

# Anomalous Hall effect — local orbital approach

## Structure of the talk:

- ▶ Experimental observations of the anomalous Hall effect, scaling of the anomalous Hall conductance
- ▶ Anomalous Hall conductance for ideal Bloch systems, Berry phase curvature corrections
- ▶ Effect of the local orbital fluctuations
- ▶ Drude-Zener type formula
- ▶ Concluding remarks

# Anomalous Hall effect — experimental observations

Anomalous Hall effect is observed on ferromagnetic systems.  
It is similar to normal Hall effect

$$\frac{U_H}{J} \rightarrow \frac{\mathcal{E}_y}{j_x} \equiv \rho_{yx} = R_H B_{\text{eff}} = R_H (B + \gamma M) \equiv R_H B + R_1 M$$

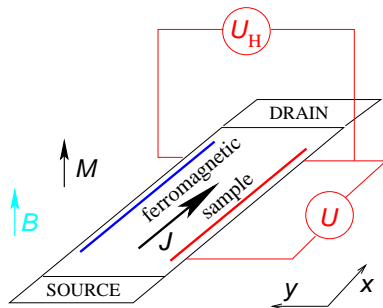
$B$  = external magnetic field

$M$  = magnetization

$$\lim_{B \rightarrow 0} U_H \neq 0$$

Another essential difference  
from the standard Hall effect:

$\gamma$  and consequently  $B_{\text{eff}}$  depends on the resistivity  $\rho = \rho_{xx}$

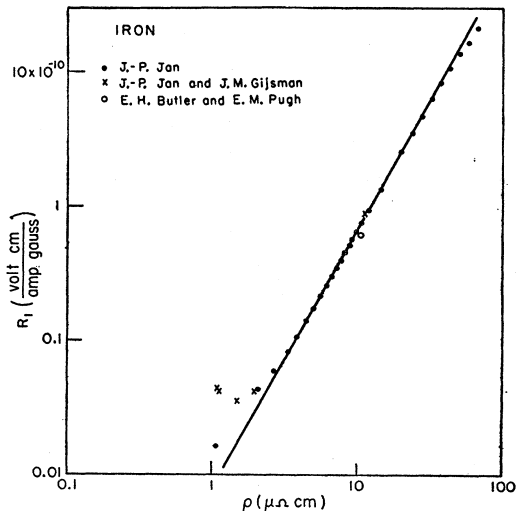


## On Fe for the first time "intrinsic anomalous Hall effect" was observed

E. H. Butler and E. M. Pugh, Phys. Rev. **57**, 916 (1940)

J.-P. Jan, Helv. Phys. Acta. **25**, 677 (1952)

J.-P. Jan and J. M. Gijnsman, Physica **18**, 339 (1952)



for Fe  $R_1 \sim \rho_{AH} \sim \rho^2$

off-diagonal  
cond. component

$$\sigma_{AH} = \frac{\rho_{AH}}{\rho^2 + \rho_{AH}^2}$$

for  $\rho \gg \rho_{AH}$

$$\sigma_{AH} \approx \frac{\rho_{AH}}{\rho^2}$$

independent  
on scattering

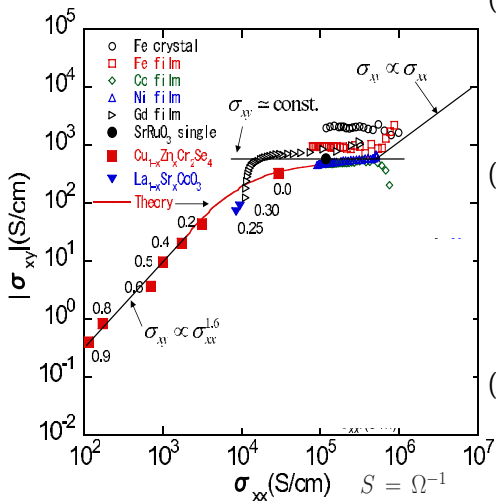


intrinsic effect

# Three broad regimes have been identified when surveying a large body of experimental data for diverse materials.

review by Nagaosa et al, Rev. Mod. Phys. **82**, 1539 (2010)

Miyasato et al, Phys. Rev. Lett. **99**, 086602 (2007)



## (i) high conductivity

$$\sigma_{xx} > 10^6 \Omega^{-1} \text{cm}^{-1}$$

$$\sigma_{xy}^{\text{AH}} \approx \sigma_{xx}^{\alpha}$$

? skew scatt. dominates ?

