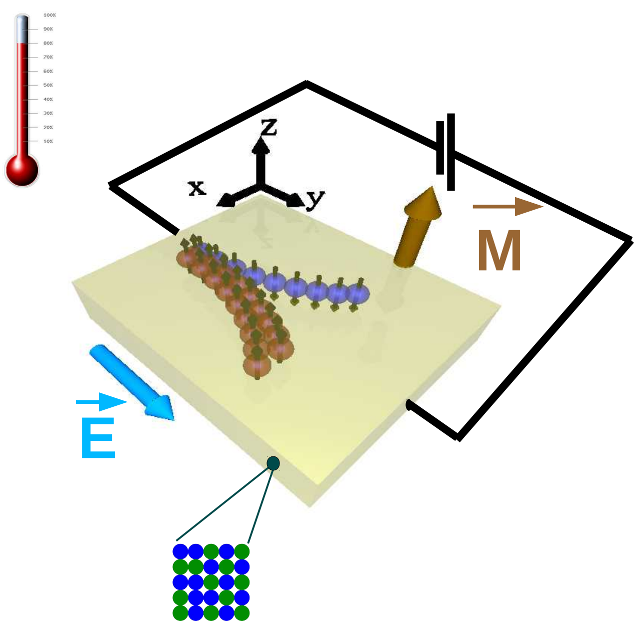
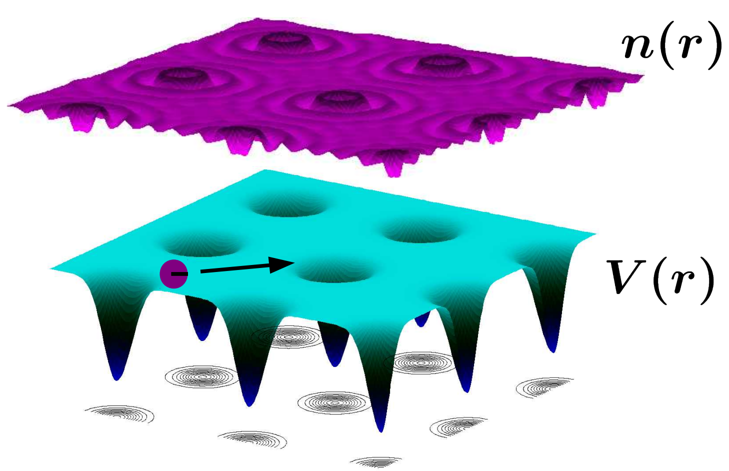
Description of galvanomagnetic transport using Kubo's linear response formalism

S. Wimmer, D. Ködderitzsch and H. Ebert
(J. Minar)





LMU
LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

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SFB 689 *Spinphänomene in reduzierten Dimensionen*

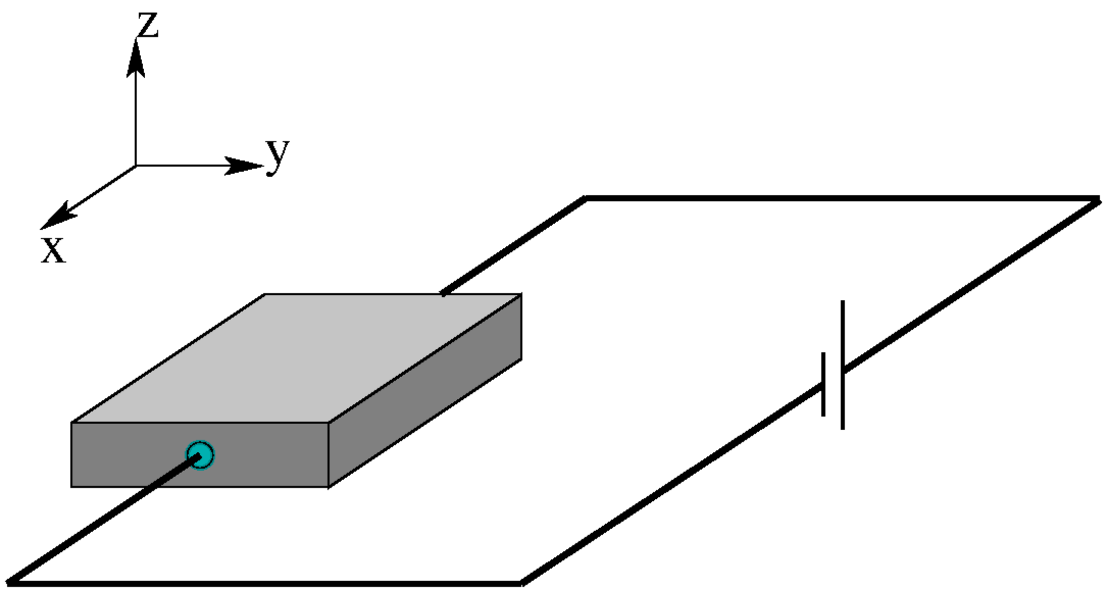
SPP 1538 *Spin Caloric Transport*

Outline

- A zoo of transport phenomena
- Transport formalism from first principles – Boltzmann
- Transport formalism from first principles – Kubo
  - longitudinal
  - transverse
  - thermogalvanic

Electronic transport – Ohm's law (linear resp.)

$$\vec{j} = \underline{\underline{\sigma}}\,\vec{E}$$



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

Introduction

Transport phenomena in linear response regime

- electrical
- spin
- heat

current density

$$\begin{pmatrix} \vec{j}_c \\ \vec{\mathcal{J}}_s \\ \vec{j}_t \end{pmatrix} = \begin{pmatrix} \underline{\underline{\sigma}}^{cc} & \underline{\underline{\sigma}}^{cs} & \underline{\underline{\sigma}}^{ct} \\ \underline{\underline{\sigma}}^{sc} & \underline{\underline{\sigma}}^{ss} & \underline{\underline{\sigma}}^{st} \\ \underline{\underline{\sigma}}^{tc} & \underline{\underline{\sigma}}^{ts} & \underline{\underline{\sigma}}^{tt} \end{pmatrix} \begin{pmatrix} \vec{E} \\ \vec{F}_s \\ \vec{\nabla} T \end{pmatrix}$$

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

Introduction

Anomalous Hall effect (AHE)
Anisotropic Magneto-Resistance (AMR)

Anisotropy of Seebeck effect (ASE)
Anomalous Nernst effect (ANE)

$$\begin{pmatrix} \underline{\underline{\sigma}}^{cc} & \underline{\underline{\sigma}}^{cs} & \underline{\underline{\sigma}}^{ct} \\ \underline{\underline{\sigma}}^{sc} & \underline{\underline{\sigma}}^{ss} & \underline{\underline{\sigma}}^{st} \\ \underline{\underline{\sigma}}^{tc} & \underline{\underline{\sigma}}^{ts} & \underline{\underline{\sigma}}^{tt} \end{pmatrix}$$

Spin Hall effect (SHE)

Spin Seebeck effect (SSE)
Spin Nernst effect (SNE)

Semi-classical approach
– Boltzmann transport theory –

Electronic structure of solids

Schrödinger equation within local (spin) density theory (LSDA)

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right]\psi_{\vec{k}}(\vec{r}) = E_{\vec{k}}\psi_{\vec{k}}(\vec{r})$$

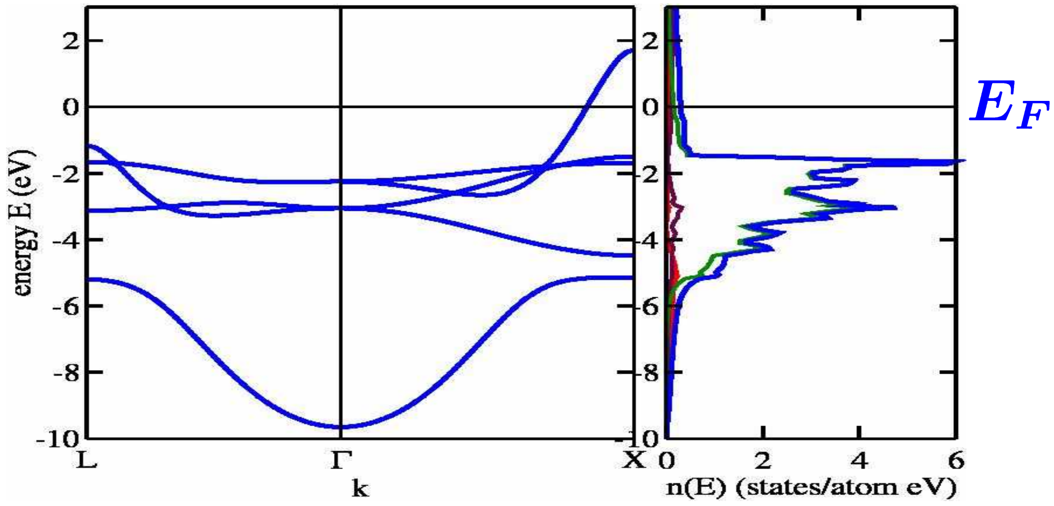
Periodic potential

$$V(\vec{r}) = V(\vec{r} + \vec{R}_n)$$

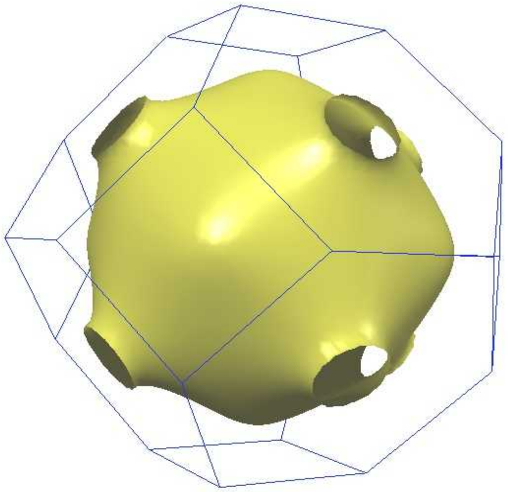
Bloch theorem

$$\psi_{\vec{k}}(\vec{r} + \vec{R}_n) = e^{i\vec{k}\vec{R}_n}\psi_{\vec{k}}(\vec{r})$$

Dispersion relation   Density of states



Fermi surface $E_{\vec{k}} = E_F$



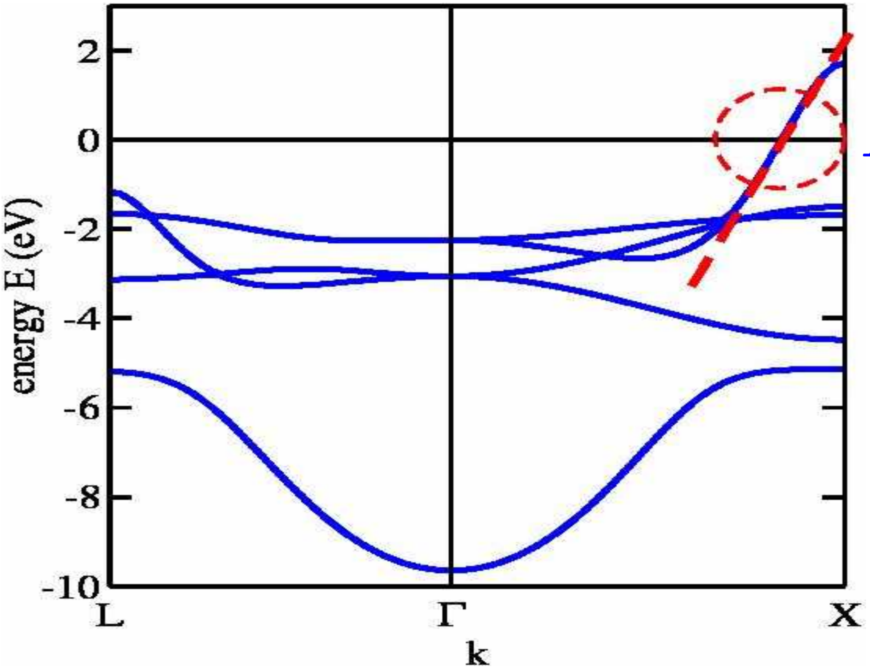
Boltzmann transport equation I

total rate in change for distribution function $f_{\vec{k}}$

$$-\left.\frac{\partial f_{\vec{k}}}{\partial t}\right|_{\text{scatt.}} + \left.\frac{\partial f_{\vec{k}}}{\partial t}\right|_{\text{field}} = 0$$

external term due to the electric field $\vec{E}$

$$\left.\frac{\partial f_{\vec{k}}}{\partial t}\right|_{\text{field}} = \frac{\mathrm{d}\vec{k}}{\mathrm{d}t}\frac{\partial f_{\vec{k}}}{\partial E_{\vec{k}}}\frac{\partial E_{\vec{k}}}{\partial \vec{k}} = -|e|\frac{\partial f_{\vec{k}}}{\partial E_{\vec{k}}}\vec{v}_{\vec{k}}\cdot\vec{E}$$



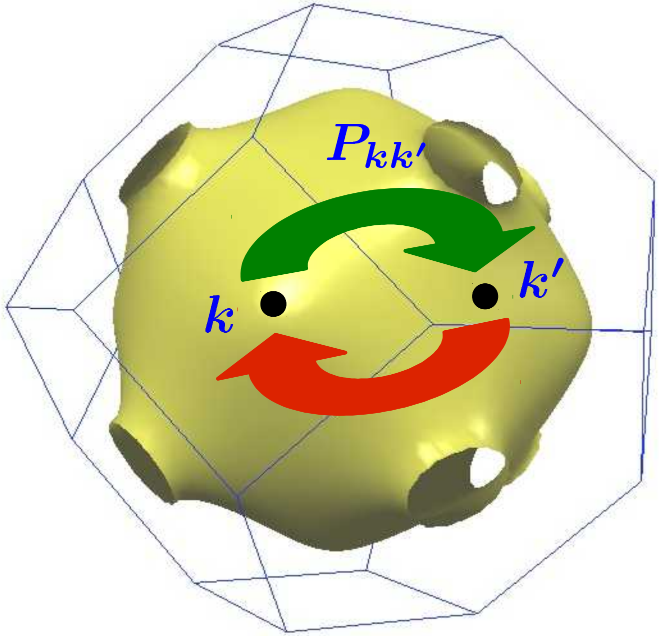
group velocity

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

Boltzmann transport equation II

scattering term

$$\left.\frac{\partial f_{\vec{k}}}{\partial t}\right|_{\text{scatt.}} = \sum_{\vec{k}'} \Big[\underbrace{f_{\vec{k}'}(1-f_{\vec{k}})P_{\vec{k}'\vec{k}}}_{\text{scattering-in}} - \underbrace{(1-f_{\vec{k}'})f_{\vec{k}}P_{\vec{k}\vec{k}'}}_{\text{scattering-out}} \Big]$$



