Transport properties calculated by means of the Kubo formalism

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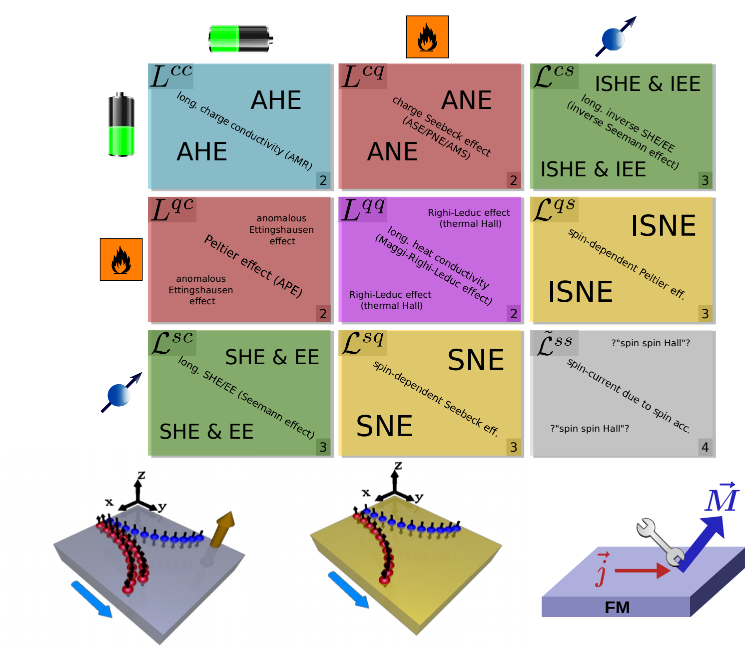
Outline

- Introduction
- Kubo-Středa vs. Kubo-Bastin
- Kubo vs. Boltzmann formalism
- Symmetry predicted properties
- Inclusion of temperature
- Summary and outlook



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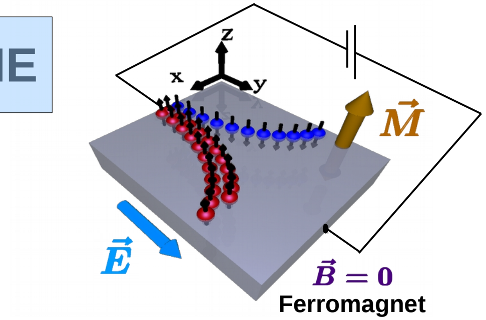
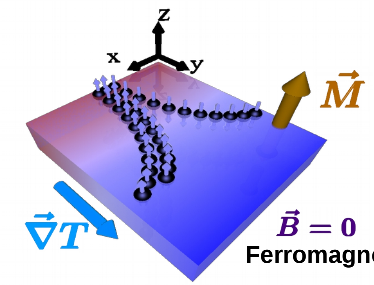
Charge, heat and spin transport with emphasis on spin-orbit induced effects

- Charge
- Heat current density
- Spin

AHE

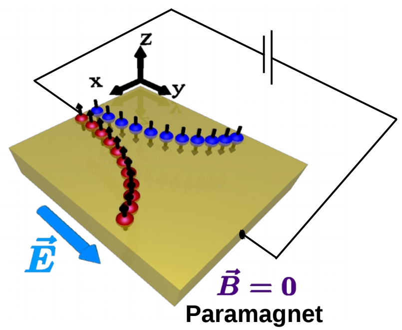


ANE

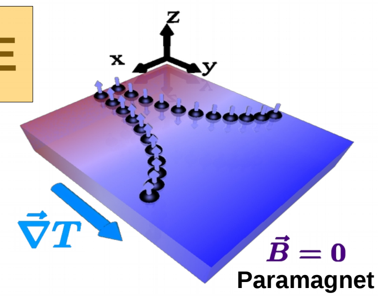


$$\begin{pmatrix} \vec{j}^{c} \\ \vec{j}^{q} \\ J^{s} \end{pmatrix} = \begin{pmatrix} L^{cc} & L^{cq} & \mathcal{L}^{cs} \\ L^{qc} & L^{qq} & \mathcal{L}^{qs} \\ \mathcal{L}^{sc} & \mathcal{L}^{sq} & \tilde{\mathcal{L}}^{ss} \end{pmatrix} \begin{pmatrix} \vec{E} \\ -\vec{\nabla}T/T \\ F^{s} \end{pmatrix}$$

SHE



SNE



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

Longitudinal effects: AMR & ASE

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

Study of pure systems and disordered alloys

Hierarchy of transport equations

Kubo

$$\sigma_{\mu\nu} = V \int_0^{(k_B T)^{-1}} d\lambda \int_0^{\infty} dt \, \left\langle \hat{j}_\nu \hat{J}_{I,\mu}(t + i\hbar\lambda) \right\rangle_c e^{i(\omega+i\delta)t}$$

Independent electron approximation, ω = 0

Bastin

$$\sigma_{\mu\nu} = \frac{i\hbar}{V} \int_{-\infty}^{\infty} dE f(E) \, \mathrm{Tr} \left\langle \hat{J}_\mu \frac{dG^+(E)}{dE} \hat{j}_\nu \delta(E - \hat{H}) - \hat{J}_\mu \delta(E - \hat{H}) \hat{j}_\nu \frac{dG^-(E)}{dE} \right\rangle_c$$

T = 0K

Kubo-Středa

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

Retaining symmetric part only

Kubo-Greenwood

$$\sigma_{\mu\nu} = \frac{\hbar}{\pi V} \mathrm{Tr} \left\langle \hat{J}_\mu \Im G^+ \hat{j}_\nu \Im G^+ \right\rangle_c$$

see also: Ködderitzsch, Lowitzer, Staunton, Ebert, phys. stat. sol. (b) **248**, 2248 (2011).

SPR-KKR-CPA electronic structure calculations

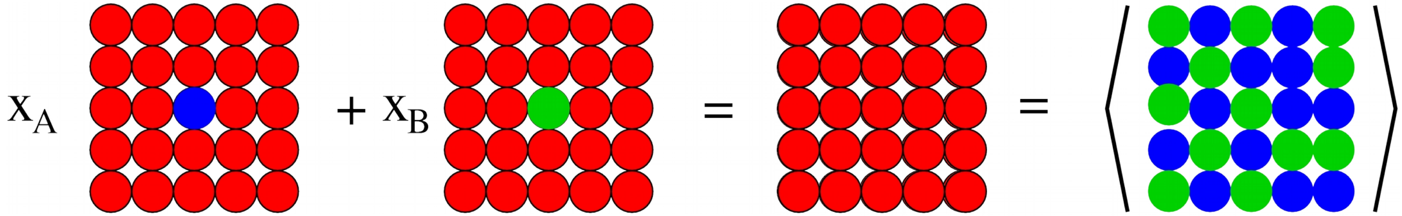
SPR: Dirac equation within LSDA

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

KKR: Green function via multiple scattering theory

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

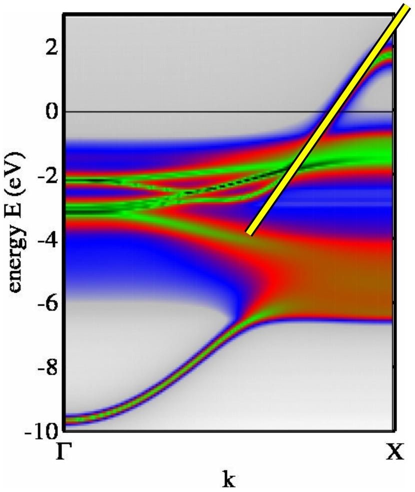
CPA: Coherent potential approximation for disorder



$$x_{\text{A}}\underline{\tau}^{nn,\text{A}}+x_{\text{B}}\underline{\tau}^{nn,\text{B}}=\underline{\tau}^{nn,\text{CPA}}$$

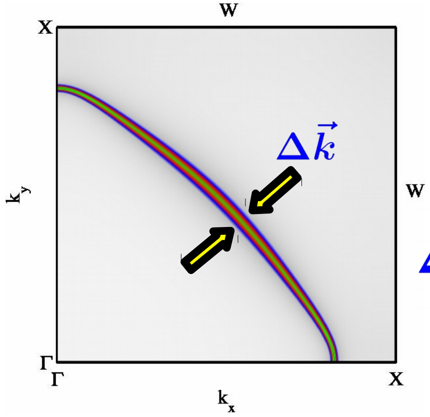
Boltzmann-formalism applied to Ag_xPd_{1-x}

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



group velocity

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

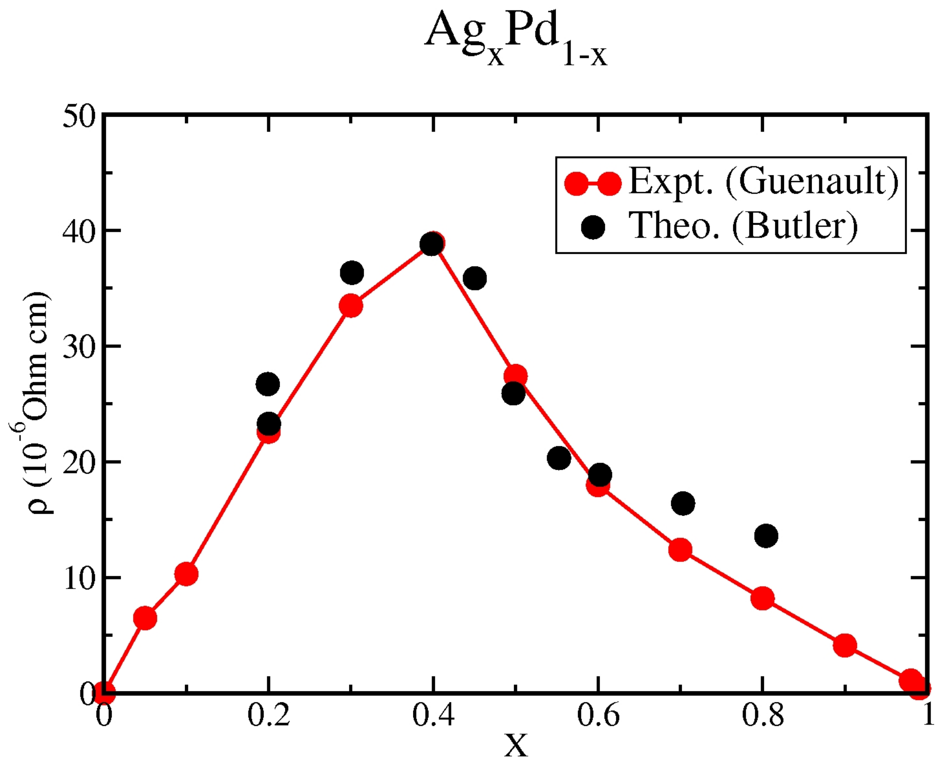


life time

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

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

Residual resistivity (T=0K)



W. H. Butler *et al.*, PRB **29**, 4217 (1984)

Neglecting scattering-in term

Kubo-Greenwood equation and Vertex corrections

Implementation within KKR-CPA

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

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

$\Lambda = (\kappa, \mu)$

relativistic quantum numbers

Vertex corrections (VC)

$\langle jG\rangle\langle jG\rangle \rightarrow \langle jGjG\rangle$

account for scattering-in processes

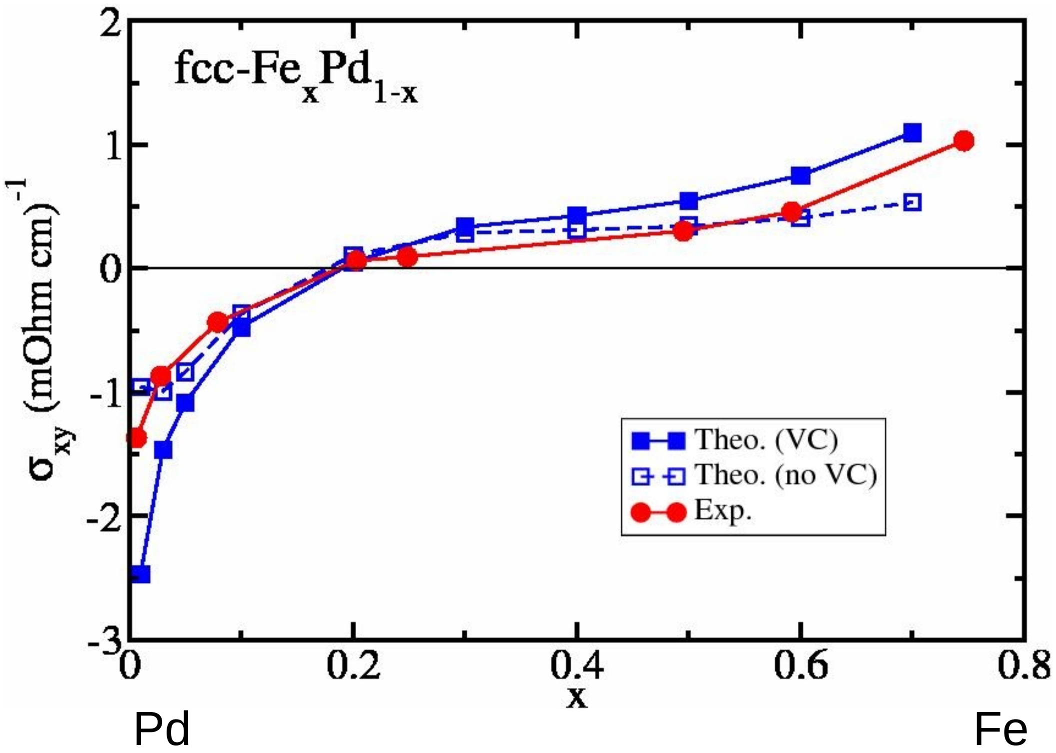
Butler, PRB **31**, 3260 (1985) (non-relativistic)
Banhart *et al.*, SSC **77**, 107 (1991) (fully-relativistic)
Turek *et al.*, PRB **65**, 125101 (2002) (LMTO-CPA)

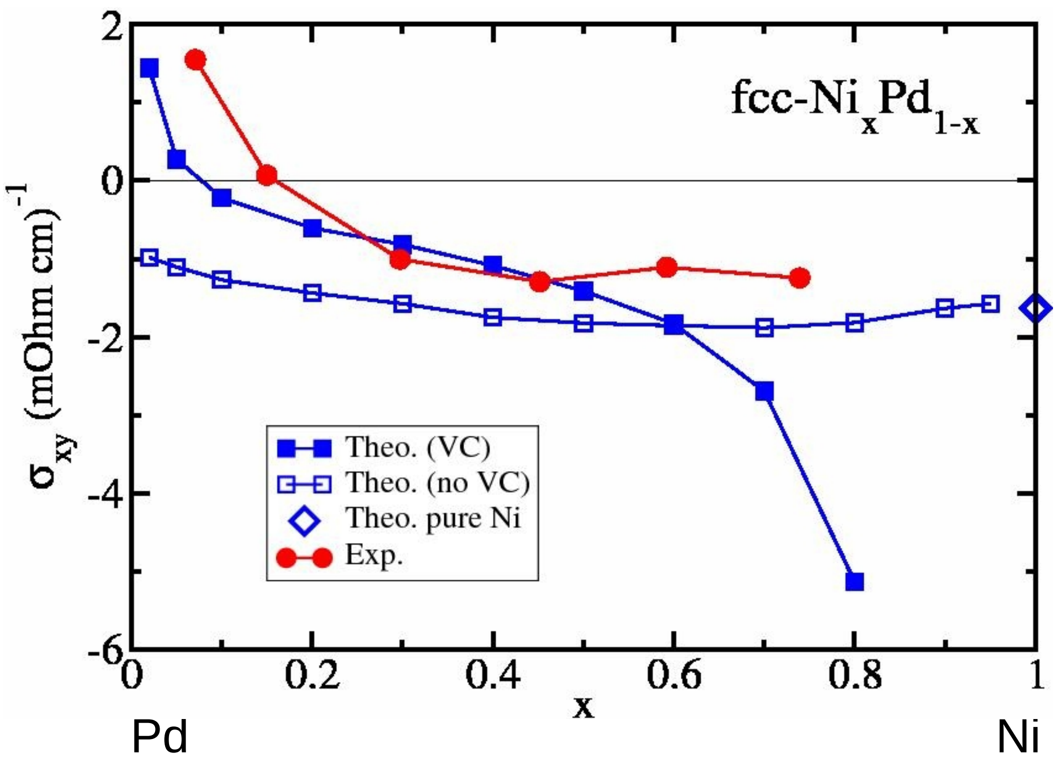
See also: Velicky, PR **184**, 614 (1969)

Kubo-Středa vs. Kubo-Bastin approach

Anomalous Hall conductivity in ferromagnetic alloys

KKR-CPA results based on Kubo-Středa equation

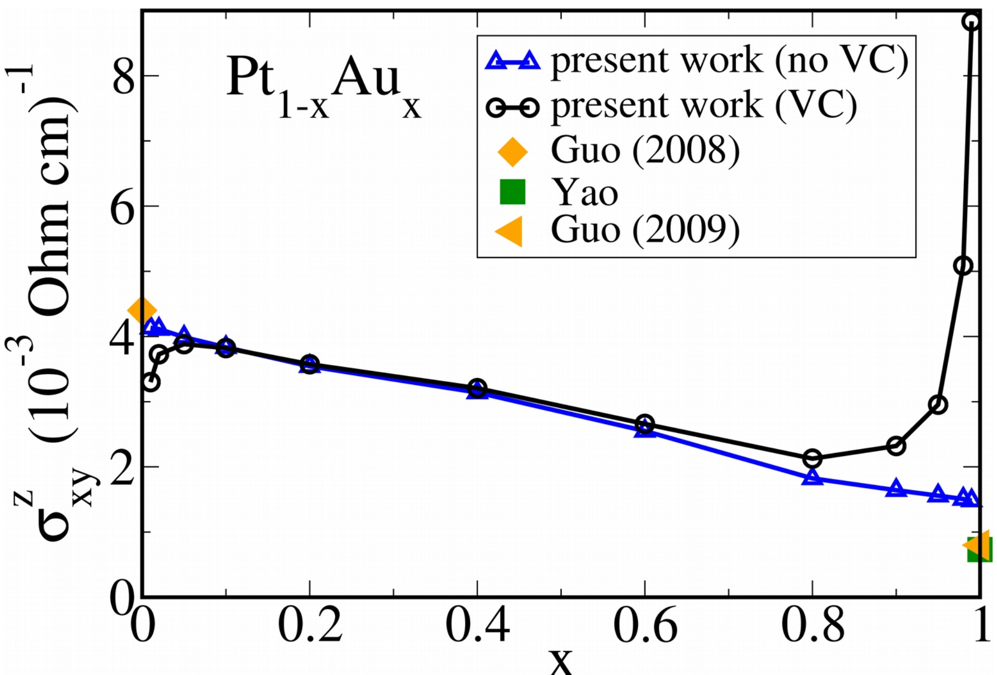


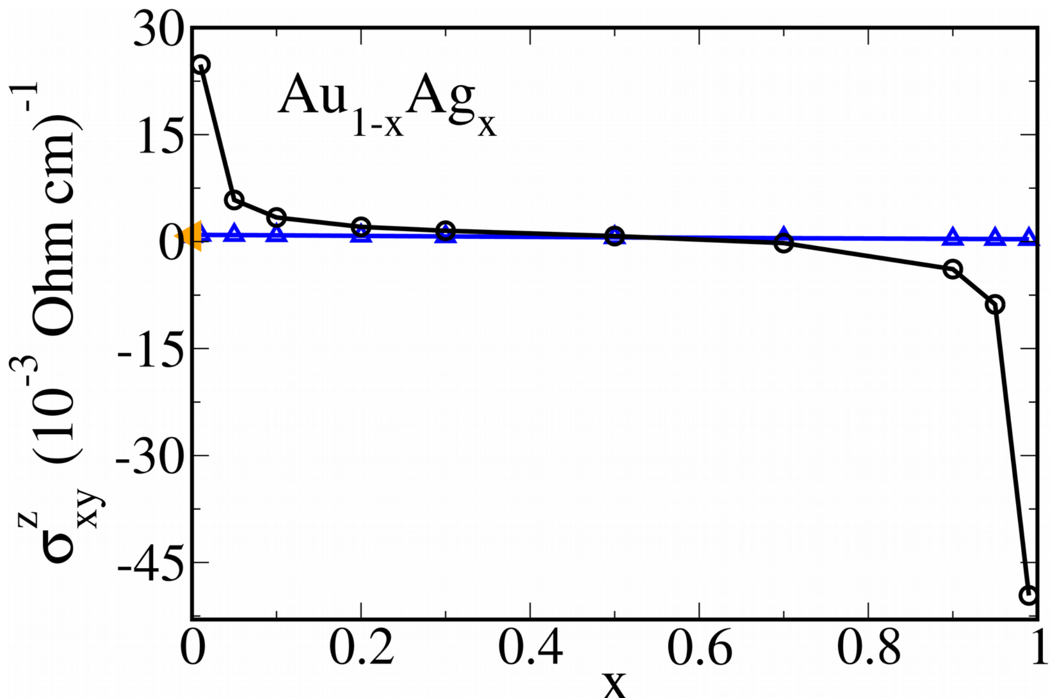


Expt.: Matveev *et al.*, Fiz. Met. Metalloved **53**, 34 (1982)
Theo.: Lowitzer *et al.*, PRL **105**, 266604 (2010)

