Topological Currents in Anomalous Hall Effect, Multiferroics, and Magnetoelectrics

Shigeki Onoda *(CREST, Dept. Applied Physics, Univ. Tokyo)*
小野田　繁樹

Collaborators:

Theoretical:

N. Nagaosa (CREST, Univ. Tokyo; CERC, AIST)
N. Sugimoto (Univ. Tokyo)
J.H. Han (SungKyunKwan; CSCMR, Seoul Univ.)
C. Jia (KIAS)

Experimental:

A. Asamitsu, T. Miyasato (CRC, Univ. Tokyo)
Y, Tokura, Y. Onose (Univ. Tokyo; CERC, AIST)

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Outline

1. Introduction

   Topological currents & the Berry's phase in the Bloch wavefunction

2. Unified theory of the anomalous Hall effect

   Band intirnsic (Berry-phase) vs. extrinsic mechanisms

   Gauge-covariant Keldysh-Dyson equation with em. Field

   Electric conductivity tensor in the bulk

   Extrinsic-to-intrinsic crossover

   A new scaling in the hopping-conduction regime

   [S. Onoda, N. Sugimoto, N. Nagaosa, Prog. Theor. Phys. **116**, 61 (2006);
   S. Onoda, N. Sugimoto, N. Nagaosa, Phys. Rev. Lett. **97**, 126602 (2006);
   T. Miyasato, et al., cond-mat/0610324]

3. Electric polarization in dielectrics, ferroelectrics, multiferroelectrics, magnetoelectrics, & spiral magnets

   Local electric dipole moments & the Berry-phase description

   [C. Jia, S. Onoda, N. Nagaosa, J.H. Han, to appear in Phys. Rev. B.
   S. Onoda, unpublished.]

Topological structure in Bloch wavefunction

Hamiltonian: H → Diagonalize it!

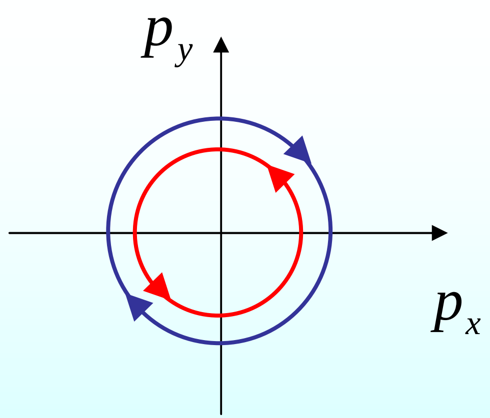
Accidentally degenerate momenta in band dispersions in 3D

[Neumann-Wigner, Herring]

For a fixed p_z

The simplest example of the band (anti-)crossing

$H = \Delta\sigma_z + p_y\sigma_x - p_x\sigma_y$: 2D Dirac fermion



Δ: perturbation

Eigenstate: vorticity (chirality) = +1, -1

Topological objects

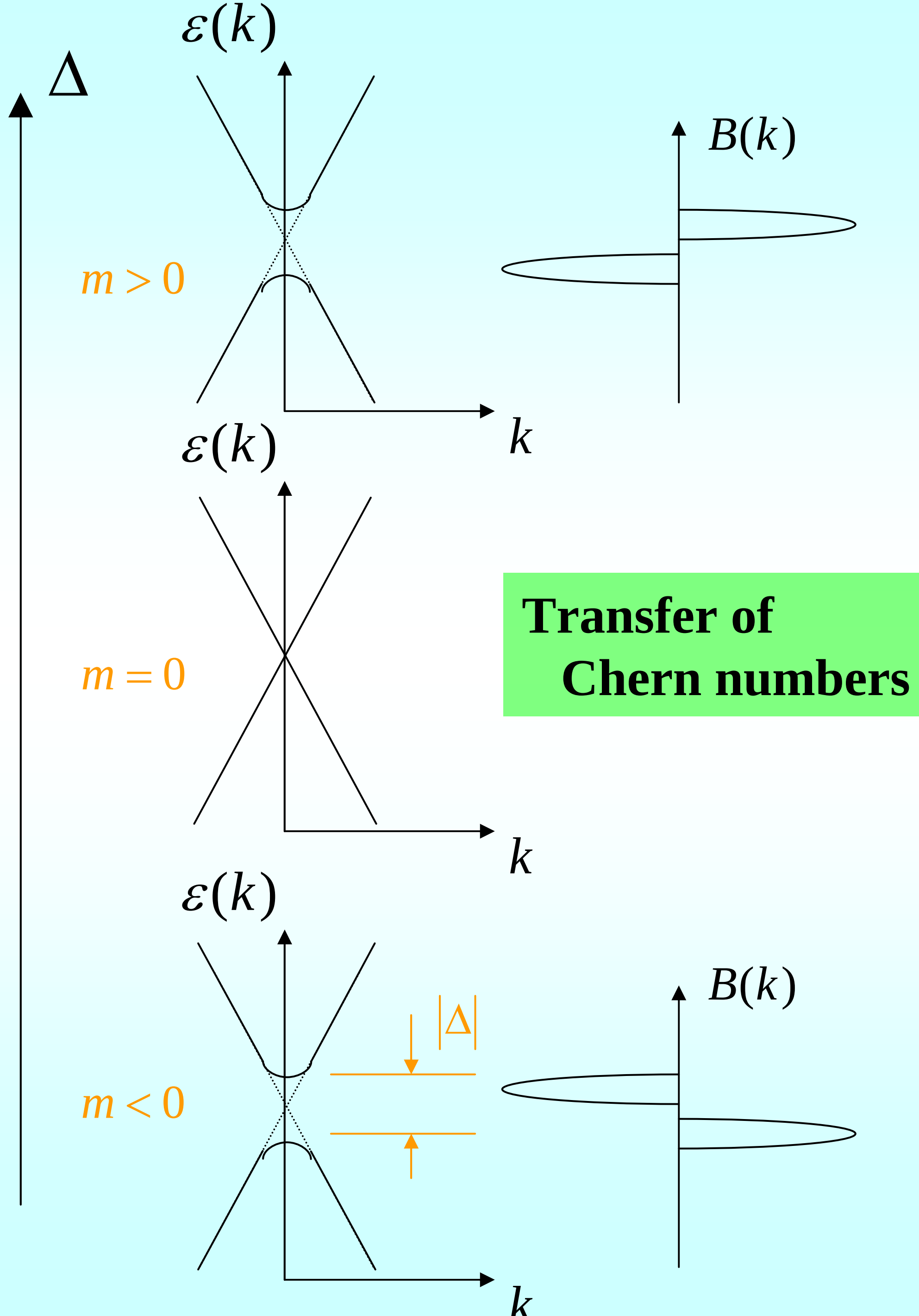
Parity anomaly
—Non-perturbative effect—

(2+1)D Dirac fermions

$$H = \Delta\sigma_z + p_x\sigma_x + p_y\sigma_y$$

$$\Rightarrow \quad \sigma_{xy} = -\frac{e^2}{2h}\,\mathrm{sgn}(\Delta)$$

You can not treat Δ perturbatively.



