Theoretical description of the anomalous and spin Hall effects in disordered alloys using the Coherent Potential Approximation

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SFB 689 *Spinphänomene in reduzierten Dimensionen*

SPP 1538 *Spin Caloric Transport*

Collaboration

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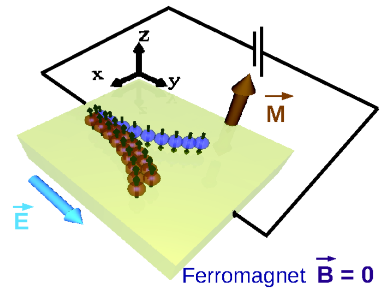
Outline

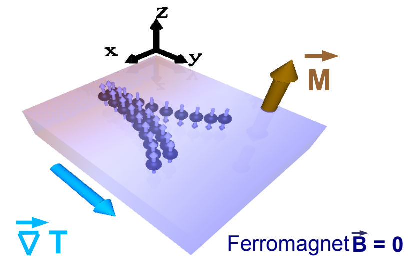
- Introduction
- Electronic structure calculations
- Response to electric field
  - Anomalous Hall Effect (**AHE**)
  - Spin Hall Effect (**SHE**)
- Response to temperature gradient
  - Anomalous Nernst Effect (**ANE**)
  - Spin Nernst Effect (**SNE**)
- Summary

Longitudinal and transverse charge, heat and spin transport in the linear response regime

- Charge
- Heat — current density
- Spin

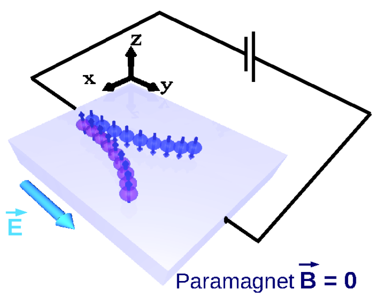


AHE

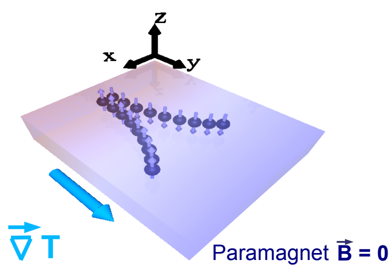


ANE

$$\begin{pmatrix} \vec{j}^{c} \\ \vec{j}^{q} \\ J^{s} \end{pmatrix} = \begin{pmatrix} L^{cc} & L^{cq} & \mathcal{L}^{cs} \\ L^{qc} & L^{qq} & \mathcal{L}^{qs} \\ \mathcal{L}^{sc} & \mathcal{L}^{sq} & \tilde{\mathcal{L}}^{ss} \end{pmatrix} \begin{pmatrix} \vec{E} \\ -\vec{\nabla} T / T \\ F^{s} \end{pmatrix}$$



SHE



SNE

- Electric field
- Temperature gradient
- Fictitious field coupling to spin

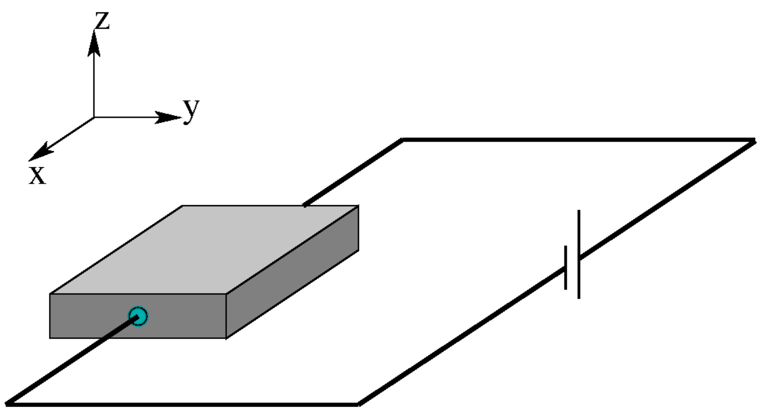
Goal: investigation treating all microscopic contributions on equal footing on first-principles level

study of pure systems and disordered alloys

Generalized Ohm's law for ferromagnets

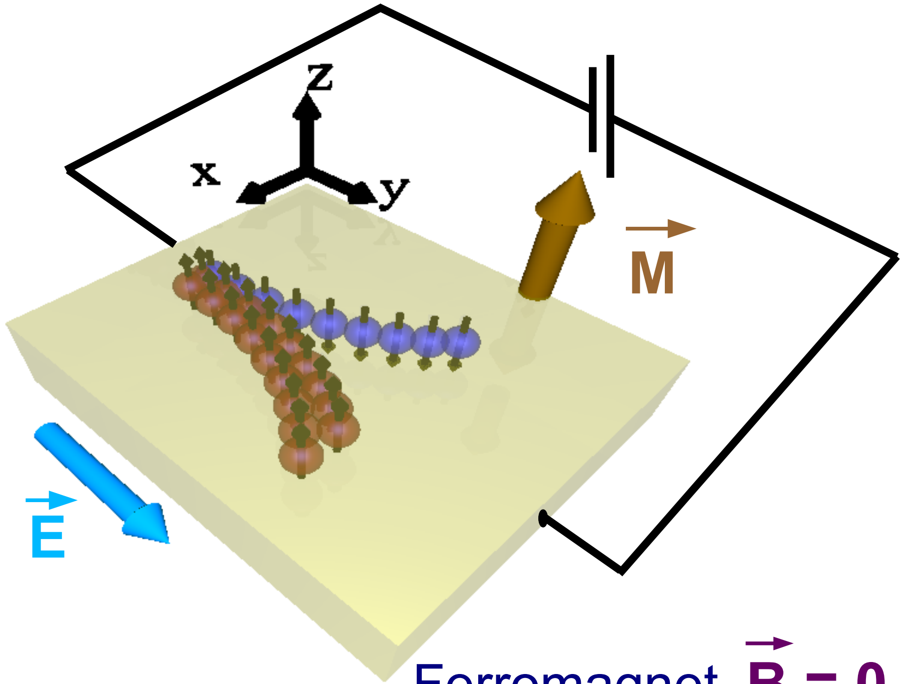
Ohm's law $\vec{j} = \underline{\underline{\sigma}}\vec{E}$

longitudinal and transverse currents



$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

Anomalous Hall Effect (AHE)



Separating charge (+ spin)

Source **relativistic** spin-orbit interaction

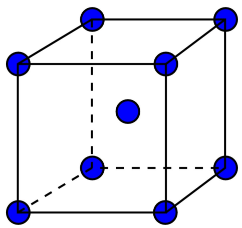
Structure of the conductivity tensor σ

Neumann's Principle

$$\sigma = S\,\sigma\,S^{\dagger} \quad \forall S \in G$$

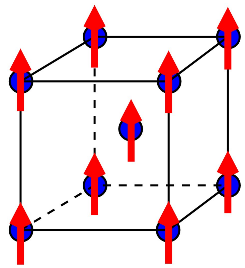
paramagnetic

G = *m3m*



ferromagnetic

G = *4/mm'm'*



$$\underline{\underline{\sigma}} = \begin{pmatrix} \sigma & 0 & 0 \\ 0 & \sigma & 0 \\ 0 & 0 & \sigma \end{pmatrix}$$

Isotropic conductivity
or resistivity

$$\underline{\underline{\sigma}} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

Galvano-magnetic effects
Anomalous Hall effect

σ_{xy} or ρ_{xy}

Anisotropic magnetoresistance AMR

$$\frac{\Delta\rho}{\bar{\rho}} = \frac{\rho_{\|} - \rho_{\perp}}{\frac{1}{3}\rho_{\|} + \frac{2}{3}\rho_{\perp}}$$

Kleiner, PR **142**, 318 (1966)

The Dirac Equation for magnetic solids

$$\Big[\frac{\hbar}{i} c\vec{\alpha}\cdot\vec{\nabla} + \beta mc^2 + \bar{V}(\vec{r}) + \underbrace{\beta\vec{\sigma}\cdot\vec{B}_{\text{eff}}(\vec{r})}_{V_{\text{spin}}(\vec{r})}\Big]\Psi(\vec{r},E) = E\,\Psi(\vec{r},E)$$

effective magnetic field

$$\vec{B}_{\text{eff}}(\vec{r}) = \frac{\delta E_{\text{xc}}[n,\vec{m}]}{\delta\vec{m}(\vec{r})}$$

is determined by the spin magnetisation $\vec{m}(\vec{r})$ within **spin density functional theory (SDFT)**

Within an atomic cell one can choose $\hat{z}'$ to have:

$$V_{\text{spin}}(\vec{r}) = \beta\sigma_{z'}\,B_{\text{eff}}(r)$$

Electronic structure calculations

Electronic structure represented by **Green's function**

$$G^{+}(\vec{r},\vec{r}\,',E) = \lim_{\epsilon\to 0}\sum_i \frac{\Psi_i(\vec{r})\Psi_i^{\dagger}(\vec{r}\,')}{E-E_i+i\epsilon}$$

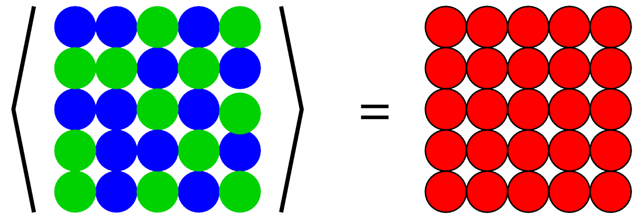
Korringa-Kohn-Rostoker (**KKR**) method
based on multiple scattering theory

$$G^{+}(\vec{r},\vec{r}\,',E) = \sum_{\Lambda\Lambda'} Z_\Lambda(\vec{r},E)\,\tau^{nm}_{\Lambda\Lambda'}(E)\,Z^{\times}_{\Lambda}(\vec{r}\,',E) - \delta_{nm}\sum_{\Lambda} Z_\Lambda(\vec{r}_<,E)\,J^{\times}_{\Lambda}(\vec{r}_>,E)$$

$Z\ (J)$	regular (irregular) solution of single-site Dirac equation
τ	scattering path operator
$\Lambda = (\kappa,\mu)$	relativistic angular momentum quantum numbers

Coherent Potential Approximation - CPA

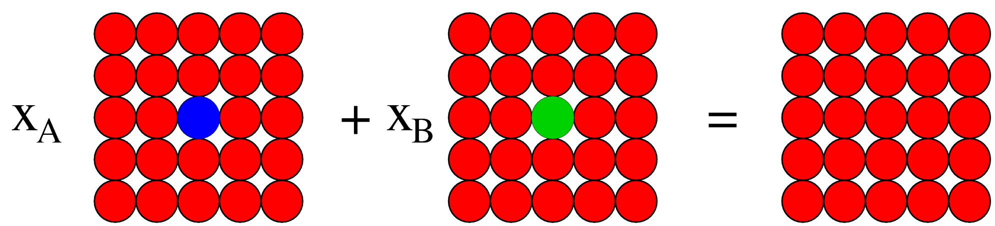
- effective CPA medium represents the electronic structure of an configurationally averaged substitutionally random alloy A_xB_{1-x}



Soven (1967)

- use mean field description – find best possible single-site scheme

Embedding of an A- or B-atom into the CPA-medium
- in the average - should not give rise to additional scattering



$$x_A \underline{\tau}^{nn,A} + x_B \underline{\tau}^{nn,B} = \underline{\tau}^{nn,CPA}$$

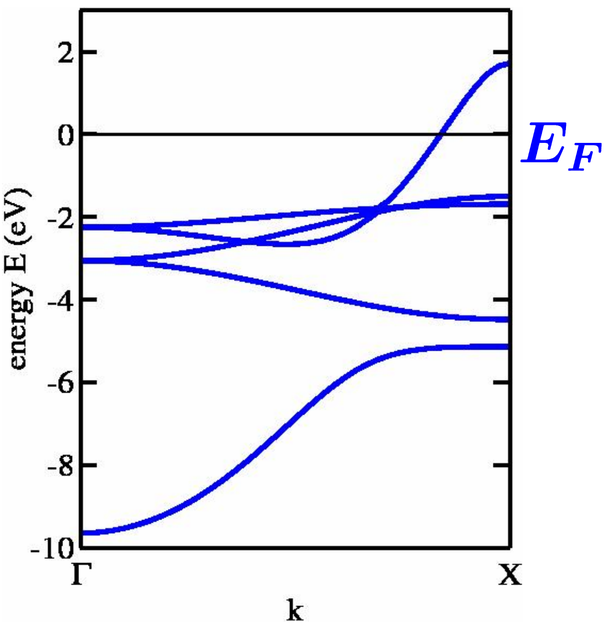
projected scattering path operator

$$\underline{\tau}^{nn,\alpha} = \underline{\tau}^{nn,CPA} \left[1 + \left(\underline{t}_\alpha^{-1} - \underline{t}_{CPA}^{-1} \right) \underline{\tau}^{nn,CPA} \right]^{-1}$$