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

KKR-CPA results based on Kubo-Středa equation





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

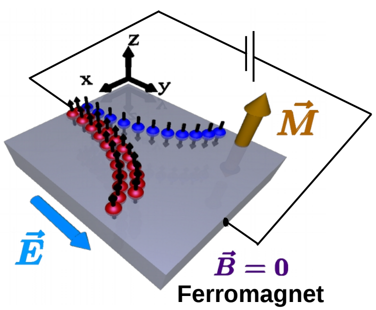
Guo *et al.*, PRL **100**, 096401 (2008)
Guo, JAP **105**, 07C701 (2009)
Yao *et al.*, PRL **95**, 156601 (2005)

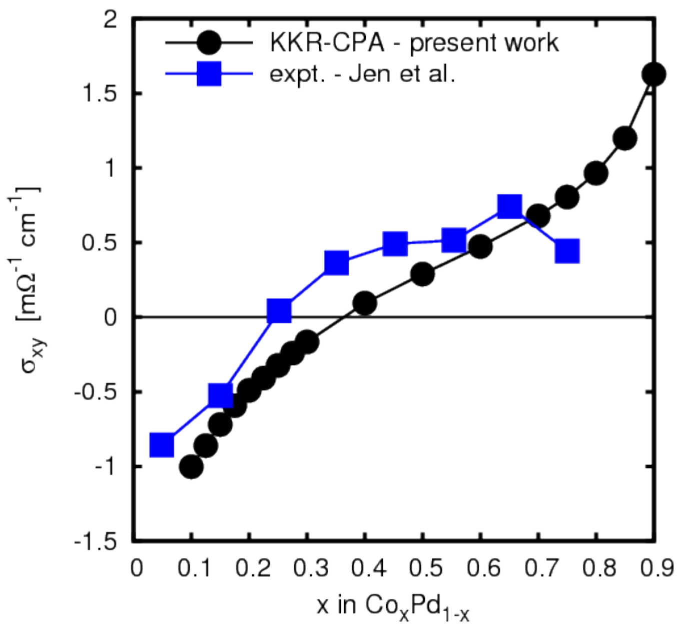
} intrinsic SHE of pure elements

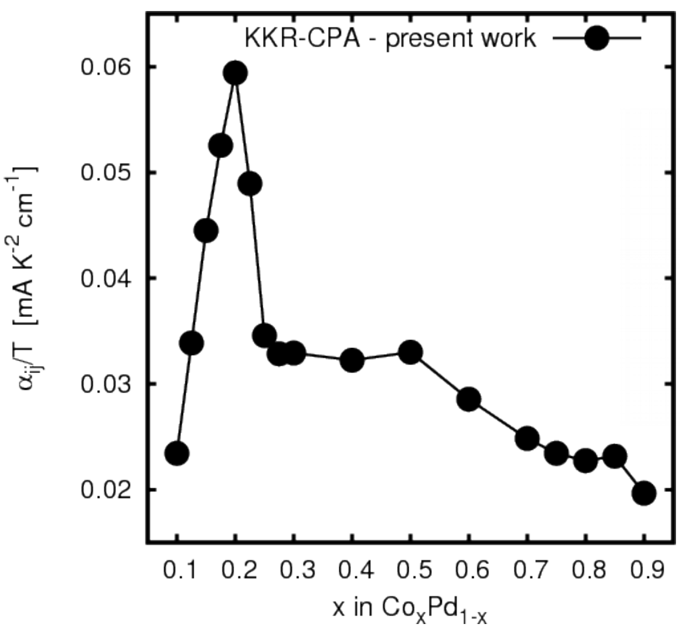
Transverse charge transport Co_xPd_{1-x} alloys

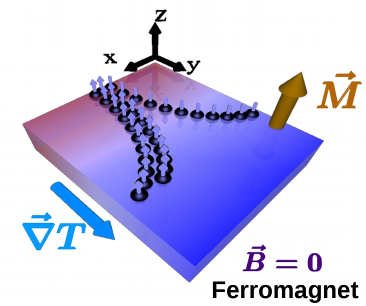
Anomalous Hall conductivity

Anomalous Nernst conductivity









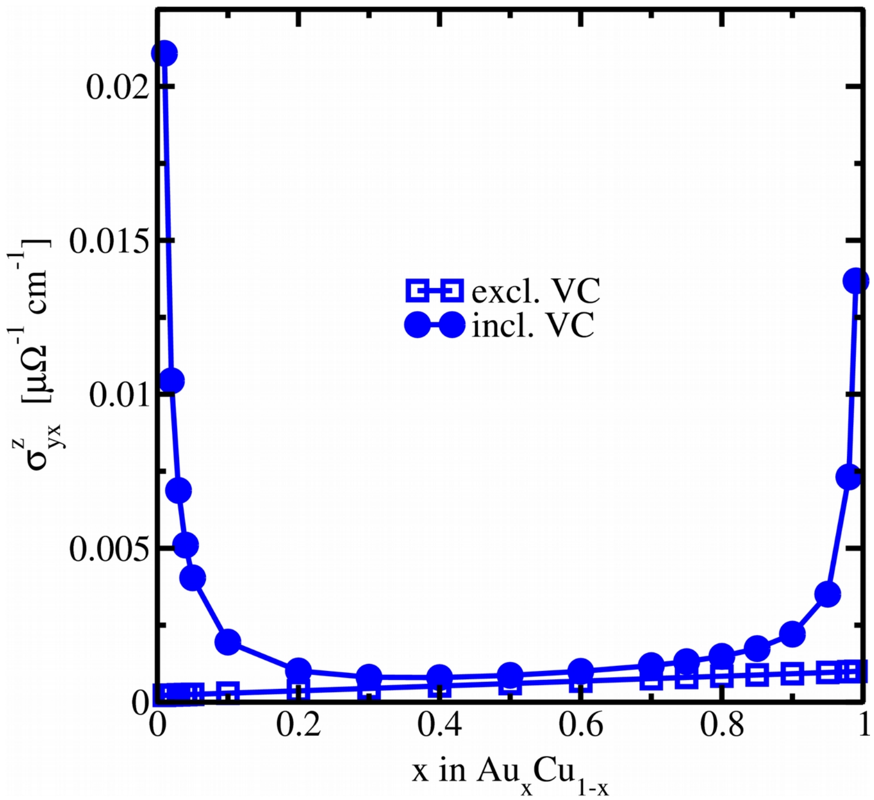
Expt.: Jen *et al.*, JAP **76**, 5782 (1994)

- No direct relation between AHC and ANC as functions of *x*
- AHC shows sign change, while ANC does not
- ANC: Maximum at x ≈ 0.2 in line with behaviour of ρ_{iso}, AMR ratio & S_{xx}

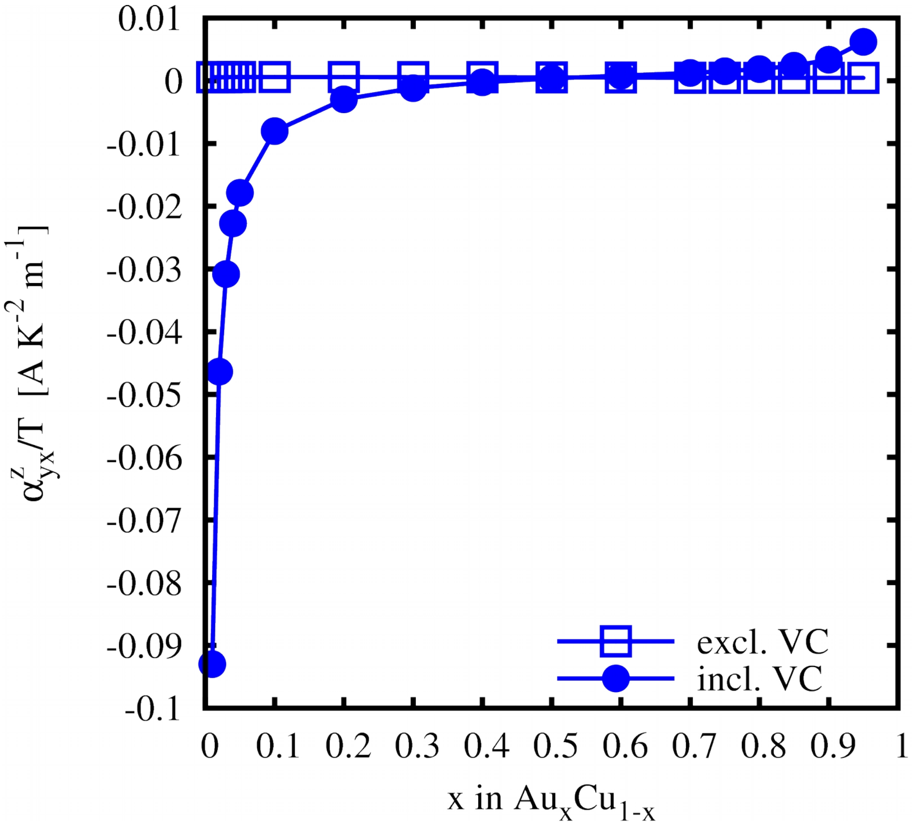
S. Wimmer, D. Ködderitzsch, and H. Ebert, Phys. Rev. B **89**, 161101(R) (2014)

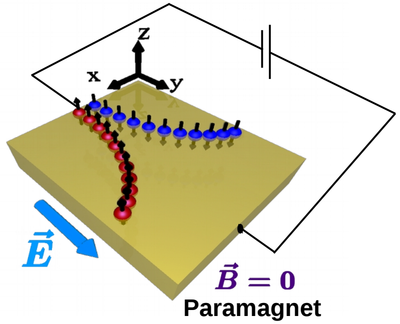
Transverse spin transport in Au_xCu_{1-x}

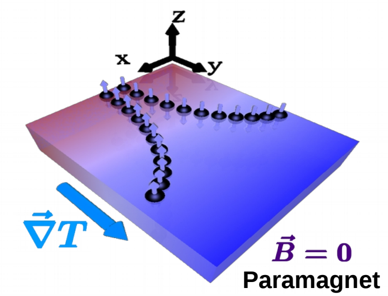
Spin Hall conductivity



(Thermal) Spin Nernst conductivity



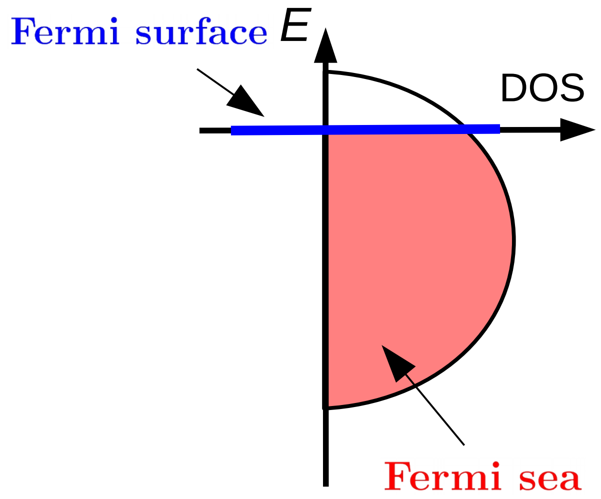




S. Wimmer, D. Ködderitzsch, K. Chadova, and H. Ebert, Phys. Rev. B **88**, 201108(R) (2013)

Kubo-Bastin formalism

$$\sigma_{\mu\nu} = \frac{i\hbar}{V}\int_{-\infty}^{\infty} dE f(E)$$
$$\mathrm{Tr}\left\langle \hat{J}_\mu \frac{dG^+(E)}{dE}\hat{j}_\nu \delta(E-\hat{H}) - \hat{J}_\mu \delta(E-\hat{H})\hat{j}_\nu \frac{dG^-(E)}{dE}\right\rangle_c$$



setting
T = 0K

$$\sigma_{\mu\nu} = \frac{1}{4}\frac{\hbar}{\pi V}\mathrm{Tr}\left\langle \hat{J}_\mu (G^+ - G^-)\hat{j}_\nu G^- - \hat{J}_\mu G^+ \hat{j}_\nu (G^+ - G^-)\right\rangle_c$$
$$+\frac{1}{4}\frac{\hbar}{\pi V}\int_{-\infty}^{E_F} d\varepsilon \mathrm{Tr}\left\langle \hat{J}_\mu G^+ \hat{j}_\nu \frac{dG^+}{d\varepsilon} - \hat{J}_\mu \frac{dG^+}{d\varepsilon}\hat{j}_\nu G^+ - \left(\hat{J}_\mu G^- \hat{j}_\nu \frac{dG^-}{d\varepsilon} - \hat{J}_\mu \frac{dG^-}{d\varepsilon}\hat{j}_\nu G^-\right)\right\rangle_c$$

- numerical difficulties (energy derivative)
- integral over δ-function like terms

→ integration in the complex plane

inclusion of vertex corrections → numerical effort

Similar approach and implementation within TB-LMTO

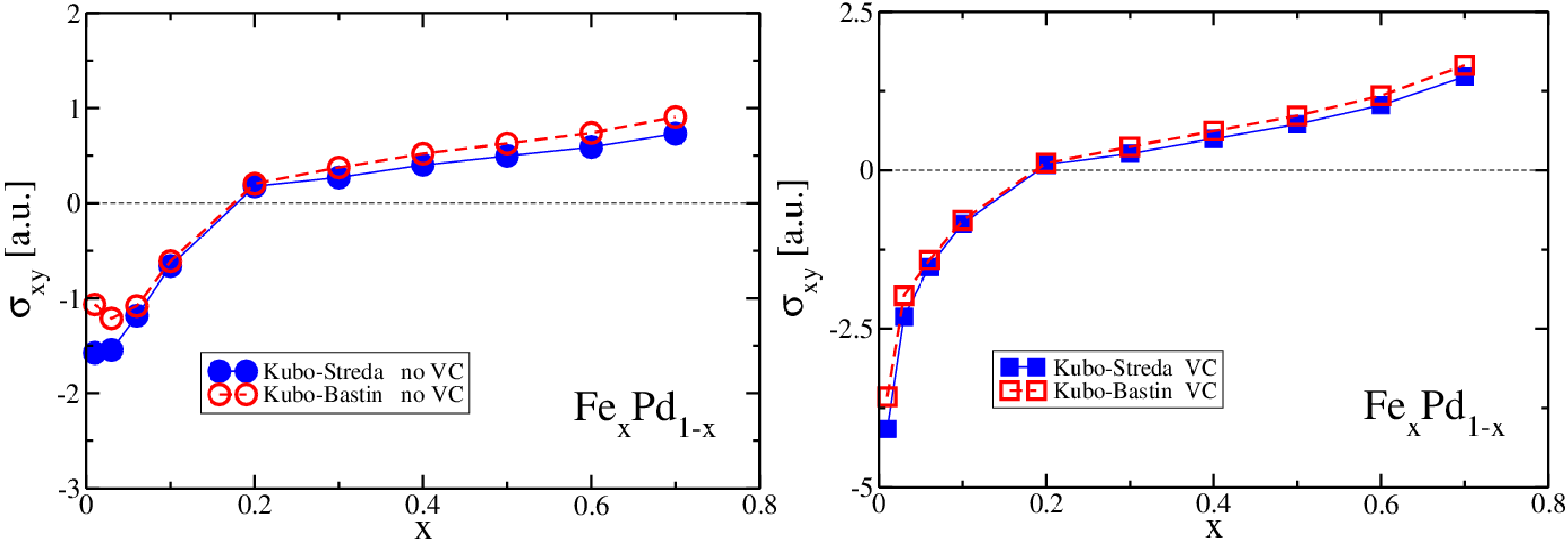
I Turek, J Kudrnovský and V Drchal, PRB **89**, 064405 (2014)

Anomalous Hall conductivity in ferromagnetic alloys

KKR-CPA results based on Bastin and Kubo-Středa equation
(numerical test for the equivalency)

without vertex corrections
(coherent part)

with vertex corrections
(total)



Kubo-Středa:
S.Lowitzer, D.Ködderitzsch, H.Ebert, PRL **105**, 266604 (2010)

Spin Hall conductivity for transition metal alloys

KKR-CPA results based on Bastin and Kubo-Středa equation
(numerical test for the equivalency)

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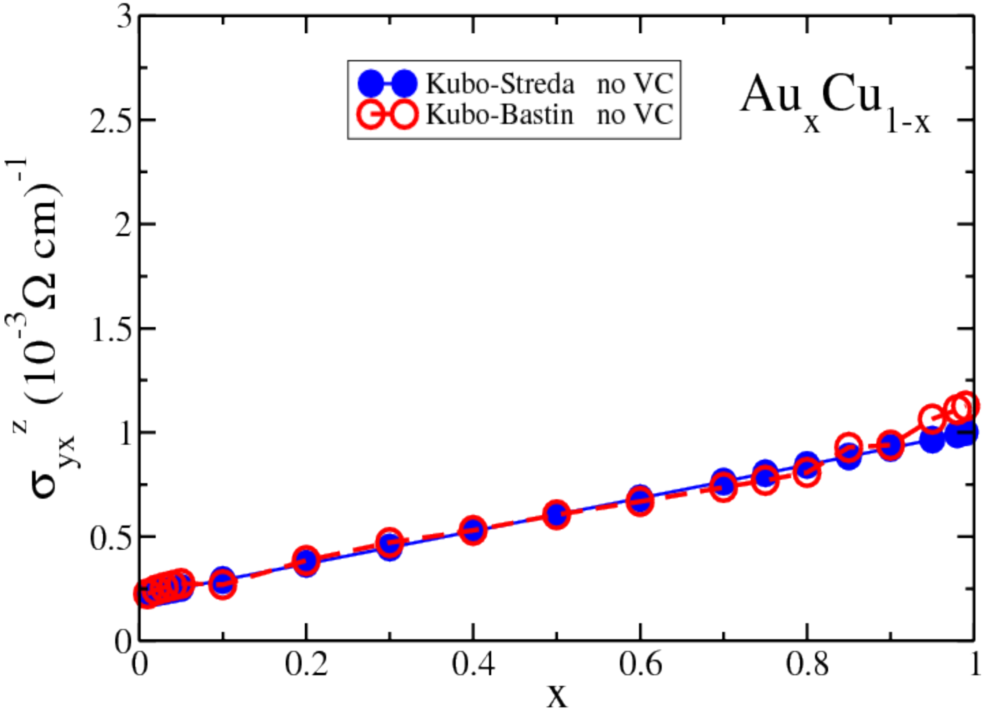
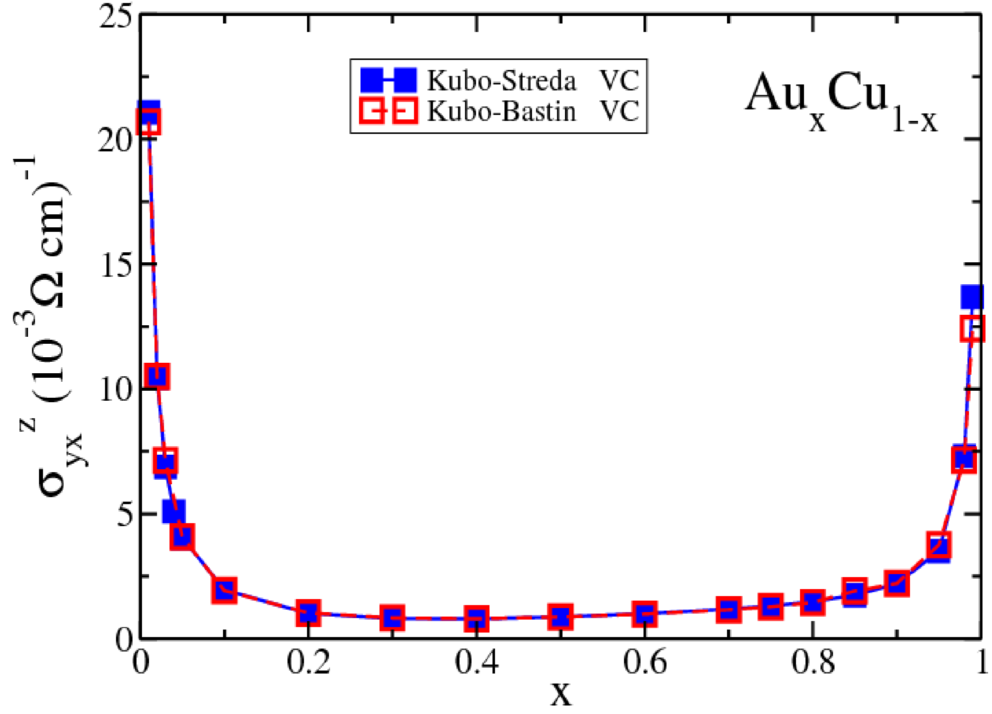


with vertex corrections
(total)