Transition propability

$$P_{\vec{k}\vec{k}'} \sim \left| \langle \psi_{\vec{k}} | V_{imp} | \psi_{\vec{k}'} \rangle \right|^2$$

with $f_{\vec{k}} = f^0_{\vec{k}} + g_{\vec{k}}$ and $g_{\vec{k}} \ll f^0_{\vec{k}}$

$$\left.\frac{\partial f_{\vec{k}}}{\partial t}\right|_{\text{scatt.}} = \sum_{\vec{k}'} P_{\vec{k}\vec{k}'} (g_{\vec{k}'} - g_{\vec{k}})$$

Boltzmann transport equation III

linear ansatz

$$g_{\vec{k}} = -|e|\,\delta(E_{\vec{k}} - E_F)\vec{\Lambda}_{\vec{k}} \cdot \vec{E}$$

$\tau_{\vec{k}}^{-1} = \sum_{\vec{k}'} P_{\vec{k}\vec{k}'}$ relaxation time

$\vec{\Lambda}_{\vec{k}}$ vector mean free path

$$\vec{\Lambda}_{\vec{k}} = \tau_{\vec{k}} \left(\vec{v}_{\vec{k}} + \sum_{\vec{k}'} P_{\vec{k}\vec{k}'} \vec{\Lambda}_{\vec{k}'} \right)$$

conductivity tensor element

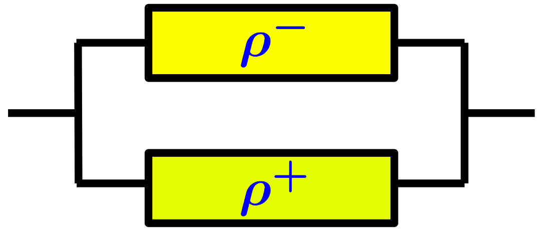
$$\sigma_{\mu\nu} = \frac{e^2}{(2\pi)^3} \sum_n \iint_{E_{\vec{k}}=E_F} dS_{\vec{k}} \frac{1}{v_{\vec{k}}^n} v_{\vec{k}}^{n,\mu} \Lambda_{\vec{k}}^{n,\nu}$$

Mertig *et al.*, Teubner (1987)

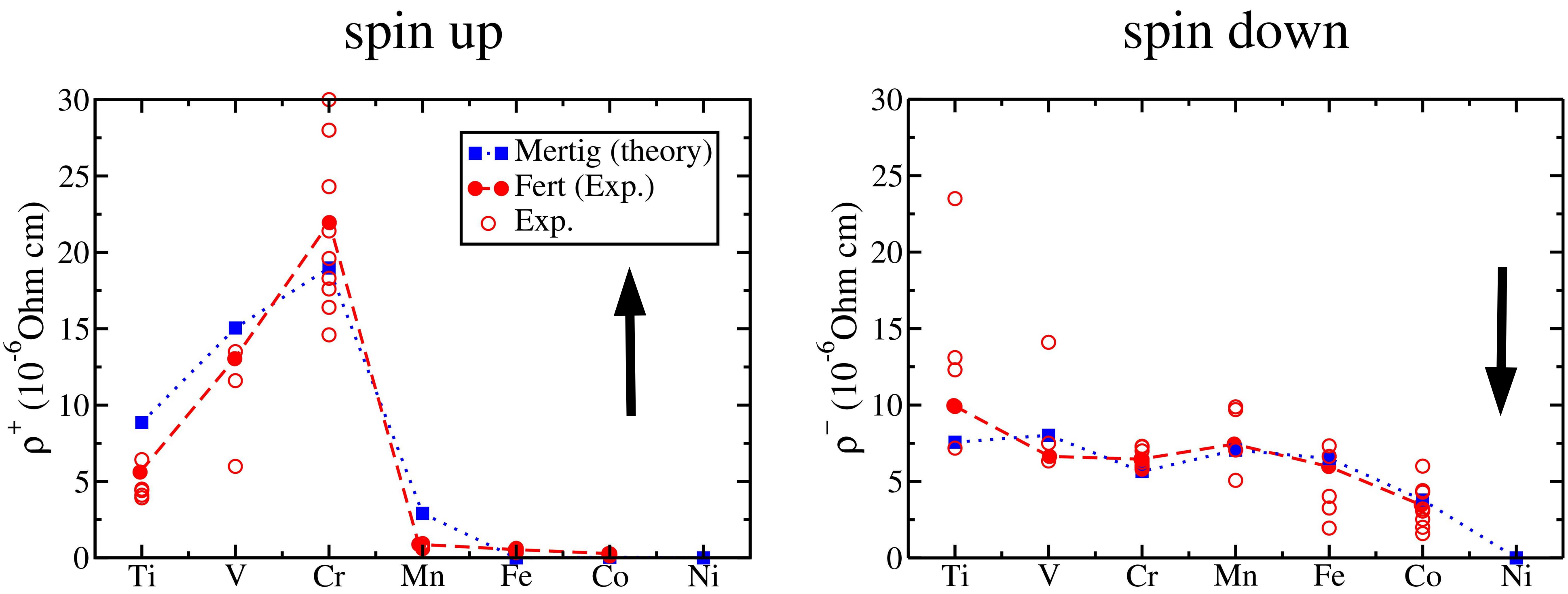
Ni with 3-*d* Transition Metal impurities (1%)

Spin projected residual resistivity based on:

- Two-current model of Mott
- Boltzmann transport formalism



$$\rho = \left(\frac{1}{\rho^+} + \frac{1}{\rho^-}\right)^{-1}$$



Experiment: A. Fert et al., PRL **21**, 1190 (1968)
Theory: I. Mertig et al., PRB **47**, 16178 (1993)

Full quantum mechanical approach
– Kubo formalism –

Kubo's formalism

Expectation value of operator $\hat{D}$ $\langle \hat{D} \rangle = \mathrm{Tr}(\rho_0 \hat{D})$

with density matrix $\rho_0 = \frac{e^{-\beta\hat{\mathcal{H}}}}{\mathrm{Tr}(e^{-\beta\hat{\mathcal{H}}})}$

To get the response to a time-dependent perturbation $\hat{W}(t)$
solve equation of motion for $\rho(t)$

$$i\hbar\frac{\partial}{\partial t}\rho(t) = [(\hat{\mathcal{H}} + \hat{W}(t)), \rho(t)]$$

To first order w.r.t. the perturbation $\hat{W}(t)$ one has

$$\begin{aligned} < \hat{D} >_t &= < \hat{D} > \\ & -i/\hbar \int_{-\infty}^{\infty} dt' \Theta(t-t') < [\hat{D}_I(t), \hat{W}_I(t')] > \end{aligned}$$

Kubo formalism applied to electric transport

perturbation $\hat{\mathbf{W}}_t = -\hat{\mathbf{P}} \cdot \mathbf{E}_t$ represents coupling of

electric dipole moment $\hat{\mathbf{P}} = \sum_{i=1}^{N} q_i \hat{\mathbf{r}}_i$ to electric field E_t

induced electric current density

$$< \hat{j}_\mu >_t \; = \; i/\hbar \sum_\nu \int_{-\infty}^{\infty} dt' \; \Theta(-t') \, < [\hat{j}_\mu, \hat{P}_{\nu,I}(t')] > e^{-i(\omega+i\delta)t'} E_{t,\nu}$$

Kubo's identity $[\hat{O}(t), \rho] = -i\hbar\rho \int_0^{(k_B T)^{-1}} d\lambda \, \dot{\hat{O}}(t - i\hbar\lambda)$

leads for the conductivity tensor to:

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

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

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

Transport from first-principles – various ingredients –

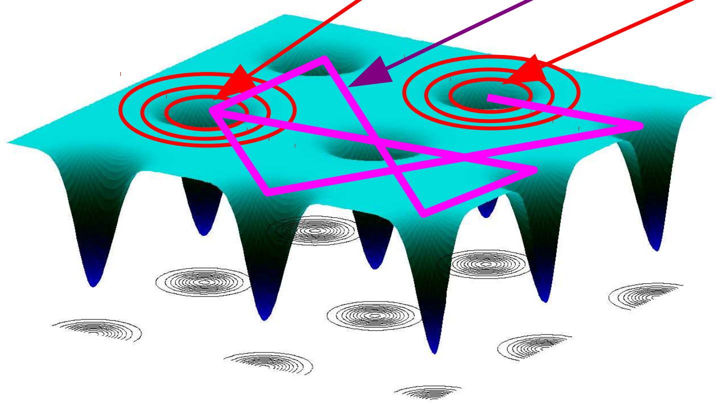
(a little detour)

Multiple scattering representation of G in KKR

$$\hat{H}^{\text{Dirac}} = c\alpha \cdot \vec{p} + \beta mc^2 + \bar{V} + \Sigma \cdot B$$

scattering path operator

$$G^{+}(\vec{r},\vec{r}\,',E) = G^{+,\text{irr}}_{nn}(\vec{r},\vec{r}\,',E) + \sum_{\Lambda\Lambda'} Z^{n}_{\Lambda}(\vec{r},E)\,\tau^{nm}_{\Lambda\Lambda'}(E)\,Z^{m\times}_{\Lambda'}(\vec{r}\,',E)$$



Muffin-Tin-Potential

numerical,
relativistic
radial solutions
&
rel. spin-angular-functions

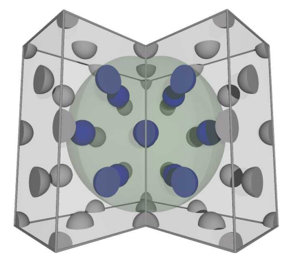
Dyson–Equation

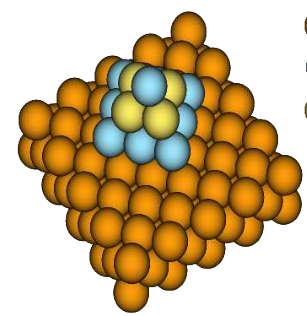
$\hat{H}_0$ Reference system

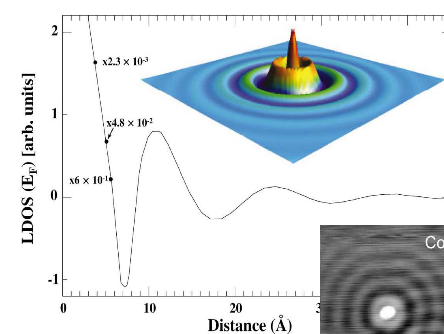
$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}$$

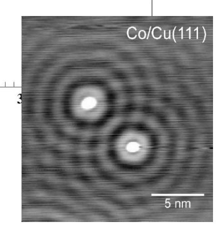
$$\hat{H} = \hat{H}_0 + V$$

- intuitive, physically transparent
- construction: Hierarchy of Dyson-Equations
- **Korringa-Kohn-Rostoker (KKR)**-GF method
  - spherical waves
  - accurate minimal basis set method
- efficient treatment of
  - impurities
  - surfaces and interfaces
  - disorder (CPA, NL-CPA)





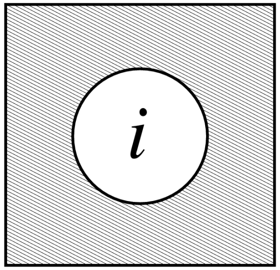




Stepanyuk *et.al,* PRB **68**, 205410 (2003)

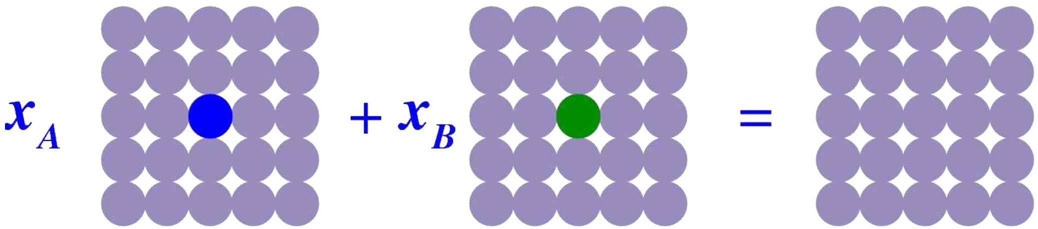
Review: Ebert, Ködderitzsch, Minár, Rep. Prog. Phys. 74, 096501 (2011)

Theory of effective media – CPA



Best single-site theory:

Coherent potential approximation (**CPA**)



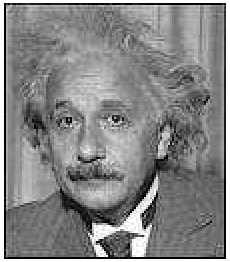
$$x_{\mathrm{A}}\underline{\tau}^{nn,\mathrm{A}} + x_{\mathrm{B}}\underline{\tau}^{nn,\mathrm{B}} = \underline{\tau}^{nn,\mathrm{CPA}}$$

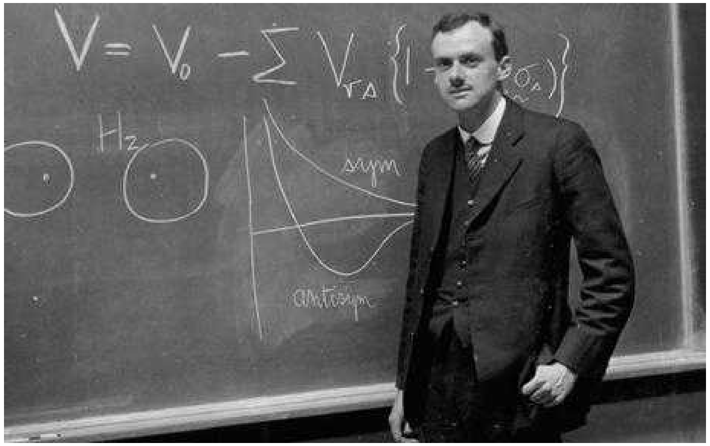
$$\underline{\tau}^{nn,\alpha} = \underline{\tau}^{nn,\mathrm{CPA}}\left[1 + \left(\underline{t}_{\alpha}^{-1} - \underline{t}_{\mathrm{CPA}}^{-1}\right)\underline{\tau}^{nn,\mathrm{CPA}}\right]^{-1}$$

self-consistent construction of the medium:

embedding of A- or B-atoms in effectiv medium
does not cause – on average – scattering

