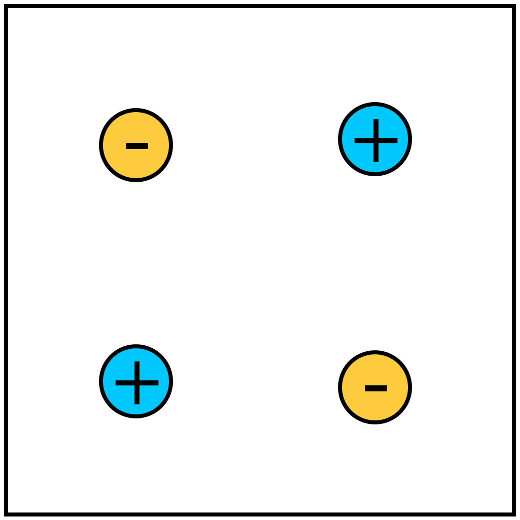


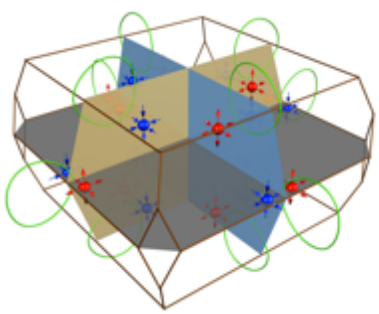
Takehito Suzuki

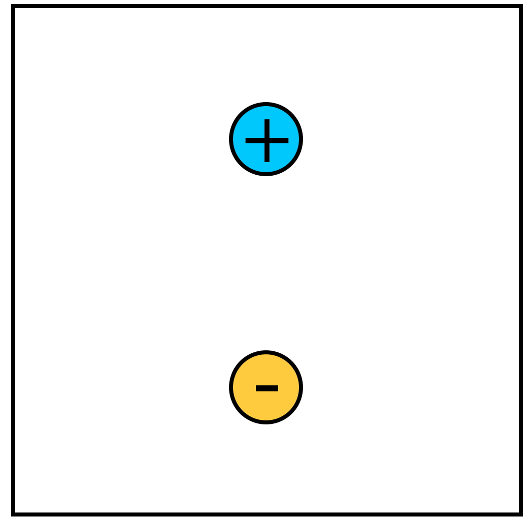
MIT

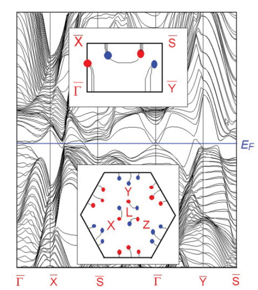
I-breaking Weyls

TR-breaking Weyls









TaAs, Na_3Bi, TaP, WTe_2,...

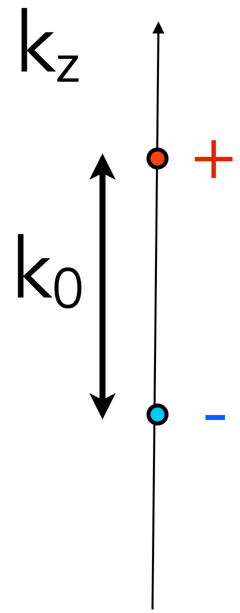
$R_2Ir_2O_7$?, Mn_3(Sn/Ge), RAlGe

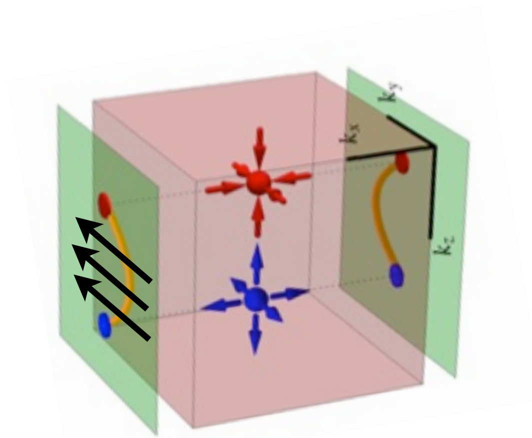
Why magnetic Weyls?

- Possibility to observe AHE
- Interesting correlation physics of magnetism
- Ability to affect electrons *in situ* by modifying magnetic configuration
- Probe static and dynamical effects of *real space* topological defects

Anomalous Hall Effect

Unique property of a magnetic Weyl semimetal





Fermi arc = chiral edge state

$$\sigma_{xy} = \frac{e^2}{h}\frac{k_0}{2\pi}$$

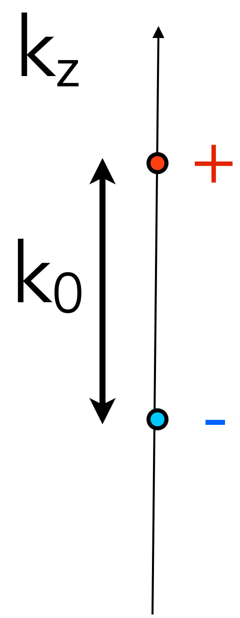
semi-quantum AHE

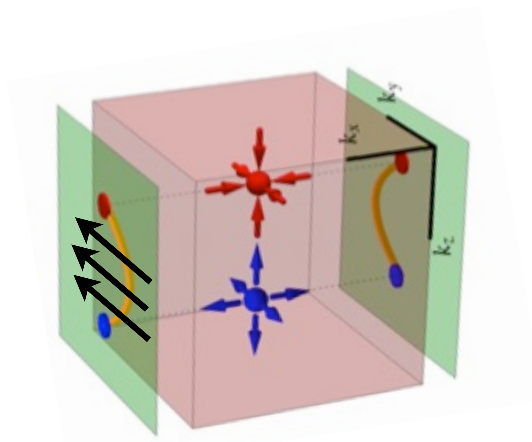
obviously breaks time-reversal symmetry

→ need a magnetic material

Anomalous Hall Effect

Unique property of a magnetic Weyl semimetal





Fermi arc = chiral edge state

$$\sigma_{\mu\nu} = \frac{e^2}{2\pi h}\epsilon_{\mu\nu\lambda}Q_\lambda$$

$$\vec{Q} = \sum_i \vec{k}_i q_i + \vec{Q}_{RLV}$$

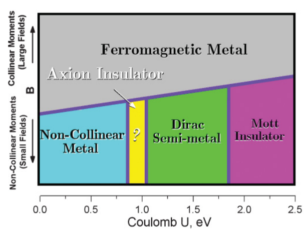
semi-quantum AHE

obviously breaks time-reversal symmetry

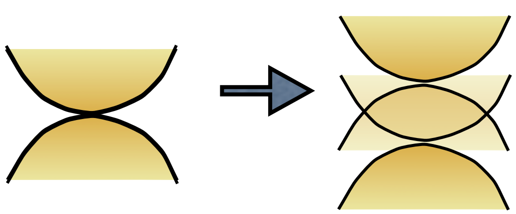
→ need a magnetic material

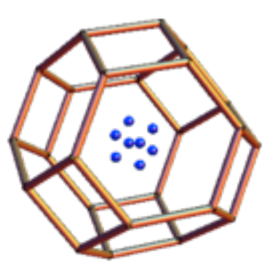
Antiferromagnetic Weyls

Pyrochlore iridates

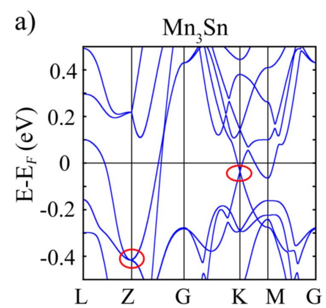


X. Wan *et al*, 2011

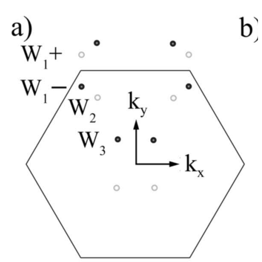




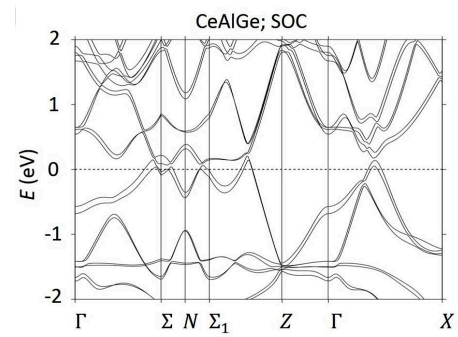
Mn_3Sn, Mn_3Ge



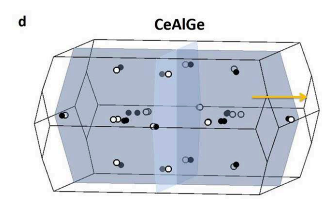
H. Yang *et al*, 2017



RAlGe



G. Chang *et al*, 2016



Quasiparticles

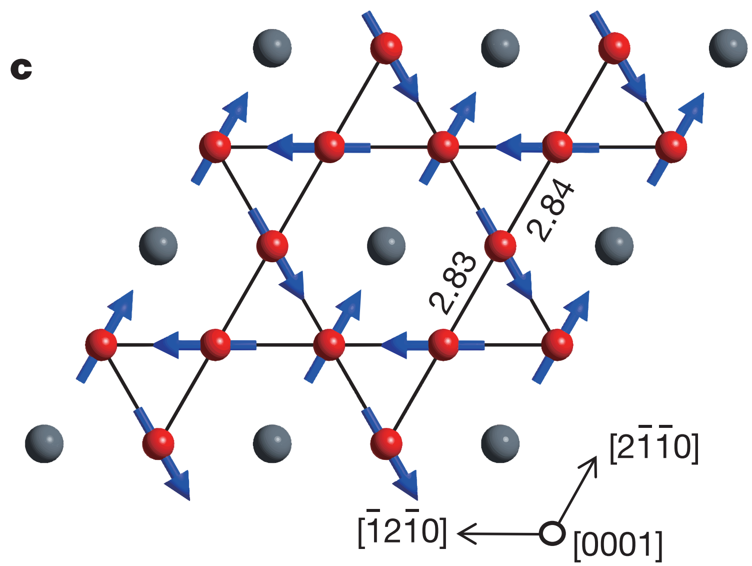
Expect that any magnetically ordered system is described at first order by mean-field quasiparticle Hamiltonian

$$H = H_{\mathrm{band}} - \sum_i \boldsymbol{h}_i \cdot c_i^\dagger \frac{\boldsymbol{\sigma}}{2} c_i$$

↑ effective Zeeman "exchange" field due to local ordered moment

Think of free-electron structure associated with each magnetic configuration

Mn_3Sn family



two kagomé layers of Mn, related by inversion

large ordered *antiferromagnetic* moment

~ 2 μ_B /Mn

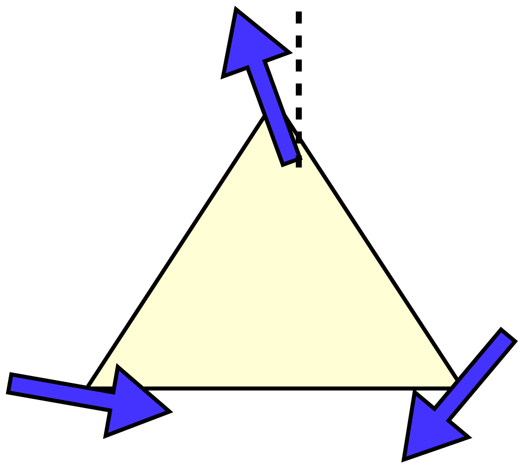
tiny FM moment:

.002 μ_B/Mn

T_N ~ 420K

Nagamiya *et al*, 1982

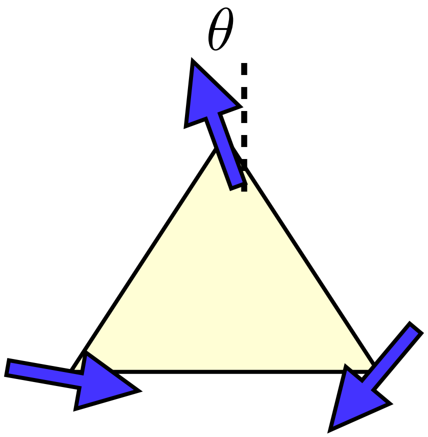
Energetics: triangle



$$E = J\left(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 + \boldsymbol{S}_2 \cdot \boldsymbol{S}_3 + \boldsymbol{S}_3 \cdot \boldsymbol{S}_1\right)$$
$$+ D\hat{\boldsymbol{z}} \cdot \left(\boldsymbol{S}_1 \times \boldsymbol{S}_2 + \boldsymbol{S}_2 \times \boldsymbol{S}_3 + \boldsymbol{S}_3 \times \boldsymbol{S}_1\right)$$
$$- K \sum_i \left(\hat{n}_i \cdot \boldsymbol{S}_i\right)^2$$

$J \gg D \gg K$ **Hierarchy of interactions**

- J: spins at 120° angles and M=0
- D: spins are "anti-chiral" in XY plane
- K: weak canting toward easy axes creates tiny moment and fixes in-plane angle