Kubo vs. Boltzmann formalism

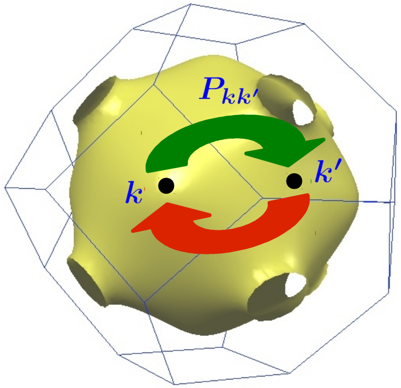
Connection with Boltzmann Formalism

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)

Connection with Boltzmann Formalism

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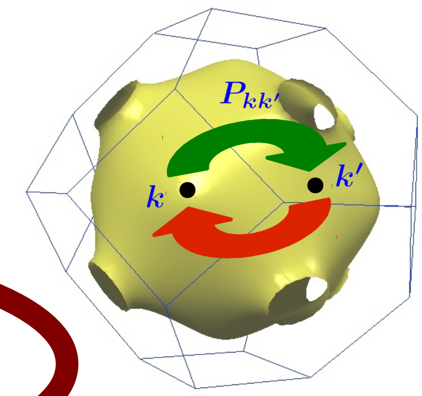


Boltzmann equation including *scattering-in term*

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

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

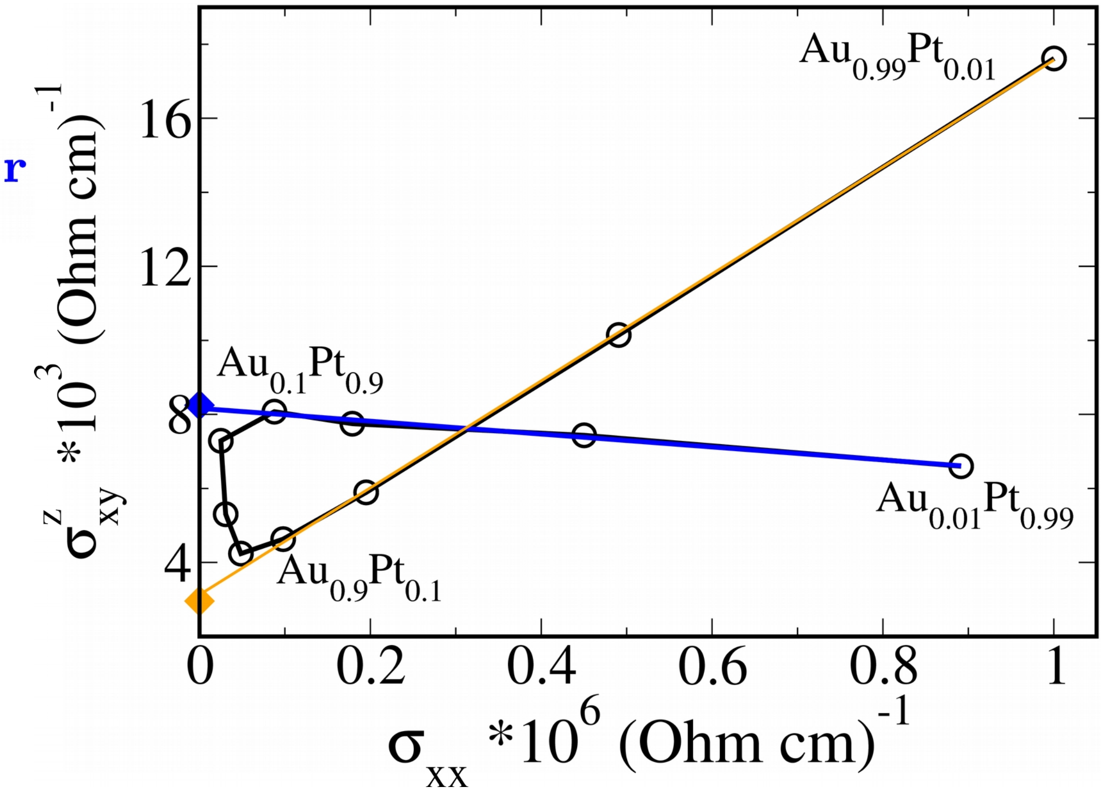
Butler, PRB **31**, 3260 (1985)

Decomposition of Spin Hall conductivity via scaling behaviour of individual contributions

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

S : skewness factor

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



Ansatz using scaling behaviour

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

linear relation on both sides of alloy system for composition

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

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

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

Description of the (Spin) Hall effect

Kubo-Středa linear response

any system

longitudinal

σ_{xx}

Decomposition

transverse

σ^{z}_{xy}

intrinsic coherent

extrinsic incoherent

scaling laws

side-jump

skew

vertex corrections

Boltzmann

dilute alloys

longitudinal

σ_{xx}

transverse

skew

scattering-in terms

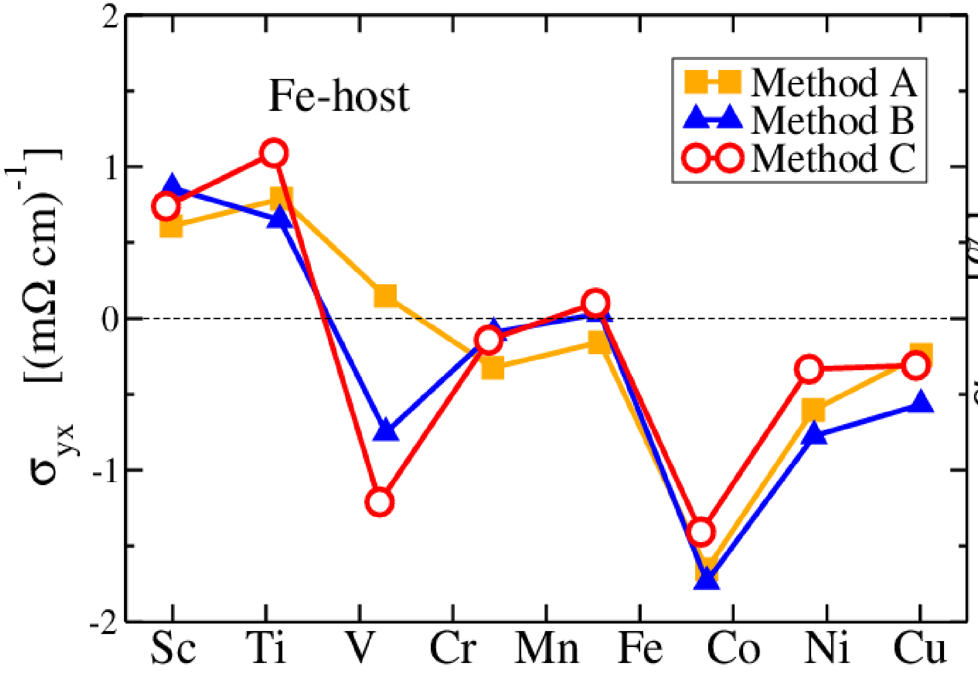
Berry curvature

pure systems

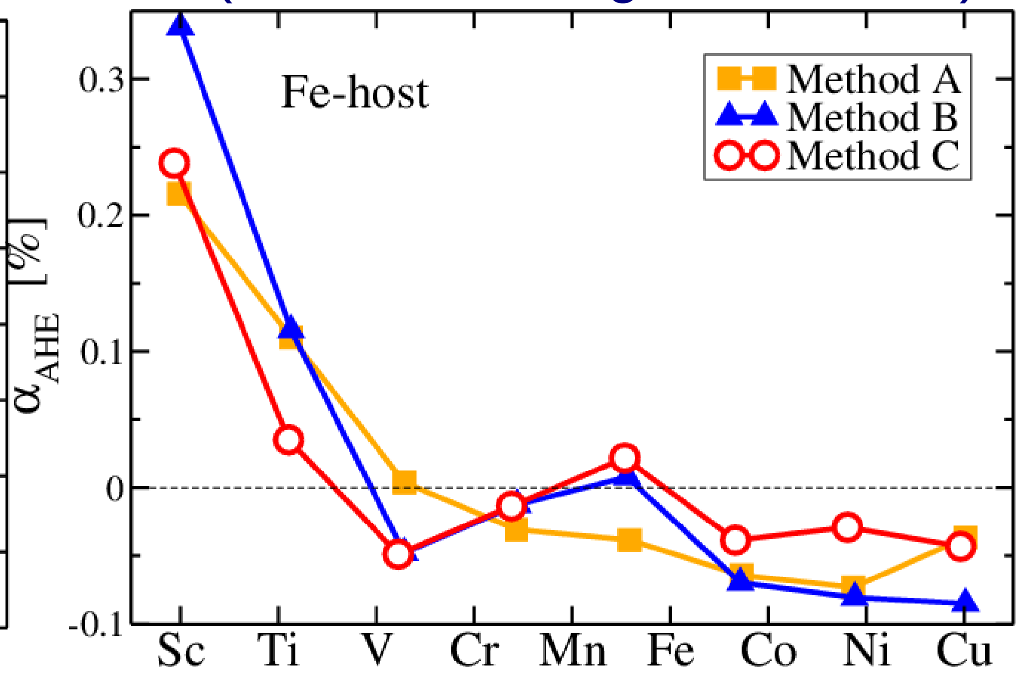
intrinsic

Ferromagnetic host doped with 3*d* impurities with concentration of 1 at.%

Skew-scattering contribution to the AHE



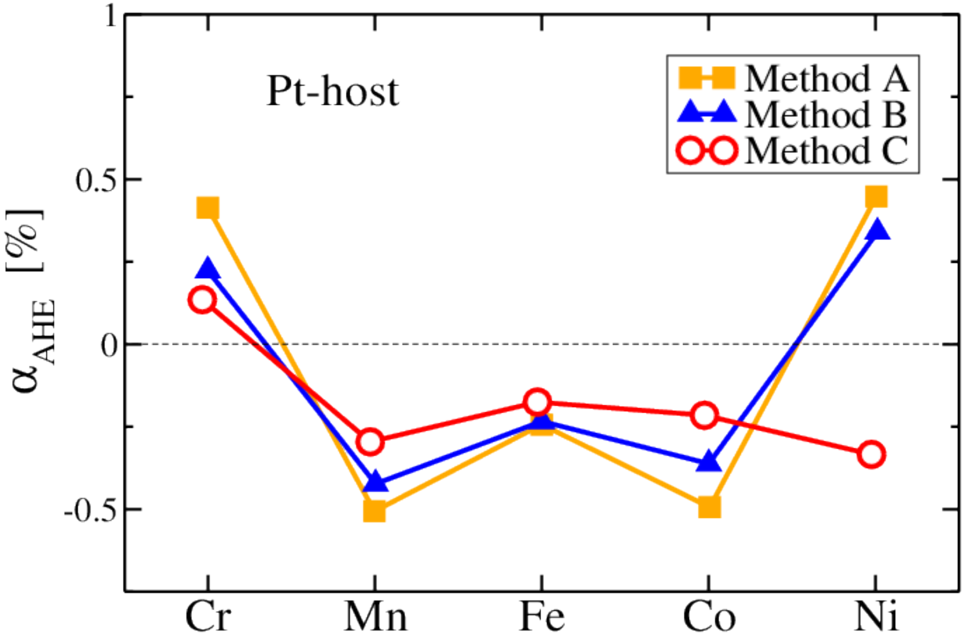
Anomalous Hall angle (skew-scattering contribution)



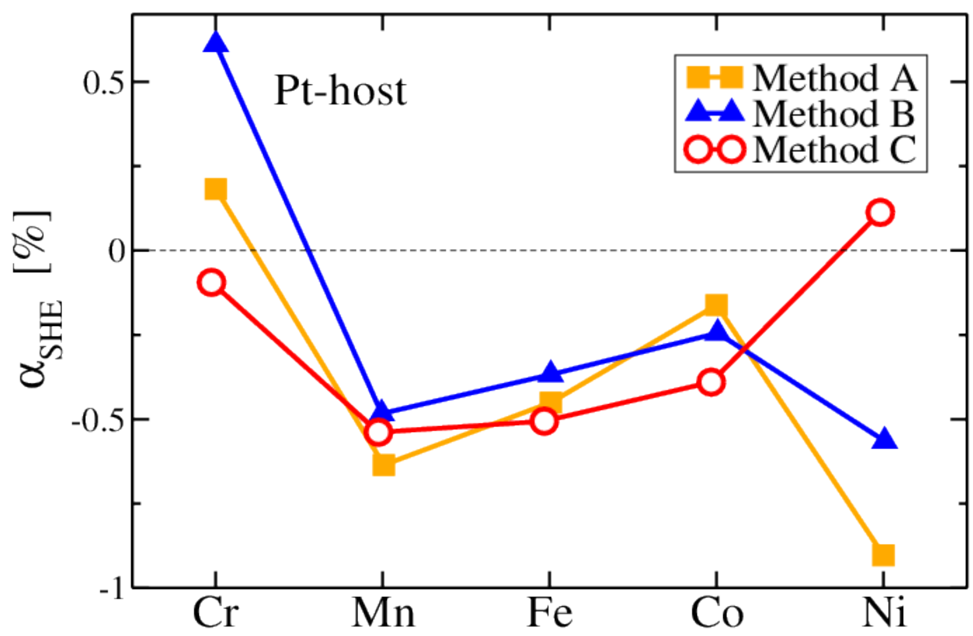
	Approach	Geometry	SOC	*group*
Method A	Boltzmann	Full potential	Pauli	*Jülich (Blügel)*
Method B	Boltzmann	ASA	Dirac	*Halle (I. Mertig)*
Method C	Kubo	ASA	Dirac	*Munich (H. Ebert)*

Paramagnetic host doped with 3*d* impurities with concentration of 1 at. %

Anomalous Hall angle (skew-scattering contribution)



Spin Hall angle



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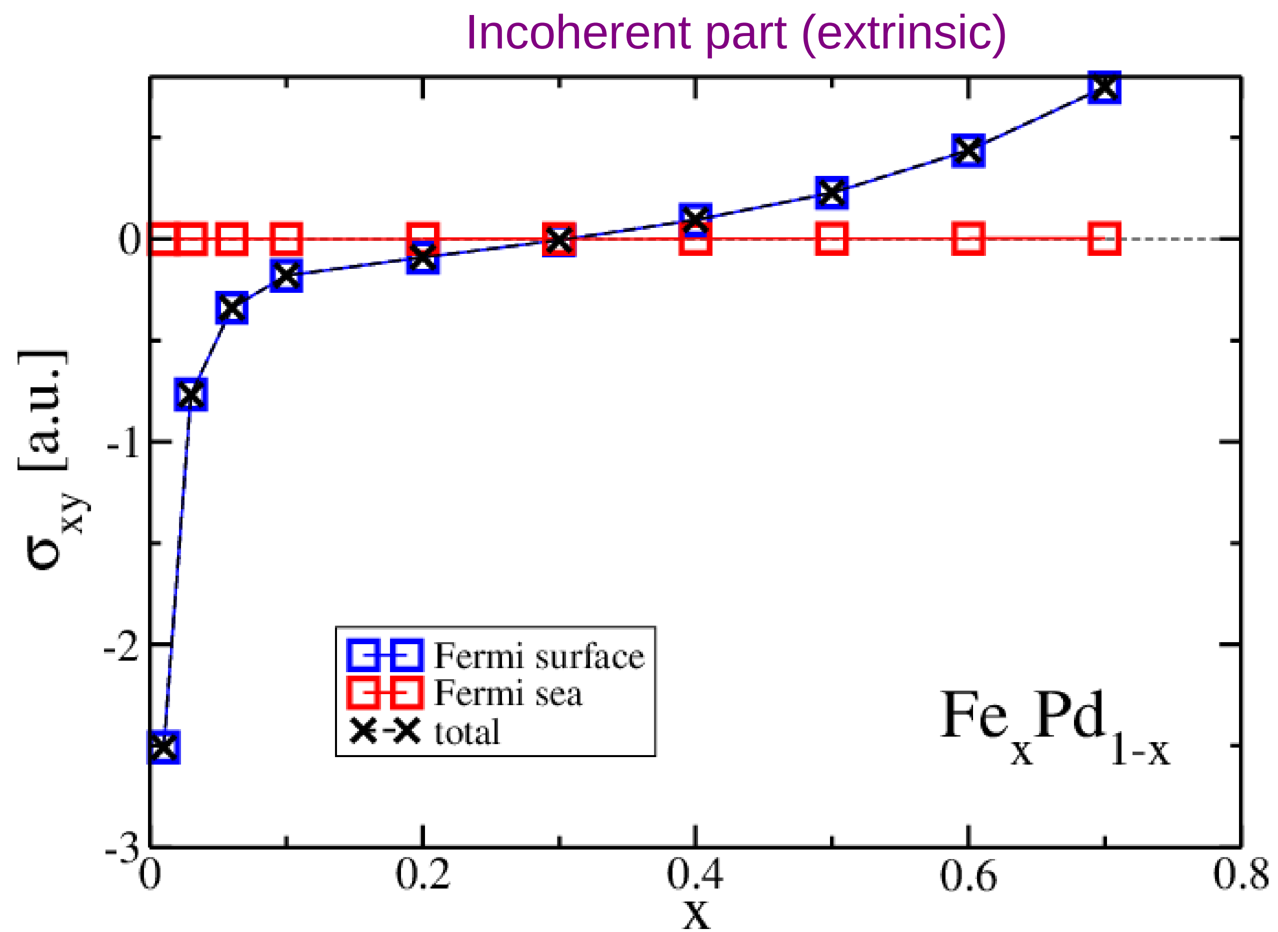
Anomalous Hall conductivity in ferromagnetic alloys

Contributions to the incoherent part of the conductivity tensor



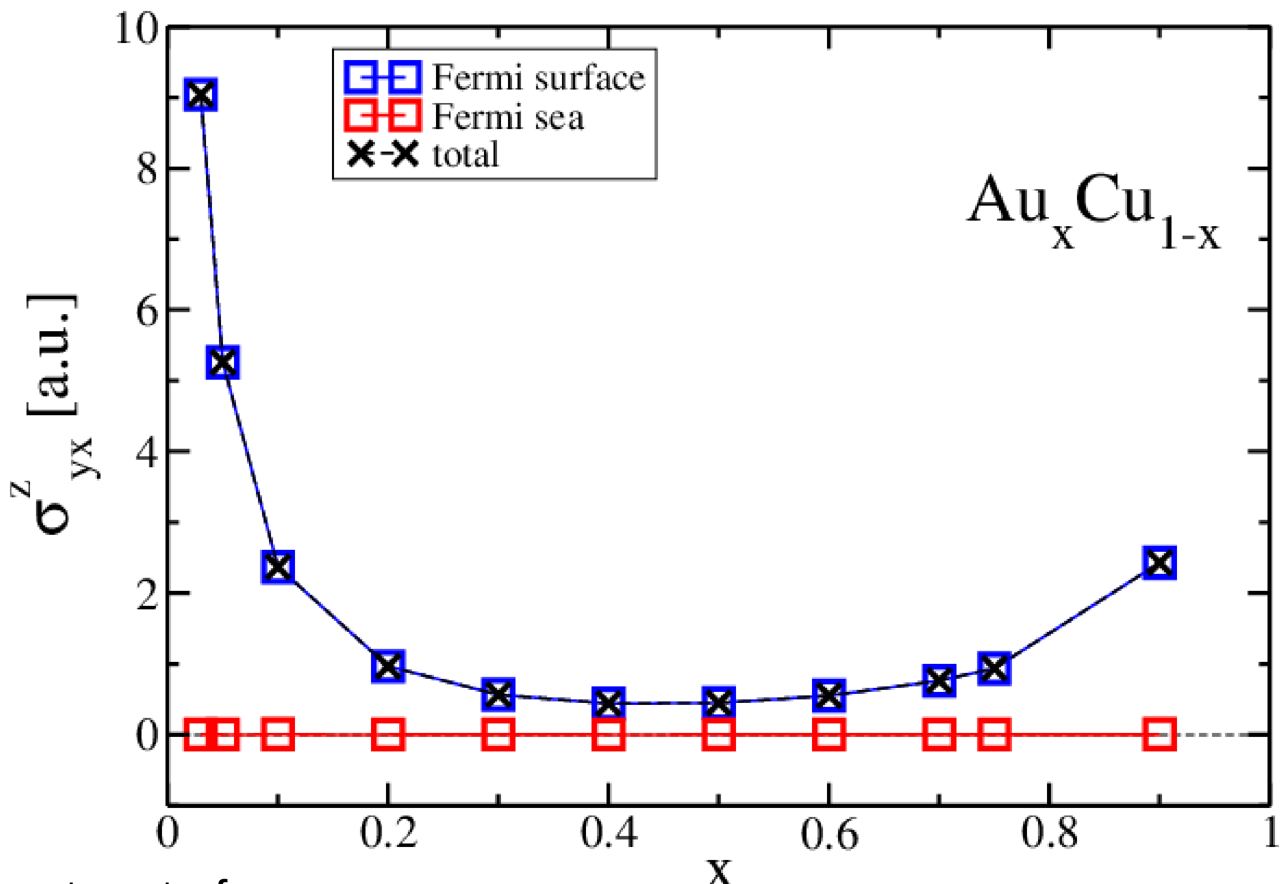
Incoherent part of Fermi sea term is negligible → justification for Kubo-Středa ↔ Boltzmann scattering

No vertex corrections for the Fermi sea term !