Theory of relativity and quantum mechanics





Westminster Abbey

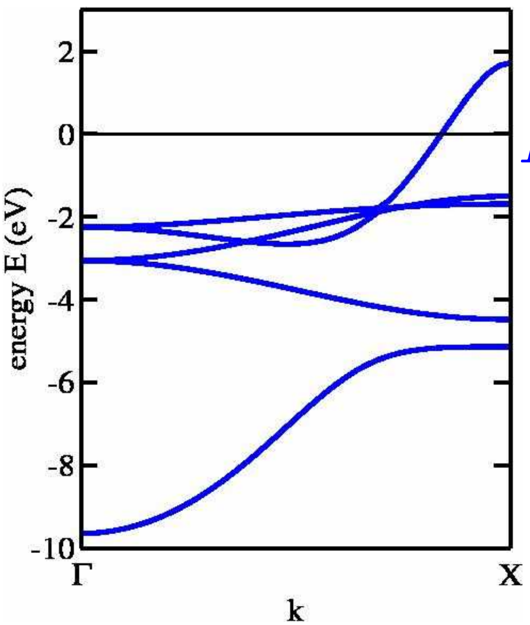
Longitudinal charge transport

Band structure of disordered alloys

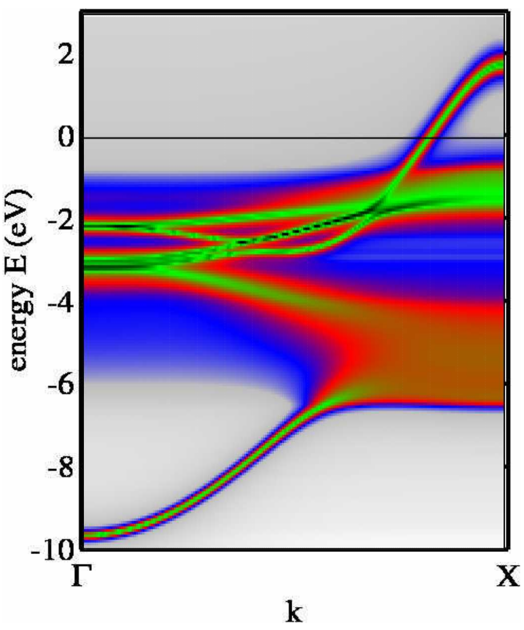
Dispersion relation of pure Cu

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

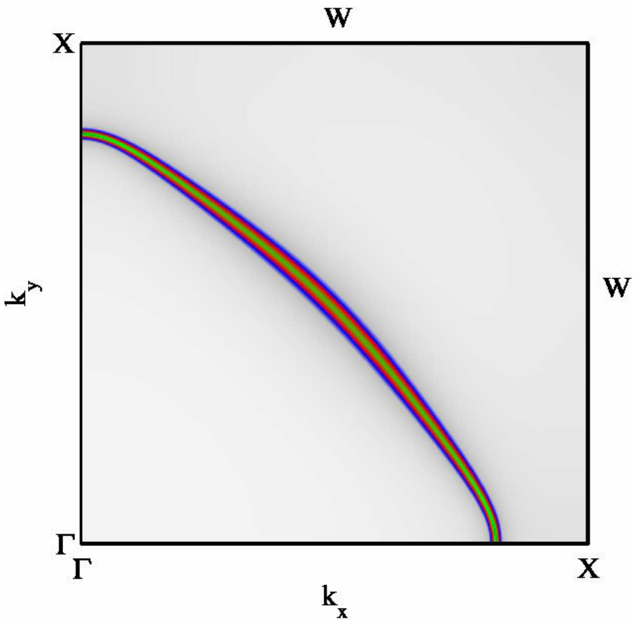
$\vec{k}$ along Γ-X



$\vec{k}$ along Γ-X



Fermi surface in Γ-X-W-plane

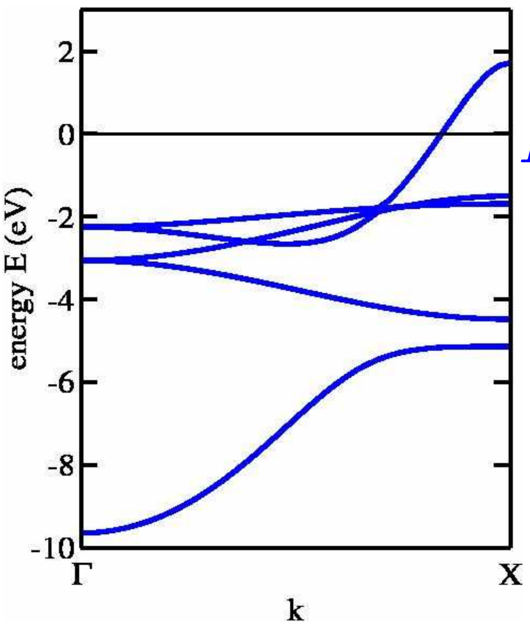


$$A_{\mathrm{B}}(\vec{k}, E) \quad = \quad -\frac{1}{\pi} \sum_{n}^{N} e^{-\imath \vec{k} \vec{R}_n} \quad \Im \int_{\Omega} d^3 r \left\langle G\left(\vec{r}, \vec{r} + \vec{R}_n, E\right)\right\rangle$$

Band structure of disordered alloys

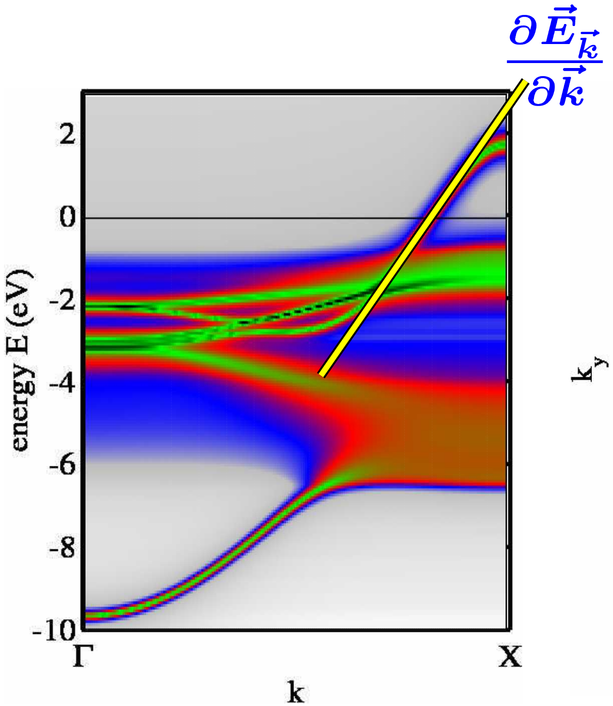
Dispersion relation of pure Cu

$\vec{k}$ along Γ-X



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

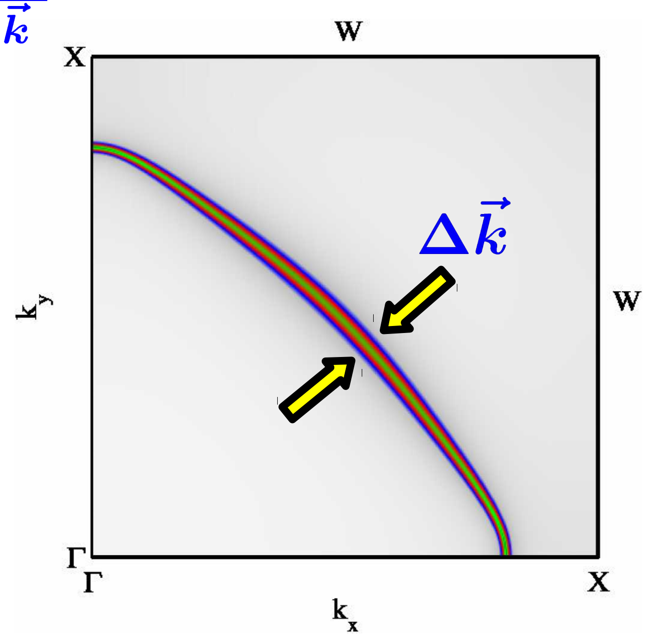
$\vec{k}$ along Γ-X



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

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

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

Boltzmann-formalism applied to Ag_xPd_{1-x}

Fermi surface of Ag_xPd_{1-x}

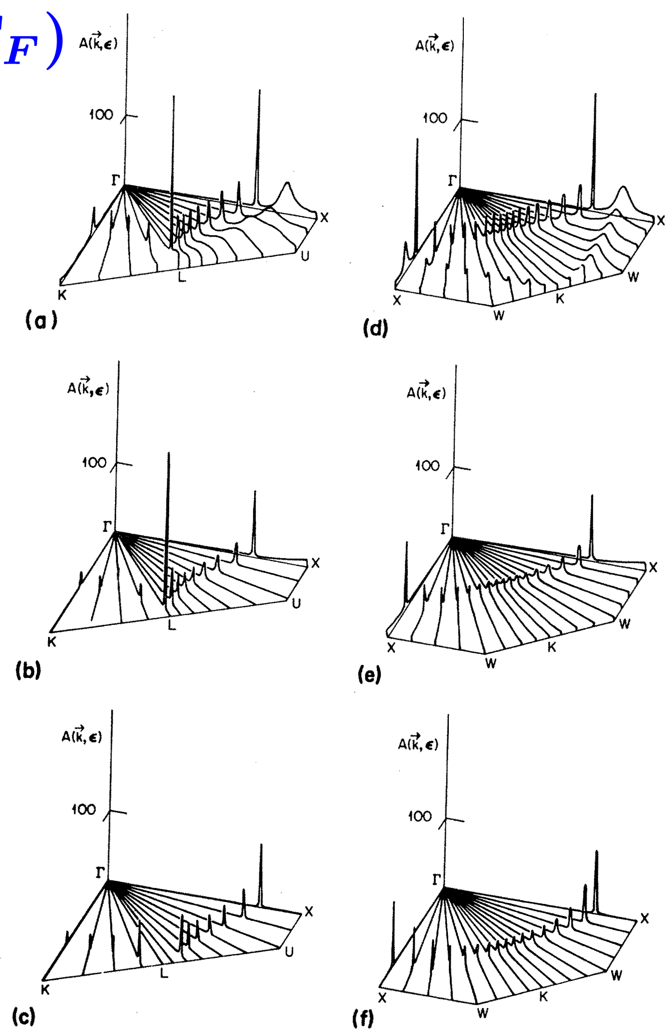
(110)-plane (001)-plane

$A_B(\vec{k}, E_F)$

$Ag_{0.2}Pd_{0.8}$

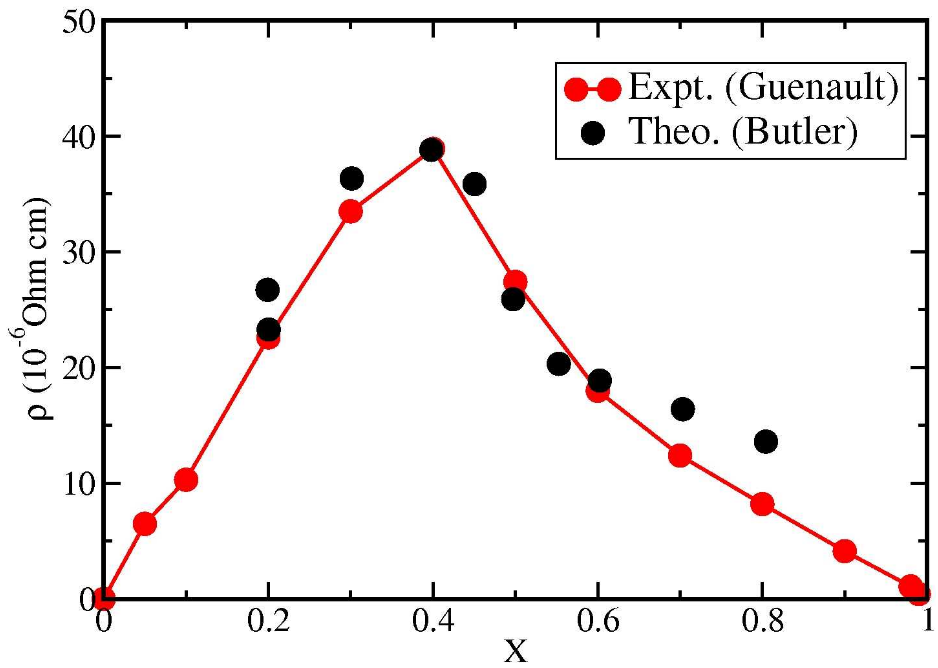
$Ag_{0.5}Pd_{0.5}$

$Ag_{0.8}Pd_{0.2}$



Residual resistivity (T=0K)

Ag_xPd_{1-x}



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

Neglecting scattering-in term

Kubo-Greenwood (KG) Equation Part I

conductivity tensor within linear response (Kubo) formalism given as **current density–current density correlation function**

$$\sigma_{\mu\nu} = \frac{\pi\hbar}{N\Omega}\left\langle \sum_{m,n} \langle m|j_\mu|n\rangle\langle n|j_\nu|m\rangle \delta(E_F - E_m)\delta(E_F - E_n) \right\rangle_c$$

current density operator $\hat{j}_\mu = -\frac{e}{m}\frac{\hbar}{i}\nabla_\mu$

$\left\langle \dots \right\rangle_c$ = average over alloy configurations

with: $\sum_m |m\rangle\langle m|\delta(E - E_m) = -\frac{1}{\pi}\lim_{\epsilon\to 0}\Im G^+(E + i\epsilon)$

$$\sigma_{\mu\nu} = -\frac{\hbar}{\pi N\Omega}\mathrm{Tr}\left\langle j_\mu \Im G^+(E_F + i\epsilon)\, j_\nu \Im G^+(E_F + i\epsilon) \right\rangle_c$$

Kubo-Greenwood Equation Part II

Implementation within KKR-CPA

$$\tilde{\sigma}_{\mu\nu} = -\frac{4m^2}{\pi\hbar^3\Omega}\left(\sum_{\alpha,\beta}\sum_{\substack{L_1,L_2\\L_3,L_4}} c^\alpha c^\beta \tilde{J}^{\alpha\mu}_{L_4,L_1}(z_2,z_1)\Big[\underbrace{\{1-\chi\omega\}^{-1}}_{\text{vertex correction}}\chi\Big]_{\substack{L_1,L_2\\L_3,L_4}} \tilde{J}^{\beta\nu}_{L_2,L_3}(z_1,z_2)\right.$$

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

$$\left. + \sum_{\alpha}\sum_{\substack{L_1,L_2\\L_3,L_4}} c^\alpha \tilde{J}^{\alpha\mu}_{L_4,L_1}(z_2,z_1)\tau^{\mathrm{CPA},00}_{L_1,L_2}(z_1) J^{\alpha\nu}_{L_2,L_3}(z_1,z_2)\tau^{\mathrm{CPA},00}_{L_3,L_4}(z_2)\right)$$

with $z_1, z_2 = \lim_{\epsilon\to 0}(E_F \pm i\epsilon)$
and the quantum numbers
$L = (l, m_l)$

Vertex corrections (VC)