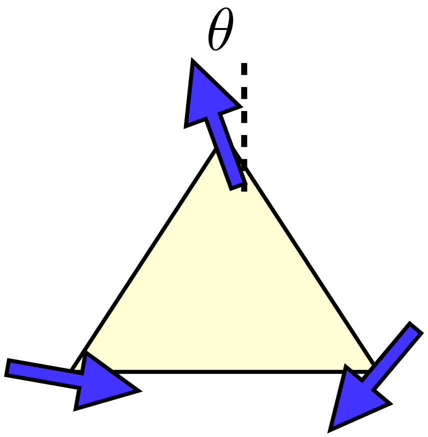


Textures

$$\psi = |\psi| e^{i\theta} \qquad F \sim \int d^3x \left\{ \frac{\rho}{2} (\nabla\theta)^2 - \lambda \cos 6\theta \right\}$$

sine-Gordon model with 6-fold anisotropy

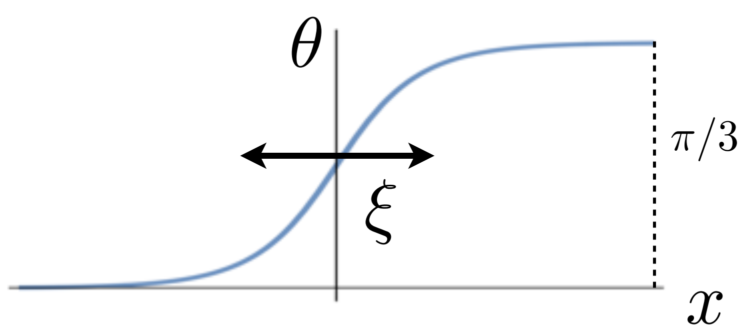
$$\rho \sim \frac{J}{a} \qquad \lambda \sim \frac{K^3}{J^2 a^3}$$



Textures

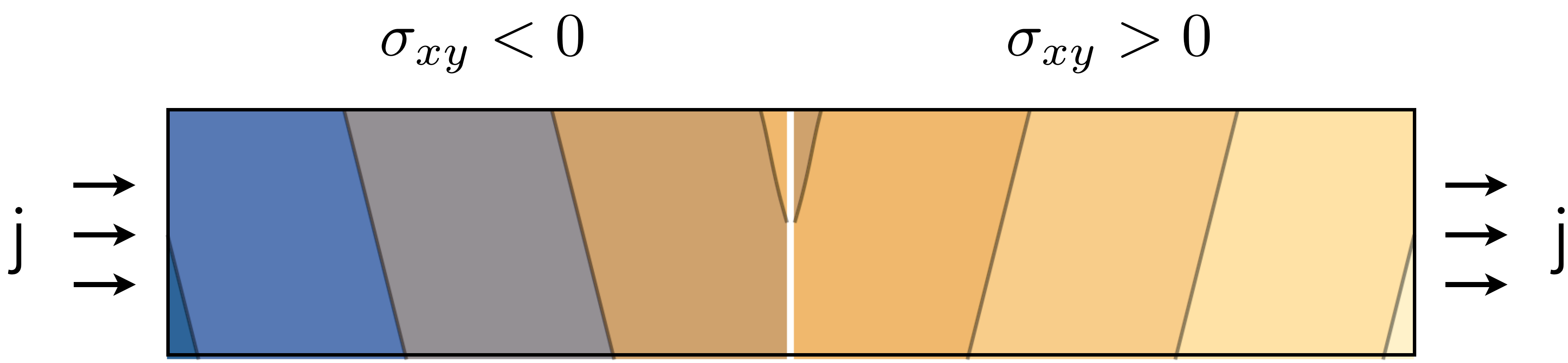
$$\psi = |\psi| e^{i\theta} \qquad\qquad F \sim \int d^3x \left\{ \frac{\rho}{2} (\nabla\theta)^2 - \lambda \cos 6\theta \right\}$$

soliton = domain wall connecting *neighboring* minima of cosine

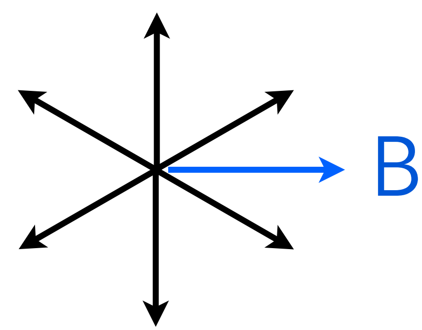


$$\theta(x) = \frac{2}{3} \tan^{-1} \exp(x/\xi) \qquad\qquad \xi = \frac{1}{6}\sqrt{\frac{\rho}{\lambda}}$$

wide
DWs

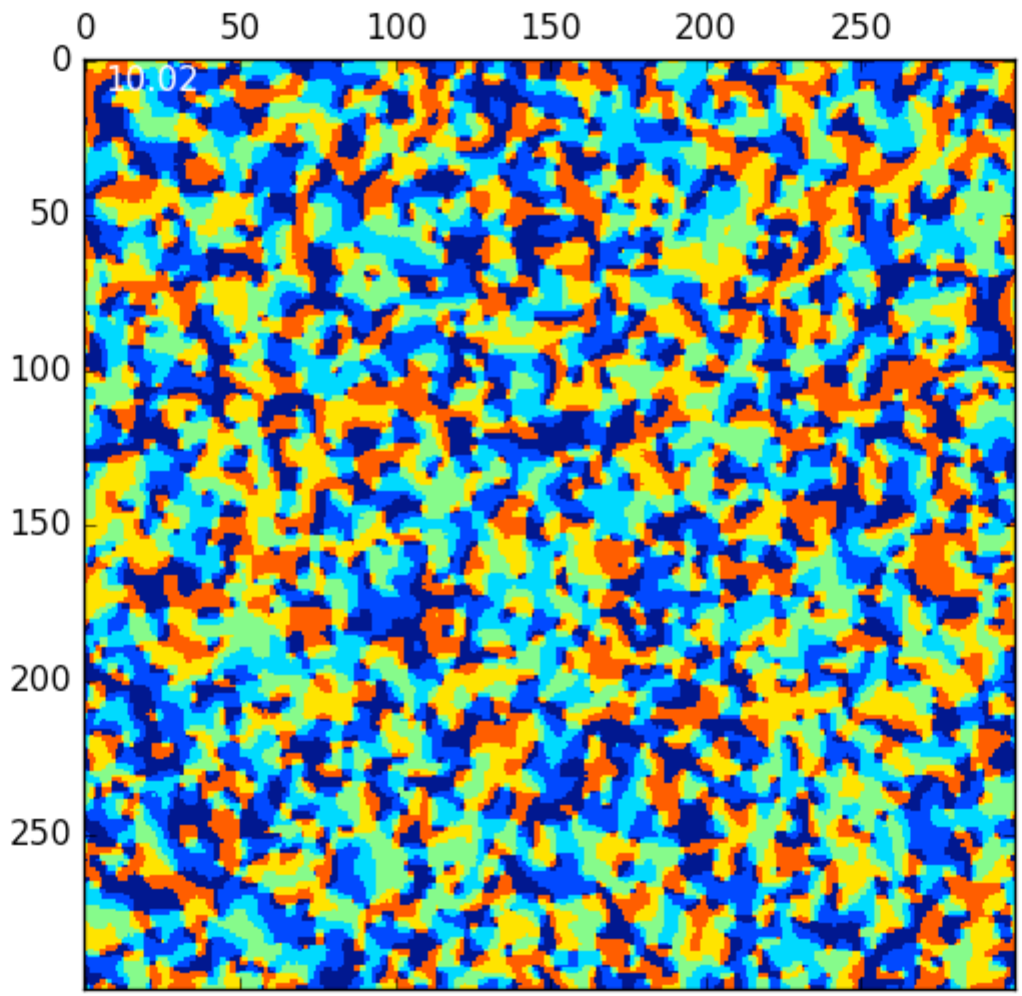


equipotentials from solution of Laplace's equation for a Hall bar with two domains



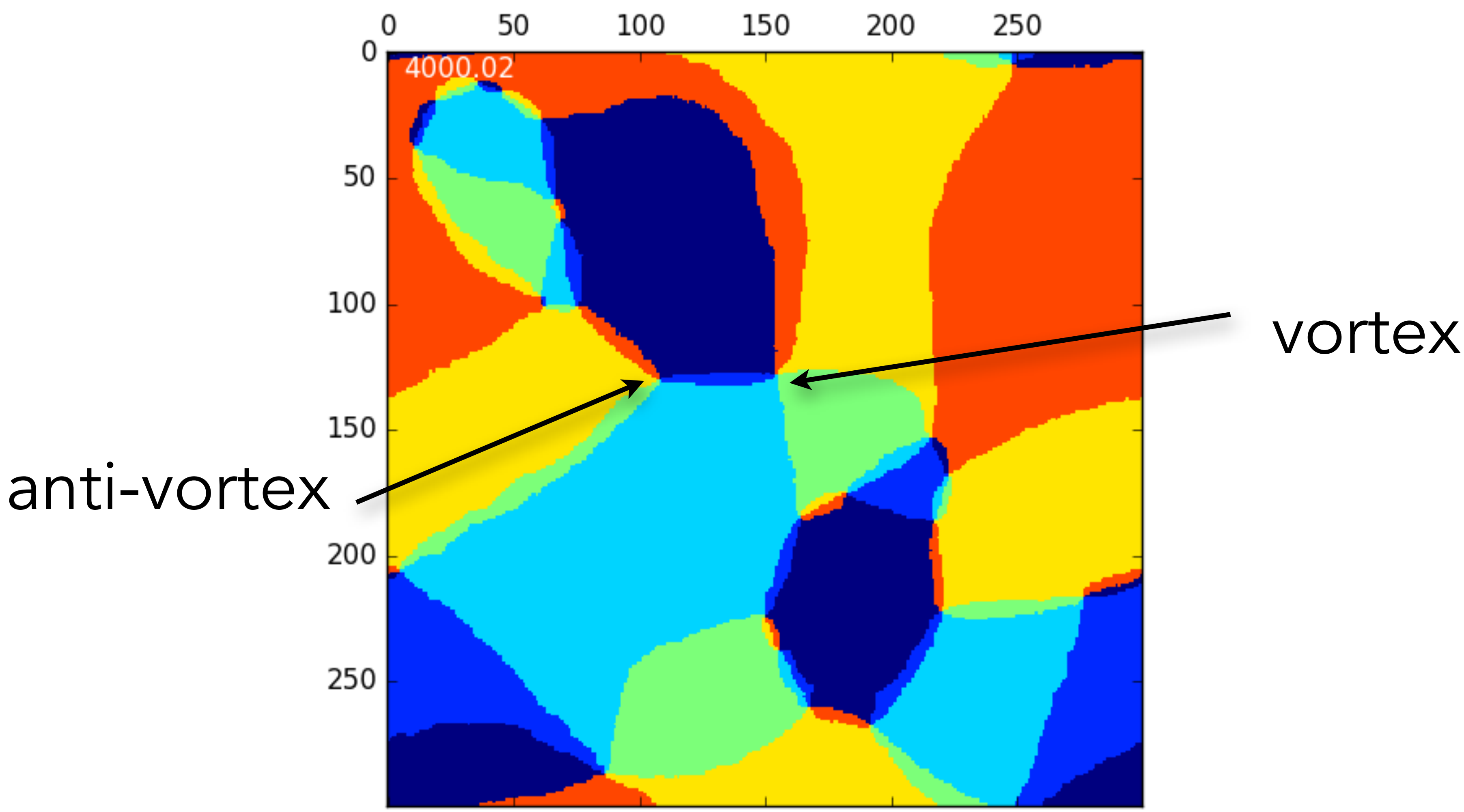
Could use this DW as a switch??

Domain formation

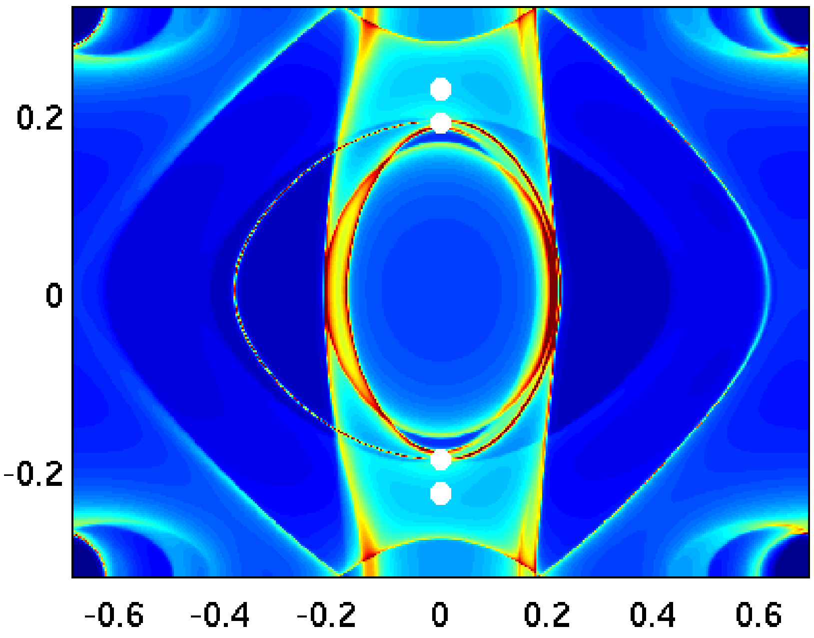


quench

Domain formation



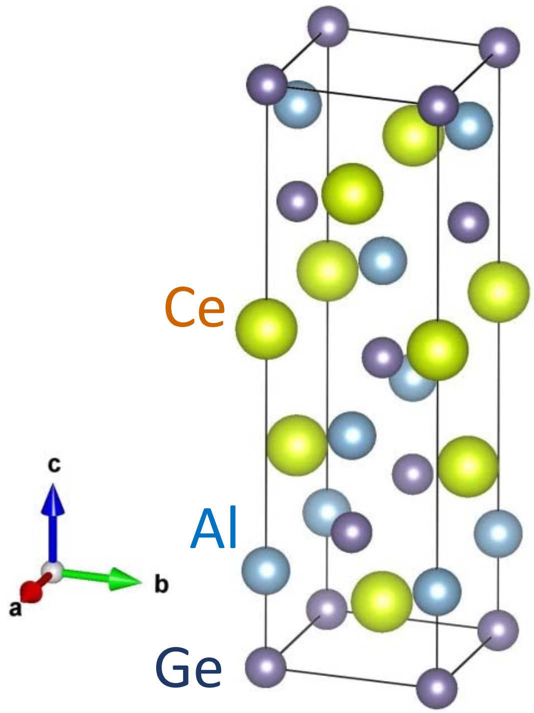
Domain wall bound states



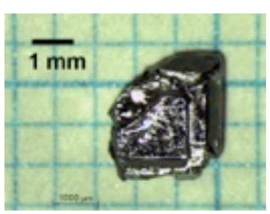
ARPES of domain wall seems challenging to say the least!