Spin Hall conductivity for transition metal alloys

Contributions to the incoherent part of the conductivity tensor

Incoherent part (extrinsic)



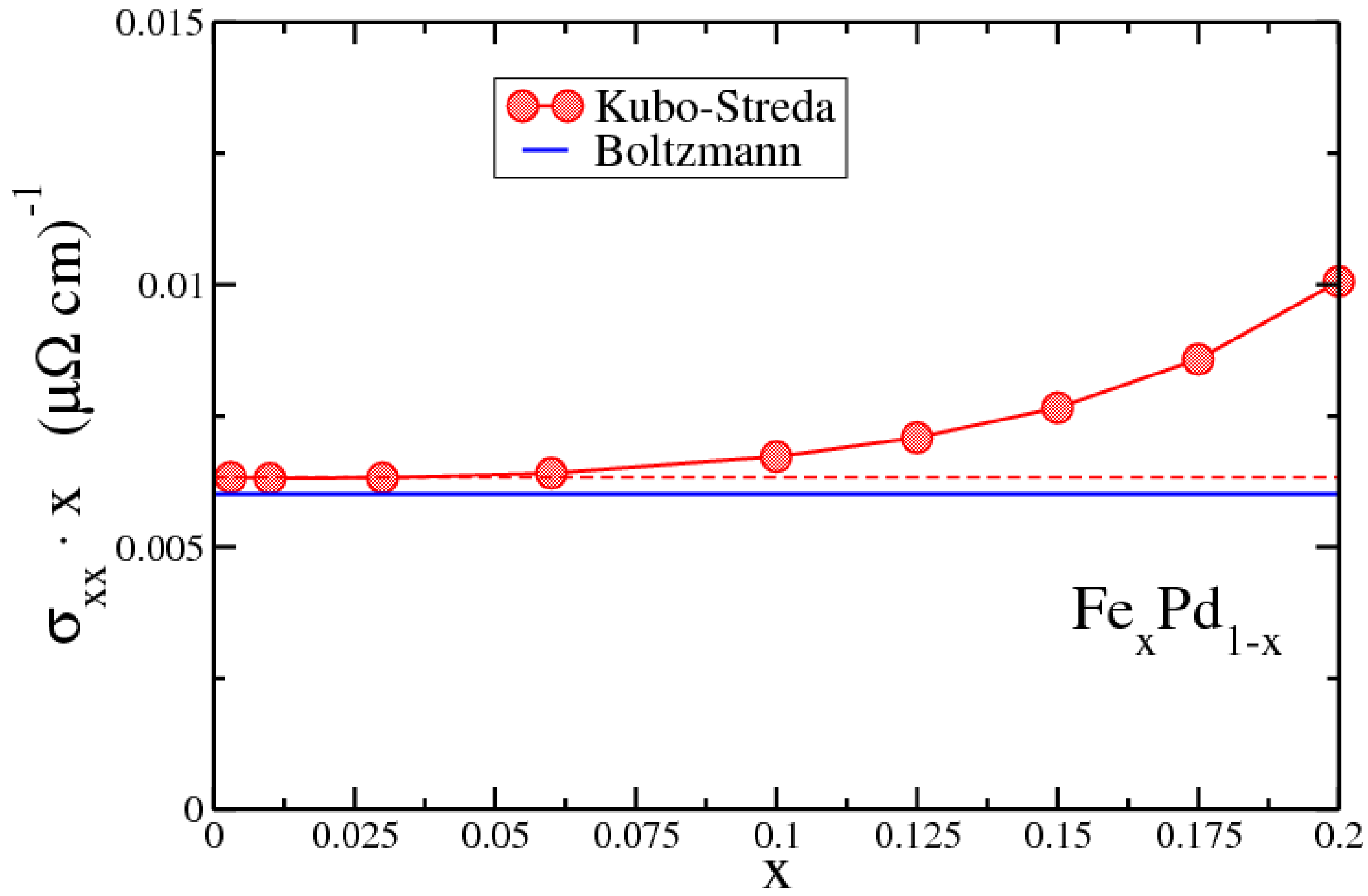
Incoherent part of Fermi sea term is negligible → justification for Kubo-Středa ↔ Boltzmann scattering

No vertex corrections for the Fermi sea term !

AHE – Boltzmann vs Kubo formalism

Comparison of results for varying concentration

longitudinal conductivity $\sigma_{xx} \times x$



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

Symmetry predicted properties

Kleiner's scheme to get the shape of the electrical conductivity tensor

$$\sigma_{ij} = \tau_{\hat{j}_i \hat{j}_j}(\omega, \vec{H}) = \int_0^\infty dt\, e^{-i\omega t} \int_0^\beta d\lambda \left(\rho(\vec{H}) \hat{j}_j \hat{j}_i (t + i\hbar\lambda; \vec{H}) \right)$$

for unitary operators *u*:

$$\sigma_{ij} = \sum_{kl} \sigma_{kl}\, D(P_R)_{ki} D(P_R)_{lj}$$

for anti-unitary operators *a*:

$$\sigma_{ij} = \sum_{kl} \sigma_{lk}\, D(P_R)^*_{ki} D(P_R)^*_{lj}$$

Pseudoalgorithm

- determine symmetry of system
- loop over symmetry operations
  - set up system of linear eqs. in elements $\{\sigma_{ij}\}$
- solution gives restrictions
  - element is linear combination of other elements
  - element is its negative → element is zero

Only the magnetic Laue group has to be considered

same transformation behavior for thermal transport ⇒ same tensor shapes

W. H. Kleiner, Phys. Rev. **142**, 318 (1966)

Electrical conductivity - tensor shapes

Results obtained by analytic computation using computer algebra system (CAS)

Non-magnetic materials

magnetic Laue group	$\underline{\tau}'$	$\underline{\sigma}$
$\bar{1}1'$	$\begin{pmatrix} \tau_{xx} & \tau_{yx} & \tau_{zx} \\ \tau_{xy} & \tau_{yy} & \tau_{zy} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix}$
$2/m1'$	$\begin{pmatrix} \tau_{xx} & 0 & \tau_{zx} \\ 0 & \tau_{yy} & 0 \\ \tau_{xz} & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & \sigma_{xz} \\ 0 & \sigma_{yy} & 0 \\ \sigma_{xz} & 0 & \sigma_{zz} \end{pmatrix}$
$mmm1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{yy} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$\bar{3}1'$, $4/m1'$, $6/m1'$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ \tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$\bar{3}1m1'$, $\bar{3}m11'$, $4/mmm1'$, $6/mmm1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$m\bar{3}1'$, $m\bar{3}m1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{xx} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$

Thermo-electrical response tensor

Electrical conductivity tensor

Magnetic materials

magnetic Laue group	$\underline{\tau}'$	$\underline{\sigma}$
$2'/m'$	$\begin{pmatrix} \tau_{xx} & -\tau_{yx} & \tau_{zx} \\ -\tau_{xy} & \tau_{yy} & -\tau_{zy} \\ \tau_{xz} & -\tau_{yz} & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ -\sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & -\sigma_{yz} & \sigma_{zz} \end{pmatrix}$
$m'm'm$	$\begin{pmatrix} \tau_{xx} & -\tau_{yx} & 0 \\ -\tau_{xy} & \tau_{yy} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/m$	$\begin{pmatrix} \tau_{yy} & -\tau_{xy} & 0 \\ -\tau_{yx} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/mm'm$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ -\tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/mmm'$	$\begin{pmatrix} \tau_{yy} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma \end{pmatrix}$
$\bar{3}1m'$, $m'1$, $4/mm'm'$, $6/mm'm'$	$\begin{pmatrix} \tau_{xx} & \tau_{xy} & 0 \\ -\tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$6'/m'$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ \tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$6'/m'm'm$, $6'/m'mm'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$m\bar{3}m'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{xx} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$

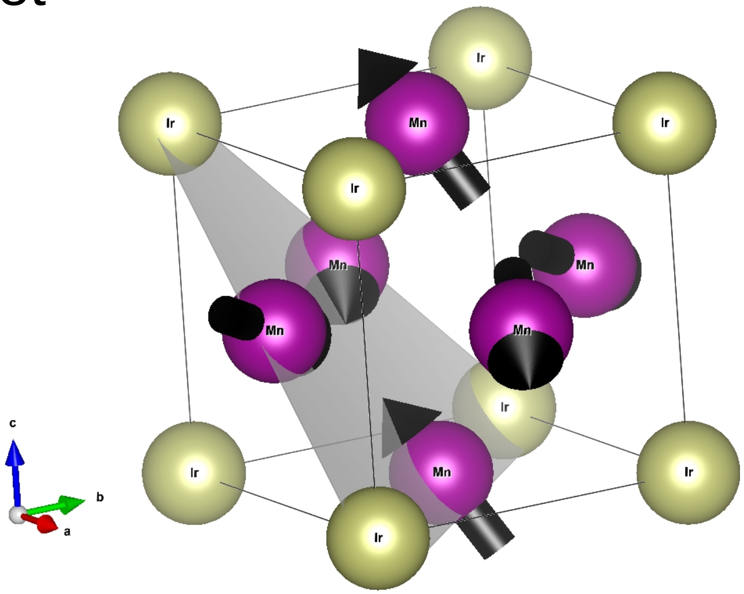
class a) contains time reversal *T*

class c) contains combined operations a=v *T*

Transverse conductivity and magneto-optics in non-collinear antiferromagnets

Mn_3Ir – a prototype non-collinear antiferromagnet

- Cu_3Au structure
- moments in (111) plane (Kagome lattice)
- magnetic space group: R$\bar{3}$m'



Prediction of **anomalous Hall effect (AHE)**

and **magneto-optical Kerr effect (MOKE)**

- based on analysis of electronic structure

  Chen, Niu, and MacDonald, PRL **112**, 017205 (2014)

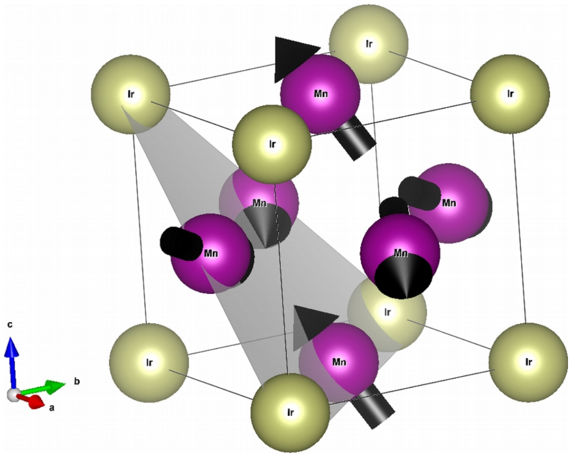
- Natural consequence of Kleiner's tables for the shape of the conductivity tensor

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

Mn_3Ir – electrical conductivity

Electrical conductivity tensor

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



z-direction along [111]

numerical work based on Kubo-Středa equation

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

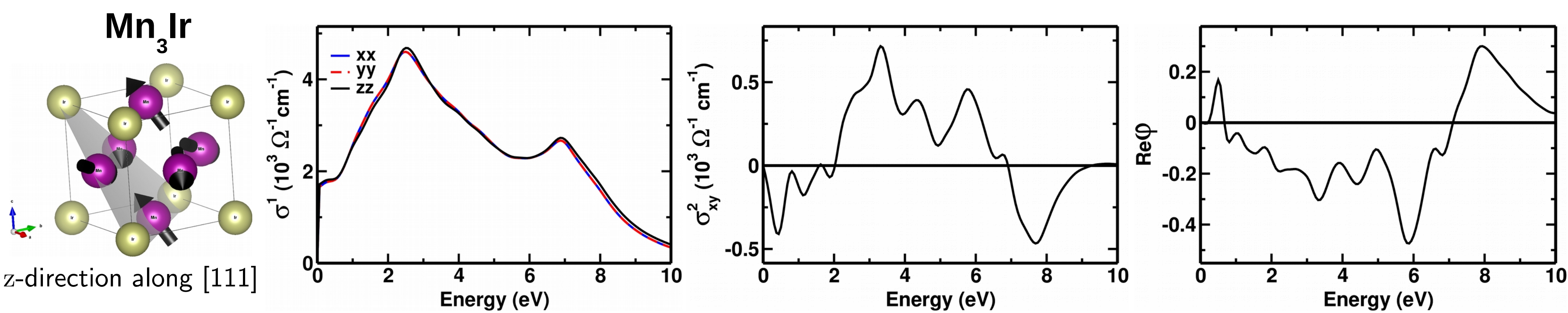
Smrčka and Středa, JPC 10, 2153 (1977)
Lowitzer *et al.*, PRL **105**, 266604 (2010)

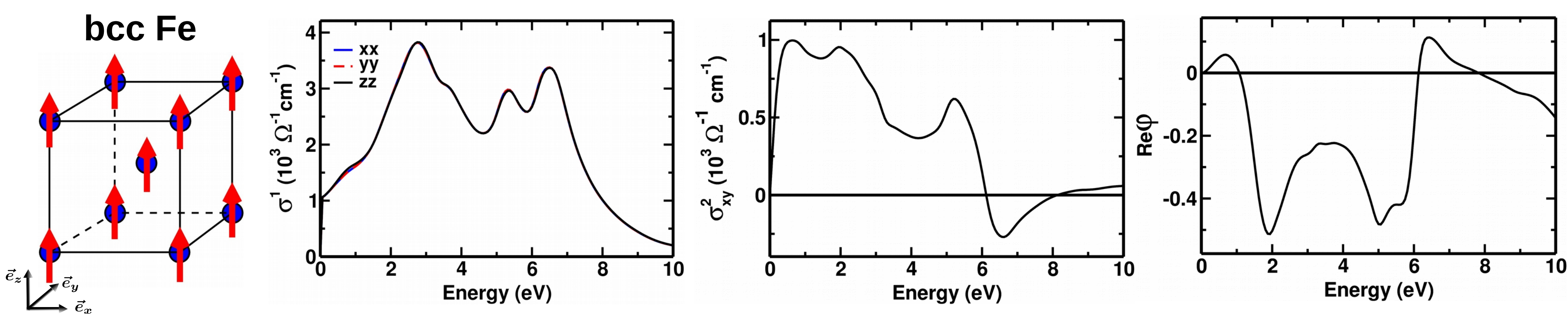
- confirms tensor shape
- Anomalous Hall conductivity

275 $(\Omega\ \mathrm{cm})^{-1}$ this work
218 $(\Omega\ \mathrm{cm})^{-1}$ Chen *et al.* (2014)

comparable in size to Fe, Co, and Ni

Mn_3Ir – optical conductivity and Kerr angle



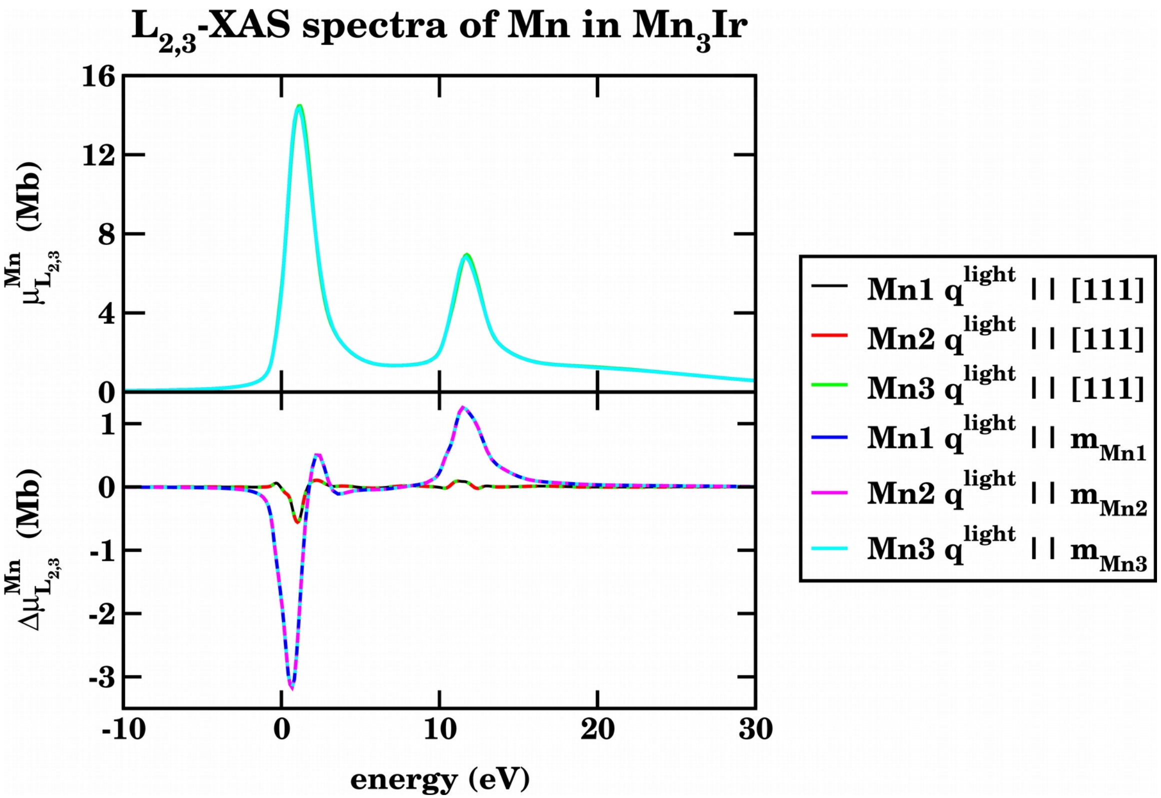


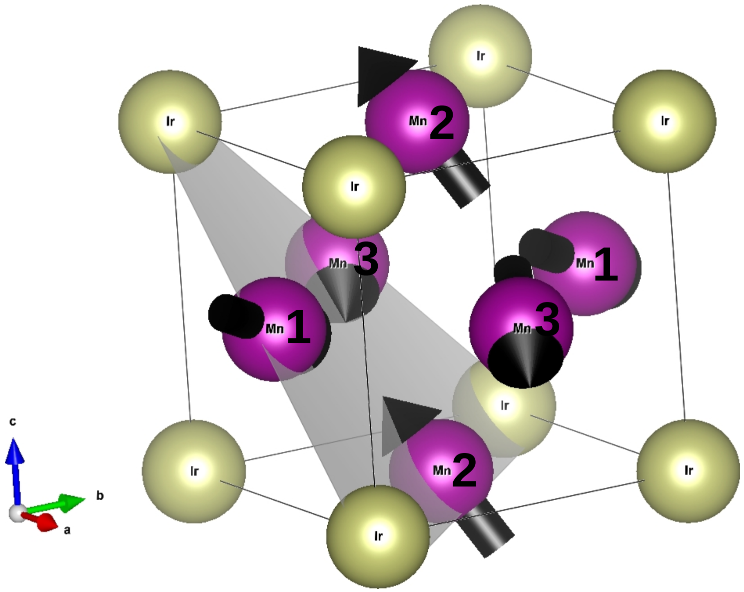
- same tensor shape as for bcc-Fe, comparable in magnitude

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

S. Wimmer, *et al.*, unpublished (2015)

Mn_3Ir – Mn $L_{2,3}$ X-ray absorption spectra





z-direction along [111]