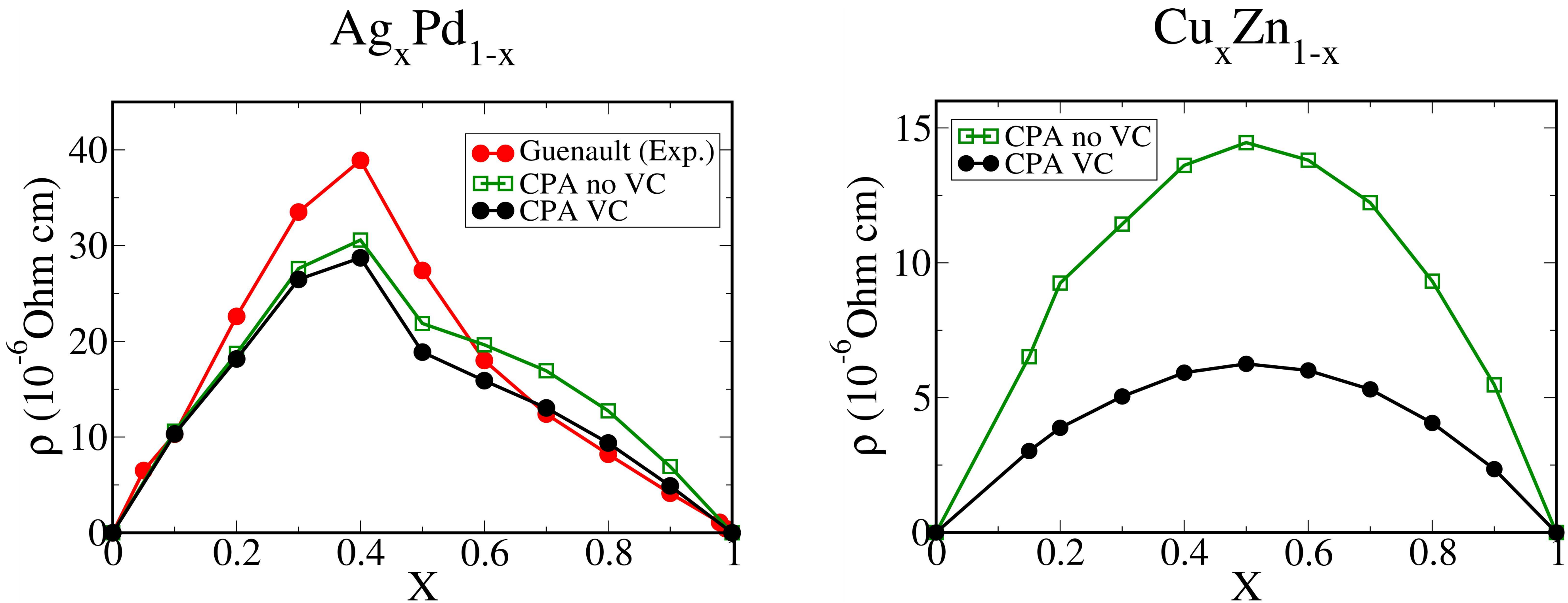
$< jGjG > - < jG >< jG >$

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)

Application to non-magnetic alloys

Residual resistivity (*T*=0K)



impact of vertex corrections (VC)

small **large**

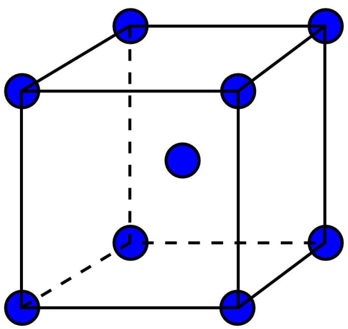
depending on alloy system and character of wave functions at Fermi level

Expt: Guénault, Phil. Mag. **30**, 641, (1974)
Theo: Tulip et al., PRB **77**, 165116 (2008)

Symmetry breaking due to magnetism

Point group for bcc-structure

paramagnetic

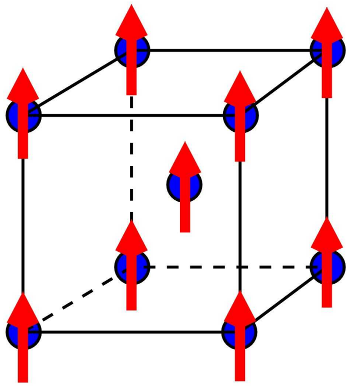


G = m3m

$$\begin{array}{llll} \mathbf{1} & \mathbf{9(2)} & \mathbf{4(\pm 3)} & \mathbf{3(\pm 4)} \\ \bar{\mathbf{1}} & \mathbf{9(\bar{2})} & \mathbf{4(\pm \bar{3})} & \mathbf{3(\pm \bar{4})} \\ \mathbf{1'} & \mathbf{9(2')} & \mathbf{4(\pm 3')} & \mathbf{3(\pm 4')} \\ \bar{\mathbf{1}}' & \mathbf{9(\bar{2}')} & \mathbf{4(\pm \bar{3}')} & \mathbf{3(\pm \bar{4}')} \end{array}$$

1': time reversal

ferromagnetic



G = 4/mm'm'

$$\begin{array}{llll} \mathbf{1} & \mathbf{2_z} & \mathbf{\pm 4_z} & \\ \bar{\mathbf{1}} & \bar{\mathbf{2}}_z & \mathbf{\pm \bar{4}_z} & \\ \mathbf{2'_x} & \mathbf{2'_y} & \mathbf{2'_{xy}} & \mathbf{2'_{-xy}} \\ \bar{\mathbf{2}}'_x & \bar{\mathbf{2}}'_y & \bar{\mathbf{2}}'_{xy} & \bar{\mathbf{2}}'_{-xy} \end{array}$$

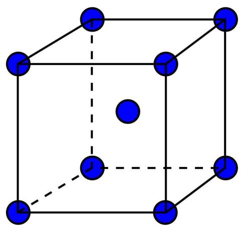
reduced symmetry due to magnetism AND spin-orbit coupling

Structure of the conductivity tensor σ

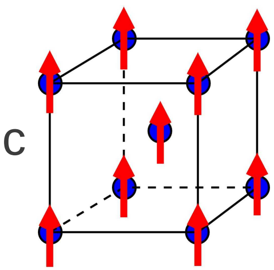
Von Neumann's Principle

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

paramagnetic



ferromagnetic



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

Isotropic conductivity
or resistivity

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

Galvano-magnetic effects
Anomalous Hall effect

σ_{xy} or ρ_{xy}

Anisotropic magnetoresistance AMR

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

The Dirac Equation for magnetic solids

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

effective magnetic field

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

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

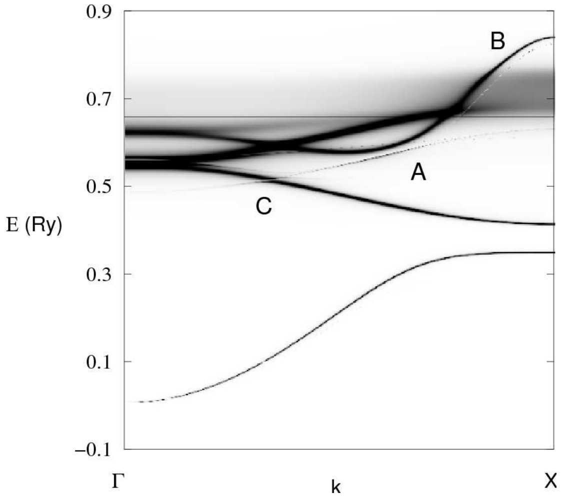
Within an atomic cell one can choose $\hat{\mathbf{z}}'$ to have:

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

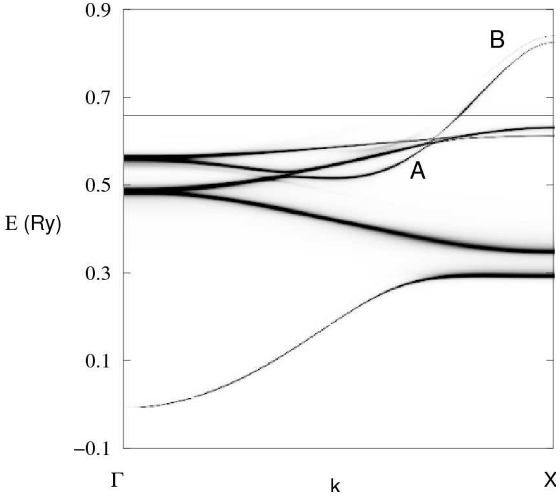
Bloch spectral function $A_{\mathrm{B}}(\vec{k}, E)$ of $Fe_{0.2}Ni_{0.8}$

$\vec{k}$ along Γ-X

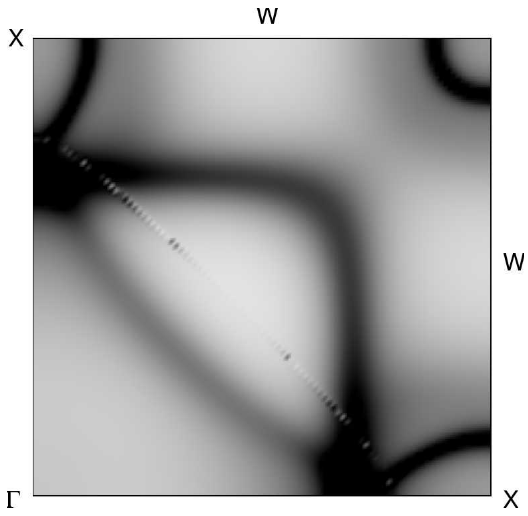
minority spin

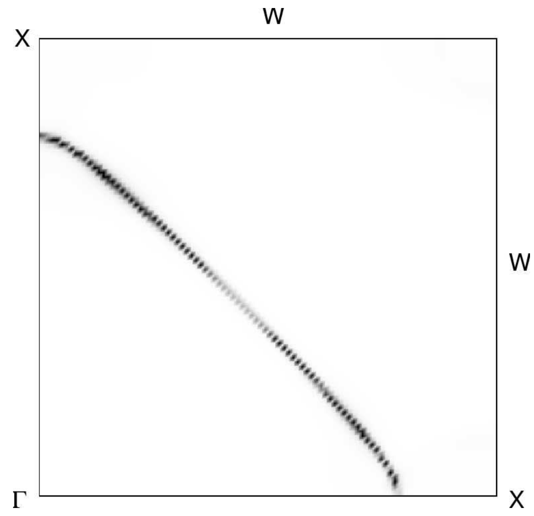


majority spin



Fermi surface
in Γ-X-W-plane





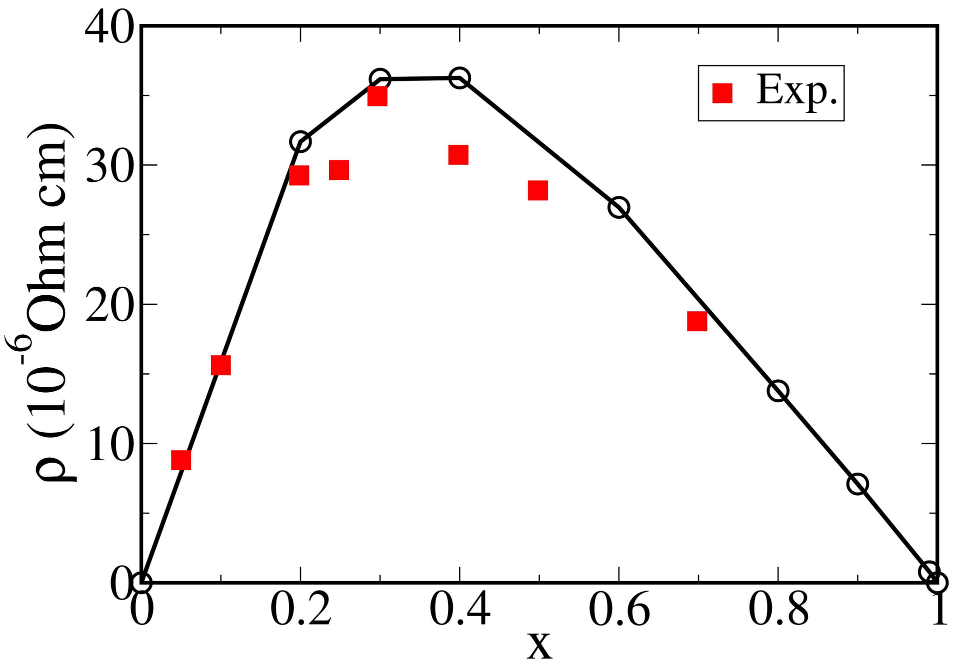
Ebert et al., SSC **104**, 243 (1997)

Residual resistivity of ferro-magnetic alloys

Isotropic residual resistivity

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

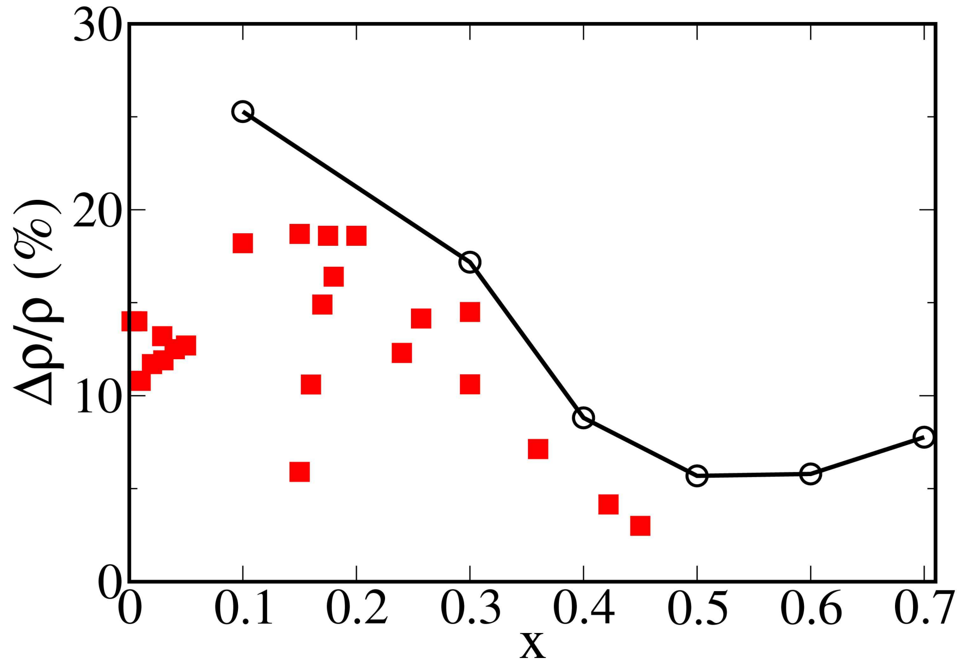
Co_xPt_{1-x}



Anisotropic magnetoresistance AMR

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

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)