- Transport: enhanced intrinsic Hall conductivity within a DW?
- STM: signatures of bound states in LDOS?

CeAlGe

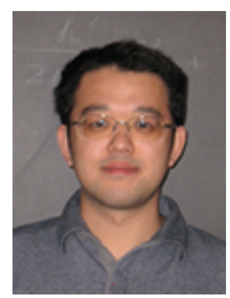


Space group: $I4_1md$



- tetragonal
- Ce $4f^1$ moments
- Semi-metallic band structure

Joe Checkelsky



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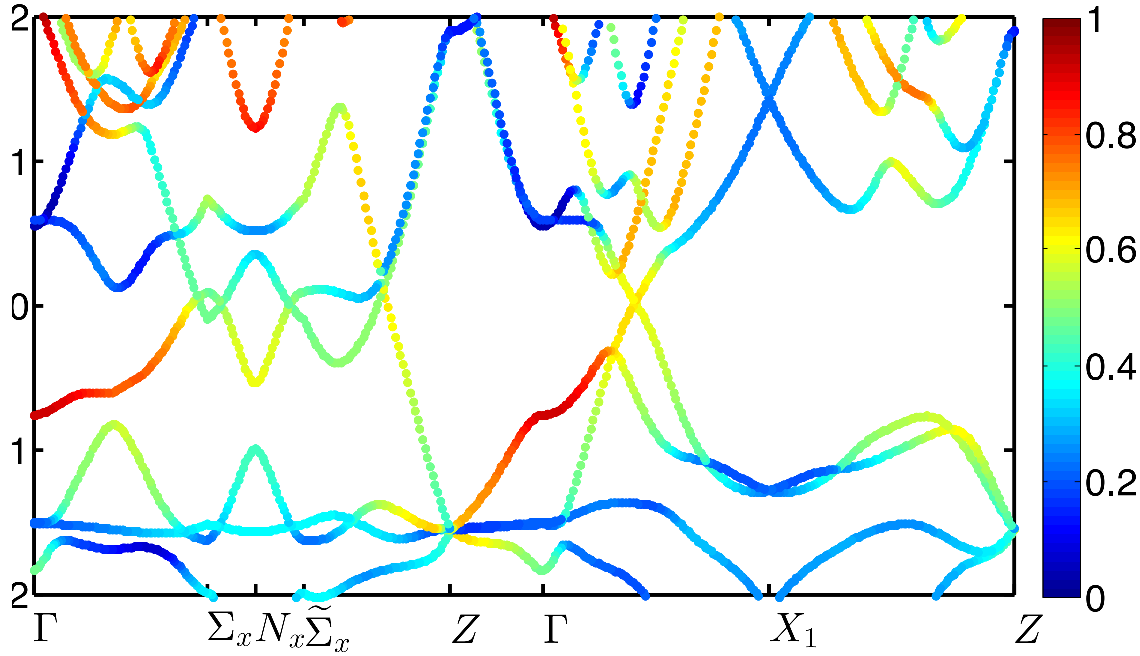
Band structure

(non-magnetic, no SOC)

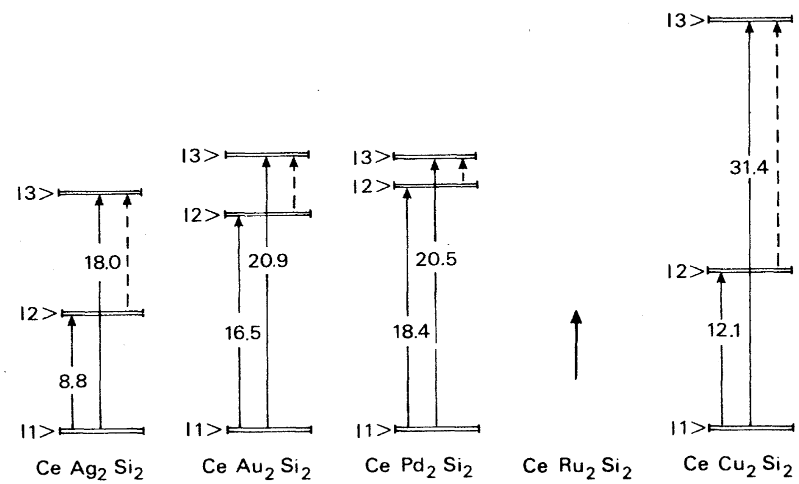


Ce d-orbital content

- bandwidth ~1eV
- no large Fermi surface: true semi-metal
- large rare-earth d-orbital content: substantial coupling to rare earth moments

Ce moments

Ce^{3+} typically Ising-like Kramers doublet

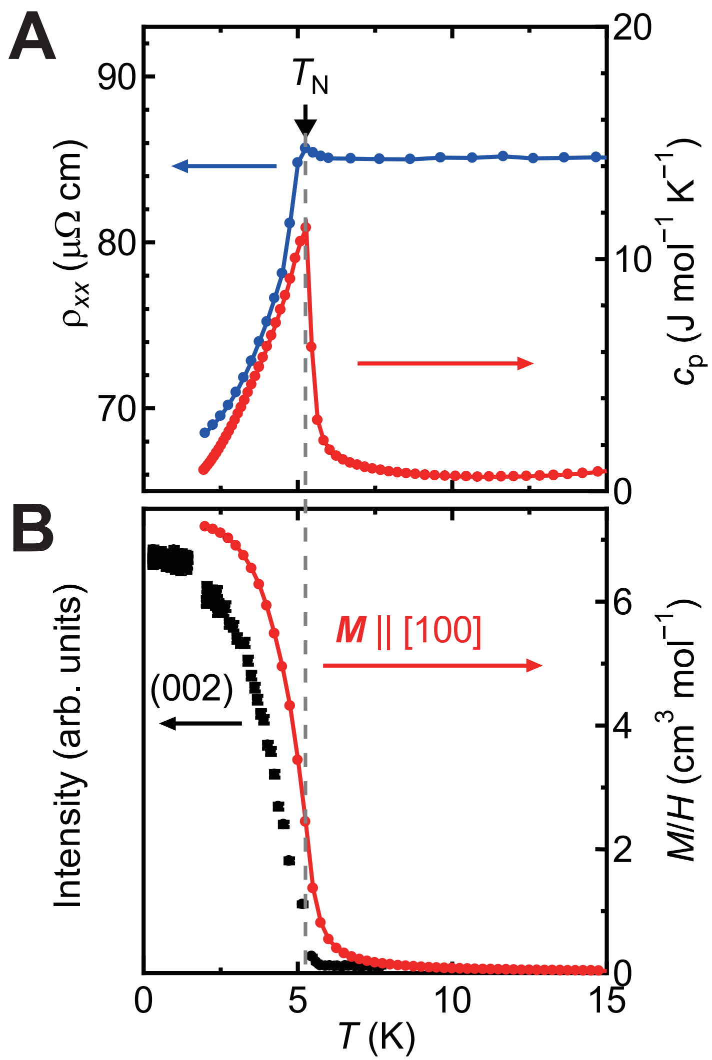


e.g. A. Severing *et al*, 1989

effective S=1/2 spin below ~10meV ~ 100K energy scale

$4f^1$ configuration: large orbital component and hence strong magnetic anisotropy

Magnetic order



Magnetic transition at 5K

2 Ce sublattices. Order does not enlarge unit cell

Kondo lattice scales

$$H = H_{\rm band} + J_K \sum_i \boldsymbol{S}_i \cdot c_i^\dagger \frac{\boldsymbol{\sigma}}{2} c_i$$

RKKY

$$J_{RKKY} \sim \frac{J_K^2}{E_F}$$

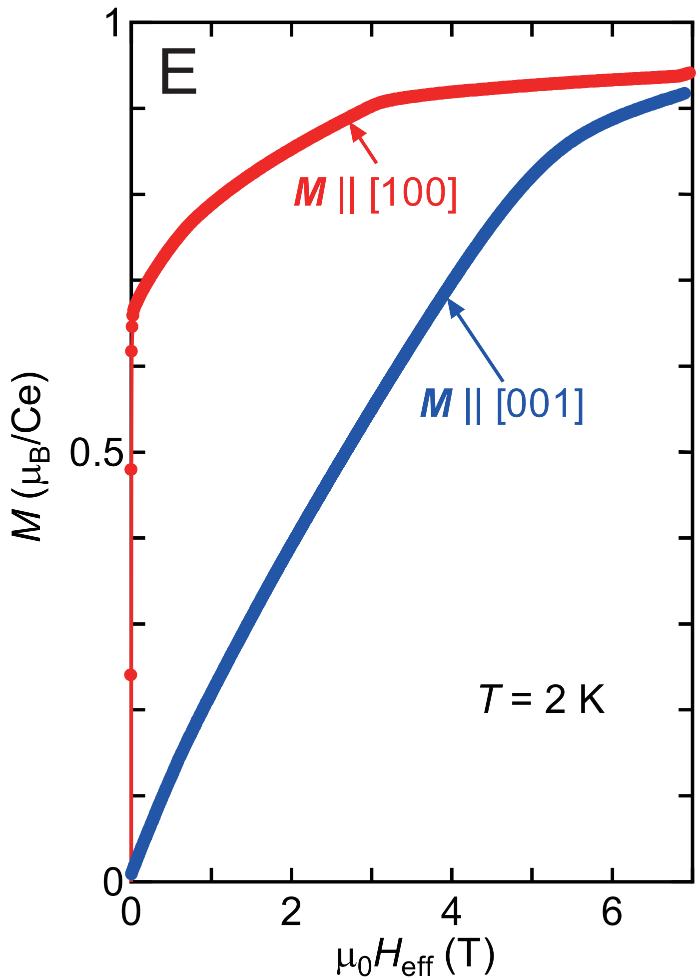
$$J_K \sim \sqrt{J_{RKKY} E_F}$$ ~100meV?

5K 1eV

Summary: key features

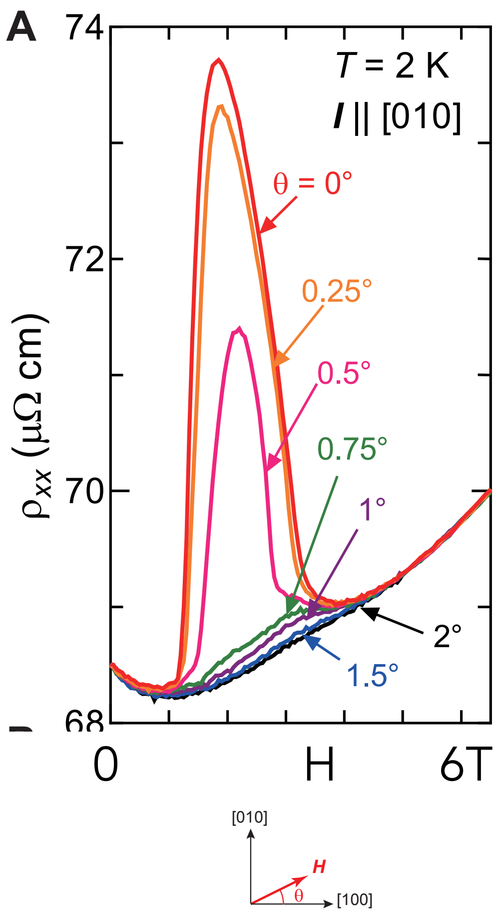
- Semi-metal
- Small bandwidth ~ 1eV
- Large J_K ~ 100meV
- Strong magnetic anisotropy/SOC
- Low T_N ~ 5K