- spectra by superposition of site-resolved abs. coeffs. $\mu^{n}_{\vec{q}\lambda}(\omega)$
- incidence $\vec{q}$ [111] vs. direction of $\vec{m}_n$ (polar geometry)
  - same total absorption
  - in **both** cases XMCD (larger for polar geometry)
- ***Results questions the XMCD sum rules***

Wimmer, *et al.*, unpublished (2015)

Extended Kleiner's scheme to get the shape of the spin-polarisation conductivity tensor

$$\tau_{(\mathcal{T}_k \hat{j}_i)\hat{j}_j}(\omega, \vec{H}) = \int_0^\infty dt\, e^{-i\omega t} \int_0^\beta d\lambda \left(\rho(\vec{H}) \hat{j}_j \mathcal{T}_k \hat{j}_i (t + i\hbar\lambda; \vec{H}) \right)$$

$$\hat{j}_j = -|e| c\, \alpha_j$$ ← Dirac matrix

Using a relativistic spin polarization operator [1,2,3]: $\mathcal{T}_k = \beta \Sigma_k - \frac{\gamma_5 \Pi_k}{mc}$

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

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

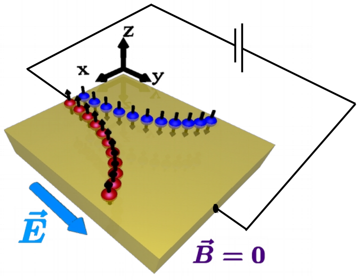
Only the magnetic Laue group has to be considered

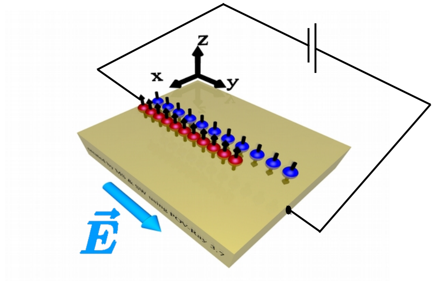
S. Wimmer *et al.*, arXiv:1502.04947, PRB RC *accepted* (2015)

[1] V. Bargmann, E. P. Wigner, Proc. Natl. Acad. Sci. U.S.A. **34**, 211 (1948)
[2] A. Vernes, B.L. Györffy, P. Weinberger, Phys. Rev. B **76**, 012408 (2007)
[3] S. Lowitzer, Ködderitzsch, H. Ebert, Phys. Rev. B **82**, 140402 (2010)

Electrical and spin-polarized conductivity tensor

magnetic Laue group	$\underline{\boldsymbol{\sigma}}$	$\underline{\boldsymbol{\sigma}}^x$	$\underline{\boldsymbol{\sigma}}^y$	$\underline{\boldsymbol{\sigma}}^z$
$m\bar{3}m1'$ e.g.: Au	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma^x_{yz} \\ 0 & -\sigma^x_{yz} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -\sigma^x_{yz} \\ 0 & 0 & 0 \\ \sigma^x_{yz} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \sigma^x_{yz} & 0 \\ -\sigma^x_{yz} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$4/mm'm'$ e.g.: FM bcc Fe	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \sigma^x_{xz} \\ 0 & 0 & \sigma^x_{yz} \\ \sigma^x_{zx} & \sigma^x_{zy} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -\sigma^x_{yz} \\ 0 & 0 & \sigma^x_{xz} \\ -\sigma^x_{zy} & \sigma^x_{zx} & 0 \end{pmatrix}$	$\begin{pmatrix} \sigma^z_{xx} & \sigma^z_{xy} & 0 \\ -\sigma^z_{xy} & \sigma^z_{xx} & 0 \\ 0 & 0 & \sigma^z_{zz} \end{pmatrix}$
$4/m1'$ e.g.: Au_4Sc	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \sigma^x_{xz} \\ 0 & 0 & \sigma^x_{yz} \\ \sigma^x_{zx} & \sigma^x_{zy} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -\sigma^x_{yz} \\ 0 & 0 & \sigma^x_{xz} \\ -\sigma^x_{zy} & \sigma^x_{zx} & 0 \end{pmatrix}$	$\begin{pmatrix} \sigma^z_{xx} & \sigma^z_{xy} & 0 \\ -\sigma^z_{xy} & \sigma^z_{xx} & 0 \\ 0 & 0 & \sigma^z_{zz} \end{pmatrix}$
$2/m1'$ e.g.: Pt_3Ge	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \sigma^x_{xz} \\ 0 & 0 & \sigma^x_{yz} \\ \sigma^x_{zx} & \sigma^x_{zy} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \sigma^y_{xz} \\ 0 & 0 & \sigma^y_{yz} \\ \sigma^y_{zx} & \sigma^y_{zy} & 0 \end{pmatrix}$	$\begin{pmatrix} \sigma^z_{xx} & \sigma^z_{xy} & 0 \\ \sigma^z_{yx} & \sigma^z_{yy} & 0 \\ 0 & 0 & \sigma^z_{zz} \end{pmatrix}$

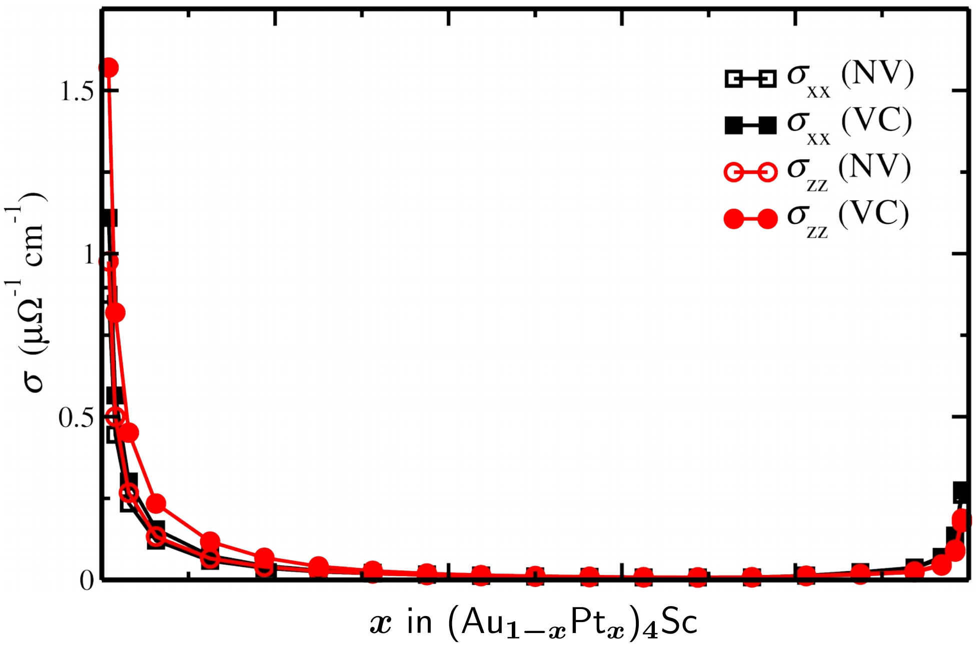




S. Wimmer *et al.*, arXiv:1502.04947, PRB RC *accepted* (2015)

Electrical conductivity & DOS of $Au_{1-x}Pt_xSc$

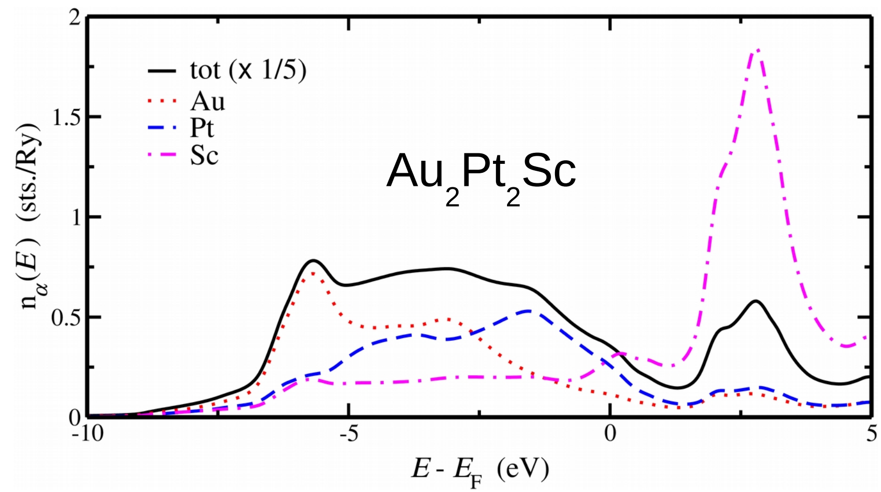
Diagonal conductivity

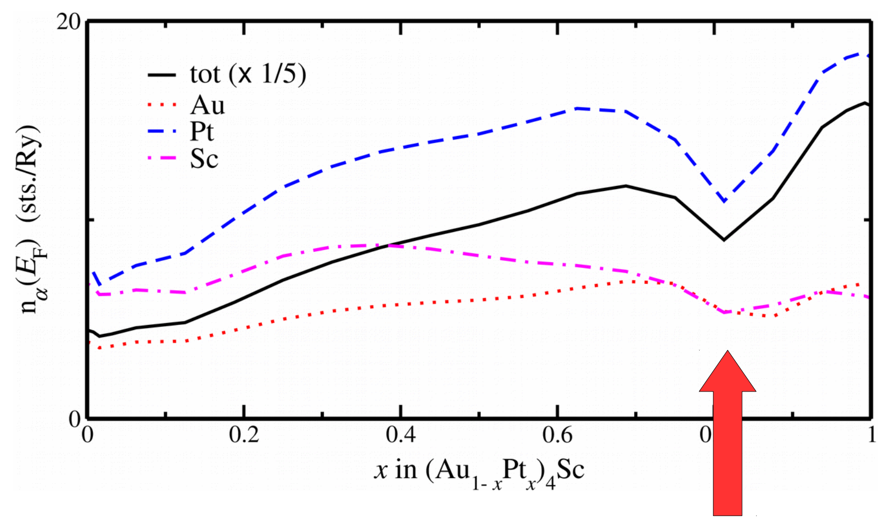


4/m1'

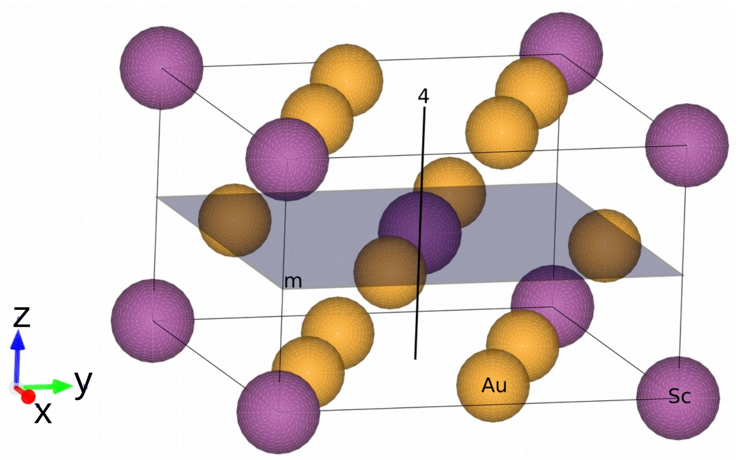
$$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

Density of states



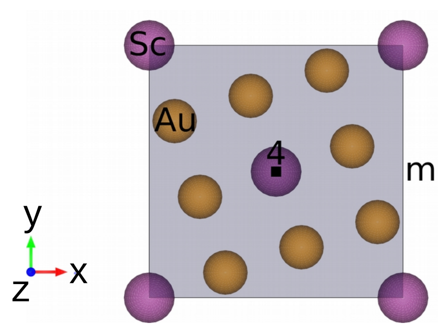


Additional transverse elements for 4/m1'



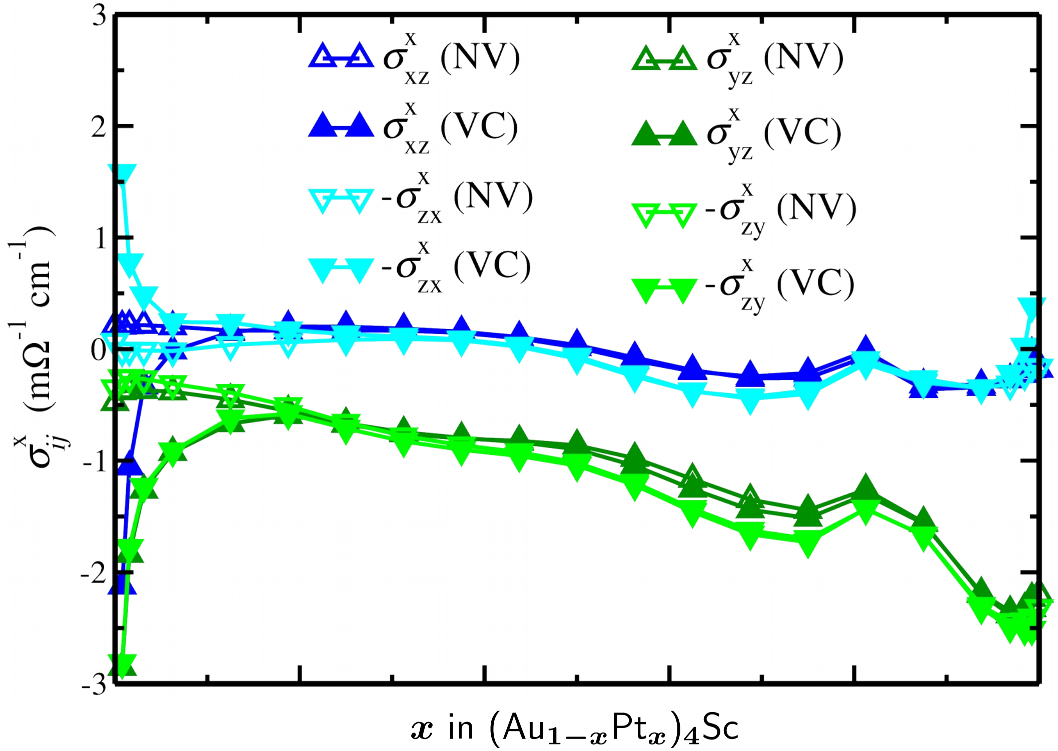
Au$_4$Mn - structure

4/m1'



$$\begin{pmatrix} 0 & 0 & \sigma^x_{xz} \\ 0 & 0 & \sigma^x_{yz} \\ \sigma^x_{zx} & \sigma^x_{zy} & 0 \end{pmatrix}$$

paramagnetic (Au$_{1-x}$Pt$_x$)$_4$Sc - alloy



Longitudinal spin polarized currents

paramagnetic

4/m1'

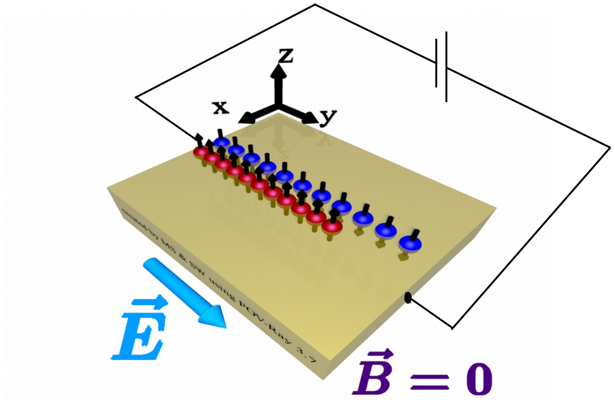
$$\begin{pmatrix} \sigma^z_{xx} & \sigma^z_{xy} & 0 \\ -\sigma^z_{xy} & \sigma^z_{xx} & 0 \\ 0 & 0 & \sigma^z_{zz} \end{pmatrix}$$

ferromagnetic

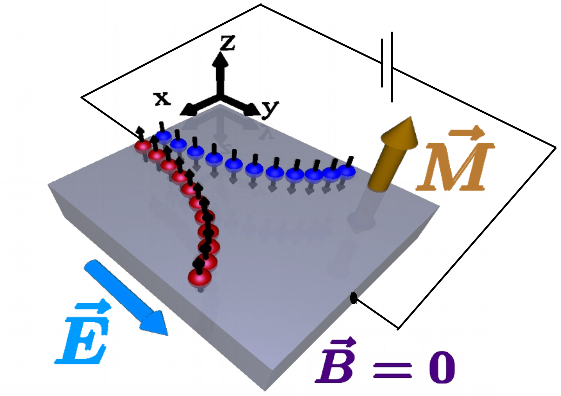
4/mm'm'

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

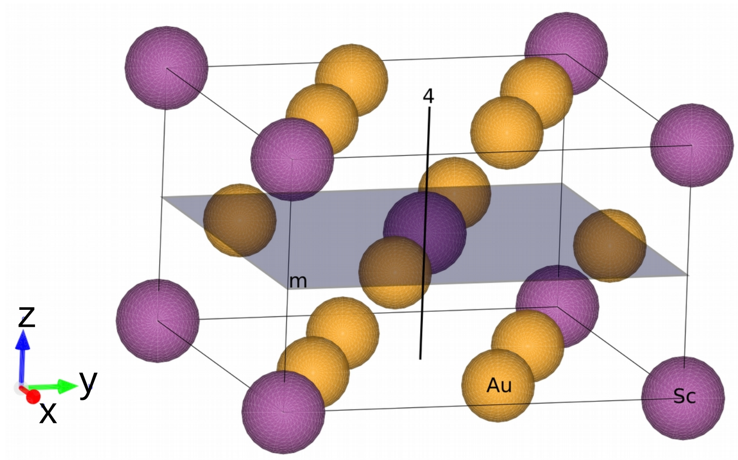
Spin Hall effect and *longitudinal* spin current
in ferromagnet
and
paramagnet



caused by spin-orbit interaction

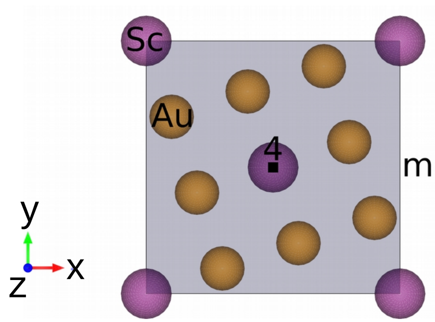


Longitudinal spin polarized currents in 4/m1'



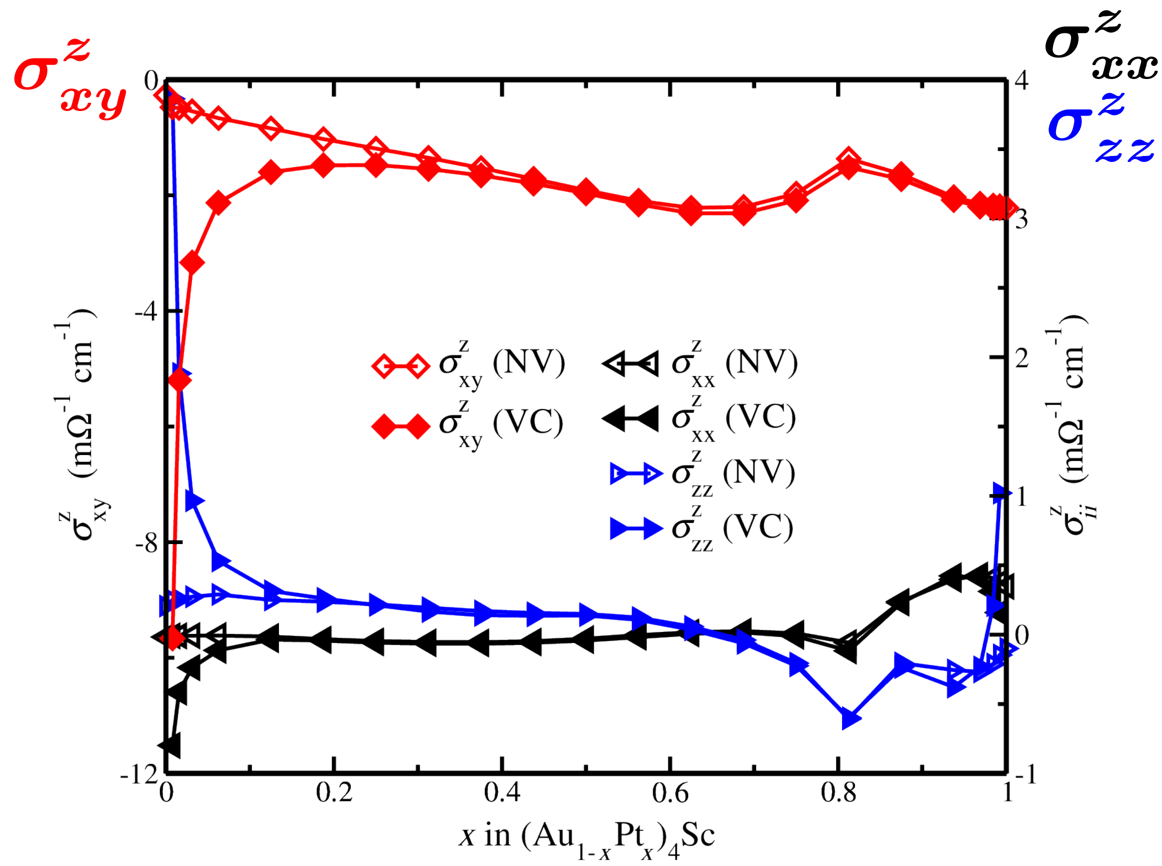
Au$_4$Mn - structure

4/m1'