## (ii) intrinsic regime

(good metal)

$$10^4 < \sigma_{xx} < 10^6 \Omega^{-1} \text{cm}^{-1}$$

$$\sigma_{xy}^{\text{AH}} \approx [\sigma_{xx}]^0$$

scattering independent

## (iii) bad metal

$$\sigma_{xx} < 10^4 \Omega^{-1} \text{cm}^{-1}$$

$$\sigma_{xy}^{\text{AH}} \approx [\sigma_{xx}]^{1.6-1.8}$$

hopping regime

# Physical origin of the anomalous Hall effect

It is generally accepted that **anomalous Hall effect**  
originates in spin-orbit coupling together with exchange interaction

They remove degeneracy of the energy spectrum and the effective single particle Hamiltonian is composed of the three terms  $H \equiv H_0 + H_{so} + H_z$  .

$$H_0 = \frac{\vec{p}^2}{2m_0} + V(\vec{r}) \quad , \quad H_{so} = \frac{\lambda_c^2}{4\hbar} \vec{\sigma} \cdot [\vec{\nabla} V(\vec{r}) \times \vec{p}] \quad , \quad H_z = -\mu_B \vec{B}_{\text{eff}} \cdot \vec{\sigma}$$

where  $\lambda_c$  denotes an effective Compton length, elements of the vector  $\vec{\sigma}$  are Pauli matrices and  $V(\vec{r})$  denotes a background potential.

Hamiltonian  $H_z$  describes Zeeman-type spin splitting due to the exchange-correlation energy represented by an effective field  $\vec{B}_{\text{eff}}$ .

Velocity operator reads

$$\vec{v} \equiv \frac{1}{i\hbar} [\vec{r}, H] = \frac{\vec{p}}{m_0} + \frac{\lambda_c^2}{4\hbar} \vec{\sigma} \times \vec{\nabla} V(\vec{r})$$

If  $V(\vec{r})$  is of the translation symmetry, eigenfunctions are of the Bloch form, and velocity expectation values are determined by the energy dispersion  $E_n(\vec{k})$

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar} \vec{\nabla}_{\vec{k}} E_n(\vec{k})$$

# Kubo formula for Hall conductivity

Hall conductivity is often presented as the sum of two ensemble averaged contributions

$$\sigma_{xy}(\mu) = \left\langle \sigma_{xy}^{(I)}(\mu) \right\rangle_{\text{av}} + \left\langle \sigma_{xy}^{(II)}(\mu) \right\rangle_{\text{av}} = -\sigma_{yx}(\mu)$$

"Fermi surface" term

$$\sigma_{xy}^{(I)}(\mu) = e^2 \frac{i\hbar}{2} \text{Tr} \left\{ \delta(\mu - H) [v_x G^+(\mu) v_y - v_y G^-(\mu) v_x] \right\}$$

and the "Fermi see" term

$$\sigma_{xy}^{(II)}(\mu) = \frac{e^2}{2} \text{Tr} \left\{ \delta(\mu - H) [x v_y - y v_x] \right\} = -e^2 \text{Tr} \left\{ \delta(\mu - H) y v_x \right\}$$

This form has been derived to get quantum Hall effect but it is not suitable if the chemical potential is located within an energy band. For perfect Bloch electron systems it can be rewritten as

$$\sigma_{xy}(\mu) = -\frac{e}{V_{\text{ws}}} \sum_n \left[ \vec{P}_n(\mu) \right]_z$$
$$\frac{\vec{P}_n(E)}{V_{\text{ws}}} \equiv -\frac{e}{8\pi^3} \int_{\text{BZ}} \delta(E_n(\vec{k}) - E) \vec{r}_n(\vec{k}) \times \vec{v}_n(\vec{k}) d^3k$$