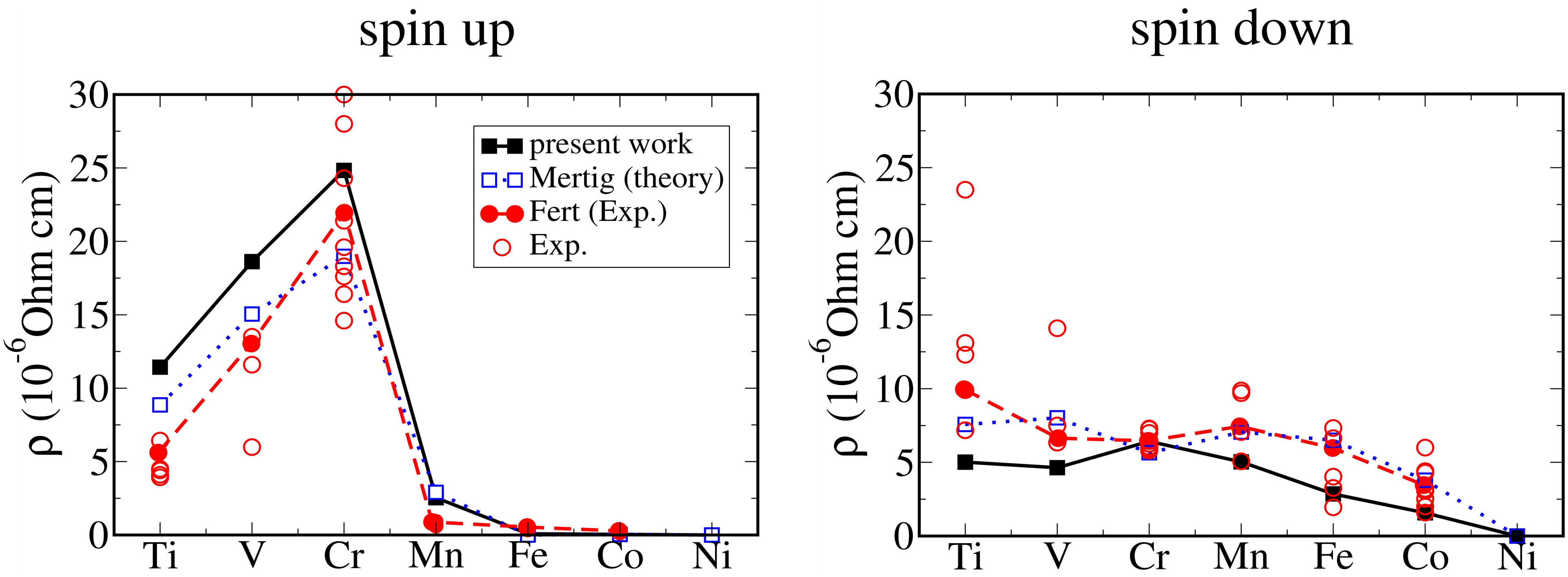
Ni with 3*d* Transition Metal impurities (1%)

Spin projected longitudinal residual resistivity

- Boltzmann transport formalism
- Two-current model of Mott

versus

- Kubo-Středa formalism
- Spin current operator



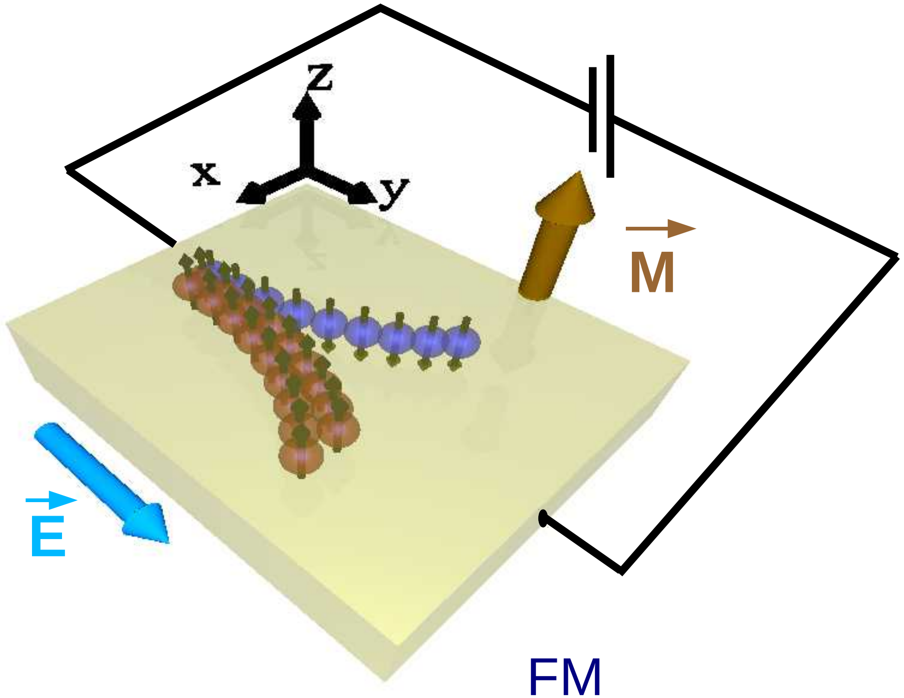
Exp. : A Fert et al., PRL **21**, 1190 (1968)

Theory:
- I Mertig et al., PRB **47**, 16178 (1993) **non-relativistic** two current model
- S Lowitzer, DK, H Ebert, PRB **82**, 140402(R) (2010), **relativistic** spin current op.

Transverse currents

Transverse charge and spin currents

Anomalous Hall Effect (AHE)

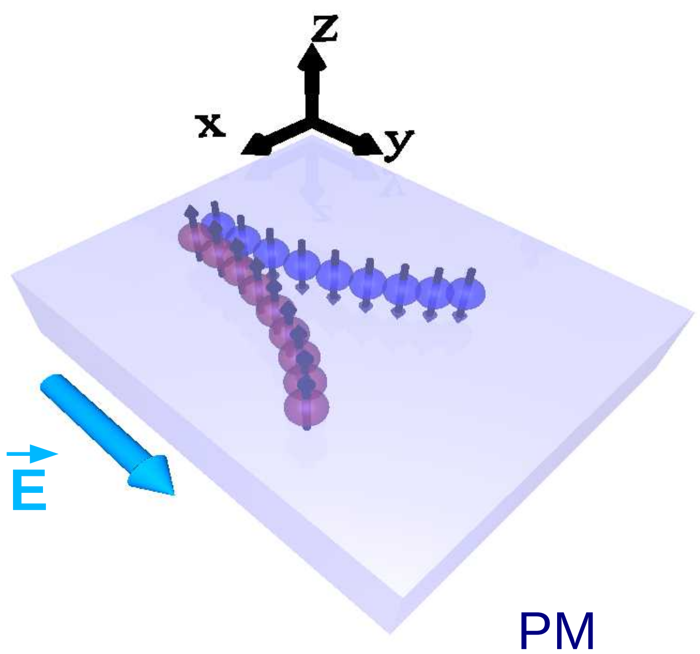


Separating charge (+ spin)

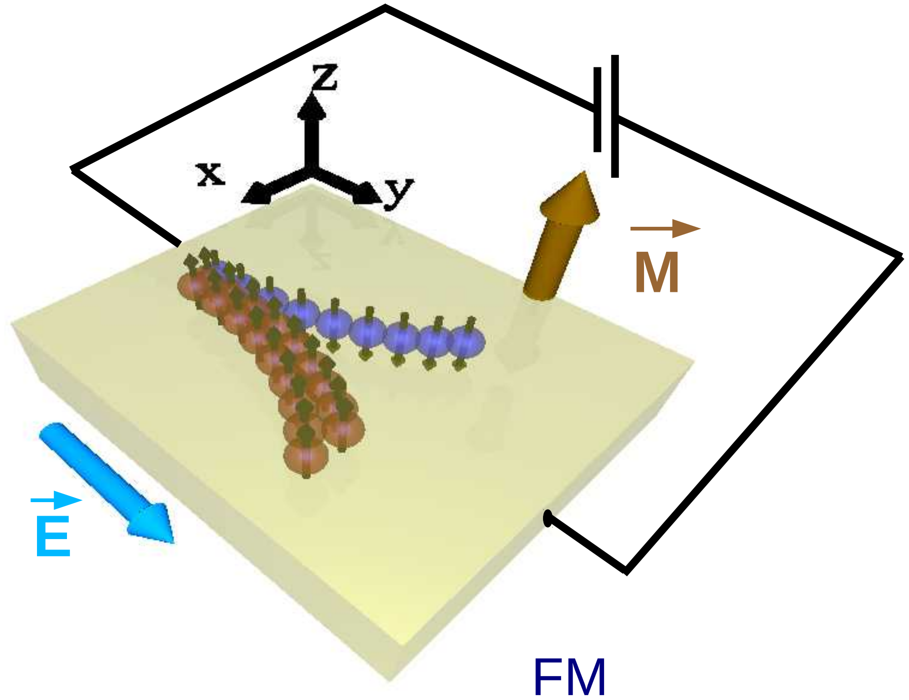
Source **relativistic** spin-orbit interaction

Transverse charge and spin currents

Spin Hall Effect (SHE)



Anomalous Hall Effect (AHE)

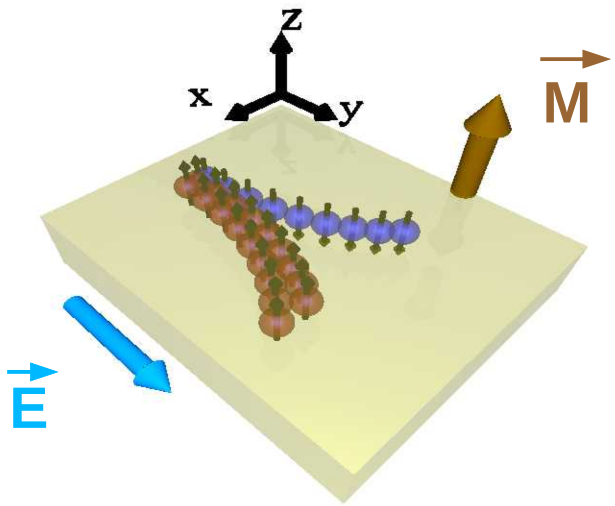


Separating spin charge (+ spin)

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

“Spintronics without magnetism”

Anomalous Hall effect (AHE)



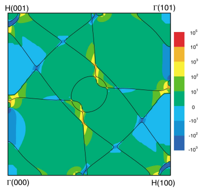
$$\underline{\underline{\sigma}}_{cc} = \begin{pmatrix} \sigma_\perp & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_\perp & 0 \\ 0 & 0 & \sigma_\parallel \end{pmatrix}$$

electrical conductivity tensor for a ferromagnetic cubic system with magnetization direction along the z-axis

Mechanisms

- Relativistics, i.e. **Spin-orbit coupling** as defining component
- Intrinsic component – interpreted in terms of Berry phase
- Extrinsic components – e.g.
  - Side-jump
  - Skew scattering

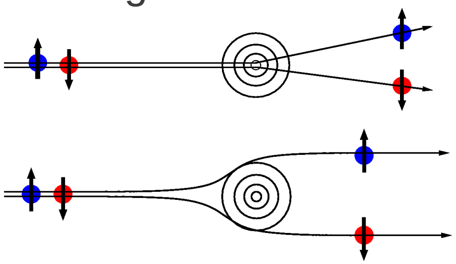
Yao et al., PRL **92**, 037204 (2004)
Sinitsyn, JPhys. Cond. Matter, **20**,023201 (2008)
Nagaosa et al., Rev. Mod. Phys, **82**, 1539 (2010)



spin dependent impurity scattering

skew (Mott-) scattering

side-jump scattering



Kubo-Středa (KS) Equation (T = 0K)

Advanced / retarded relativistic Green function

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

with the current density operators

Dirac matrix

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

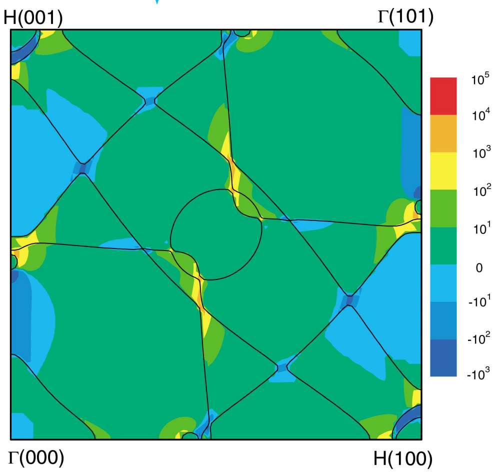
spin $\hat{J}^z_\mu = c\alpha_\mu T_z$

Spinprojektionsop. [1,2,3] $\mathcal{P}_z^{\pm,\mathcal{T}} = \frac{1}{2}\left[1 \pm \left(\beta\Sigma_z - \frac{\gamma_5 \Pi_z}{mc}\right)\right]$

[1] Bargmann & Wigner, Proc. Natl. Acad. Sci. **34**, 211 (1948)
[2] Vernes, Györffy, Weinberger, PRB **76**, 12408 (2007)
[3] Lowitzer, Ködderitzsch, Ebert, PRB **82**, 140402(R) (2010)

Intrinsic AHE of 3*d* metals

σ_{xy} $(\Omega cm)^{-1}$	bcc Fe	fcc Ni	hcp Co	
SPR-KKR	727	-2115	343	Kubo-Středa
Roman et al. (2009)			481	Berry curvature
Yao et al. (2004)	753	-2073	492	
Wang et al. (2007)	751	-2203		
Dheer (1967)	1032			Experiment
Lavine (1961)		-646		
Miyasato et al. (2007)			480	



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

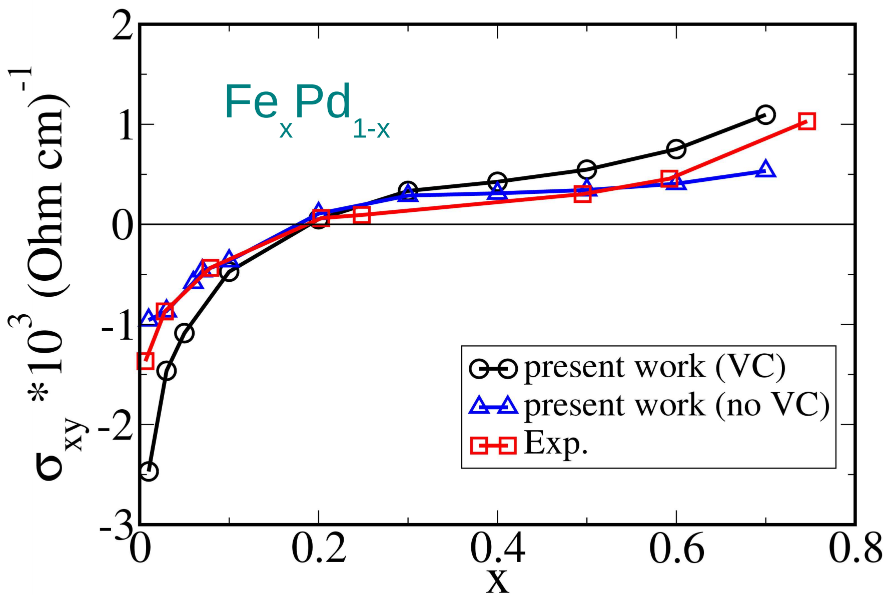
$$\sigma_{xy}^{\mathrm{intr}} = -e^2\hbar \sum_n \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\, f_n\, \Omega_n(\mathbf{k})$$