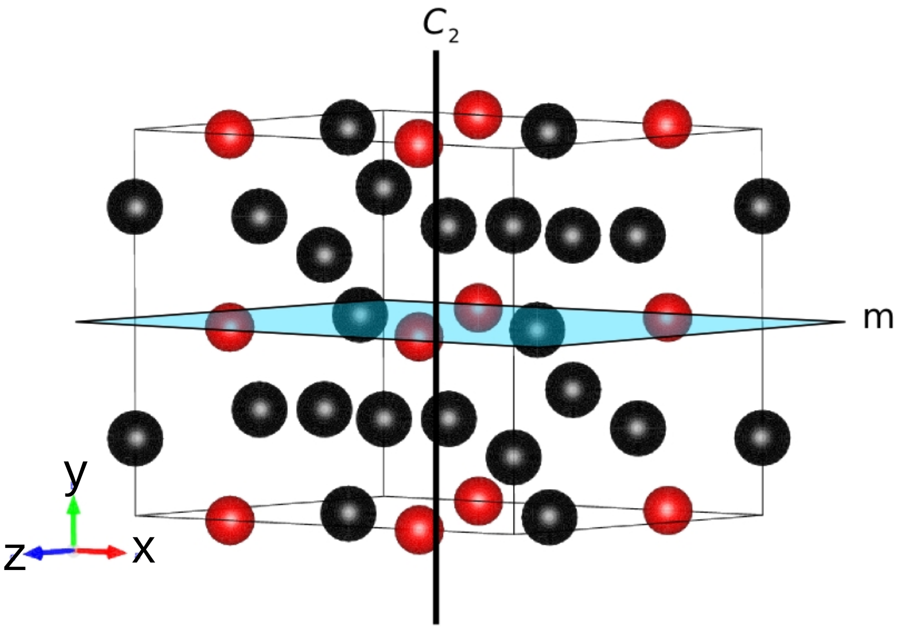
$$\begin{pmatrix} \sigma^z_{xx} & \sigma^z_{xy} & 0 \\ -\sigma^z_{xy} & \sigma^z_{xx} & 0 \\ 0 & 0 & \sigma^z_{zz} \end{pmatrix}$$

paramagnetic (Au$_{1-x}$Pt$_x$)$_4$Sc - alloy



S. Wimmer *et al.*, arXiv:1502.04947, PRB RC *accepted* (2015)

Longitudinal spin polarized currents in 2/m1'

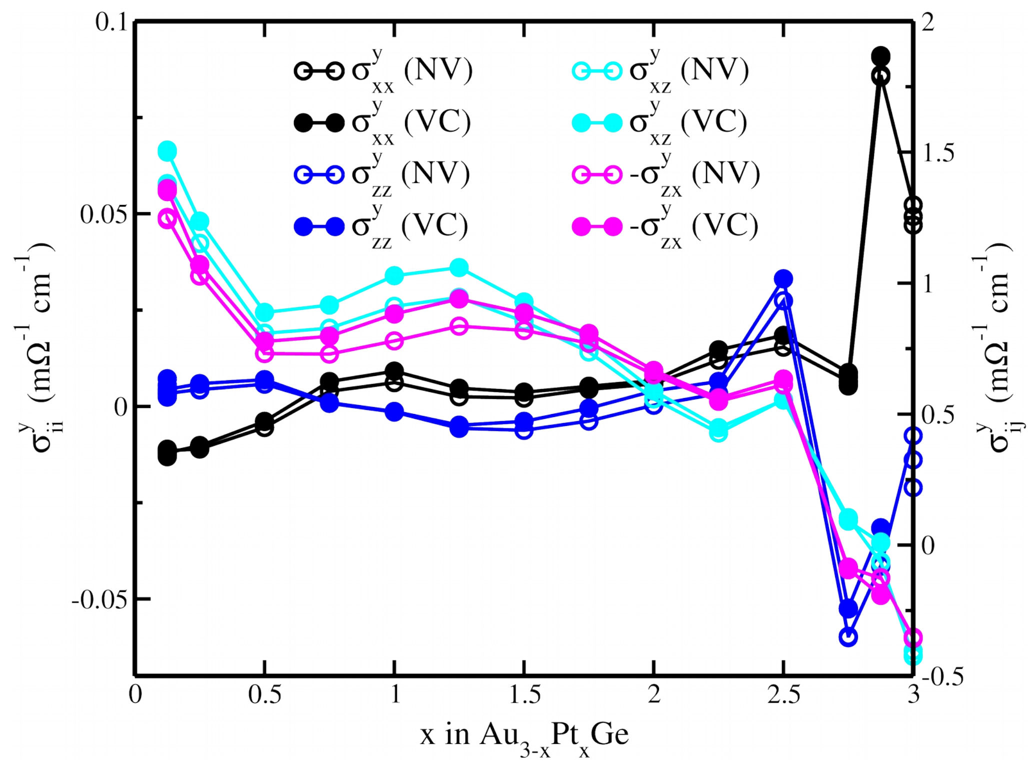


Pt$_3$Ge - structure

2/m1'

$$\begin{pmatrix} \sigma^y_{xx} & 0 & \sigma^y_{xz} \\ 0 & \sigma^y_{yy} & 0 \\ \sigma^y_{zx} & 0 & \sigma^y_{zz} \end{pmatrix}$$

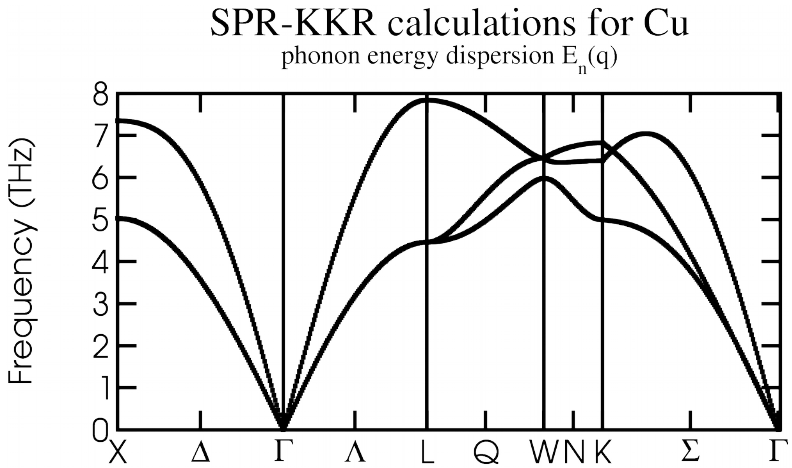
paramagnetic (Pt$_{1-x}$Au$_x$)$_3$Ge - alloy



S. Wimmer *et al.*, (unpublished)

Inclusion of temperature

Phonon dispersion relation of Cu

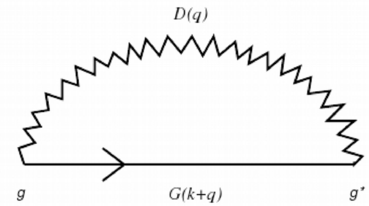


Selfenergy
$$\tilde{\Sigma}_k(E) = 2\int \Sigma^{Einst}(E,\omega)\alpha^2 F_k(\omega)d\omega$$

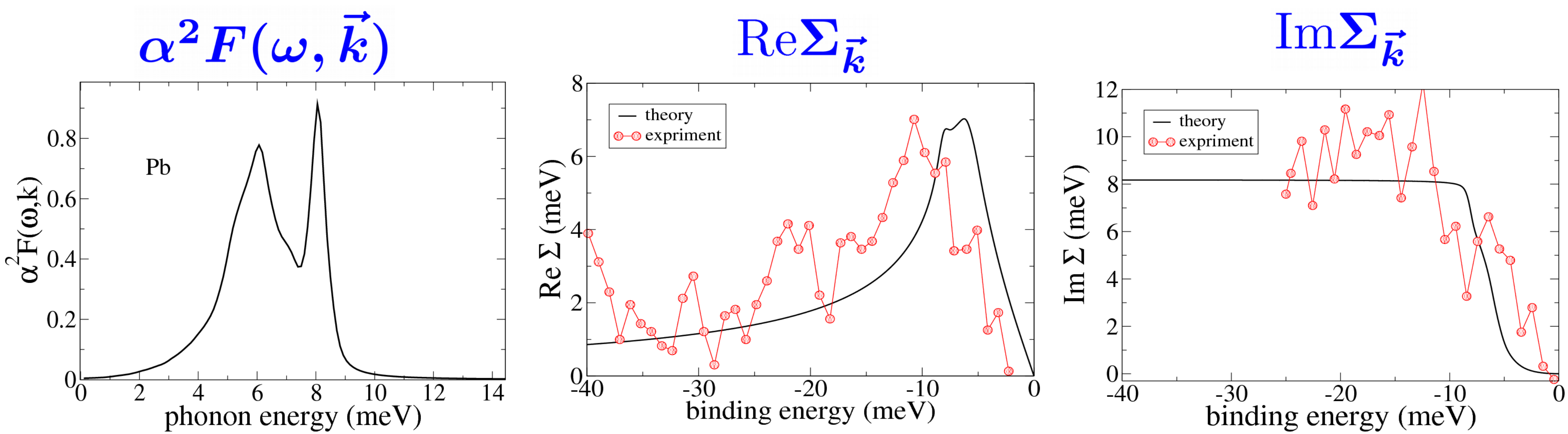
Eliashberg function
$$\alpha^2 F_k(\omega) = \sum_{\vec{q},\lambda} |g^{\lambda}_{\vec{k},\vec{k}-\vec{q}}|^2 \delta(\omega - \omega^{\lambda}_{\vec{q}})\delta(E_{\vec{k}} - E_F)\delta(E_{\vec{k}-\vec{q}} - E_F)$$

Renormalisation of electron structure

$$\tilde{G}(E) = \frac{1}{E - E^0_k - \tilde{\Sigma}_k(E)}$$



Electron-phonon self energy Σ_k for fcc-Pb



Experiment: at T = 8K

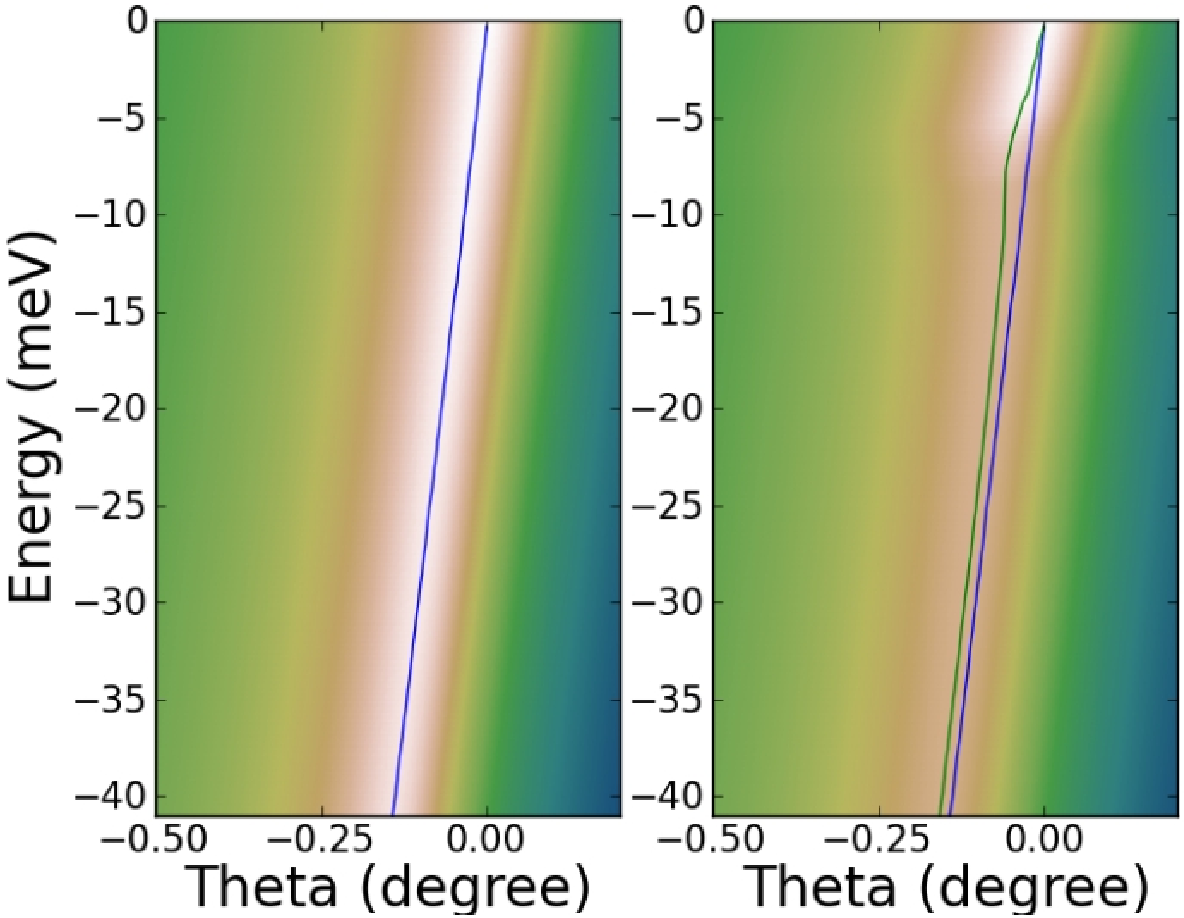
F. Reinert *et al., PRL* **91**, 186406 (2003)

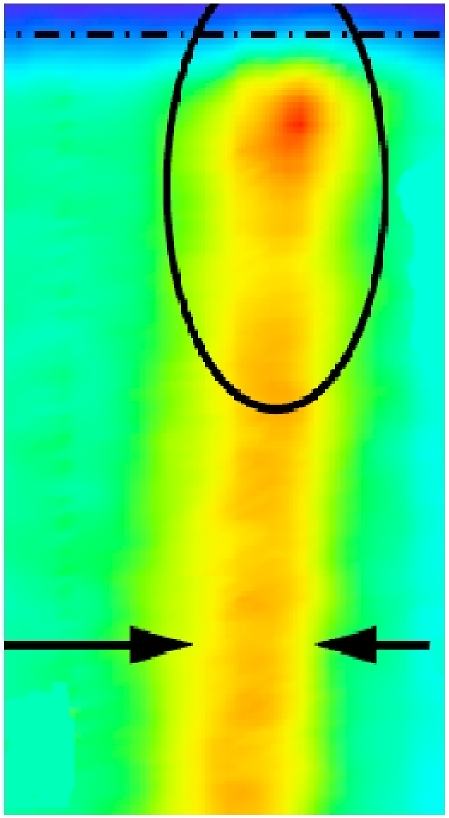
Minar *et al., JESRP* **184**, 91 (2011)

ARPES from Pb(110)

Calculated ARPES spectra

Without SE | Including SE | Experiment





Minar *et al.*, *JESRP* **184**, 91 (2011)

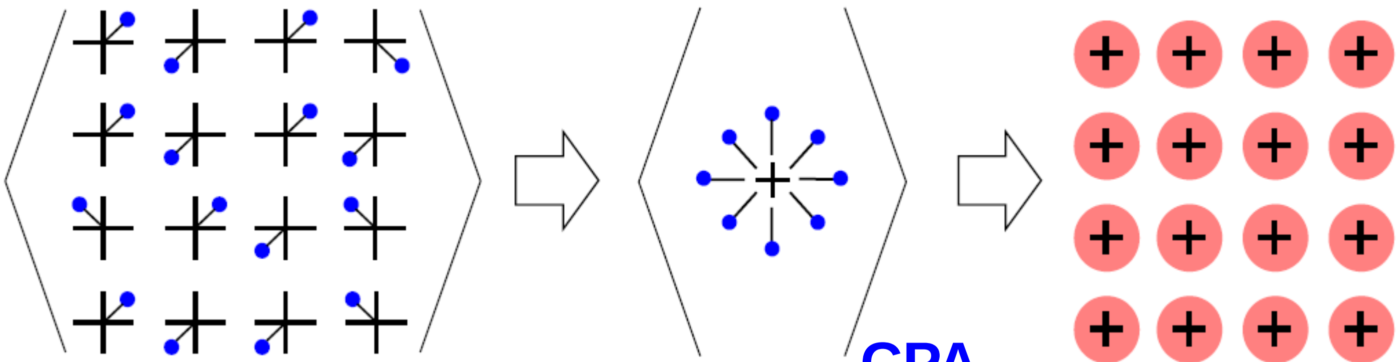
$E_{h\nu}$ = 21.1 eV

Expt: F. Reinert *et al.* *PRL* **91**, 186406 (2003)

Alloy analogy model for thermal vibrations

Representation of thermal vibrations

by temperature dependent, quasi-static, descrete set of dispacements



Multi-component CPA equations

$$\underline{\tau}^{nn}_{\mathrm{CPA}} = \sum_{v=1}^{N_v} x_v \underline{\tau}^{nn}_v$$

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

$$\underline{\tau}^{nn}_{\mathrm{CPA}} = \frac{1}{\Omega_{\mathrm{BZ}}} \int_{\Omega_{\mathrm{BZ}}} d^3k \left[(\underline{t}_{\mathrm{CPA}})^{-1} - \underline{G}(\mathbf{k}, E) \right]^{-1}$$

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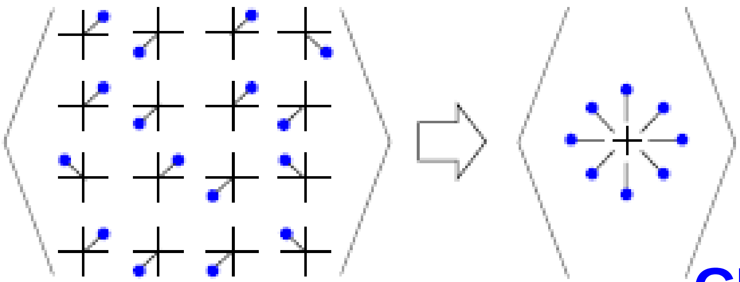
Models for thermal displacements

Fixing the descrete set of dispacements

via temperature dependent root square displacement



CPA

$$\frac{1}{N_v}\sum_{v=1}^{N_v}|\Delta\mathbf{R}_v^q(T)|^2 = \langle u_q^2\rangle_T$$

root square displacement from Debye model

$$\langle u^2\rangle_T = \frac{1}{4}\frac{3h^2}{\pi^2 M k_{\mathrm{B}}\Theta_D}\left[\frac{\Phi(\Theta_D/T)}{\Theta_D/T}+\frac{1}{4}\right]$$

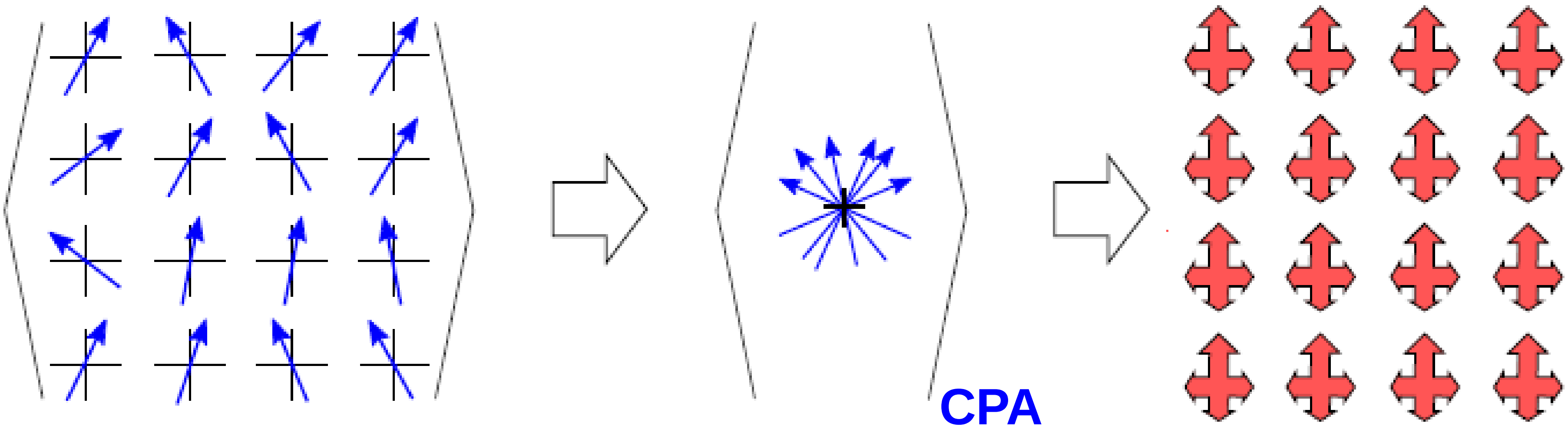
root square displacement from phonon calculations

$$\langle u_{i,\mu}^2\rangle_T = \frac{3\hbar}{2M_i}\int_0^\infty d\omega\, g_{i,\mu}(\omega)\frac{1}{\omega}\coth\frac{\hbar\omega}{2k_{\mathrm{B}}T}$$