# Intrinsic AHE in terms of the Berry phase curvature

$$\begin{aligned}\sigma_{xy}(\mu) &= -\frac{e^2}{8\pi^3} \sum_n \left[ \int_{\text{BZ}} \frac{df_0}{d\mu} \vec{v}_n(\vec{k}) \times \vec{r}_n(\vec{k}) d^3k \right]_z = \\ &= \frac{e^2}{h} \frac{1}{4\pi^2} \sum_n \left[ \int_{\text{BZ}} [\vec{\nabla}_{\vec{k}} f_0] \times \vec{r}_n(\vec{k}) d^3k \right]_z\end{aligned}$$

Periodic part of Bloch functions  $u_{n,\vec{k}}(\vec{r})$  can be expressed via Wannier functions  $\phi_n(\vec{r} - \vec{R}_l)$  and for coordinate expectation value  $\vec{r}_n(\vec{k})$  we get

$$u_{n,\vec{k}}(\vec{r}) = \sum_{l=1}^N \frac{e^{i\vec{k}(\vec{R}_l - \vec{r})}}{\sqrt{N}} \phi_n(\vec{r} - \vec{R}_l) \Rightarrow \vec{r}_n(\vec{k}) = -\text{Im} \int_{V_{\text{ws}}} u_{n,\vec{k}}^+(\vec{r}) \vec{\nabla}_{\vec{k}} u_{n,\vec{k}}(\vec{r}) d^3r$$

Integration per parts gives the expression already derived by Karplus and Luttinger [PR **95**, 1154 (1954)]

$$\sigma_{xy}(\mu) = -\frac{e^2}{h} \frac{1}{4\pi^2} \sum_n \int_{\text{BZ}} f_0 (E_n(\vec{k}) - \mu) [\vec{\Omega}_n(\vec{k})]_z d^3k$$

where the Berry phase curvature  $\vec{\Omega}_n(\vec{k})$  of Bloch states reads

$$\vec{\Omega}_n(\vec{k}) \equiv -\text{Im} \langle \vec{\nabla}_{\vec{k}} u_{n,\vec{k}} | \times | \vec{\nabla}_{\vec{k}} u_{n,\vec{k}} \rangle$$

# Orbital polarization momentum

For perfect Bloch electron system Hall conductivity reads

$$\sigma_{xy}(\mu) = -\frac{e}{V_{\text{ws}}} \sum_n \left[ \vec{P}_n(\mu) \right]_z$$
$$\frac{\vec{P}_n(E)}{V_{\text{ws}}} \equiv -\frac{e}{8\pi^3} \int_{\text{BZ}} \delta(E_n(\vec{k}) - E) \vec{r}_n(\vec{k}) \times \vec{v}_n(\vec{k}) d^3k$$

Quantity  $\vec{P}_n(\mu)$  represents Fermi electron contribution to the part of the local orbital magnetization, often called as **Berry phase correction to the orbital magnetization**.

It is responsible for current induced charge polarization

since mass-center positions of states having opposite velocity do not coincide. It can thus also be called as **orbital polarization momentum**.

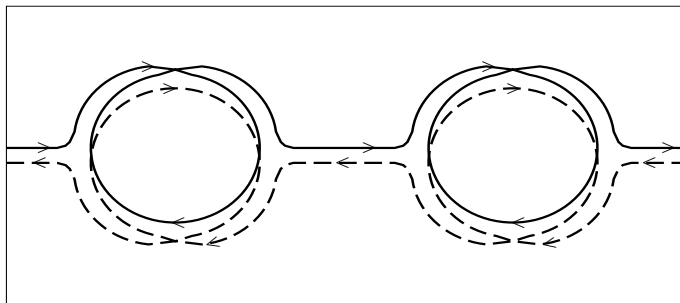
For imperfect systems the above result have to be averaged over the ensemble of the background potential fluctuations

$$\sigma_{xy}(\mu) = -\frac{e}{V_{\text{ws}}} \left\langle \sum_n \left[ \vec{P}_n(\mu) \right]_z \right\rangle_{\text{av}}$$