Band structure of disordered alloys

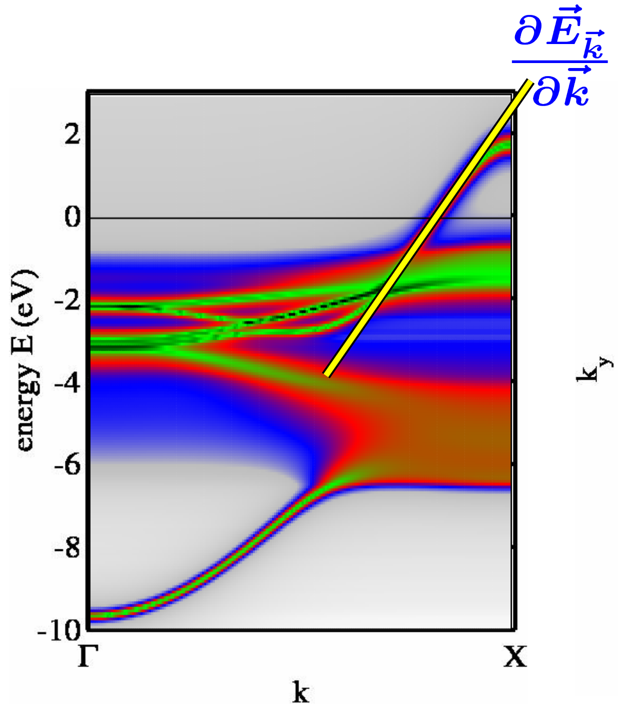
Dispersion relation of pure Cu

$\vec{k}$ along Γ-X



Bloch spectral function $A_{\mathrm{B}}(\vec{k}, E)$ of $Cu_{0.80}Pd_{0.20}$

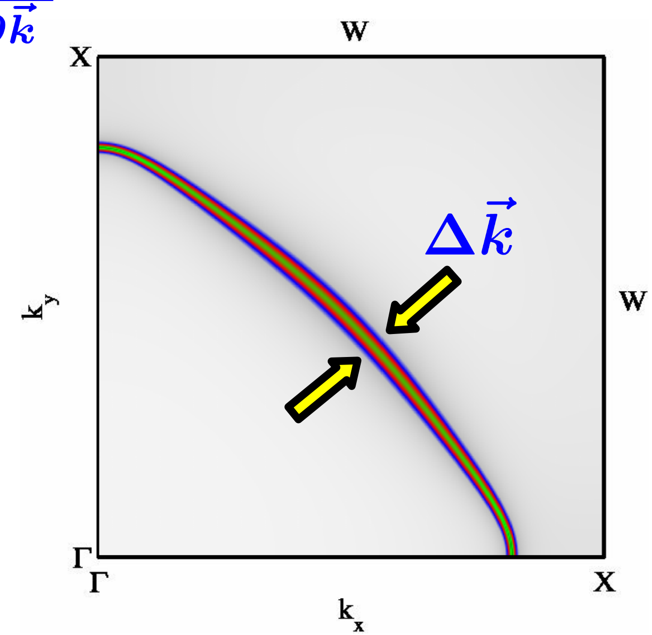
$\vec{k}$ along Γ-X



group velocity

$$\vec{v}_{\vec{k}} = \frac{1}{\hbar} \frac{\partial \vec{E}_{\vec{k}}}{\partial \vec{k}}$$

Fermi surface in Γ-X-W-plane



life time

$$\tau_{\vec{k}} = \hbar / \Delta E_{\vec{k}}$$

$$\Delta E_{\vec{k}} = \Delta\vec{k} \frac{\partial E_{\vec{k}}}{\partial \vec{k}}$$

Kubo-Středa (KS) equation (T = 0 K)

$$\sigma_{\mu\nu} = \frac{\hbar}{4\pi\Omega}\mathrm{Tr}\left\langle \hat{j}_\mu(G^+ - G^-)\hat{j}_\nu G^- - \hat{j}_\mu G^+ \hat{j}_\nu (G^+ - G^-)\right\rangle_c + \frac{|e|}{4\pi i\Omega}\mathrm{Tr}\left\langle (G^+ - G^-)(\hat{r}_\mu \hat{j}_\nu - \hat{r}_\nu \hat{j}_\mu)\right\rangle_c$$

Smrčka and Středa, JPC **10**, 2153 (1977)

with current density operator $\hat{j}_\mu = -|e|c\,\alpha_\mu$

allows calculation of the full conductivity tensor

$$\sigma = \begin{pmatrix} \sigma_\perp & -\sigma_\mathrm{H} & 0 \\ \sigma_\mathrm{H} & \sigma_\perp & 0 \\ 0 & 0 & \sigma_\parallel \end{pmatrix} \quad \text{for } \vec{M}||\hat{z} \text{ and } G = 4/mm'm'$$

Kubo-Greenwood equation and Vertex corrections

Implementation within KKR-CPA

$$\tilde{\sigma}_{\mu\nu} = -\frac{4m^2}{\pi\hbar^3\Omega} \Bigg\{ \sum_{\alpha,\beta} \sum_{\substack{\Lambda_1,\Lambda_2\\ \Lambda_3,\Lambda_4}} c^\alpha c^\beta \tilde{J}^{\alpha\mu}_{\Lambda_4,\Lambda_1} \Big(\underbrace{[1-\chi\omega]^{-1}}_{\text{vertex correction}} \chi \Big)_{\substack{\Lambda_1,\Lambda_2\\ \Lambda_3,\Lambda_4}} \tilde{J}^{\beta\nu}_{\Lambda_2,\Lambda_3}$$

$$+ \sum_{\alpha} \sum_{\substack{\Lambda_1,\Lambda_2\\ \Lambda_3,\Lambda_4}} c^\alpha \, \tilde{J}^{\alpha\mu}_{\Lambda_4,\Lambda_1} \, \tau^{\mathrm{CPA},00}_{\Lambda_1,\Lambda_2} \, J^{\alpha\nu}_{\Lambda_2,\Lambda_3} \, \tau^{\mathrm{CPA},00}_{\Lambda_3,\Lambda_4} \Bigg\}$$

$\Lambda = (\kappa, \mu)$
relativistic quantum numbers

Vertex corrections (VC)

$$< jG >< jG > \rightarrow < jGjG >$$

account for
scattering-in processes

Butler, PRB **31**, 3260 (1985) (non-relativistic)
Banhart *et al.*, SSC **77**, 107 (1991) (fully-relativistic)
Turek *et al.*, PRB **65**, 125101 (2002) (LMTO-CPA)

See also: Velicky, PR **184**, 614 (1969)

Connection with Boltzmann Formalism

Kubo-Greenwood equation within KKR-CPA

$$\tilde{\sigma}^{1}_{\mu\nu} = \frac{-4m^2}{\pi\hbar^3\Omega} \sum_{\alpha,\beta} c^\alpha c^\beta \sum_{K,K'} \tilde{J}^{\alpha\mu}_{K} \left(\left[1 - \chi w\right]^{-1} \chi \right)_{KK'} \tilde{J}^{\beta\nu}_{K'}$$

Neglecting the vertex corrections gives
Boltzmann equation without scattering-in term

$$\sigma^{\mathrm{NVC}}_{\mu\nu}(\varepsilon) = \frac{e^2}{(2\pi)^3} \int_\varepsilon \frac{dS_{\vec{k}}}{\hbar v_{\vec{k}}} v^\mu_{\vec{k}} v^\nu_{\vec{k}} \tau^B_{\vec{k}}$$

Boltzmann equation including scattering-in term

$$\sigma_{\mu\nu}(\varepsilon_F) = e^2 \sum_{\vec{k},\vec{k}'} v^\mu_{\vec{k}} \left[1 - \tau^B P\right]^{-1}_{\vec{k}\vec{k}'} v^\nu_{\vec{k}'} \tau^B_{\vec{k}'} \delta(\varepsilon_F - \varepsilon_{\vec{k}'})$$

Inverse lifetime $(\tau^B_{\vec{k}})^{-1} = \sum_{\vec{k}'} P_{\vec{k}\vec{k}'}$

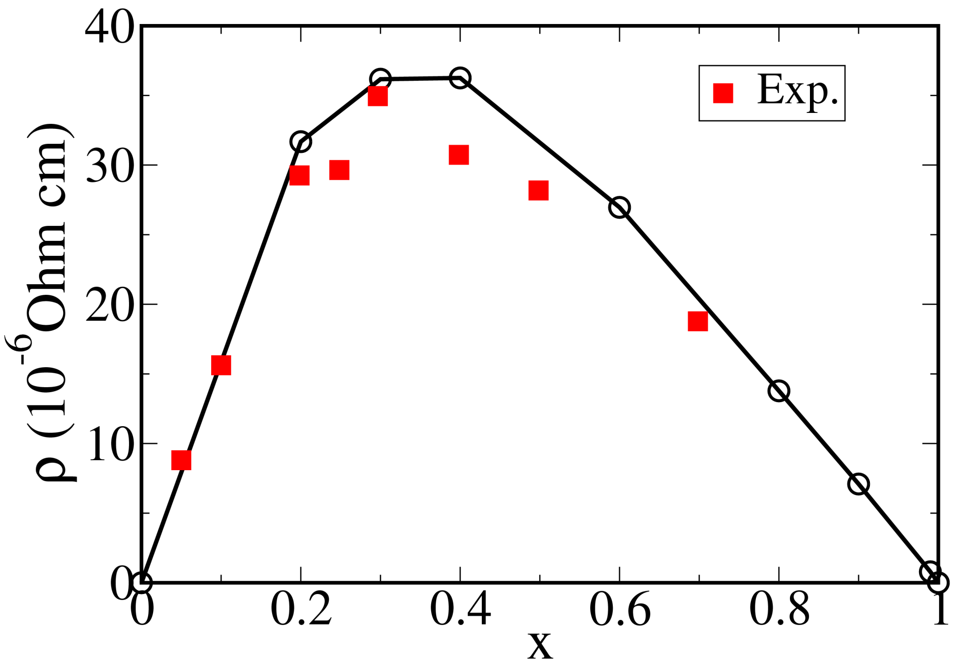
Butler, PRB **31**, 3260 (1985)

Longitudinal residual resistivity of ferromagnetic alloys

Isotropic residual resistivity

$$\rho = \frac{1}{3}\rho_{\parallel} + \frac{2}{3}\rho_{\perp}$$

Co_xPt_{1-x}

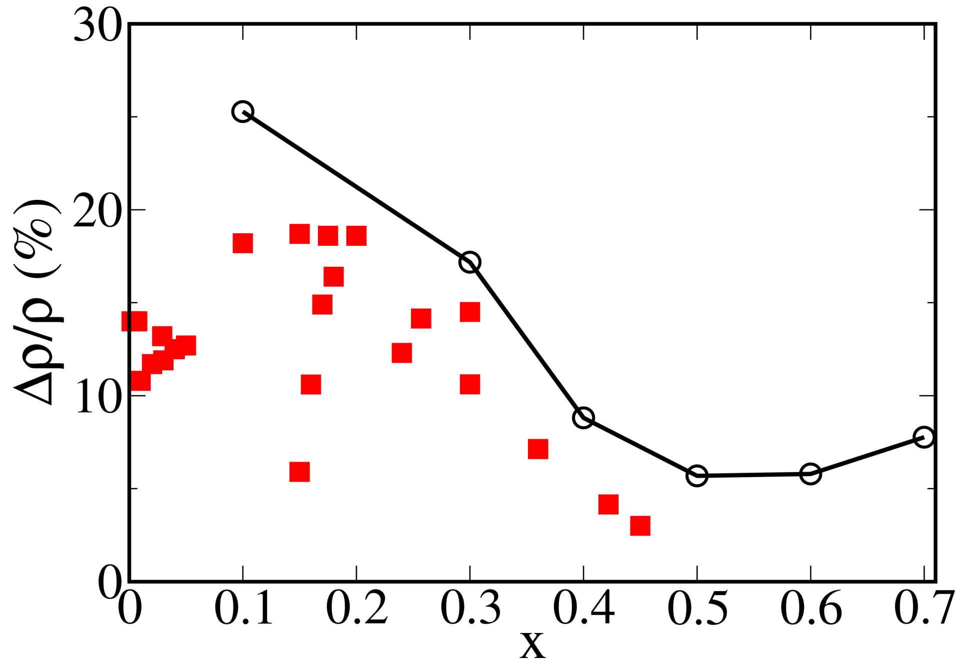


see also:
Ebert *et al.*, PRB **54**, 8479 (1996)

Anisotropic magnetoresistance AMR

$$\frac{\Delta\rho}{\rho} = \frac{\rho_{\parallel} - \rho_{\perp}}{\frac{1}{3}\rho_{\parallel} + \frac{2}{3}\rho_{\perp}}$$

