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Linear response functions for finite temperatures on the basis of the alloy analogy model

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Deutsche Forschungsgemeinschaft DFG

SFB689

Finite temperature transport

KKR Green function based calculation of the **response function** within the **Kubo formalism**

$$\chi_{\mu\nu} \sim Trace\left\langle \hat{O}_\mu \Im G^+(E_F) \hat{O}_\nu \Im G^+(E_F) \right\rangle$$

- Transport: $\hat{O}_\mu = \hat{j}_\mu \rightarrow \chi_{\mu\nu} = \sigma_{\mu\nu}$
- Gilbert damping: $\hat{O}_\mu = \hat{T}_\mu \rightarrow \chi_{\mu\nu} = \alpha_{\mu\nu}$

$\langle \dots \rangle$ - **thermal average** over temperature-induced **spin fluctuations and lattice vibrations**

Retarded Green function

$$G^+(\vec{r},\vec{r}',E) = \sum_{\Lambda\Lambda'} Z^m_\Lambda(\vec{r},E)\tau^{mn}_{\Lambda\Lambda'}(E)Z^{n\times}_{\Lambda'}(\vec{r}',E) - \delta_{mn}\sum_\Lambda Z^n_\Lambda(\vec{r},E)J^{n\times}_{\Lambda'}(\vec{r}',E)\Theta(r'_n - r_n) + J^n_\Lambda(\vec{r},E)Z^{n\times}_{\Lambda'}(\vec{r}',E)\Theta(r_n - r'_n)$$

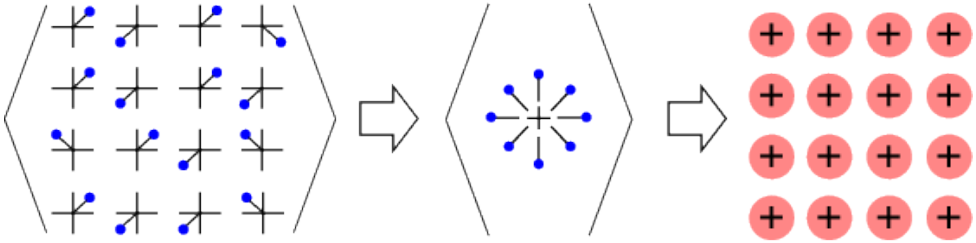
T≠0: configurational average via CPA

Lattice vibrations: alloy analogy model

- lattice vibrations are localized on atomic sites and non-correlated
- lattice vibrations are slow → **adiabatic approximation**

- t-matrix transformation $\underline{t}_v(\vec{s}_v) = \underline{U}(\vec{s}_v)\underline{t}_0\underline{U}^{-1}(\vec{s}_v)$

Thermal average → configurational average via CPA



Linear response: **configurational average** via CPA

$$\chi_{\mu\nu} \sim Trace \left\langle \hat{O}_\mu \Im G^+(E_F) \hat{O}_\nu \Im G^+(E_F) \right\rangle$$

requires vertex corrections (Butler, PRB 31, 3260 (1985)) to go beyond :

$$\chi_{\mu\nu} \sim Trace \left\langle \hat{O}_\mu \Im G^+(E_F) \right\rangle \left\langle \hat{O}_\nu \Im G^+(E_F) \right\rangle$$

Lattice vibrations

- displacement vectors $\vec{s}_v^{\,q}(T)$ with weighting factor $x_v = 1/N_v$

$$\sum_{v=1}^{N_v} x_v |\vec{s}_v^{\,q}(T)|^2 = \frac{1}{N_v} \sum_{v=1}^{N_v} |\vec{s}_v^{\,q}(T)|^2 = \langle u_q^2 \rangle_T$$

- Root mean square (rms) displacement: $(\langle u^2 \rangle_T)^{1/2}$
- rms displacement via phonon calculations

