A first-principles description of the anomalous and spin Hall effects in disordered alloys

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Financial support Deutsche Forschungsgemeinschaft DFG

SFB 689 *Spinphänomene in reduzierten Dimensionen*

SPP 1538 *Spin Caloric Transport*

Collaboration

Martin Gradhand
Diema Fedorov
Ingrid Mertig
University of Halle (Germany)

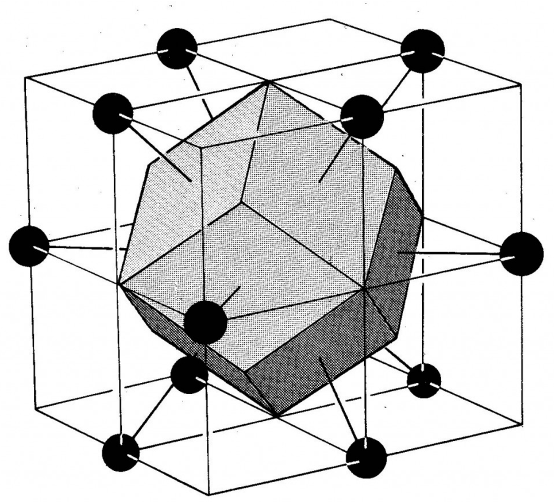
Relation to the work of E. P. Wigner

The title

A first-principles description of the anomalous and spin Hall effects in disordered alloys

might remind one to

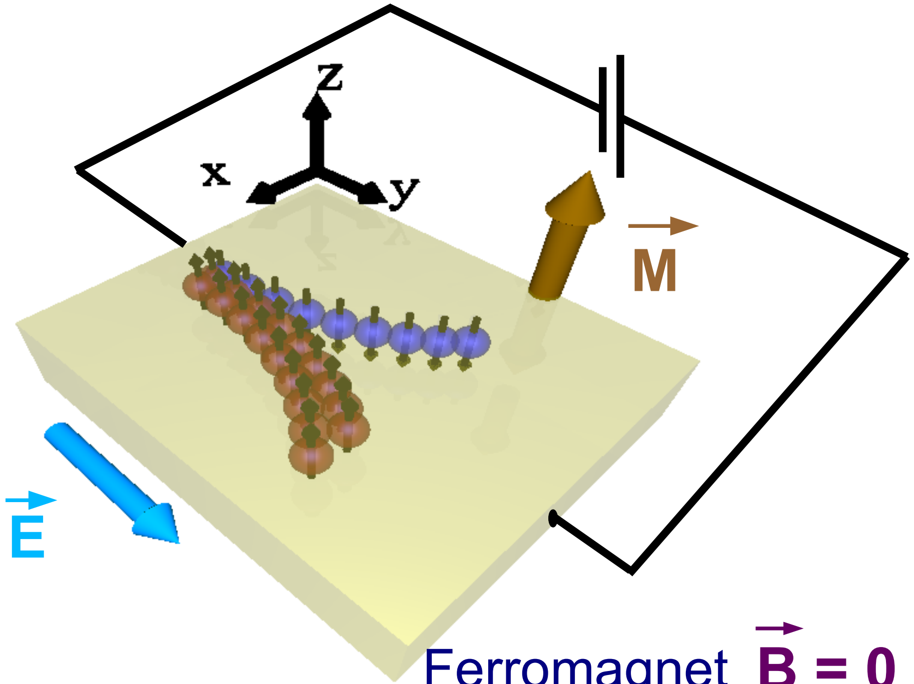
- **Wigner-Seitz cell**
- **Wigner-Seitz radius**
- **Wigner Seitz cellular method**
- **Wigner D-matrix**
- **…**



but there is much more

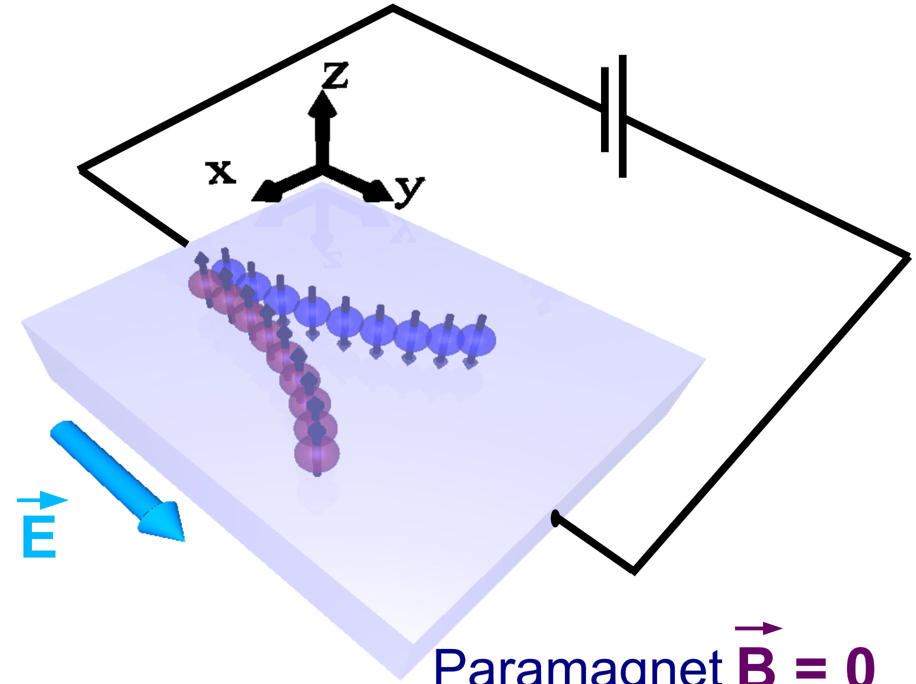
Transverse charge and spin currents

Anomalous Hall Effect (AHE)



Ferromagnet $\vec{B} = 0$

Spin Hall Effect (SHE)



Paramagnet $\vec{B} = 0$

Separating charge (+ spin) spin

Source in both cases **relativistic** spin-orbit interaction

"Spintronics without magnetism"

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

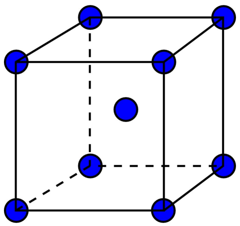
Structure of the conductivity tensor σ

Neumann's Principle

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

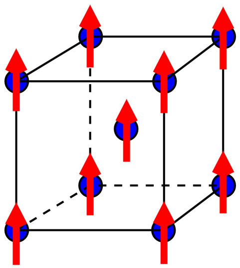
paramagnetic

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)

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Anti-unitary symmetry operators

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 1, NUMBER 5 SEPTEMBER–OCTOBER, 1960

Normal Form of Antiunitary Operators

EUGENE P. WIGNER
Palmer Physical Laboratory, Princeton University, Princeton, New Jersey

(Received April 25, 1960)

Antiunitary operators are characterized in a manner similar to the characterization of unitary operators by their characteristic vectors and characteristic values. It is shown that a complete orthonormal set of vectors can be defined, some of which are invariant under the antiunitary operator. The rest of the vectors, which are always even in number, form pairs in such a way that the antiunitary operator transforms each member of a pair into a multiple of the other member of the same pair [Eq. (11)]. The extent to which the vectors of the orthonormal set are determined by the antiunitary operator is ascertained and the number of free parameters in the various cases of degeneracy found.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 1, NUMBER 5 SEPTEMBER–OCTOBER, 1960

Phenomenological Distinction between Unitary and Antiunitary Symmetry Operators

EUGENE P. WIGNER
Palmer Physical Laboratory, Princeton University, Princeton, New Jersey

(Received April 25, 1960)

It is well known that one always can find as many orthogonal states (i.e., states between which the transition probability is zero) as the Hilbert space has dimensions which are invariant under a given unitary transformation. The corresponding vectors are characteristic vectors of the unitary operator. In contrast, most antiunitary operators leave not more than one state invariant. However, if there are two orthogonal invariant states, a consideration of the states for which the transition probability is $\frac{1}{2}$ into both invariant states surely provides a distinction. In the antiunitary case, one of these states is also invariant, another one is transformed into an orthogonal state, the rest are in between. In the unitary case, the transition probability between original state and transformed state is the same for all states for which the transition probability is $\frac{1}{2}$ into two orthogonal states. This provides a "directly observable" distinction between unitary and antiunitary transformations.