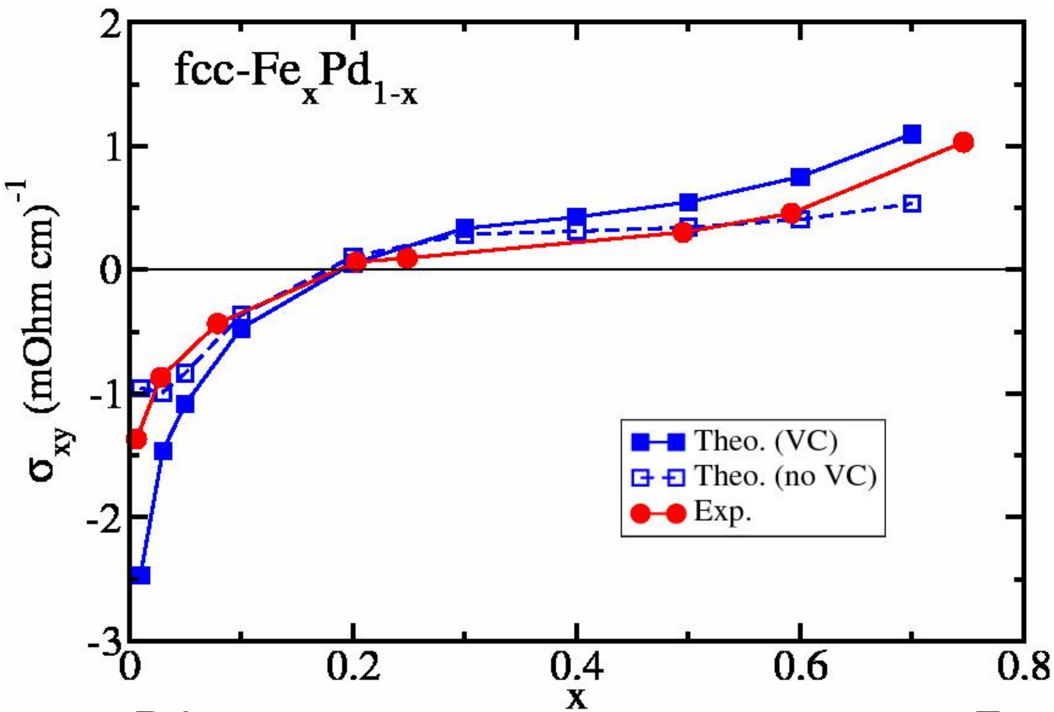
Fe_xNi_{1-x}

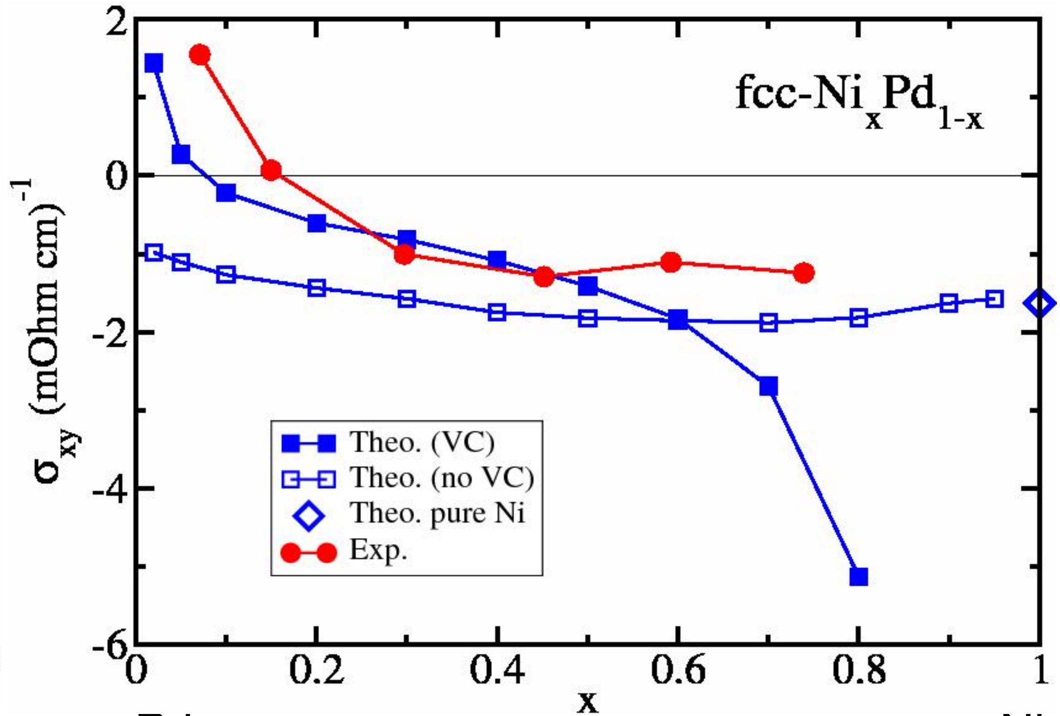


see also :
Banhart *et al.*, PRB **56**, 10165 (1997)
Khmelevskyi *et al.*, PRB **68**, 012402 (2003)
Turek *et al.*, JPCS **200**, 052029 (2010)
& PRB **86**, 014405 (2012)

Anomalous Hall conductivity in ferromagnetic alloys

KKR-CPA results based on Kubo-Středa equation

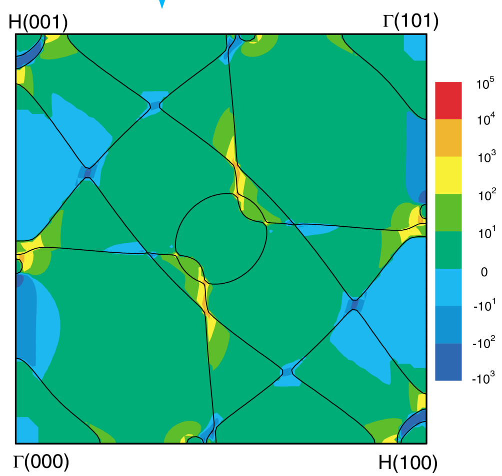




Expt.: Matveev *et al.*, Fiz. Met. Metalloved **53**, 34 (1982)
Theo.: Lowitzer *et al.*, PRL **105**, 266604 (2010)

Intrinsic AHE of pure 3*d* metals

σ_{xy} $(\Omega cm)^{-1}$	bcc Fe	fcc Ni	hcp Co	
SPR-KKR, LSDA	685	-2062	325	Kubo-Středa
SPR-KKR, LSDA+*U*	703	-1092	390	
Roman et al. (2009)			481	Berry curvature
Yao et al. (2004)	751	-2073	492	
Wang et al. (2007)	753	-2203	477	
Dheer (1967)	1032			Experiment
Lavine (1961)		-646 (RT)		
Ye et al. (2012)		-1100 (5 K)		
Volkenshtein (1961)			813	
Miyasato et al. (2007)			480	



Yao *et al.*, PRL **92**, 037204 (2004)

Intrinsic Hall conductivity in terms of the Berry curvature

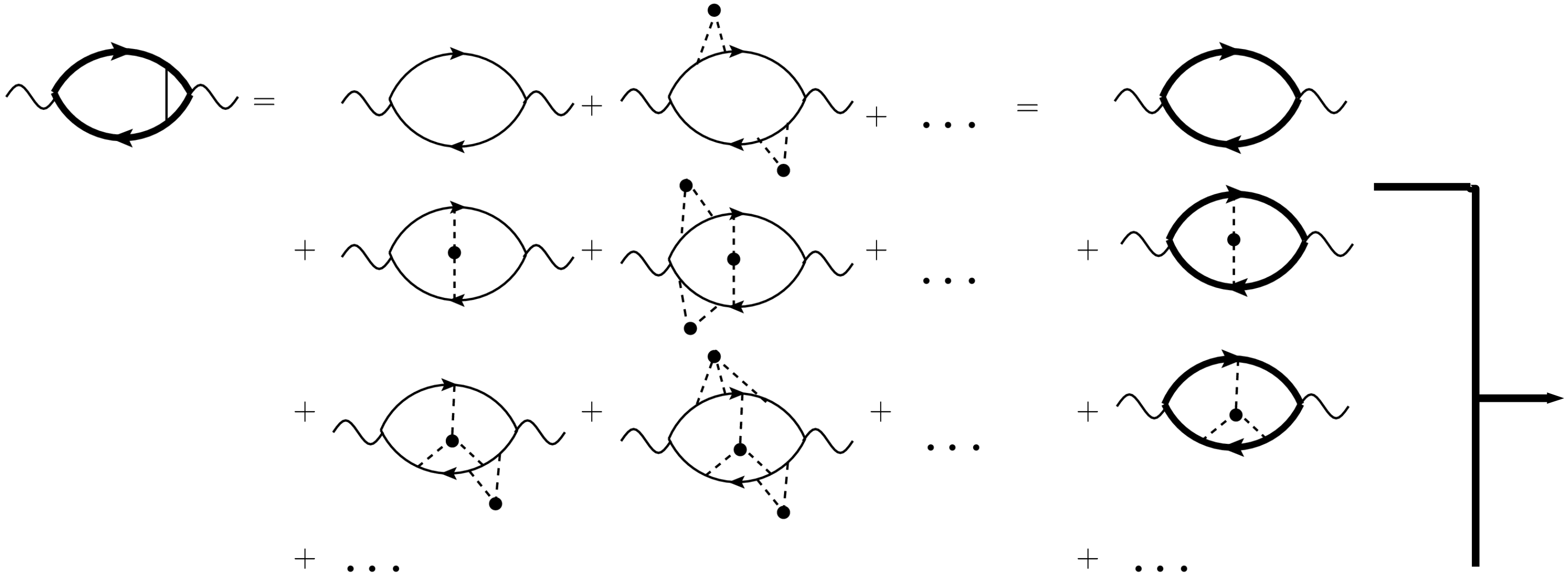
$$\sigma_{xy}^{\mathrm{intr}} = -e^2\hbar \sum_n \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\, f_n\, \Omega_n(\mathbf{k})$$

$$\Omega_n(\mathbf{k}) = -\sum_{n'\neq n} \frac{2\Im\langle\psi_{n\mathbf{k}}|v_x|\psi_{n'\mathbf{k}}\rangle\langle\psi_{n'\mathbf{k}}|v_y|\psi_{n\mathbf{k}}\rangle}{(E_{n'}-E_n)^2}$$

Equivalence of Kubo and Berry curvature formulation
See e.g. Naito *et al.*, PRB **81** 195111 (2010)

Diagrammatic representation of the KS equation

$$\sigma_{\mu\nu} = \frac{e^2\hbar}{2\pi V}\,\mathrm{Tr}\left\langle \hat{j}_\mu G^+[1+\ldots]\hat{j}_\nu G^-[1+\ldots]\right\rangle_c$$



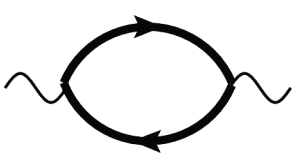
vertex diagrams

intrinsic

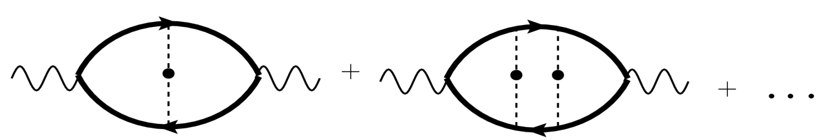
extrinsic

scaling

$\rho_{xx} \propto x$

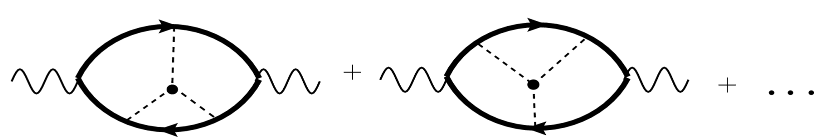


side-jump scattering



$\rho_{xy}^{sj} \propto x^2$

skew scattering



$\rho_{xy}^{skew} \propto x - 3x^2$

Crepieux *et al.*, PRB **64**, 014416 (2001)

Decomposition of the Hall conductivity via scaling behaviour of individual contributions

Superclean limit
skew scattering should dominate with

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

S : skewness factor

decomposition of σ_{xy}

$$\sigma_{xy} = \sigma_{xx} S + \sigma_{xy}^{\text{sj}} + \sigma_{xy}^{\text{intr}}$$

For diluted alloys with concentration x as implicit parameter

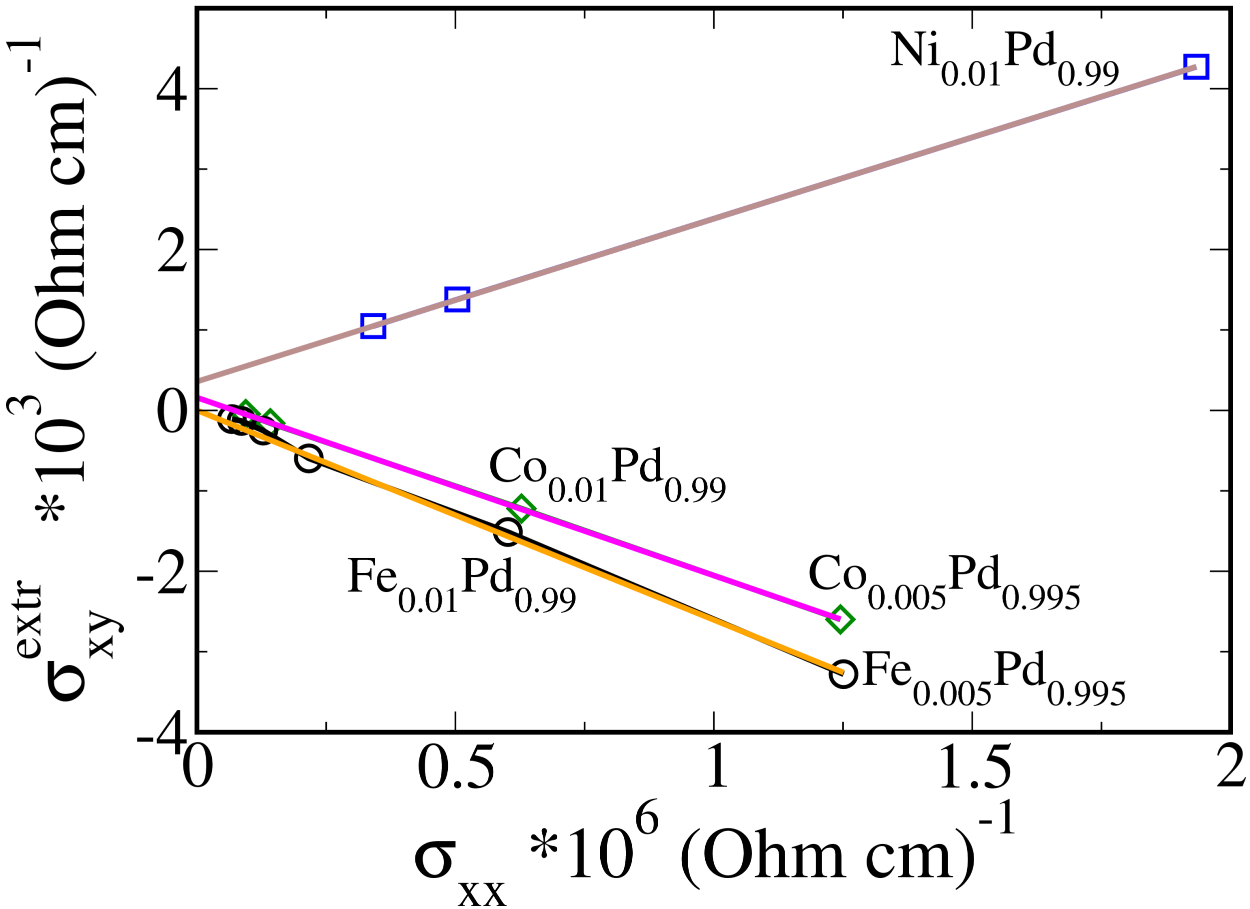
$$\sigma_{xy}^{\text{sj}} + \sigma_{xy}^{\text{intr}} \approx \text{const}$$