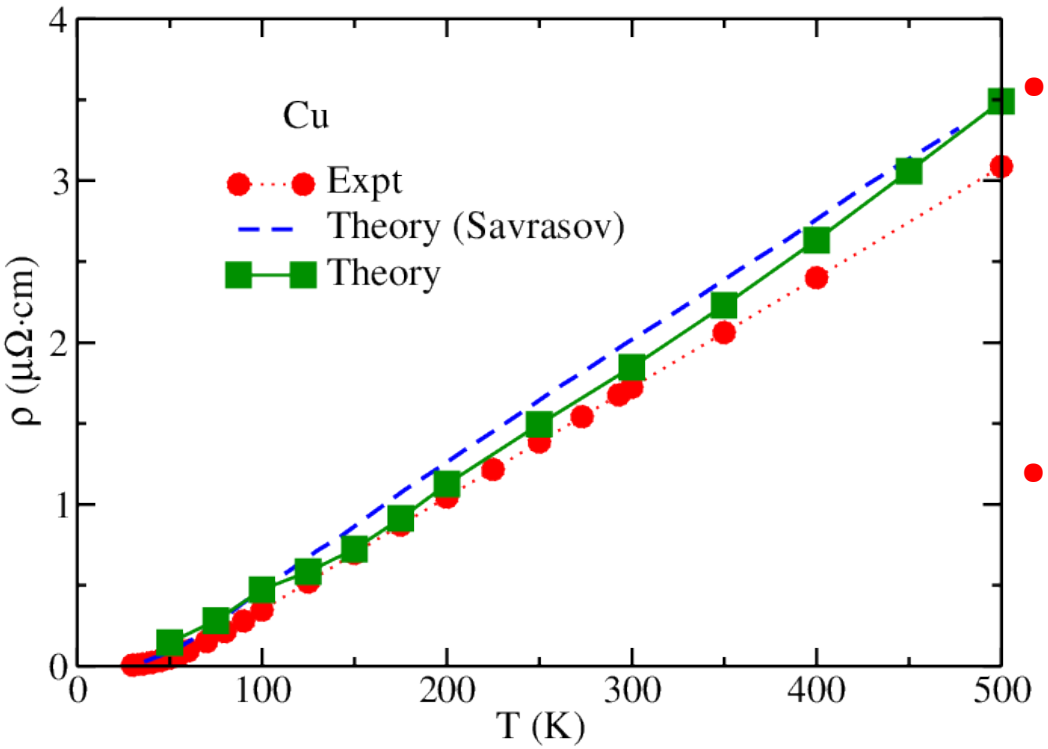
$$\langle u_{i,\mu}^2 \rangle_T = \frac{3\hbar}{2M_i} \int_0^\infty d\omega g_{i,\mu}(\omega) \frac{1}{\omega} \coth \frac{\hbar\omega}{2k_B T}$$

- Isotropic rms displacement obtained using Debye's theory

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

Resistivity due to thermal lattice vibrations

Cu resistivity vs temperature



Textbook: resistivity due to electron-phonon scattering

- $T >> \Theta_D$:
  - the vibration quantization - not important
  - electron scattering is proportional to the square of lattice displacements. This gives

$$\rho \sim T \quad (T >> \Theta_D)$$

- $T << \Theta_D$:
  - quantized lattice vibrations – phonons.
  - electron scattering on phonons:

$$\mathbf{k} + \mathbf{q} \leftarrow \mathbf{k}' \quad \text{or} \quad \mathbf{k} + \mathbf{q} \rightarrow \mathbf{k}'$$