Magnetization



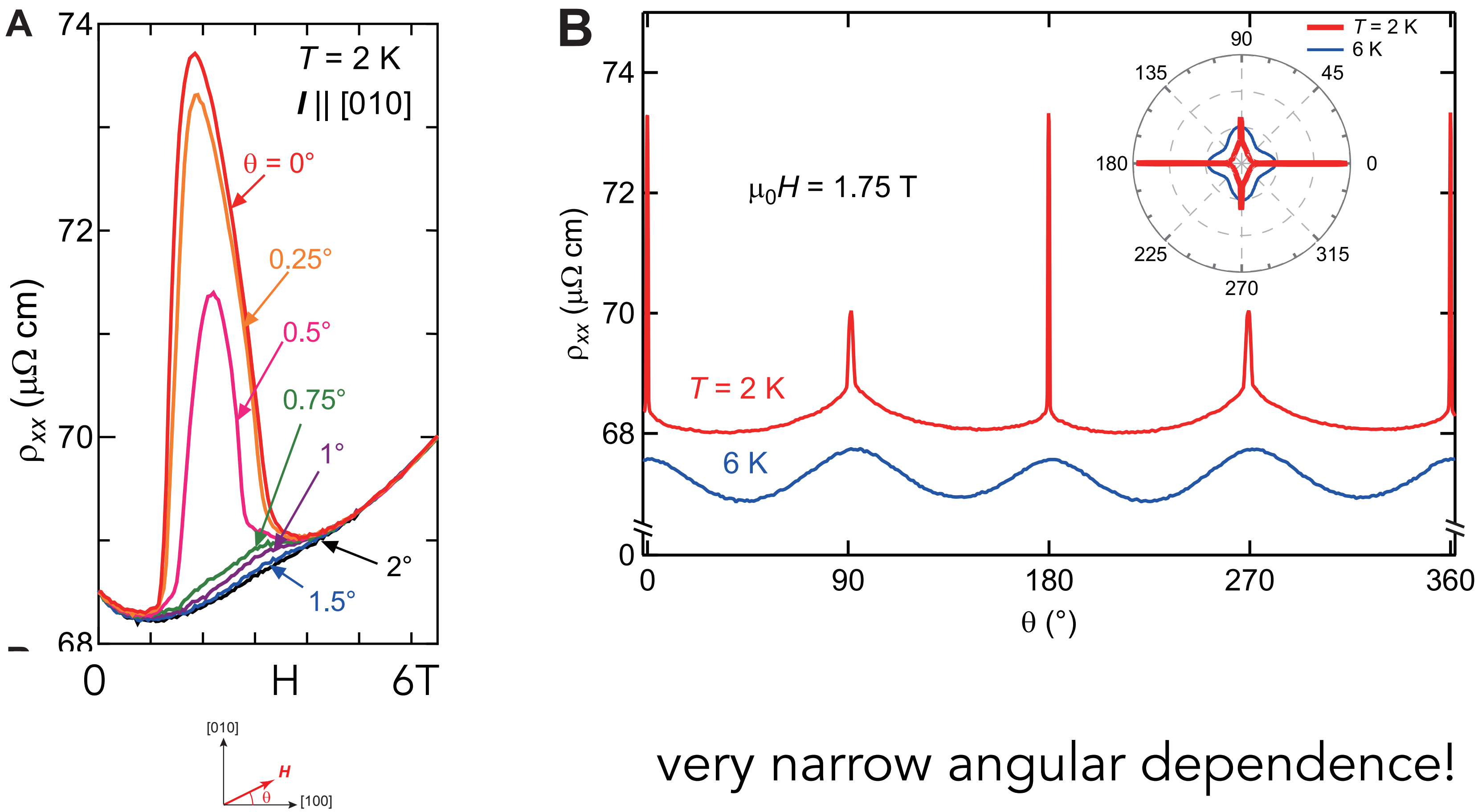
- In-plane field shows ferromagnetic component
- Out of plane field paramagnetic
- If you look carefully, hints of more transitions

Resistivity



resistivity enhancement at intermediate fields and low T

Resistivity



very narrow angular dependence!

Suzuki Angular Magneto-Resistance

~~Suzuki~~ Angular Magneto-Resistance

Savary Angular Magneto-Resistance

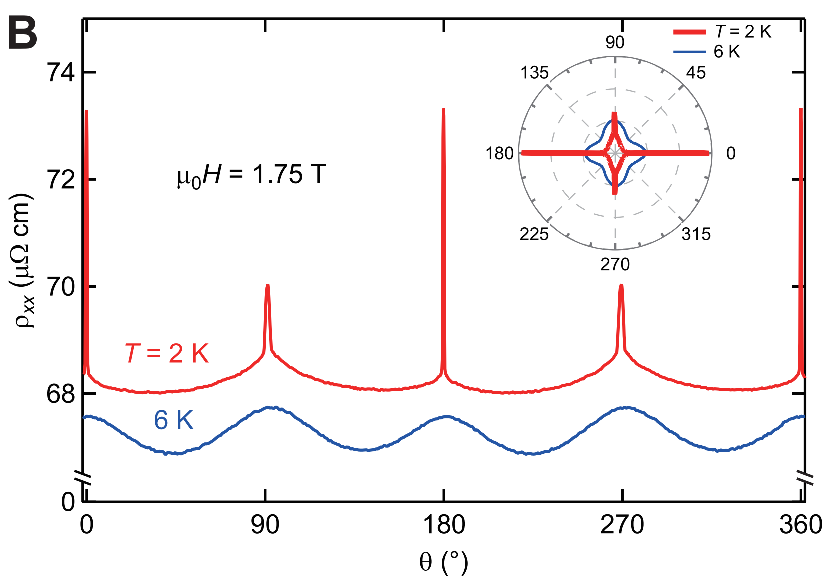
~~Suzuki~~ Angular Magneto-Resistance

~~Savary~~ Angular Magneto-Resistance

Singular Angular Magneto-Resistance

SAMR

Symmetry



Effect is tied to crystalline axes. Yet appears only below critical temperature.

Must be some effect of space group symmetry breaking. Unique to <100> axis?

Symmetry

symmetry	(h^x, h^y, h^z)	**h** doesn't break sym. explicitly if	(N_x, N_y, N_z)	**N** breaks spont. if
TR	$(-h_x, -h_y, -h_z)$	$\mathbf{h} = \mathbf{0}$	$(-N_x, -N_y, -N_z)$	$\mathbf{N} \neq \mathbf{0}$
C_2	$(-h_x, -h_y, h_z)$	$h_x = h_y = 0$	$(-N_x, -N_y, N_z)$	$N_x \neq 0$ or $N_y \neq 0$
m_{010}	$(-h_x, h_y, -h_z)$	$h_x = h_z = 0$	$(-N_x, N_y, -N_z)$	$N_x \neq 0$ or $N_z \neq 0$
$m_{100}\times$TR	$(-h_x, h_y, h_z)$	$h_x = 0$	$(-N_x, N_y, N_z)$	$N_x \neq 0$
m_{100}	$(h_x, -h_y, -h_z)$	$h_y = h_z = 0$	$(N_x, -N_y, -N_z)$	$N_y \neq 0$ or $N_z \neq 0$
$m_{010}\times$TR	$(h_x, -h_y, h_z)$	$h_y = 0$	$(N_x, -N_y, N_z)$	$N_y \neq 0$
$C_2\times$TR	$(h_x, h_y, -h_z)$	$h_z = 0$	$(N_x, N_y, -N_z)$	$N_z \neq 0$
$m_{110}{}^* \times C_2$	$(-h_y, -h_x, -h_z)$	$h_y = -h_x$ and $h_z = 0$	(N_y, N_x, N_z)	$N_x \neq N_y$
$m_{110}{}^*\times$TR	$(-h_y, -h_x, h_z)$	$h_y = -h_x$	$(N_y, N_x, -N_z)$	$N_x \neq N_y$ or $N_z \neq 0$
$C_4C_4C_4{}^*\times$TR	$(-h_y, h_x, -h_z)$	$\mathbf{h} = \mathbf{0}$	$(N_y, -N_x, N_z)$	$N_x \neq 0$ or $N_y \neq 0$
$C_4{}^*$	$(-h_y, h_x, h_z)$	$h_x = h_y = 0$	$(N_y, -N_x, -N_z)$	$\mathbf{N} \neq \mathbf{0}$
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$C_4C_4C_4{}^*$	$(h_y, -h_x, h_z)$	$h_x = h_y = 0$	$(-N_y, N_x, -N_z)$	$\mathbf{N} \neq \mathbf{0}$
$m_{110}{}^*$	$(h_y, h_x, -h_z)$	$h_x = h_y$ and $h_z = 0$	$(-N_y, -N_x, N_z)$	$N_y \neq -N_x$
$m_{110}{}^* \times C_2\times$TR	(h_y, h_x, h_z)	$h_x = h_y$	$(-N_y, -N_x, -N_z)$	$N_y \neq -N_x$ or $N_z \neq 0$

Table 2: All transformations for **h**.

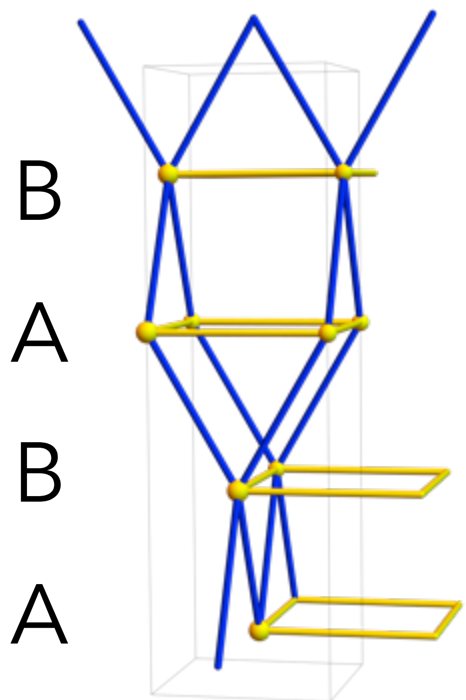
Symmetry

symmetry	(h^x, h^y, h^z)	**h** doesn't break sym. explicitly if	(N_x, N_y, N_z)	**N** breaks spont. if
TR	$(-h_x, -h_y, -h_z)$	$\mathbf{h} = \mathbf{0}$	$(-N_x, -N_y, -N_z)$	$\mathbf{N} \neq \mathbf{0}$
C_2	$(-h_x, -h_y, h_z)$	$h_x = h_y = 0$	$(-N_x, -N_y, N_z)$	$N_x \neq 0$ or $N_y \neq 0$
m_{010}	$(-h_x, h_y, -h_z)$	$h_x = h_z = 0$	$(-N_x, N_y, -N_z)$	$N_x \neq 0$ or $N_z \neq 0$
$m_{100} \times$TR	$(-h_x, h_y, h_z)$	$h_x = 0$	$(-N_x, N_y, N_z)$	$N_x \neq 0$
m_{100}	$(h_x, -h_y, -h_z)$	$h_y = h_z = 0$	$(N_x, -N_y, -N_z)$	$N_y \neq 0$ or $N_z \neq 0$
$m_{010} \times$TR	$(h_x, -h_y, h_z)$	$h_y = 0$	$(N_x, -N_y, N_z)$	$N_y \neq 0$
$C_2 \times$TR	$(h_x, h_y, -h_z)$	$h_z = 0$	$(N_x, N_y, -N_z)$	$N_z \neq 0$
$m_{110}{}^* \times C_2$	$(-h_y, -h_x, -h_z)$	$h_y = -h_x$ and $h_z = 0$	(N_y, N_x, N_z)	$N_x \neq N_y$
$m_{110}{}^* \times$TR	$(-h_y, -h_x, h_z)$	$h_y = -h_x$	$(N_y, N_x, -N_z)$	$N_x \neq N_y$ or $N_z \neq 0$
$C_4C_4C_4{}^* \times$TR	$(-h_y, h_x, -h_z)$	$\mathbf{h} = \mathbf{0}$	$(N_y, -N_x, N_z)$	$N_x \neq 0$ or $N_y \neq 0$
$C_4{}^*$	$(-h_y, h_x, h_z)$	$h_x = h_y = 0$	$(N_y, -N_x, -N_z)$	$\mathbf{N} \neq \mathbf{0}$
$C_4{}^* \times$TR	$(h_y, -h_x, -h_z)$	$\mathbf{h} = \mathbf{0}$	$(-N_y, N_x, N_z)$	$N_x \neq 0$ or $N_y \neq 0$
$C_4C_4C_4{}^*$	$(h_y, -h_x, h_z)$	$h_x = h_y = 0$	$(-N_y, N_x, -N_z)$	$\mathbf{N} \neq \mathbf{0}$
$m_{110}{}^*$	$(h_y, h_x, -h_z)$	$h_x = h_y$ and $h_z = 0$	$(-N_y, -N_x, N_z)$	$N_y \neq -N_x$
$m_{110}{}^* \times C_2 \times$TR	(h_y, h_x, h_z)	$h_x = h_y$	$(-N_y, -N_x, -N_z)$	$N_y \neq -N_x$ or $N_z \neq 0$

Table 2: All transformations for **h**.