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

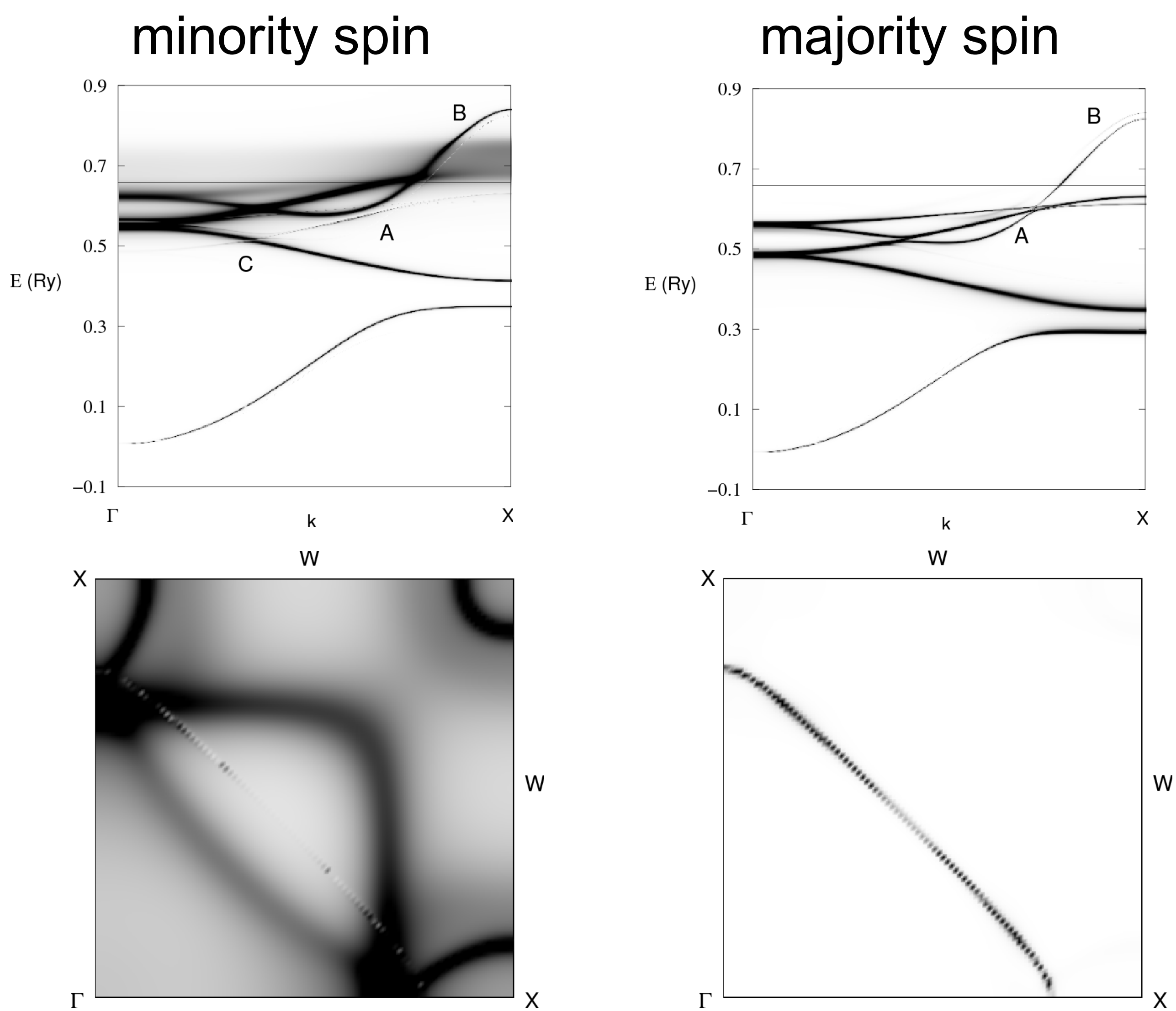
allows calculation of the full conductivity tensor

Bloch spectral function $A_B(\vec{k}, E)$

Relativistic KKR-CPA applied to disordered $Fe_{0.2}Ni_{0.8}$

$\vec{k}$ along Γ-X

Fermi surface
in Γ-X-W-plane



Ebert *et al.*, SSC **104**, 243 (1997)

Kubo-Greenwood equation and Vertex corrections

Implementation within KKR-CPA

$$\tilde{\sigma}_{\mu\nu} = -\frac{4m^2}{\pi\hbar^3\Omega}\left\{\sum_{\alpha,\beta}\sum_{\substack{\Lambda_1,\Lambda_2\\\Lambda_3,\Lambda_4}} c^\alpha c^\beta \tilde{J}^{\alpha\mu}_{\Lambda_4,\Lambda_1}\left(\underbrace{[1-\chi\omega]^{-1}}_{\text{vertex correction}}\chi\right)_{\substack{\Lambda_1,\Lambda_2\\\Lambda_3,\Lambda_4}} \tilde{J}^{\beta\nu}_{\Lambda_2,\Lambda_3} + \sum_{\alpha}\sum_{\substack{\Lambda_1,\Lambda_2\\\Lambda_3,\Lambda_4}} c^\alpha\, \tilde{J}^{\alpha\mu}_{\Lambda_4,\Lambda_1}\, \tau^{\mathrm{CPA},00}_{\Lambda_1,\Lambda_2}\, J^{\alpha\nu}_{\Lambda_2,\Lambda_3}\, \tau^{\mathrm{CPA},00}_{\Lambda_3,\Lambda_4}\right\}$$

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

relativistic quantum numbers

Vertex corrections (VC)

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

account for scattering-in processes

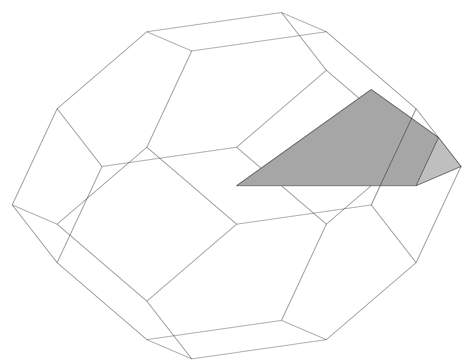
Butler, PRB **31**, 3260 (1985) (non-relativistic)
Banhart *et al.*, SSC **77**, 107 (1991) (fully-relativistic)
Turek *et al.*, PRB **65**, 125101 (2002) (LMTO-CPA)

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

Brillouin zone integration

Symmetry allows to reduce the integration regime Ω_{BZ} to an irreducible wedge

$$
\begin{aligned}
&\frac{1}{V_{BZ}}\int_{V_{BZ}} d^3k\,\tau^{\alpha'\beta'}_{\Lambda\Lambda'}(\vec{k})\,\tau^{\beta'\alpha'}_{\Lambda''\Lambda'''}(\vec{k}) \\
&\quad = \frac{1}{V_{BZ}} \sum_{j=1,\dots,n_U} \sum_{l=0,\dots,n'_{BZ}} \int_{V^*_{IBZ}} d^3k\,\tau^{\alpha'\beta'}_{\Lambda\Lambda'}(\underline{U}^j \underline{S}^l \vec{k})\,\tau^{\beta'\alpha'}_{\Lambda''\Lambda'''}(\underline{U}^j \underline{S}^l \vec{k}) + \sum_{k=1,\dots,n^*_A} \tau^{\alpha'\beta'}_{\Lambda\Lambda'}(\underline{U}^j \underline{\tilde{U}}^k \underline{S}^l \vec{k})\,\tau^{\beta'\alpha'}_{\Lambda''\Lambda'''}(\underline{U}^j \underline{\tilde{U}}^k \underline{S}^l \vec{k}) \\
&\quad = \sum_{j=1,\dots,n_U} \sum_{l=0,\dots,n'_{BZ}} \frac{1}{V_{BZ}} \int_{V^*_{IBZ}} d^3k \left(\underline{U}^j \underline{\tau}^{\alpha\beta}(\underline{S}^l \vec{k})\underline{U}^{j-1}\right)_{\Lambda\Lambda'} \left(\underline{U}^j \underline{\tau}^{\beta\alpha}(\underline{S}^l \vec{k})\underline{U}^{j-1}\right)_{\Lambda''\Lambda'''} \\
&\qquad + \sum_{k=1,\dots,n^*_A} \left(\underline{U}^j \underline{\tilde{U}}^k \underline{\tau}^{\beta''\alpha''T}(\underline{S}^l \vec{k})\underline{\tilde{U}}^{k-1}\underline{U}^{j-1}\right)_{\Lambda\Lambda'} \left(\underline{U}^j \underline{\tilde{U}}^k \underline{\tau}^{\alpha''\beta''T}(\underline{S}^l \vec{k})\underline{\tilde{U}}^{k-1}\underline{U}^{j-1}\right)_{\Lambda''\Lambda'''} . \qquad (44)
\end{aligned}
$$