# Classical view - chain of atomic states

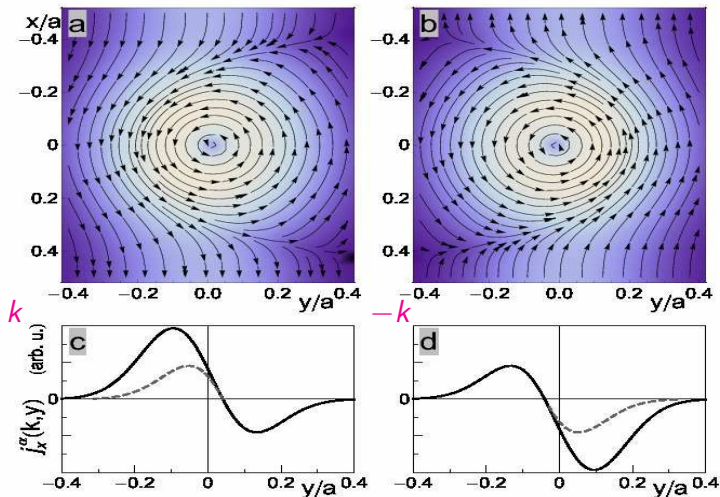
Electron moving within a chain of tight-binding states, say along  $\hat{x}$  direction, has a **finite dwell time that it spends within the unit cell area**. There are two states with  $\pm k_F$  at the Fermi energy.



Part of the current originally circulating within atoms is now forming an outer paths loop of the macroscopic length. It leads to the mass-center separation of states at the Fermi energy having opposite velocity

$$\Delta Y_n(k_F) = \langle n, k_F | y | n, k_F \rangle - \langle n, -k_F | y | n, -k_F \rangle \equiv Y_n(k_F) - Y_n(-k_F)$$

# Current distribution for $p$ -states: $m = -1$ , $s_z = 1/2$



Non-equilibrium occupation of states induces charge polarization.

# Single-band model of the perfect Bloch electron system

If the potential  $V(\vec{r})$  is translationally invariant the considered Hamiltonian

$$H = \frac{\vec{p}^2}{2m_0} + V(\vec{r}) + \frac{\lambda_c^2}{4\hbar} \vec{\sigma} \cdot [\vec{\nabla} V(\vec{r}) \times \vec{p}] - \mu_B \vec{B}_{\text{eff}} \cdot \vec{\sigma}$$

can be for a particular energy band written as follows

$$H = \sum_l |l\rangle E_a \langle l| + \sum_{l,m}^{l \neq m} |l\rangle t_{lm} \langle m|$$

where  $|l\rangle$  and  $|m\rangle$  are Wannier functions representing atomic-like orbitals of the energy  $E_a$  associated with lattice sites  $\vec{R}_l$  and  $\vec{R}_m$ , respectively.

Instead of considering a specific form of the band dispersion it will be assumed that it gives an elliptical density of states which normalized per Wigner-Seitz volume  $V_{\text{ws}}$  reads

$$g(E) = \frac{2}{\pi w^2} \sqrt{w^2 - (E - E_a)^2} \text{ if } |E - E_a| \leq w \quad ; \quad g(E) = 0 \text{ if } |E - E_a| > w$$

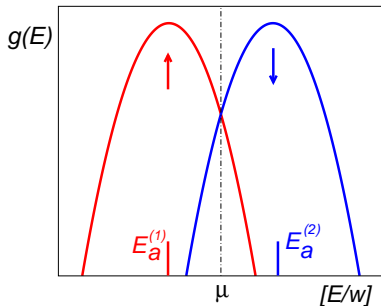
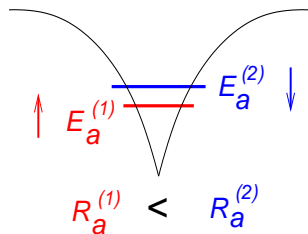
$2w$  = band width. The corresponding mean Fermi velocity reads

$$v_F = \frac{w^2}{2\hbar} \left(\frac{\pi}{2}\right)^{2/3} \tilde{a} g(\mu),$$

where  $\tilde{a} \equiv V_{\text{ws}}^{1/3}$  just equals to the lattice constant for the simple cubic lattice.

