

Overview and special topics in magnetism

J.Kübler

1. Spin density functional theory
2. Basic applications of SDFT: Curie T etc
3. The anomalous Hall effect (AHE) and topology

1. SDFT

- We need to write down a few definitions
- Operator for density

$$\hat{n}(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i)$$

- Density matrix: let

$$\Phi(r_1, r_2, \dots, r_N) \quad (r_i = \mathbf{r}_i, \sigma_i)$$

be the groundstate **wave function** of the N-particle system.

Then the density matrix is defined as follows:

$$\rho(r'_1, r'_2, \dots, r'_N | r_1, r_2, \dots, r_N) = \sum_{\ell=1}^n c_{\ell} \Phi_{\ell}(r'_1, \dots, r'_N) \Phi_{\ell}^*(r_1, \dots, r_N) ,$$

with $0 \leq c_{\ell} \leq 1$ and $\sum_{\ell} c_{\ell} = 1$.

n: degeneracy of state /

The electron density

is obtained from

$$n(\mathbf{r}) = \text{Tr} \langle \rho \hat{n}(\mathbf{r}) \rangle =$$
$$\sum_{\alpha=1}^2 \int dr_2 \dots dr_N \rho(\mathbf{r}\alpha, r_2, \dots, r_N | \mathbf{r}\alpha, r_2, \dots, r_N)$$

The spin density matrix

has elements $n_{\alpha\beta}(\mathbf{r})$ given by

$$n_{\alpha\beta}(\mathbf{r}) = N \int dr_2 \dots dr_N \rho(\mathbf{r}\alpha, r_2, \dots, r_N | \mathbf{r}\beta, r_2, \dots, r_N)$$

Definition:

$$\tilde{n}(\mathbf{r}) = \begin{pmatrix} n_{11}(\mathbf{r}) & n_{12}(\mathbf{r}) \\ n_{12}^*(\mathbf{r}) & n_{22}(\mathbf{r}) \end{pmatrix}$$

Density and magnetization

- Density

$$n(\mathbf{r}) = \text{Tr } \tilde{n}(\mathbf{r})$$

- Magnetization

$$\mathbf{m}(\mathbf{r}) = \text{Tr } \vec{\sigma} \tilde{n}(\mathbf{r}) ,$$

where components of $\vec{\sigma}$ are
Pauli spin matrices

Basic assertion:

The electronic structure is unambiguously determined by the density. We do not need to determine the wave function.

Hohenberg, Kohn, Kohn, Sham

The Kohn-Sham-Schrödinger equations

Consider the total energy

- Essential step: the total ground-state energy is a functional of the density matrix \tilde{n}

$$E[\tilde{n}] = F[\tilde{n}] + V^{\text{ext}}[\tilde{n}] ,$$

$$F[\tilde{n}] = T[\tilde{n}] + \iint \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' + E_{\text{xc}}[\tilde{n}] ,$$

$$V^{\text{ext}}[\tilde{n}] = \sum_{\alpha\beta} \int v_{\alpha\beta}^{\text{ext}}(\mathbf{r}) n_{\beta\alpha}(\mathbf{r}) d\mathbf{r} ,$$

$T[\tilde{n}]$ being the kinetic energy.

- Essential step : for any many-electron system the energy functional has a **minimum** equal to the ground-state energy at the ground-state density matrix.
- This step leads to a **variational principle** to approximate the total energy and the density matrix.
- The corresponding Euler–Lagrange equations are called the **Kohn-Sham** equations („effective single particle Schrödinger equations“).

Euler-Lagrange / Kohn-Sham Equations

- as

$$\sum_{\beta=1}^2 \left[-\delta_{\alpha\beta} \nabla^2 + v_{\alpha\beta}^{\text{eff}}(\mathbf{r}) - \varepsilon_i \delta_{\alpha\beta} \right] \psi_{i\beta}(\mathbf{r}) = 0$$

- Lagrange parameter ε_i and

$$v_{\alpha\beta}^{\text{eff}}(\mathbf{r}) = v_{\alpha\beta}^{\text{ext}}(\mathbf{r}) + 2\delta_{\alpha\beta} \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \frac{\delta E_{\text{xc}}}{\delta n_{\beta\alpha}(\mathbf{r})}$$

The local density approximation

- The gas of interacting electrons is used for exchange-correlation density, then

$$E_{xc} = \int d\mathbf{r} [ne_{xc}(n)]_{n=n(\mathbf{r})}$$

- whence

$$v_{\alpha}^{xc}(\mathbf{r}) = \frac{\delta E_{xc}}{\delta n_{\alpha}(\mathbf{r})} = \left[\frac{d}{dn_{\alpha}} ne_{xc}(n_{\uparrow}, n_{\downarrow}) \right]_{n=n(\mathbf{r})}$$

The self-consistency problem

- Solutions of the Kohn-Sham equations give the density matrix

$$n_{\alpha\beta}(\mathbf{r}) = \sum_{i=1}^N \psi_{i\beta}(\mathbf{r}) \psi_{i\alpha}^*(\mathbf{r})$$

- which determines the effective potential
- More -- we diagonalize the density matrix:

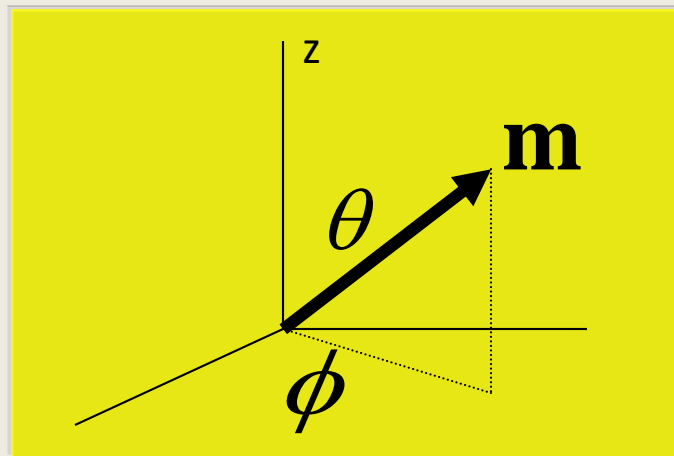
Diagonalize the density matrix

- Choose spin-1/2 rotation matrix to do the job:

$$U\tilde{n}U^+ = \begin{pmatrix} n_{\uparrow} & 0 \\ 0 & n_{\downarrow} \end{pmatrix}$$

Spin rotation matrix defines the directions of magnetic moments

$$U = \begin{pmatrix} \exp\left(\frac{i\phi}{2}\right) \cos \frac{\theta}{2} & \exp\left(\frac{-i\phi}{2}\right) \sin \frac{\theta}{2} \\ -\exp\left(\frac{i\phi}{2}\right) \sin \frac{\theta}{2} & \exp\left(\frac{-i\phi}{2}\right) \cos \frac{\theta}{2} \end{pmatrix}$$



Global vs. local frame of reference

- Kohn-Sham equations in **global** frame

$$(-\hbar^2 \nabla^2 + \mathbf{v}^{\text{eff}}) \psi_i = \varepsilon_i \psi_i$$

- Potential

$$\mathbf{v}^{\text{eff}}(\mathbf{r}) = \sum_{n\nu} U^+(\theta_\nu, \phi_\nu) \begin{pmatrix} v^{\text{eff}}_{\uparrow\nu}(\mathbf{r}_{n\nu}) & 0 \\ 0 & v^{\text{eff}}_{\downarrow\nu}(\mathbf{r}_{n\nu}) \end{pmatrix} U(\theta_\nu, \phi_\nu)$$

$$\mathbf{r}_{n\nu} = \mathbf{r} - \mathbf{R}_n - \vec{\tau}_\nu$$

2. Basic applications of the SDF approximation to the problem of magnetism in solids

Theory of Itinerant Electron Magnetism, Oxford University Press, 2009

Magnetic Susceptibility

- Assume magnetic field ΔB . It induces magnetization Δm and leads to
- change of exchange correlation potential = effective increase of applied field:

Enhanced magnetic susceptibility, I :

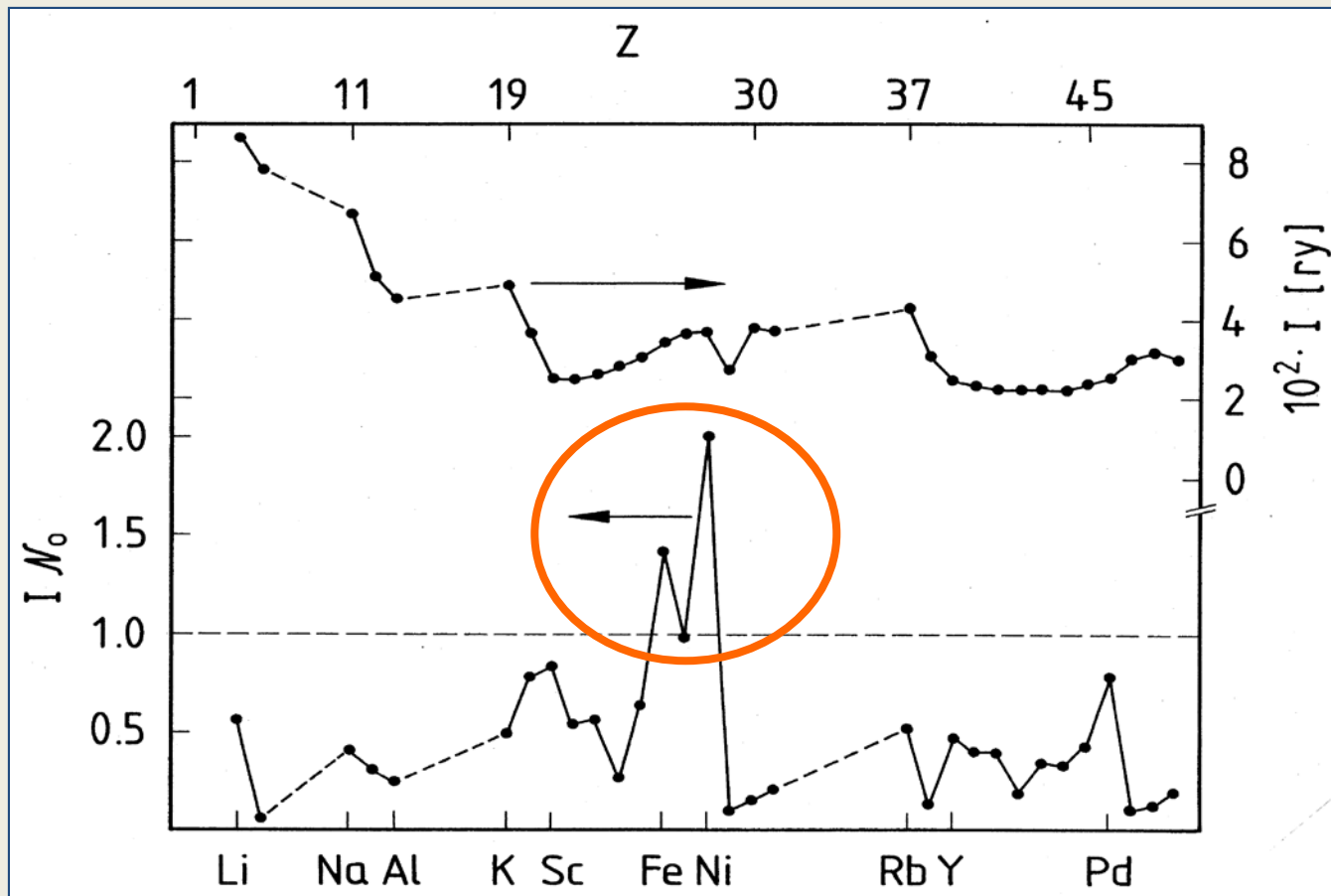
Stoner exchange const.