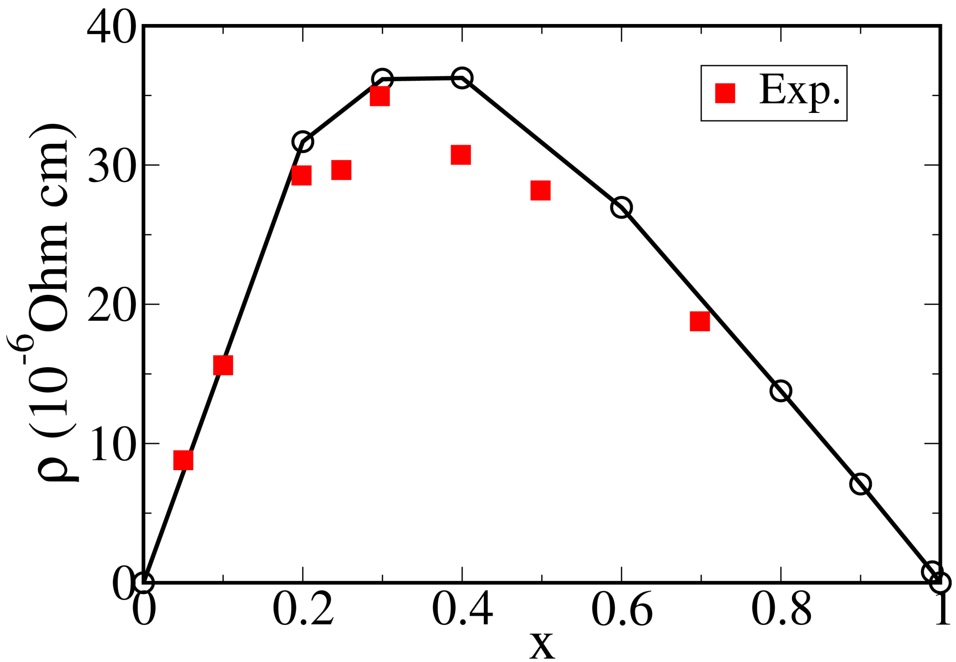


Longitudinal residual resistivity of ferromagnetic alloys

Isotropic residual resistivity

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

Co_xPt_{1-x}

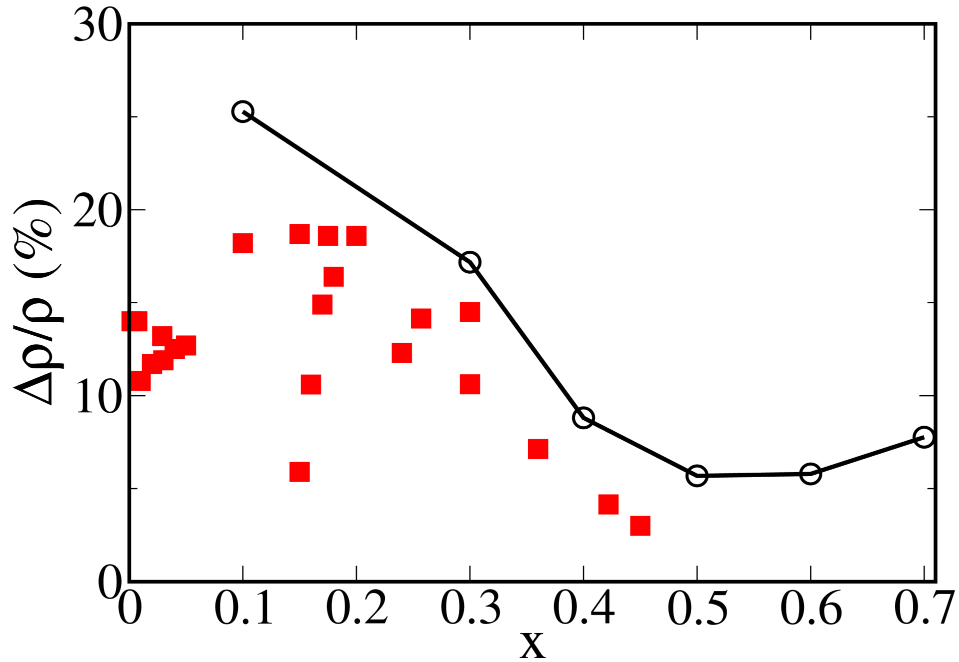


see also:
Ebert *et al.,* PRB **54**, 8479 (1996)