Topological structure in Bloch wavefunction

Electric current operator: $\boldsymbol{J} = e\dot{\boldsymbol{x}} = (i\hbar)^{-1}[\boldsymbol{x}, H] = \nabla_k H$

Dissipationless topological current in the Quantum Hall effect

$$\sigma_{ij} = e^2\hbar \sum_{n \neq n'} \int \frac{d^d \boldsymbol{p}}{(2\pi\hbar)^d} f(\varepsilon_n(\boldsymbol{p})) \frac{\langle \Phi_{nk} | J_k^i | \Phi_{n'k} \rangle \langle \Phi_{n'k} | J_k^j | \Phi_{nk} \rangle}{(E_{nk} - E_{nk'})^2}$$

Kubo formula

in the case without dissipation

$$= -2e^2\hbar \sum_n \int \frac{d^d \boldsymbol{p}}{(2\pi\hbar)^d} f(\varepsilon_n(\boldsymbol{p}))\varepsilon_{ijl} b_{n\boldsymbol{k}}^l$$

Thouless-Kohmoto-Nightingale-Nijs (TKNN) formula

Adiabatic Berry-phase connection: $\boldsymbol{a}_{nk} = -i\langle \Phi_{nk} | \nabla_k | \Phi_{nk} \rangle$

Berry-phase curvature: $\boldsymbol{b}_{nk} = \nabla_k \times \boldsymbol{a}_{nk} = -i\langle \nabla_k \Phi_{nk} | \times | \nabla_k \Phi_{nk} \rangle$

c.f. Ferroelectric polarization in cystalline insulators (the second topic)
[Vanderbilt, Martin, Resta, …]

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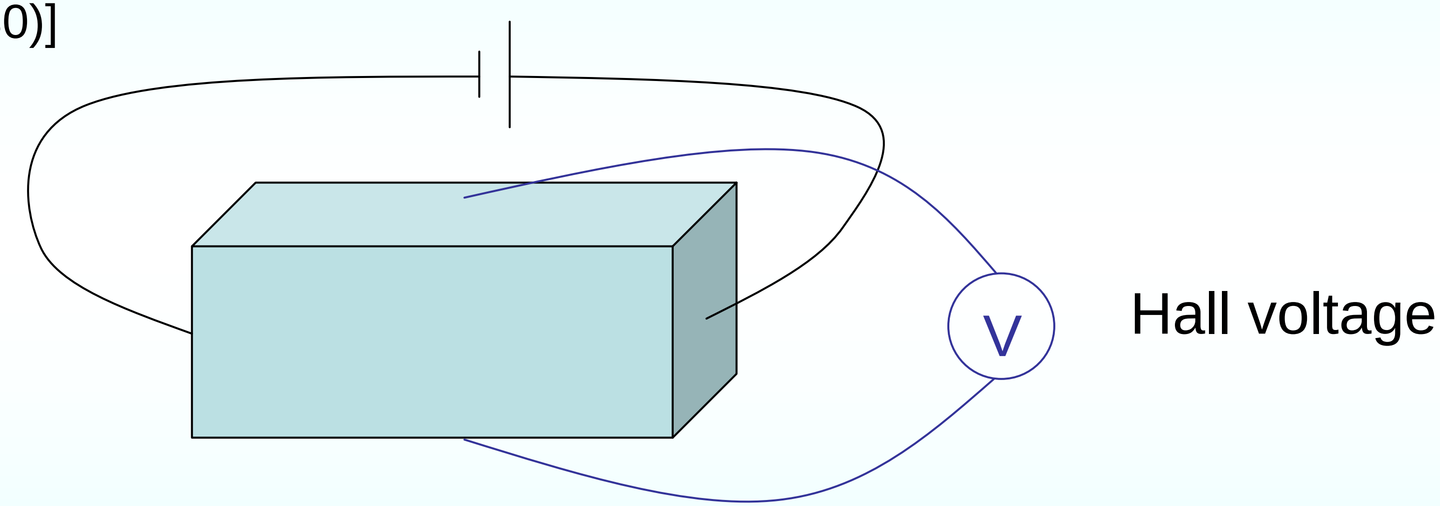
4. Summary

History of experiments and theories on the AHE

[Hurd, *The Hall Effect in Metals and Alloys* (1972)]

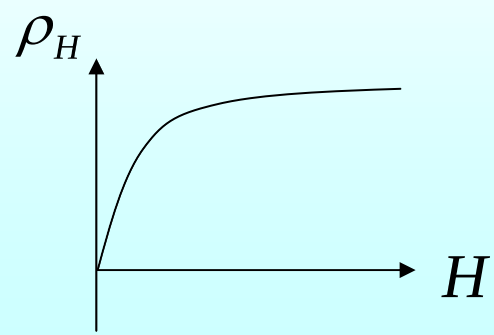
1. Voltage drop perpendicular to the current in ferromagnets
   → orders of magnitude larger than the Lorentz force
   [Hall (1879, 1880)]



2. Empirical relation from experiments [Pugh & coworkers (1930)]

$$\rho_H = R_0 H + R_s M$$

$$R_0 = 1/ne$$



[Pugh & Rostoker, Rev. Mod. Phys. **25**, (1953) 151]

Band-intrinsic mechanism of the AHE

Spin-orbit interaction (SOI) & magnetization:

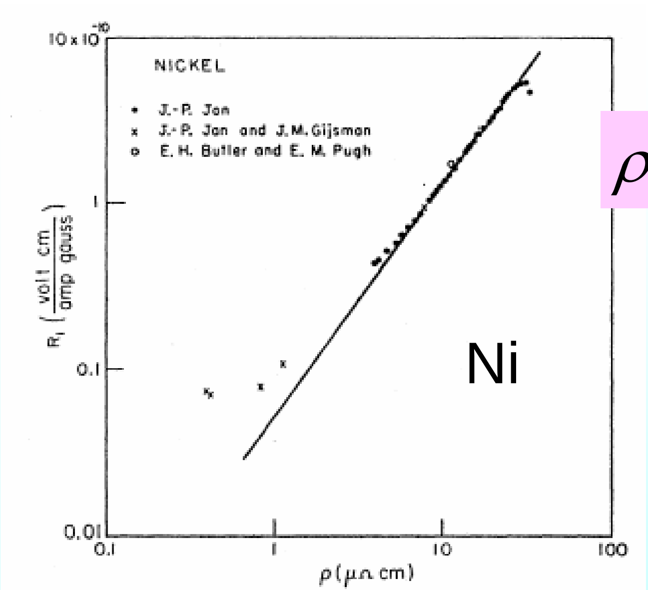
→ Thermodynamic Hall current due to inter-band matrix elements of the current.

$\rho_H \propto \rho^2$ explains the experiments. [Karplus & Luttinger (1954)]

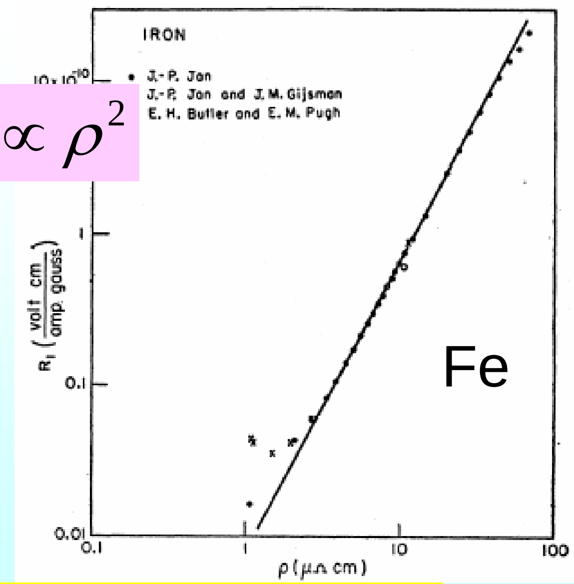
→ Anomalous velocity [Adams & Blount (1959)]