$$\Delta m = \chi_0 \Delta B + \chi_0 I \Delta m$$

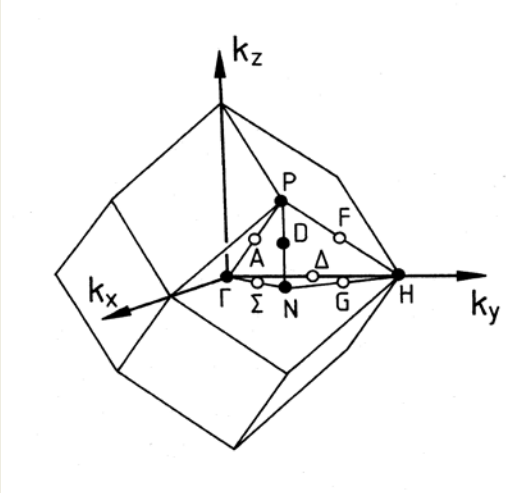
$$(1 - \chi_0 I) \Delta m = \chi_0 \Delta B$$

$$\therefore \chi = \frac{\chi_0}{1 - \chi_0 I}$$

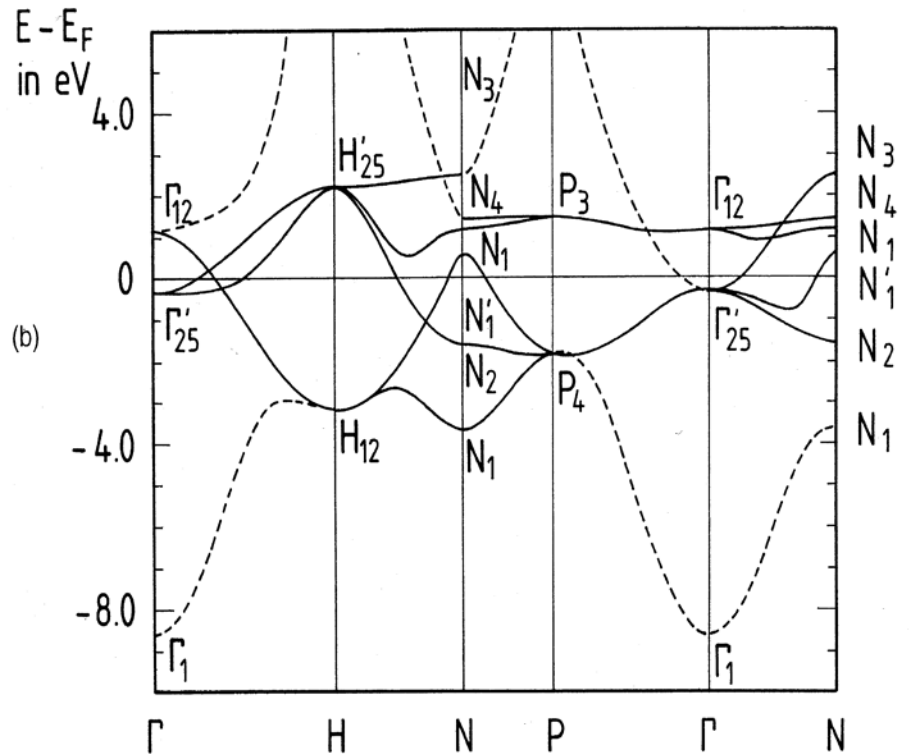
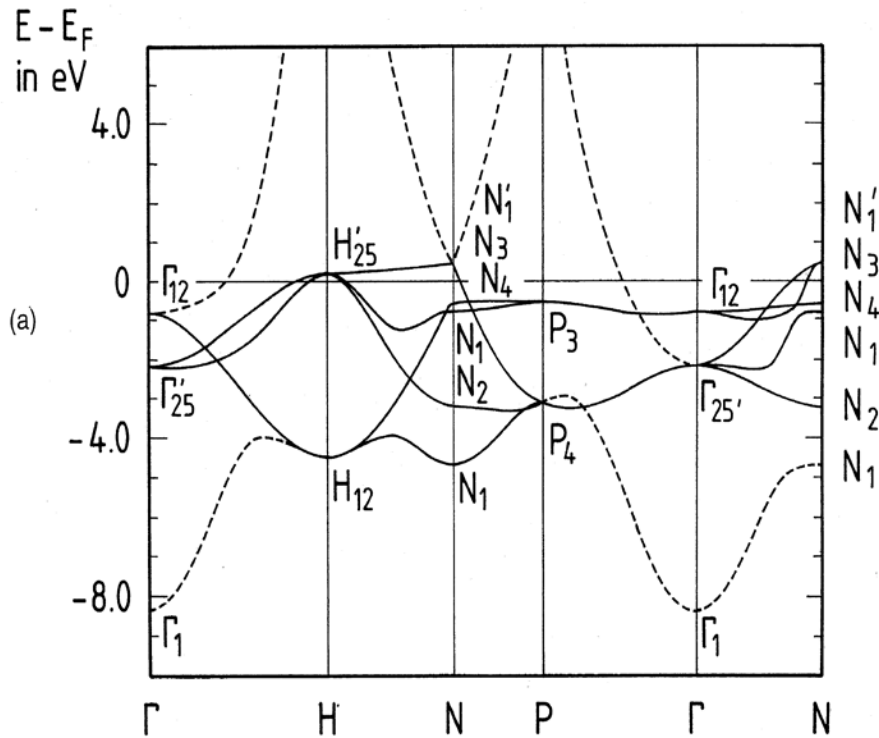
Linear response theory for susceptibility



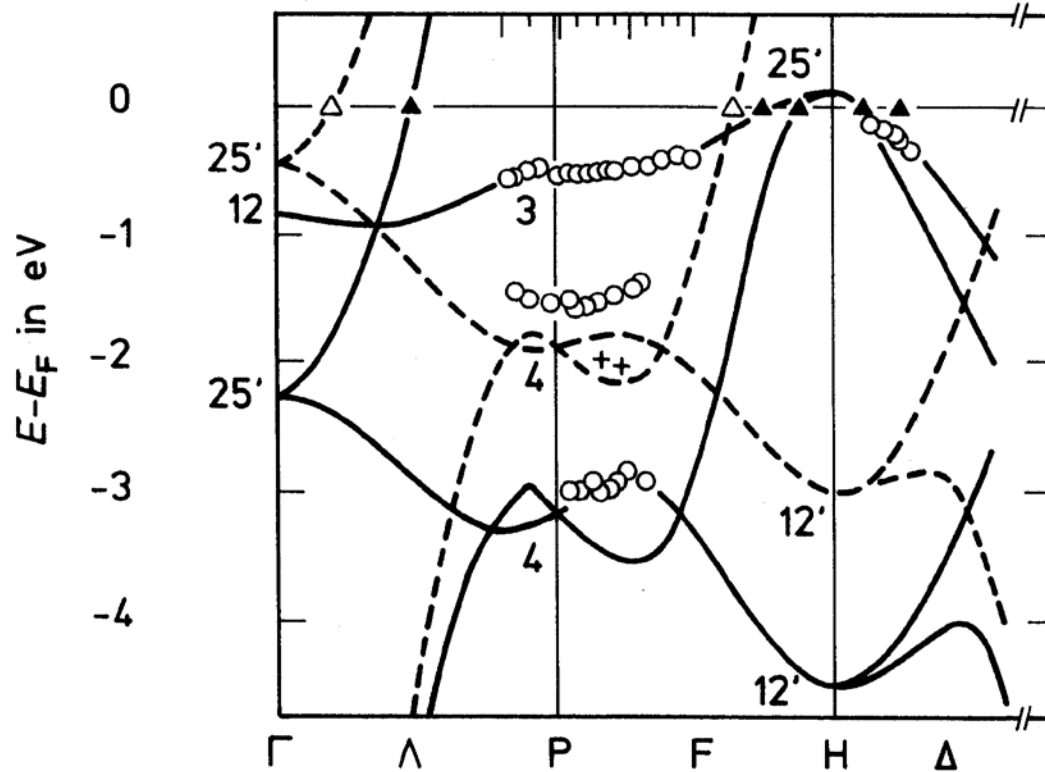
Iron
spin \uparrow



Iron
spin \downarrow



Energy eigenvalues



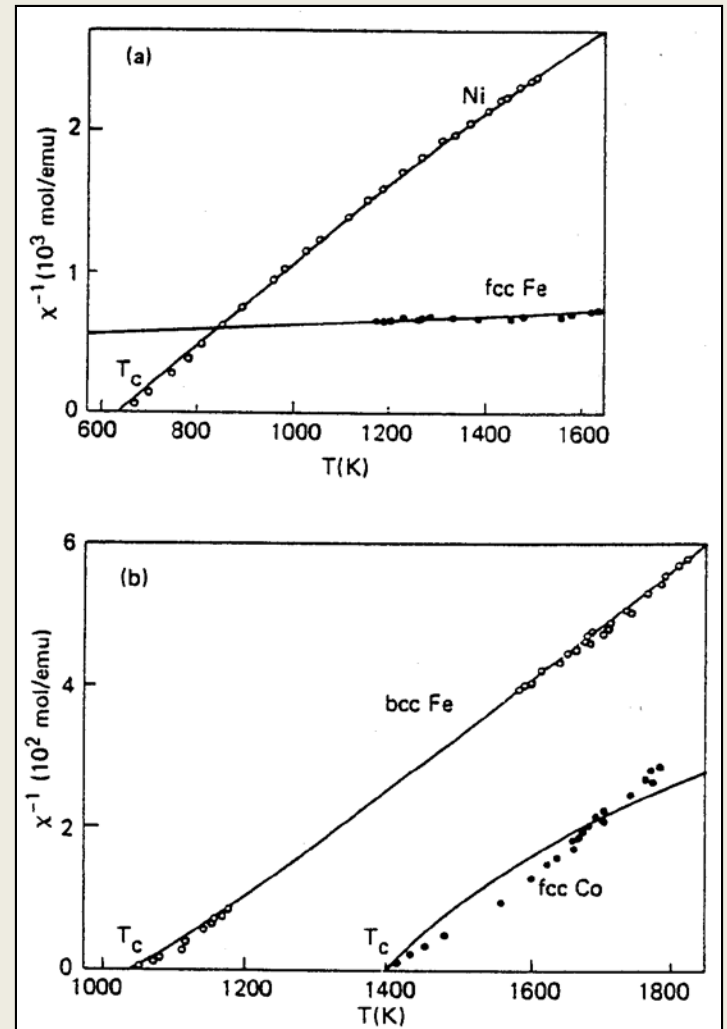
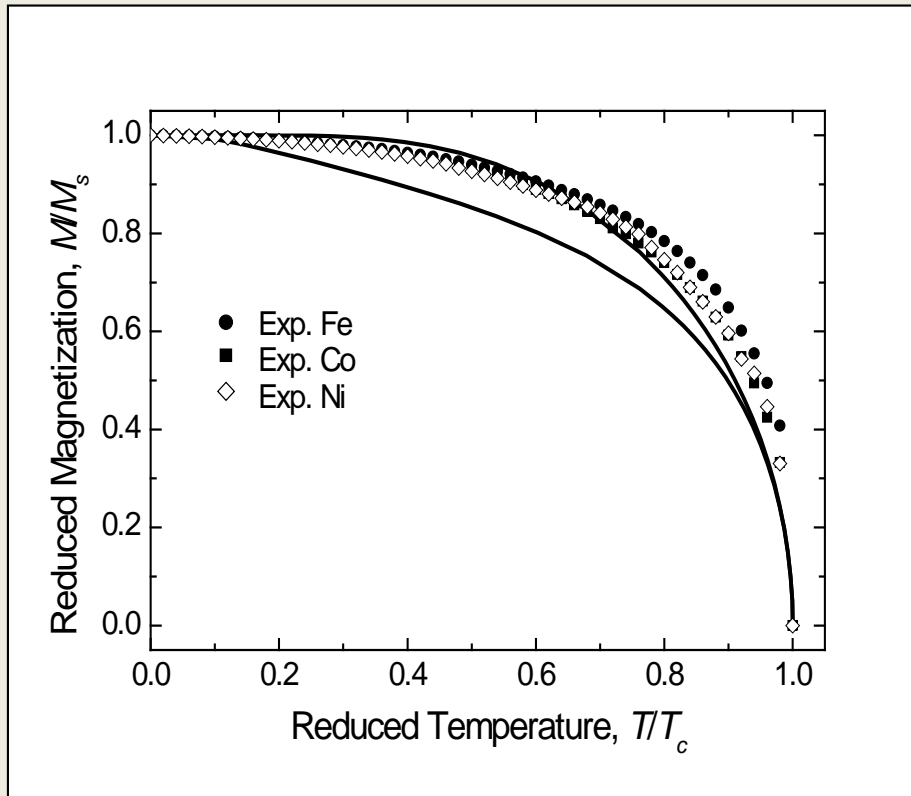
bcc-Fe

Angle-resolved photoemission,
Eastman et al (1979)

Thermodynamics

Curie-Weiss susceptibilities

Order parameter



The Classical Heisenberg Hamiltonian

$$H_{mag} = -\sum_{ij} J_{ij} \vec{\sigma}_i \cdot \vec{\sigma}_j + \dots$$

J_{ij} are the exchange interaction parameters (the energy of changing from parallel to antiparallel alignment of spins in i and j sites).