Anisotropic magnetoresistance AMR

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

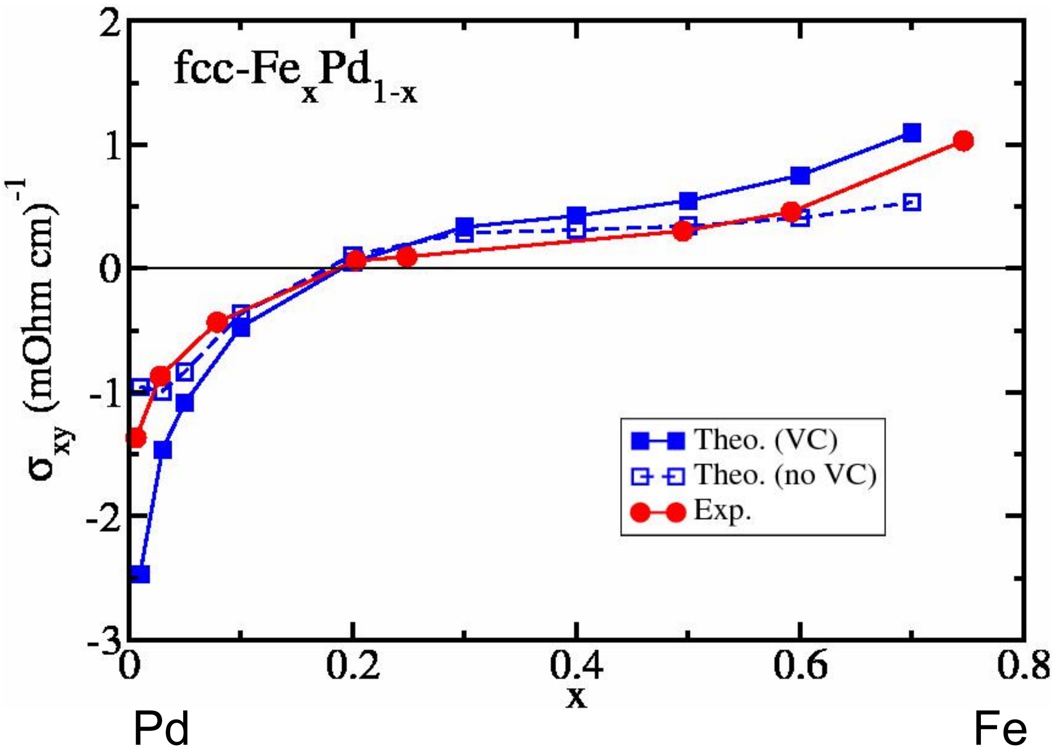
Fe_xNi_{1-x}

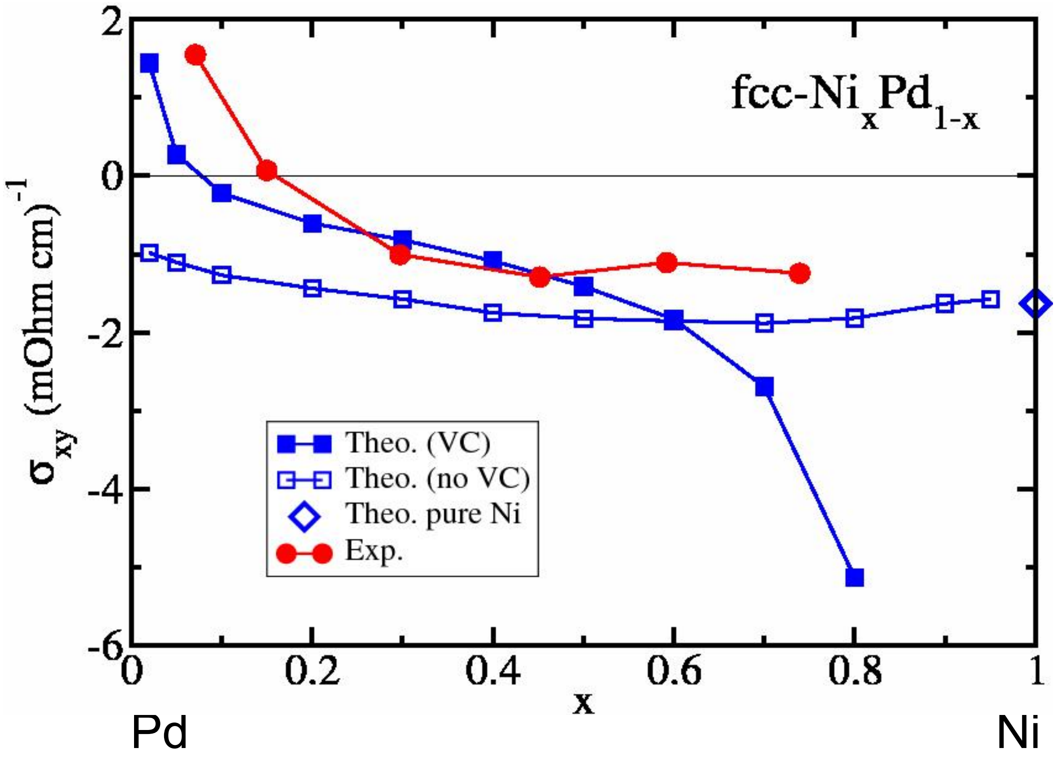


see also :
Banhart *et al.,* PRB **56**, 10165 (1997)
Khmelevskyi *et al.*, PRB **68**, 012402 (2003)
Turek *et al.*, JPCS **200**, 052029 (2010)
& PRB **86**, 014405 (2012)

Anomalous Hall conductivity in ferromagnetic alloys

KKR-CPA results based on Kubo-Středa equation

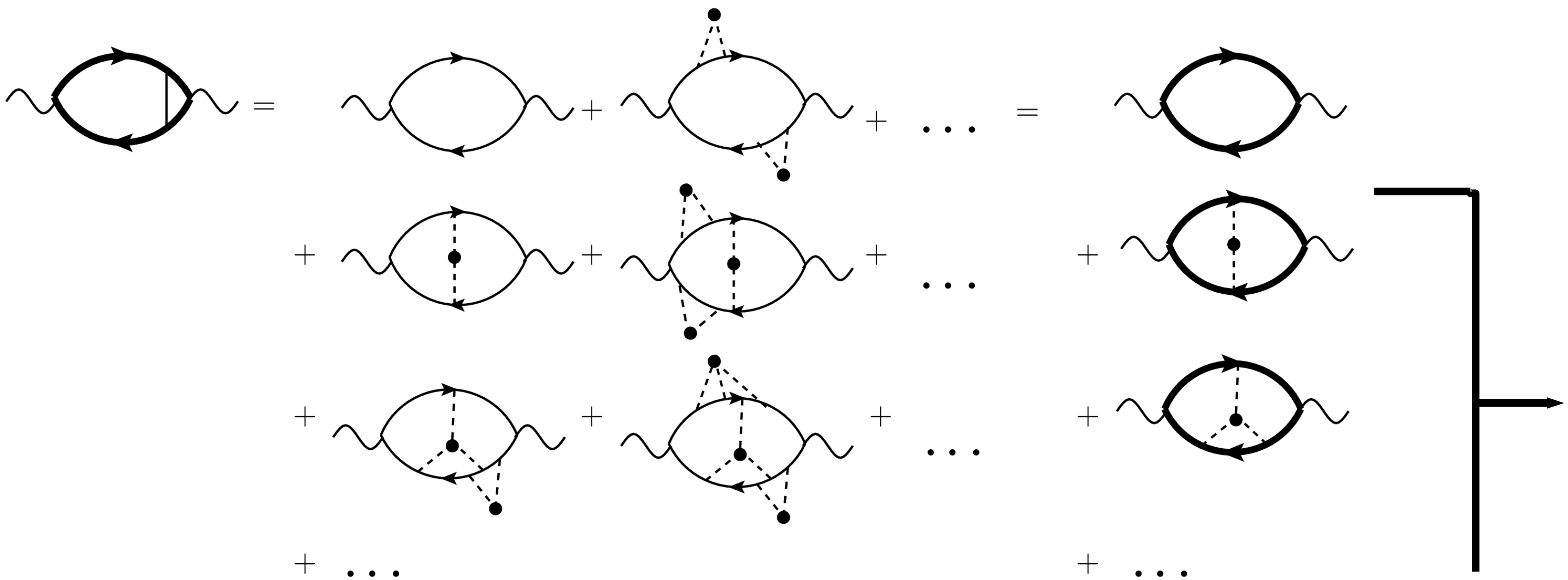




Expt.: Matveev *et al.*, Fiz. Met. Metalloved **53**, 34 (1982)
Theo.: Lowitzer *et al.*, PRL **105**, 266604 (2010)

Diagrammatic representation of the KS equation

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



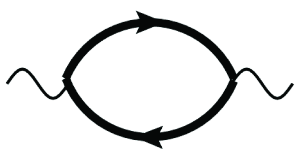
vertex diagrams

intrinsic

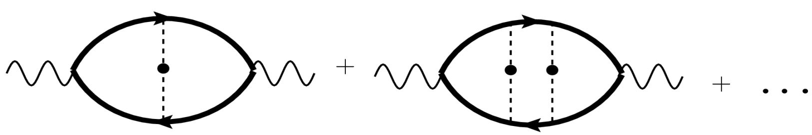
extrinsic

scaling

$\rho_{xx} \propto x$

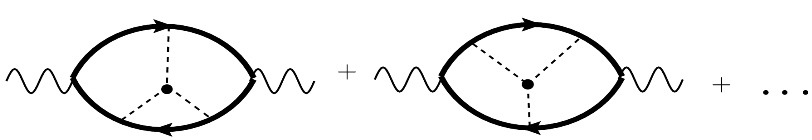


side-jump scattering



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

skew scattering



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

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

Decomposition of the extrinsic AHE via scaling behaviour of individual contributions