  - this restriction results in

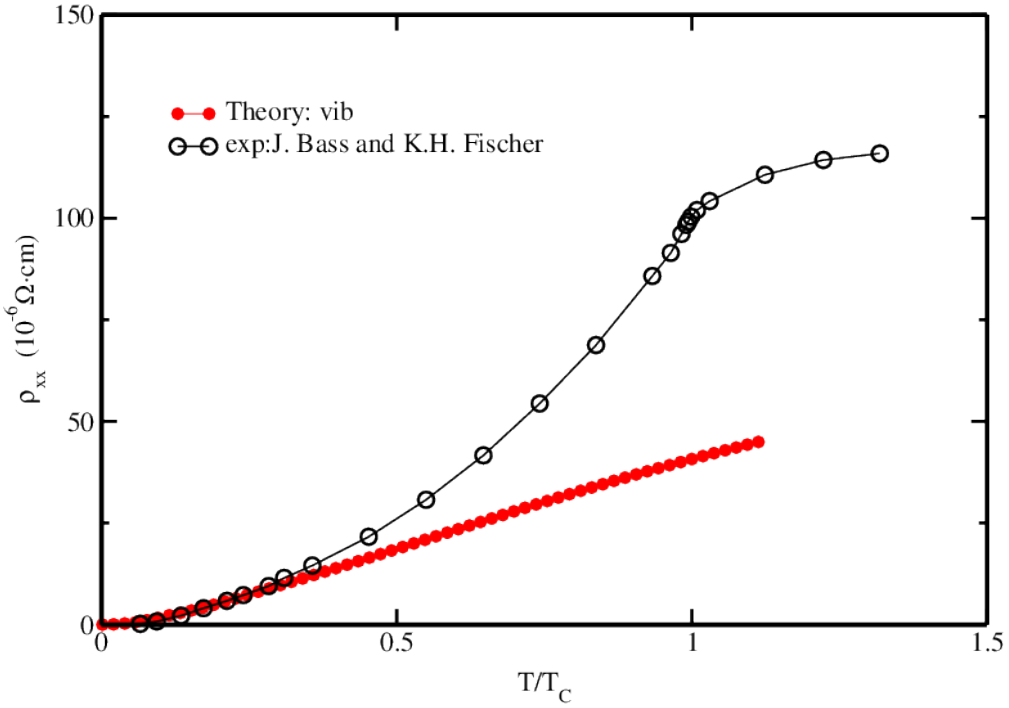
$$\rho \sim T^5 \quad (T << \Theta_D)$$

- **Intermediate T - ?**

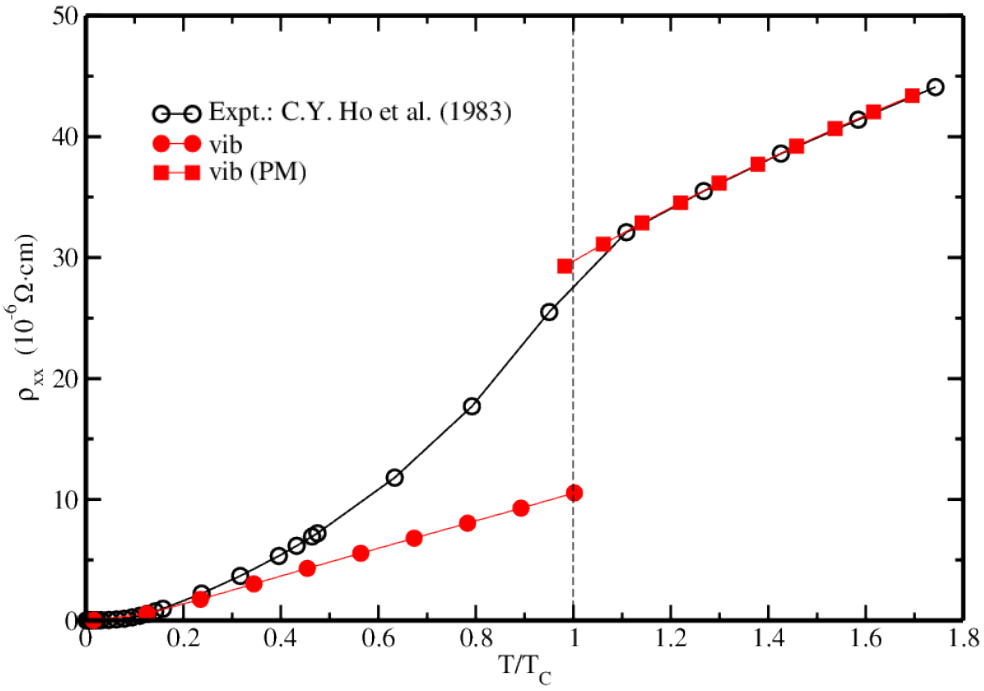
- Calculations: **Cu resistivity vs temperature linear down to $T < \Theta_D$**
  – in agreement with experiment

Fe: resistivity due to thermal lattice vibrations

Fe resistivity vs temperature



Ni resistivity vs temperature



- **FM** Fe, Ni: Strong discrepancy with the experiment at increasing temperature
- **PM** Ni: agreement between theory and experiment

