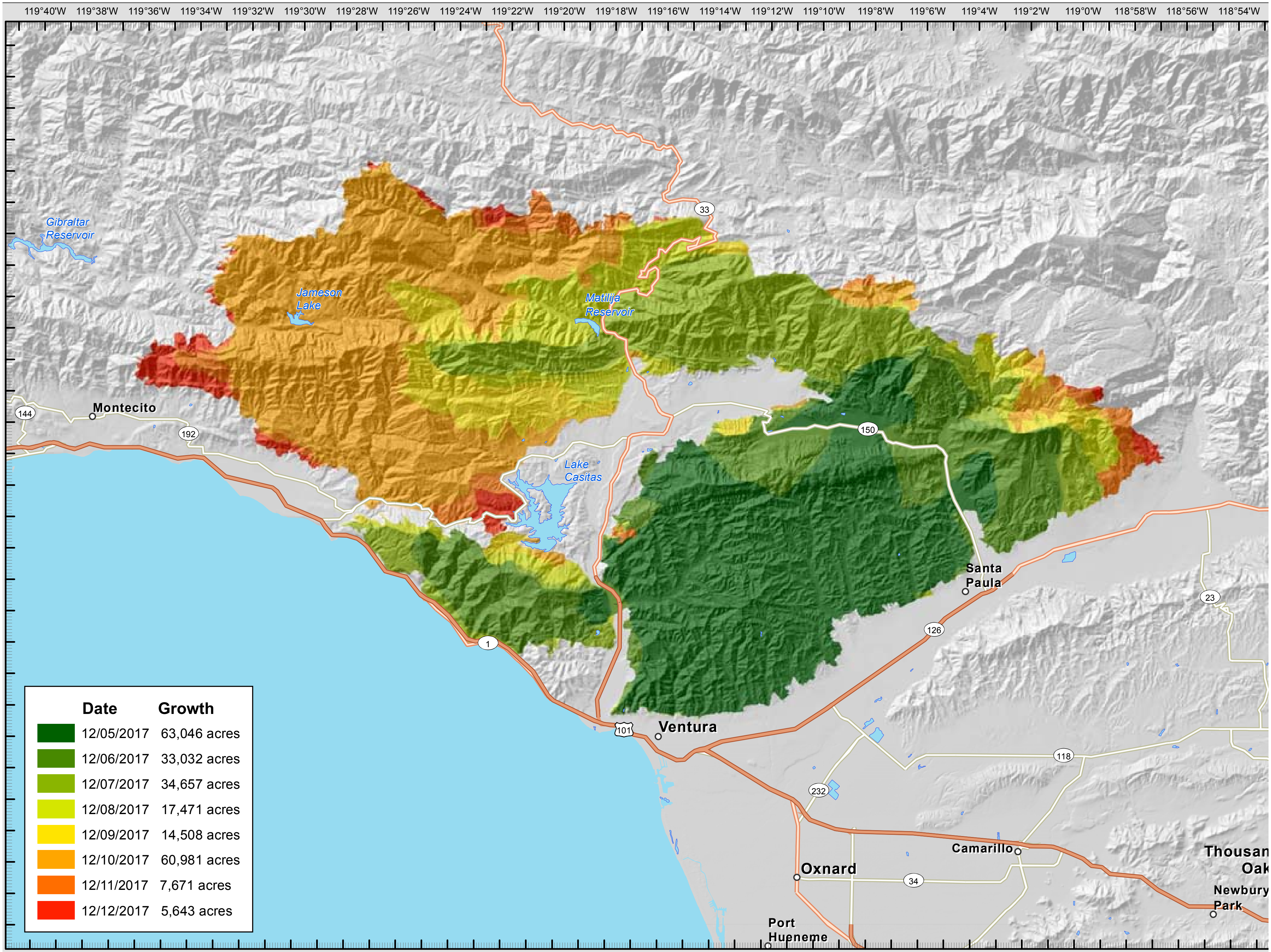
not necessarily

Magnetic ~~topological~~ semimetals

Leon Balents, KITP



119°40'W
119°38'W
119°36'W
119°34'W
119°32'W
119°30'W
119°28'W
119°26'W
119°24'W
119°22'W
119°20'W
119°18'W
119°16'W
119°14'W
119°12'W
119°10'W
119°8'W
119°6'W
119°4'W
119°2'W
119°0'W
118°58'W
118°56'W
118°54'W
Gibraltar Reservoir
Jameson Lake
Matilija Reservoir
Lake Casitas
Montecito
Ventura
Santa Paula
Oxnard
Camarillo
Port Hueneme
Thousan
Oak
Newbury Park
33
144
192
150
1
101
126
23
118
232
34
Date
Growth
12/05/2017 63,046 acres
12/06/2017 33,032 acres
12/07/2017 34,657 acres
12/08/2017 17,471 acres
12/09/2017 14,508 acres
12/10/2017 60,981 acres
12/11/2017 7,671 acres
12/12/2017 5,643 acres

Collaborators

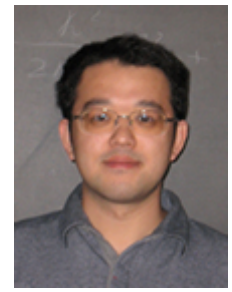
Jianpeng Liu

KITP

Lucile Savary

ENS Lyon

Joe Checkelsky



Takehito Suzuki

MIT

Topological semimetals

- Band touching at some points/lines in momentum space
- May be protected by topology and/or symmetry
- 2d: graphene
- 3d: Weyl points, Dirac points, nodal lines…

Weyl semimetal

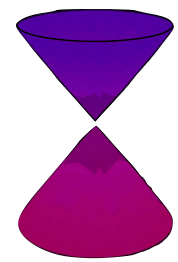
937 PHYSICAL REVIEW

Accidental Degeneracy in the Energy Bands of Crystals

CONYERS HERRING
Princeton University, Princeton, New Jersey
(Received June 16, 1937)

For a crystal without an inversion center, the energy separation $\delta E(\mathbf{k}+\boldsymbol{\kappa})$ in the neigborhood of a point $\mathbf{k}$ where contact of equivalent manifolds occurs may be expected to be of the order of κ as $\kappa\rightarrow 0$, for all directions of $\boldsymbol{\kappa}$.

$$H = v\vec{\sigma}\cdot\vec{k}$$



A two-component spinor in three dimensions: “half” of a Dirac fermion. Weyl fermions have a chirality and *must* be massless

Weyl semimetal

937 PHYSICAL REVIEW

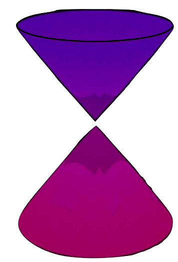
Accidental Degeneracy in the Energy Bands of Crystals

CONYERS HERRING
Princeton University, Princeton, New Jersey

(Received June 16, 1937)

For a crystal without an inversion center, the energy separation $\delta E(\mathbf{k}+\boldsymbol{\kappa})$ in the neigborhood of a point $\mathbf{k}$ where contact of equivalent manifolds occurs may be expected to be of the order of κ as $\kappa \to 0$, for all directions of $\boldsymbol{\kappa}$.

$$H = v\vec{\sigma} \cdot \vec{k}$$



A Weyl point is a "topological defect" in momentum space: a monopole for the Berry curvature

$$\boldsymbol{\nabla}_{\boldsymbol{k}} \cdot \mathcal{B} = \pm 2\pi q$$

Weyl semimetal

937 PHYSICAL REVIEW

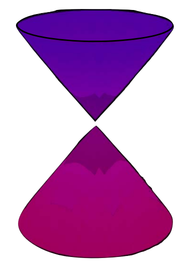
Accidental Degeneracy in the Energy Bands of Crystals

CONYERS HERRING
Princeton University, Princeton, New Jersey

(Received June 16, 1937)

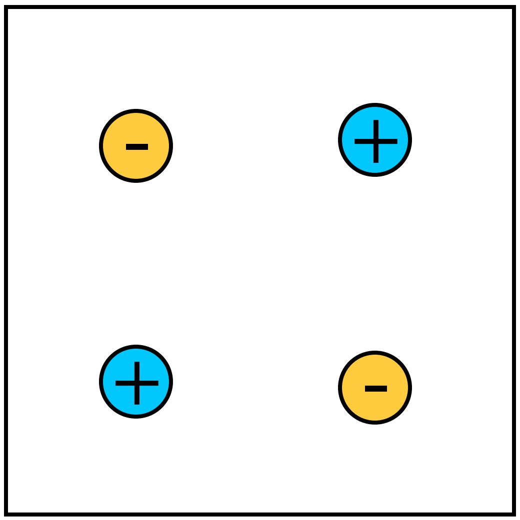
For a crystal without an inversion center, the energy separation $\delta E(\mathbf{k}+\boldsymbol{\kappa})$ in the neigborhood of a point $\mathbf{k}$ where contact of equivalent manifolds occurs may be expected to be of the order of κ as $\kappa \rightarrow 0$, for all directions of $\boldsymbol{\kappa}$.

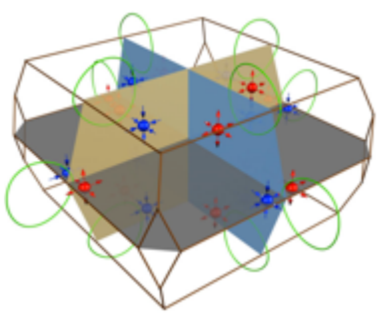
$$H = v\vec{\sigma} \cdot \vec{k}$$



Weyl point is "symmetry prevented": needs *broken* inversion and/or time-reversal

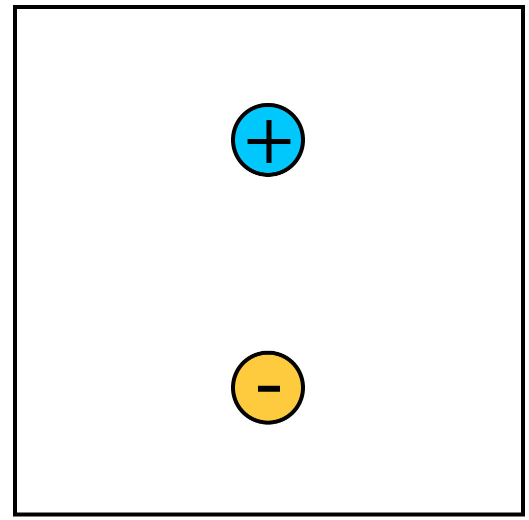
I-breaking Weyls

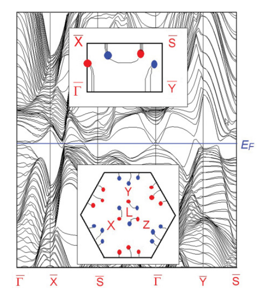




TaAs, Na_3Bi, TaP, WTe_2,...

TR-breaking Weyls





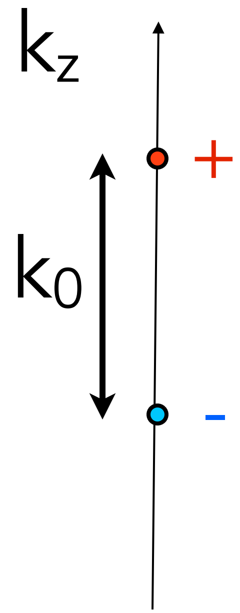
$R_2Ir_2O_7$?, $Mn_3(Sn/Ge)$, RAlGe

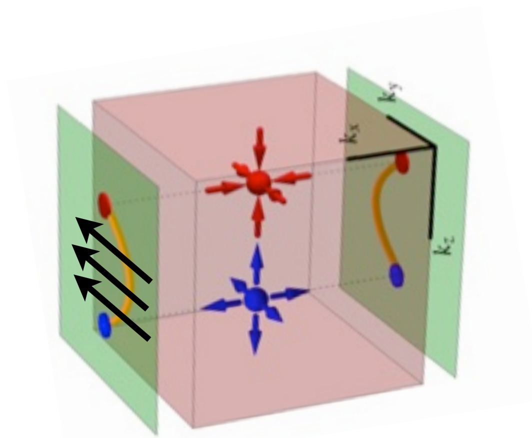
Why magnetic Weyls?