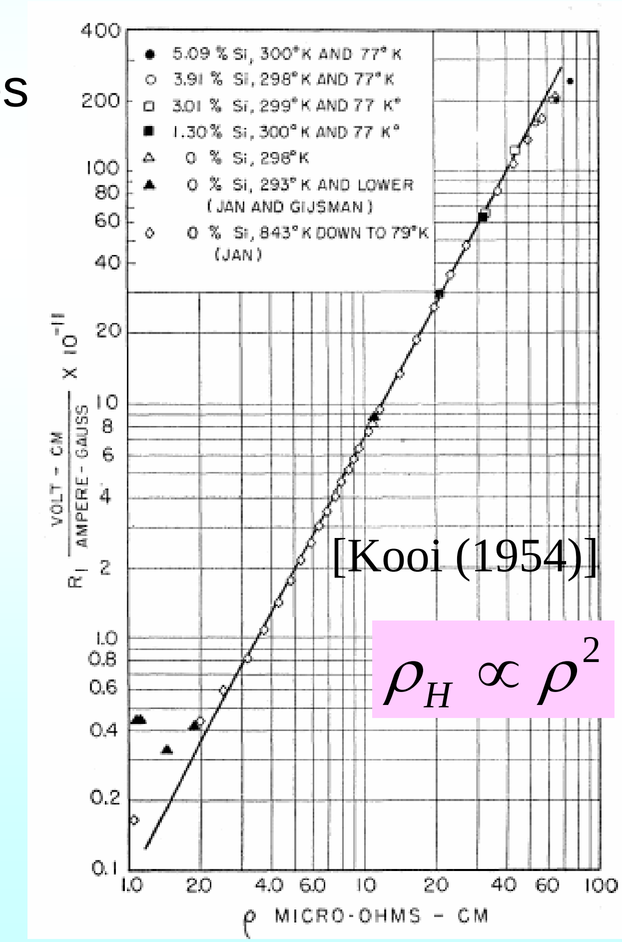
→ The sum of the Berry-phase over the occupied states

(Topological current in an analogy to the QHE)



$\rho_H \propto \rho^2$





$\rho_H \propto \rho^2$

But, they ignored the impurity scattering!

Extrinsic mechanisms of the AHE

- Skew scattering [Smit (1955, 1958)] or Mott scattering
  Scattering by impurity potential with the SOI bends the electron motion
  → non-equilibrium transport Hall current $\rho_H \propto \rho$

- Side jump mechanism [Berger (1970,1972)]
  SIO due to the impurity potential shifts the momentum.

- Crossover from skew-scattering to side-jump [Noziere-Lewiner (1973)]

- Expansion of the conductivity tensor in the impurity potential *v*

Kohn-Luttinger

$$\sigma^{ij} = v^{-2} g^{ij}_{(-2)} + v^{-1} g^{ij}_{(-1)} + v^{0} g^{ij}_{(0)} + \cdots$$

[Luttinger (1958)]

$$\sigma^{xy} = v^{-1} g^{xy}_{(-1)} + v^{0} g^{xy}_{(0)} + \cdots$$

$v^{-1} g^{xy}_{(-1)}$ → **Skew-scattering contribution**

$v^{0} g^{xy}_{(0)}$ → intrinsic contributions and others

Rashba model: Sinitsyn et al., Dugaev et al., Inoue et al.→ a part of the story

Expansion of σ_{xy} in the impurity potential v_{imp}, & (spin-orbit coupling)x(magnetization)

Luttinger (1958) $\sigma_{xy} = v_{imp}^{-1} g_{xy}^{(-1)} + v_{imp}^{0} g_{xy}^{(0)} + \cdots$

$\rho_H \propto \rho$

Extrinsic Skew (or Mott)-scattering
[Smit (1955, 1958)]

$$\sigma_{xy}^{skew} = S\sigma_{xx} \sim \frac{e^2}{ha}\frac{\varepsilon_{SO}\tau}{\hbar} \qquad S \approx \frac{\varepsilon_{SO} v_{imp}}{W^2}$$

Intrinsic [Karplus-Luttinger (1954)]
Side jump [Berger (1970)]

$\rho_H \propto \rho^2$

$$\sigma_{xy}^{\text{Int}}, \sigma_{xy}^{\text{Side jump}} \cong \frac{e^2}{ha}\frac{\varepsilon_{SO}}{E_F} = \frac{e^2}{ha}\frac{\varepsilon_{SO}\tau}{\hbar}\left(\frac{E_F\tau}{\hbar}\right)^{-1}$$

3 energy scales in the problem

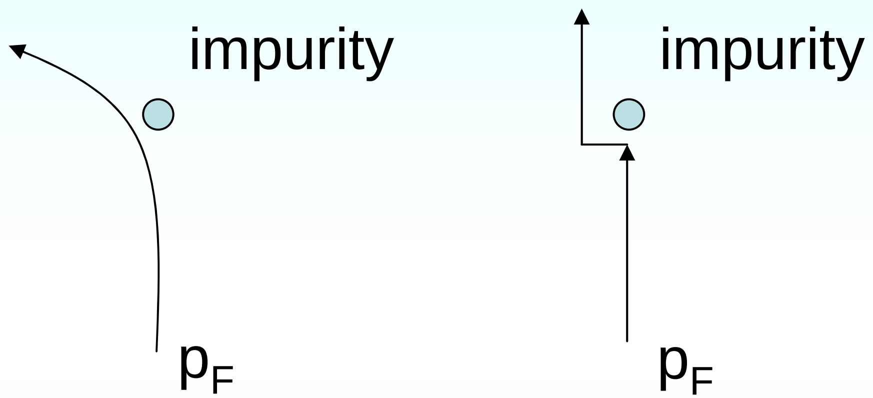
E_F or W	Bandwidth
h/τ	Relaxation rate
ε_{SO}	Spin-orbit interaction energy

But, $\varepsilon_F\tau$ is the only controlling parameter.
Is it true? -No.

Claim: The intrinsic AHE is a topological and non-perturbative effect in ε_{SO}

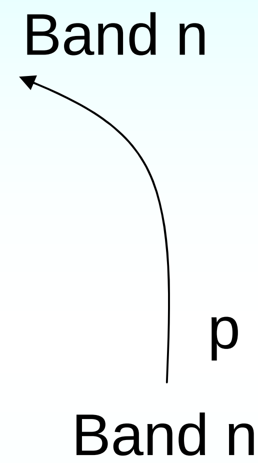
Intuitive view of electron motion in ferromagents

Simple classical Boltzmann picture



Skew scattering
[Smit]

Side jump
[Berger]



Adiabatic Berry phase
[Sundaram-Niu,
M.Onoda-Nagaosa,
Jungwirth-MacDonald]

Extrinsic mechanisms

Intrinsic mechanism

can be calculated *ab initio*.

A unified theory

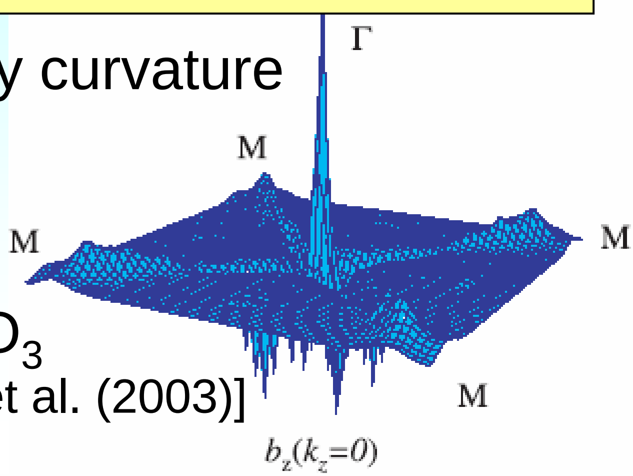
Generic model for anti-crossing of band dispersions

Anti-crossing of band dispersions due to the spin-orbit interaction in the presence of M>0