Resistivity due to spin fluctuations

Magnetization vs temperature

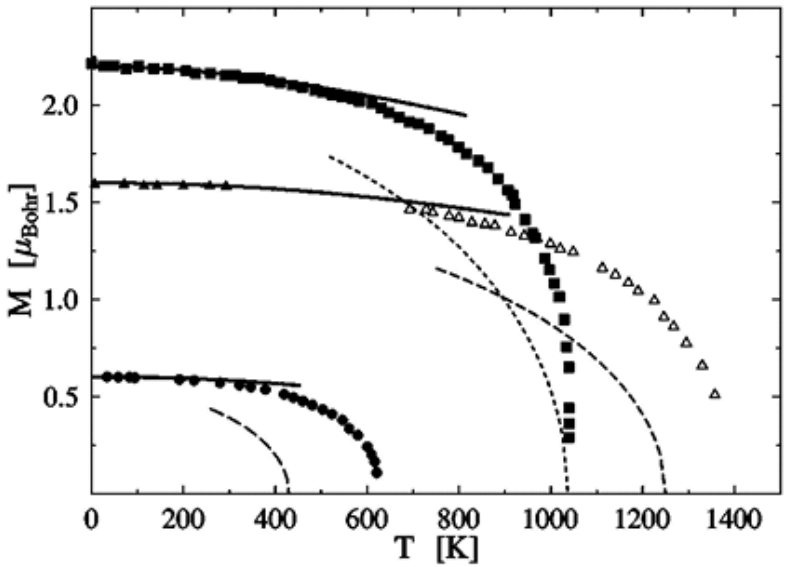


FIG. 8. Magnetization vs temperature of Fe [squares (Ref. 34)], Co [full triangles hcp (Ref. 35), open triangles fcc (Ref. 34)], and Ni [balls (Ref. 36)]. Solid lines: calculated from magnon spectra. Dashed lines: mean-field results.

Literature: resistivity due to electron-magnon scattering

- Low T << T_c:
  - quantized lattice vibrations – magnons.
  - electron scattering on magnons:

$$\mathbf{k}+\mathbf{q} \leftarrow \mathbf{k}' \quad \text{or} \quad \mathbf{k}+\mathbf{q} \rightarrow \mathbf{k}'$$

  - this restriction results in

$$\rho \sim T^2 \quad (T << T_C)$$

- High T ~ T_c:
  - s-d model
  - MFT for local magnetic moments

$$\rho \approx \frac{m^2 k_F N}{\pi n e^2 \hbar^3} \mathrm{J}^2 S(S+1)\left[1-\frac{|<M_S>|^2}{S(S+1)}\right] \quad (T \sim T_C)$$

- **Intermediate T - ?**

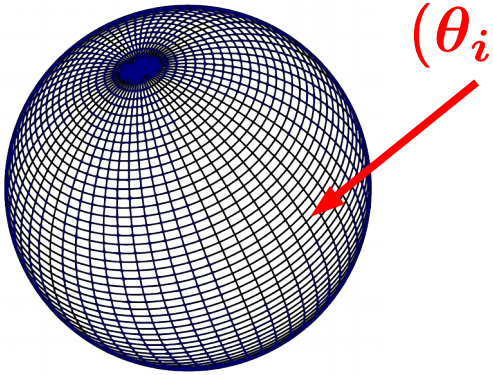
T≠0: configurational average via CPA

Spin moment fluctuations (MFA): alloy analogy model

Approximations

- spin fluctuations $\{\hat{e}_f\}$ are localized on atomic sites and non-correlated
- spin fluctuations are slow → **adiabatic approximation**

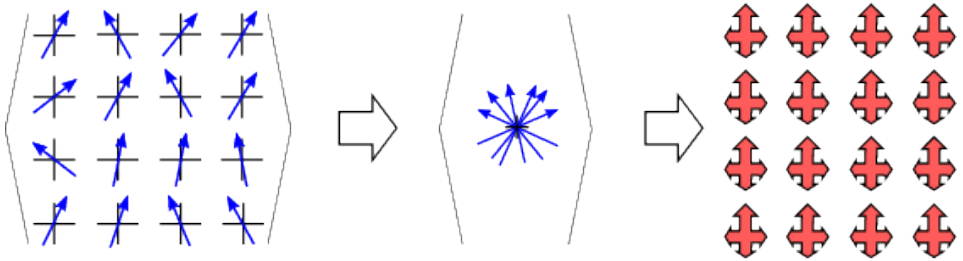
- Generate a grid on sphere (θ_i, ϕ_j) for directions of magnetic moments $\hat{e}_f(\theta,\phi)$