- 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

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

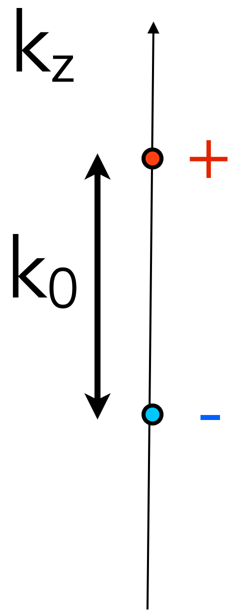
semi-quantum AHE

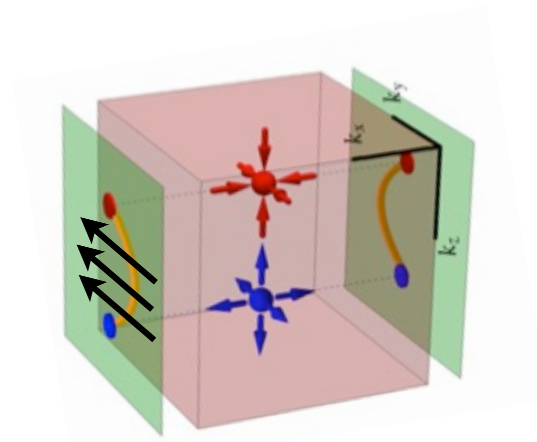
obviously breaks time-reversal symmetry

→ need a magnetic material

Anomalous Hall Effect

Unique property of a magnetic Weyl semimetal





Fermi arc = chiral edge state

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

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

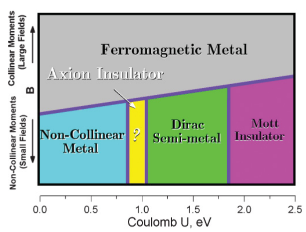
semi-quantum AHE

obviously breaks time-reversal symmetry

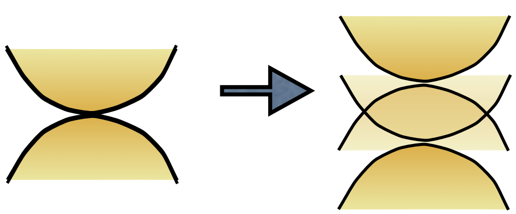
→ need a magnetic material

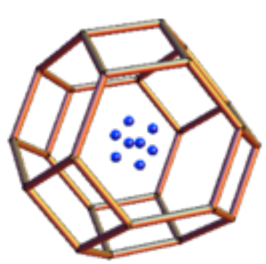
Antiferromagnetic Weyls

Pyrochlore iridates

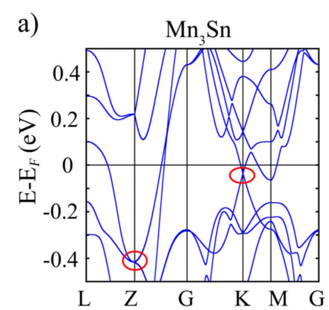


X. Wan *et al*, 2011

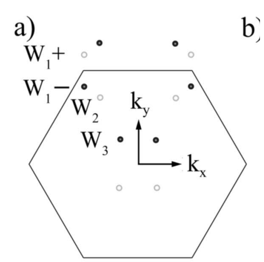




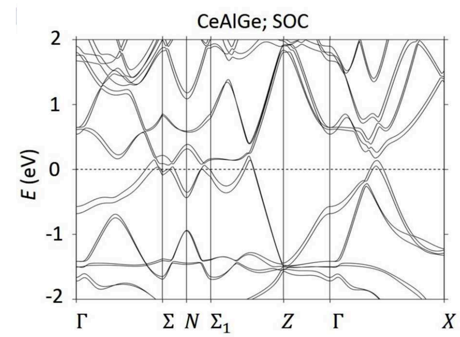
Mn_3Sn, Mn_3Ge



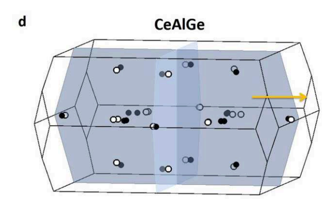
H. Yang *et al*, 2017



RAlGe



G. Chang *et al*, 2016



Quasiparticles

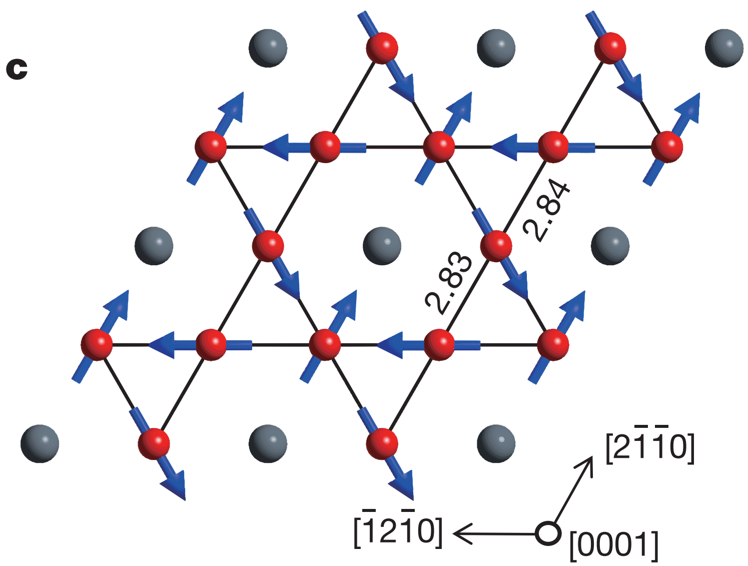
Expect that any magnetically ordered system is described at first order by mean-field quasiparticle Hamiltonian

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

↑ 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

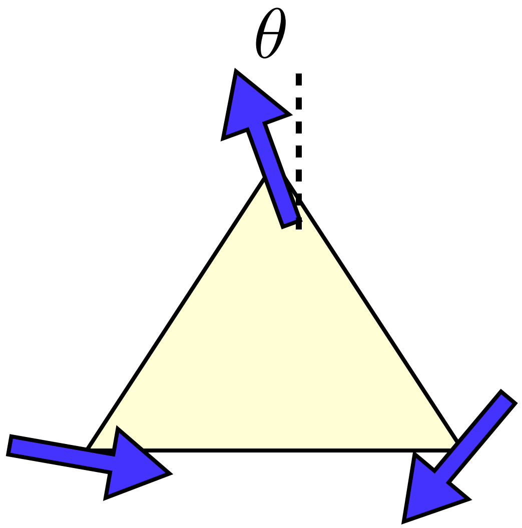
tiny FM moment:

.002 μ_B/Mn

T_N ~ 420K

Nagamiya *et al*, 1982

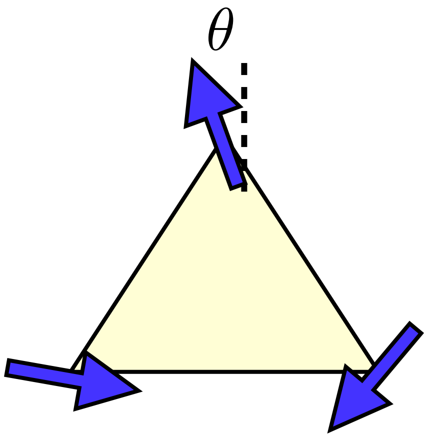
Energetics: triangle



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

$J \gg D \gg K$ **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

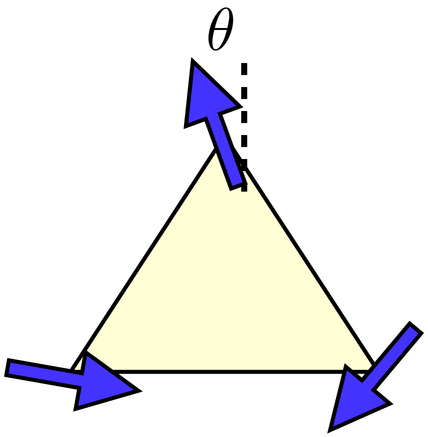


Textures

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

sine-Gordon model with 6-fold anisotropy

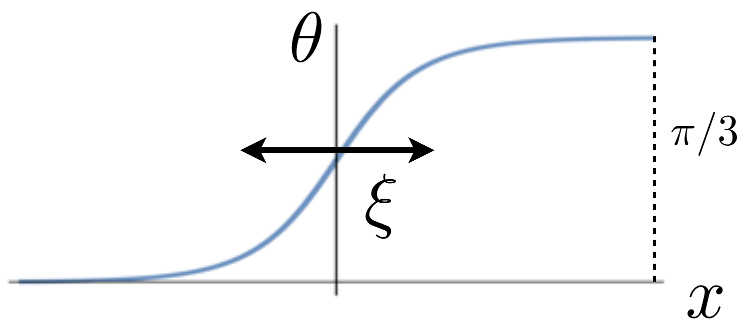
$$\rho \sim \frac{J}{a} \qquad \lambda \sim \frac{K^3}{J^2 a^3}$$



Textures

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

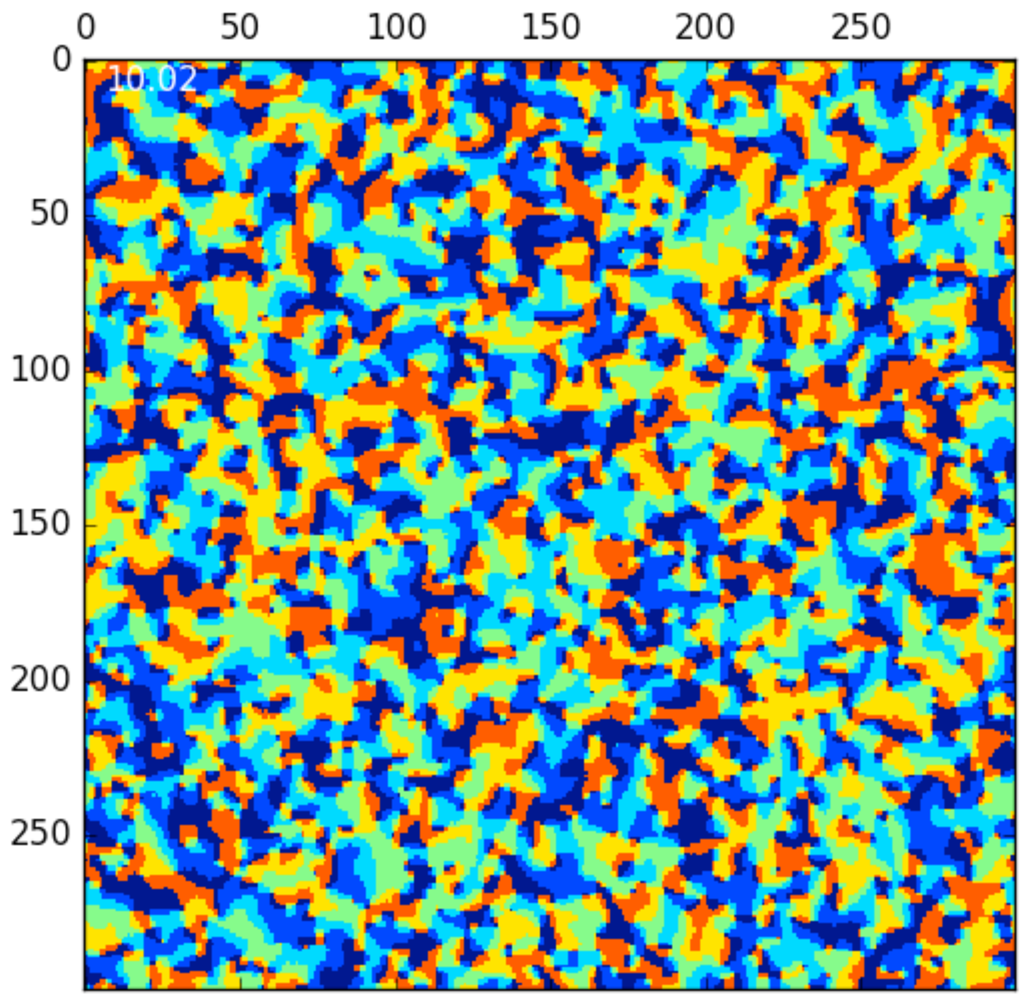
soliton = domain wall connecting *neighboring* minima of cosine