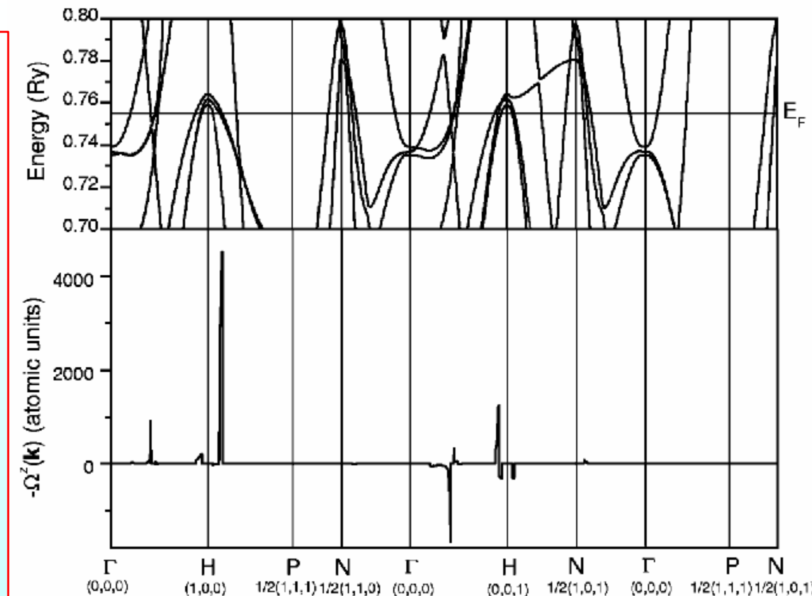
↓

Berry curvature

Berry curvature



$SrRuO_3$
[Fang et al. (2003)]



bcc Fe [Yao et al. (2004)]

Focus on an anti-crossing of two dispersions

$$H = H_0 + V$$

$$= -\Delta_0 \hat{\sigma}^z - \lambda \boldsymbol{p} \cdot \hat{\boldsymbol{\sigma}} \times \boldsymbol{e}_z + \frac{\boldsymbol{p}^2}{2m} + V_{imp} \sum_{\boldsymbol{r}_{imp}} \delta(\boldsymbol{r} - \boldsymbol{r}_{imp})$$

$\hat{\boldsymbol{\sigma}} \equiv (\hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z)$: Pauli matrices

m : electronic effective mass

λ : "Dirac - fermion" velocity

$\Delta_0 = \varepsilon_{SO}$: splitting at the anti - crossing

Linear response theory

S. Onoda, N. Sugimoto, N. Nagaosa, Prog. Theor. Phys. 116, 61 (2006)

Fermi-surface contribution | **Quantum contribution from the occupied states**

$$\hat{G}^{<}_{E_i}(\varepsilon,\mathbf{p}) = \hat{G}^{<,I}_{E_i}(\varepsilon,\mathbf{p})\partial_\varepsilon f(\varepsilon) + \left(\hat{G}^{A}_{E_i}(\varepsilon,\mathbf{p}) - \hat{G}^{R}_{E_i}(\varepsilon,\mathbf{p})\right) f(\varepsilon)$$

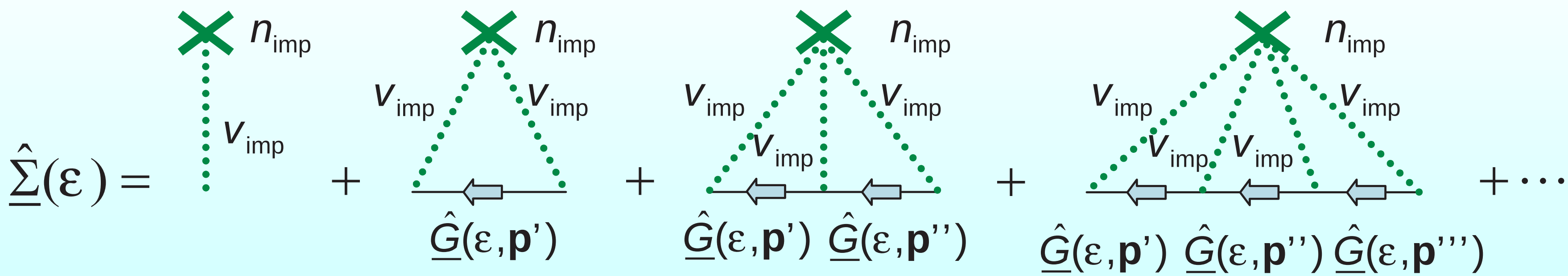
$$\sigma^{tot}_{ij} = e^2\hbar\int\frac{d\varepsilon}{2\pi i}\int\frac{d^d\mathbf{p}}{(2\pi\hbar)^d} Tr\left[\hat{v}_i(\mathbf{p})\hat{G}^{<}_{E_i}(\varepsilon,\mathbf{p})\right] = \sigma^{I}_{ij}+\sigma^{II}_{ij} \Rightarrow$$

Gauge-covariant

Streda formula (1982)