Onoda *et al.*, PRB **77**, 165103 (2008) , Crepieux *et al.*, PRB **64**, 014416 (2001)

Decomposition of the extrinsic AHE via scaling behaviour of individual contributions

KKR-CPA results based on Kubo-Středa equation

$$\sigma_{xy}^{\text{extr}} = \sigma_{xy}^{\text{skew}} + \sigma_{xy}^{\text{sj}}$$
$$= \sigma_{xx} S + \sigma_{xy}^{\text{sj}}$$



⇒ side-jump contribution is negligible for these systems

Description of the Anomalous Hall effect

Kubo-Středa linear response

any system

longitudinal

σ_{xx}

transverse

σ_{xy}

Decomposition

intrinsic coherent

extrinsic incoherent

scaling laws

side-jump

skew

vertex corrections

Boltzmann

dilute alloys

longitudinal

σ_{xx}

transverse

skew

scattering-in terms

Berry curvature

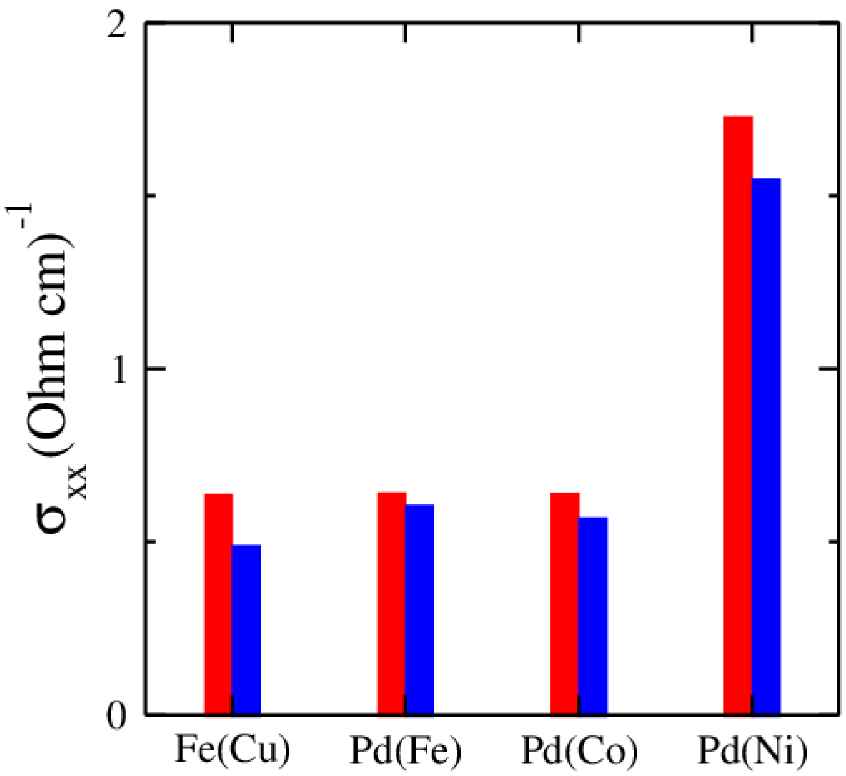
pure systems

intrinsic

Boltzmann vs Kubo formalism

Comparison of results for diluted alloys (1%)

longitudinal conductivity σ_{xx}

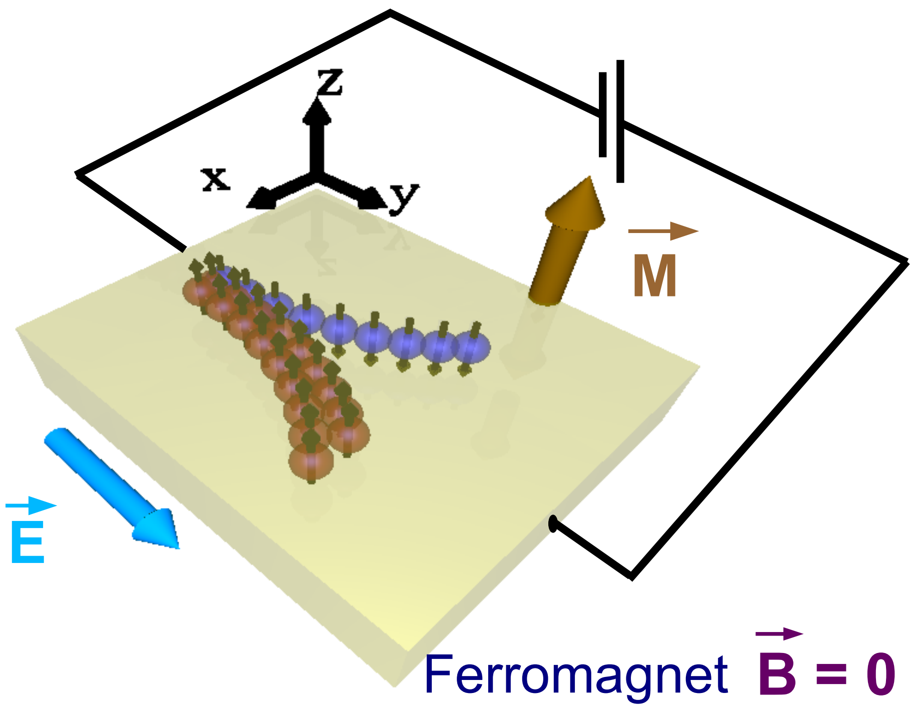


Boltzmann-based calculations:
Gradhand, Fedorov, Mertig, unpublished (2013)

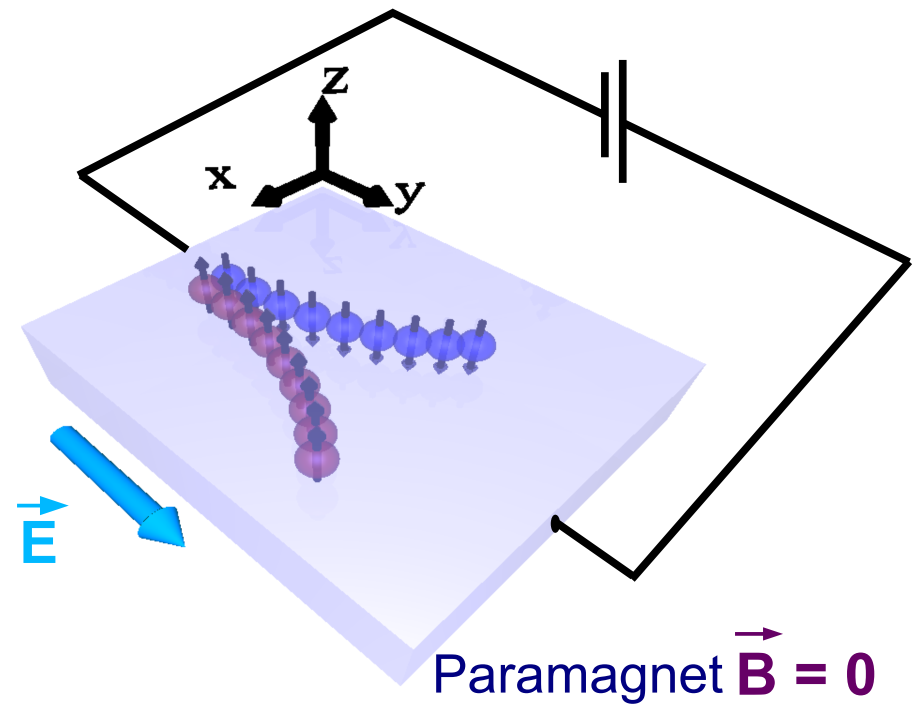
PRELIMINARY RESULTS !

Transverse charge and spin currents

Anomalous Hall Effect (AHE)



Spin Hall Effect (SHE)



Separating	charge (+ spin)	spin
Source	in both cases **relativistic** spin-orbit interaction	

"Spintronics without magnetism"

Kubo-Středa (KS) for spin conductivity tensor

$$\sigma^z_{\mu\nu} = \frac{\hbar}{4\pi N\Omega}\mathrm{Tr}\left\langle \hat{J}^z_\mu(G^+ - G^-)\hat{j}_\nu G^- - \hat{J}^z_\mu G^+\hat{j}_\nu(G^+ - G^-)\right\rangle_c + \frac{e}{4\pi i N\Omega}\mathrm{Tr}\left\langle (G^+ - G^-)(\hat{r}_\mu\hat{J}^z_\nu - \hat{r}_\nu\hat{J}^z_\mu)\right\rangle_c$$

with current density operator

charge $\hat{j}_\mu = -|e|c\,\alpha_\mu$

spin $\hat{J}^z_\mu = c\alpha_\mu T_z$

Lowitzer *et al.*, PRB **82**, 140402(R) (2010)
Lowitzer *et al.*, PRL **106**, 056601 (2011)

spin polarization four-vector $\mathcal{T}$ for particle in field $\vec{T} = \beta\vec{\Sigma} - \frac{1}{mc}\gamma_5\vec{\Pi}$

$$T_4 = \frac{i}{mc}\vec{\Sigma}\cdot\vec{\Pi}$$

with kinetic momentum $\vec{\Pi} = \frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}$

based on:

[1] Bargmann & Wigner, Proc. Natl. Acad. Sci. **34**, 211 (1948)
[2] Vernes *et al.*, PRB **76**, 012408 (2007)

Structure of the spin conductivity tensor

Extension of Kleiner's scheme

Kleiner, PR **142**, 318 (1966)

unitary symmetry operation

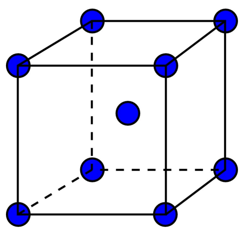
$$\sigma^k_{ij} = \sum_{lmn} D(P_R)_{li} D(P_R)_{mj} D(P_R)_{nk}\, \sigma^n_{lm}$$

anti-unitary symmetry operation

$$\sigma^k_{ij} = -\sum_{lmn} D(P_R)_{li} D(P_R)_{mj} D(P_R)_{nk}\, \sigma'^n_{lm}$$

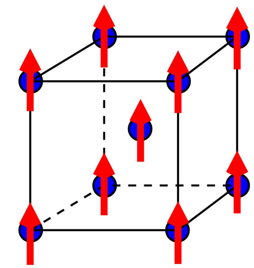
paramagnetic

G = *m3m*



ferromagnetic

G = *4/mm'm'*



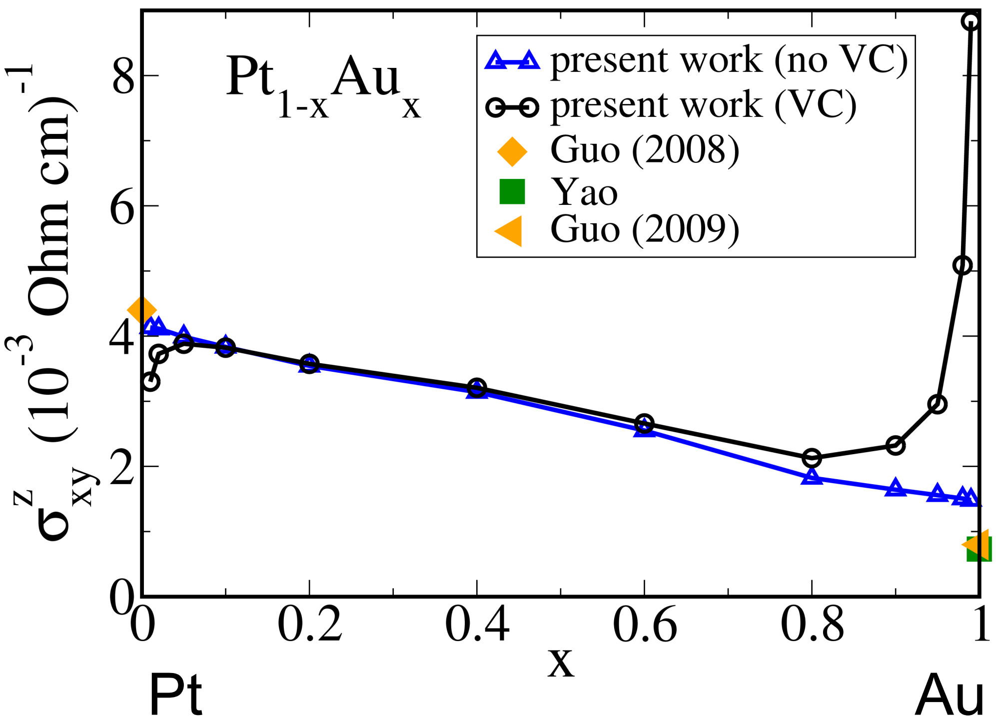
$$\underline{\underline{\sigma}}^x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma^z_{xy} \\ 0 & -\sigma^z_{xy} & 0 \end{pmatrix} \qquad \underline{\underline{\sigma}}^x = \begin{pmatrix} 0 & 0 & \sigma^x_{xz} \\ 0 & 0 & \sigma^x_{yz} \\ \sigma^x_{zx} & \sigma^x_{zy} & 0 \end{pmatrix}$$