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

- for each direction $\hat{e}_f(\theta,\phi)$
  - t-matrix $\underline{t}_f(\hat{e}_f) = \underline{R}(\hat{e}_f)\underline{t}(\hat{z})\underline{R}^{-1}(\hat{e}_f)$
  - weighting factor at temperature *T* $x_f(\theta,\phi,T)$

- Thermal average → configurational average via CPA



T≠0: configurational average via CPA

Monte Carlo simulations => Mean Field approach

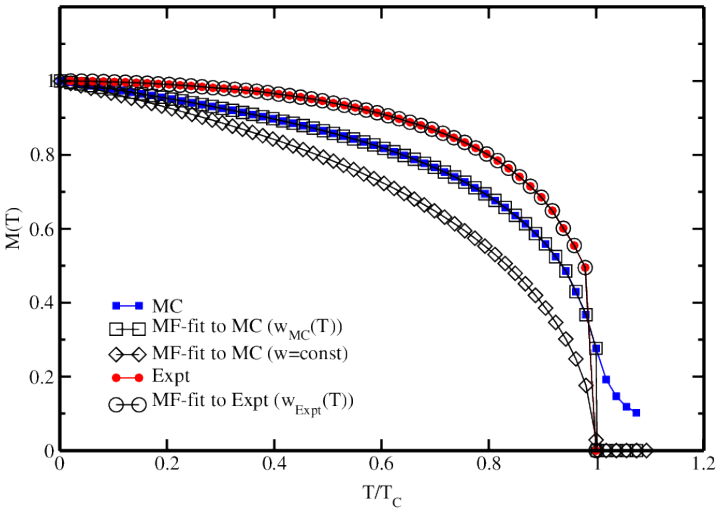
- Within MFA for each direction $\hat{e}_f(\theta,\phi)$ weighting factor at temperature T

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

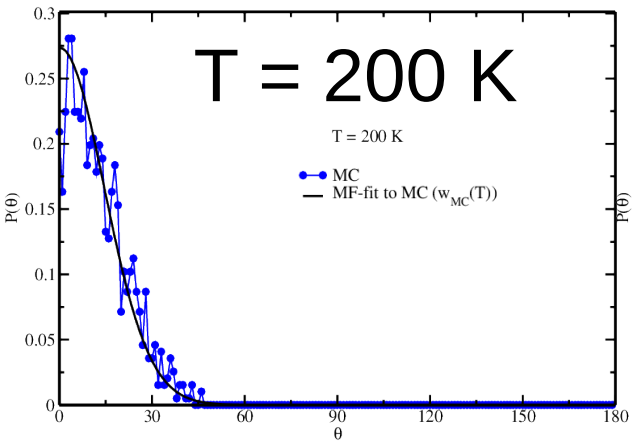
To use the results of MC simulations or experiment: $\lim_{w\to w(T)} M(T) = M_{MC}(T)$

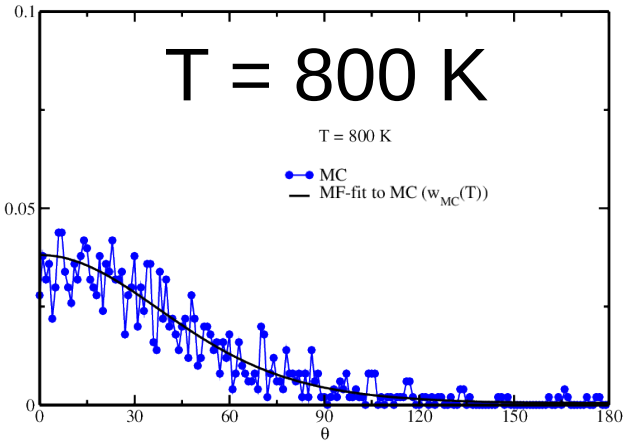
where $M(T) = L\left(\frac{wm_0^2M(T)}{k_{\mathrm{B}}T}\right)$ and Weiss field (**fitting**) parameter $w(T)$