+ vertex corrections

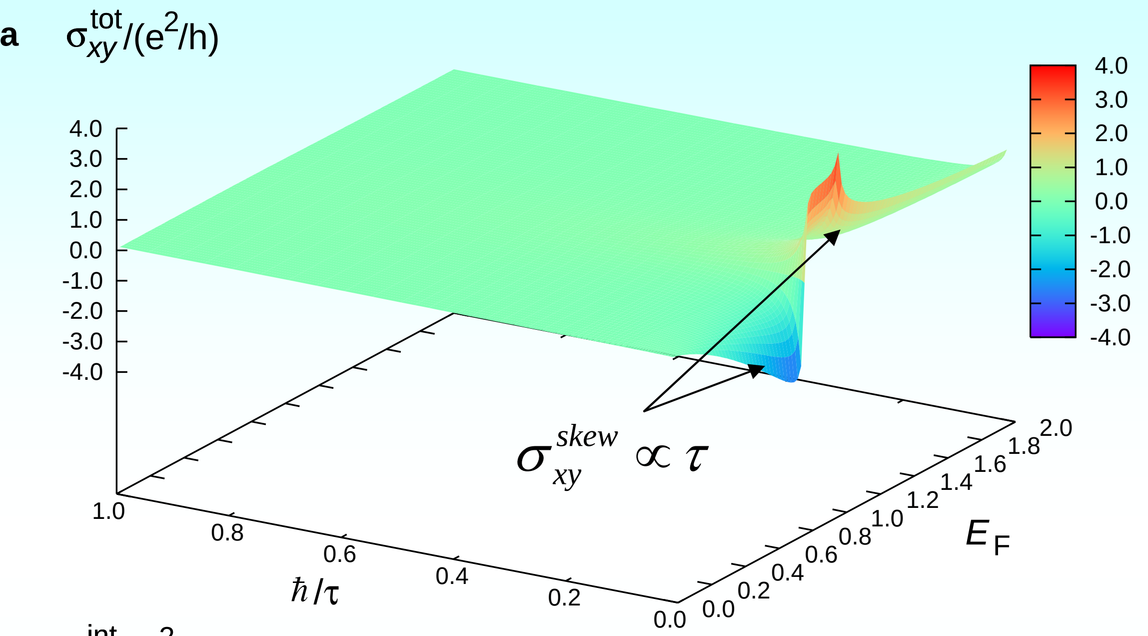
Self-consistent T-matrix approximation

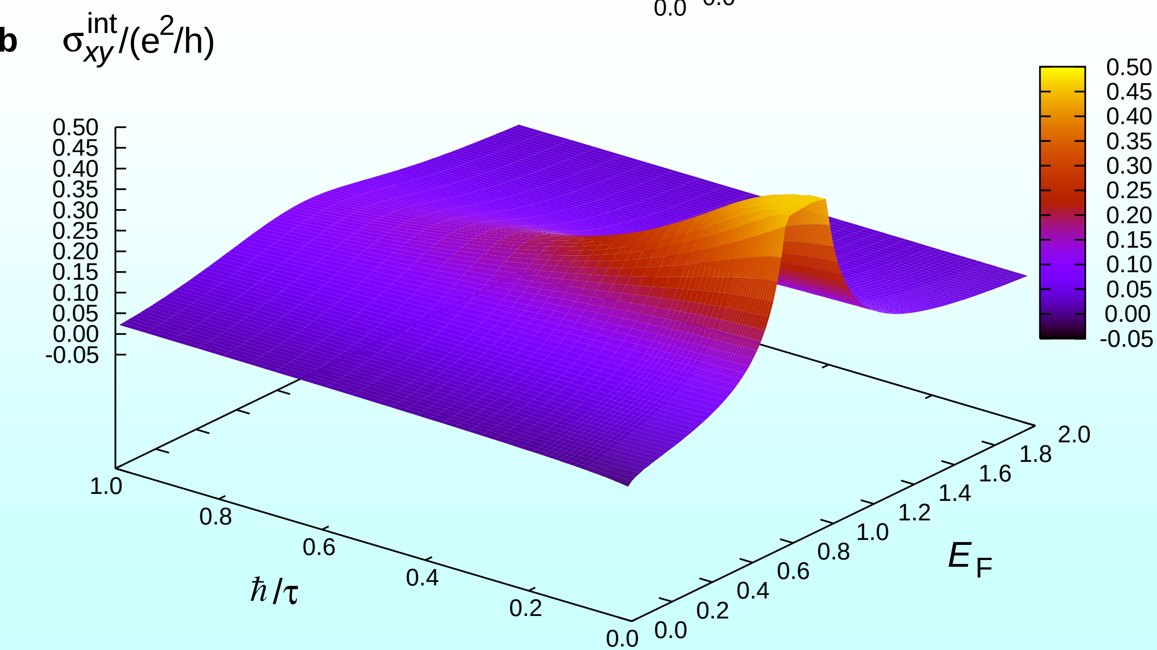


Include all orders in v_{imp} !

Accessible to dirty systems.

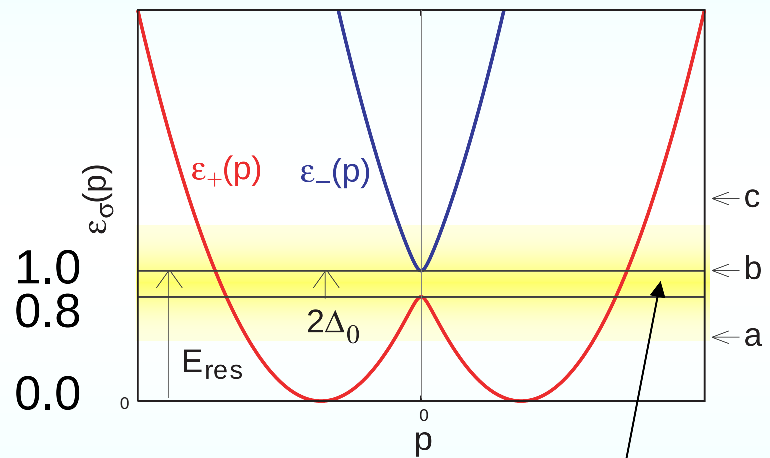
Anomalous Hall conductivity: σ_{xy}^{tot} & σ_{xy}^{int}





S. Onoda, N. Sugimoto, N. Nagaosa, Phys. Rev. Lett. **97**, 126602 (2006).

Total anomalous Hall conductivity



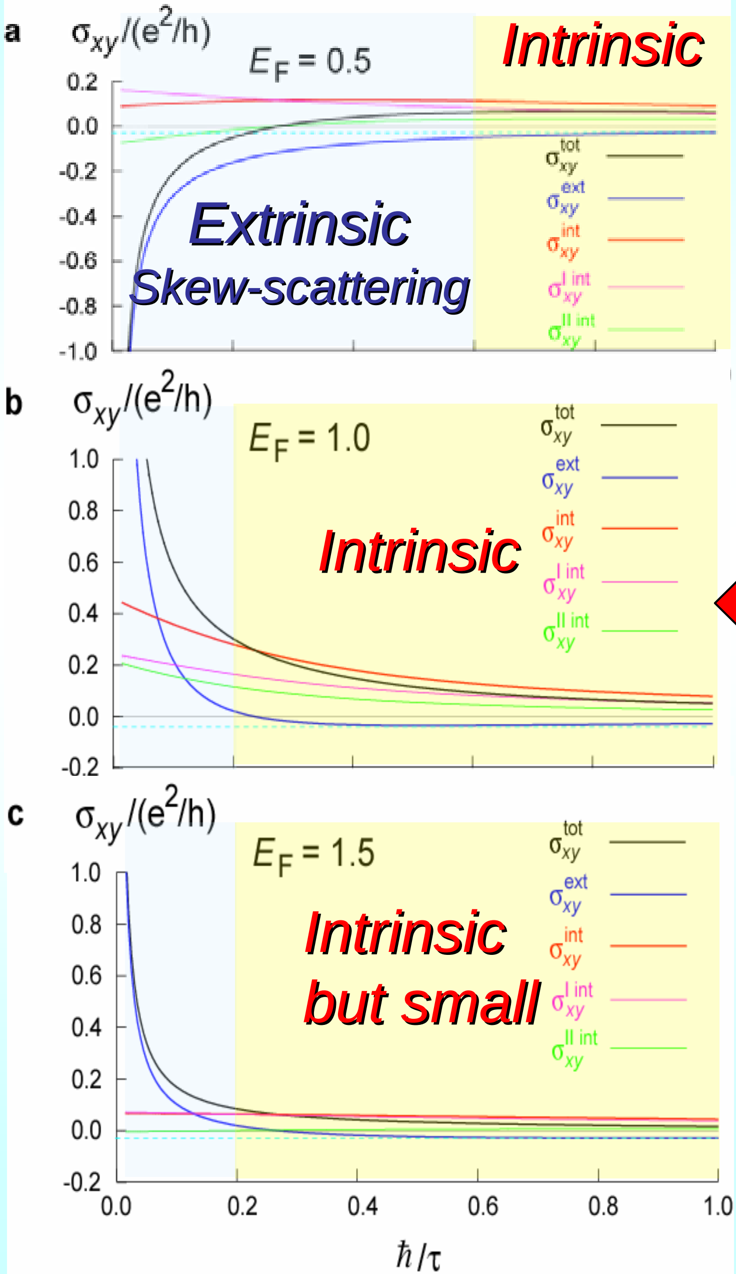
Intrinsic part

$$\sigma_{xy}^{\text{int}} \sim \frac{e^2}{2\hbar}$$

with the resonant condition for E_F.

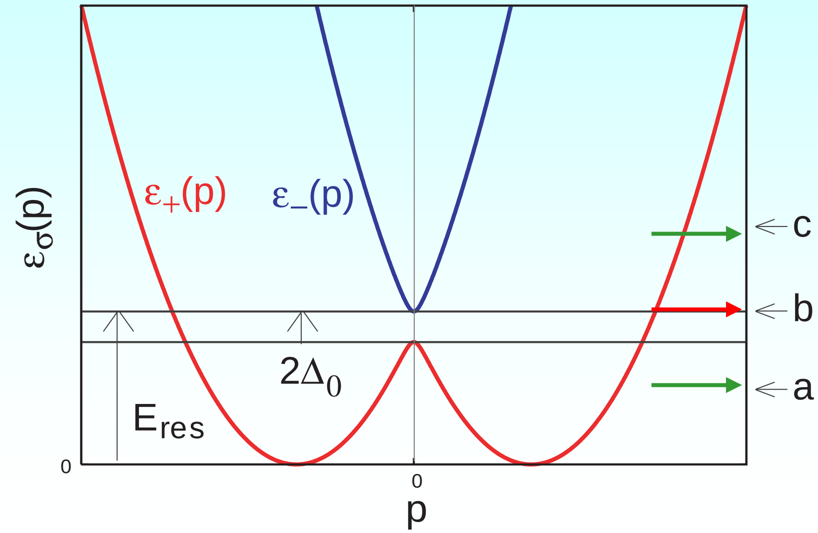
Gradual decrease as $\tau \to 0$.