There are several ways to obtain J_{ij} from ab initio calculations.
(A. Lichtenstein, M. Katsnelson, 1984) (JK 2009)

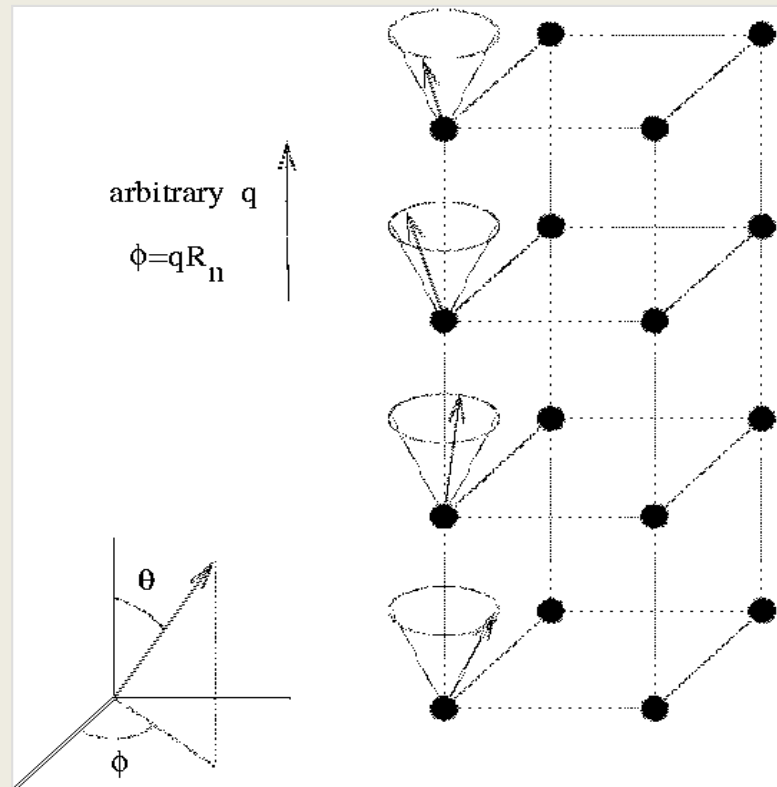
A useful non-collinear moment arrangement

Spinspiral

$$\mathbf{M}_n = M [\cos(\mathbf{q} \cdot \mathbf{R}_n) \sin \theta, \sin(\mathbf{q} \cdot \mathbf{R}_n) \sin \theta, \cos \theta]$$

Consider symmetry
(Sandratskii, Herring)

Optain from total energy
differences $j(\mathbf{q})$



The determination of $j(\mathbf{q})$ is simple for elementary ferromagnets such as Fe, Co and Ni, but is somewhat involved for compounds.

For the former:

$$\Delta E = M^2 \sin^2 \theta j(\mathbf{q}) \doteq \Delta E(\mathbf{q}, \theta) ,$$

Spin-wave dispersion relation

$$\omega(\mathbf{q}) = \lim_{\theta \rightarrow 0} \frac{4}{M} \frac{\Delta E(\mathbf{q}, \theta)}{\sin^2 \theta} .$$

Mean-field theory

$$\mathcal{H} = \sum'_{i,j} M^2 J_{ij} \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j ,$$

$$\langle \mathcal{H} \rangle_0 = \sum'_{i,j} M^2 J_{ij} m_i m_j$$

„Molecular“ or „mean field“

$$h_i = - \frac{\partial \langle \mathcal{H} \rangle_0}{\partial m_i} ,$$

$$h = 2M^2 m \sum_{\mathbf{q}} j(\mathbf{q}) .$$

$$\chi(T) = \frac{1}{3k_{\text{B}}T - 2M^2 \sum_{\mathbf{q}} j(\mathbf{q})} .$$

Mean-field approximation for Curie Temperature

$$k_{\text{B}}T_c = \frac{2}{3} \sum_{\mathbf{q}} M^2 j(\mathbf{q}) .$$

Quality of mean-field approximation

	bcc Fe	fcc Co	fcc Ni
$\sum_{\mathbf{q}} M^2 j(\mathbf{q})$ [mRy]	12.5	14.8	6.1
T_{Lang} [K]	1316	1558	642
T_c [K]	1044	1388	627

Mean-field Curie temperature



$$k_{\text{B}}T_c = \frac{2}{3} \sum_{\mathbf{q}} M^2 j(\mathbf{q}) .$$

Quick fix:

$$k_{\text{B}}T_c = \frac{2}{3} \sum_{\tau} \mathcal{L}_{\tau}^2 \left[\sum_{\mathbf{k}n} \frac{1}{j_n(\mathbf{k})} \right]^{-1} .$$

So-called spherical approximation

To derive the quick fix one can use

the **partition** function
proposed by Moriya

and

the spherical approximation, also as
proposed by Moriya

Partition function

$$\exp(-F / k_B T) = \int dL^2 \int \prod_{\mathbf{q}} d\mathbf{M}_{\mathbf{q}} \exp[-\Psi(M, L^2, \mathbf{M}_{\mathbf{q}}) / k_B T]$$

L^2 Length of magnetic moment

$\mathbf{M}_{\mathbf{q}}$ Fluctuation vector $\mathbf{M}_{\mathbf{q}} = (m_{x\mathbf{q}}, m_{y\mathbf{q}}, m_{z\mathbf{q}})$

M Order parameter (magnetization)

Functional details

Functional Ψ

$$\Psi = \sum_{\mathbf{q}} j(L^2, \mathbf{q}) |\mathbf{M}_{\mathbf{q}}|^2 + E(M, L^2)$$

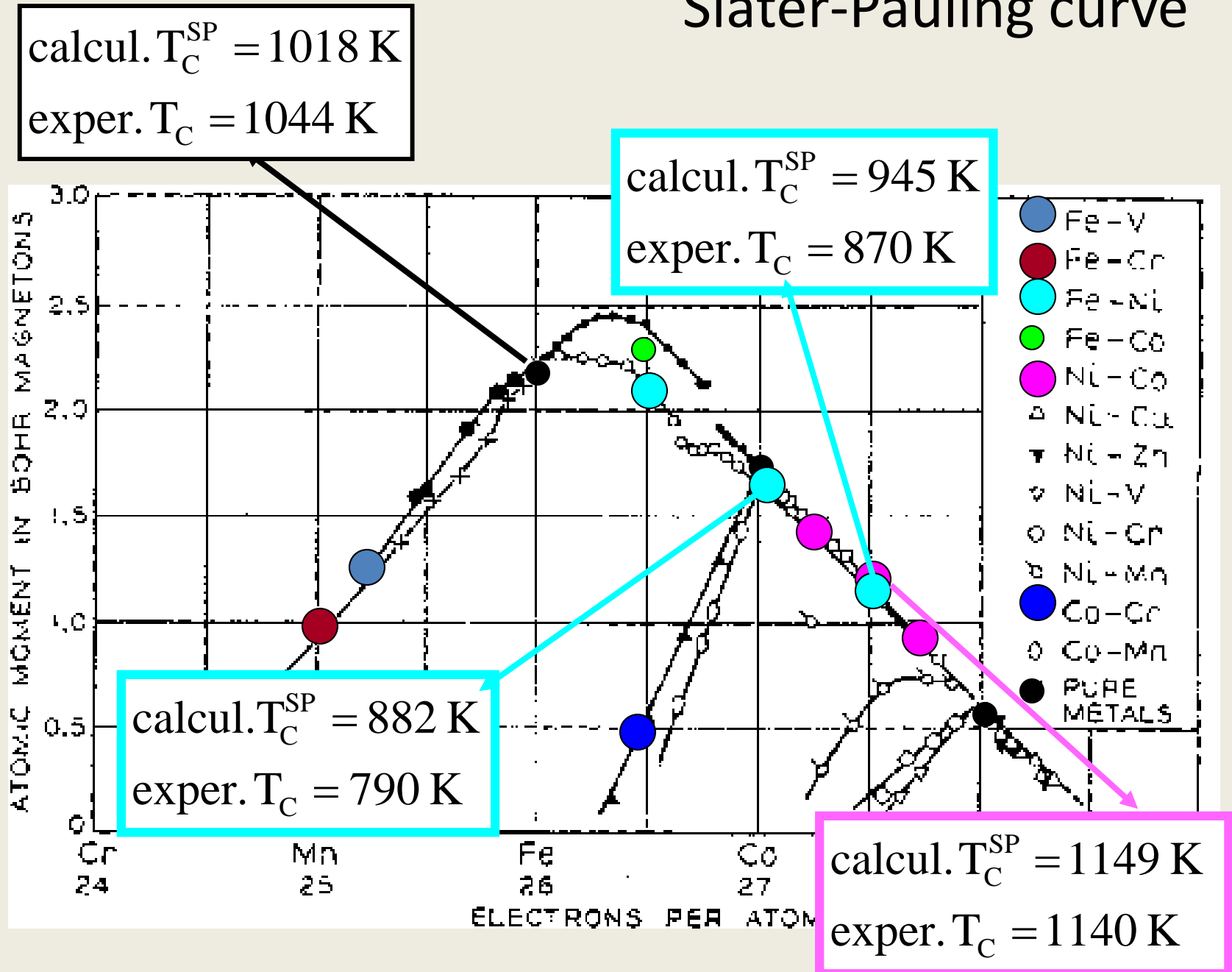
$$+ \sum_{\alpha=1}^3 \lambda_{\alpha} (L_{\alpha}^2 + \delta_{\alpha z} M^2 - \sum_{\mathbf{q}} |m_{\alpha\mathbf{q}}|^2)$$

Lagrange multiplier -> spherical approximation

A Usefull formula derivable from
Moriya's theory in the spherical approximation
Also called RPA

$$k_{\text{B}}T_{\text{C}} = \frac{2}{3} \sum_{\tau} L_{\tau}^2 \left[\frac{1}{N} \sum_{\mathbf{q}} \sum_n \frac{1}{j_n(\mathbf{q})} \right]^{-1}$$

Slater-Pauling curve



Another example: and application for Heusler compounds

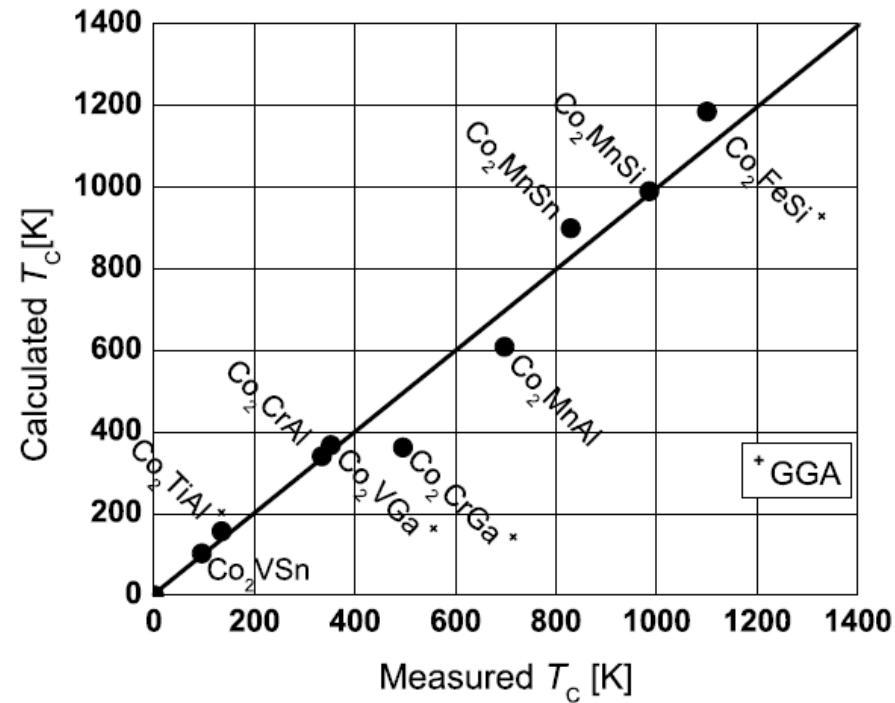


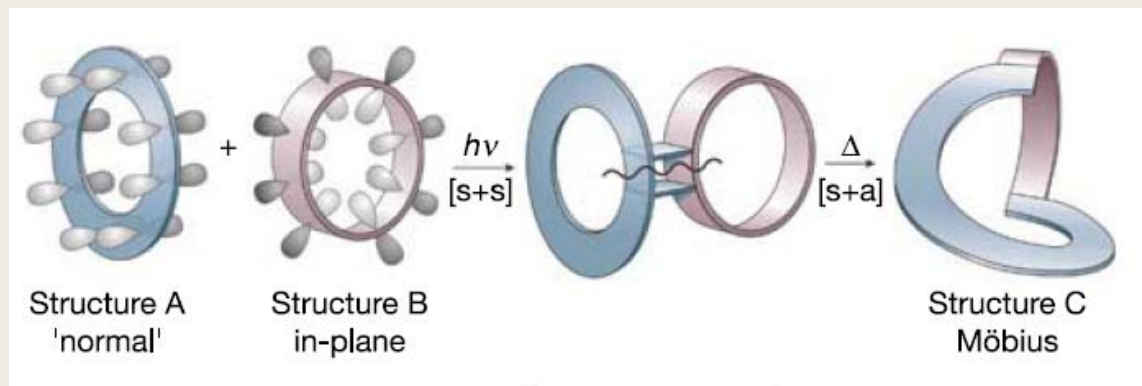
FIG. 5.17. Calculated versus measured Curie temperatures of a collection of Co_2 -Heusler compounds. For the calculations the spherical approximation was used. From Kübler *et al.* (2007).