$M(T)$



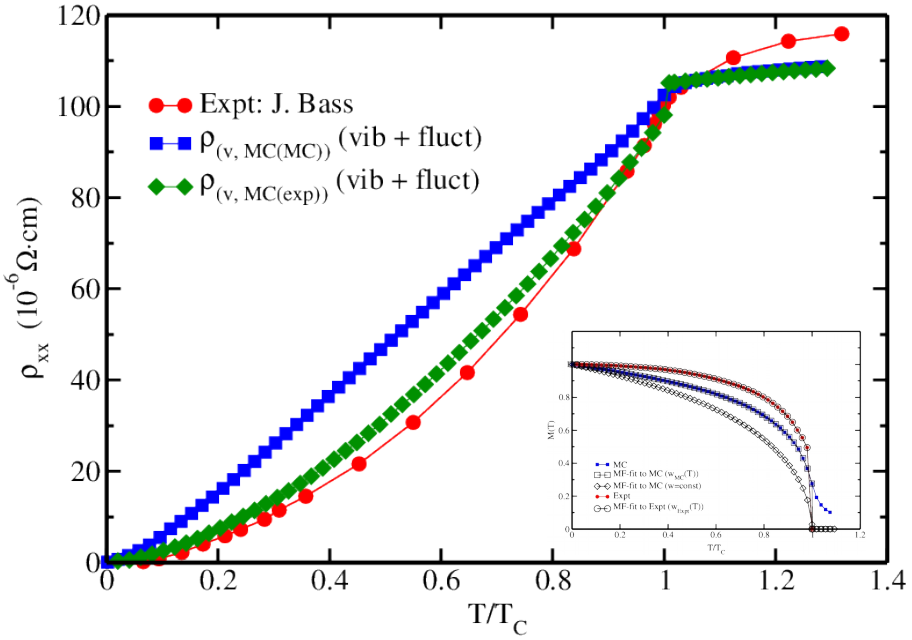
Angular distribution P(θ)