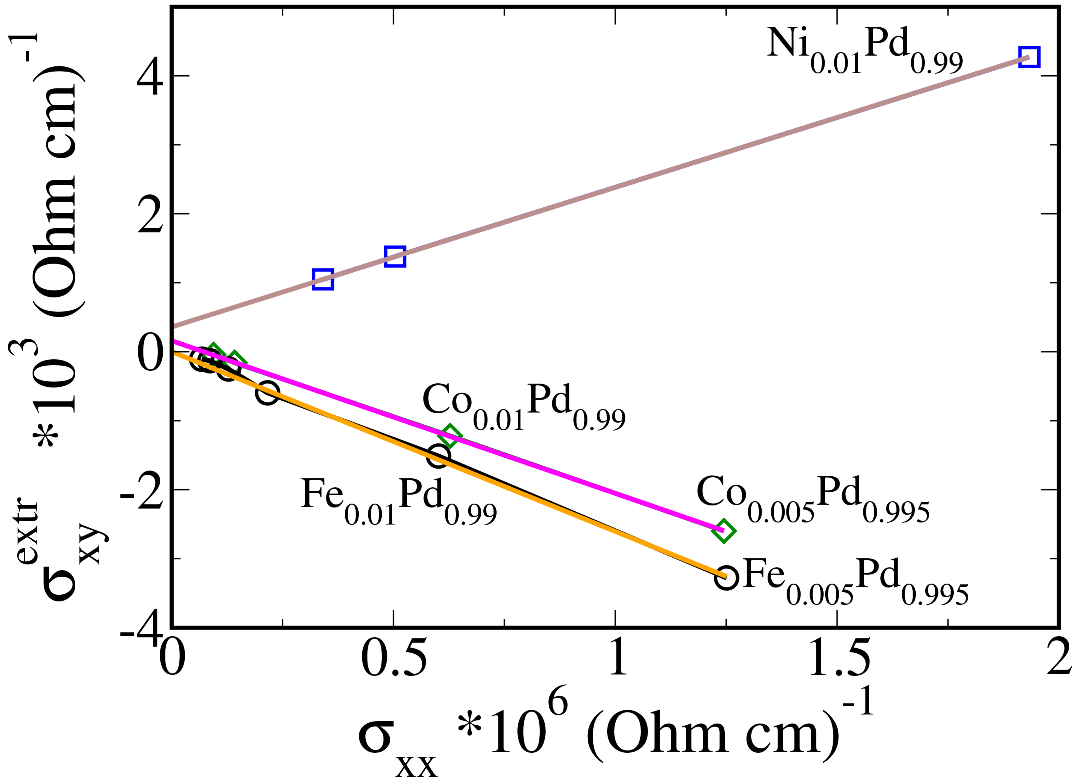
Scaling of skew scattering part

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

S : skewness factor

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

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

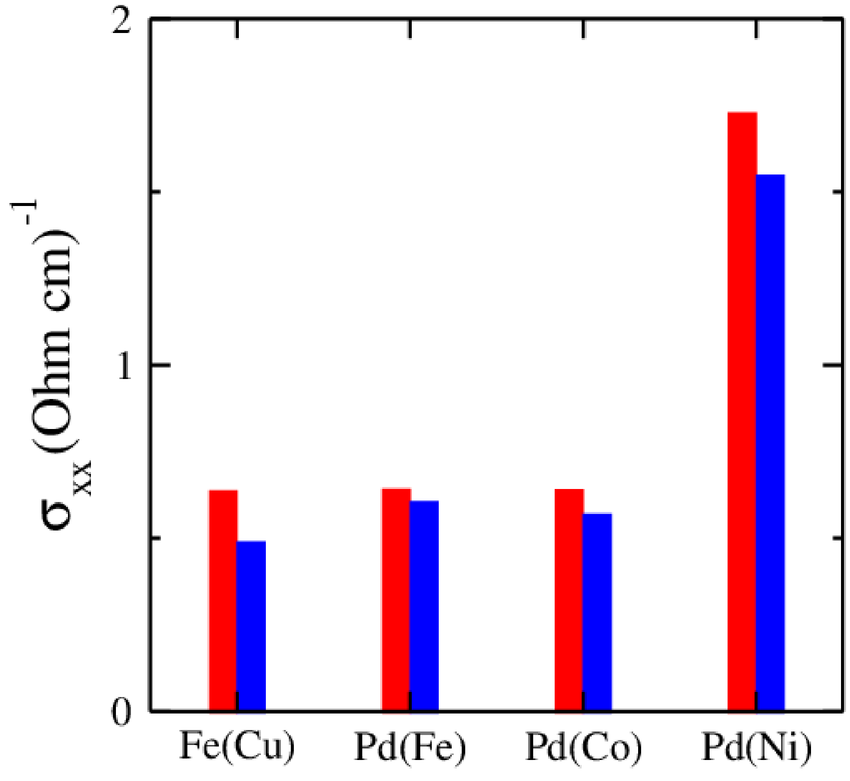


⇒ side-jump contribution is negligible for these systems

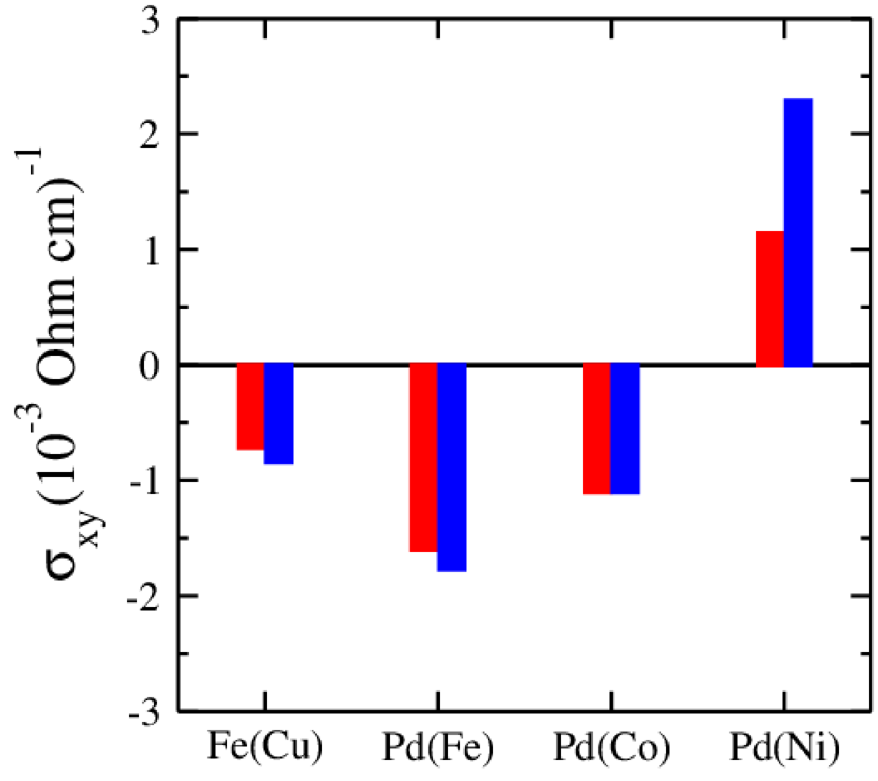
AHE – Kubo vs Boltzmann formalism

Comparison of results for diluted alloys (1%)

longitudinal conductivity σ_{xx}



transverse conductivity σ_{xy}
(**Kubo**: *total*, **Boltzmann**: *skew only*)