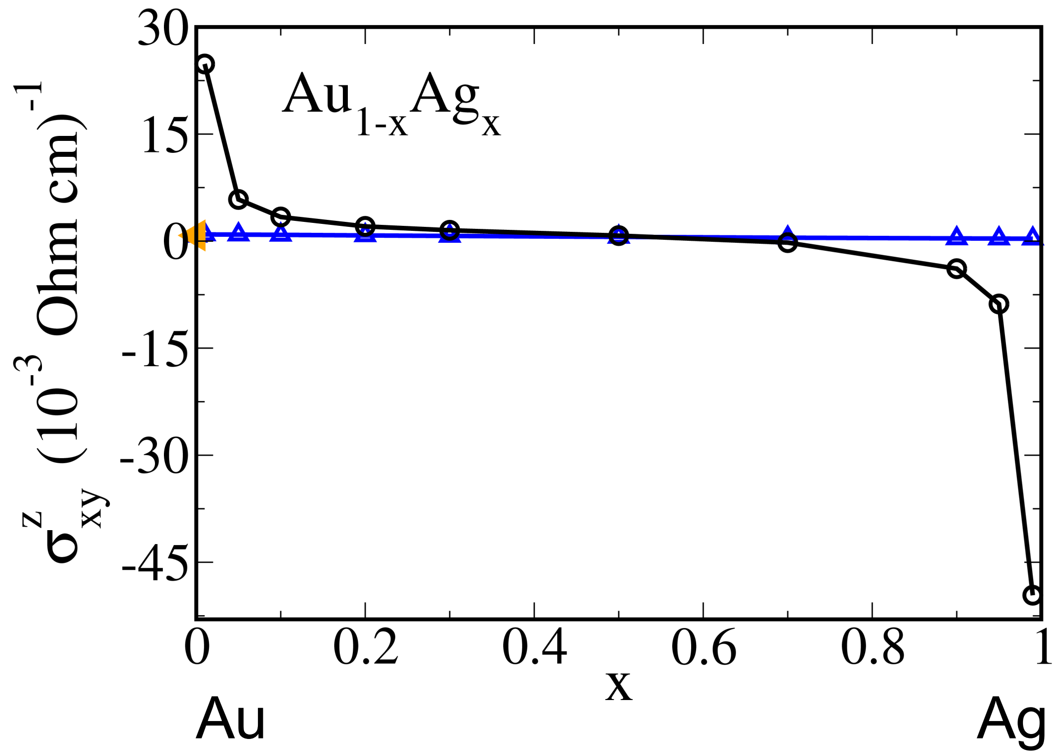
$$\underline{\underline{\sigma}}^y = \begin{pmatrix} 0 & 0 & -\sigma^z_{xy} \\ 0 & 0 & 0 \\ \sigma^z_{xy} & 0 & 0 \end{pmatrix} \qquad \underline{\underline{\sigma}}^y = \begin{pmatrix} 0 & 0 & -\sigma^x_{yz} \\ 0 & 0 & \sigma^x_{xz} \\ -\sigma^x_{zy} & \sigma^x_{zx} & 0 \end{pmatrix}$$

$$\underline{\underline{\sigma}}^z = \begin{pmatrix} 0 & \sigma^z_{xy} & 0 \\ -\sigma^z_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \underline{\underline{\sigma}}^z = \begin{pmatrix} \sigma^z_{xx} & \sigma^z_{xy} & 0 \\ -\sigma^z_{xy} & \sigma^z_{xx} & 0 \\ 0 & 0 & \sigma^z_{zz} \end{pmatrix}$$

SHE for 4d- and 5d-transition metal alloys

KKR-CPA results based on Kubo-Středa equation





Lowitzer *et al.*, PRL 106, 056601 (2011)

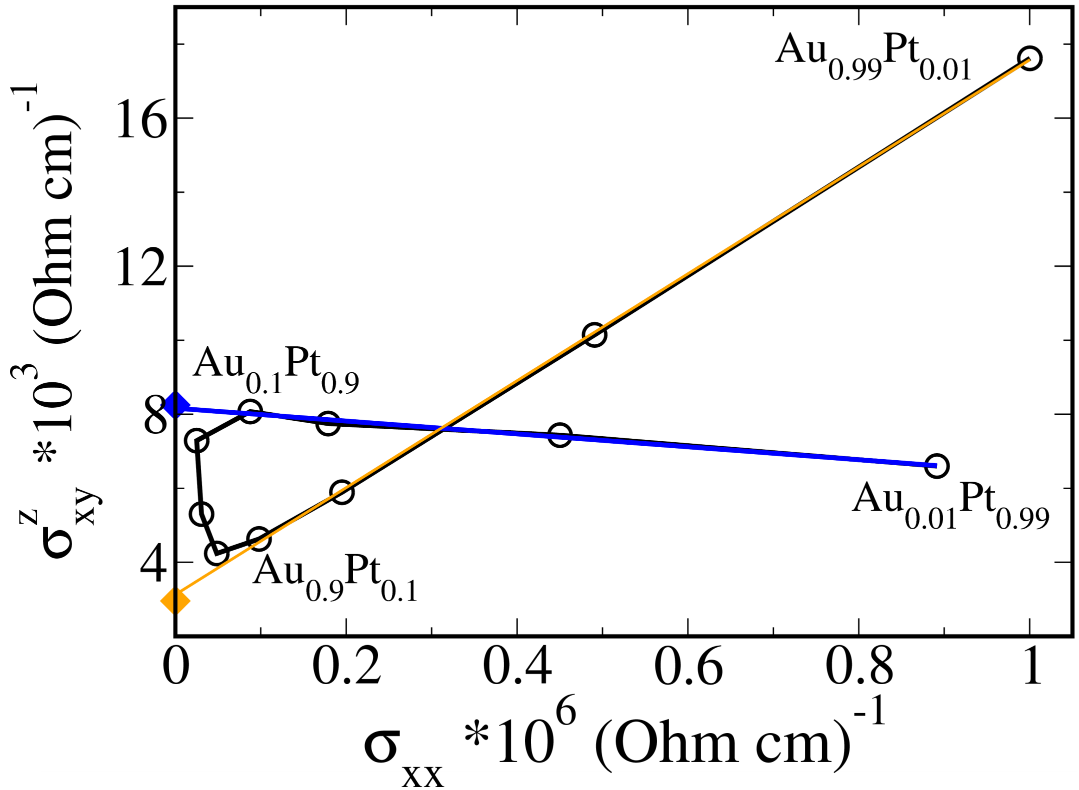
Guo *et al.*, PRL **100**, 096401 (2008)
Guo, JAP **105**, 07C701 (2009)
Yao *et al.*, PRL **95**, 156601 (2005)
} intrinsic SHE of pure elements

Decomposition of Spin Hall conductivity via scaling behaviour of individual contributions

Ansatz in analogy to AHE

$$\sigma^{z}_{xy} = \sigma_{xx} S + \sigma^{z,\mathrm{sj}}_{xy} + \sigma^{z,\mathrm{intr}}_{xy}$$

KKR-CPA results for $Au_{1-x}Pt_x$



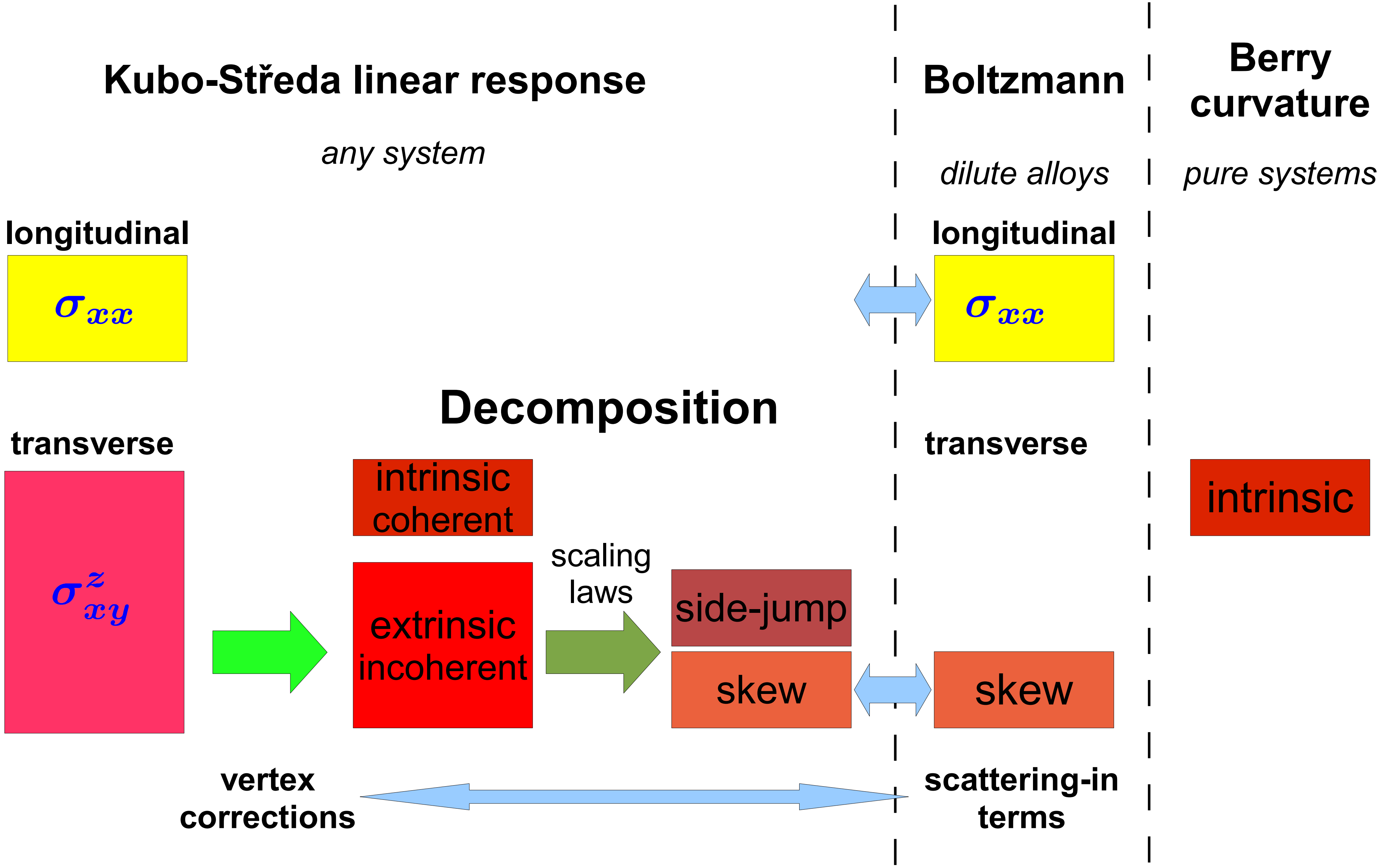
linear relation on both sides of alloy system for composition

$$x_{\mathrm{Au}}(x_{\mathrm{Pt}}) \leq 0.1$$

Extrapolation to $\sigma_{xx} \rightarrow 0$

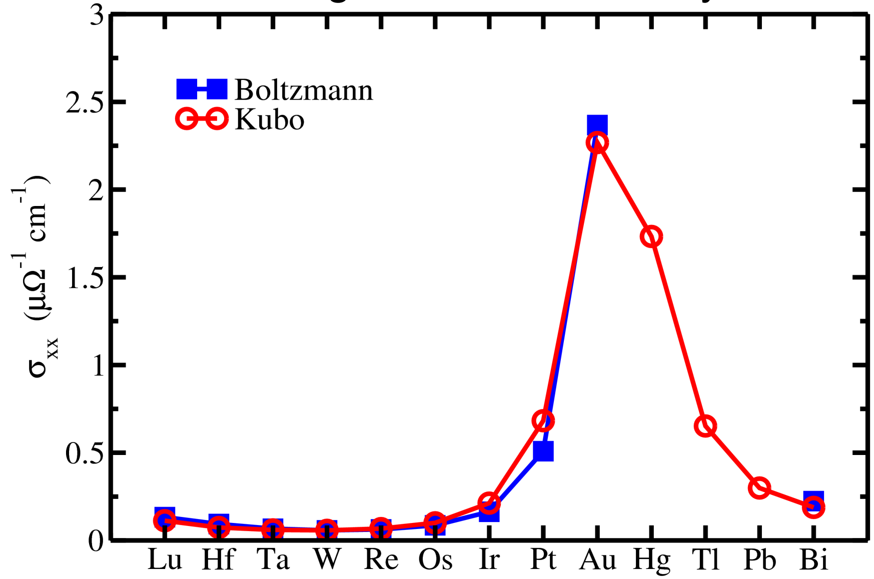
$$\sigma^{z}_{xy} = \sigma^{z,\mathrm{sj}}_{xy} + \sigma^{z,\mathrm{intr}}_{xy}$$