Extrinsic & intrinsic contributions



σ_{xy}^{tot}

σ_{xy}^{int}



Resonant enhancement of intrinsic contributions

$\sigma_{xy}^{int} \sim e^2/2h$

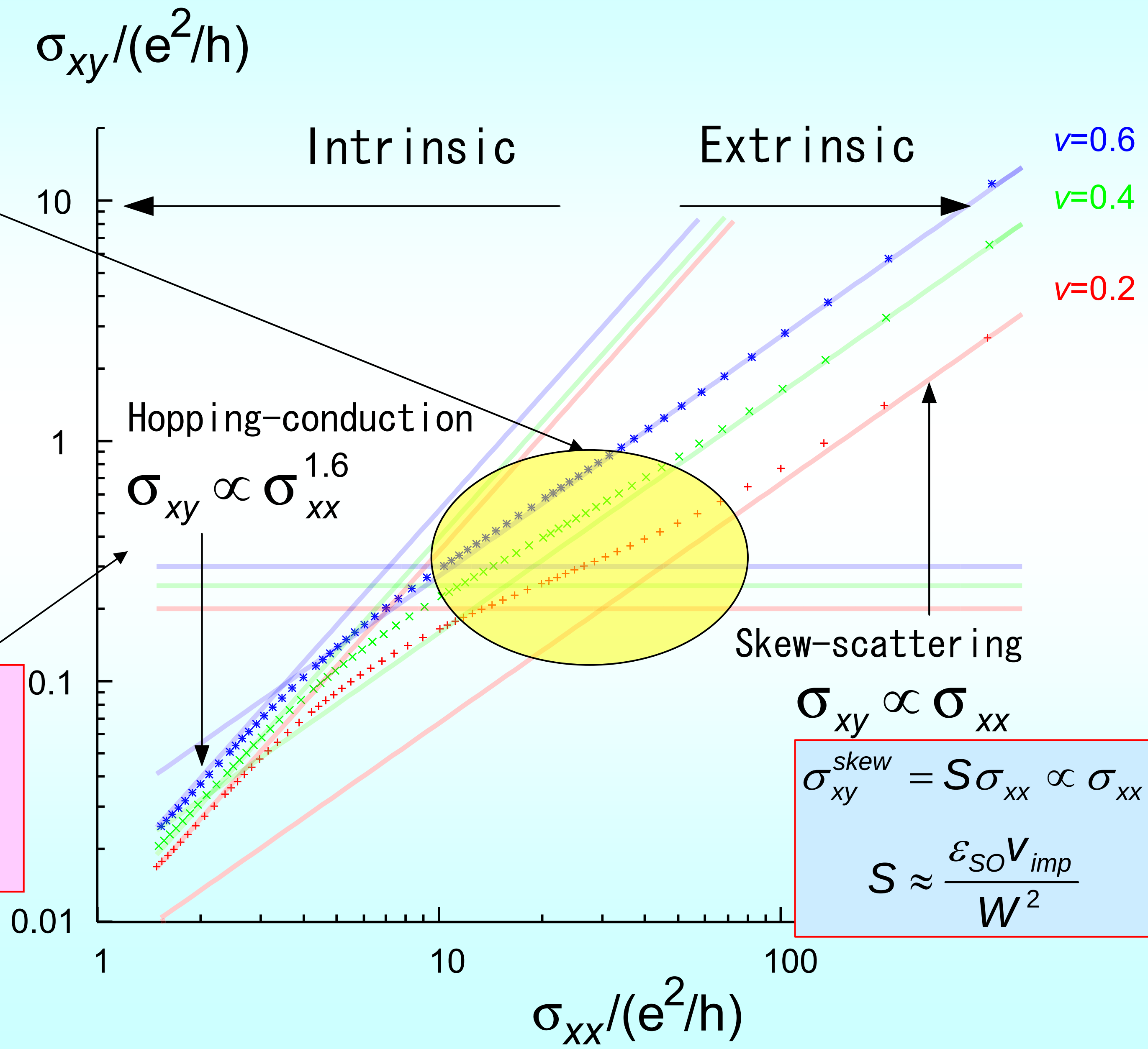
$$\sigma_{xy}^{I\,int} = -e^2\hbar \int \frac{d\boldsymbol{p}}{(2\pi\hbar)^d} \sum_{n,n'} \partial_\varepsilon f(\varepsilon_n(\boldsymbol{p})) \times (\varepsilon_n(\boldsymbol{p}) - \varepsilon_{n'}(\boldsymbol{p})) \Im\left[\langle n\boldsymbol{p}|\partial_{p_x}|n'\boldsymbol{p}\rangle\langle n'\boldsymbol{p}|\partial_{p_y}|n\boldsymbol{p}\rangle\right]$$

appears from the Fermi surface.

Dominant in dirtier case and off the resonance.

Scaling relations

σ_{xy} = constant
in the limit of $v_{imp} \rightarrow 0$
at a fixed $1/\tau$.
Berry-phase contribution