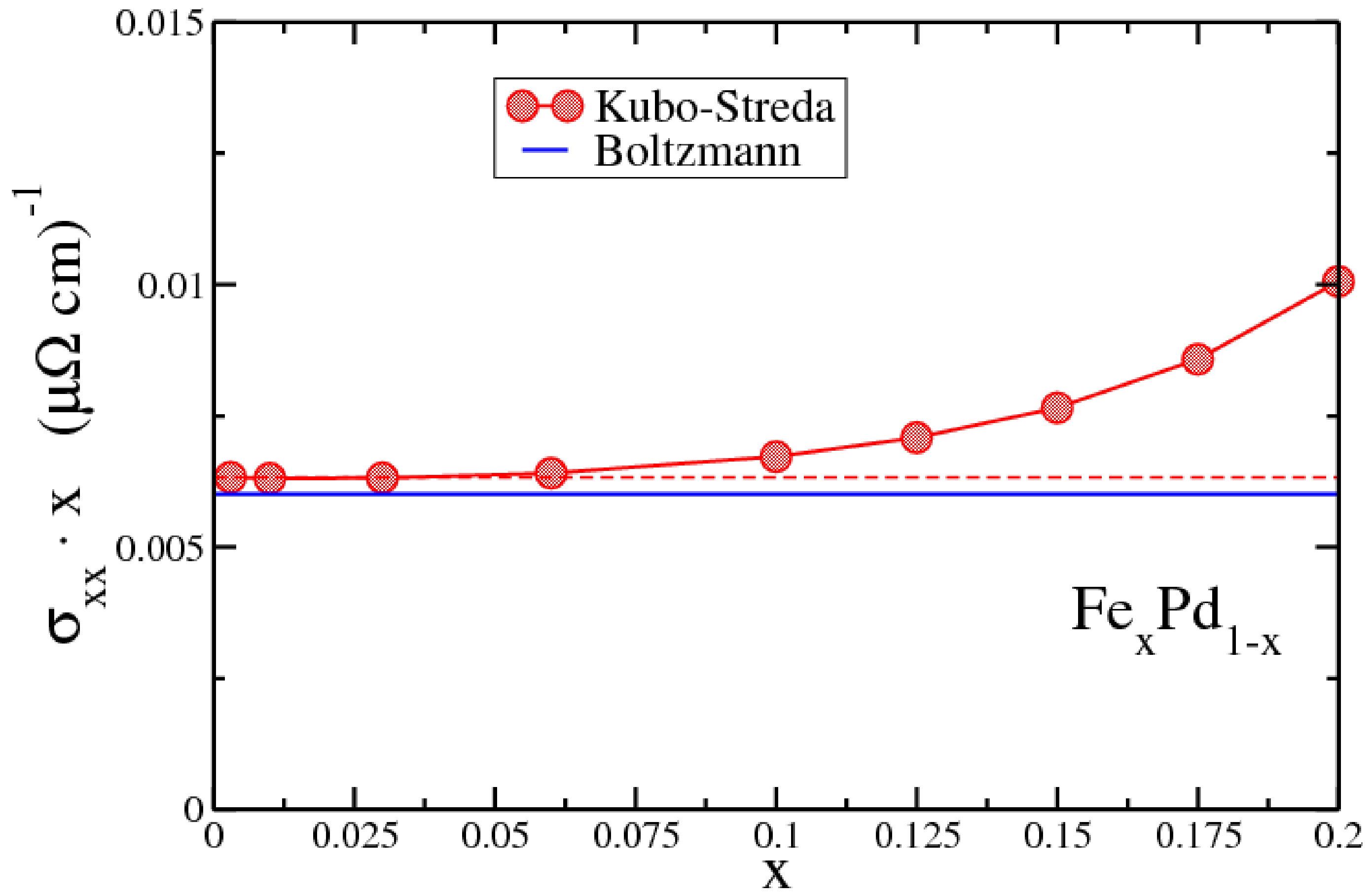


Boltzmann-based calculations:
Gradhand, Fedorov, Mertig, unpublished (2013)
Mokrousov *et al.*, unpublished (2013)

AHE – Boltzmann vs Kubo formalism

Comparison of results for varying concentration

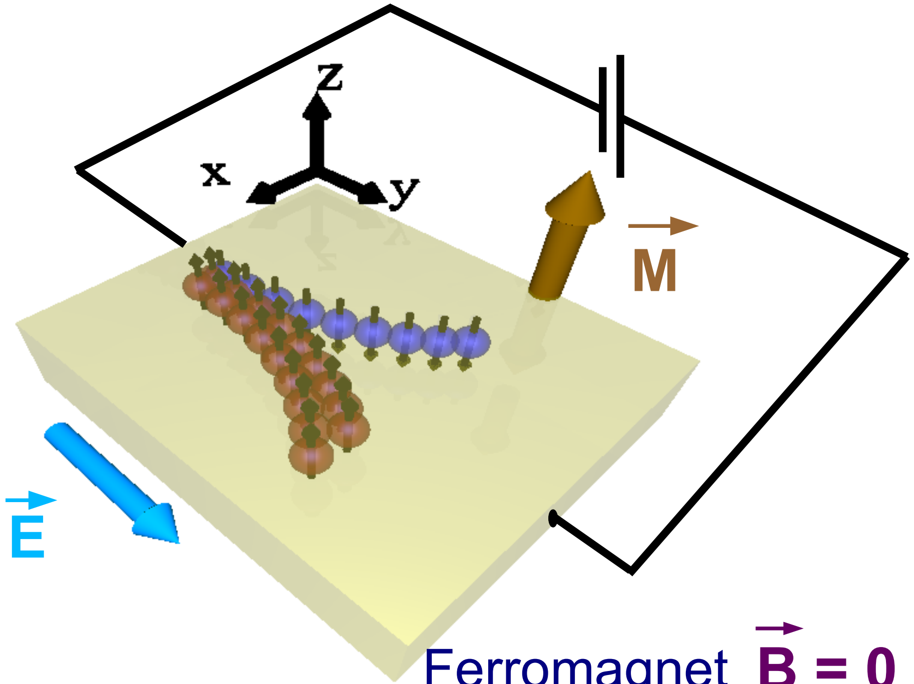
longitudinal conductivity σ_{xx} . x



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

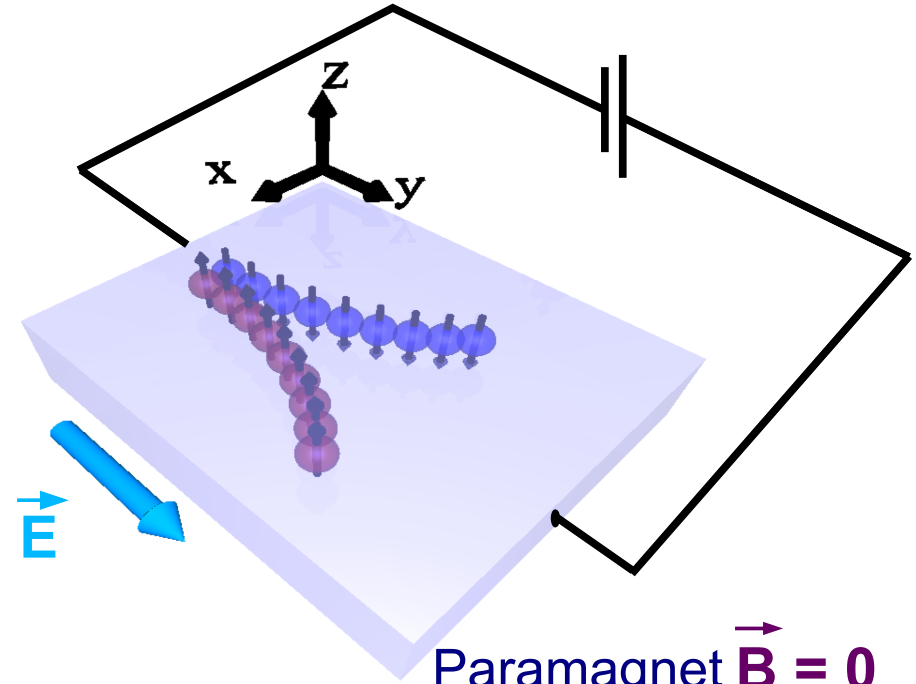
Transverse charge and spin currents

Anomalous Hall Effect (AHE)



Ferromagnet $\vec{B} = 0$

Spin Hall Effect (SHE)



Paramagnet $\vec{B} = 0$

	AHE	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)

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Spin polarisation and current density operators

Vol. 34, 1948 PHYSICS: BARGMANN AND WIGNER 211

GROUP THEORETICAL DISCUSSION OF RELATIVISTIC WAVE EQUATIONS

By V. Bargmann and E. P. Wigner

Princeton University

Read before the Academy, November 18, 1947

Introduction.[1]—The wave functions, ψ, describing the possible states of a quantum mechanical system form a linear vector space **V** which, in general, is infinite dimensional and on which a positive definite inner product (ϕ, ψ) is defined for any two wave functions ϕ and ψ (i.e., they form a Hilbert space). The inner product usually involves an integration over the whole configuration or momentum space and, for particles of higher spin, a summation over the spin indices.

If the wave functions in question refer to a free particle and satisfy relativistic wave equations, there exists a correspondence between the wave functions describing the same state in different Lorentz frames.