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

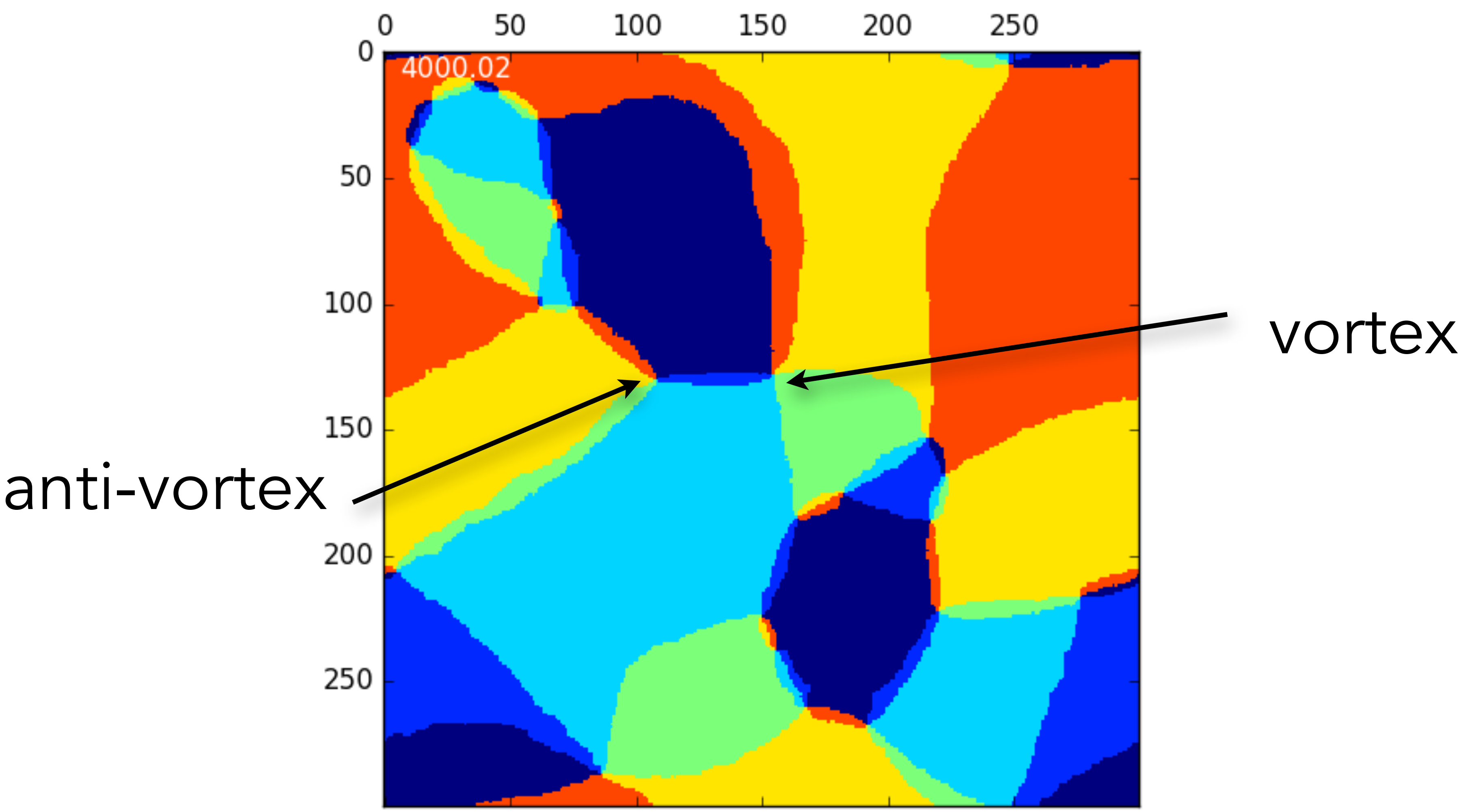
wide
DWs

Domain formation

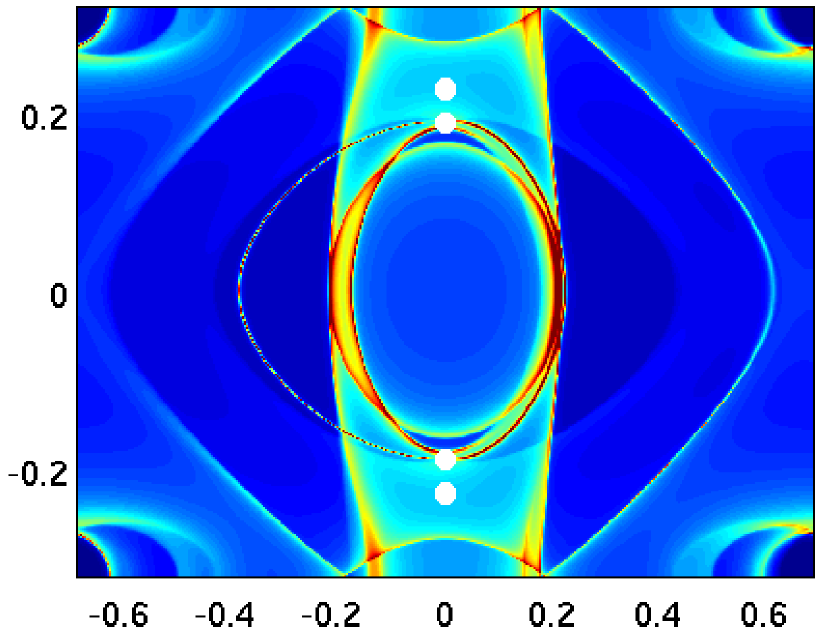


quench

Domain formation



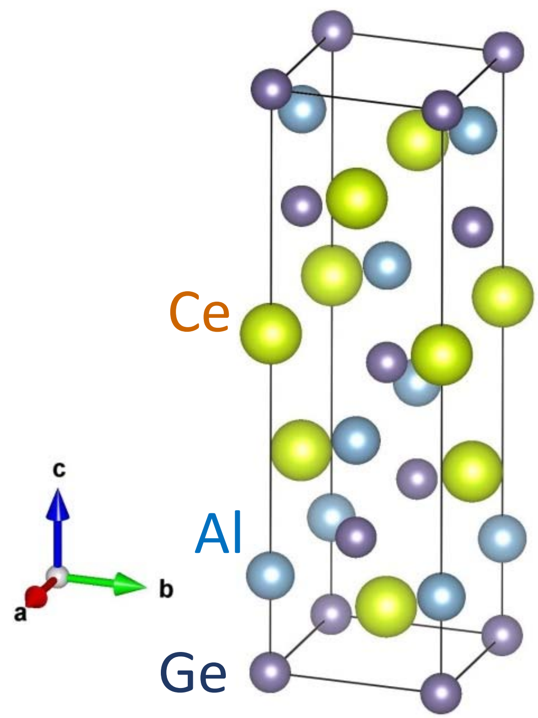
Domain wall bound states



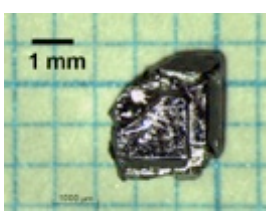
ARPES of domain wall seems challenging to say the least!

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

CeAlGe

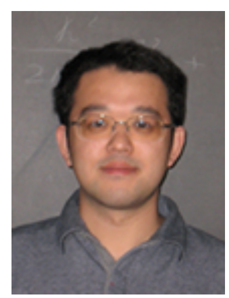


Space group: $I4_1md$



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

Joe Checkelsky



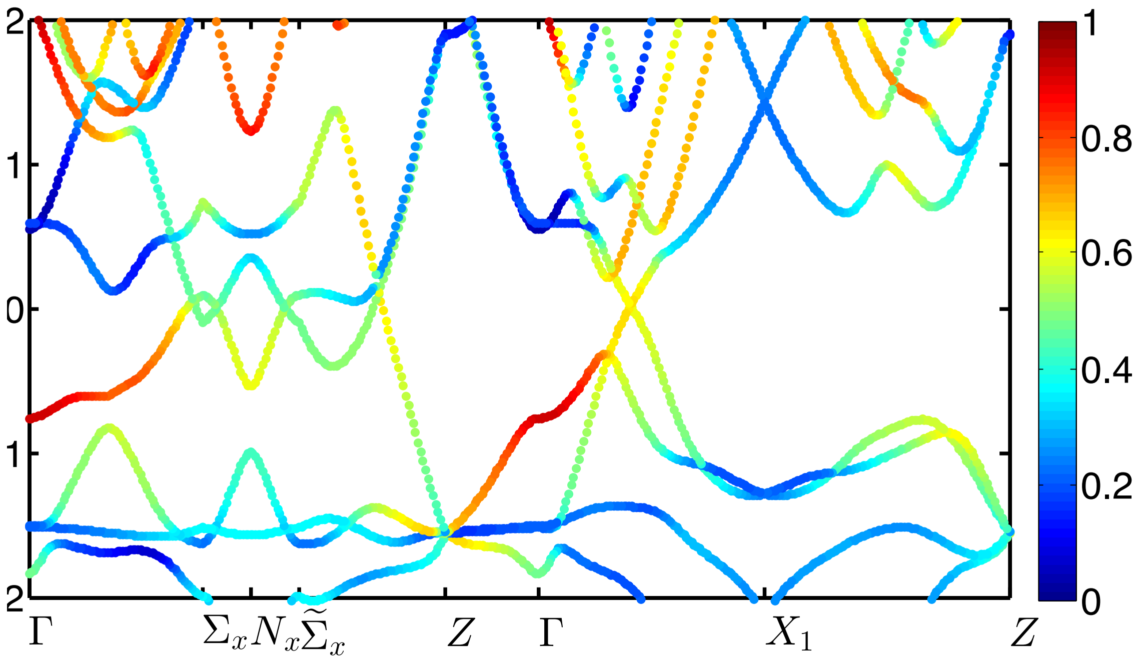
Takehito Suzuki

Lucile Savary

Jianpeng Liu

Band structure

(non-magnetic, no SOC)