The topics that now follow are not
contained in my book

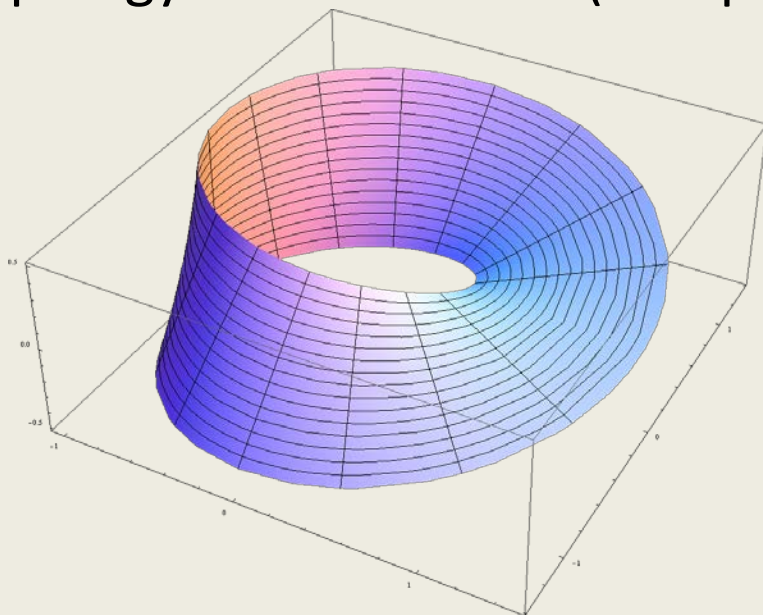
3. The anomalous Hall effect (AHE)

Topology

Topology in chemistry, example from Ajami et al. Nature 426, 819 (2003)



Topology from textbook (Wikipedia): Möbius strip



Topology in real space

- The Berry connection

Insulators

- The Berry curvature

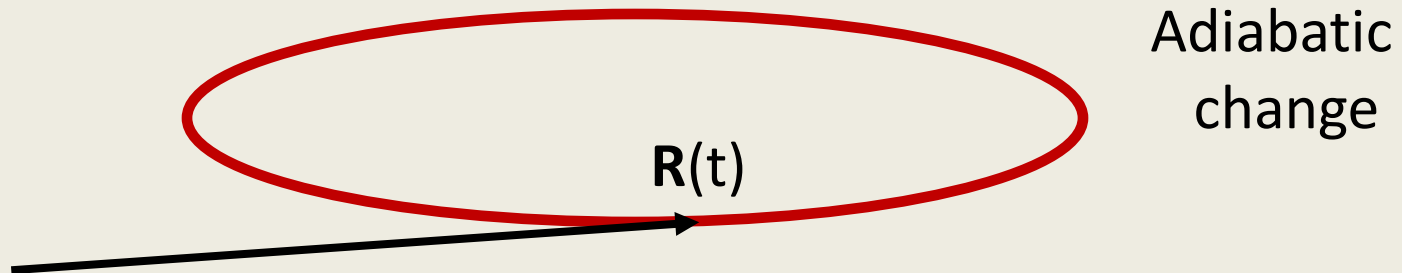
Metals

Topological properties

Berry phase

Proc. Roy. Soc. A 392 (1984) 45

Parameter space



$$H(\mathbf{R}) \dot{\psi}(t) = i \dot{\psi}(t)$$

$$H(\mathbf{R}) |n(\mathbf{R})\rangle = E_n(\mathbf{R}) |n(\mathbf{R})\rangle$$

Berry phase

Proc. Roy. Soc. A 392 (1984) 45

Parameter space



$$H(\mathbf{R}) \dot{\psi}(t) = i \dot{\psi}(t)$$

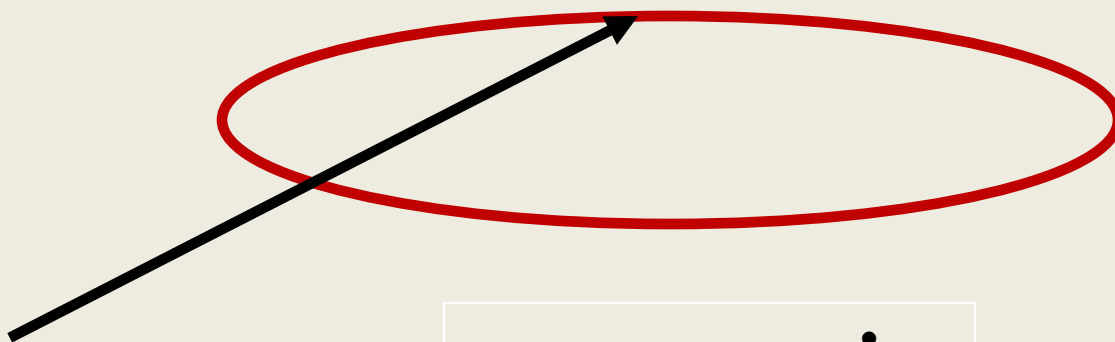
$$H(\mathbf{R}) |n(\mathbf{R})\rangle = E_n(\mathbf{R}) |n(\mathbf{R})\rangle$$

Berry phase

Proc. Roy. Soc. A 392 (1984) 45

Parameter space

$\mathbf{R}(t)$



Adiabatic
change

$$H(\mathbf{R}) \psi(t) = i \dot{\psi}(t)$$

$$H(\mathbf{R}) |n(\mathbf{R})\rangle = E_n(\mathbf{R}) |n(\mathbf{R})\rangle$$

Time development:

$$\psi(t) = e^{\left[-i \int_0^t E_n(\mathbf{R}(t')) dt' \right]} e^{[i\gamma_n(t)]} |n(\mathbf{R})\rangle$$

Dynamical phase

Berry's geometrical phase

*Substitute into time-dependent
Schrödinger equation*

$$\frac{d}{dt}\gamma(t) = i\langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle \frac{d}{dt} \mathbf{R}(t)$$

Going around the circuit C

$$\gamma(C) = i \oint \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle d\mathbf{R}$$



Called Berry phase

Specify parameter space

Density functional theory:
Single-particle Schrödinger
equation

$$\left[\frac{p^2}{2m} + V_{eff} \right] \psi_n = E_n \psi_n$$

for crystal periodic systems

$$\psi_n(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} u_n(\mathbf{r}) \quad \longrightarrow$$

$$\left[\frac{(\mathbf{p} + \mathbf{k})^2}{2m} + V_{eff}(\mathbf{r}) \right] u_{n\mathbf{k}}(\mathbf{r}) = E_{n\mathbf{k}} u_{n\mathbf{k}}(\mathbf{r})$$

$$\gamma_n(C) = i \oint \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle d\mathbf{k}$$

Berry connection

$$\mathbf{A}(\mathbf{k}) = i \sum_{n \text{ occup}} \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle$$

Physics?

The connection of the polarization
with the Berry connection
is the origin
of the modern theory
for the macroscopic electric polarization

King-Smith, Vanderbilt and
Resta (RMP 66, 899 (1994))

Overview:

Di Xiao, M-C. Chang, Q. Niu: Rev. Mod. Phys.
82,1959 (2010)

The derivation starts with the Kubo
formula and uses the idea that the
polarization originates from an
adiabatic current flow

Details: another talk

From the Berry phase to the Berry curvature

The Hall effect

$$\rho_{xy} = R_0 H_z + R_S M_z$$



Hall resistivity



Anomalous Hall effect

The new discovery is an added term to the velocity
obtained by optimizing (Euler –Lagrange) a wave package

$$\dot{\mathbf{r}} = \mathbf{v}(\mathbf{k}) = \frac{\partial \varepsilon(\mathbf{k})}{\hbar \partial \mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k})$$

so that with the equation

$$\hbar \dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B}$$

we get a Hall effect without a magnetic field \mathbf{B}

$$\mathbf{v}(\mathbf{k}) = \frac{\partial \varepsilon(\mathbf{k})}{\hbar \partial \mathbf{k}} + \frac{e}{\hbar} \mathbf{E} \times \boldsymbol{\Omega}(\mathbf{k})$$

$$\sigma_{xy} = -\frac{e^2}{\hbar} \frac{1}{V} \sum_{(B.Z.)} \Omega(\mathbf{k})_z f(\mathbf{k})$$

$$\boldsymbol{\Omega}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}(\mathbf{k})$$

Berry curvature

Di Xiao et al. Rev. Mod. Phys. 82, 1959 (2010)

From Gradhand *et al.*
J. Phys. CM 24, 213212
(2012)

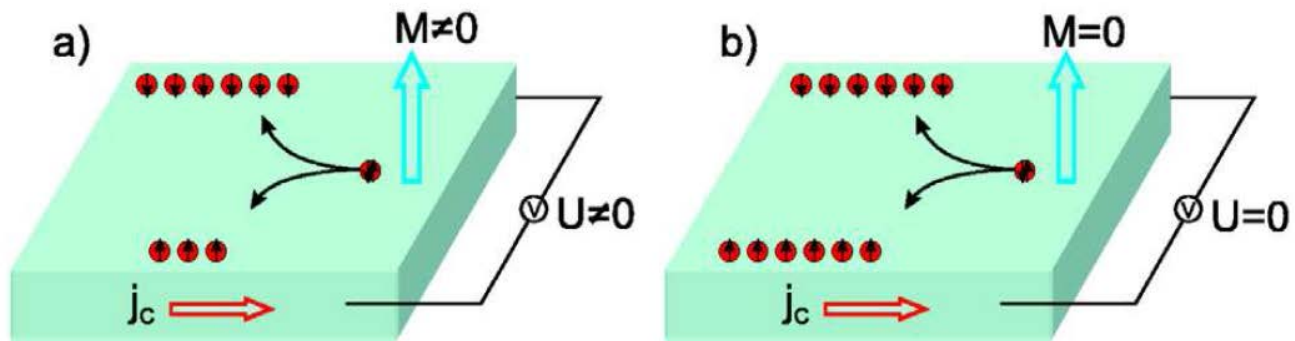


Figure 1. (a) The anomalous Hall effect and (b) the spin Hall effect.

Complications
Degeneracy of bands
Non-abelian Berry phase

So how do we quickly
compute the abelian
Berry connection and
curvature?