Description of the Spin Hall effect

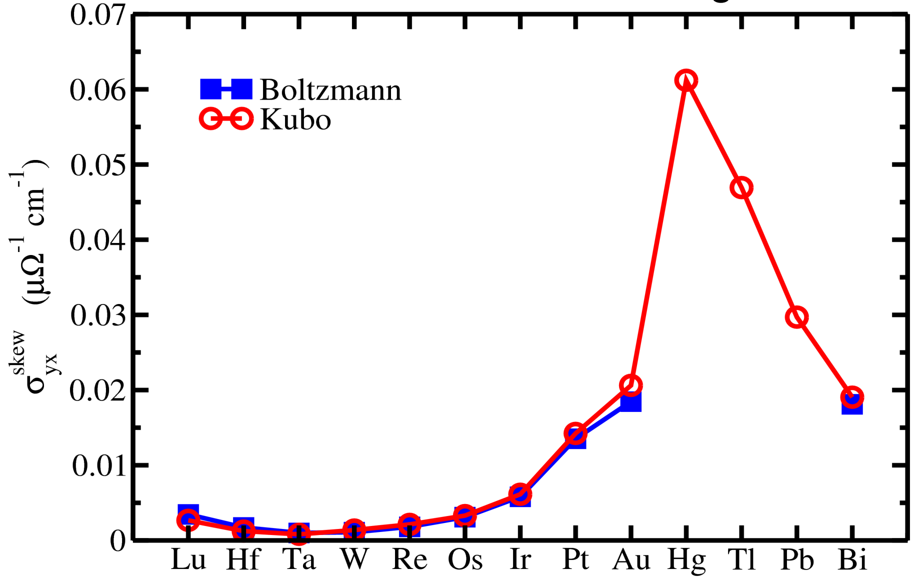


Comparison between Kubo and Boltzmann for $Cu_{0.99}M_{0.01}$ with M = Lu … Bi

Longitudinal conductivity

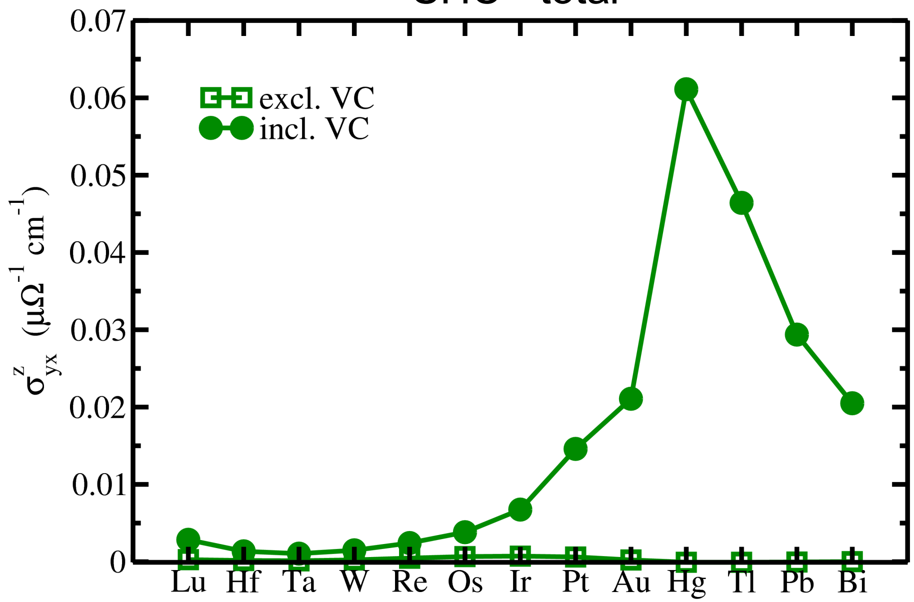


SHC – skew scattering



Boltzmann results:
C. Herschbach *et al.*, arXiv:1308.4012v1

SHC - total



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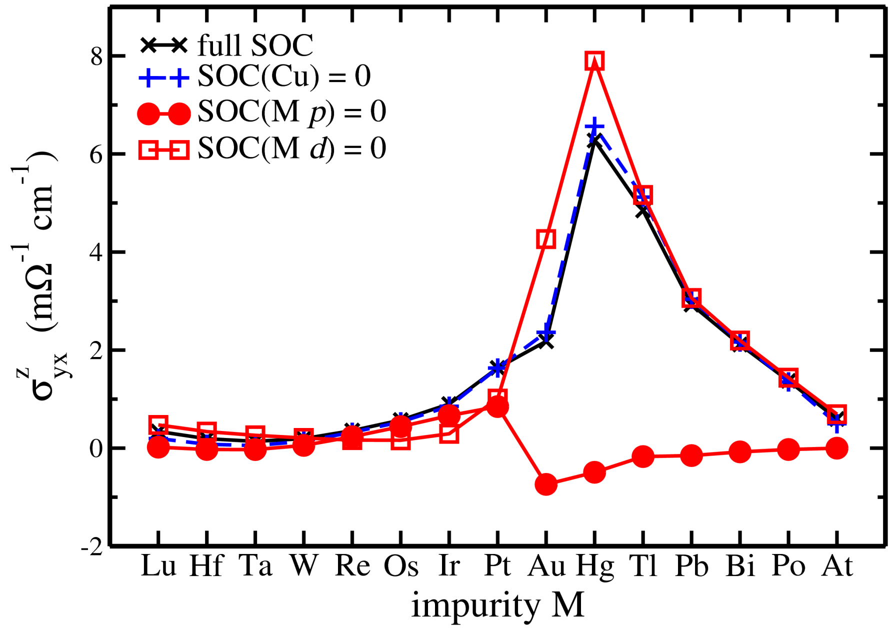
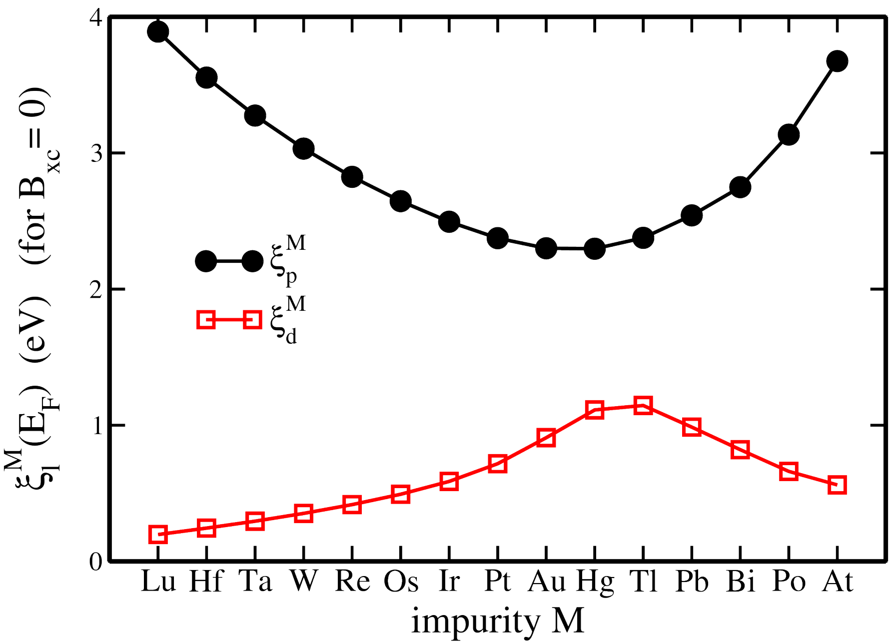
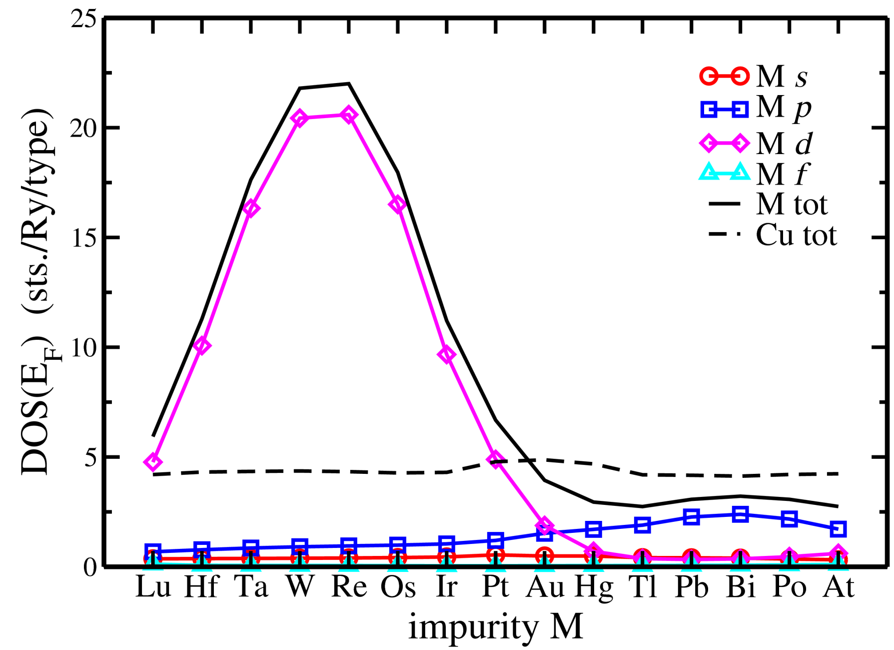
Influence of SOC + DOS on SHC σ in $Cu_{0.99}M_{0.01}$





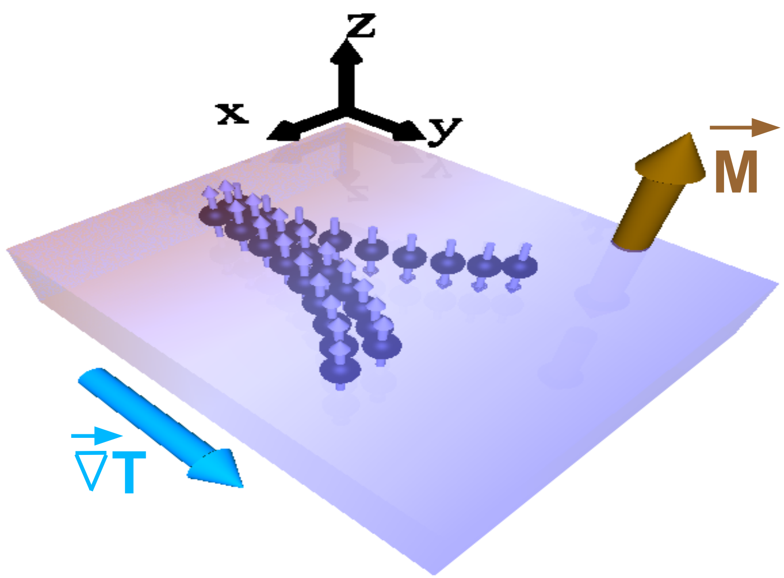
- SHC caused primarily by SOC of M
- Mostly *p*- but also *d*-states relevant around maximum

- Crossover of dominance of *d*- to *p*-states at E_F between M = Au and Hg
- SOC strength maximal in *d*-channel and minimal in *p*-channel, but larger in the latter



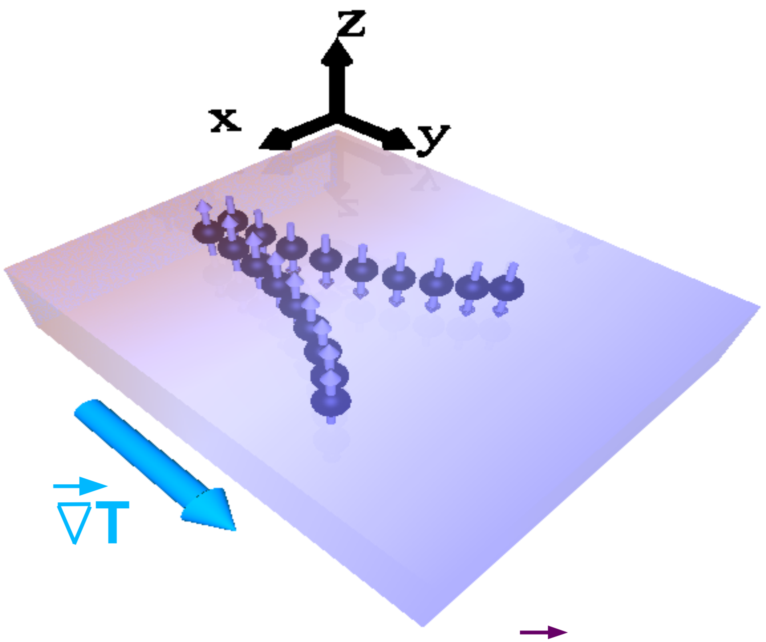
Transverse thermogalvanic charge and spin conductivity

Anomalous Nernst Effect (ANE)



Ferromagnet $\vec{B} = 0$

Spin Nernst Effect (SNE)



Paramagnet $\vec{B} = 0$

Thermal analogues to

Anomalous Hall and **Spin Hall effect**

Charge, heat and spin transport due to electric field and thermal gradient

Currents induced by gradient of electrochemical potential $\vec{\nabla}\mu = \vec{\mu}_c - e\vec{E}$

and temperature gradient $\vec{\nabla}T$:

charge $\vec{j}^c = -L^{cc}\vec{\nabla}\mu - L^{cq}\vec{\nabla}T/T$

heat $\vec{j}^q = -L^{qc}\vec{\nabla}\mu - L^{qq}\vec{\nabla}T/T$

spin $J^s = -\mathcal{L}^{sc}\vec{\nabla}\mu - \mathcal{L}^{sq}\vec{\nabla}T/T$

with response functions

$$(L/\mathcal{L})^{(s/c)c(,\xi)}_{\mu\nu}(T) = -\frac{1}{e}\int dE\,\sigma^{(s/c)c(,\xi)}_{\mu\nu}(E)\left(-\frac{\partial f(E,T)}{\partial E}\right)$$