# Ferromagnetic system — two-band model

The simplest model of the ferromagnetic system is to consider two fully polarized energy bands.



Expectation value of the radius vector can be approximated by the radius  $R(E_a)$  of the given orbital which is an energy dependent quantity

$$\frac{R(E_a)}{\tilde{a}} \approx \frac{R_0}{\tilde{a}} \left( 1 + \kappa \frac{E_a - E_0}{w} \right) ; \quad [\vec{r}_n(\vec{k}) \times \vec{v}_n(\vec{k})]_z \sim R(E_a) v_F$$

# Disordered systems

The simplest possible approach to model disorder is to assume the so called single-site fluctuations, i.e. a variation of the orbital energy  $E_a$ .

- ▶ Static disorder like impurities, dislocations, grain boundaries and other crystal imperfections,  $E_a \rightarrow E_a + \delta_i$  controlled by an probability distribution  $p(\delta_i)$ .
- ▶ Dynamical disorder like lattice vibrations (temperature fluctuations) represented by the deformation potential,  $E_a \rightarrow E_a + \delta_{\text{th}}$  controlled by the normal probability distribution  $p(\delta_{\text{th}}) \sim \exp(-\delta_{\text{th}}^2/2\Gamma^2)$ .

Numerical results will be presented for Lorentzian distribution

$$p(\delta, \Gamma) = \frac{1}{\pi} \frac{\Gamma}{\delta^2 + \Gamma^2} \Rightarrow \langle \text{Tr} \delta(H + \delta - E) \rangle_{\text{av}} = \frac{1}{\pi} \frac{\Gamma}{[E_n(\vec{k}) - E]^2 + \Gamma^2}$$

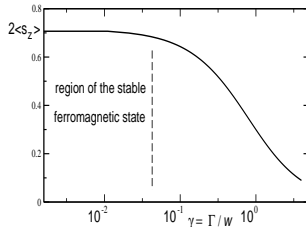
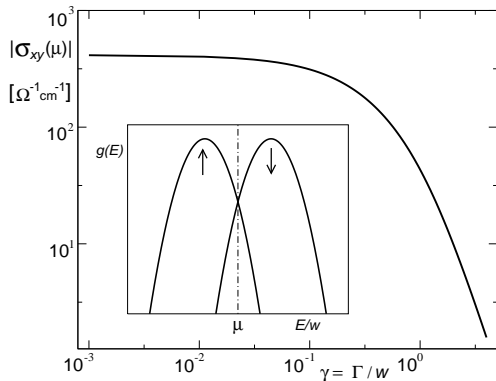
allowing to relate  $\Gamma$  to the electron life time  $\tau = \hbar/2\Gamma$ .

Note that this single-site model fluctuations are not applicable to high conductivity regime for which vertex corrections cannot be neglected.

They vanish in this model!

# Numerical example

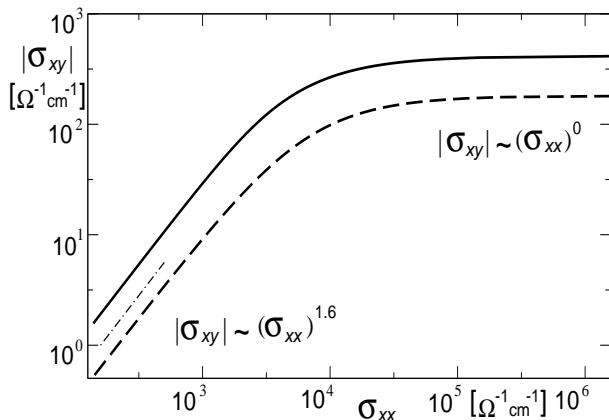
Following set of parameters has been used:  $\tilde{a} = 3\text{\AA}$ ,  $R_a(0)/\tilde{a} = 0.3$ ,  $\kappa = 1$ , and  $(E_a^{(2)} - E_a^{(1)})/w = 0.6$ .