My numerics

$$\mathcal{A}(\mathbf{k}) = i \sum_n \langle u_{\mathbf{k},n} | \nabla_{\mathbf{k}} | u_{\mathbf{k},n} \rangle,$$

$$\Omega(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}(\mathbf{k}).$$

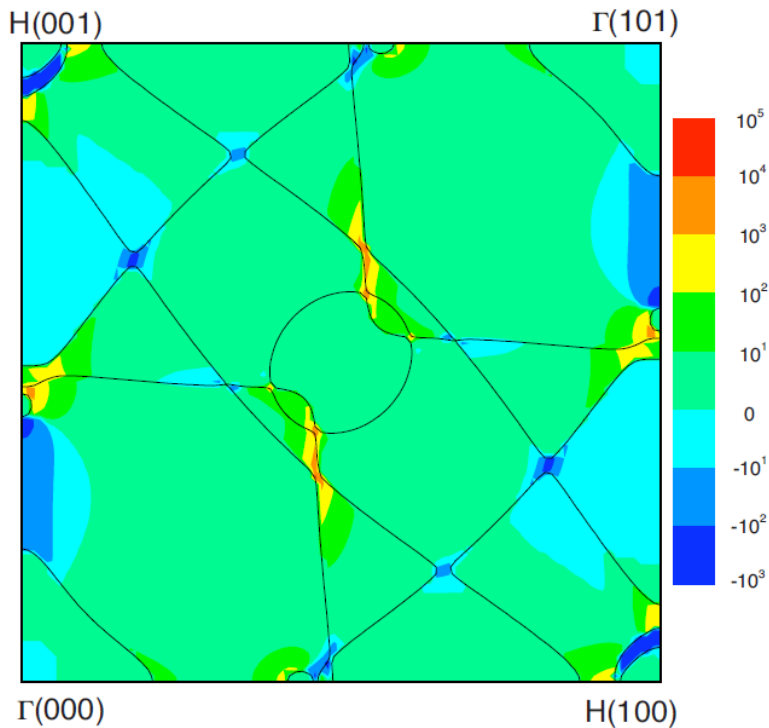
n, m in occupied states

$$U_j(\mathbf{k}) = \det[\langle u_{n\mathbf{k}} | u_{m\mathbf{k}+j} \rangle],$$

$$\mathcal{A}_j(\mathbf{k}) = \text{Im} \ln U_j(\mathbf{k}),$$

$$\Omega_z(\mathbf{k}) = \text{Im} \ln \frac{U_y(\mathbf{k} + \hat{\mathbf{k}}_x) U_x(\mathbf{k})}{U_y(\mathbf{k}) U_x(\mathbf{k} + \hat{\mathbf{k}}_y)}.$$

$$\det \exp A = \exp \text{tr} A$$



bcc Iron

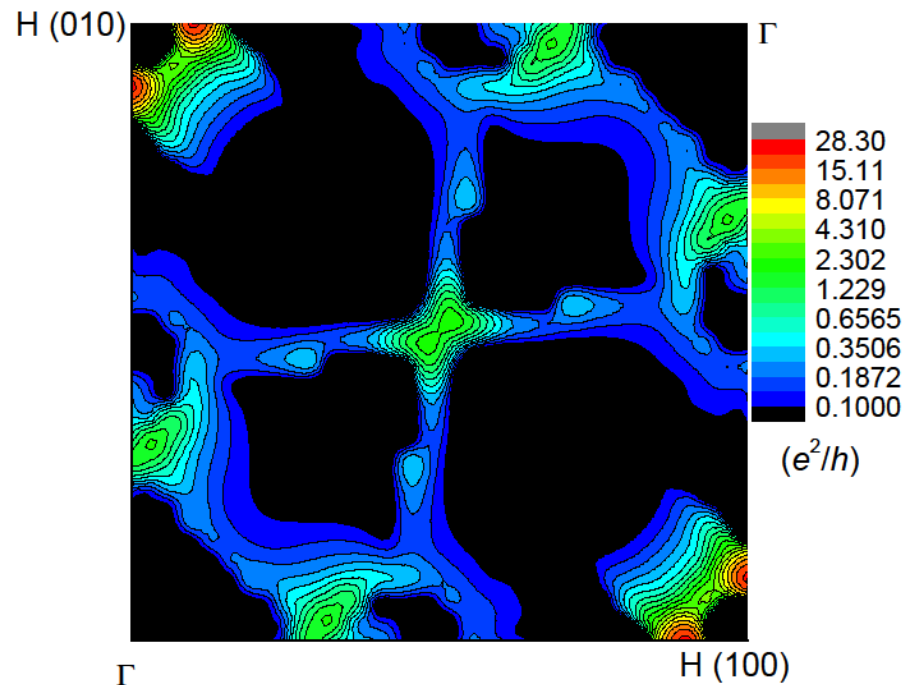
Calculated value (our)
600 S/cm

Our calculation

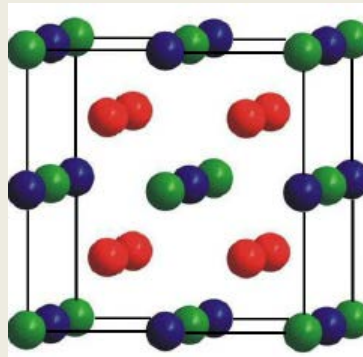
“ Kubo ”

bcc-Fe from Yao et al.
PRL 92, 037204 (2004)

Calculated value 700 S/cm
Experiment about 1000 S/cm



Heusler Compounds



PHYSICAL REVIEW B **85**, 012405 (2012)

Berry curvature and the anomalous Hall effect in Heusler compounds

Jürgen Kübler^{1,*} and Claudia Felser²

AHE in half metallic ferromagnets

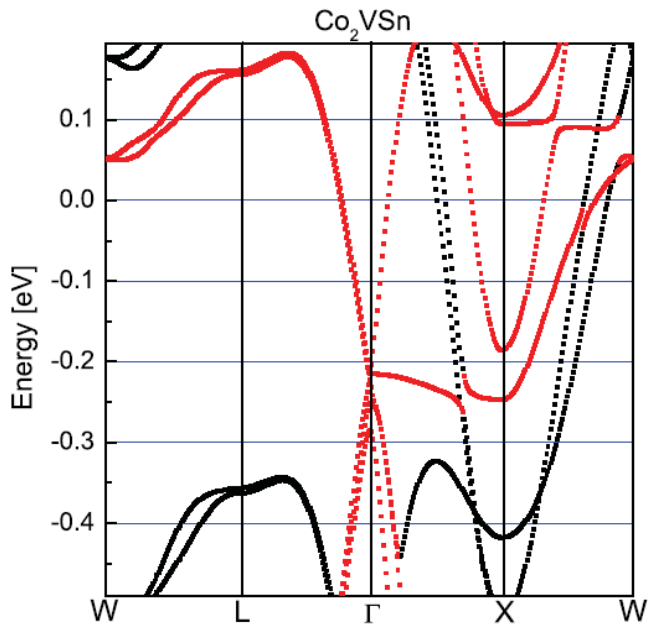


FIG. 4. (Color online) Band structure near the Fermi edge of Co₂VSn. Majority-spin electron states appear in red, minority-spin states in black. Note the Dirac cone at the Γ point at about -0.22 eV.

Compound ^a	N_V	a (nm)	M^{exp}	M^{calc}	σ_{xy}	P (%)
Co ₂ VGa	26	0.5779	1.92	1.953	66	65
Co ₂ CrAl	27	0.5727	1.7	2.998	438	100
Co ₂ VSn	27	0.5960	1.21	1.778	-1489	35
Co ₂ MnAl	28	0.5749	4.04	4.045	1800	75
Rh ₂ MnAl	28	0.6022		4.066	1500	94
Mn ₂ PtSn ^b	28	0.4509 (1.3477)		6.66	1108	91
Co ₂ MnSn	29	0.5984	5.08	5.00	118	82
Co ₂ MnSi	29	0.5645	4.90	4.98	228	100

Why so large?

Weyl nodes

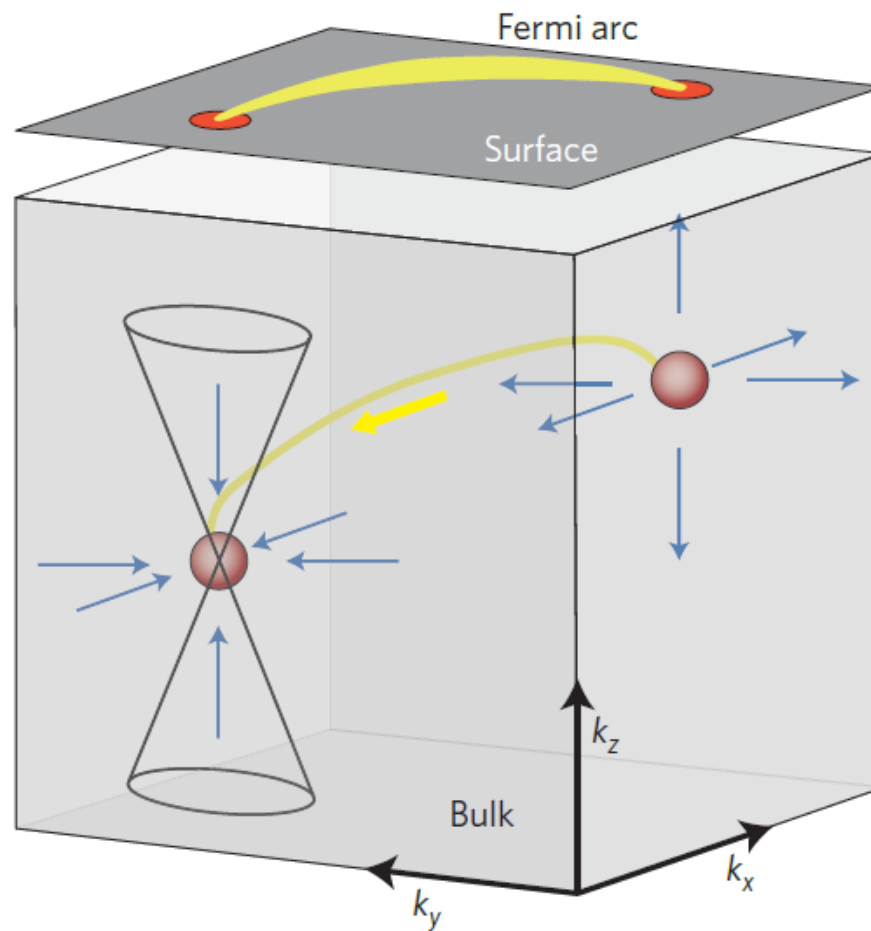


Figure 1 | Weyl semimetals in momentum space. Two Weyl nodes (red) act as monopoles, which have linear band dispersions (black) and are connected by a Dirac string (yellow). The top plane (grey) shows the two-dimensional projection, which has a Fermi arc (yellow) that connects the nodes and can be observed in photoemission experiments.

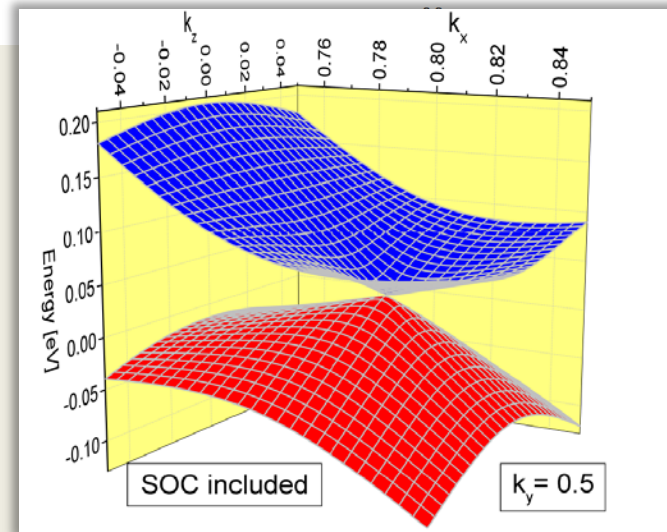
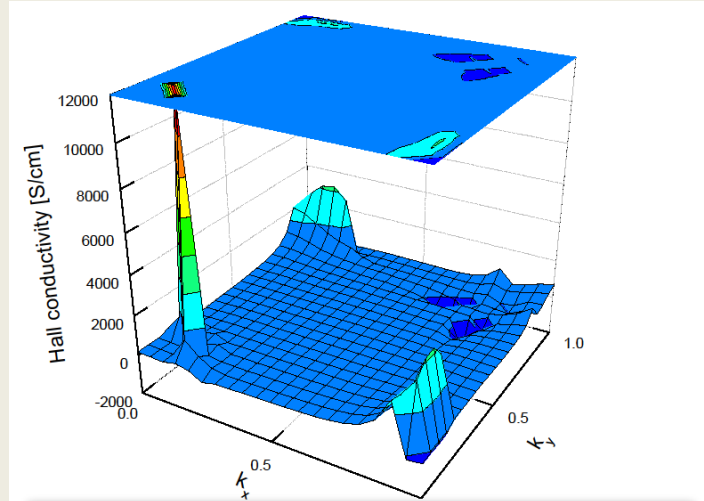
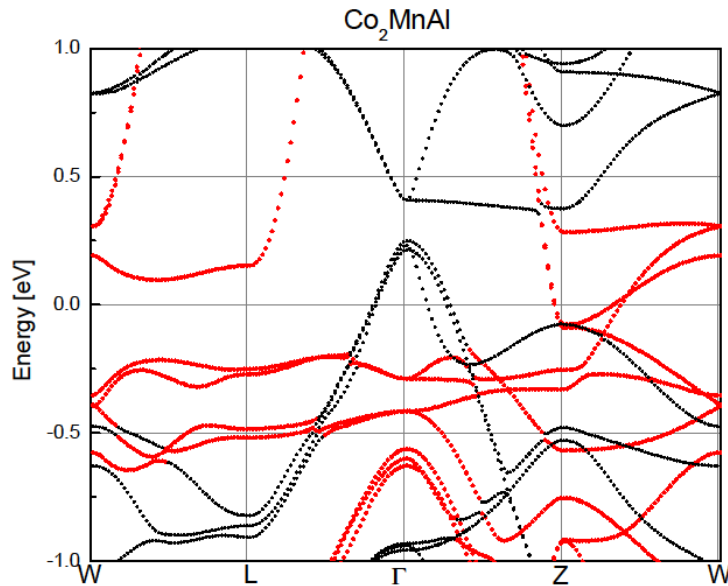
Bernevig 2015
Nature