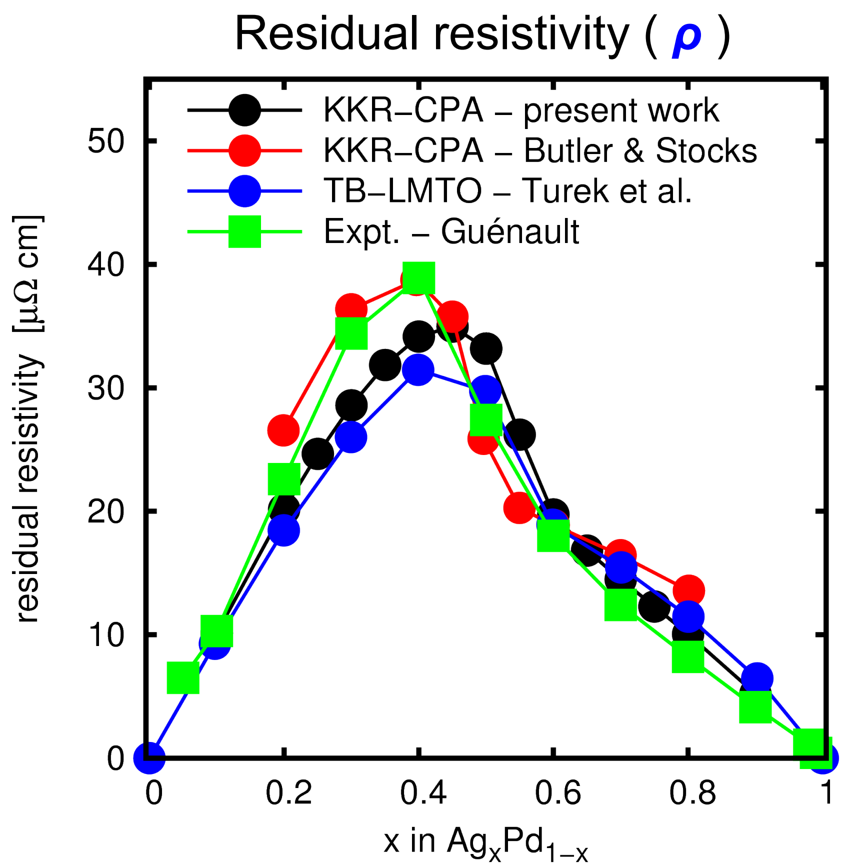
$$(L/\mathcal{L})^{(s/c)q(,\xi)}_{\mu\nu}(T) = -\frac{1}{e}\int dE\,\sigma^{(s/c)c(,\xi)}_{\mu\nu}(E)\left(-\frac{\partial f(E,T)}{\partial E}\right)(E-E_F)$$

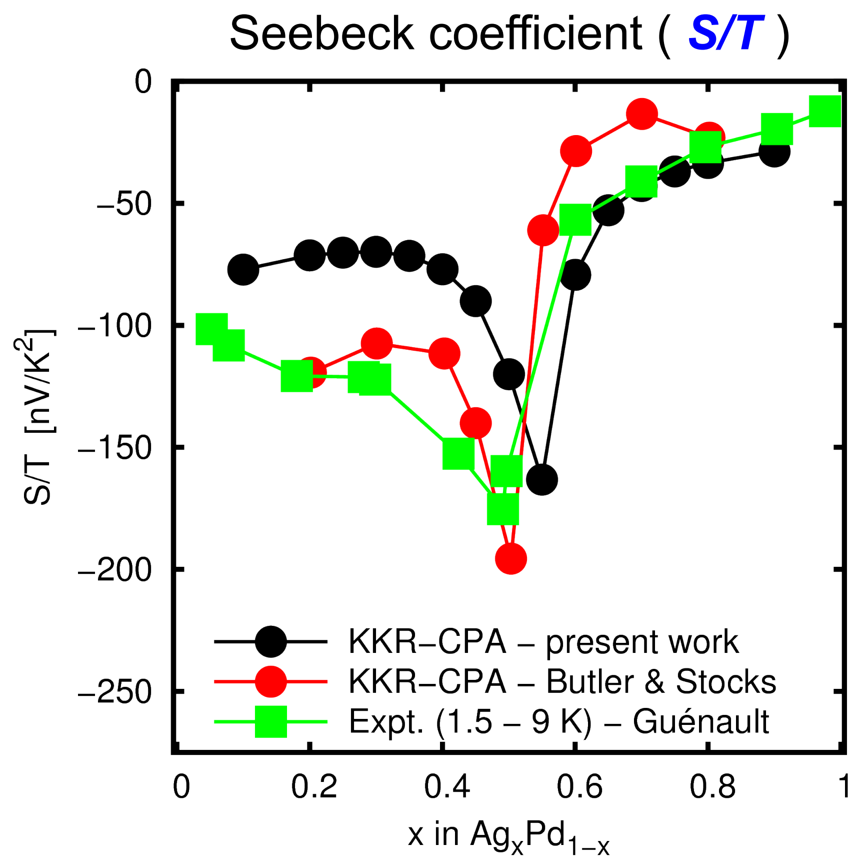
$$L^{qq}_{\mu\nu}(T) = -\frac{1}{e}\int dE\,\sigma^{cc}_{\mu\nu}(E)\left(-\frac{\partial f(E,T)}{\partial E}\right)(E-E_F)^2$$

where L^{ab} and L^{ba} are connected via Onsager symmetry relations

and $\sigma^{cc} \equiv -eL^{cc}$, $\sigma^{sc} \equiv -e\mathcal{L}^{sc}$ **for** $T \to 0$

Residual resistivity and Seebeck coefficient of Ag_xPd_{1-x} alloys





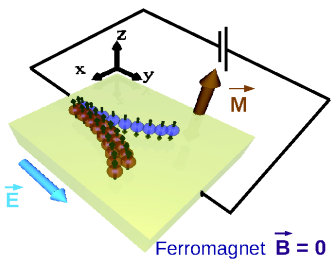
- Butler & Stocks: ρ obtained from BSF, without vertex corrections

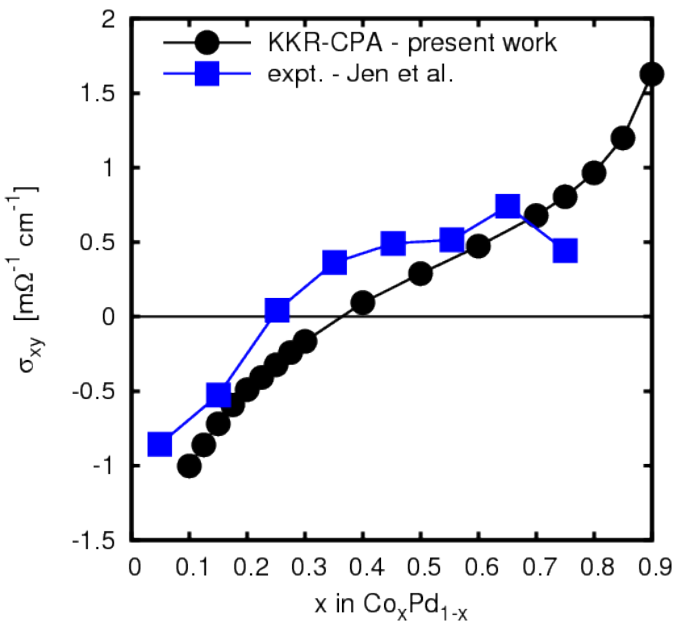
Theory: Butler and Stocks, PRB **29**, 4217 (1984), I. Turek *et al.*, PRB **65**, 125101 (2002)

Experiment: Guénault, PM **30**, 641 (1974)

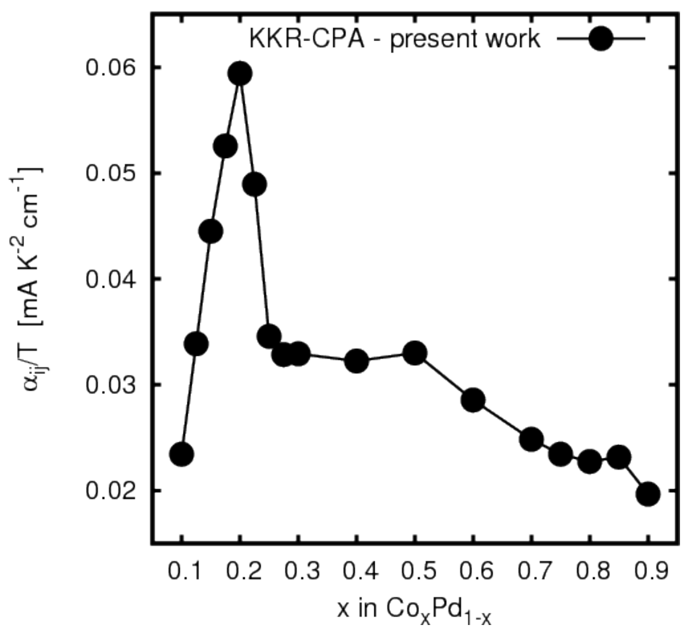
Transverse charge transport Co_xPd_{1-x} alloys

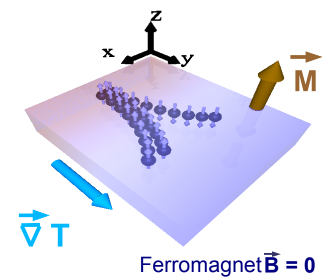
Anomalous Hall conductivity





Anomalous Nernst conductivity



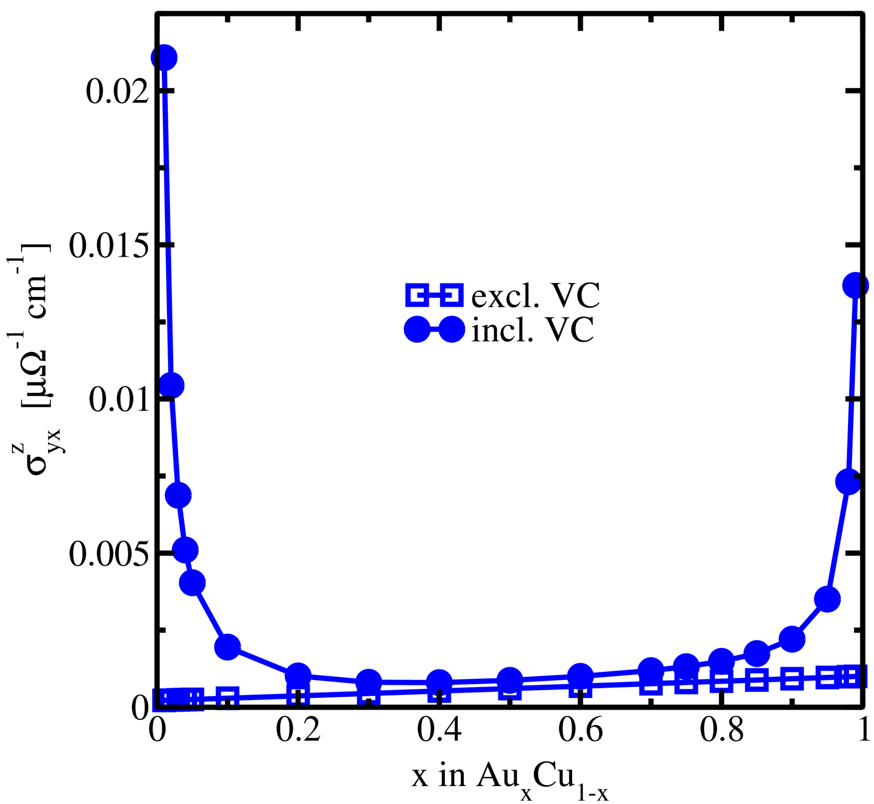


- No direct relation between AHC and ANC
- AHC shows sign change, while ANC does not
- ANC: Maximum at $x \approx 0.2$ in line with behaviour of ρ, AMR ratio & S

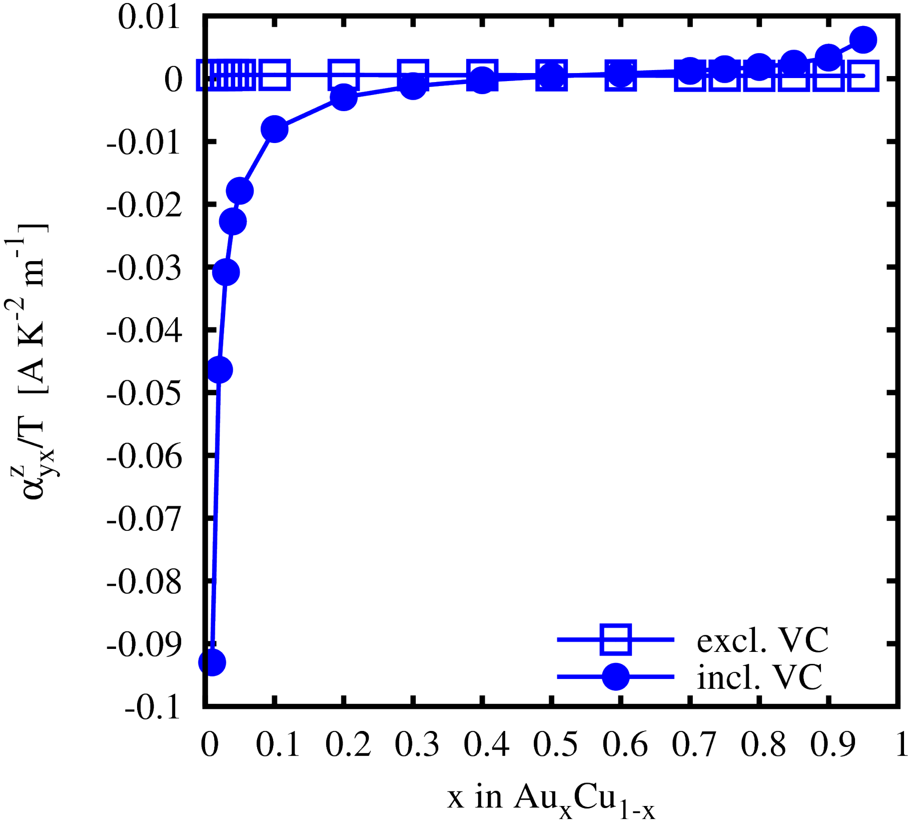
Expt.: Jen *et al.*, JAP **76**, 5782 (1994)