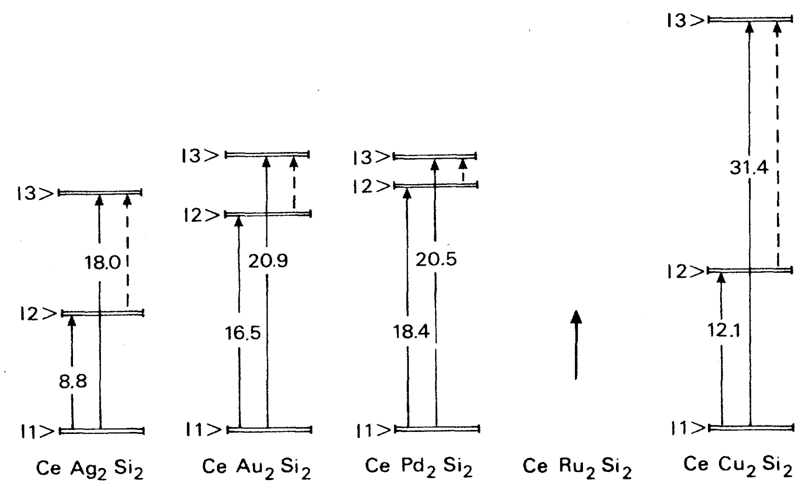


Ce d-orbital content

- 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

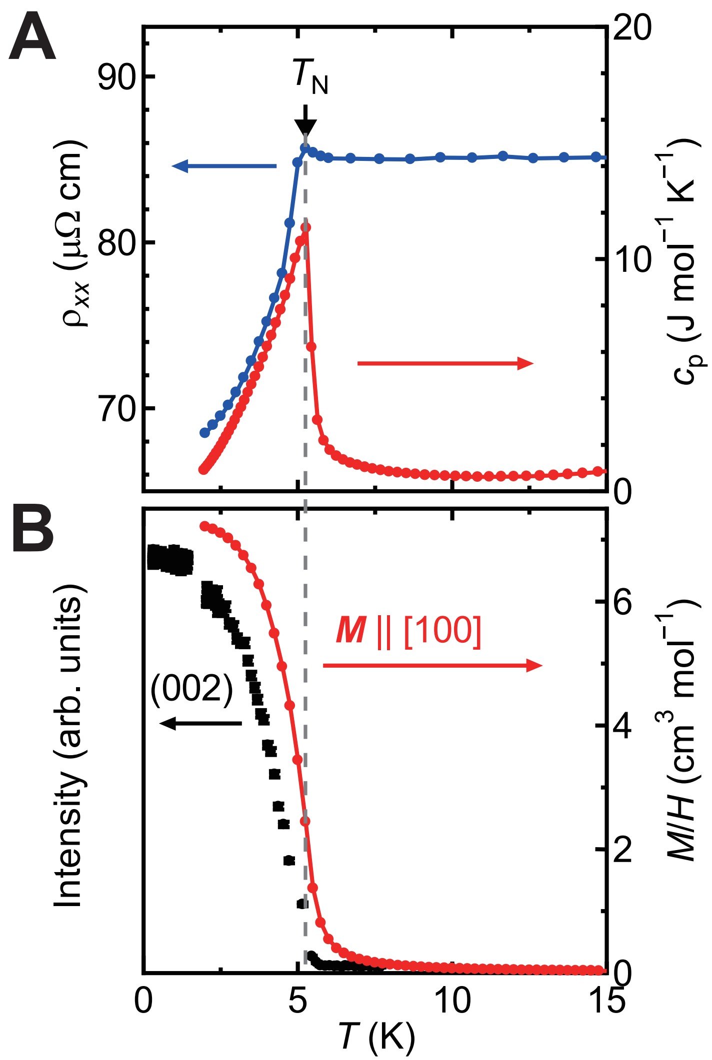


e.g. A. Severing *et al*, 1989

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

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

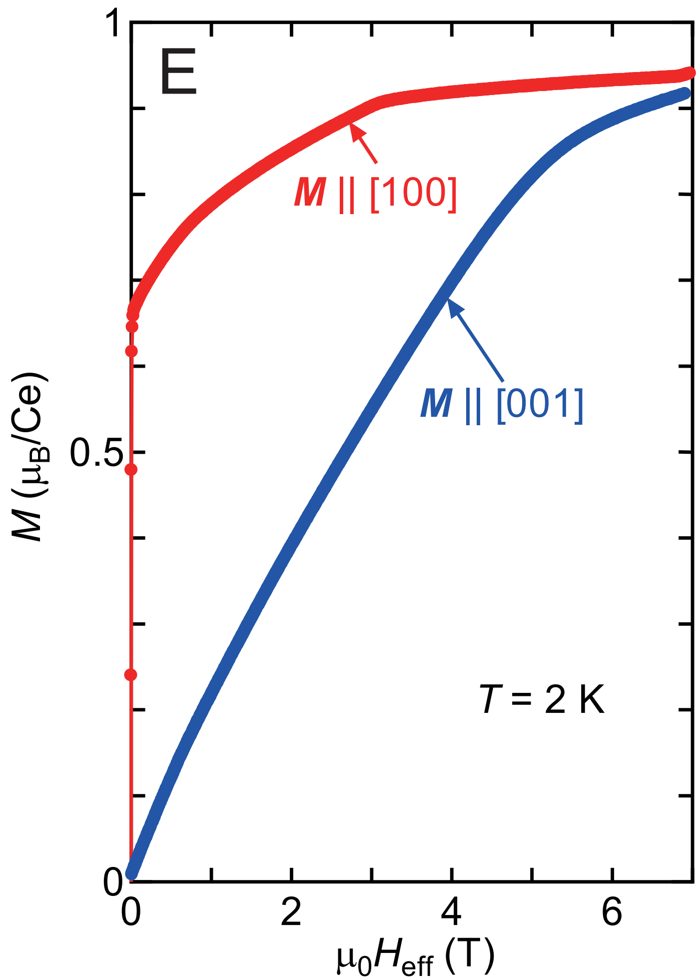
$$J_K \sim \sqrt{J_{RKKY} E_F}$$ ~100meV?

5K 1eV

Summary: key features

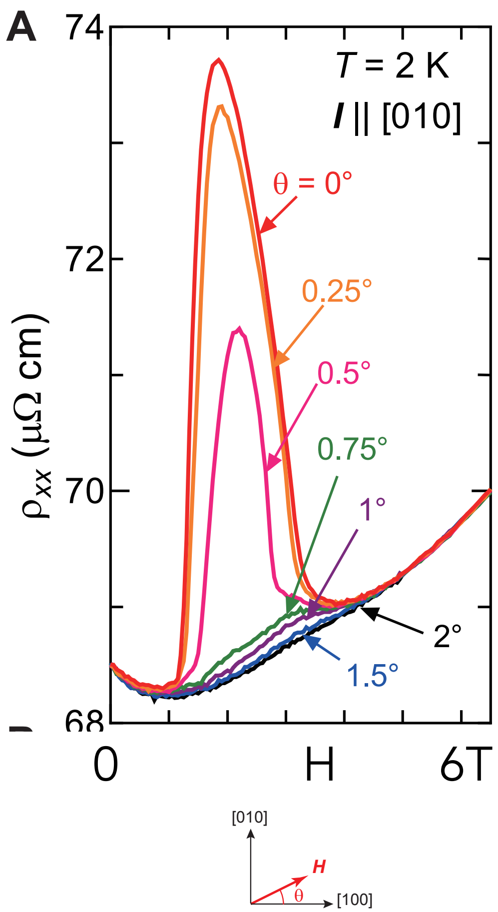
- Semi-metal
- Small bandwidth ~ 1eV
- Large J_K ~ 100meV
- Strong magnetic anisotropy/SOC
- Low T_N ~ 5K

Magnetization



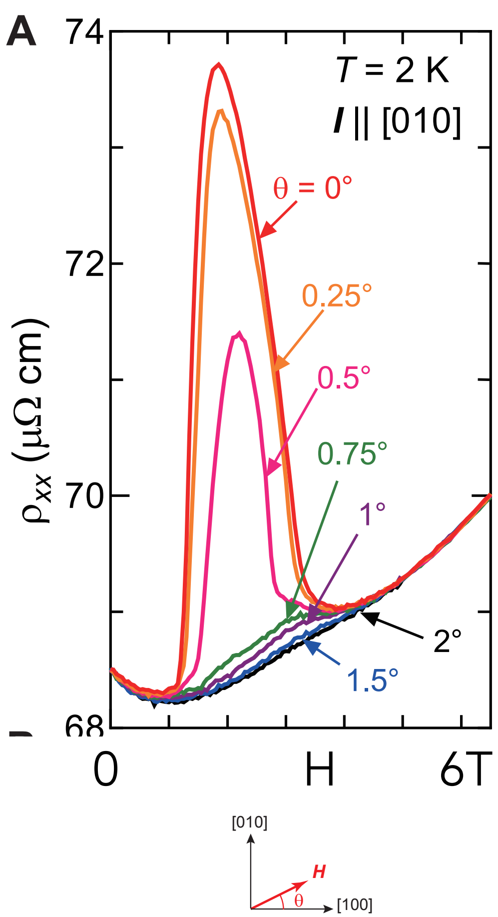
- In-plane field shows ferromagnetic component
- Out of plane field paramagnetic
- If you look carefully, hints of more transitions

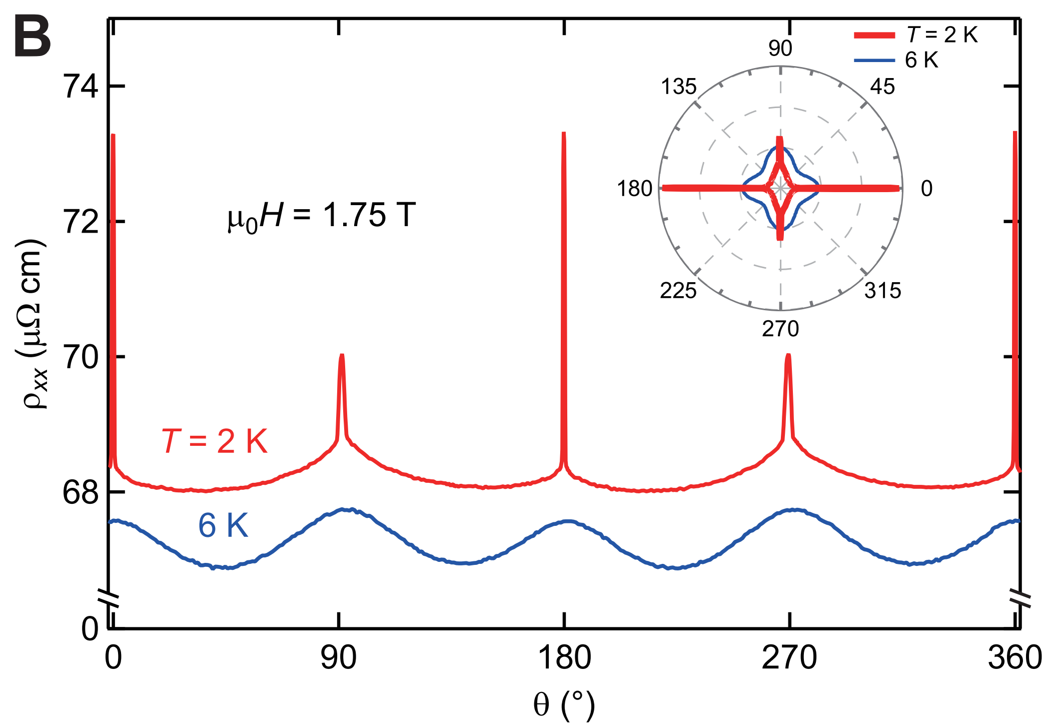
Resistivity



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

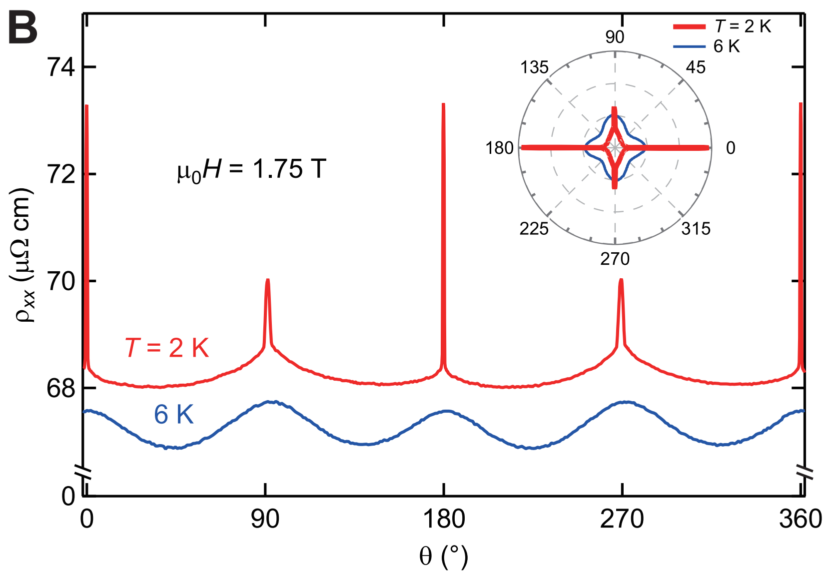
~~Suzuki~~ Angular Magneto-Resistance

~~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)	$\mathbf{h}$ doesn't break sym. explicitly if	(N_x, N_y, N_z)	$\mathbf{N}$ 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 $N_z \neq 0$
$C_4C_4{C_4}^*\times$TR	$(-h_y, h_x, -h_z)$	$\mathbf{h} = \mathbf{0}$	$(N_y, -N_x, N_z)$	$N_x \neq 0$ or $N_y \neq 0$
${C_4}^*$	$(-h_y, h_x, h_z)$	$h_x = h_y = 0$	$(N_y, -N_x, -N_z)$	$\mathbf{N} \neq \mathbf{0}$
${C_4}^*\times$TR	$(h_y, -h_x, -h_z)$	$\mathbf{h} = \mathbf{0}$	$(-N_y, N_x, N_z)$	$N_x \neq 0$ or $N_y \neq 0$
$C_4C_4{C_4}^*$	$(h_y, -h_x, h_z)$	$h_x = h_y = 0$	$(-N_y, N_x, -N_z)$	$\mathbf{N} \neq \mathbf{0}$
${m_{110}}^*$	$(h_y, h_x, -h_z)$	$h_x = h_y$ 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 $\mathbf{h}$.