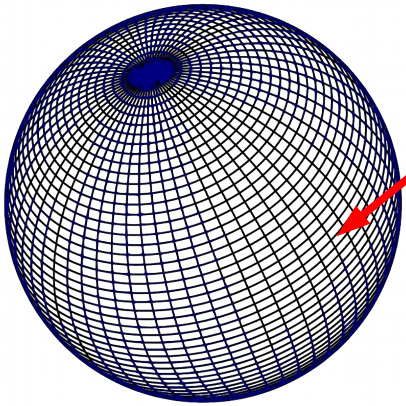
Alloy analogy model for thermal spin fluctuations

Representation of thermal spin fluctuations

by temperature dependent, quasi-static, descrete set of non-collinear spin orientations



Spin fluctuations from Monte Carlo simulations



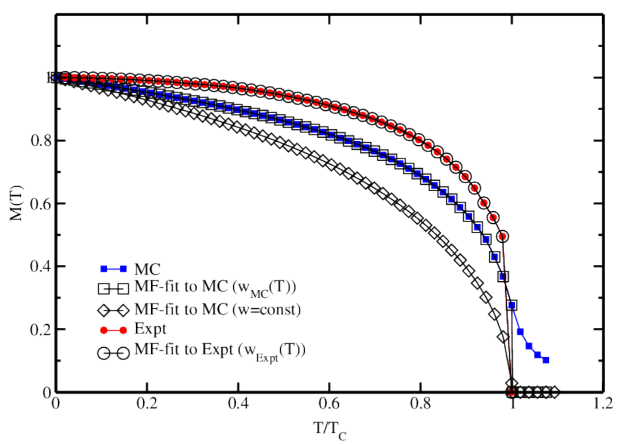
(θ_i, ϕ_j)

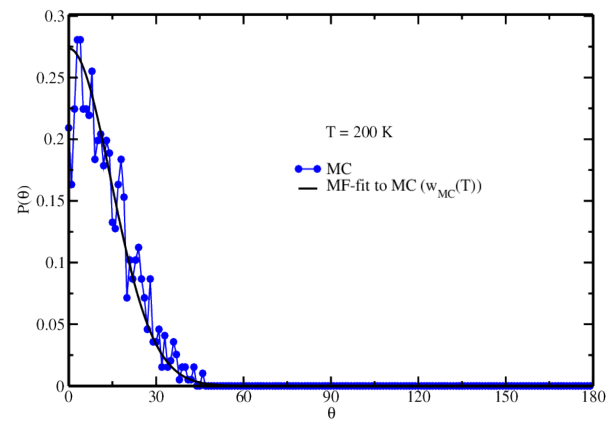
$\hat{e}_f(\theta, \phi)$ is defined on the grid:

$$\theta_i, i = 1, \ldots, N_\theta$$
$$\phi_j, j = 1, \ldots, N_\phi$$

weighting factor at temperature *T*

$$x_f = \frac{\sin(\theta_f) \exp[w(T)\hat{z} \cdot \hat{e}_f / k_\mathrm{B}T]}{\sum_{f'} \sin(\theta_{f'}) \exp[w(T)\hat{z} \cdot \hat{e}_{f'} / k_\mathrm{B}T]}$$

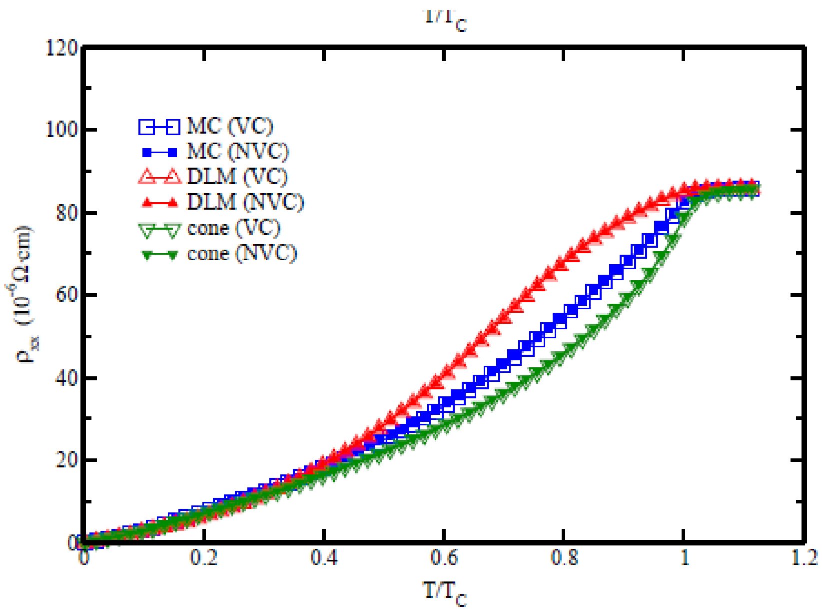




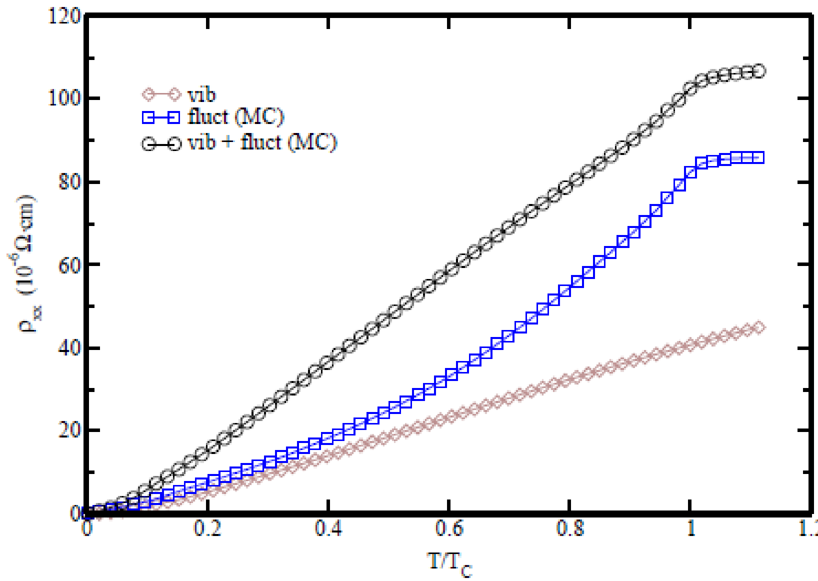
Fitting of Weiss field parameter $\lim_{w \to w(T)} M(T) = M_{MC}(T)$

Temperature dependent resisitivity of ferromagnetic solids – bcc-Fe

Comparison of different models of spin disorder



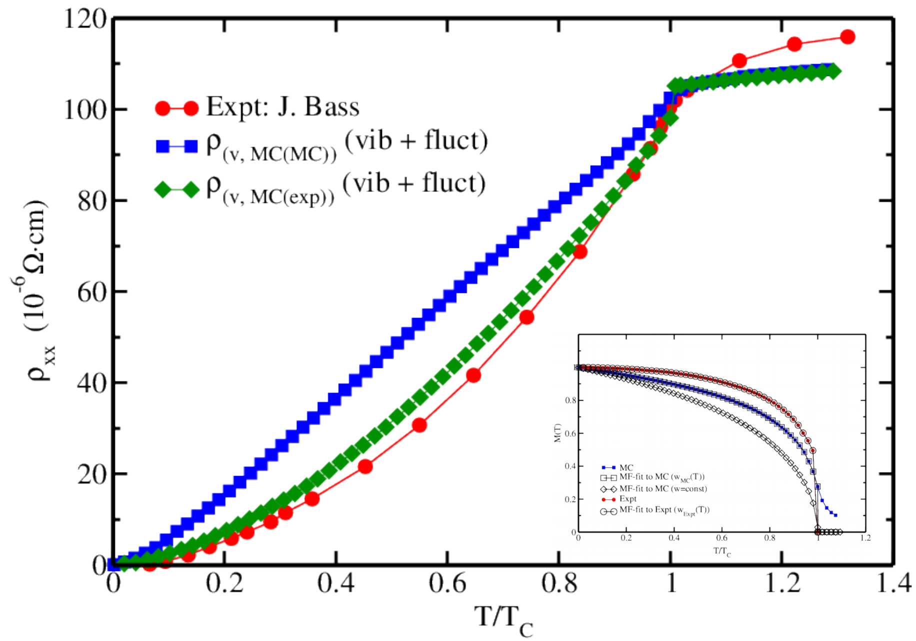
Combination of thermal lattice vibrations and spin fluctuations



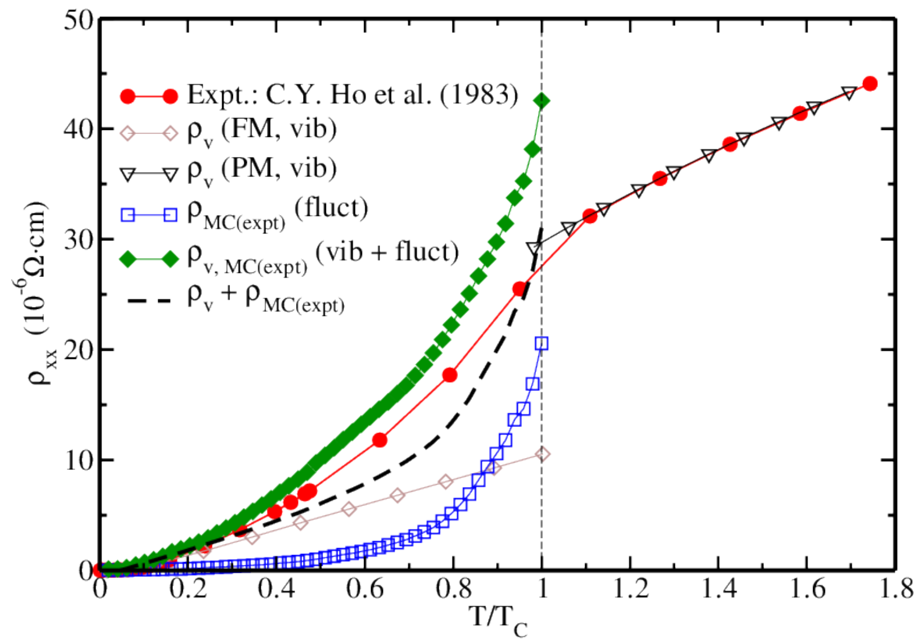
- **Transverse spin fluctuations important for spin disorder**
- **Impact of thermal lattice vibrations and spin fluctuations are not additive**

Resistivity: theory vs experiment

Fe bcc: resistivity vs temperature



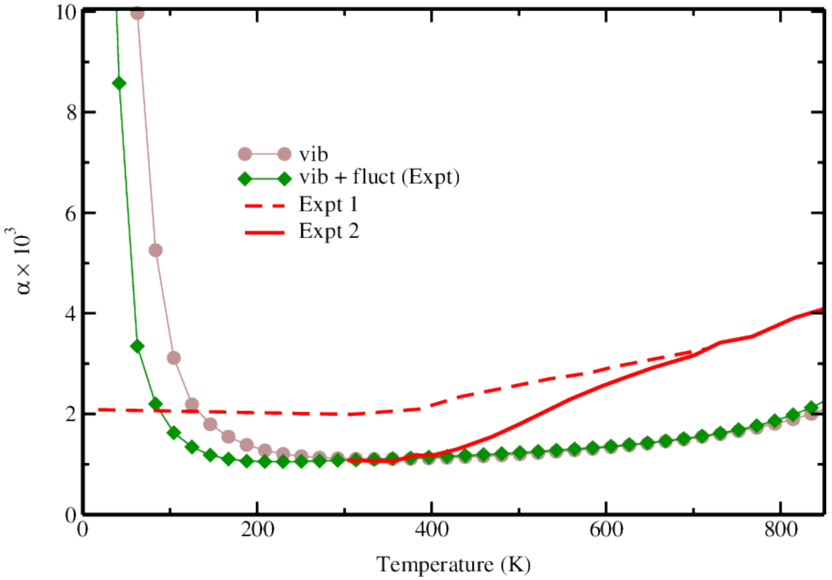
Ni fcc: resistivity vs temperature

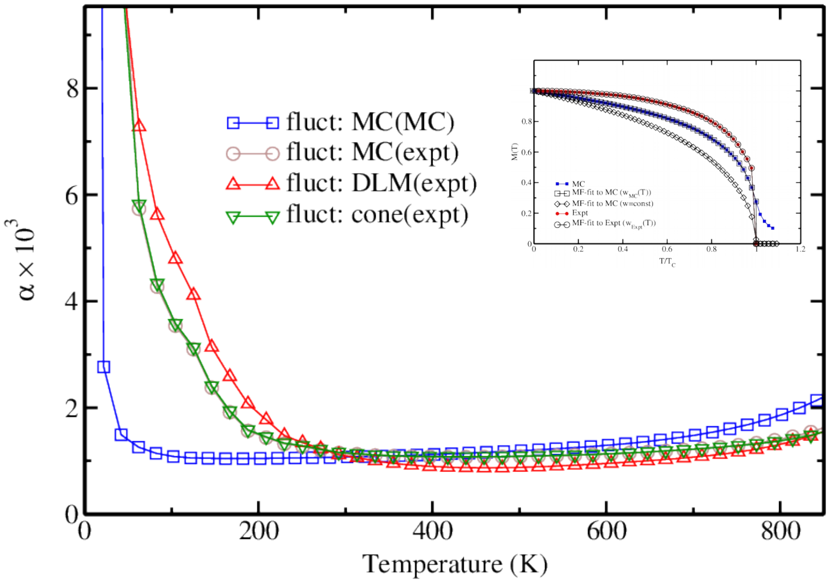


- Fe: MC $M(T)$: magnetic fluctuation effect is overestimated
- Crucial role of $M(T)$ dependence → discrepancies between the resistivity results based on MC and experimental $M(T)$
- Ni: Longitudinal fluctuations should be taken into account near T_C

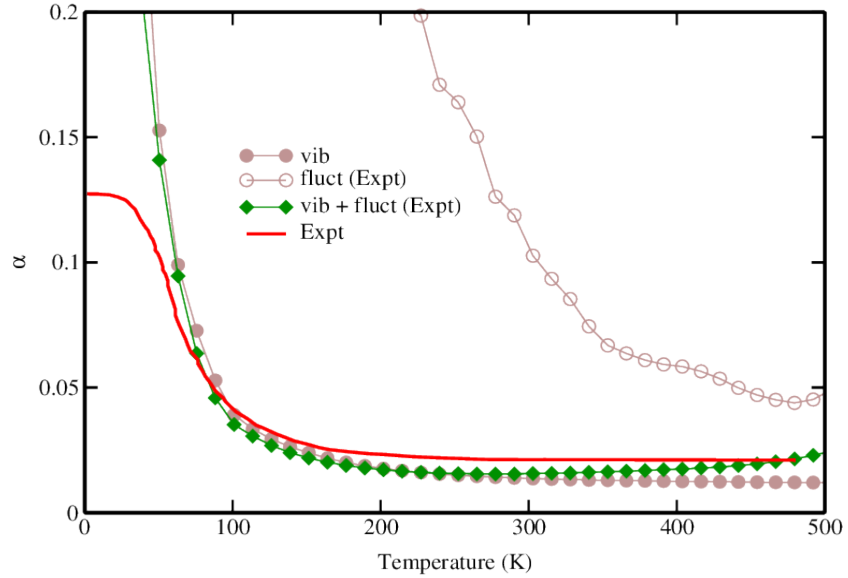
Gilbert damping

Gilbert damping for Fe





Gilbert damping for Ni

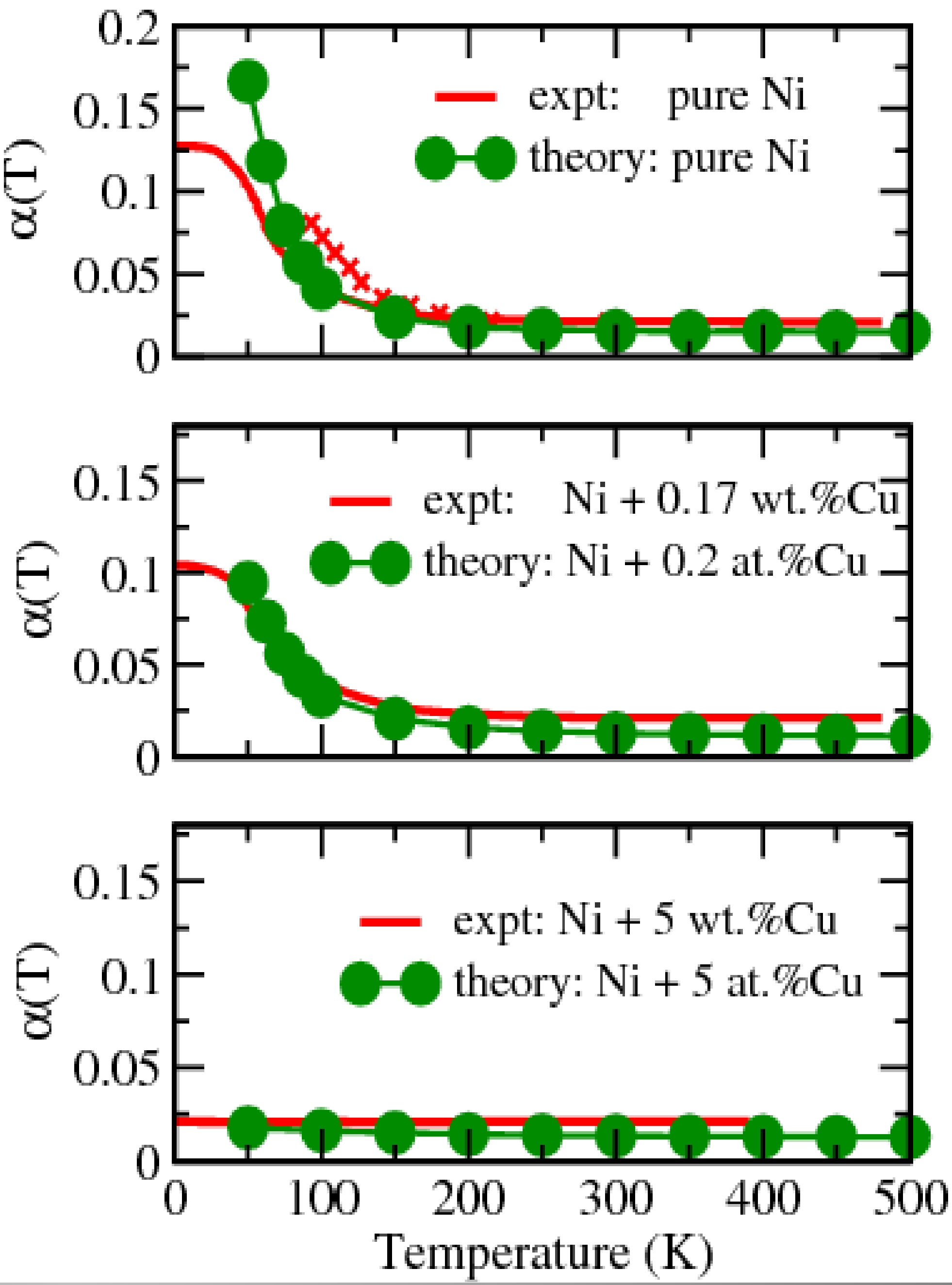


- Fe: comparable contributions of lattice vibrations and spin fluctuations
- Ni: main contribution – from lattice vibrations