PHYSICAL REVIEW B 76, 012408 (2007)

Spin currents, spin-transfer torque, and spin-Hall effects in relativistic quantum mechanics

A. Vernes,[1] B. L. Györffy,[1,2] and P. Weinberger[1]

[1]*Center for Computational Materials Science, Technical University Vienna, Gumpendorferstrasse 1a, A-1060 Vienna, Austria*

[2]*H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom*

(Received 25 June 2007; published 26 July 2007)

Structure of the spin conductivity tensor

Extension of Kleiner's scheme

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

unitary symmetry operation

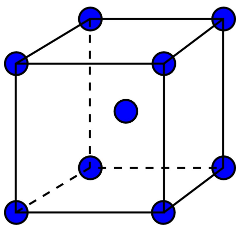
$$\sigma^k_{ij} = \sum_{lmn} D(P_R)_{li} D(P_R)_{mj} D(P_R)_{nk}\, \sigma^n_{lm}$$

anti-unitary symmetry operation

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

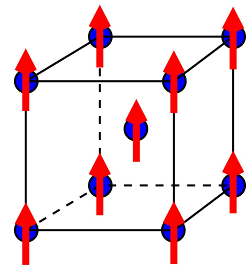
paramagnetic

G = *m3m*



ferromagnetic

G = *4/mm'm'*



$$\underline{\underline{\sigma}}^x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma^z_{xy} \\ 0 & -\sigma^z_{xy} & 0 \end{pmatrix}$$

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

$$\underline{\underline{\sigma}}^y = \begin{pmatrix} 0 & 0 & -\sigma^z_{xy} \\ 0 & 0 & 0 \\ \sigma^z_{xy} & 0 & 0 \end{pmatrix}$$

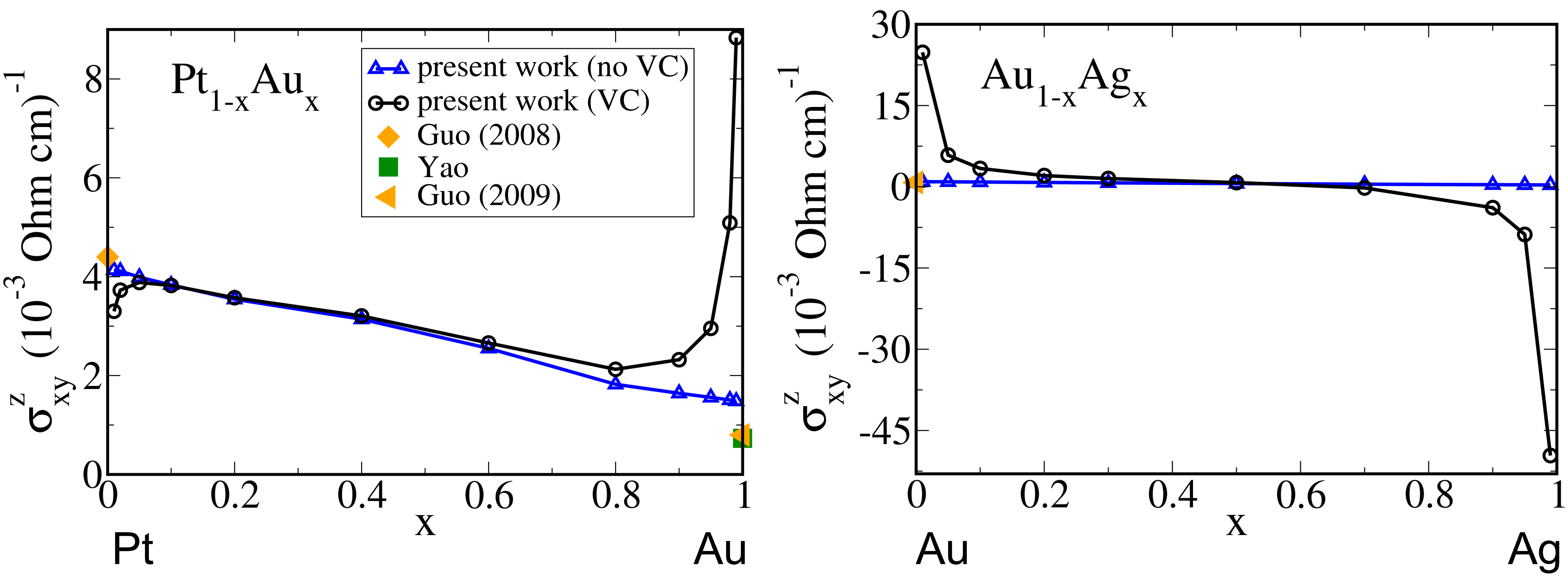
$$\underline{\underline{\sigma}}^y = \begin{pmatrix} 0 & 0 & -\sigma^x_{yz} \\ 0 & 0 & \sigma^x_{xz} \\ -\sigma^x_{zy} & \sigma^x_{zx} & 0 \end{pmatrix}$$

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

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

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)

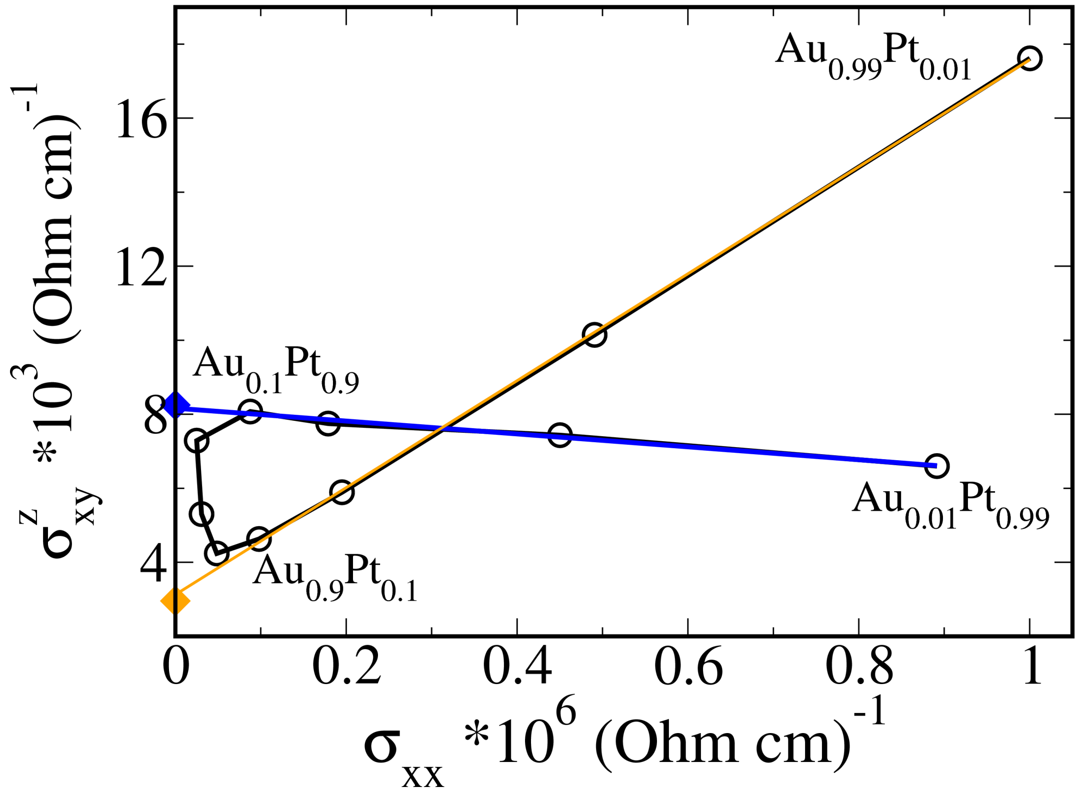
} intrinsic SHE of pure elements

Decomposition of Spin Hall conductivity via scaling behaviour of individual contributions

Ansatz in analogy to AHE

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

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



linear relation on both sides of alloy system for composition

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

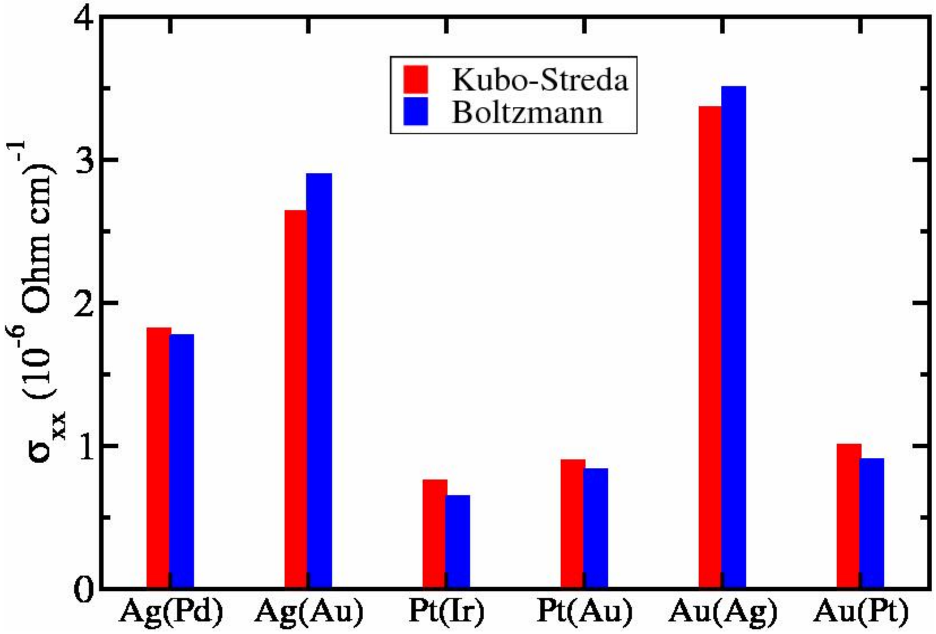
Extrapolation to $\sigma_{xx} \rightarrow 0$