AHE in half metallic ferromagnets

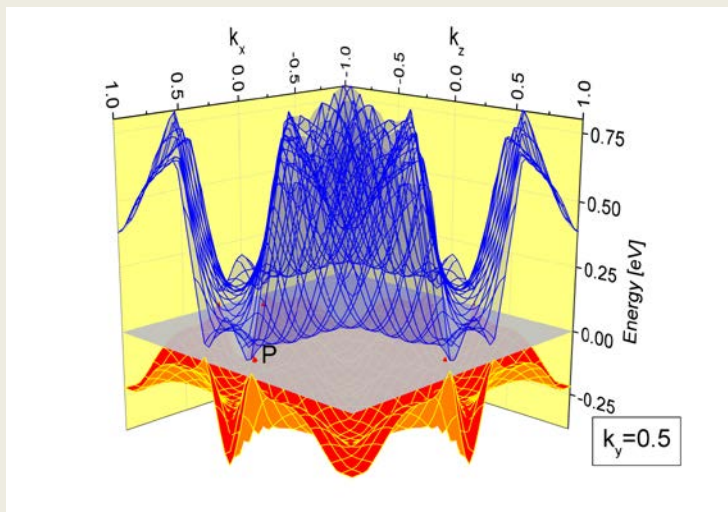
Huge Hall conductivity

$$\sigma_{xy} = 1800 \text{ S/cm calc.}$$

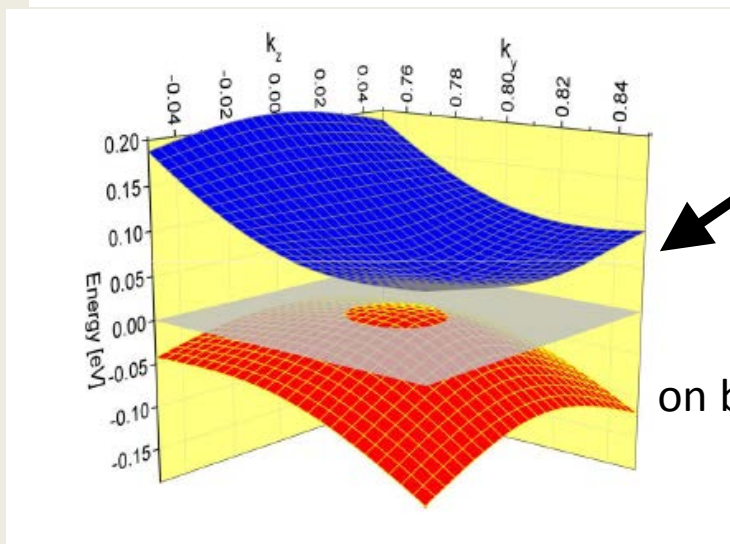
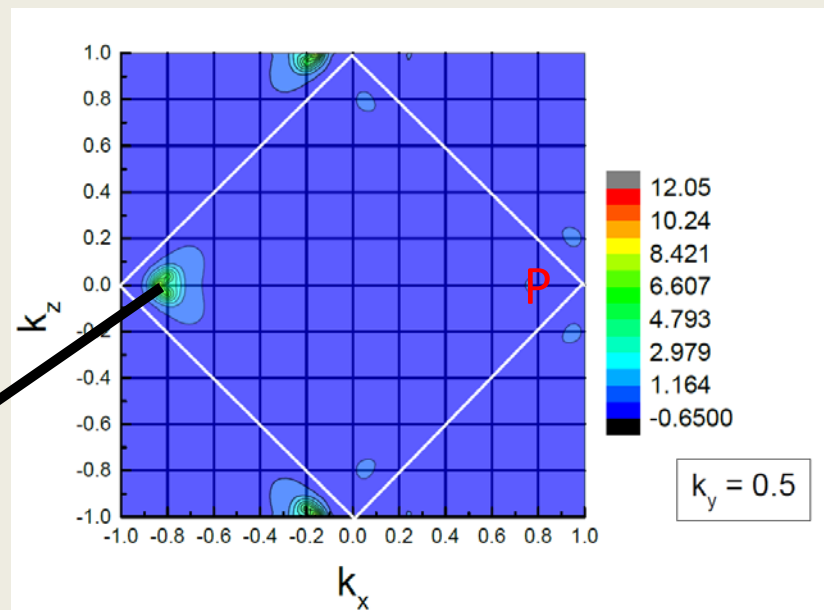
$$\sigma_{xy} \approx 2000 \text{ S/cm meas.}$$



Weyl points are the origin for a large Berry phase

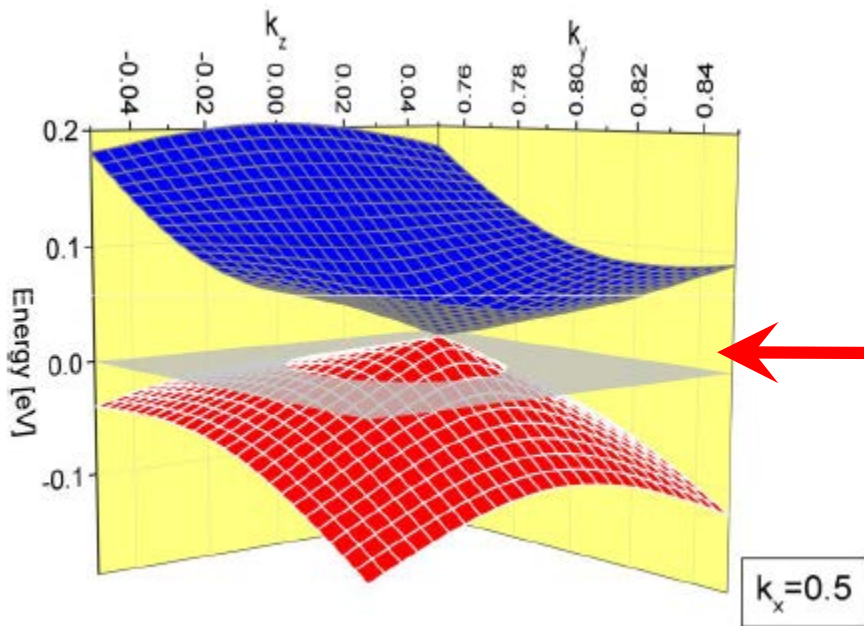


Berry curvature



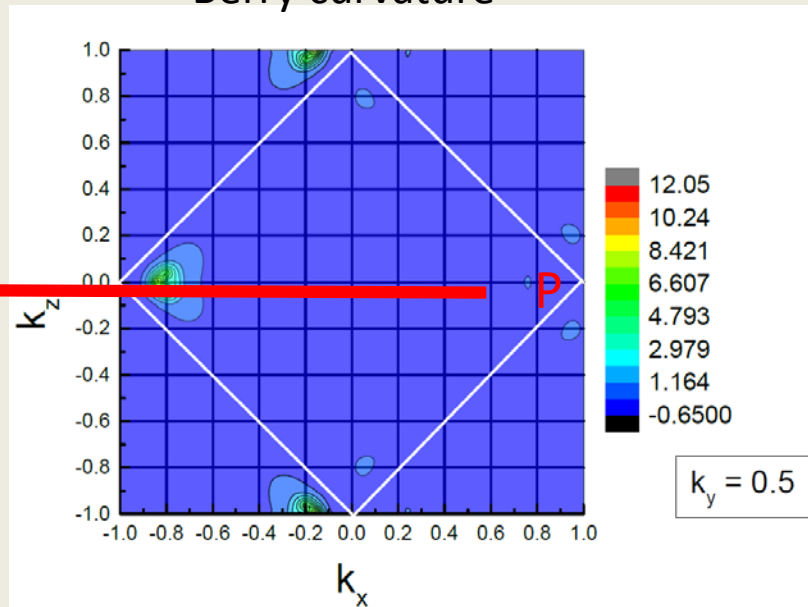
Zoom
in
on band structure

Band structure

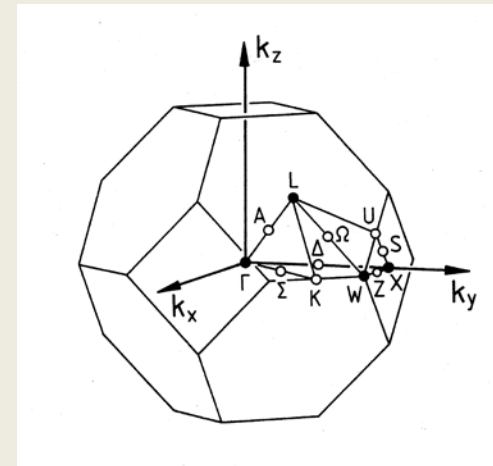
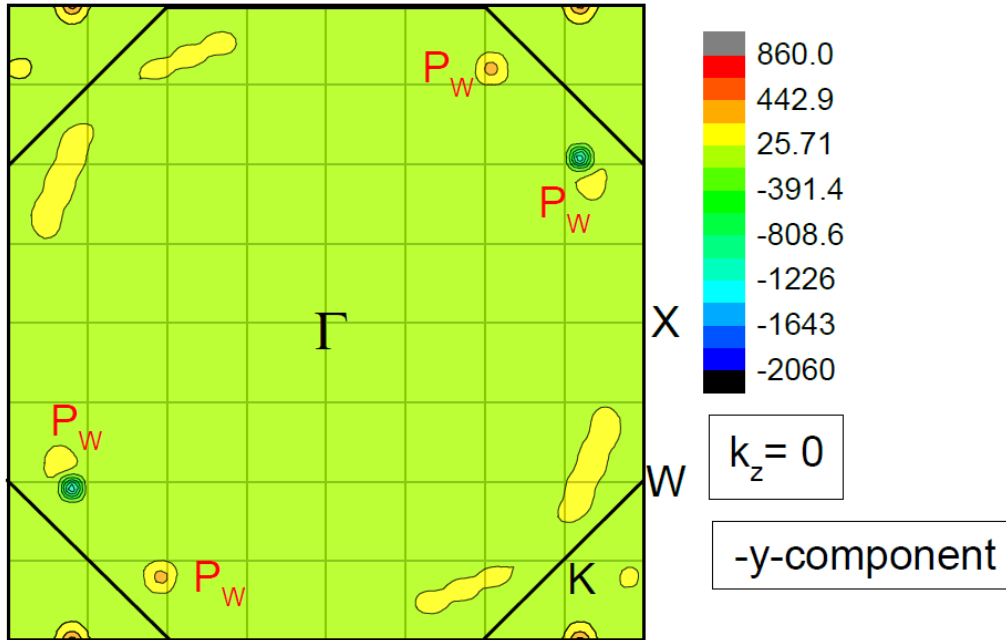


Weyl point

Berry curvature



Berry curvature with Fermi energy shifted to Weyl point



Positive and negative chirality

$$H_{Weyl} = \pm c p \sigma$$

Chern-number

Chirality = sign det(velocity tensor)

The **Chern** vector

$$\frac{1}{2\pi} \int_{BZ} \Omega_n^p(k) d^3k = C_n G_n^p$$

Integral is over a non-degenerate band labelled n ,
 p is the vector component.