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

$\Omega_n(\mathbf{k})$ Berry curvature

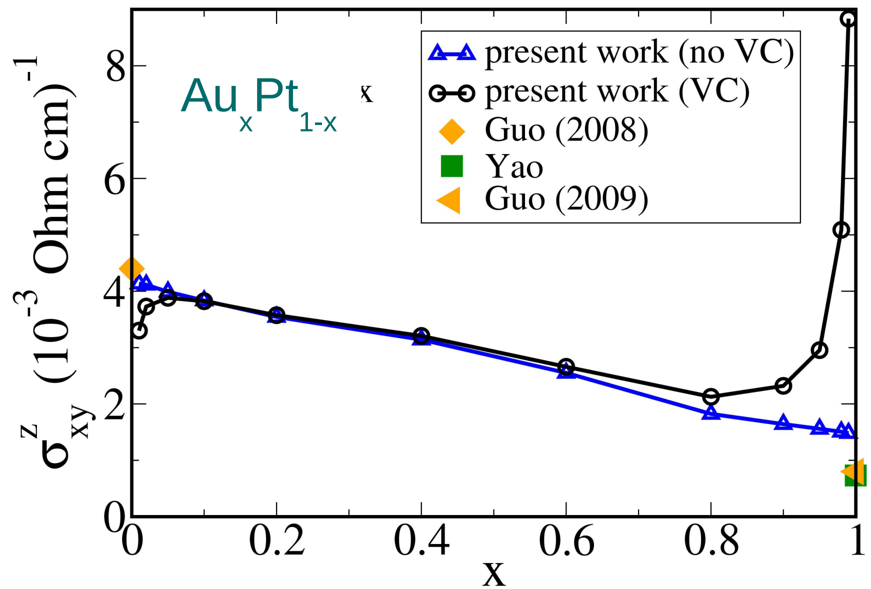
AHE and SHE in alloys

Anomalous Hall-Effect



Exp.: Matveev *et al.*, Fiz. Met. Metalloved **53**, 34 (1982)

Spin-Hall-Effect



Lowitzer, Ködderitzsch, Ebert,
Phys. Rev Lett. **105**, 266604 (2010)

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

Lowitzer, Gradhand, Ködderitzsch, *et al.*
Phys. Rev. Lett. **106**, 056601 (2011)

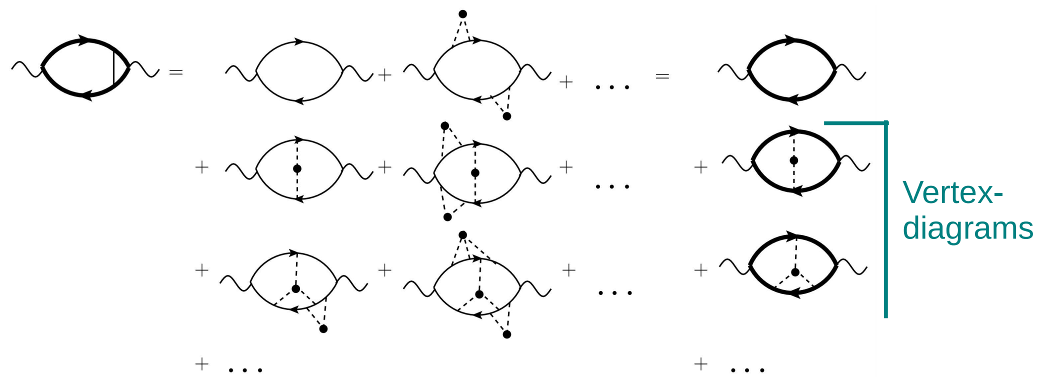
Classification of contributions

First-principles calculation:
KKR-GF-Kubo-Středa

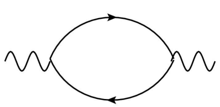
- intrinsic
  - calculation without vertex corrections
- extrinsic
  - with vertex corrections
  - assume scaling
  - extract values

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

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



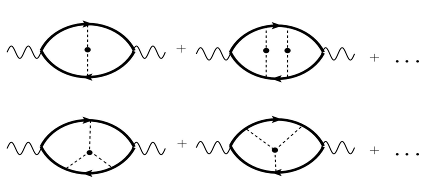
intrinsic

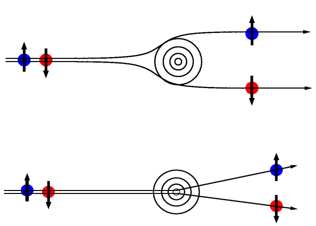


extrinsic

side-jump

skew



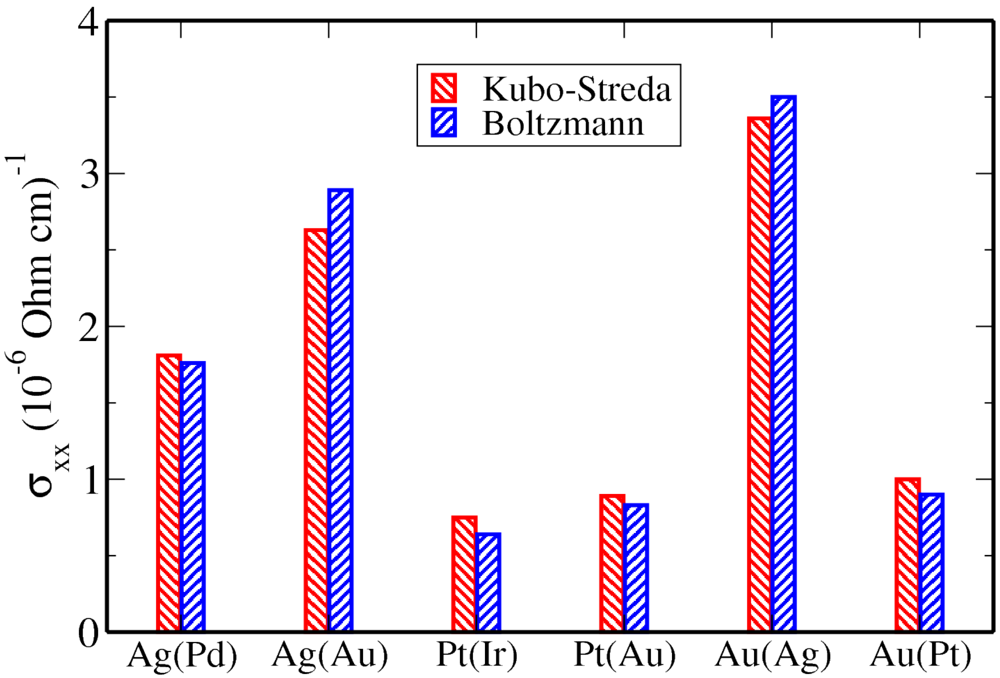


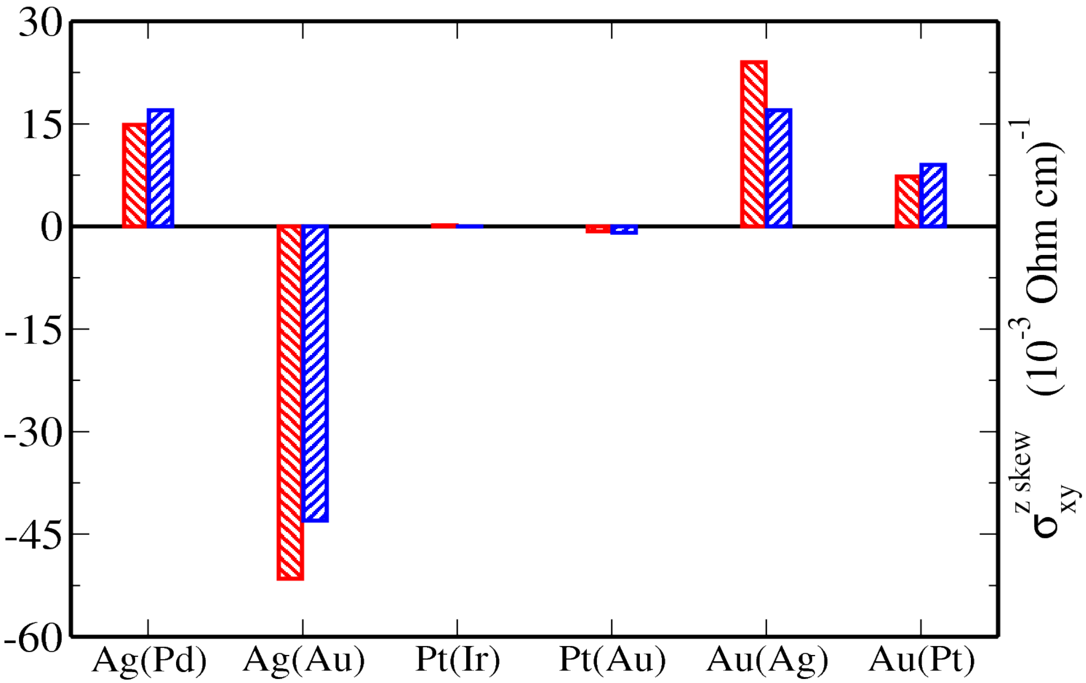
Crepieux, Bruno, PRB **64**, 014416 (2001)

SHE: Kubo-Středa vs. Boltzmann-Formalism

Comparison of results for
(impurity concentration 1%)

longitudinal conductivity σ_{xx} skew scattering $\sigma_{xy}^{z,\mathrm{skew}}$





Boltzmann-based calculations:
Collaboration with Gradhand, Fedorov, Mertig Uni Halle-Wittenberg

Lowitzer, Gradhand, Ködderitzsch, *et al.*
Phys. Rev. Lett. **106**, 056601 (2011)

Summary

First-principles, parameter-free, material specific electronic structure determination

- Spin-density-functional theory
- KKR-Green function method
- Disorder (CPA)
- relativistic effects

Transport formalisms

- Boltzmann
  - semi-classical
  - dilute alloys
- Kubo(-Středa)
  - full quantum mechanical

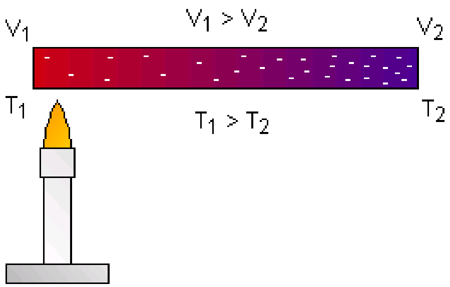
Transport phenomena

- Longitudinal
  - conductivity
  - spin-decomposition
  - AMR
  - Seebeck
- Transverse
  - Spin-Hall
  - Anomalous Hall
  - Spin-Nernst
  - Anomalous Nernst

Thermogalvanic transport

Thermogalvanic coefficients

Flashback: talk by Ch. Heiliger (yesterday)



$$S = \frac{V}{\triangle T}$$

$$\vec{E} = S\vec{\nabla}T$$

Seebeck effect

Thomas J. Seebeck
(1770-1831)

Electrical and thermal current in linear response theory

$$\begin{aligned} \vec{j}^{1}_{\mu} &= L^{11}_{\mu\nu}[-(1/T)\nabla_{\nu}(\mu + eV)] + L^{12}_{\mu\nu}\nabla_{\nu}(1/T) \\ \vec{j}^{2}_{Q,\mu} &= L^{21}_{\mu\nu}[-(1/T)\nabla_{\nu}(\mu + eV)] + L^{22}_{\mu\nu}\nabla_{\nu}(1/T)) \end{aligned}$$

Response functions by Kubo formulas in Matsubara notation

$$L^{ij}(i\omega) = -\frac{iT}{(i\omega)d\Omega}\int_0^{\beta} d\tau e^{i\omega\tau}\langle T_{\tau}\vec{j}^{i}(\tau)\vec{j}^{j}(0)\rangle$$

Jonson & Mahan, PRB **21**, 4223 (1980); Kontani, PRB 67, 014408 (2003)

Thermogalvanic coefficients via Mott's rule

- for constant μ: $\sigma = \frac{e^2 L^{11}}{T}$, $S = \frac{1}{eT}\frac{L^{12}}{L^{11}}$
- S from integral (T-dependence via Fermi distr.)

$$S = \frac{1}{eT}\frac{\int dE(E-\mu)\sigma(E)(-\frac{df}{dE})}{\int dE\sigma(E)(-\frac{df}{dE})} \xrightarrow[\text{(low T)}]{\text{Sommerfeld}} S = \frac{\pi^2 k_B^2 T}{3e}\left.\frac{d\ln\sigma(E)}{dE}\right|_{E_F}$$

Mott's formula for the thermoelectric power
with conductivity calculated via Kubo-Středa

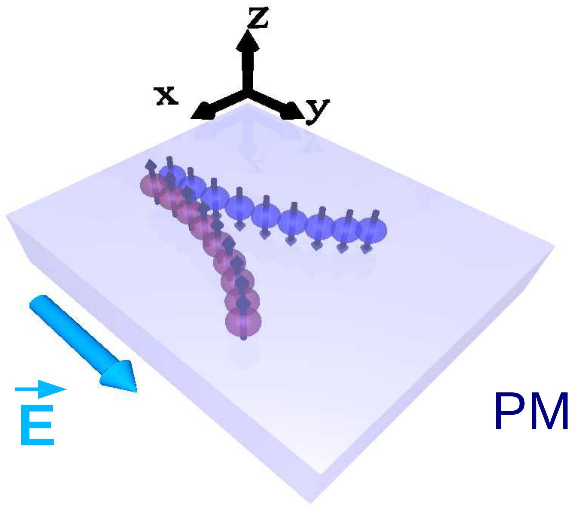
- Seebeck (diagonal) $S_{ii} \propto \frac{1}{\sigma_{ii}(E_F)}\left.\frac{d\sigma_{ii}(E)}{dE}\right|_{E_F}$
- Anomalous Nernst conductivity (off-diagonal)

Variation of $\underline{\underline{\sigma}}$ at Fermi energy

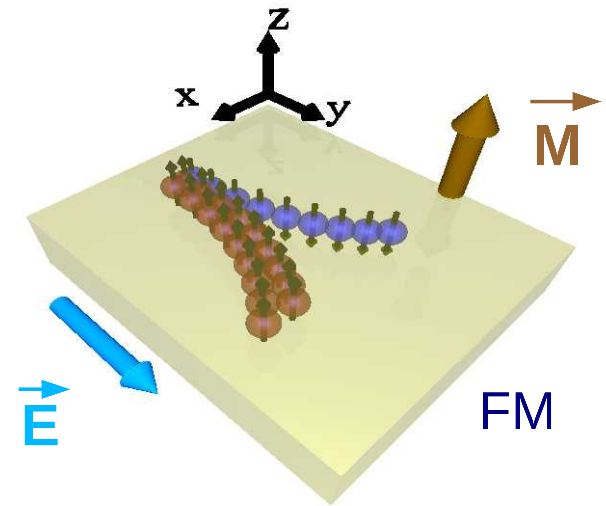
$$\underline{\underline{S}} = \underline{\underline{\sigma}}^{-1}\,\underline{\underline{\alpha}} \qquad \alpha_{ij} \propto \left.\frac{d\sigma_{ij}(E)}{dE}\right|_{E_F}$$

Thermogalvanic coefficients – nomenclature

Spin Hall Effect (SHE)