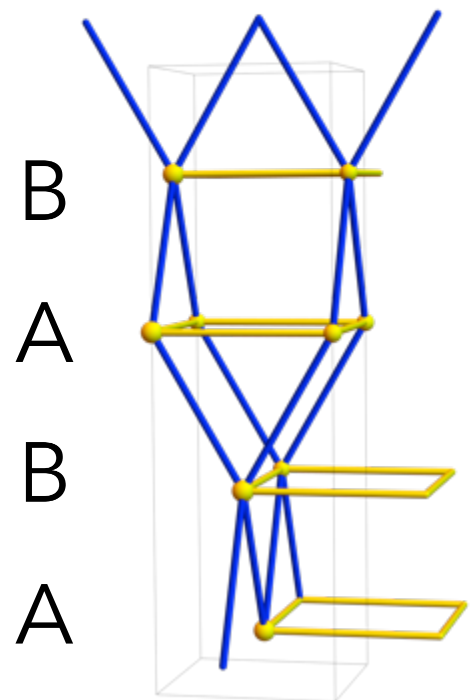
Symmetry

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

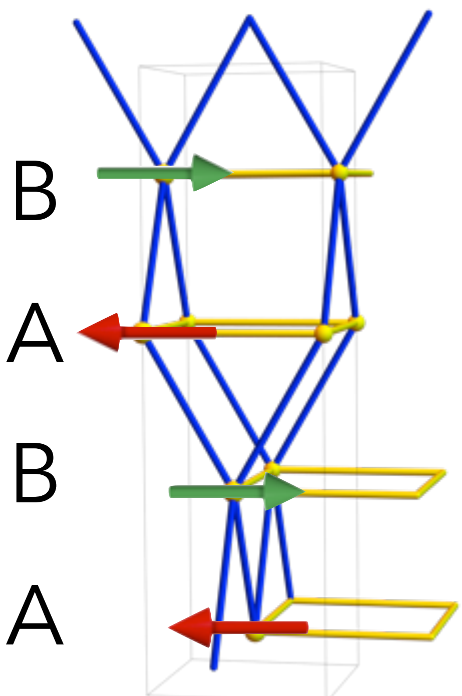


Two Ce sublattices

“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

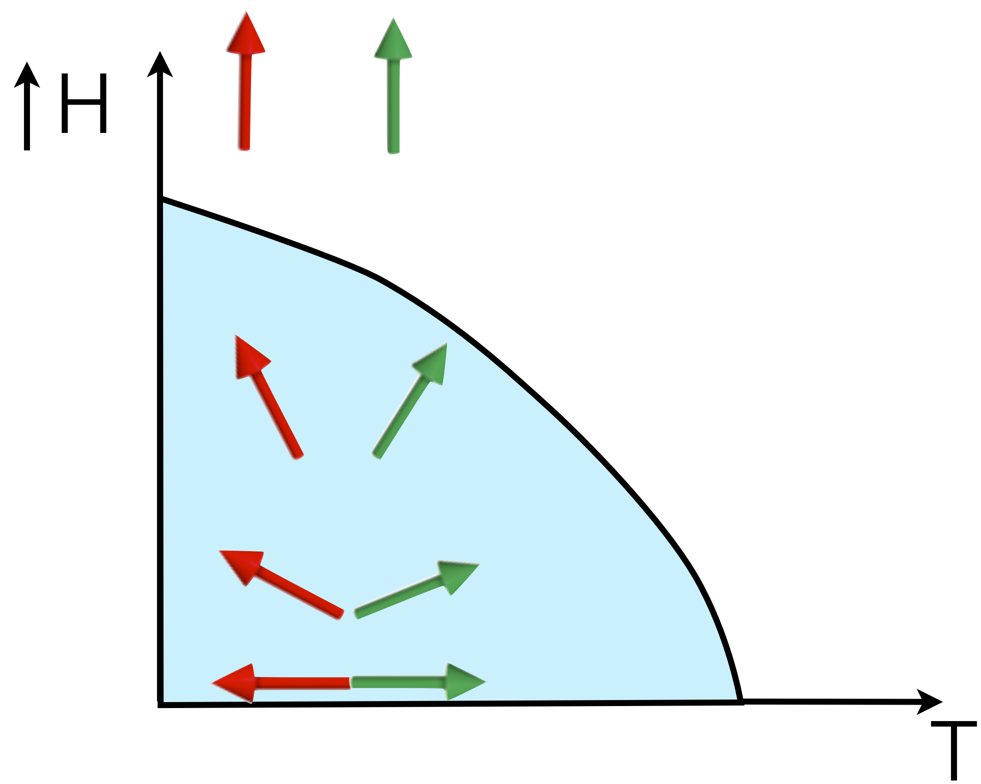
"intra-unit cell antiferromagnet"

$$E = J_{\perp}(S^x_{\mathrm{A}} S^x_{\mathrm{B}} + S^y_{\mathrm{A}} S^y_{\mathrm{B}}) + J_z S^z_{\mathrm{A}} S^z_{\mathrm{B}} + \sum_{\alpha} \left[D \left(S^z_{\alpha} \right)^2 \right.$$

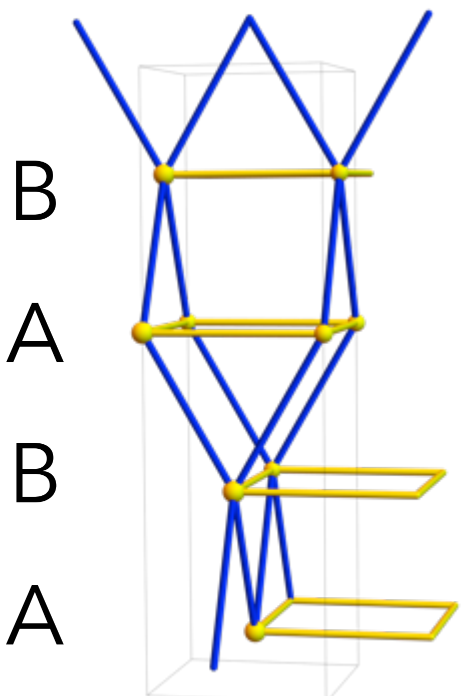
$2D > J_z - J_p$ → in-plane (XY) spins

Spin Flop

Standard
Heisenberg or XY
antiferromagnet



Minimal model



Two Ce sublattices

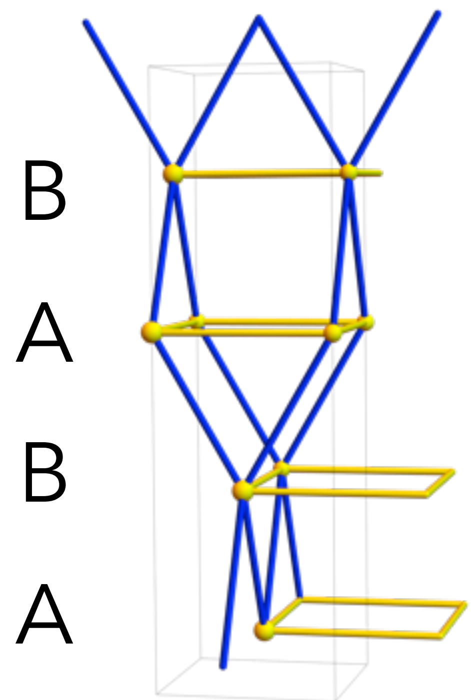
"intra-unit cell antiferromagnet"

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

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"

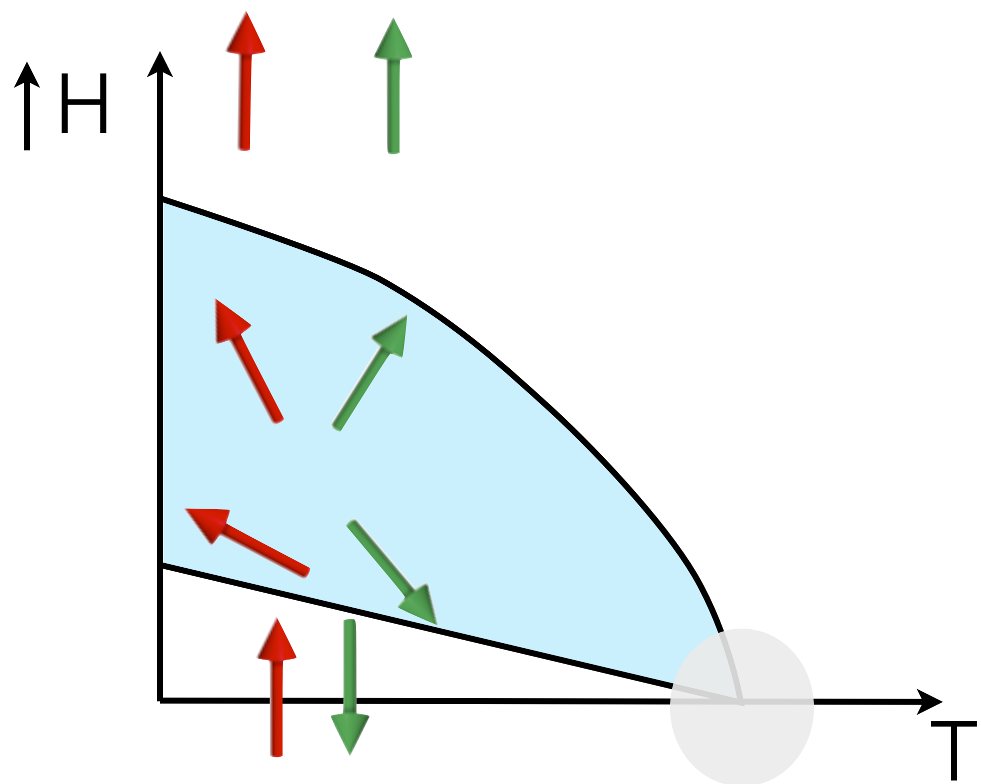
$$E = J_{\perp}(S_{\mathrm{A}}^{x}S_{\mathrm{B}}^{x} + S_{\mathrm{A}}^{y}S_{\mathrm{B}}^{y}) + J_{z}S_{\mathrm{A}}^{z}S_{\mathrm{B}}^{z} + \sum_{\alpha}\left[D\left(S_{\alpha}^{z}\right)^{2} - \mathbf{H}\cdot\mathbf{m}_{\alpha}\right],$$

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

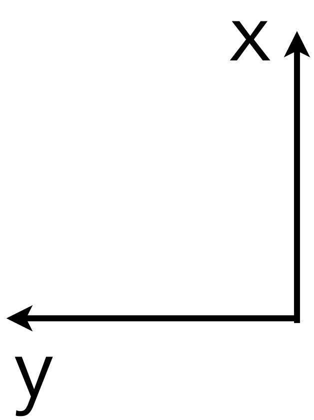
$$E = J_{\perp}(S_{A}^{x}S_{B}^{x} + S_{A}^{y}S_{B}^{y}) - H(g_{x}S_{A}^{x} + g_{y}S_{B}^{x})$$

Spin Flop

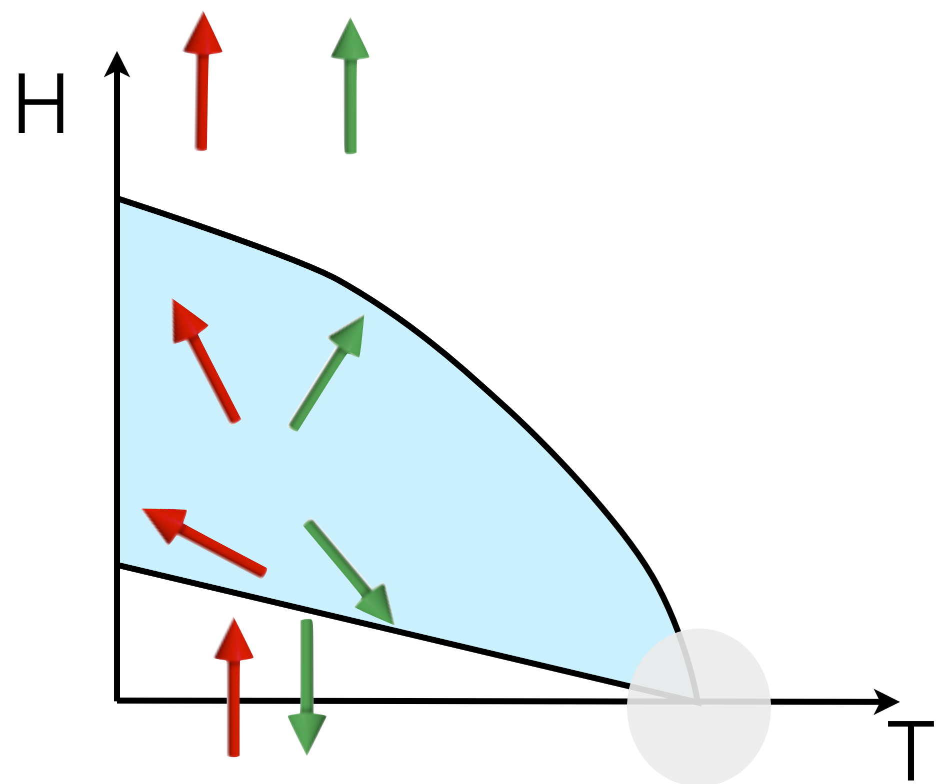
With g-factor anisotropy *and* H along (100)