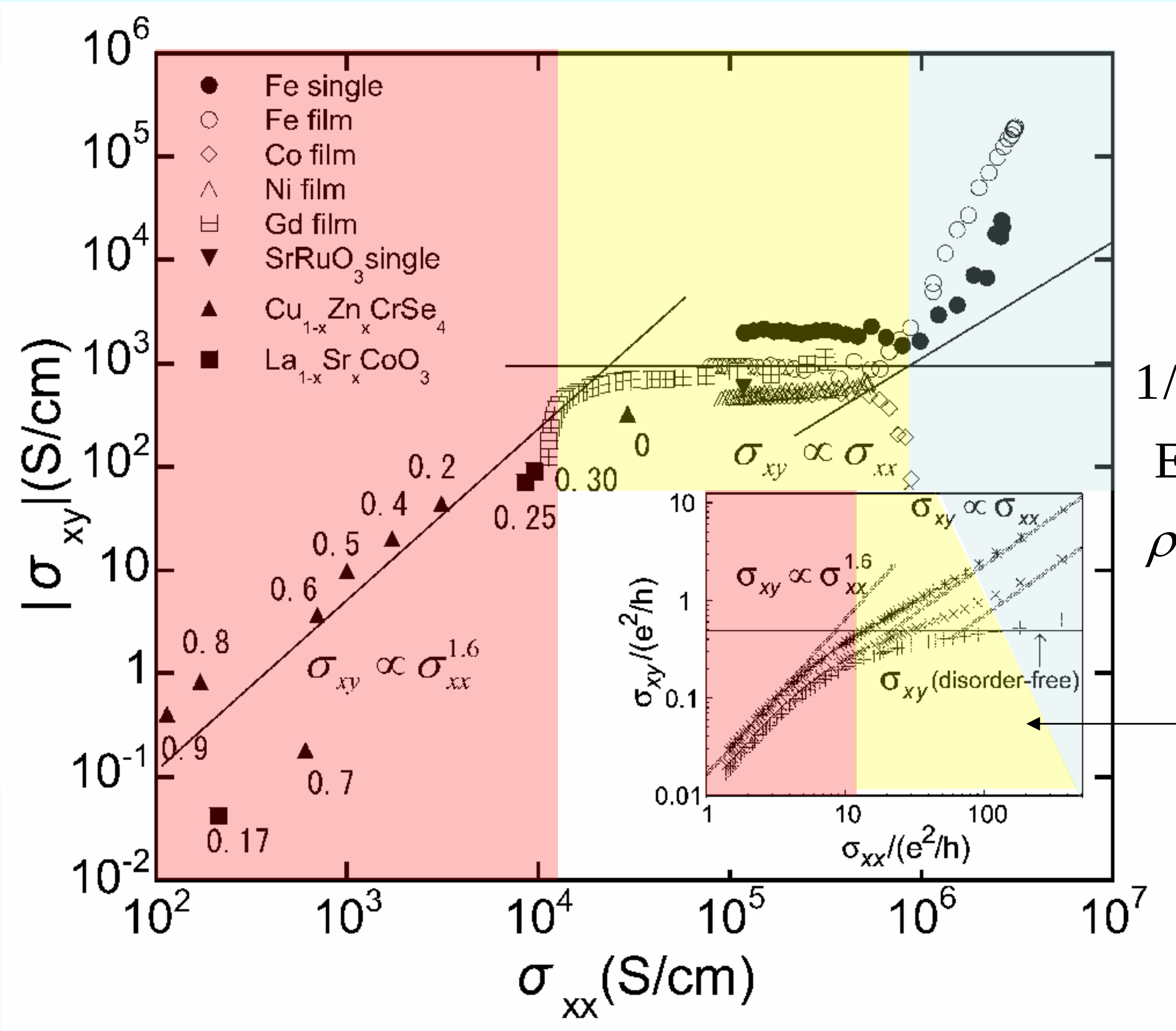


Consistent with the scaling for the insulating behavior of quantum Hall systems [Pryadko-Auerbach (1998)]

$$\sigma_{xy}^{skew} = S\sigma_{xx} \propto \sigma_{xx}$$

$$S \approx \frac{\varepsilon_{SO} v_{imp}}{W^2}$$

Experimental evidence on the crossovers



T. Miyasato, et al., cond-mat/0610324

Extrinsic-intrinsic Crossover around

$$1/\tau \sim \Delta_0 \sim 20\,\mathrm{meV}$$

$$E_F \sim W\ (\text{bandwidth}) \sim 5\,\mathrm{eV}$$

$$\rho_{xx} \sim 2\,\mu\Omega\,\mathrm{cm}$$

Present theory

Summary: unified theory of AHE

Novel crossover in quantum transport (AHE) in multi-band systems as a function of $1/\tau$

$1/\tau$ **Clean**

Extrinsic skew-scattering mechanism. $\rho_H \propto \rho$

Impurity potential and vertex correction are crucial.

ε_{SO}

Intrinsic Berry-phase contribution $\rho_H \propto \rho^2$
in the resonant case (near band-crossing around FS)

Vertex correction rapidly decays.

E_F

Dirty (hopping-conduction)

Damped intrinsic contribution from the FS.
Insulating scaling $\rho_H \propto \rho^{1.6}$

How generic is the model?
→ Clarification of near band-crossing in various systems is required.

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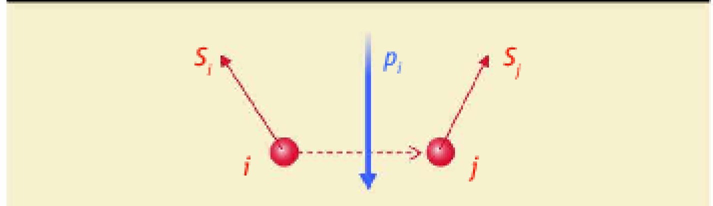
MATERIALS SCIENCE

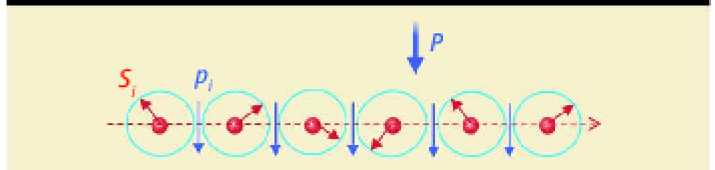
Multiferroics as Quantum Electromagnets

Yoshinori Tokura

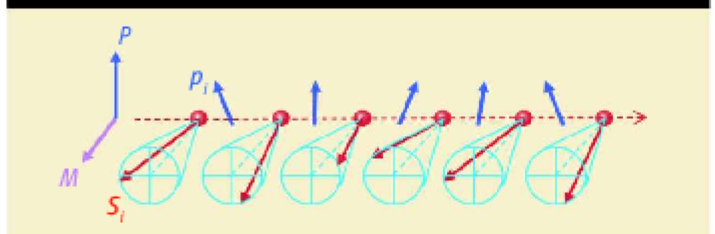
Canted spins on neighboring atomic sites can produce an electronic polarization (p_i) due to overlap of the electronic wave functions (the spin-exchange interaction) and the spin-orbit interaction.



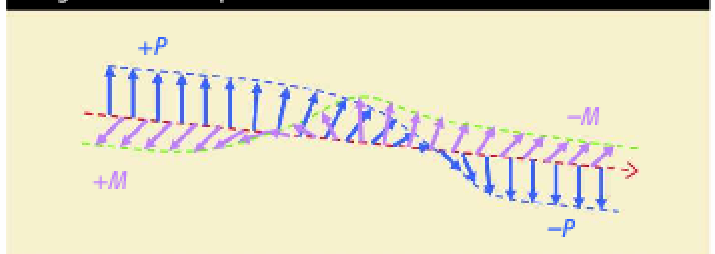
Spiral spin structure can produce a uniform overall polarization P, which is the sum of individual polarizations (p_i).



Conical spin structure allows both uniform magnetization M and polarization P, producing a multiferroic state of purely magnetic origin.



Clamping of ferromagnetic and ferroelectric domain walls may allow electric (or magnetic) field–induced reversal of magnetization (or polarization).



<u>Multiferroics</u>

Ferroelectric, ferromagnetic, ...

<u>Uniform polarization in spiral spin structure</u>

- Dzyaloshinskii-Moriya interaction

  (spatial inversion symmetry breaking)

  [Sergienko-Daggotto]

- Spin-current induced polarization

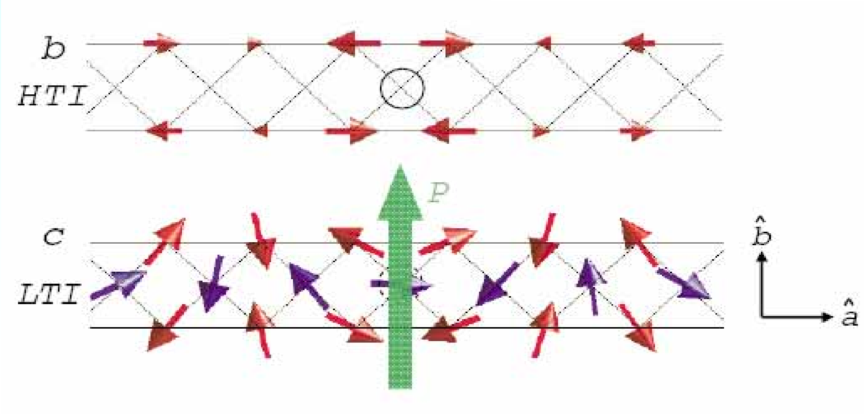
  (ferroelectrics due to non-collinear magnetism)

  [Katsura-Nagaosa-Balatsky]