Fields along <100> axes preserve this "magnetic mirror" symmetry

Minimal model

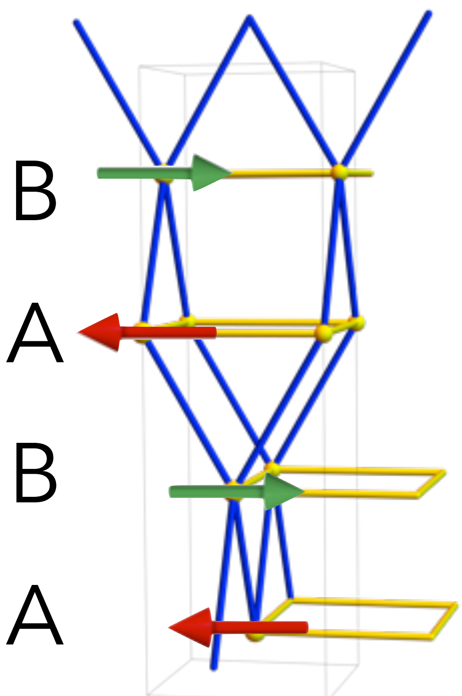


Two Ce sublattices

"intra-unit cell antiferromagnet"

$$E = J_{\perp}(S_{\mathrm{A}}^{x} S_{\mathrm{B}}^{x} + S_{\mathrm{A}}^{y} S_{\mathrm{B}}^{y}) + J_{z} S_{\mathrm{A}}^{z} S_{\mathrm{B}}^{z} + \sum_{\alpha} \left[D \left(S_{\alpha}^{z} \right)^{2} \right.$$

Minimal model



Two Ce sublattices

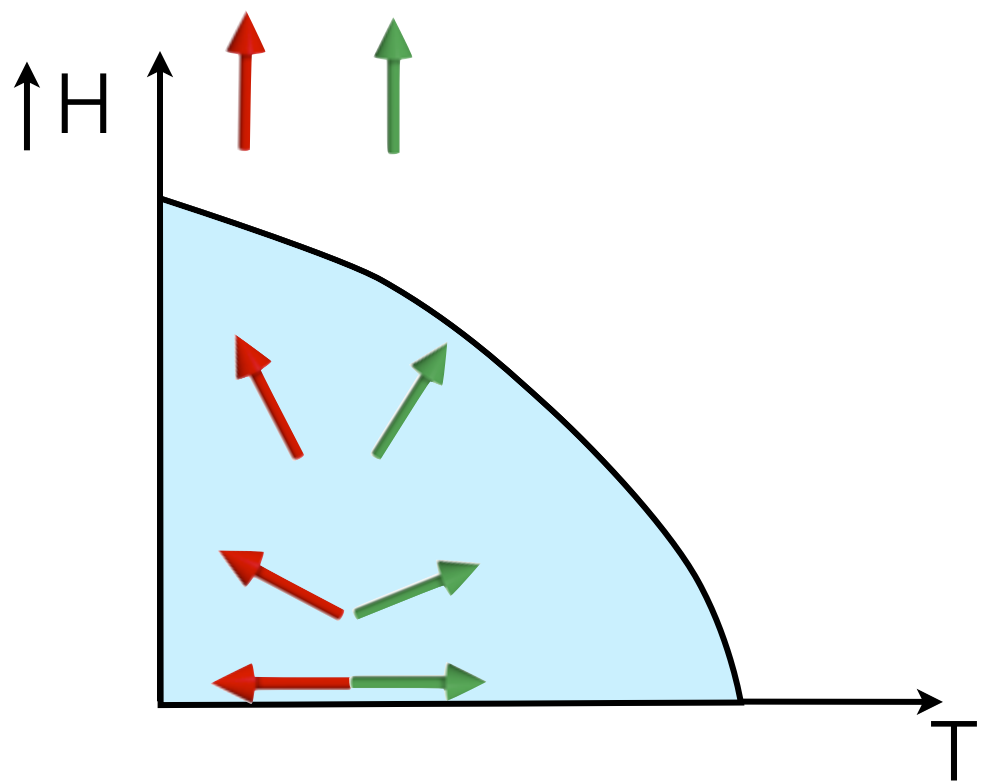
“intra-unit cell antiferromagnet”

$$E = J_{\perp}(S_{\mathrm{A}}^{x} S_{\mathrm{B}}^{x} + S_{\mathrm{A}}^{y} S_{\mathrm{B}}^{y}) + J_{z} S_{\mathrm{A}}^{z} S_{\mathrm{B}}^{z} + \sum_{\alpha} \left[D \left(S_{\alpha}^{z} \right)^{2} \right.$$

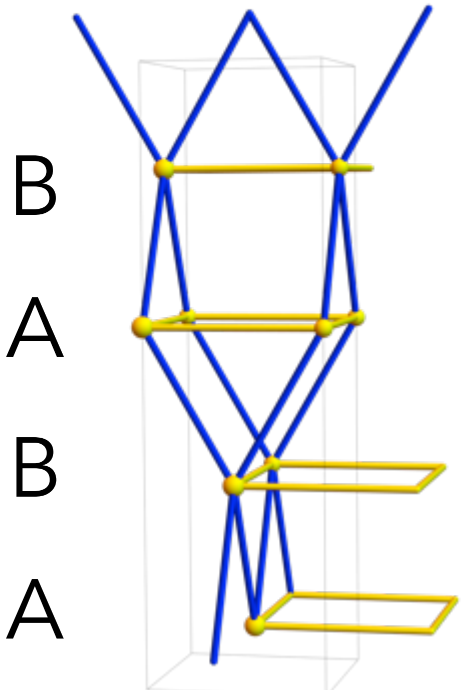
$2D > J_z - J_p$ ⟶ in-plane (XY) spins

Spin Flop

Standard
Heisenberg or XY
antiferromagnet



Minimal model



Two Ce sublattices

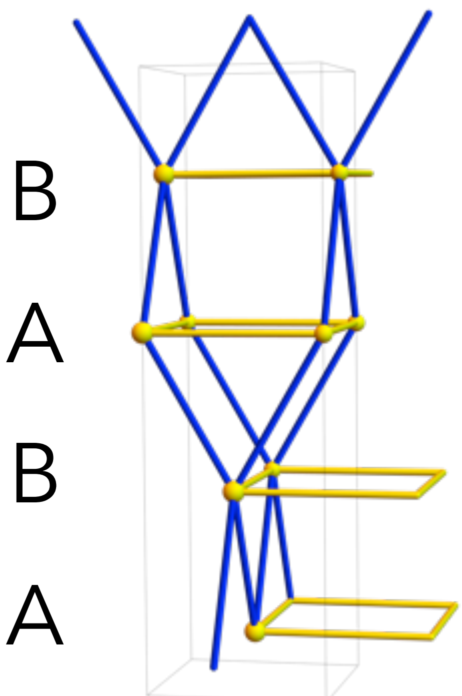
“intra-unit cell antiferromagnet”

$$E = J_{\perp}(S^x_{\mathrm{A}} S^x_{\mathrm{B}} + S^y_{\mathrm{A}} S^y_{\mathrm{B}}) + J_z S^z_{\mathrm{A}} S^z_{\mathrm{B}} + \sum_{\alpha} \left[D \left(S^z_{\alpha} \right)^2 - \mathbf{H} \cdot \mathbf{m}_{\alpha} \right],$$

g-tensor anisotropy

$$\boldsymbol{m}_{\alpha} = g_{\alpha} \boldsymbol{S}_{\alpha} \qquad g_A = \begin{pmatrix} g_x & & \\ & g_y & \\ & & g_z \end{pmatrix} \qquad g_B = \begin{pmatrix} g_y & & \\ & g_x & \\ & & g_z \end{pmatrix}$$

Minimal model



Two Ce sublattices

"intra-unit cell antiferromagnet"

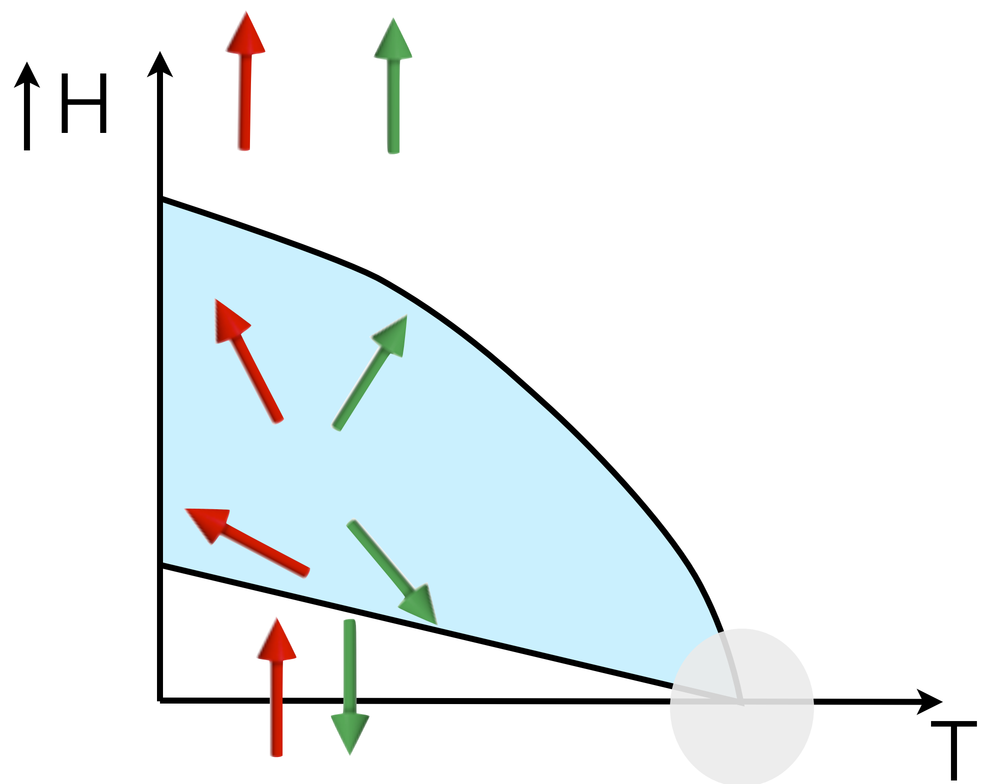
$$E = J_\perp (S_\mathrm{A}^x S_\mathrm{B}^x + S_\mathrm{A}^y S_\mathrm{B}^y) + J_z S_\mathrm{A}^z S_\mathrm{B}^z + \sum_\alpha \left[D \left(S_\alpha^z \right)^2 - \mathbf{H} \cdot \mathbf{m}_\alpha \right],$$

$$\boldsymbol{H} = (H, 0, 0)$$

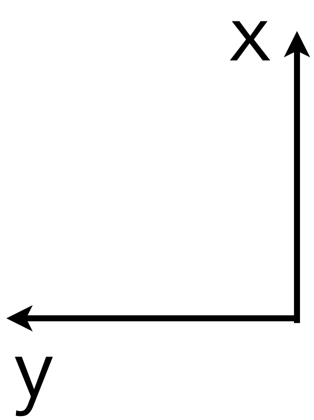
$$E = J_\perp (S_A^x S_B^x + S_A^y S_B^y) - H(g_x S_A^x + g_y S_B^x)$$

Spin Flop

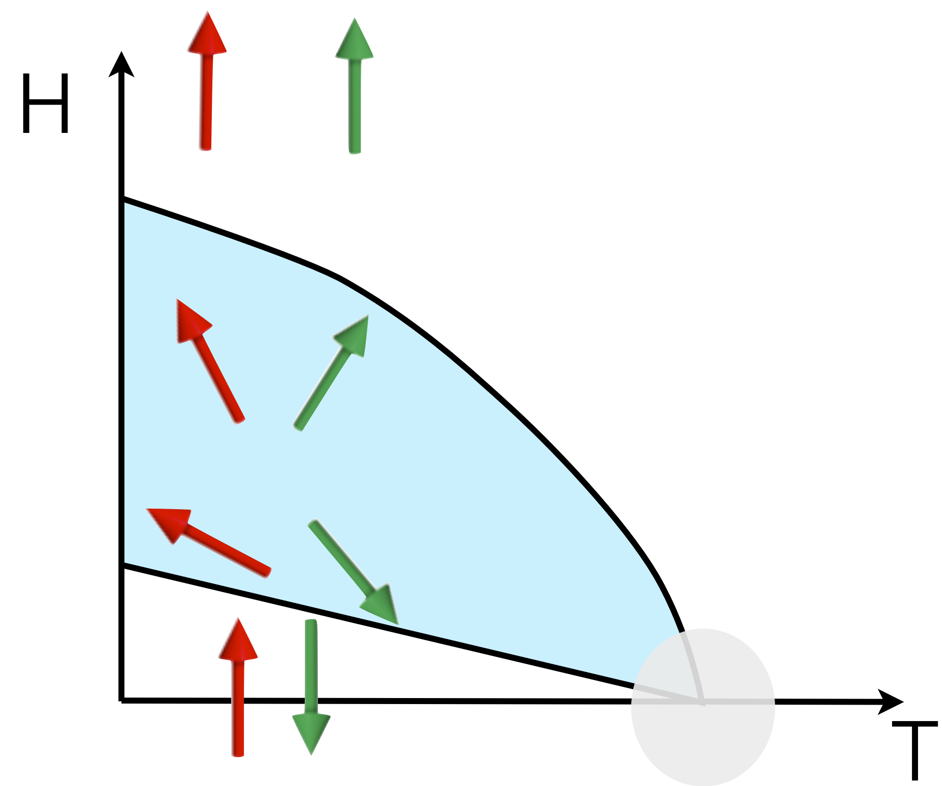
With g-factor anisotropy *and* H along (100)