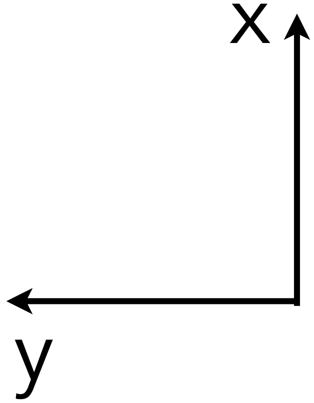
Spin Flop



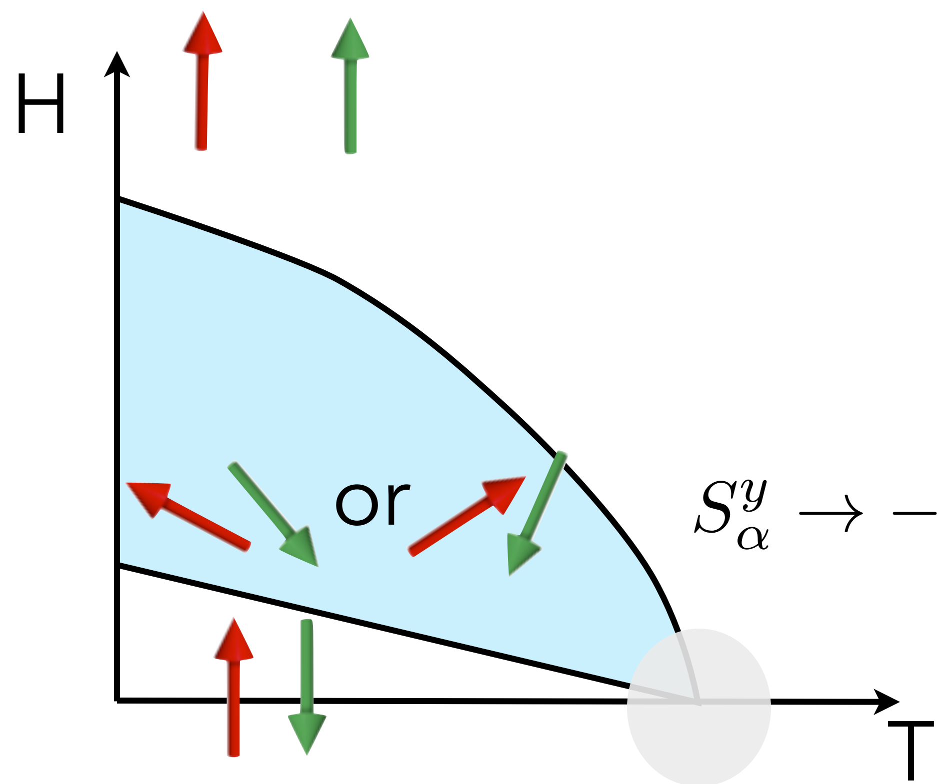
$m_{010} \times \mathrm{TR}$
broken



Domains

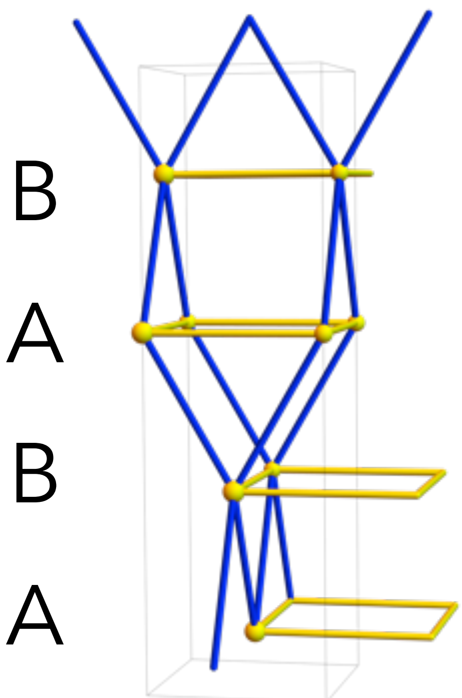


$m_{010} \times \mathrm{TR}$
broken



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

Minimal model



Two Ce sublattices

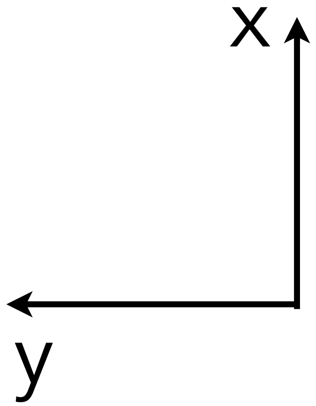
“intra-unit cell antiferromagnet”