<u>Magneto-electric effect</u>

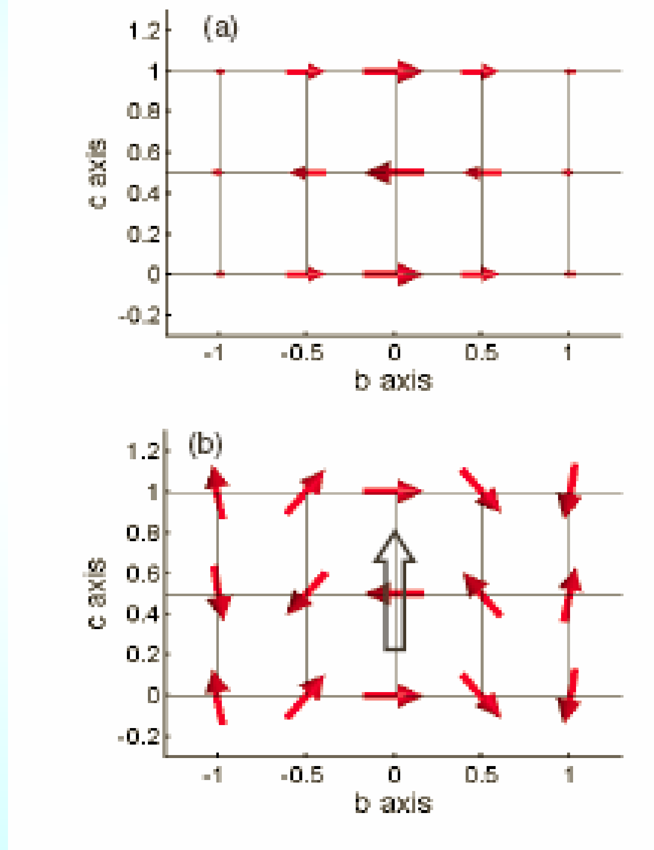
Ferroelectrics due to Non-collinear magnetism

$Ni_3V_2O_8$ [Lawes et al. (2005)]



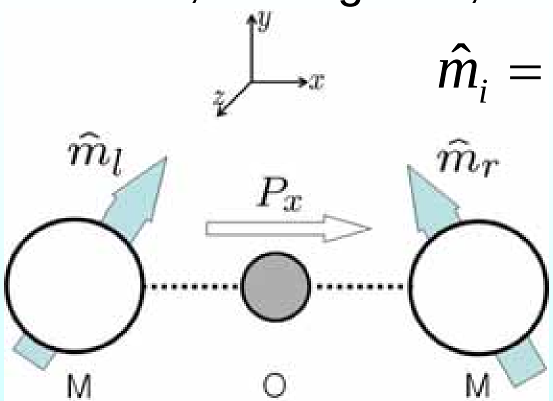
TbMnO$_3$

[Kenzelman et al. (2005)]

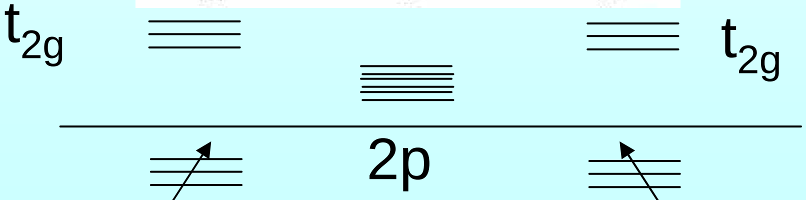


[C. Jia, S. Onoda, N. Nagaosa, J.H. Han, PRB in press]

$$\hat{m}_i = m(\cos\phi_i, \sin\phi_i)$$



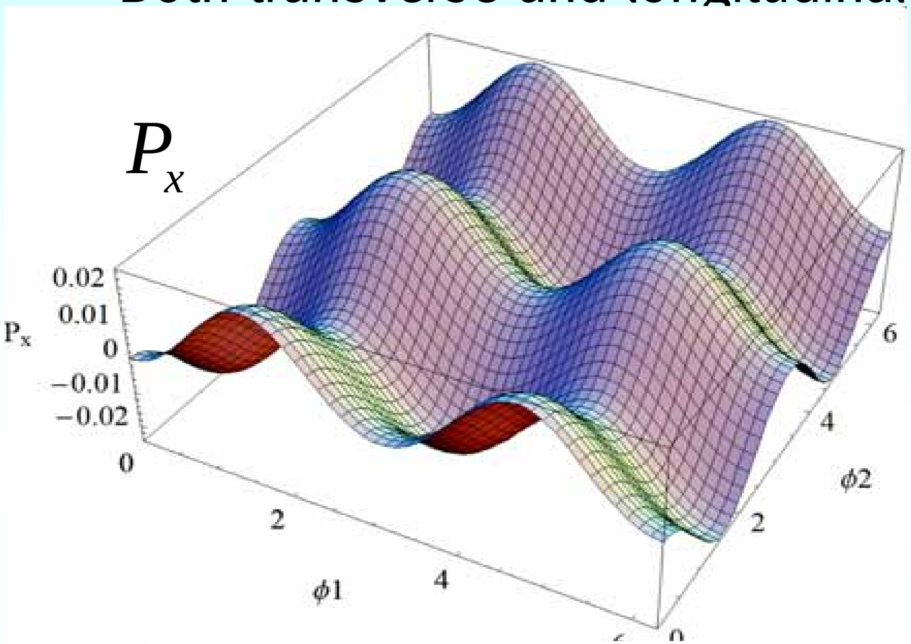
Spin-orbit int.

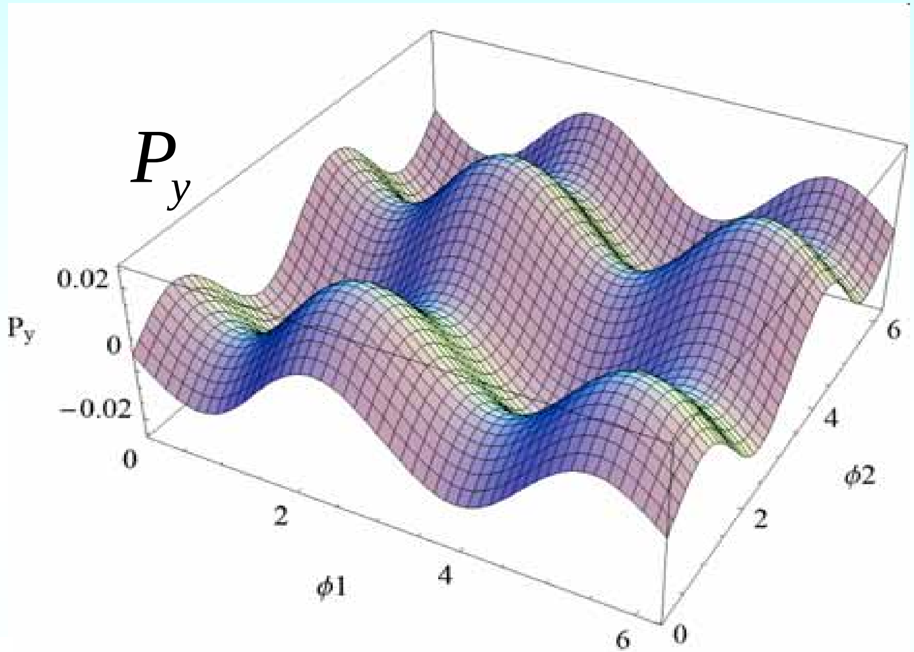


c.f. Katsura-Nagaosa-Balatsky

One hole per magnetic ion (t_{2g} orbital)

Both transverse and longitudinal dipole moments are induced.





$$P_x/L = A\left[\cos(2\phi_r) - \cos(2\phi_l)\right]$$

$$P_y/L = -B_1 \sin(\phi_r - \phi_l) + B_2\left[\sin(2\phi_r) - \sin(2\phi_l)\right]$$

Rotating with half the periodicity

Spin-current

$A \sim B_2 \sim 200\ \mathrm{nC/cm^2}$

$B_1 \sim 80\ \mathrm{nC/cm^2}$