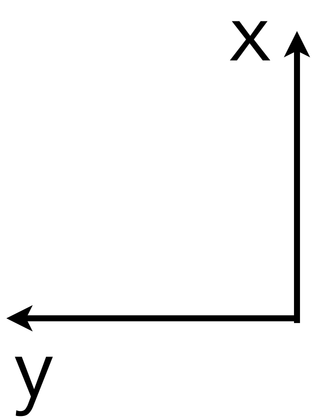
Spin Flop



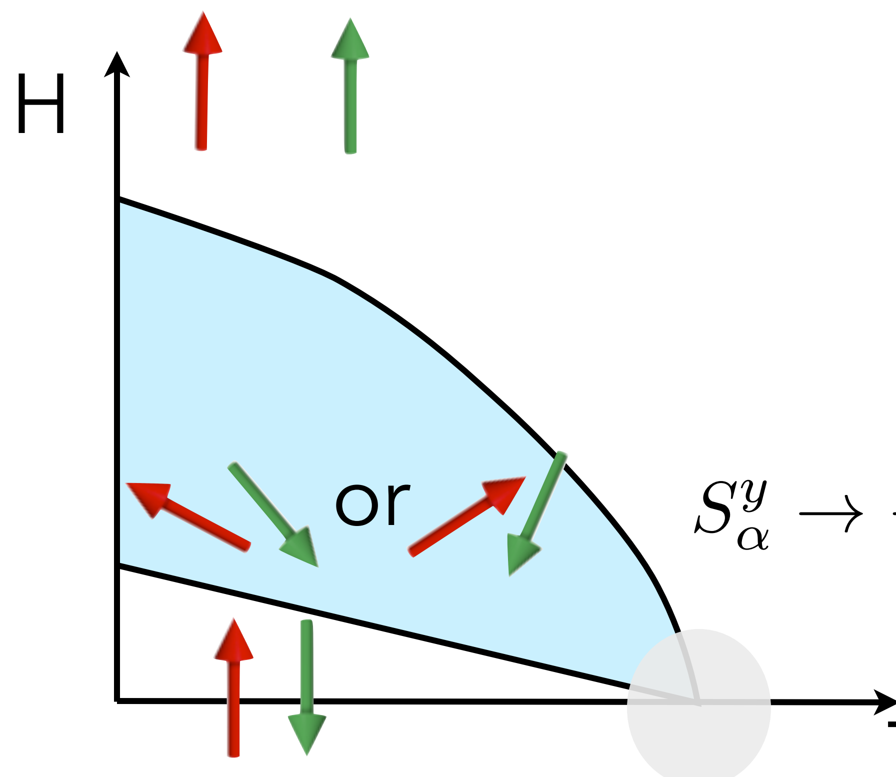
$m_{010} \times \mathrm{TR}$
broken



Domains

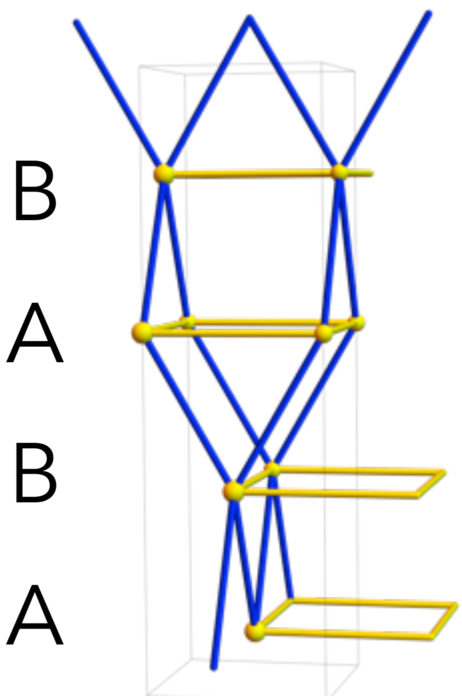


$m_{010} \times \mathrm{TR}$
broken



$S^y_\alpha \to -S^y_\alpha$

Minimal model



Two Ce sublattices

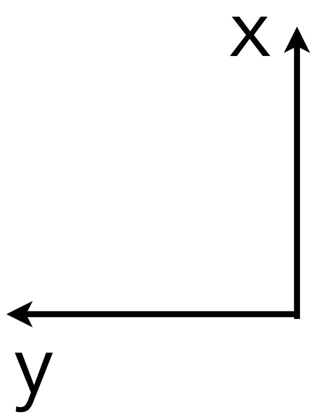
"intra-unit cell antiferromagnet"

$$E = J_\perp (S_A^x S_B^x + S_A^y S_B^y) + J_z S_A^z S_B^z + \sum_\alpha \left[D\,(S_\alpha^z)^2 - \mathbf{H} \cdot \mathbf{m}_\alpha \right],$$

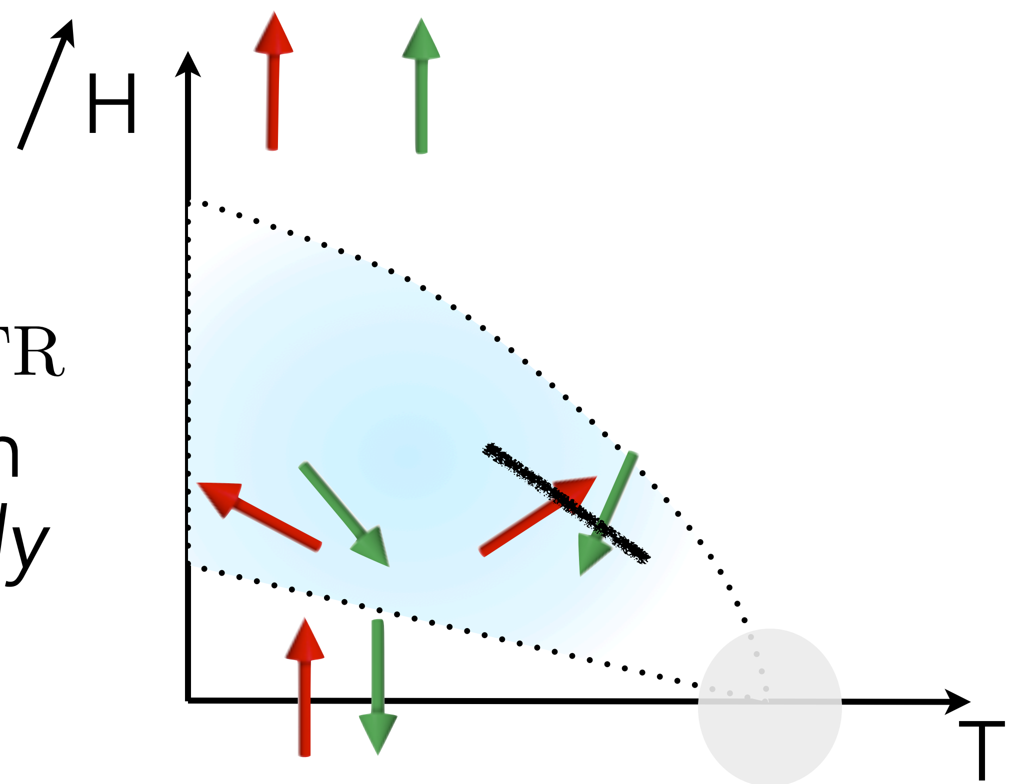
g-tensor anisotropy

$$\boldsymbol{m}_\alpha = g_\alpha \boldsymbol{S}_\alpha \qquad g_A = \begin{pmatrix} g_x & & \\ & g_y & \\ & & g_z \end{pmatrix} \qquad g_B = \begin{pmatrix} g_y & & \\ & g_x & \\ & & g_z \end{pmatrix}$$