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

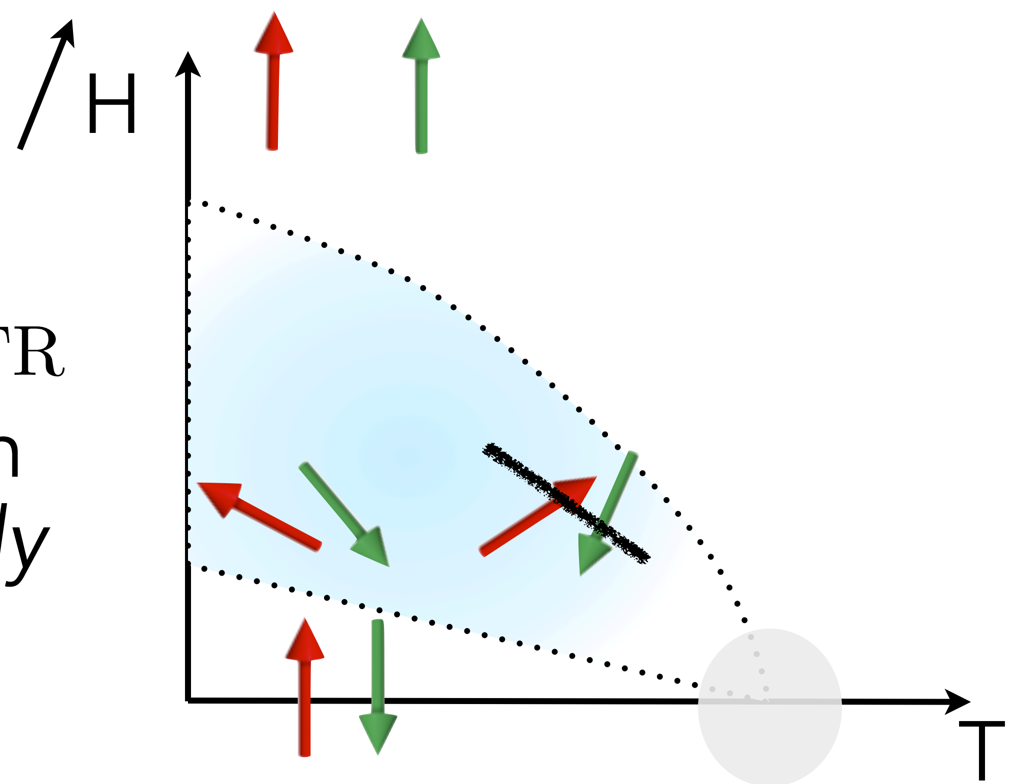
g-tensor anisotropy

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

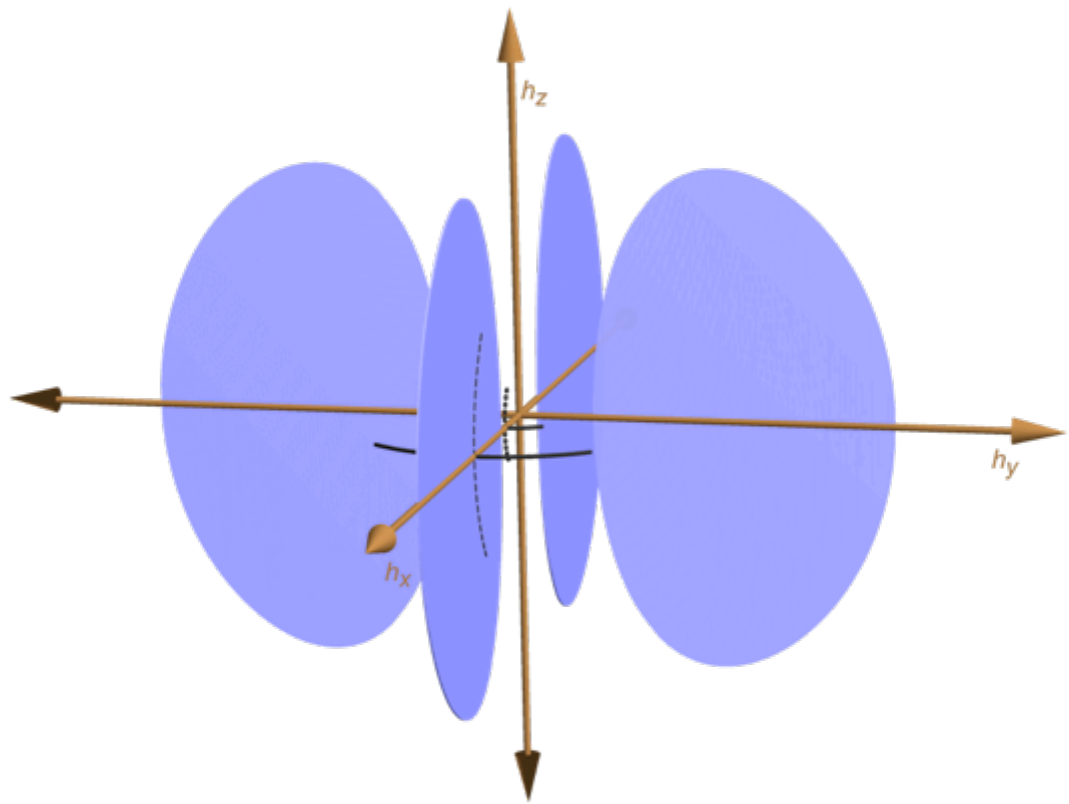
Domains



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

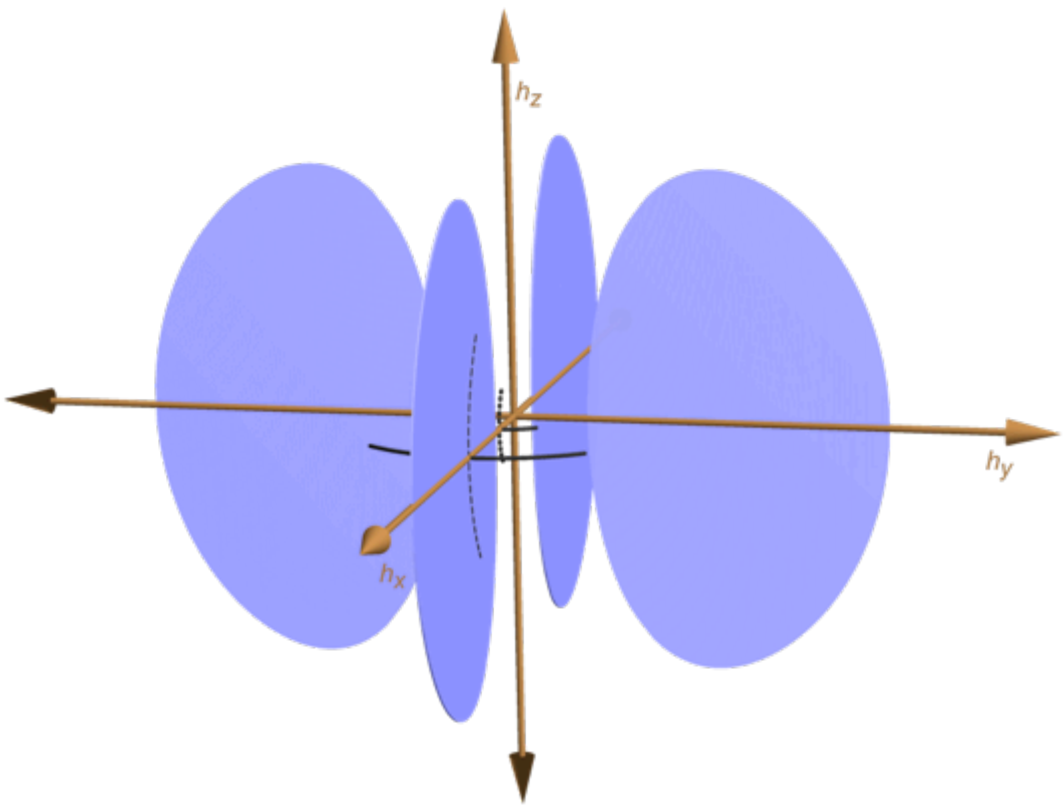


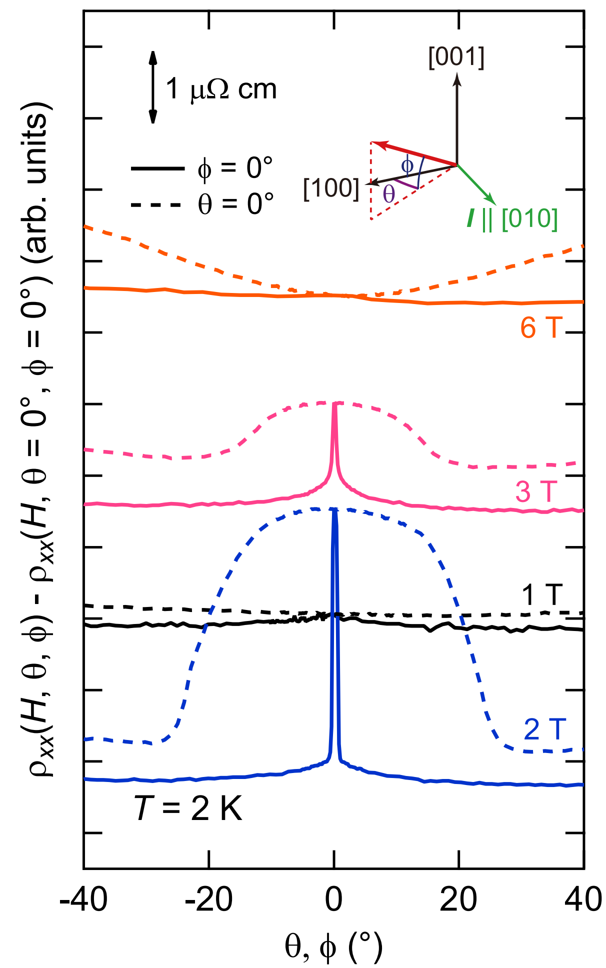
Phase diagram



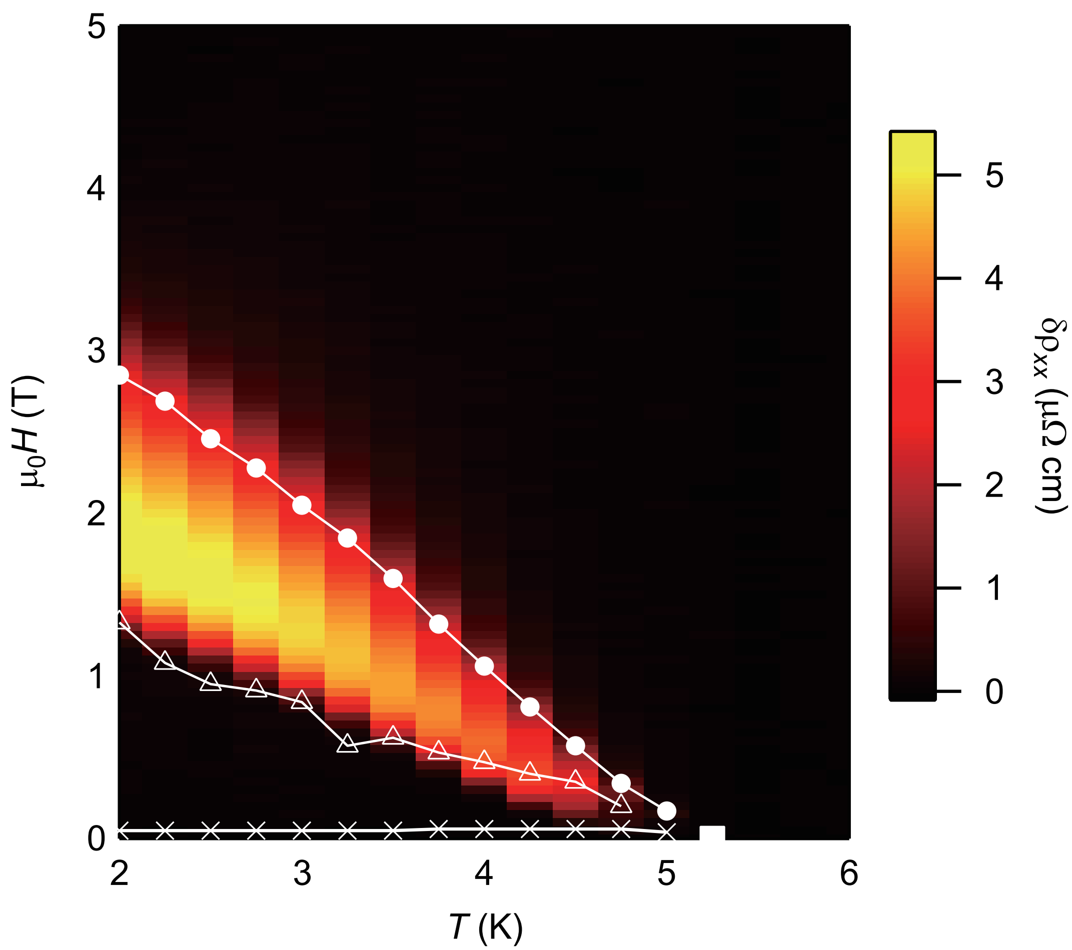
Canted phase forms 4 “infinitely thin” wedges

Phase diagram



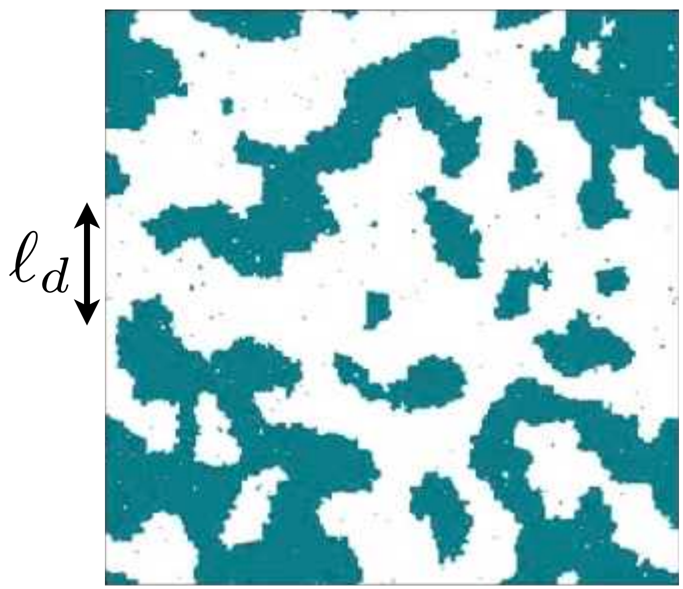


Phase Diagram



Resistivity

Extra resistance comes from *domain walls*



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

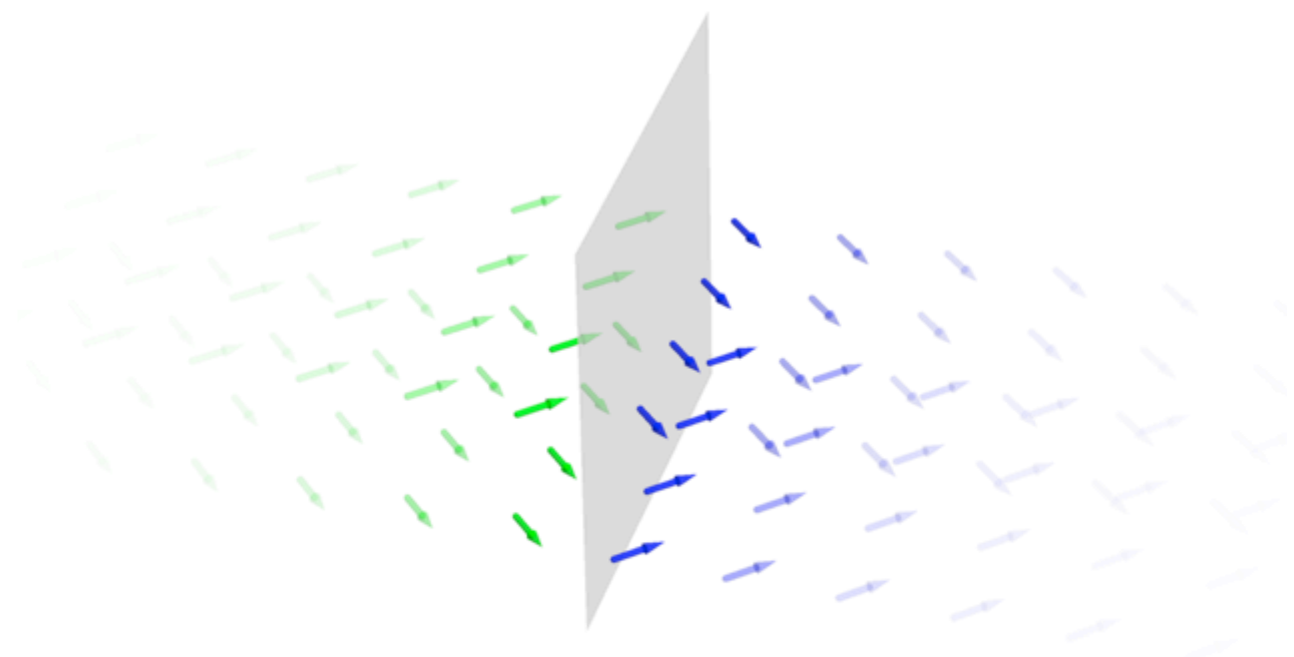
$$V_{\text{dw}} = \tilde{\rho}_{\text{dw}} j$$

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

Domain wall

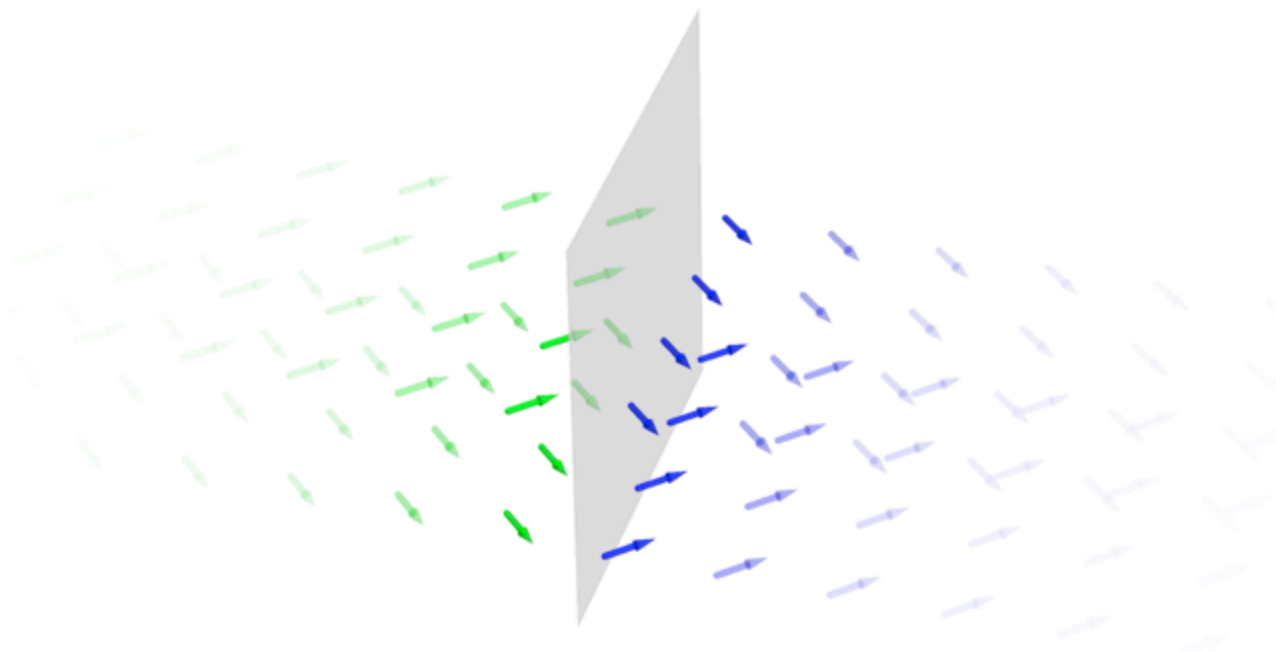
Strong anisotropy/Ising order:

narrow domain walls



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

Phase space



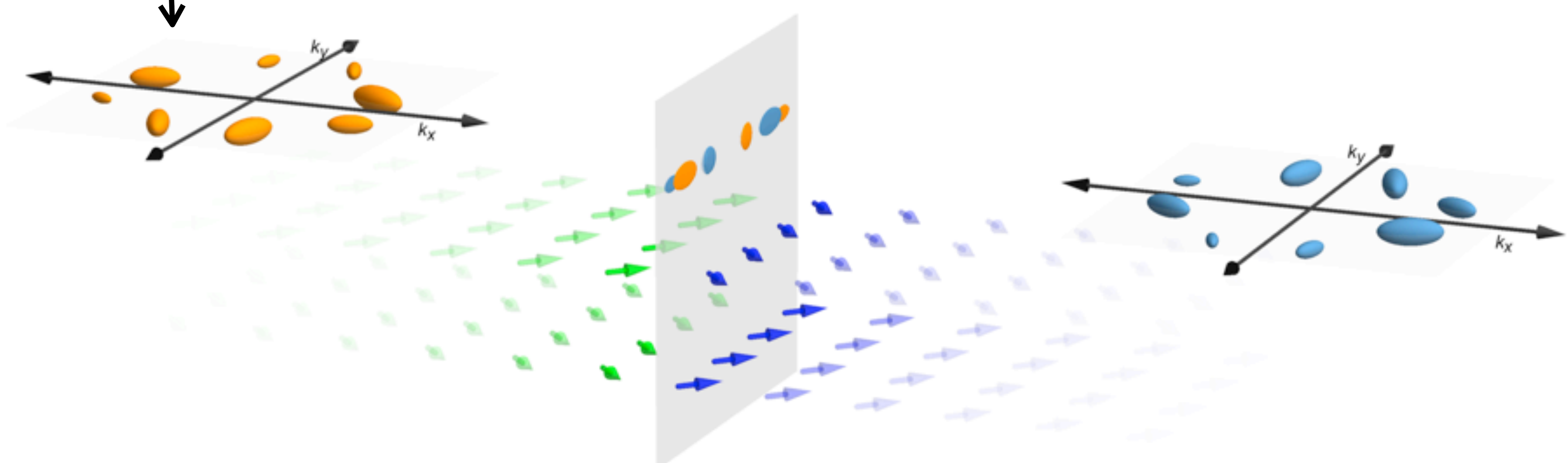
Landauer-Büttiker: one channel for each transverse momenta