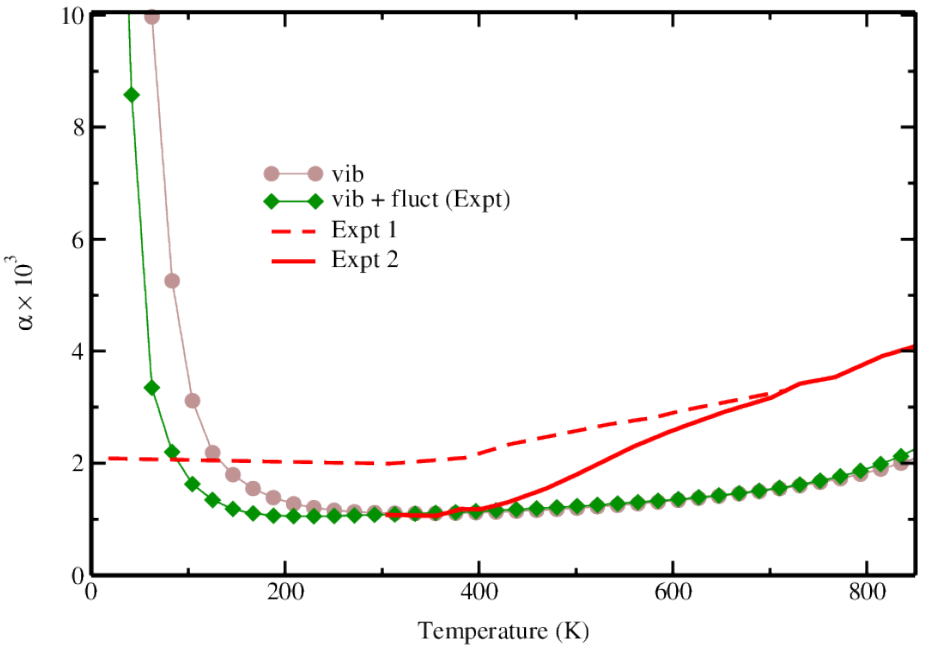


bcc Fe: effect of lattice and spin excitations

Fe bcc: resistivity vs temperature



Fe bcc: Gilbert damping vs temperature

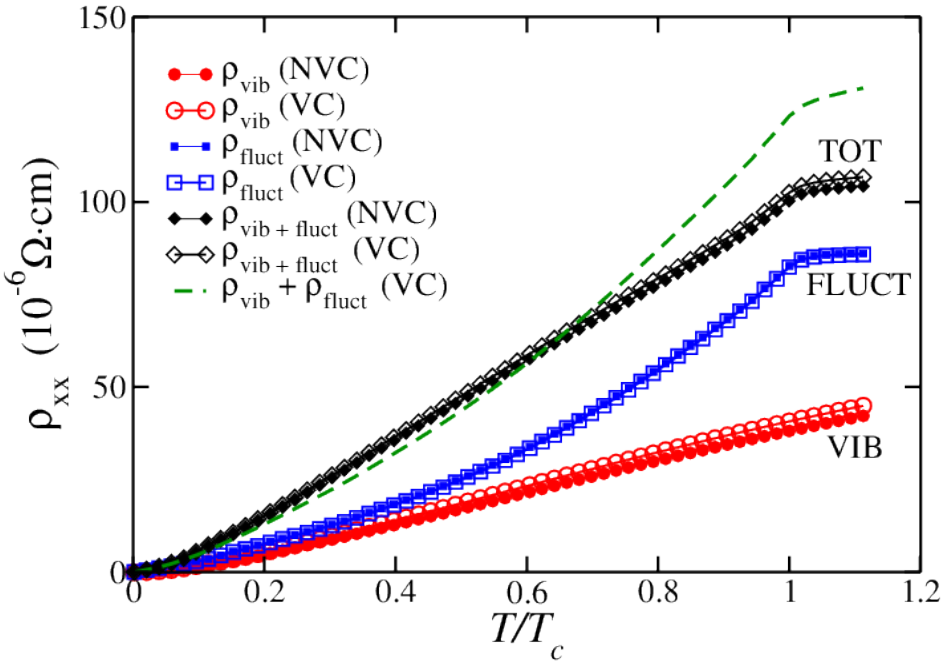


- **Monte Carlo** *M*(*T*): **magnetic fluctuation effect is overestimated**
- Crucial role of *M*(*T*) dependence → discrepancies between the resistivity results based on MC and experimental *M*(*T*)

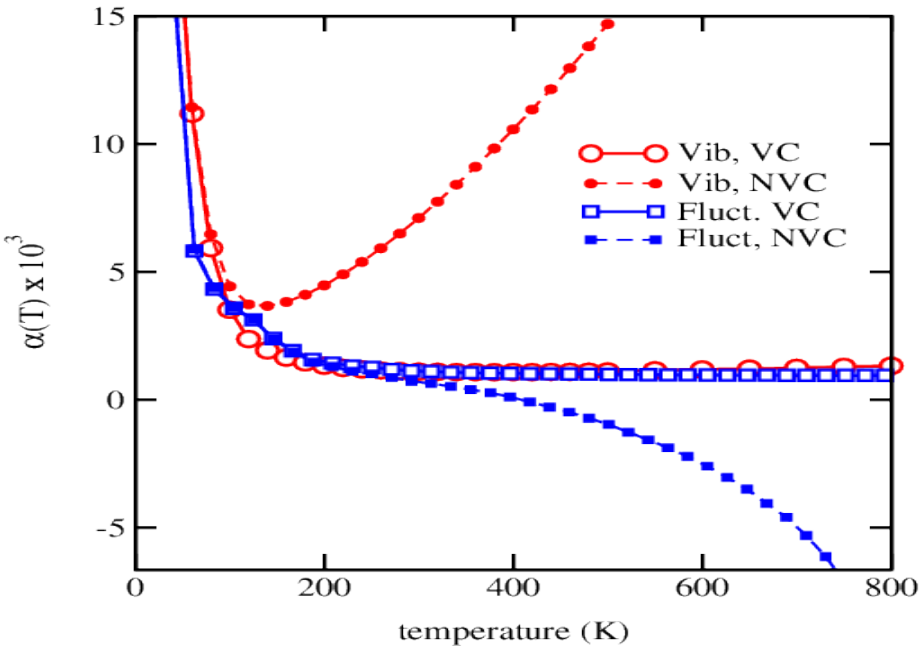
H. Ebert, S. Mankovsky, K. Chadova, S. Polesya, J. Minár, and D. Ködderitzsch, PRB **91**, 165132 (2015)