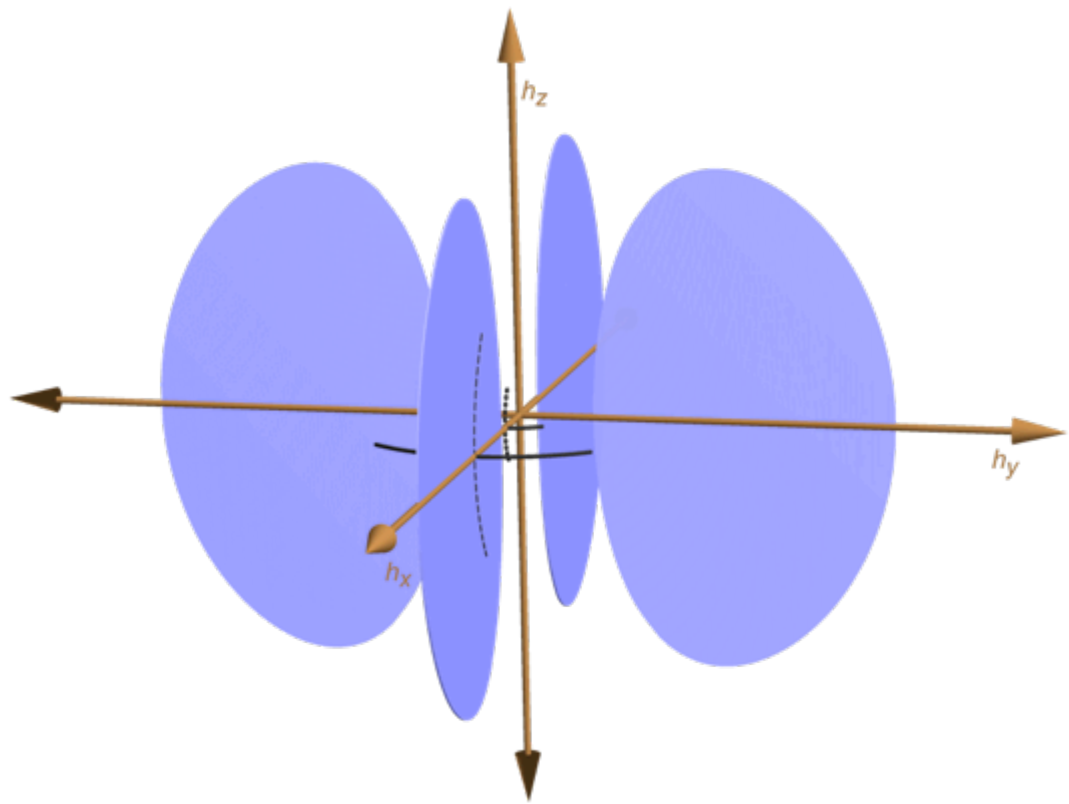
Domains



$m_{010} \times \mathrm{TR}$
broken
explicitly

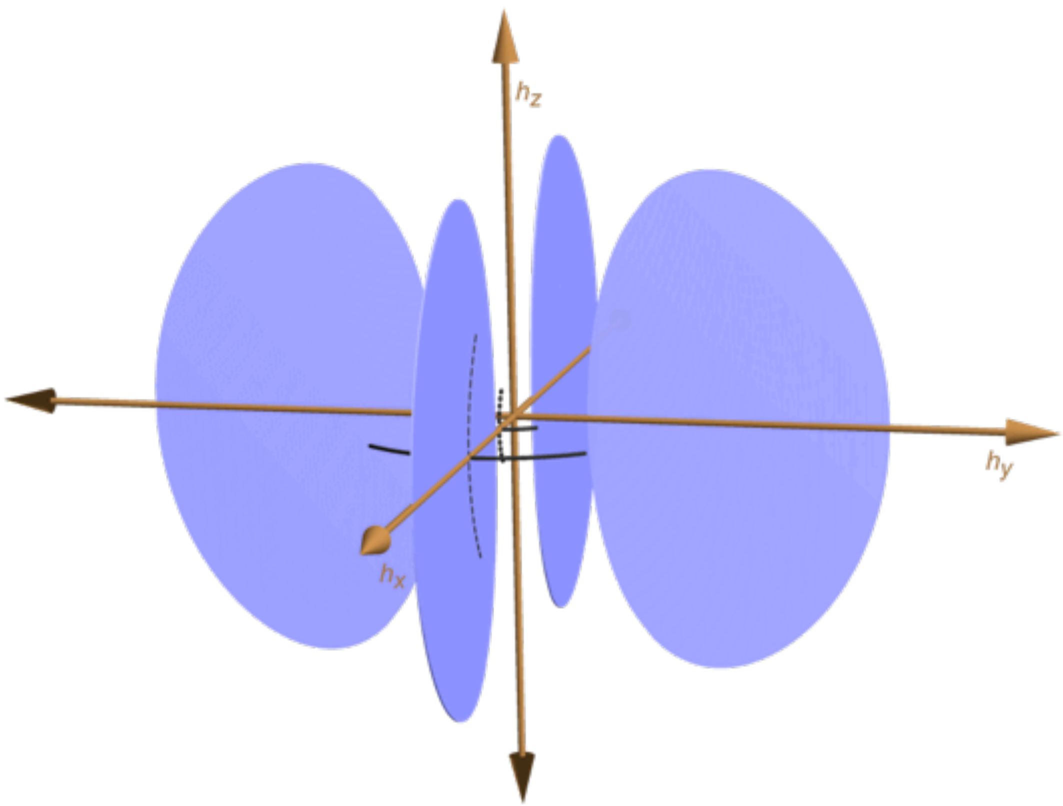


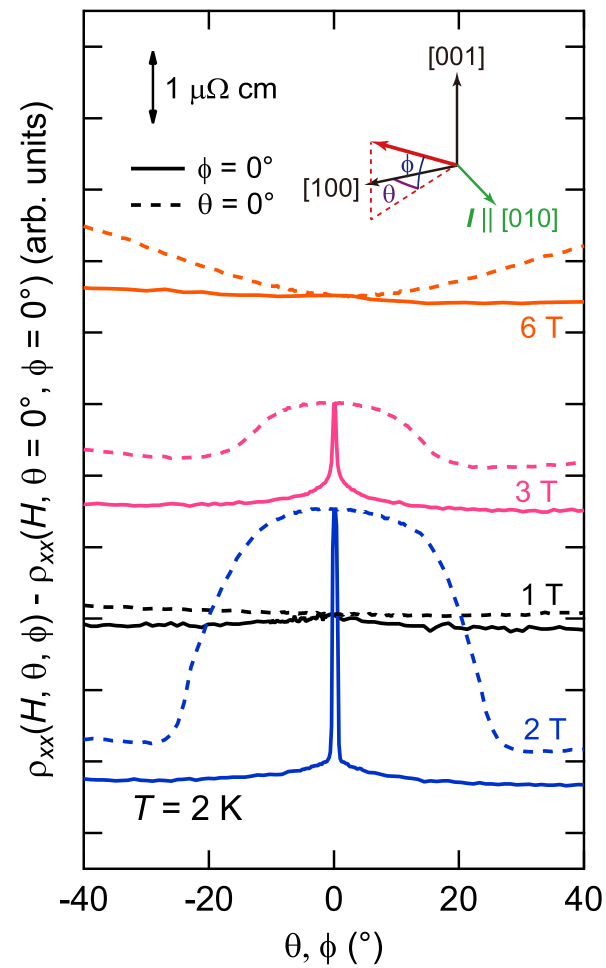
Phase diagram



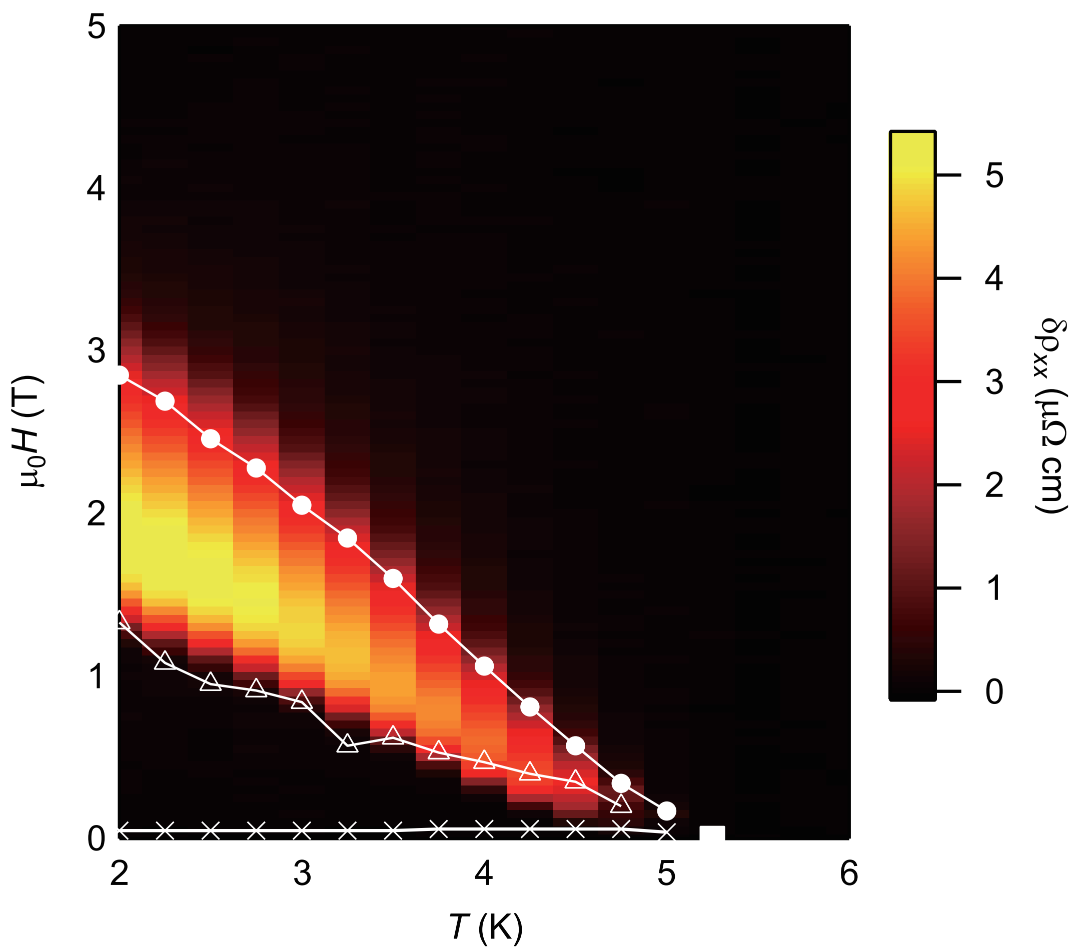
Canted phase forms 4 “infinitely thin” wedges

Phase diagram



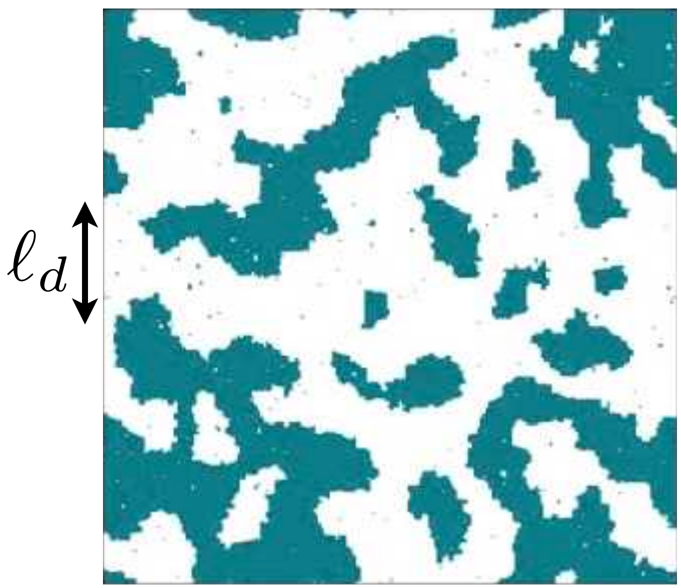


Phase Diagram



Resistivity

Extra resistance comes from *domain walls*



$$\rho_{\text{eff}} = \rho + \frac{\tilde{\rho}_{\text{dw}}}{\ell_d}$$

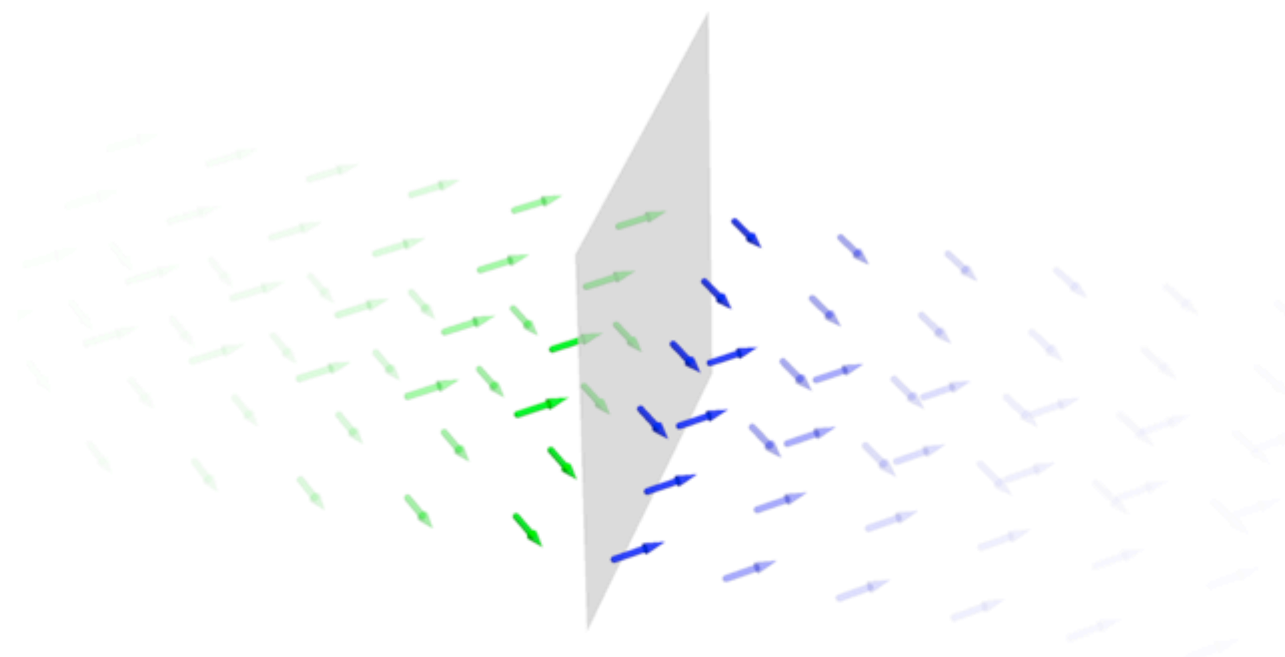
$$V_{\text{dw}} = \tilde{\rho}_{\text{dw}} j$$

Size of the effect depends on size of $\tilde{\rho}_{dw}$

Domain wall

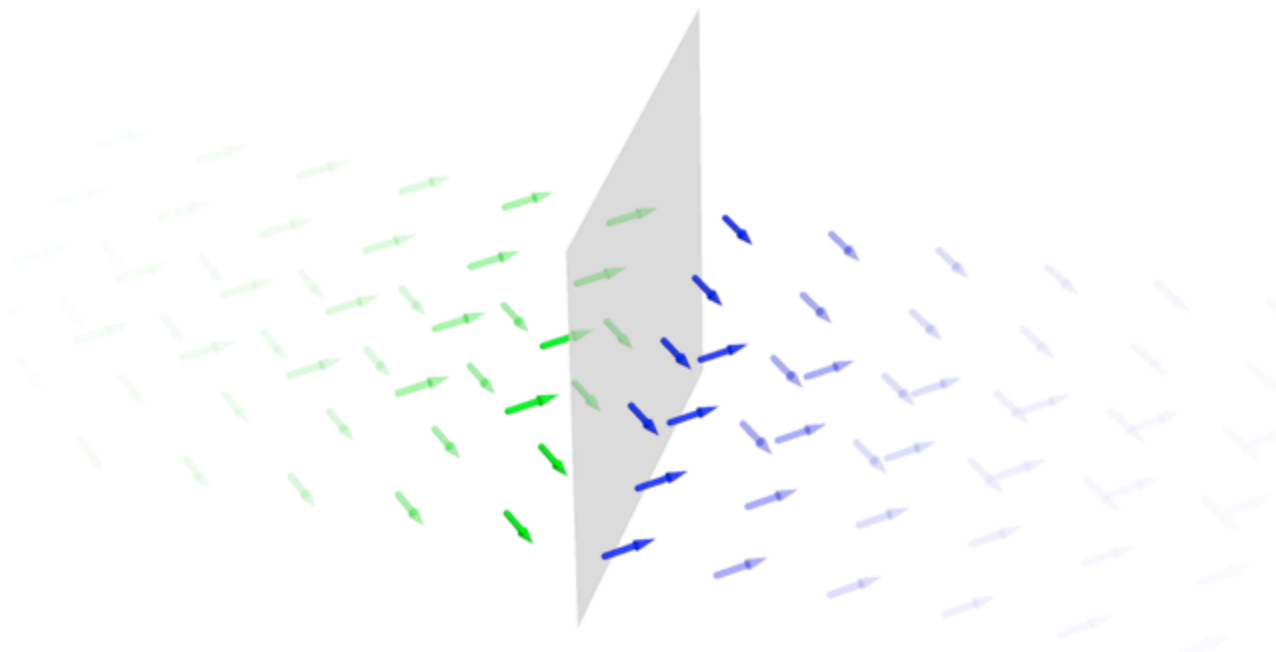
Strong anisotropy/Ising order:

narrow domain walls



Crudely, effective potential for electrons is "abrupt": strong scattering if Fermi energy is low

Phase space



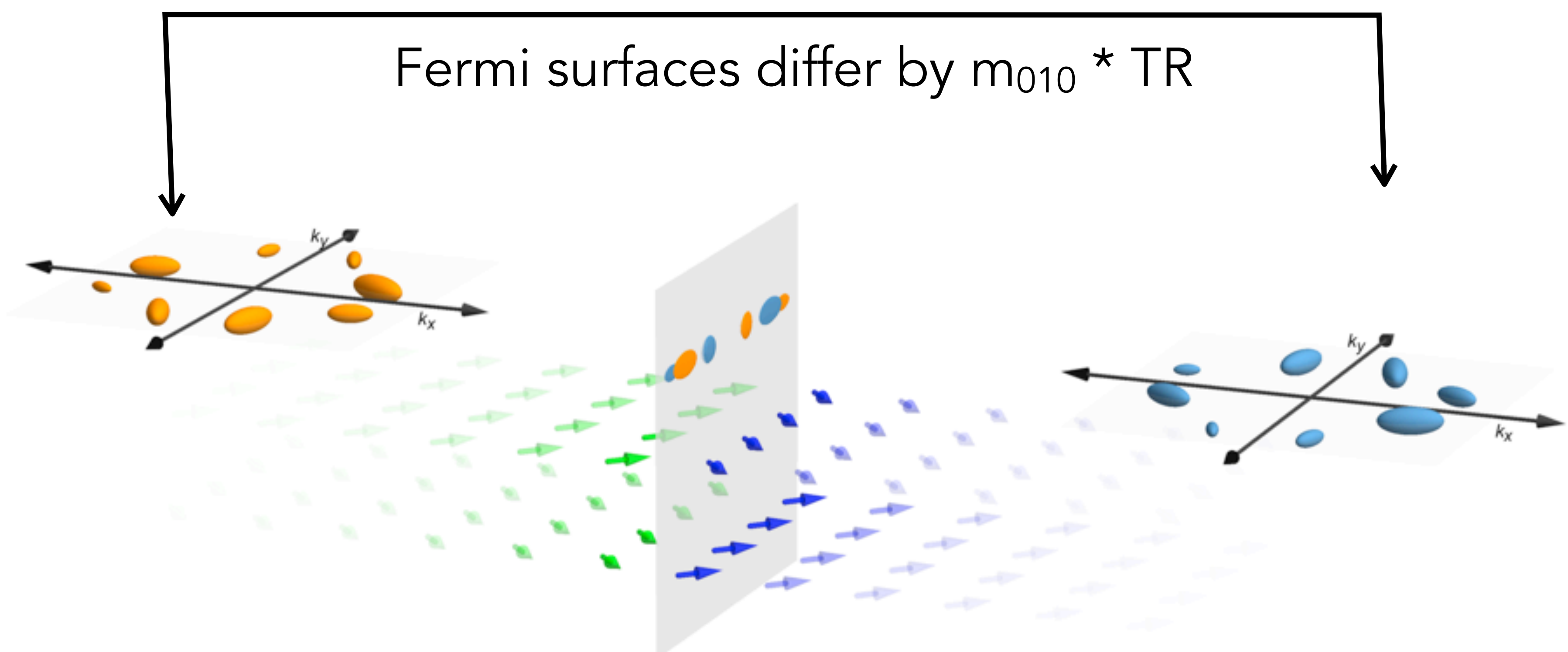
Landauer-Büttiker: one channel for each transverse momenta