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

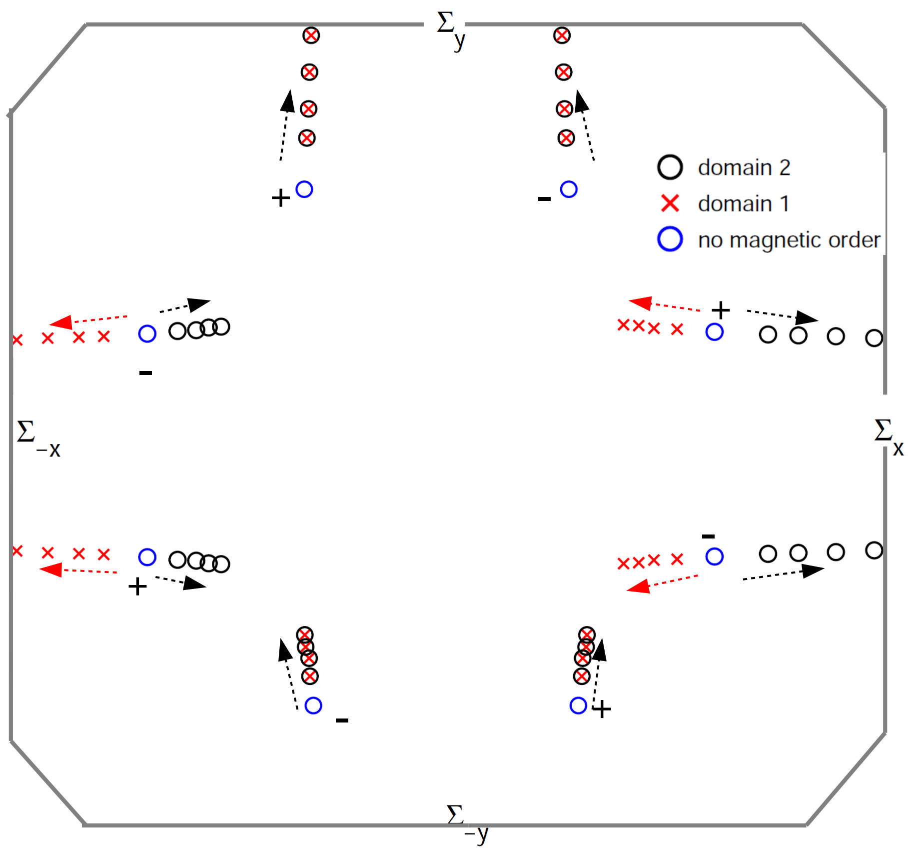
BUT sum only includes modes that exist at Fermi energy on both sides

Phase space

Fermi surfaces differ by m_{010} * TR



Weyl points

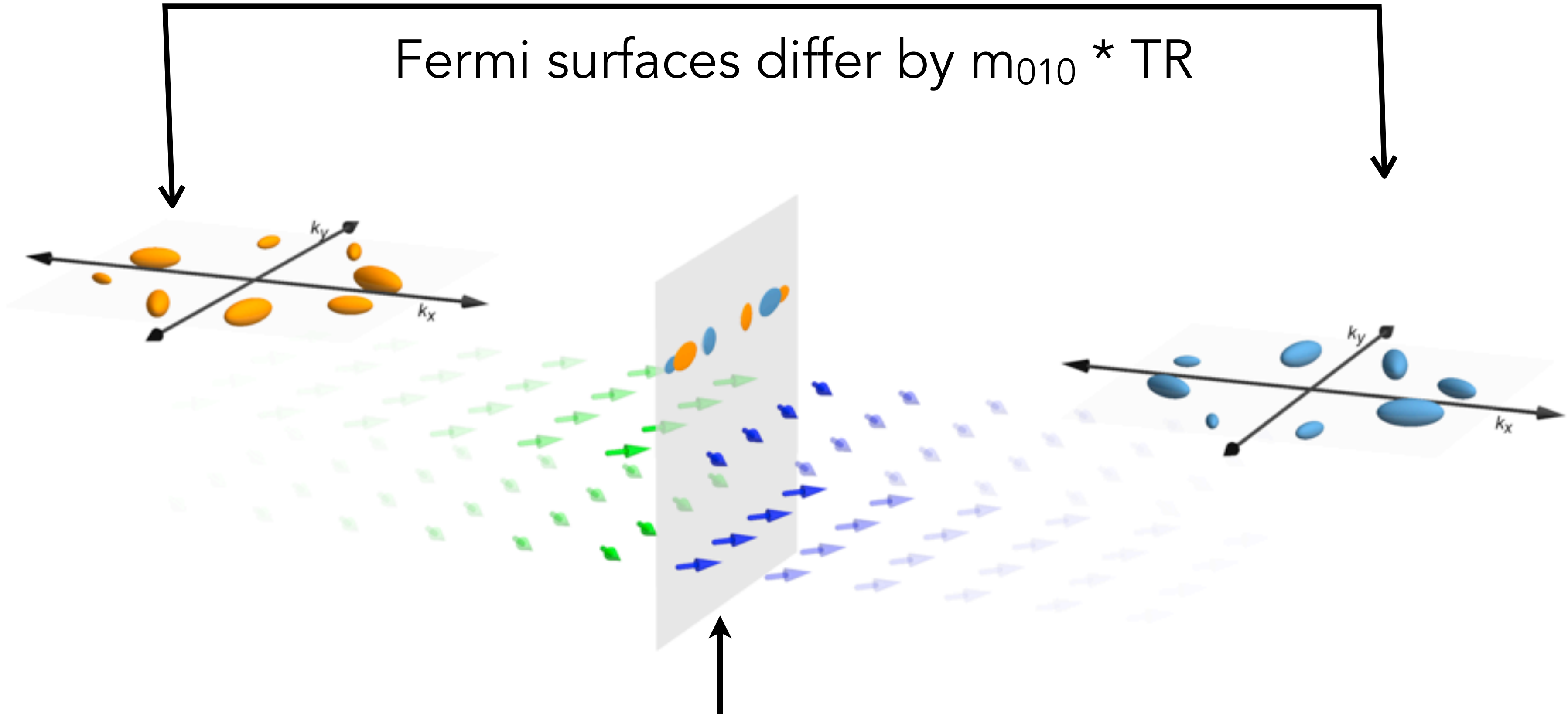


Low symmetry, SOC: Weyl point locations depend on domain

(from DFT-fit tight-binding model)

Phase space

Fermi surfaces differ by m_{010} * TR

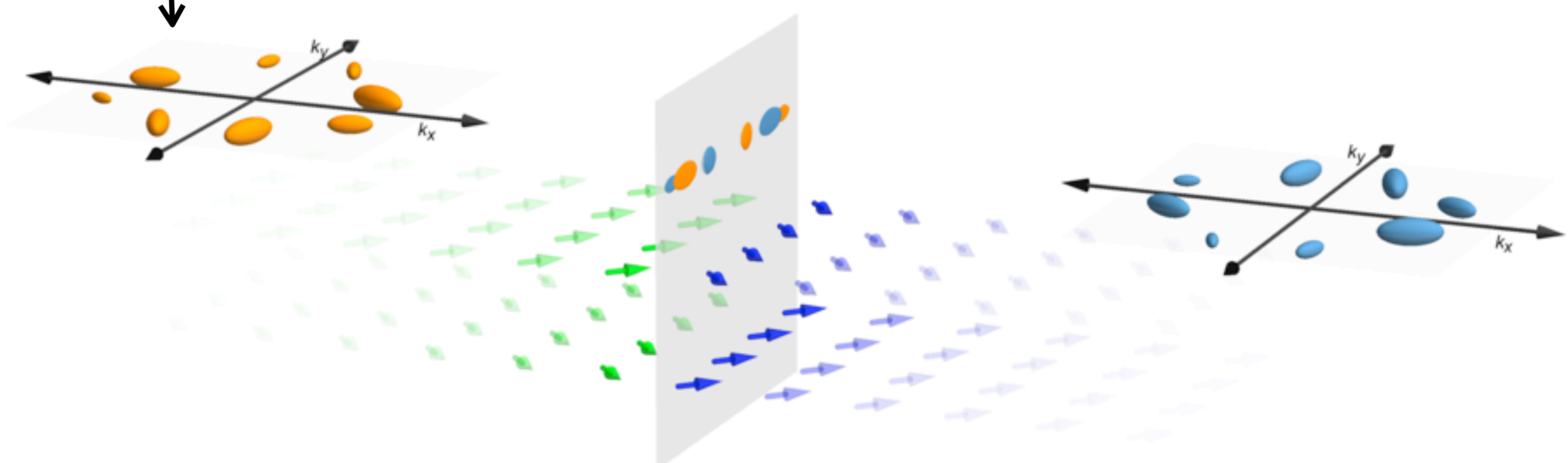


projection to interface BZ

Only overlapping portions contribute!

Phase space

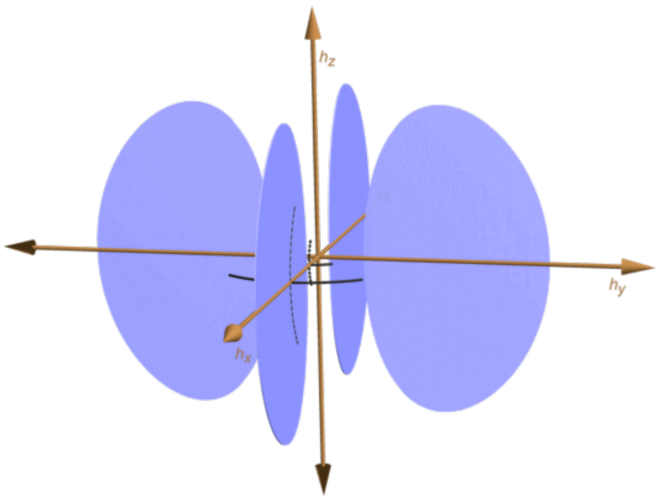
Fermi surfaces differ by m_{010} * TR

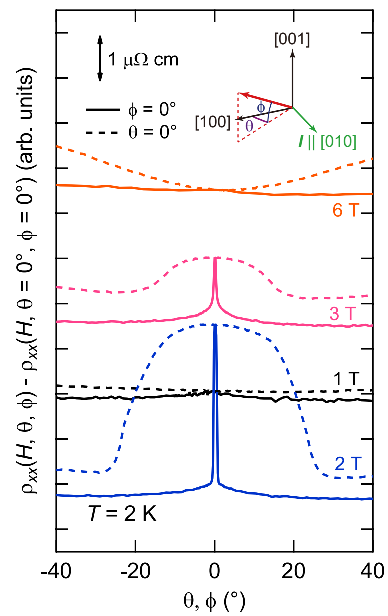


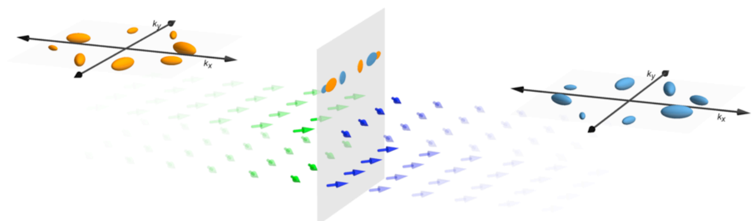
$$G = L^2 \frac{\mathcal{A}_{int}}{(2\pi)^2} T \frac{e^2}{h}$$

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

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?