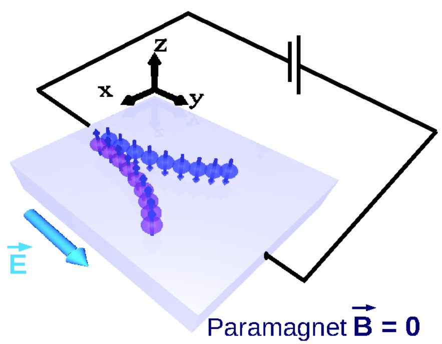
Transverse spin transport in Au_xCu_{1-x}

Spin Hall conductivity

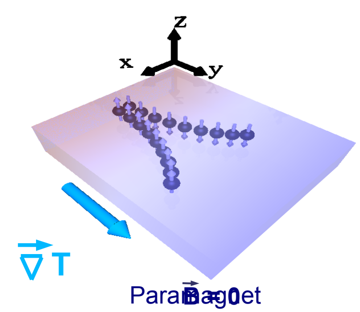


(Thermal) Spin Nernst conductivity



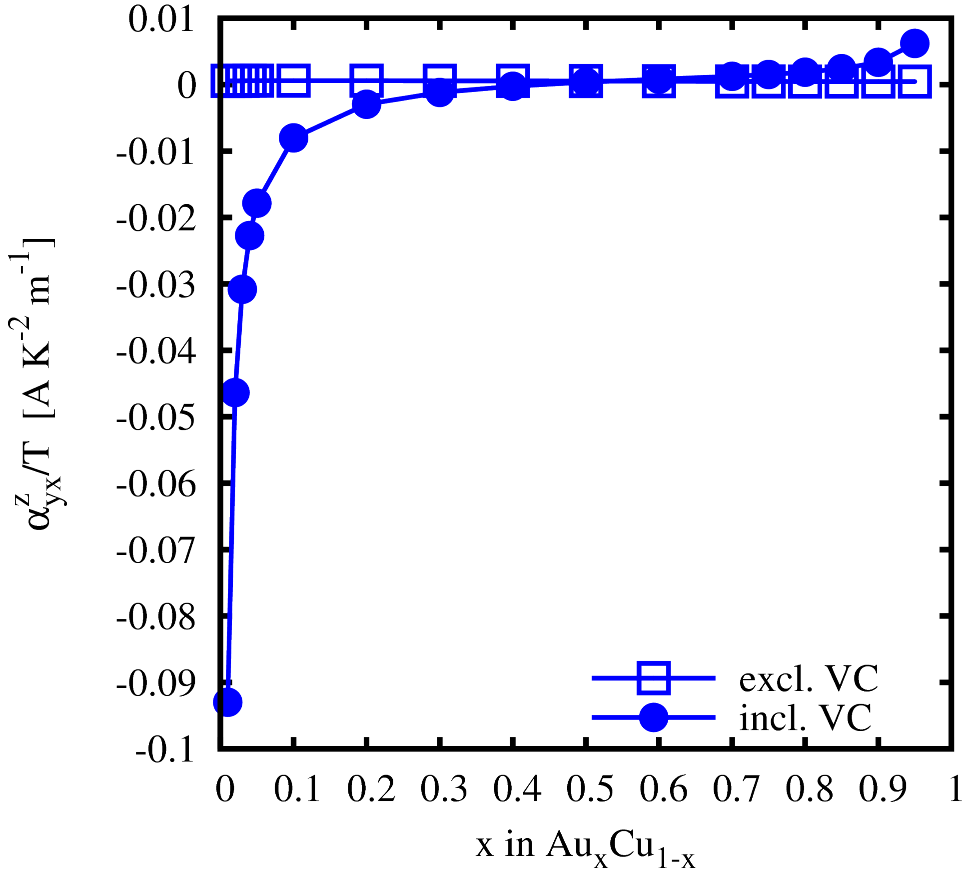


Wimmer et al. arXiv:1306.0621

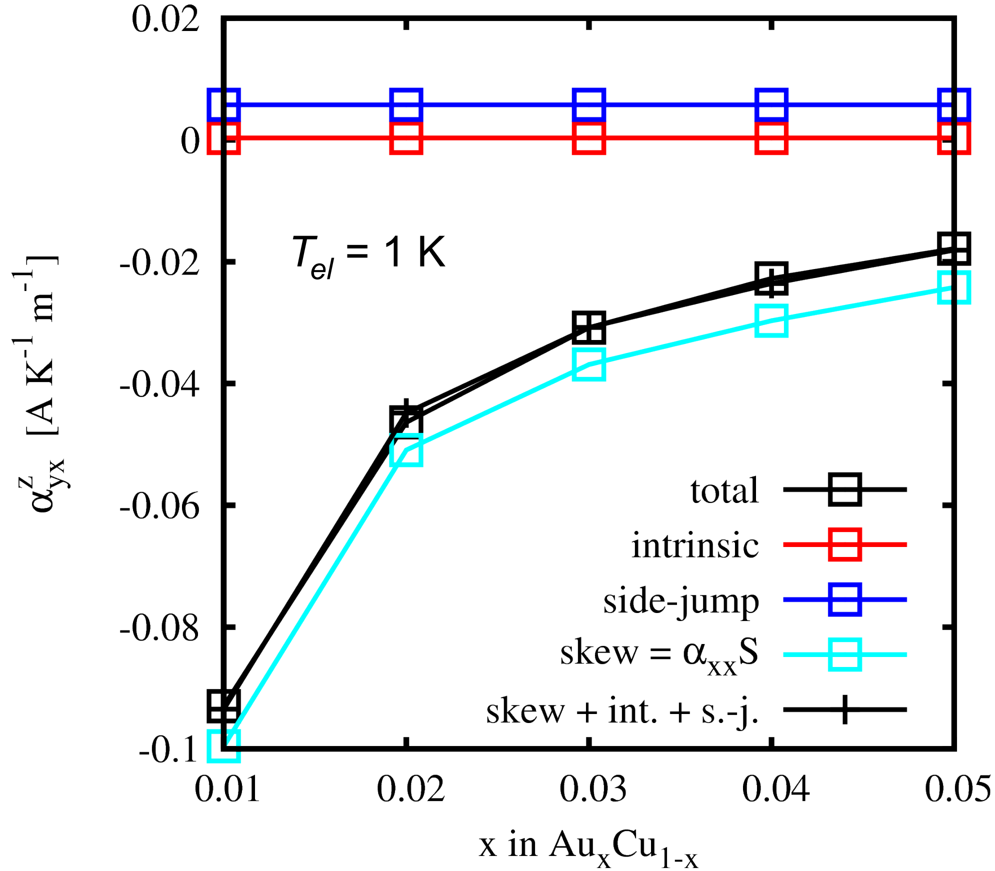


Spin Nernst Conductivity in Au_xCu_{1-x} and its decomposition via scaling behaviour

(Thermal) Spin Nernst conductivity σ^T_{SN}



Decomposition of SNC for Cu-rich alloys



$$\alpha^z_{yx} = \alpha_{xx} S + \alpha^{z,\mathrm{sj}}_{yx} + \alpha^{z,\mathrm{intr}}_{yx}$$

Transverse spin transport in an open circuit

Open circuit condition implies

$$\vec{E} \;=\; -\frac{1}{eT}(L^{cc})^{-1}L^{cq}\vec{\nabla}T = S\,\vec{\nabla}T$$

leading to the spin current density

$$\begin{aligned} J^s &= \mathcal{L}^{sc}(-e\vec{E}) + \mathcal{L}^{sq}(-\vec{\nabla}T/T) \\ &= \alpha^{scq}\,\vec{\nabla}T \end{aligned}$$

with the combined response tensor

$$\alpha^{scq} \;=\; -e\mathcal{L}^{sc}S - \mathcal{L}^{sq}/T$$

consisting of an **electrical** and a **thermal** contribution.

The transverse element with polarization normal to driving forces and response

$$\begin{aligned} \alpha^{scq,z}_{yx} &= -e\mathcal{L}^{sc,z}_{yx}S_{xx} - \frac{1}{T}\mathcal{L}^{sq,z}_{yx} \\ &= \alpha^{sc,z}_{yx} + \alpha^{sq,z}_{yx} \end{aligned}$$

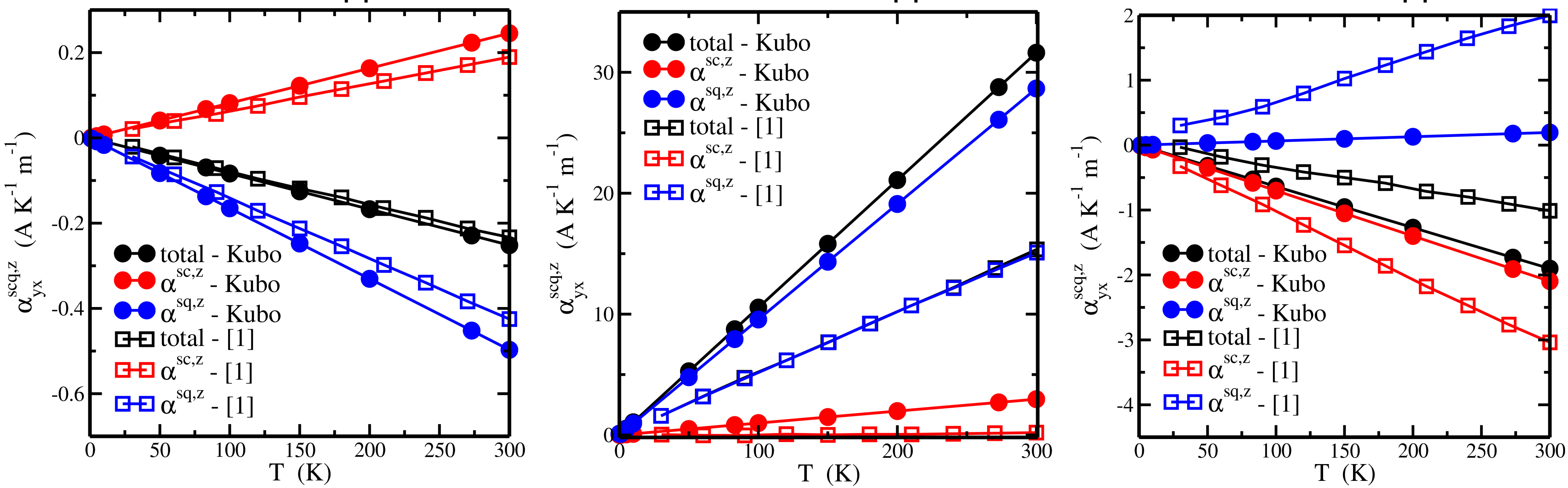
is the **spin Nernst conductivity**.

see also: Tauber *et al.*, PRL **109**, 026601 (2012).

Spin Nernst conductivity and its components

- Comparison to calculations using Boltzmann transport theory [1]

1 % Ti in copper | 1 % Au in copper | 1 % Bi in copper



$$\alpha_{yx}^{scq,z} = \alpha_{yx}^{sc,z} + \alpha_{yx}^{sq,z}$$

"proper" Spin Nernst conductivity

Spin Hall contribution due to electric field created by longitudinal Seebeck effect

[1] Tauber *et al.*, PRL **109**, 026601 (2012).

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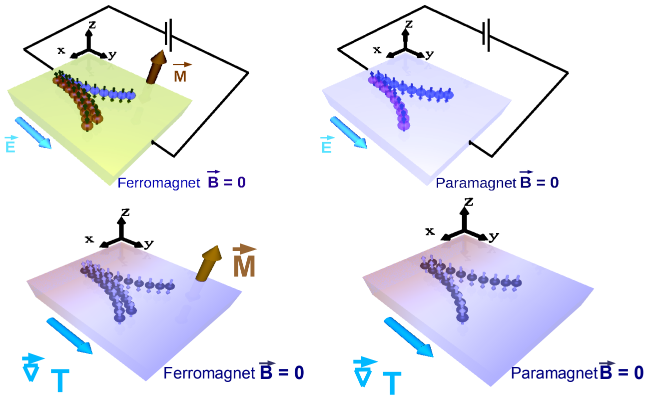
Summary

- A relativistic implementation of the Kubo-Středa formalism on the basis of the KKR-CPA formalism was presented

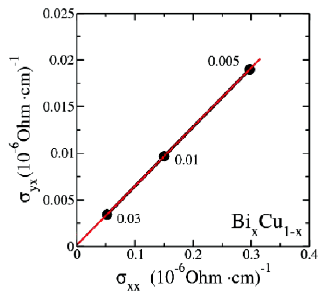
$$\sigma^z_{\mu\nu} = \frac{\hbar}{4\pi N\Omega} \mathrm{Tr} \left\langle \hat{J}^z_\mu (G^+ - G^-) \hat{j}_\nu G^- - \hat{J}^z_\mu G^+ \hat{j}_\nu (G^+ - G^-) \right\rangle_c + \frac{e}{4\pi i N\Omega} \mathrm{Tr} \left\langle (G^+ - G^-)(\hat{r}_\mu \hat{J}^z_\nu - \hat{r}_\nu \hat{J}^z_\mu) \right\rangle_c$$

- Applications to concentrated alloys for investigations on
  - Anomalous Hall Effect
  - Spin Hall Effect
  - Anomalous Nernst Effect
  - Spin Nernst Effect



- Decomposition into intrinsic and extrinsic contributions based on vertex corrections

- Skew- and side-jump contributions identified via scaling behaviour



- Results for diluted alloys in full coherence with results based on Boltzmann formalism