$$G = \sum_{n=1}^{L^2} g_n \frac{e^2}{h},$$

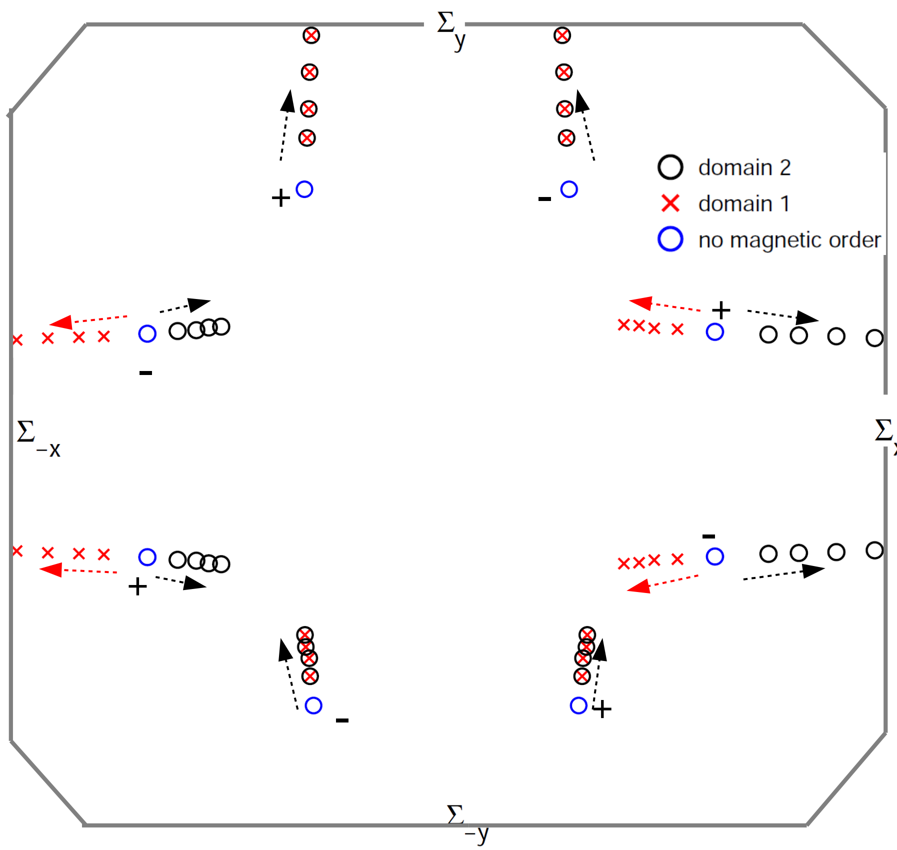
BUT sum only includes modes that exist at Fermi energy on both sides

Phase space

Fermi surfaces differ by m_{010} * TR



Weyl points

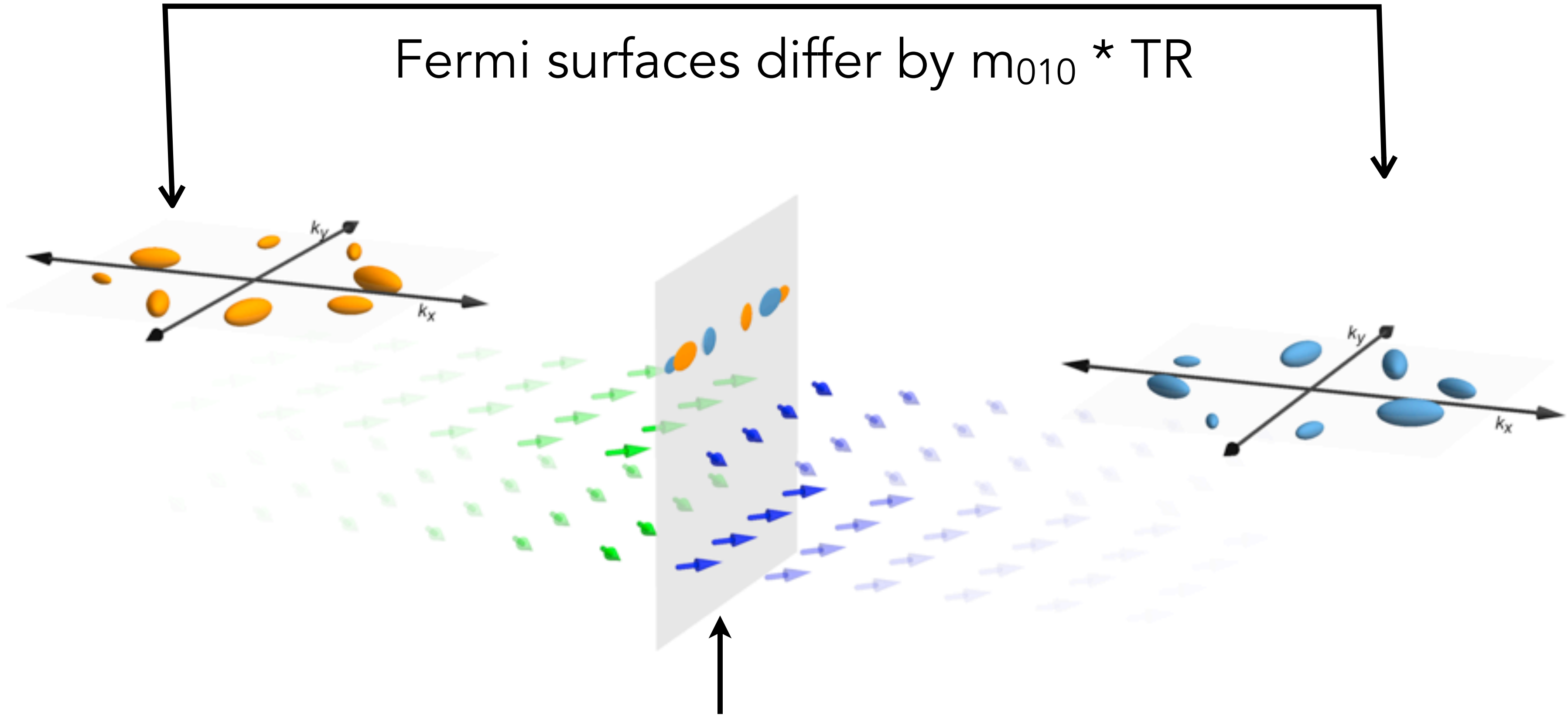


Low symmetry, SOC: Weyl point locations depend on domain

(from DFT-fit tight-binding model)

Phase space

Fermi surfaces differ by m_{010} * TR

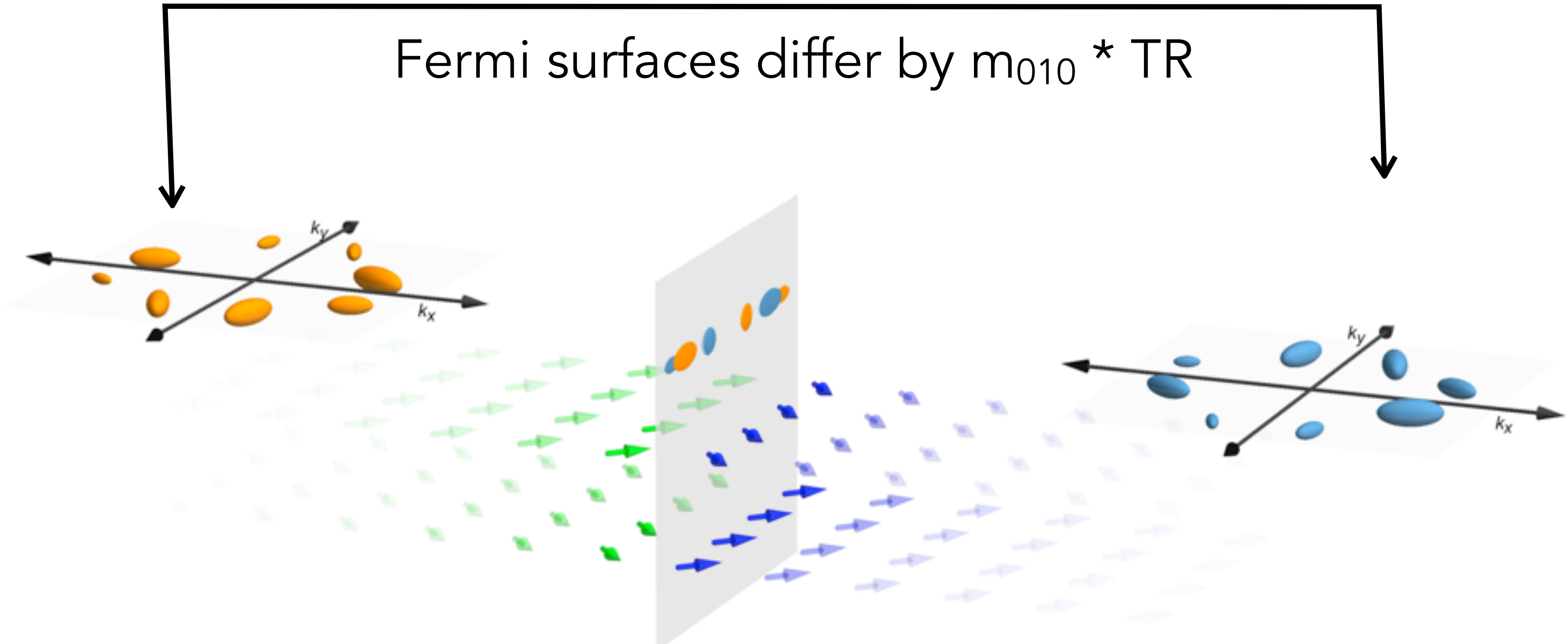


projection to interface BZ

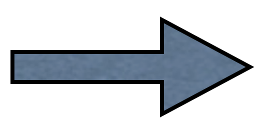
Only overlapping portions contribute!

Phase space

Fermi surfaces differ by m_{010} * TR

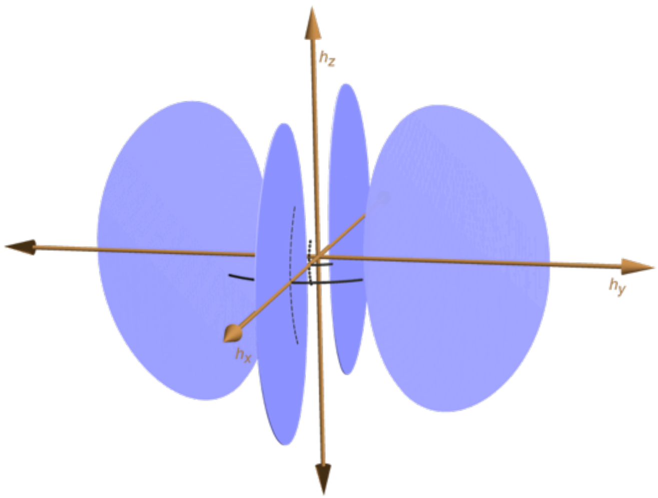


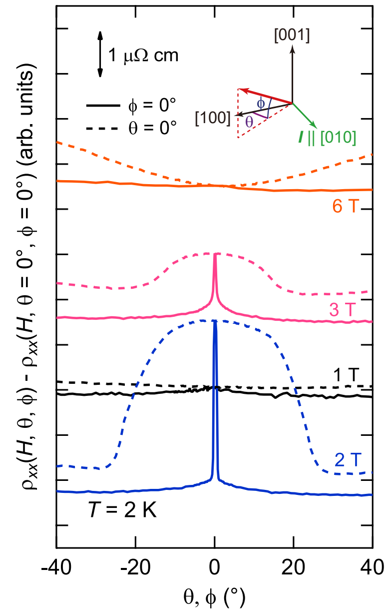
$$G = L^2 \frac{\mathcal{A}_{int}}{(2\pi)^2} T \frac{e^2}{h}$$

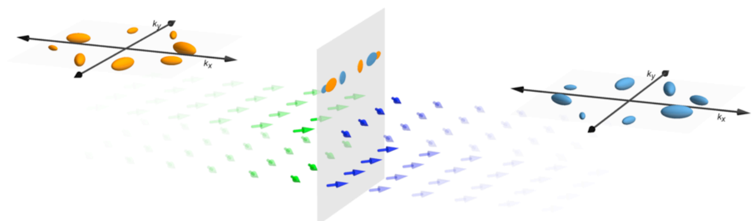


$$\frac{\rho_{\text{eff}} - \rho}{\rho} \sim \frac{1}{k_F^2 \mathcal{A}_{int}} \frac{\ell}{\ell_d} T^{-1}$$

End







Super **A**mazing **M**agneto-**R**esistance: a new effect in a SOC semimetal

?*One of many new effects related to topological defects in semimetals*?