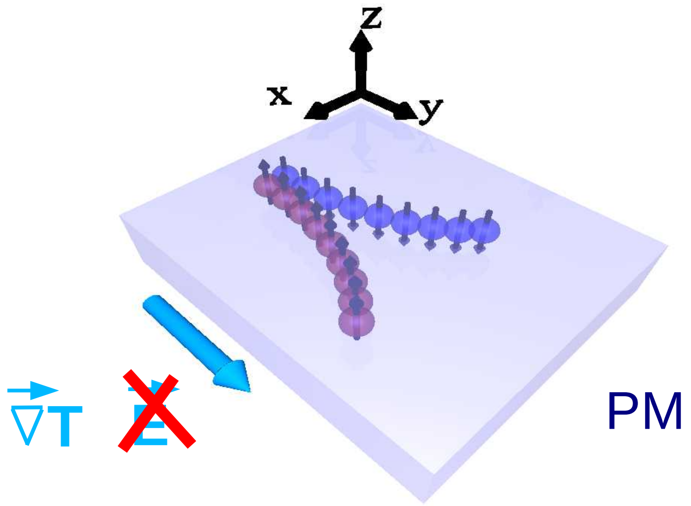


Anomalous Hall Effect (AHE)

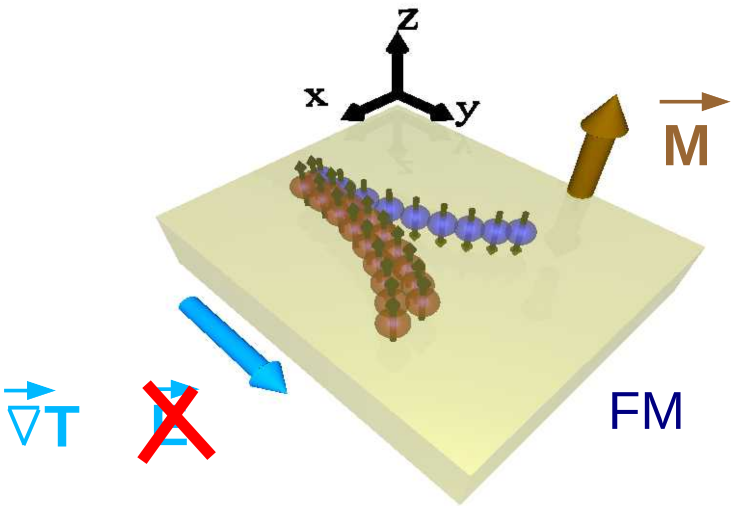


Thermogalvanic coefficients – nomenclature

Spin ~~Hall~~ Effect (SHE) Nernst



Anomalous ~~Hall~~ Effect (AHE) Nernst

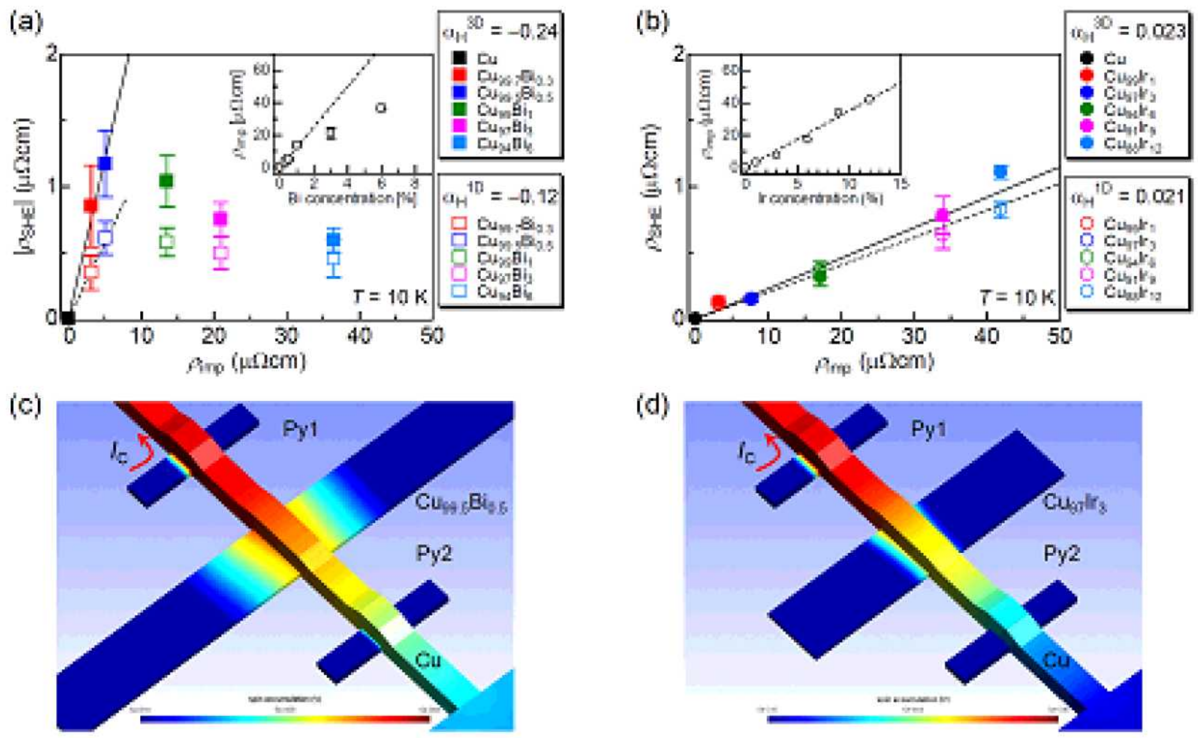


	H≠0 M=0	H=0 M≠0	H=0 M=0
$\vec{E}$	Hall effect	AHE	SHE
∇T	Nernst effect	ANE	SNE

Spin-Hall Effect for Cu-Ir and Cu-Bi

Spin-Hall resistivity versus longitudinal resistivity

Cu-Bi Cu-Ir



Niimi et al., PRL, accepted (2012)

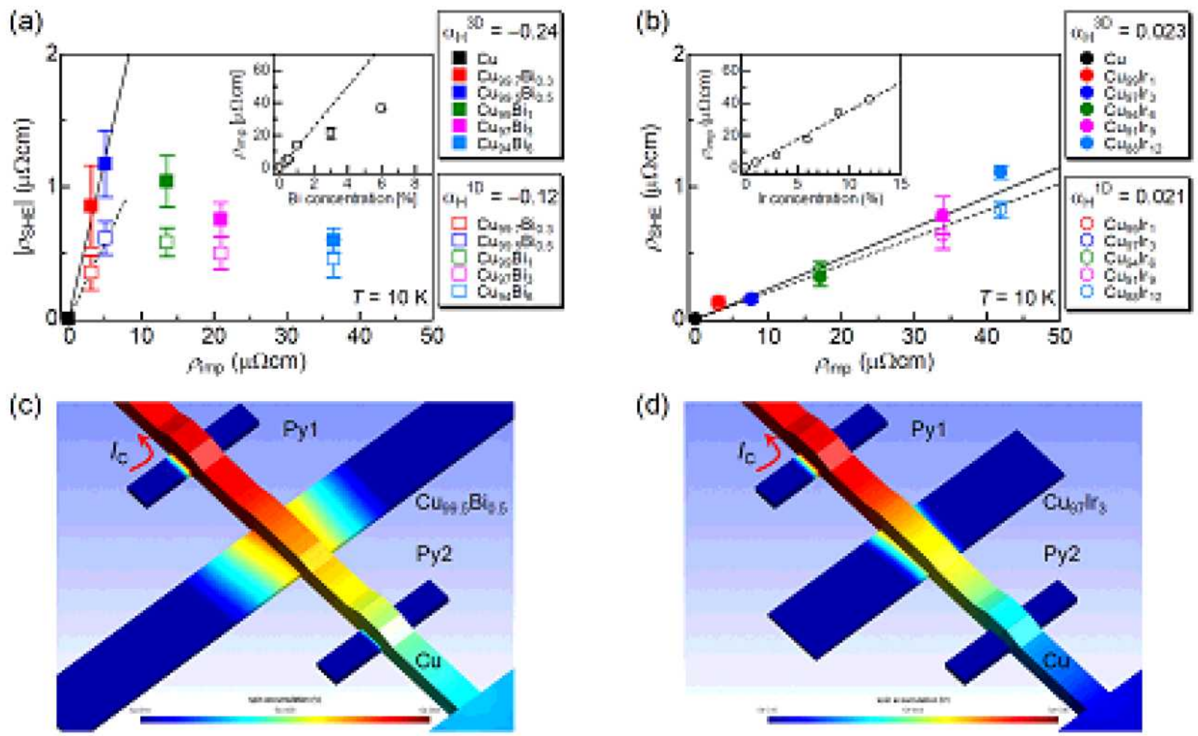
Gigantic SHE

Spin Hall angle $S_{exp} = \frac{\sigma_{yx}}{\sigma_{xx}} = -0.24$

Spin-Hall Effect for Cu-Ir and Cu-Bi

Spin-Hall resistivity versus longitudinal resistivity

Cu-Bi Cu-Ir



Spin Nernst?

Niimi et al., PRL, accepted (2012)

Gigantic SHE

Spin Hall angle $S_{exp} = \frac{\sigma_{yx}}{\sigma_{xx}} = -0.24$

Spin dependent thermogalvanic coefficients

- Linear transport coefficients: $L_n^{\uparrow} = \int dE(E-\mu)^n \sigma^{\uparrow}(E)(-\frac{df}{dE})$
- Spin-dependent thermopowers $\frac{\nabla\mu^{\uparrow}}{T} = S^{\uparrow} = \frac{1}{eT}(L_0^{\uparrow})^{-1}L_1^{\uparrow}$
- Charge Seebeck coefficient $S = \frac{1}{2}(S^{\uparrow} + S^{\downarrow})$
- Spin-polarised Seebeck coefficient: $S^{sp} = \frac{1}{2}(S^{\uparrow} - S^{\downarrow})$

  off-diagonal component: $S^{sp}_{yx} = \frac{1}{eT}\frac{L^{\uparrow}_{0,xx}L^{\uparrow}_{1,yx} - L^{\uparrow}_{0,yx}L^{\uparrow}_{1,xx}}{(L^{\uparrow}_{0,xx})^2 + (L^{\uparrow}_{0,yx})^2}$

  describes the spin accumulation transverse to a temperature gradient

- Spin Nernst conductivity

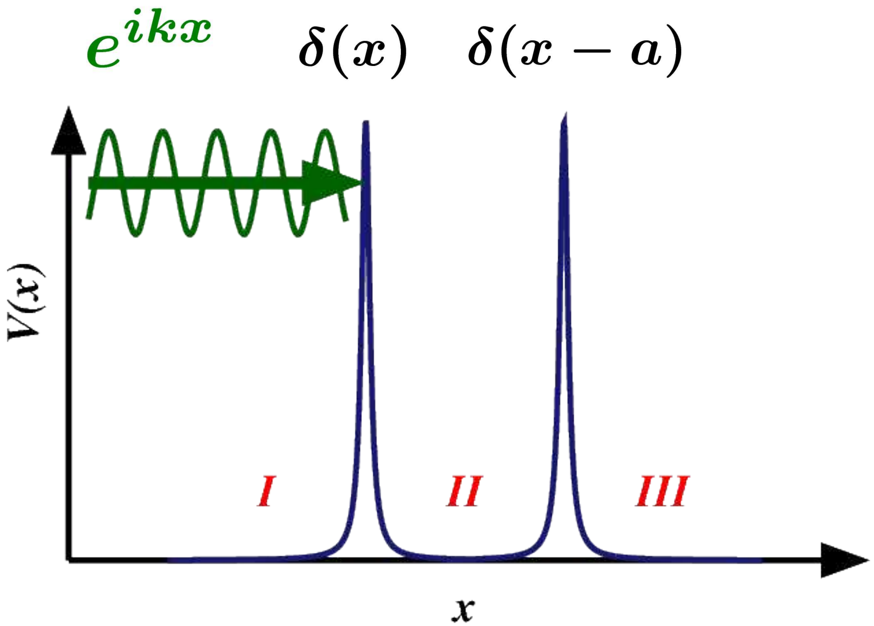
See talk Sebastian Wimmer

$$j_y^{sp} = \sigma_{SN}\nabla_x T$$

$$\sigma_{SN} = \sigma^E_{SN} + \sigma^T_{SN} = -2eS_{xx}L^{\uparrow}_{0,yx} - \frac{2}{T}L^{\uparrow}_{1,yx}$$

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

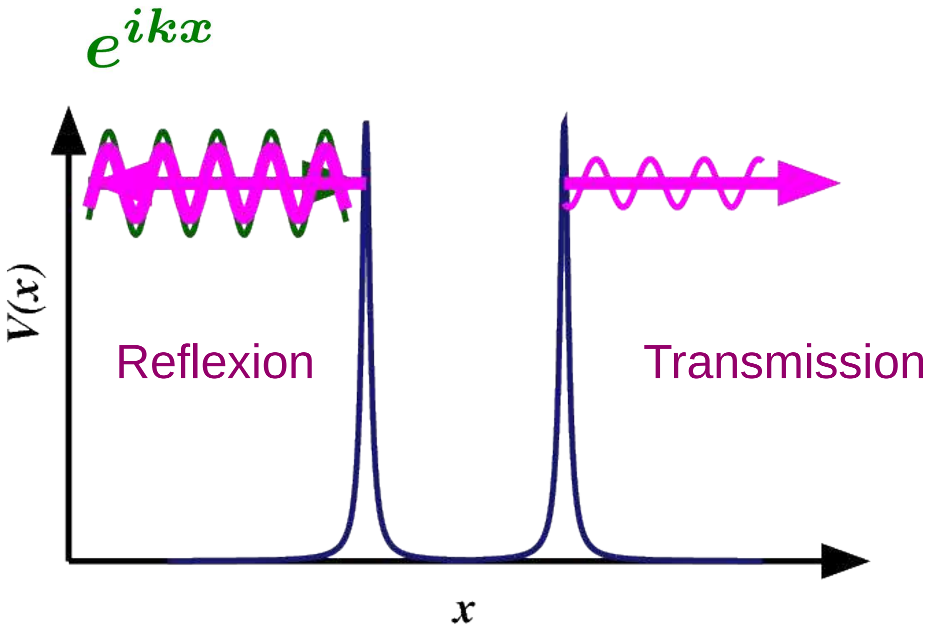
Vielfachstreutheorie



Doppel-Delta-Barriere

- Traditionelle Lösung
  - Schrödingergleichung in ***I,II,III***
  - Wellenfunktion anpassen
  - Gleichungssystem lösen

Vielfachstreutheorie



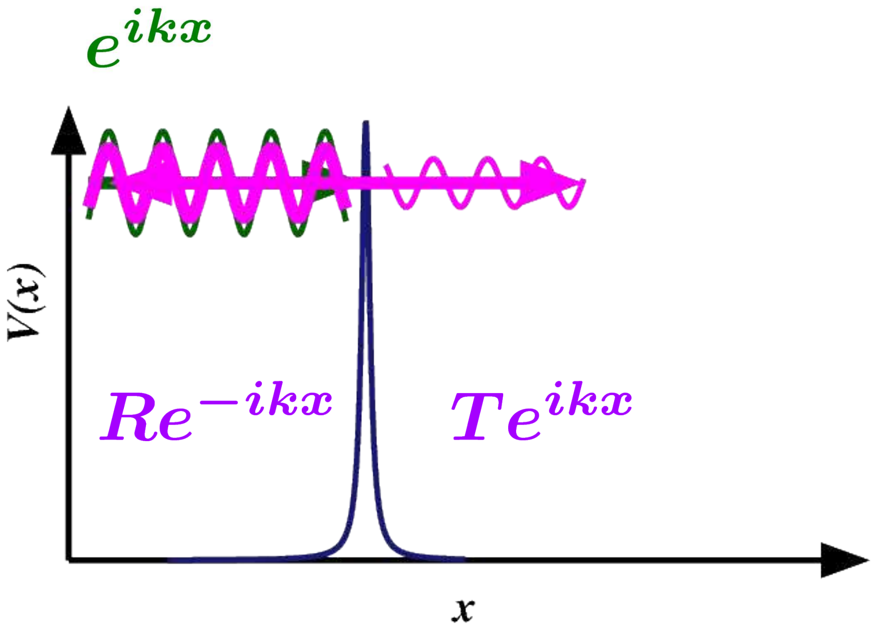
- Traditionelle Lösung
  - Schrödingergleichung: ***I,II,III***
  - Wellenfunktion anpassen
  - Gleichungssystem lösen

Ist es möglich, aus den Eigenschaften der Einzelbarrieren die Lösung zu bestimmen ?