The right hand side is the Chern number times
a reciprocal lattice vector

(Kohmoto, Halperin, Wu PRB 45, 13488 (1992))

Return to basic relation

$$\rho_{xy} = R_0 H_z + R_S M_z$$

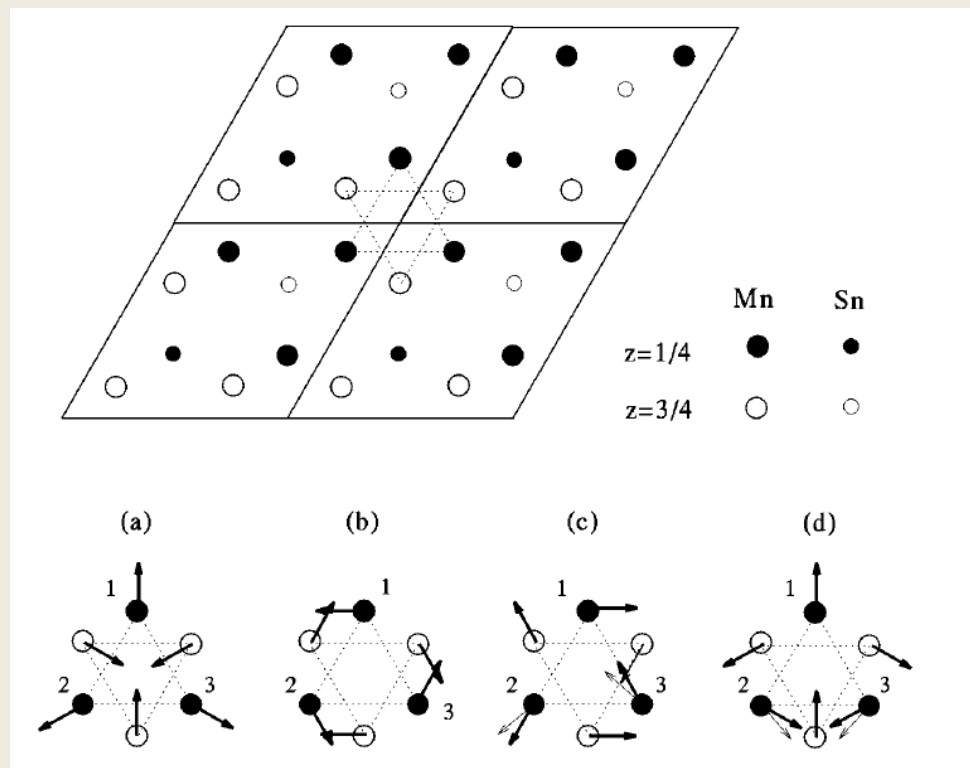
Antiferromagnet ?

Role of Orbital Polarization in Weak Ferromagnetism

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(Received 8 December 1995)



Also: Sticht, Höck, JK: J. Phys. CM 1, 8155 (1989)

EPL, 108 (2014) 67001

Non-collinear antiferromagnets and the anomalous Hall effect

J. KÜBLER¹ and C. FELSER²

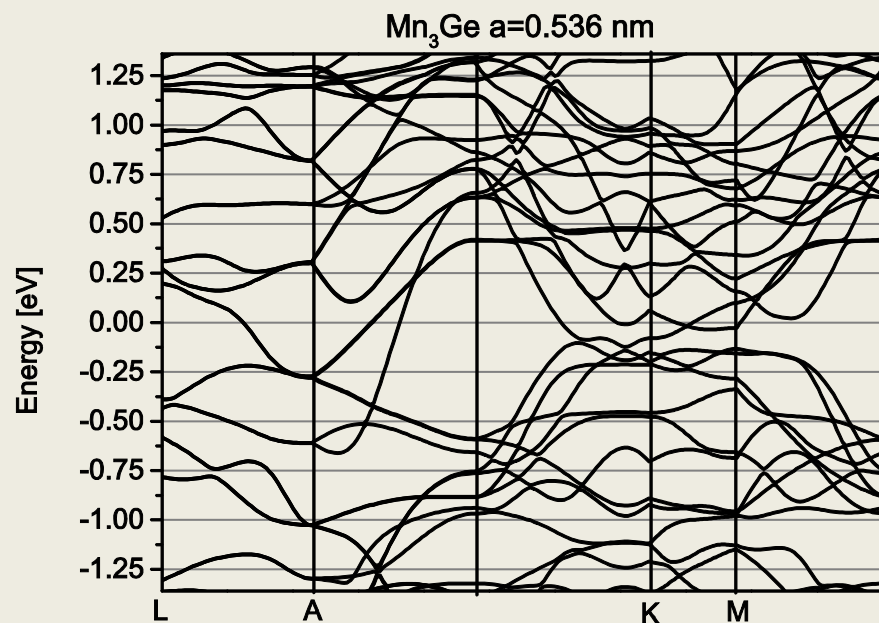
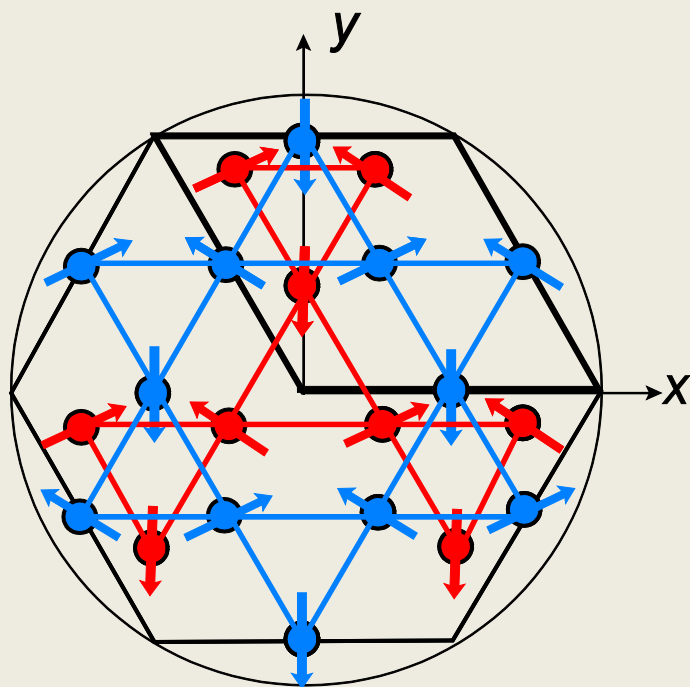
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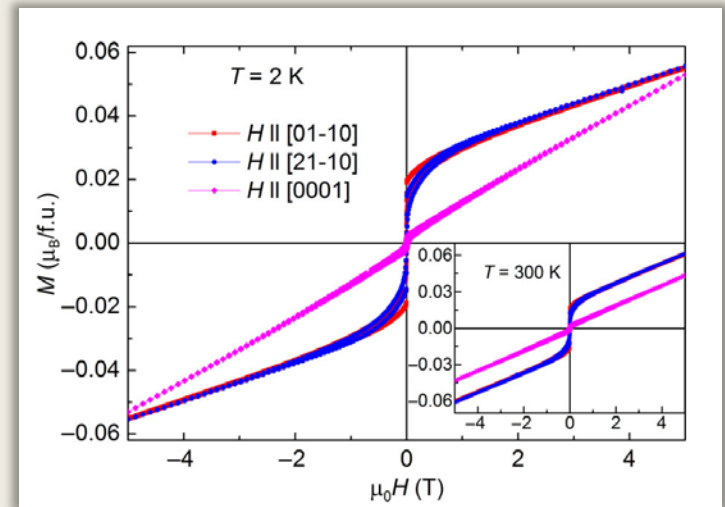
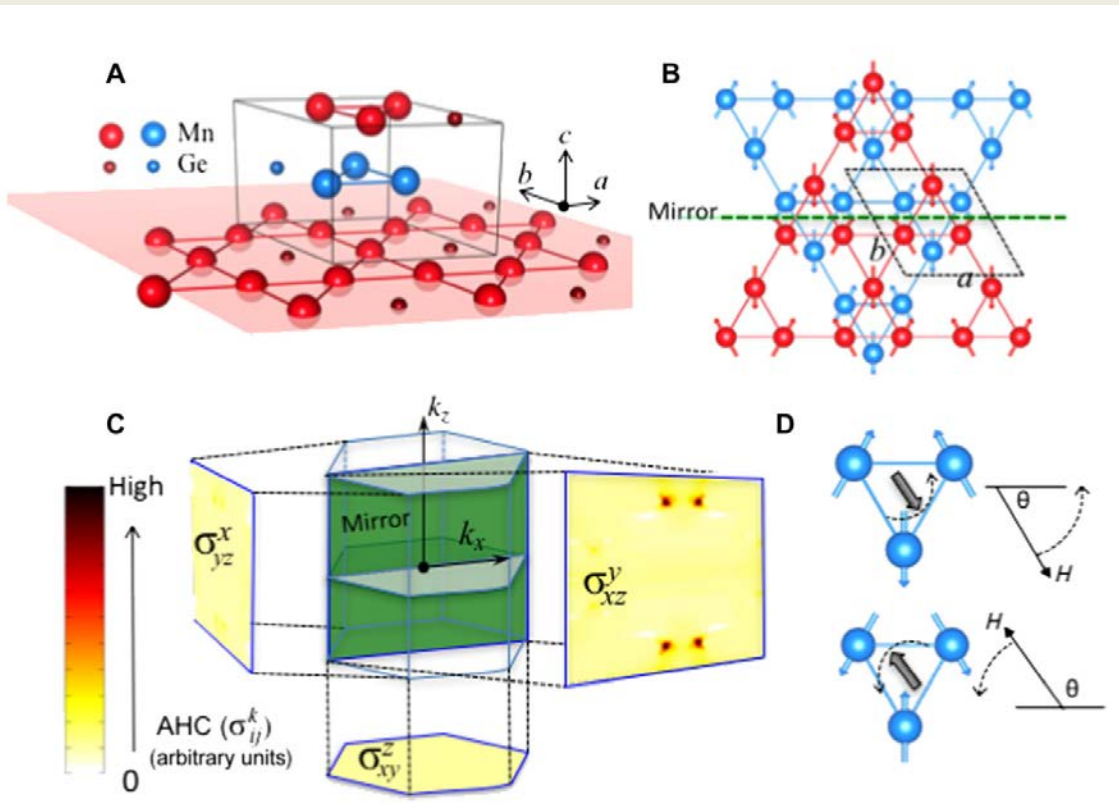
The ground-state configuration and the band structure along symmetry lines



$$\sigma_{zx} = 531 \text{ S/cm}$$

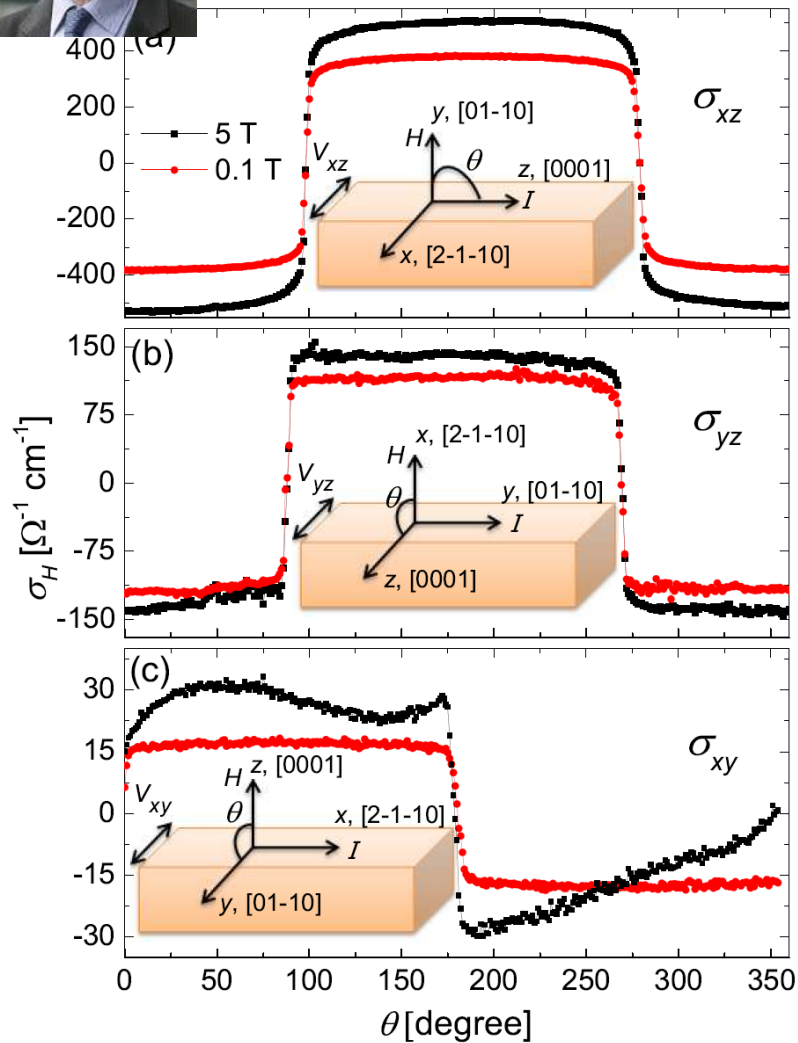
(all other components are zero)