Gilbert damping: Temperature effects

Ni-rich $Ni_{1-x}Cu_x$ alloys

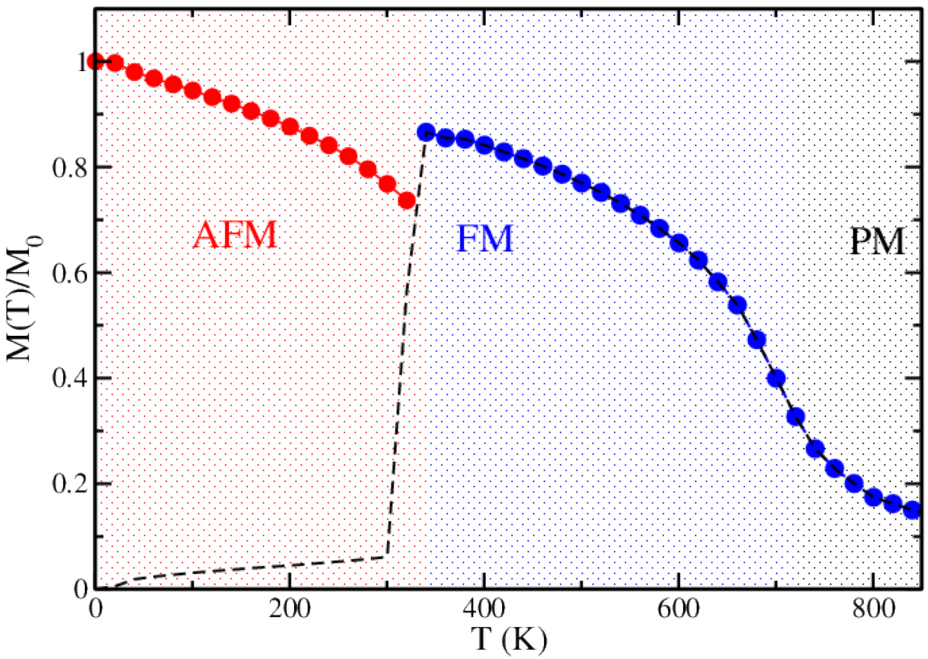
- Pure Ni: conductivity-like behaviour for low temperatures
- Less than 1 % Cu strongly damp low temperature singularity
- With more than 5 % Cu the temperature dependence is nearly suppressed



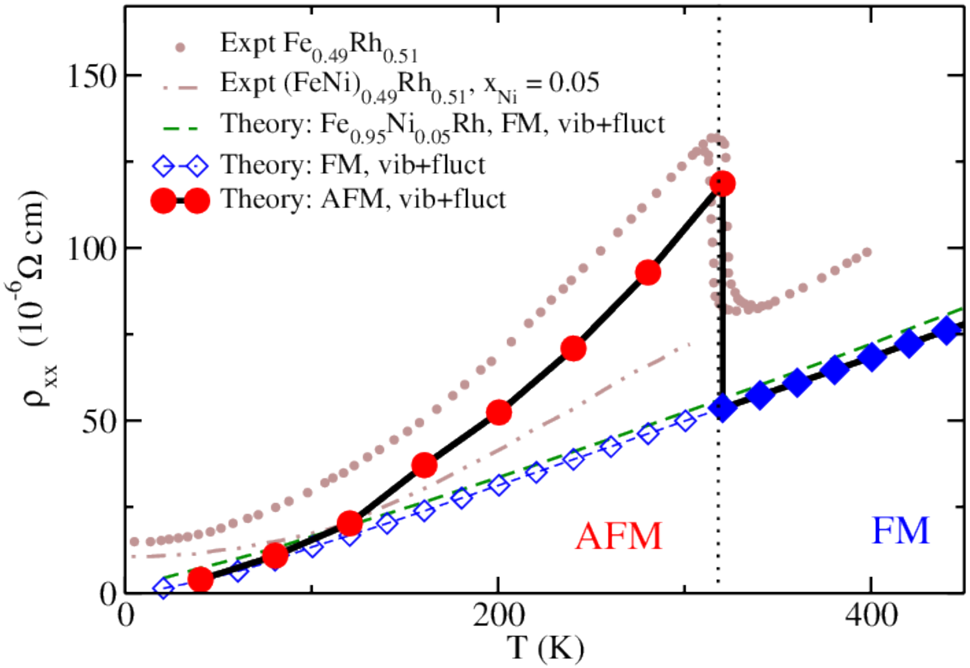
Expt: Bhagat and Lubitz,
Phys. Rev. B **10**, 179, (1974)

FeRh: electrical resistivity

MC: $M(T)/M_0$ for **one Fe sublattice**



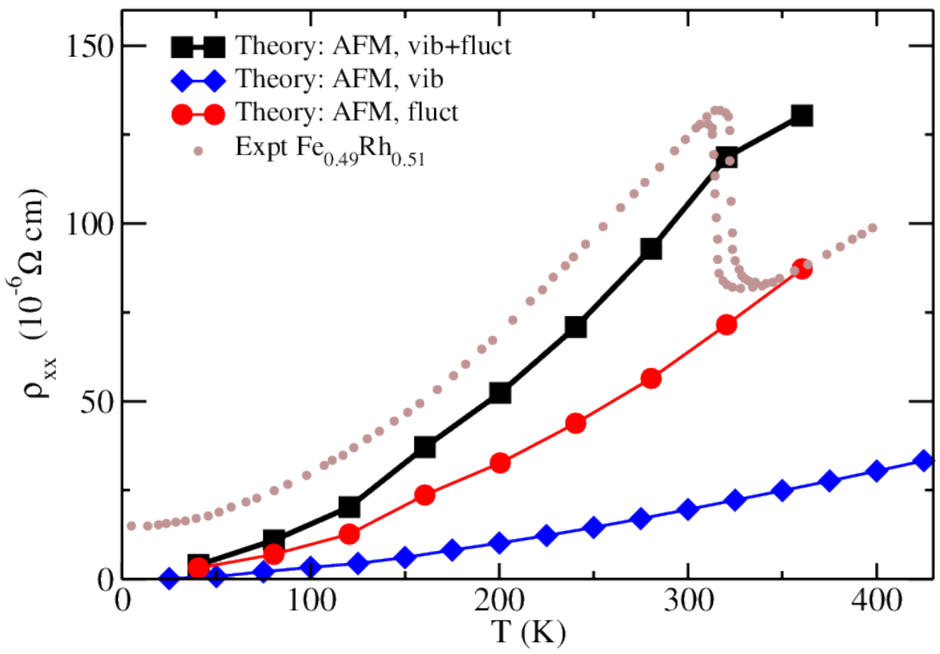
Expt vs theory: resistivity vs T



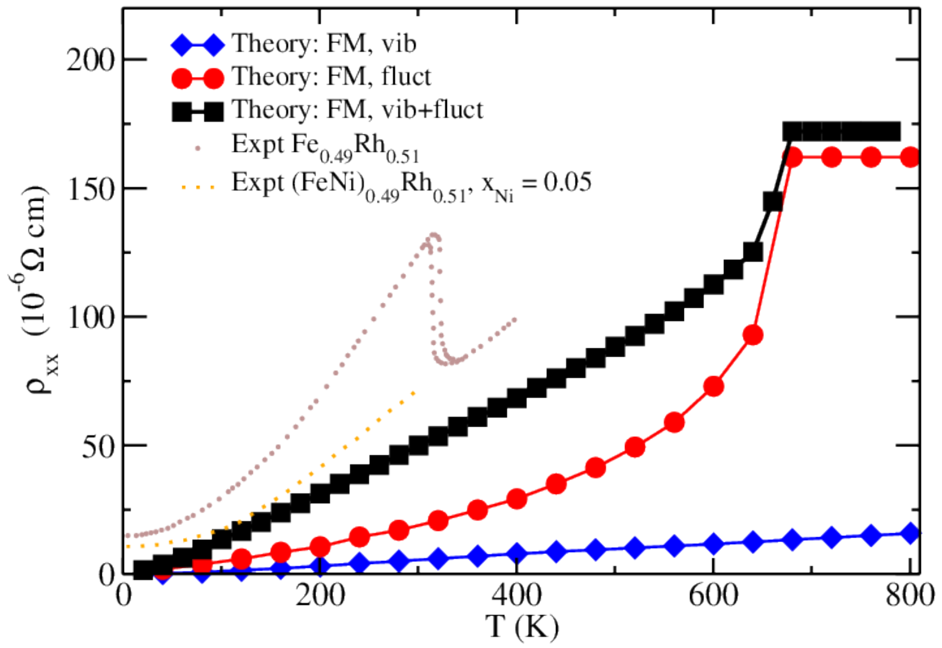
- Monte Carlo simulations: Temperature dependent **magnetization** of AFM-aligned **sublattices** of Fe
- **AFM** state: Faster decrease of Fe sublattice magnetization (**stronger spin fluctuations**) → **steeper increase of resistivity**

FeRh: electrical resistivity

FeRh, AFM: contributions



FeRh, FM: contributions

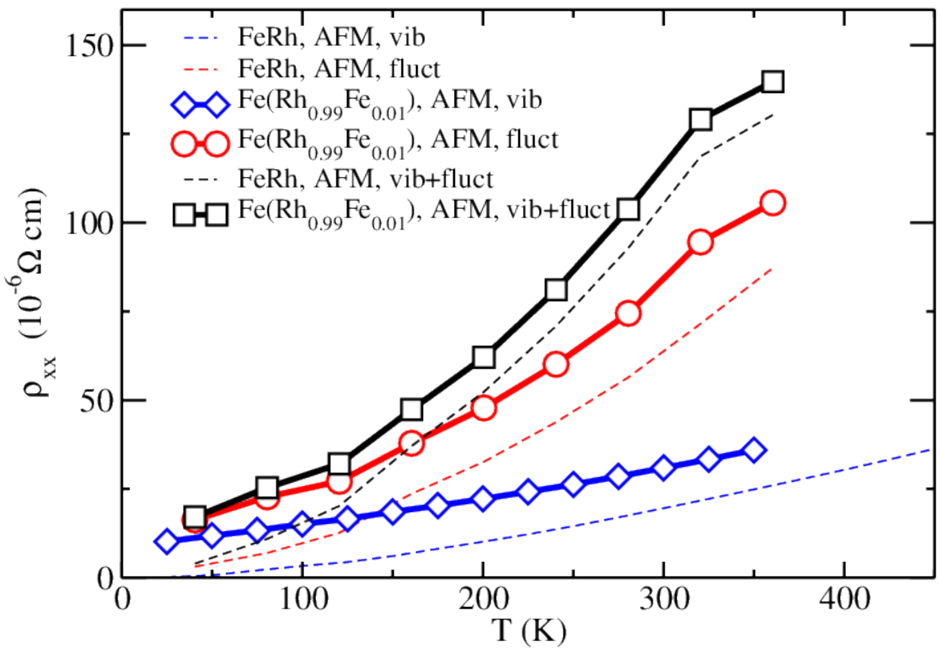


- **FM** state: **Weak** contribution to the resistivity from the scattering due to **lattice vibrations**.
- **AFM** state: **stronger spin fluctuations**

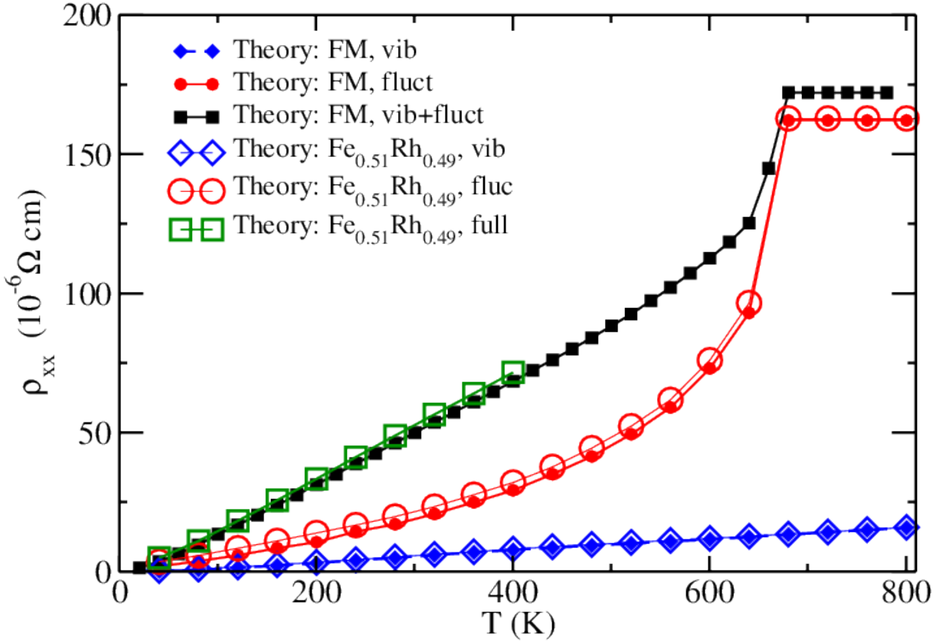
  → **steeper increase of resistivity**

Fe(Rh,Fe): electrical resistivity

Fe(Rh,Fe), AFM: contributions



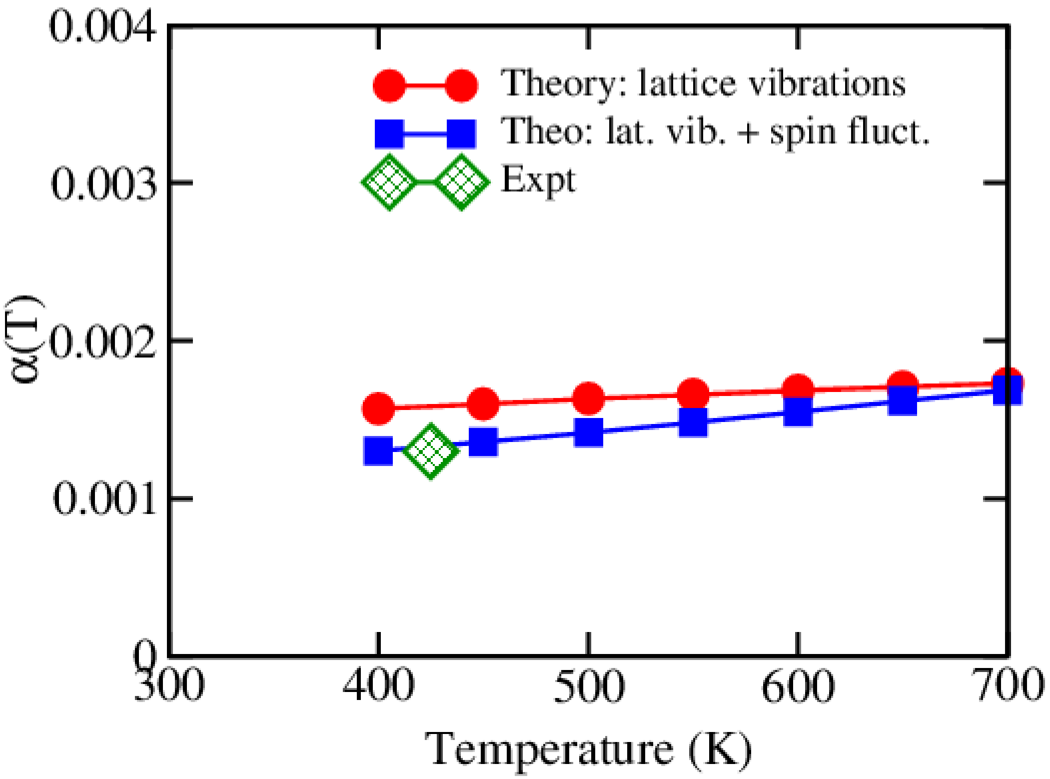
Fe(Rh,Fe), FM: contributions



- **FM** state: **Weak** effect of Fe impurities in Rh sublattice
- **AFM** state: **strong** effect of Fe impurities in Rh sublattice

FeRh: Gilbert damping

FeRh, FM

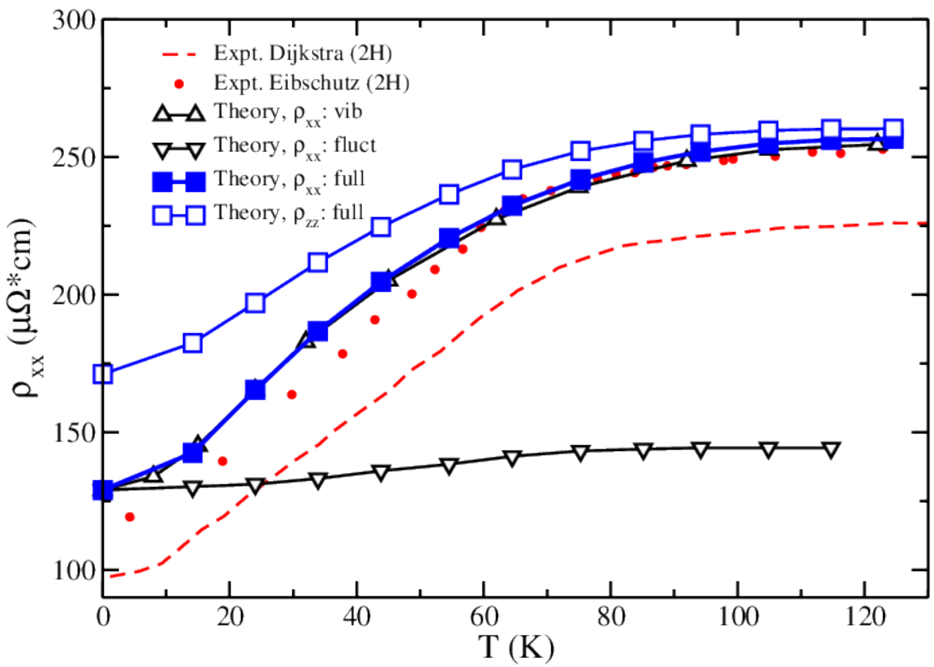


- Main temperature effect: *lattice vibrations*

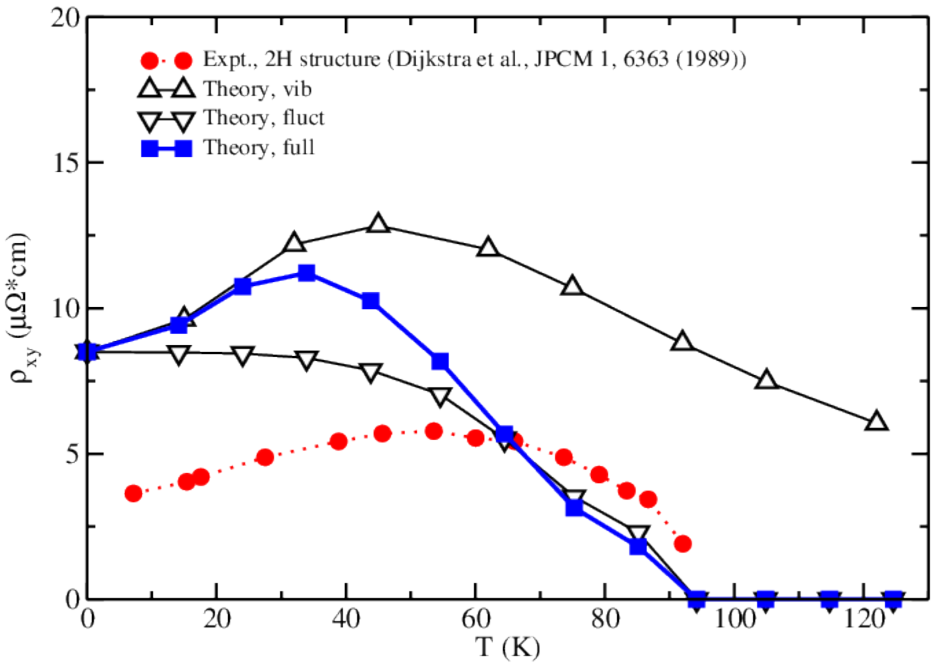
Expt: E. Mancini et al. J. Phys. D: Appl. Phys. **46** (2013) 245302

$2H\text{-}Fe_{0.28}TaS_2$: transport proprties

Electrical resistivity vs T



AHE vs T



- Small contribution of spin fluctuations to the electrical resistivity
- AHE: increase of $\rho_{xy}(T)$ at low temperature – due to phonon contribution
- AHE: Crucial effect of temperature induced magnetic disorder for $\rho_{xy}(T)$

Summary

- Kubo-Středa vs. Kubo-Bastin
  - Numerical equivalency demonstrated
- Kubo vs. Boltzmann formalism
  - Coherent results in the dilute limit
- Symmetry predicted properties
  - New phenomena identified
- Inclusion of temperature
  - Description of thermal lattice vibrations and spin fluctuations via alloy analogy model

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Spin Caloric Transport