Ja!

Alternative: Vielfachstreuung und Greensche Funktion

Vielfachstreutheorie und Greensche Funktion G



$$G_0(x,x') = \frac{\frac{2m}{\hbar^2} e^{ik|x-x'|}}{2ik}$$

t – Matrix Operator

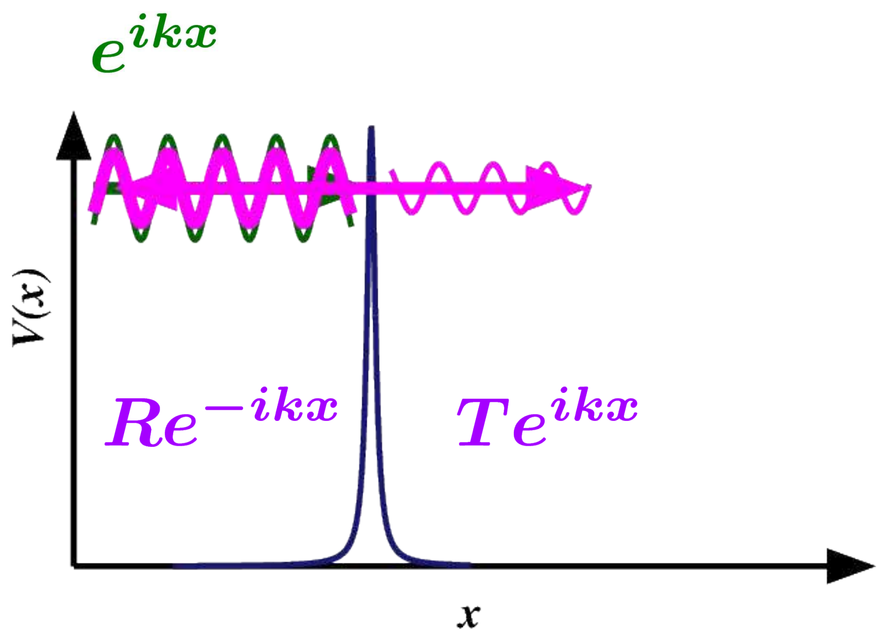
$$\hat{t} = \hat{v}(1 + \hat{G}_0 \hat{t}) \qquad (*)$$

$$|\psi\rangle = |k\rangle + \hat{G}_0 \hat{t} |k\rangle$$

Greensche Funktion ohne Barriere (Potential)

$$\hat{G}_0 = \lim_{\varepsilon \to 0} \frac{1}{E + i\varepsilon - \hat{H}_0}$$

Vielfachstreutheorie und Greensche Funktion G



$$G_0(x,x') = \frac{\frac{2m}{\hbar^2} e^{ik|x-x'|}}{2ik}$$

t – Matrix Operator

$$\hat{t} = \hat{v}(1 + \hat{G}_0 \hat{t}) \qquad (*)$$

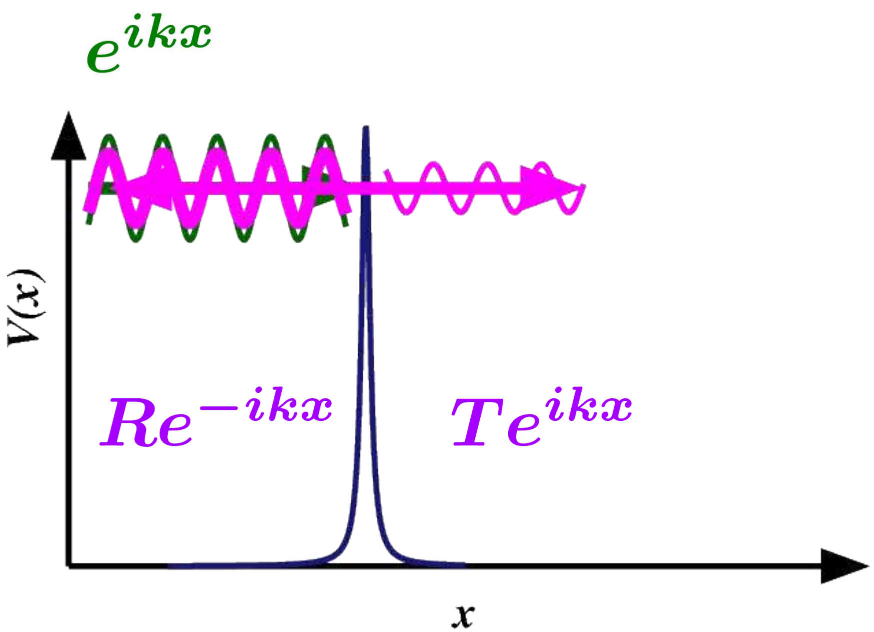
$$|\psi\rangle = |k\rangle + \hat{G}_0 \hat{t} |k\rangle$$

Greensche Funktion ohne Barriere (Potential)

$$\hat{G}_0 = \lim_{\varepsilon \to 0} \frac{1}{E + i\varepsilon - \hat{H}_0}$$

Iteriere (*) → $\hat{t}$ → $|\psi\rangle$ → Reflexion R, Transmission T

Vielfachstreutheorie und Greensche Funktion G



$$G_0(x,x') = \frac{\alpha e^{ik|x-x'|}}{2ik}$$

t – Matrix Operator

$$\hat{t} = \hat{v}(1 + \hat{G}_0\hat{t}) \qquad (*)$$

$$|\psi\rangle = |k\rangle + \hat{G}_0\hat{t}|k\rangle$$

Greensche Funktion ohne Barriere (Potential)

$$\hat{G}_0 = \lim_{\varepsilon\to 0} \frac{1}{E + i\varepsilon - \hat{H}_0}$$

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Äquivalent: Konstruktion der Greenschen Funktion $\hat{G}$ des Systems mit Barriere

Vielfachstreutheorie und Greensche Funktion G

Äquivalent: Konstruktion der Greenschen Funktion $\hat{G}$ des Gesamtsystems

↓

Erwartungswert einer Einteilchenobservable (Operator $\mathcal{A}$)

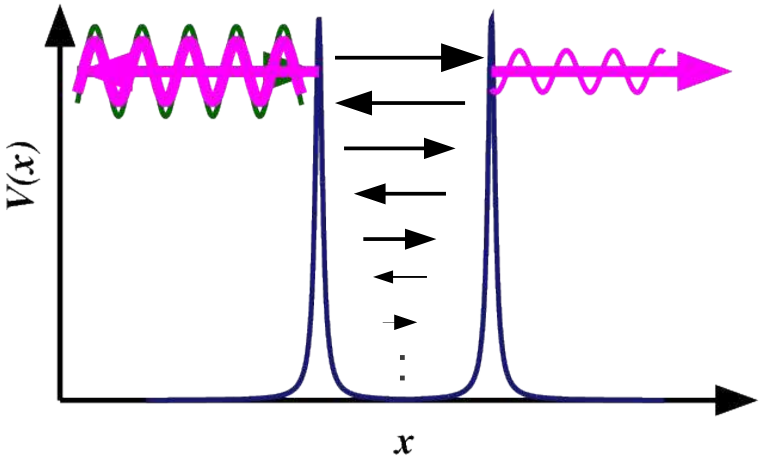
$$\langle \mathcal{A} \rangle = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{\infty} f_{\mathrm{FD}}(E)\ \mathcal{A}\ \hat{G}(E)$$

Dyson–Gleichung

Greensche Funktion des Gesamtsystems

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}$$

Vielfachstreutheorie und Greensche Funktion



$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}$$
$$= \hat{G}_0 + \hat{G}_0 \hat{T} \hat{G}_0$$

$$\begin{aligned}
\hat{T} = \; & \hat{t}_1[1 + \hat{G}_0\hat{t}_2\hat{G}_0\hat{t}_1 + (\hat{G}_0\hat{t}_2\hat{G}_0\hat{t}_1)^2 + \ldots] \\
& + \hat{t}_2[1 + \hat{G}_0\hat{t}_1\hat{G}_0\hat{t}_2 + (\hat{G}_0\hat{t}_1\hat{G}_0\hat{t}_2)^2 + \ldots] \\
& + \hat{t}_1\hat{G}_0\hat{t}_2[1 + \hat{G}_0\hat{t}_2\hat{G}_0\hat{t}_1 + (\hat{G}_0\hat{t}_2\hat{G}_0\hat{t}_1)^2 + \ldots] \\
& + \hat{t}_2\hat{G}_0\hat{t}_1[1 + \hat{G}_0\hat{t}_1\hat{G}_0\hat{t}_2 + (\hat{G}_0\hat{t}_1\hat{G}_0\hat{t}_2)^2 + \ldots] \\
= \; & \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \hat{T}_4 \\
= \; & \sum_{mn} \hat{\tau}^{mn}
\end{aligned}$$

Streupfadoperator

Dyson–Gleichung

$\hat{H}_0$ Referenzsystem

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}$$

$$\hat{H} = \hat{H}_0 + V$$

Vielfachstreudarstellung von G in der KKR

$$\hat{H}^{\mathrm{Dirac}} = c\alpha \cdot \vec{p} + \beta m c^2 + \bar{V} + \Sigma \cdot B$$

$$\updownarrow$$

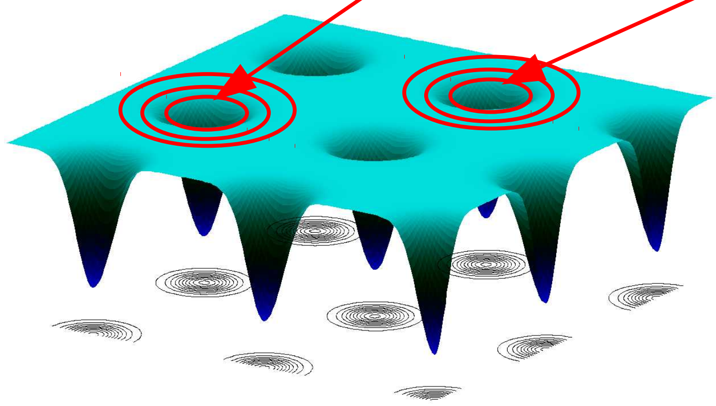
$$G^{+}(\vec{r},\vec{r}\,',E) = G^{+,\mathrm{irr}}_{nn}(\vec{r},\vec{r}\,',E) + \sum_{\Lambda\Lambda'} Z^{n}_{\Lambda}(\vec{r},E)\,\tau^{nm}_{\Lambda\Lambda'}(E)\,Z^{m\times}_{\Lambda'}(\vec{r}\,',E)$$

Vielfachstreudarstellung von G in der KKR

$$\hat{H}^{\text{Dirac}} = c\alpha \cdot \vec{p} + \beta m c^2 + \bar{V} + \Sigma \cdot B$$

$\Updownarrow$

$$G^{+}(\vec{r},\vec{r}\,',E) = G^{+,\text{irr}}_{nn}(\vec{r},\vec{r}\,',E) + \sum_{\Lambda\Lambda'} Z^{n}_{\Lambda}(\vec{r},E)\, \tau^{nm}_{\Lambda\Lambda'}(E)\, Z^{m\times}_{\Lambda'}(\vec{r}\,',E)$$



Muffin-Tin-Potenzial

numerische,
relativistische
Radialwellen
&
rel. Spin-Winkel-Funktionen

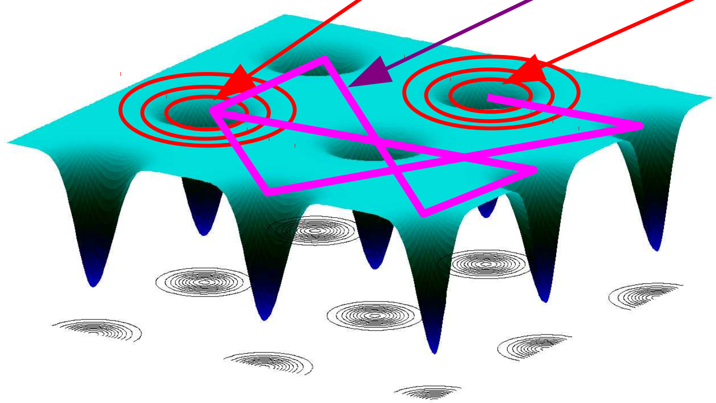
Vielfachstreudarstellung von G in der KKR

$$\hat{H}^{\text{Dirac}} = c\boldsymbol{\alpha}\cdot\vec{p} + \beta mc^2 + \bar{V} + \boldsymbol{\Sigma}\cdot\boldsymbol{B}$$

↕

Streupfadoperator

$$G^+(\vec{r},\vec{r}\,',E) = G^{+,\text{irr}}_{nn}(\vec{r},\vec{r}\,',E) + \sum_{\Lambda\Lambda'} Z^n_\Lambda(\vec{r},E)\,\tau^{nm}_{\Lambda\Lambda'}(E)\,Z^{m\times}_{\Lambda'}(\vec{r}\,',E)$$



Muffin-Tin-Potenzial

numerische,
relativistische
Radialwellen
&
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Vielfachstreudarstellung

$$
\begin{aligned}
G^{+}(\vec{r},\vec{r}\,',E) &= \sum_{\Lambda\Lambda'} Z^{n}_{\Lambda}(\vec{r},E)\,\tau^{nm}_{\Lambda\Lambda'}(E)\,Z^{m\times}_{\Lambda'}(\vec{r}\,',E) \\
&\quad -\delta_{nm}\sum_{\Lambda}\Big[Z^{n}_{\Lambda}(\vec{r},E)\,J^{n\times}_{\Lambda}(\vec{r}',E)\theta(r'_n-r_n) \\
&\qquad +J^{n}_{\Lambda}(\vec{r},E)\,Z^{n\times}_{\Lambda}(\vec{r}',E)\theta(r_n-r'_n)\Big]
\end{aligned}
$$