Note, that qualitative features of the anomalous Hall conductivity as function of the inverse electron life-time are not affected by the use of different probability distribution functions.

# Scaling of the anomalous Hall conductivity

Following set of parameters has been used:  $\tilde{a} = 3\text{\AA}$ ,  $R_a(0)/\tilde{a} = 0.3$ ,  $\kappa = 1$  (0.5), and  $(E_a^{(2)} - E_a^{(1)})/w = 0.6$  (0.4).



high  
conductivity  
regime

???

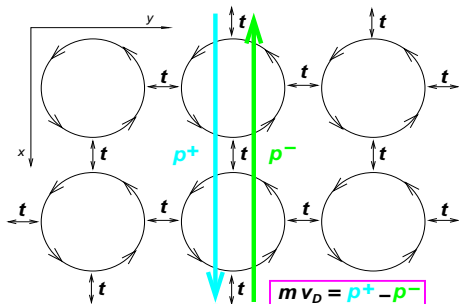
bad metal (hopping) regime || good metal (intrinsic) regime

Qualitative agreement with experimental observations has been obtained!

# Intrinsic AHE — Drude-Zener type formula

Scattering independent anomalous Hall conductivity can be understood by using classical arguments. In the steady state the total force has to vanish

$$\vec{F} = -e N_e \vec{\mathcal{E}} - \frac{1}{c} N_e \vec{v} \times \vec{B} - \left( \frac{\partial \vec{p}}{\partial t} \right)_{\text{scatt}} = 0$$



$$\left( \frac{\partial \vec{p}}{\partial t} \right)_{\text{scatt}} \approx \frac{\vec{p} - \vec{p}_0}{\tau}$$

$\vec{p}_0$  is the momentum density corresponding to the non-dissipative Hall current

$$\begin{aligned} \text{e.g. } j_x^{(H)} &= e^2 v_F g(\mu) \Delta Y \mathcal{E}_y \\ &= -v_F \{ -e g(\mu) \Delta Y e \mathcal{E}_y \} \\ &\quad \text{dipole charge density} \end{aligned}$$

Defining  $\vec{p}_0 \equiv -\frac{m}{e} \vec{j}^{(H)}$  we get

$$\begin{aligned} \text{Generally } \vec{j}^{(H)} &= e \vec{\mathcal{P}} \times \vec{\mathcal{E}} \\ \vec{\mathcal{P}} &= -e g(E_F) \vec{R} \times \vec{v}_F(\vec{R}) \end{aligned}$$

$$\vec{j} - \tau \vec{\omega}_c \times \vec{j} = \frac{e^2 \tau N_e}{m} \vec{\mathcal{E}} + e \vec{\mathcal{P}} \times \vec{\mathcal{E}}, \quad \vec{\omega}_c \equiv e \vec{B} / m c$$



# Concluding remarks

- ▶ **Anomalous Hall effect is determined by** the orbital polarization momentum (Berry phase correction to the orbital momentum of Fermi electrons) giving rise to **the local charge polarization induced by the applied current.**
- ▶ Despite of the model simplicity it describes **qualitative features of** the two experimentally observed regimes: **bad metal (hopping) regime and good metal (intrinsic - scattering independent) regime.**
- ▶ **Quantitative agreement could be obtained by using exact form of Wannier functions together with the fluctuation model relevant for the considered material which should be treated by using coherent potential approach.**
- ▶ Used single-site model fluctuations is not acceptable **for the high conductivity regime** for which so called **vertex corrections have to be taken into account.**

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- ▶ **Quantitative agreement could be obtained by using exact form of Wannier functions together with the fluctuation model relevant for the considered material which should be treated by using coherent potential approach.**
- ▶ Used single-site model fluctuations is not acceptable **for the high conductivity regime** for which so called **vertex corrections have to be taken into account.**
- ▶ **!!!** Observed properties of the high conductivity regime are puzzling for me since for ideal Bloch systems theory predicts values given by the Berry phase correction to the orbital magnetization which seems to be smaller in the most cases **!!!**