Non-collinear AFM in metallic Mn₃Ge



Kübler and Felser EPL 108 (2014) 67001

Non-collinear AFM Mn₃Ge/Mn₃Sn



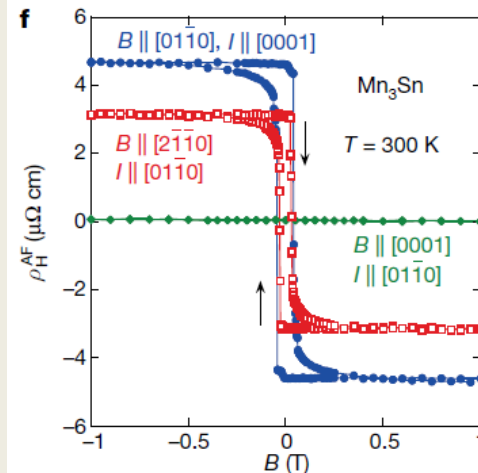
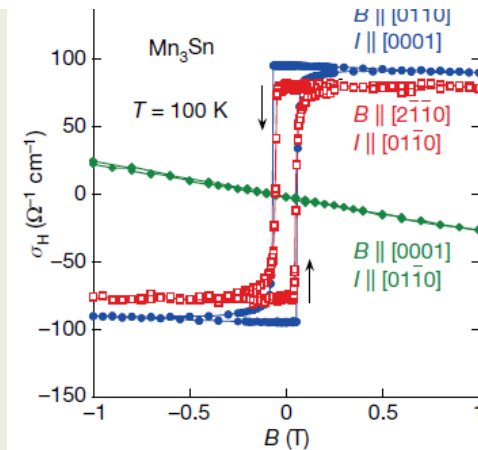
Nayak et al. *Science Advances* 2 (2016) e1501870
 Kiyohara, Nakatsuji, preprint: arXiv:1511.04619, PRX
 2016

LETTER

doi:10.1038/nature15723

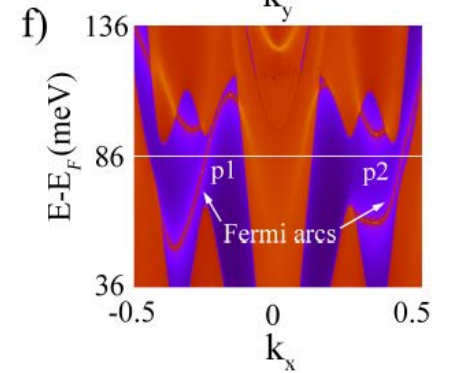
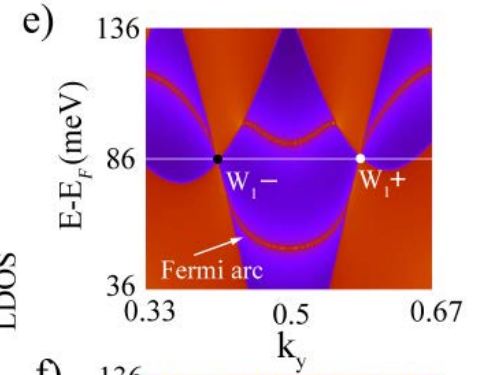
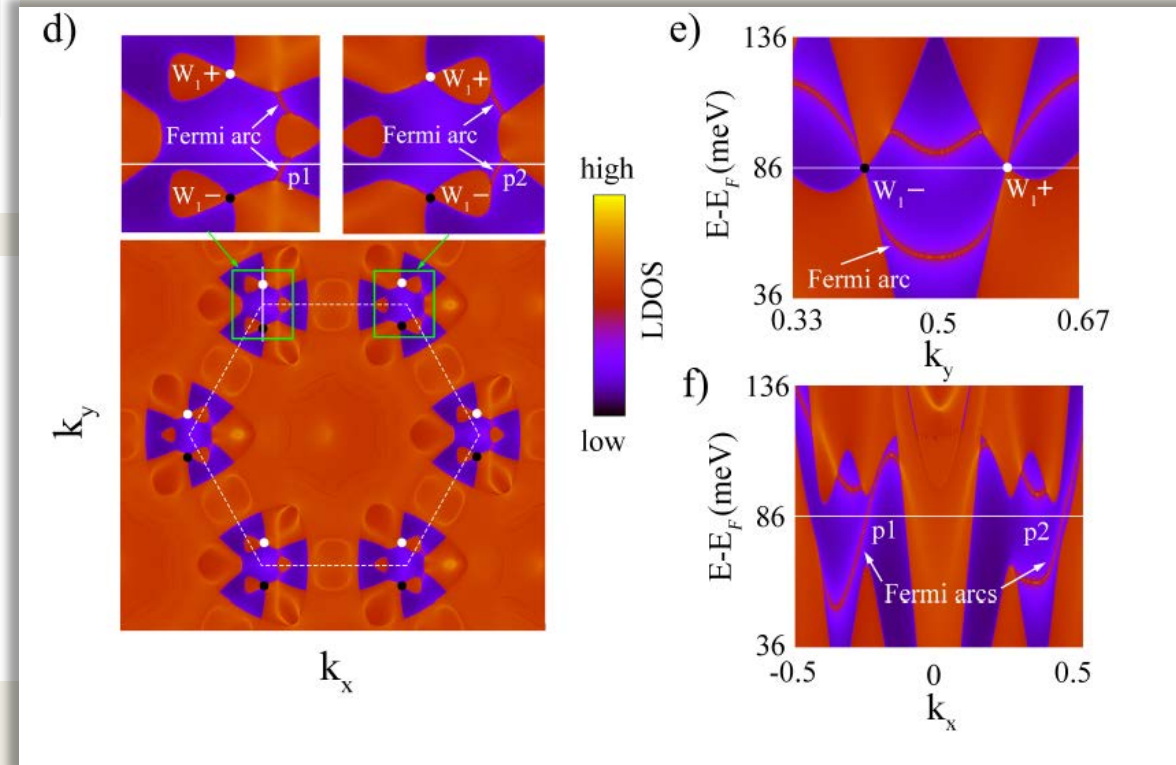
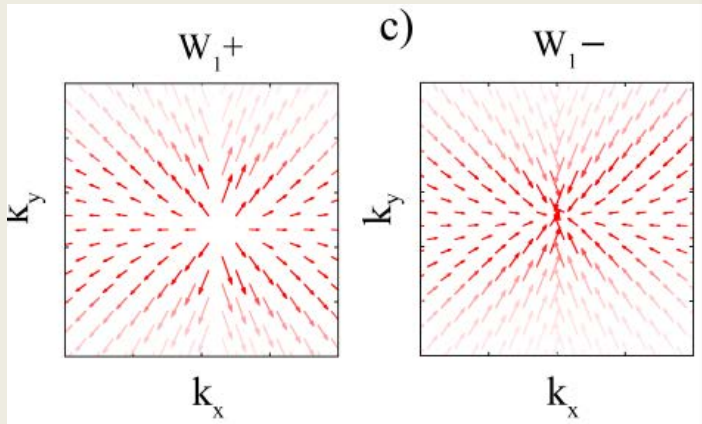
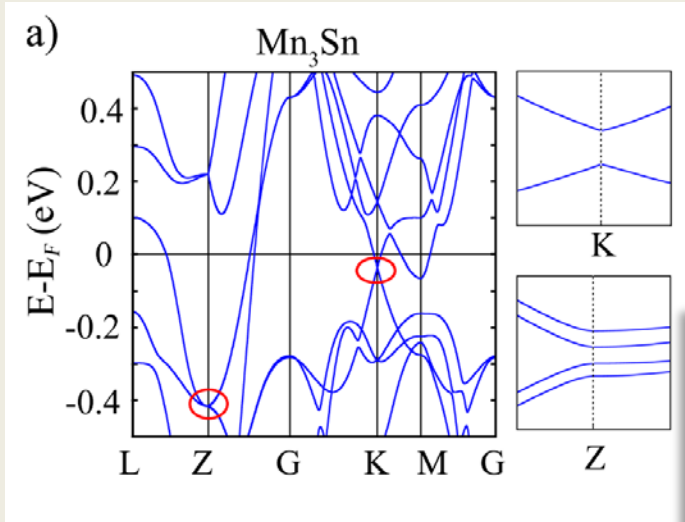
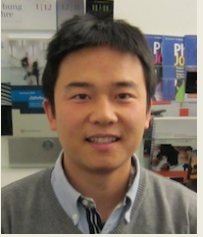
Large anomalous Hall effect in a non-collinear antiferromagnet at room temperature

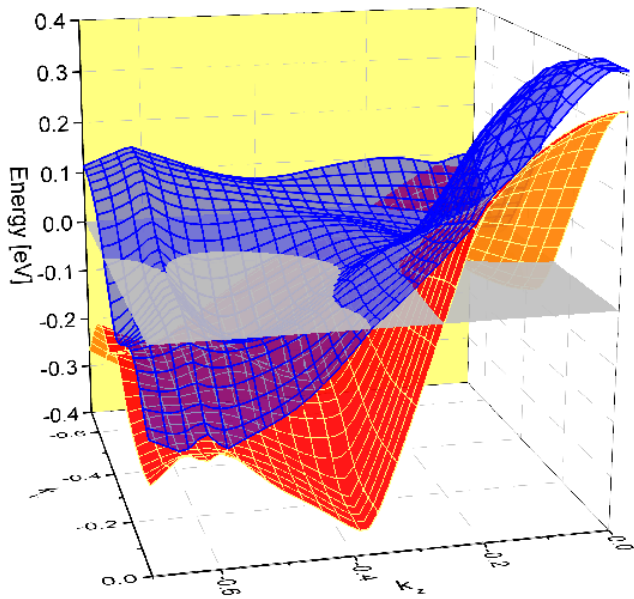
Satoru Nakatsuji^{1,2}, Naoki Kiyohara¹ & Tomoya Higo¹



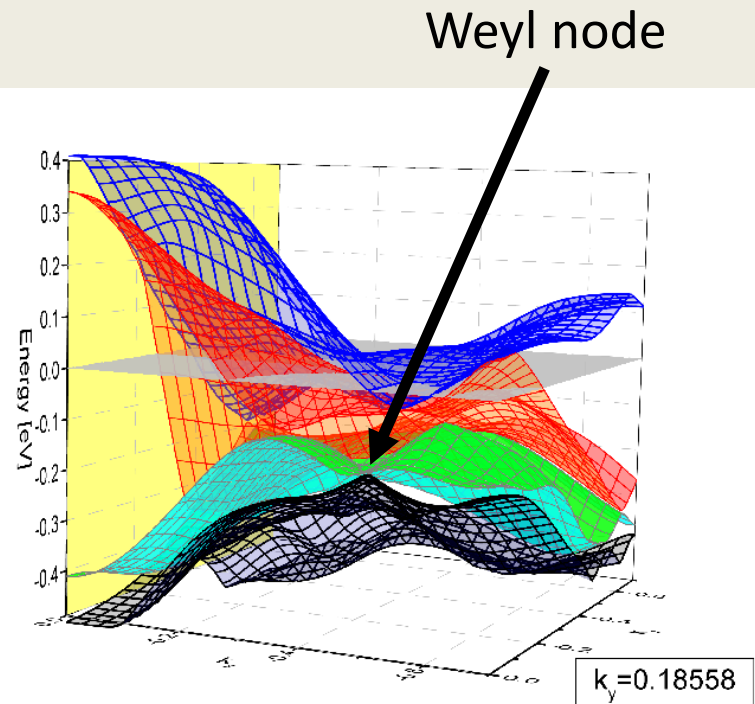
Nakatsuji, Kiyohara, & Higo, *Nature*,
 doi:10.1038/nature15723

Fermiarcs in the Weyl AFM





Bands at the Fermi energy



Bands below the Fermi energy

Thanks for
hanging on