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

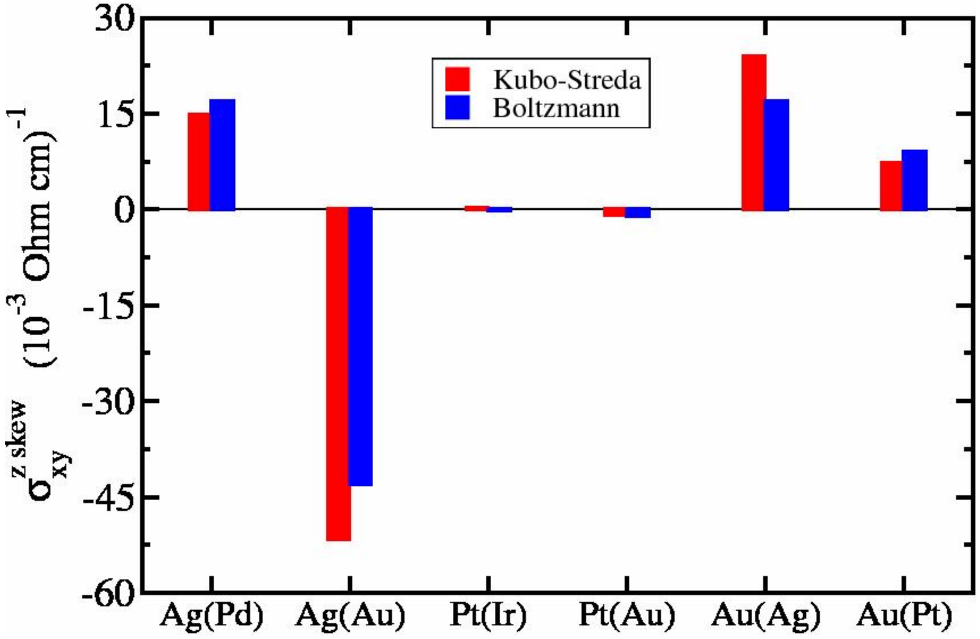
Kubo vs. Boltzmann-Formalism

Comparison of results for diluted alloys (1%)

longitudinal conductivity σ_{xx}



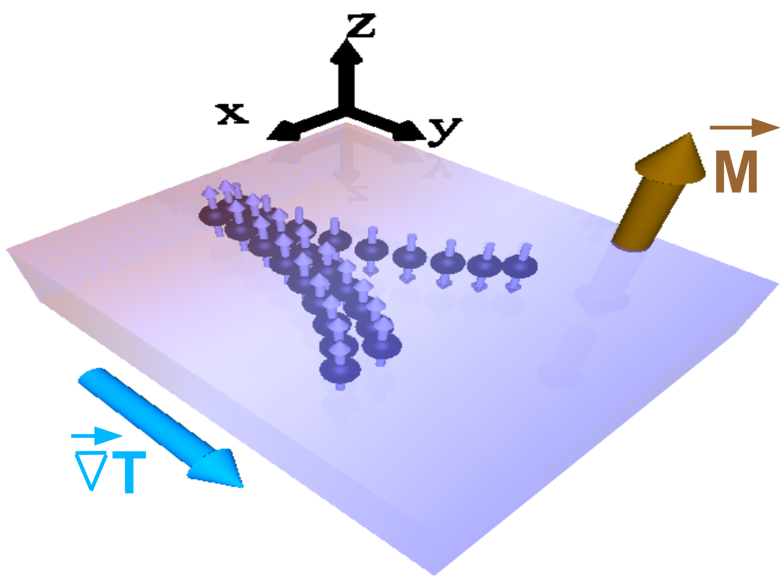
skew scattering $\sigma_{xy}^{z,\mathrm{skew}}$



Boltzmann-based calculations:
Gradhand, Fedorov, Mertig, (2010)

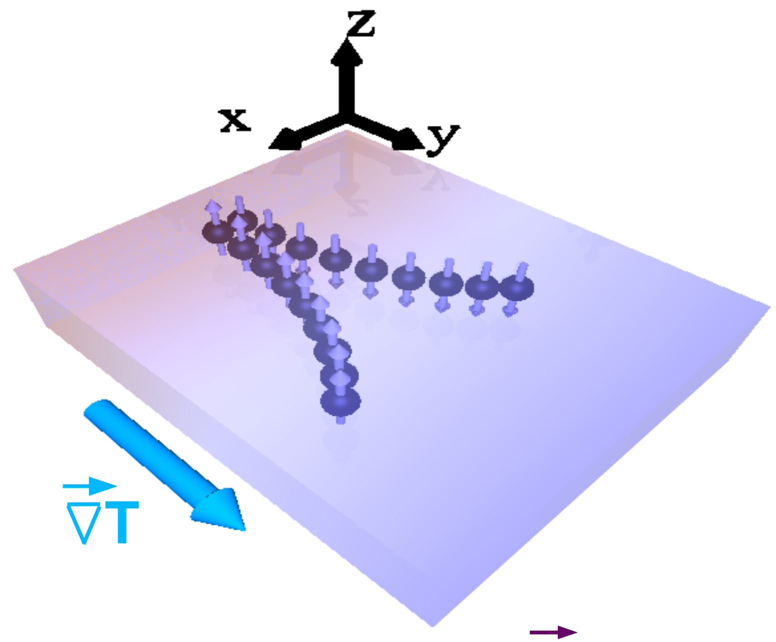
Transverse thermogalvanic charge and spin transport

Anomalous Nernst Effect (ANE)



Ferromagnet $\vec{B} = 0$

Spin Nernst Effect (SNE)



Paramagnet $\vec{B} = 0$

Thermal analogues to

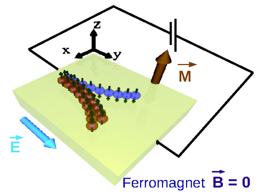
Anomalous Hall and **Spin Hall effect**

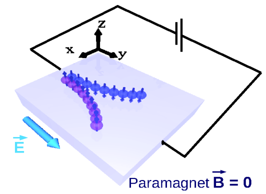
Summary

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

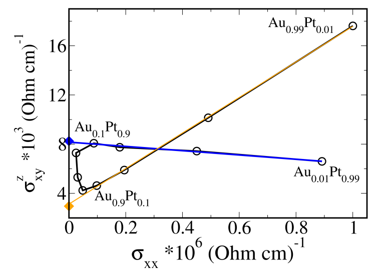
$$\sigma^z_{\mu\nu} = \frac{\hbar}{4\pi N\Omega}\mathrm{Tr}\left\langle \hat{J}^z_\mu (G^+ - G^-)\hat{j}_\nu G^- - \hat{J}^z_\mu G^+ \hat{j}_\nu (G^+ - G^-)\right\rangle_c + \frac{e}{4\pi i N\Omega}\mathrm{Tr}\left\langle (G^+ - G^-)(\hat{r}_\mu \hat{J}^z_\nu - \hat{r}_\nu \hat{J}^z_\mu)\right\rangle_c$$

- Applications to alloys on
  - Anomalous Hall Effect
  - Spin Hall Effect

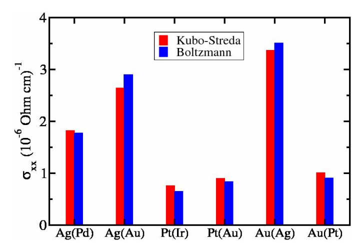




- Decomposition into intrinsic and extrinsic contributions based on vertex corrections



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



- Dilute alloys: very good agreement with Boltzmann formalism

- ***We owe much more to Wigner than the Wigner-Seitz cell***