bcc Fe: effect of vertex corrections

Electrical resistivity vs T



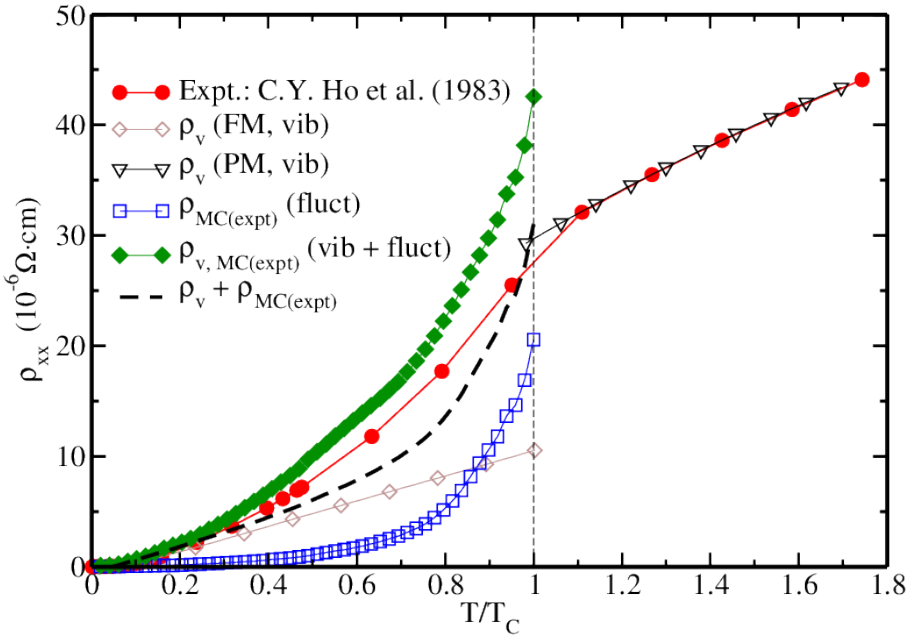
Gilbert damping vs T



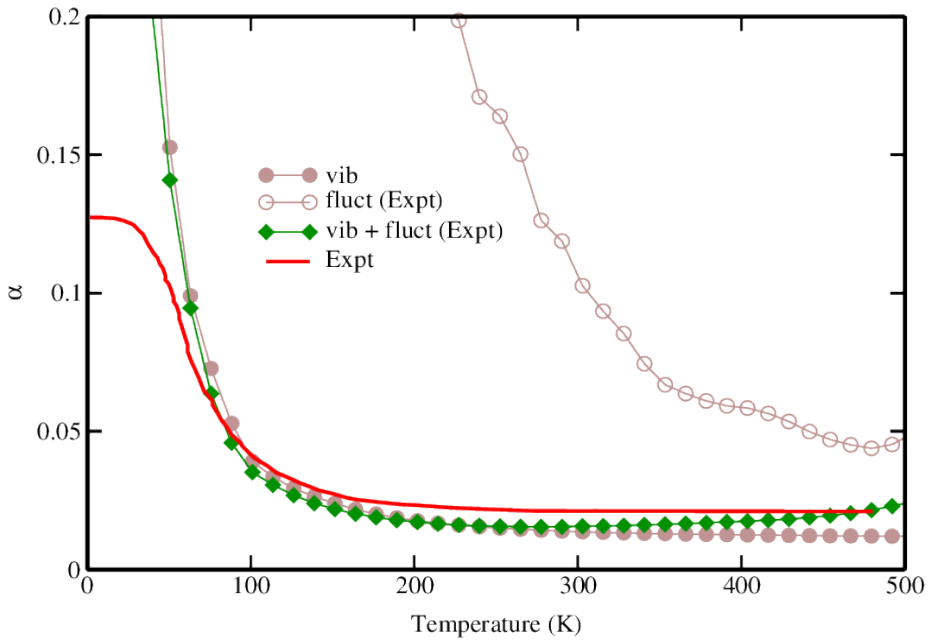
- Non-additive contributions of lattice vibrations and spin moment fluctuations
- Comparable contributions of lattice vibrations and spin fluctuations
- **Small effect** of vertex corrections for **resistivity**
- **Very strong effect** of vertex corrections for Gilbert damping at the increasing temperature

fcc Ni: effect of lattice and spin excitations

Ni fcc: resistivity vs temperature



Ni fcc: Gilbert damping vs temperature

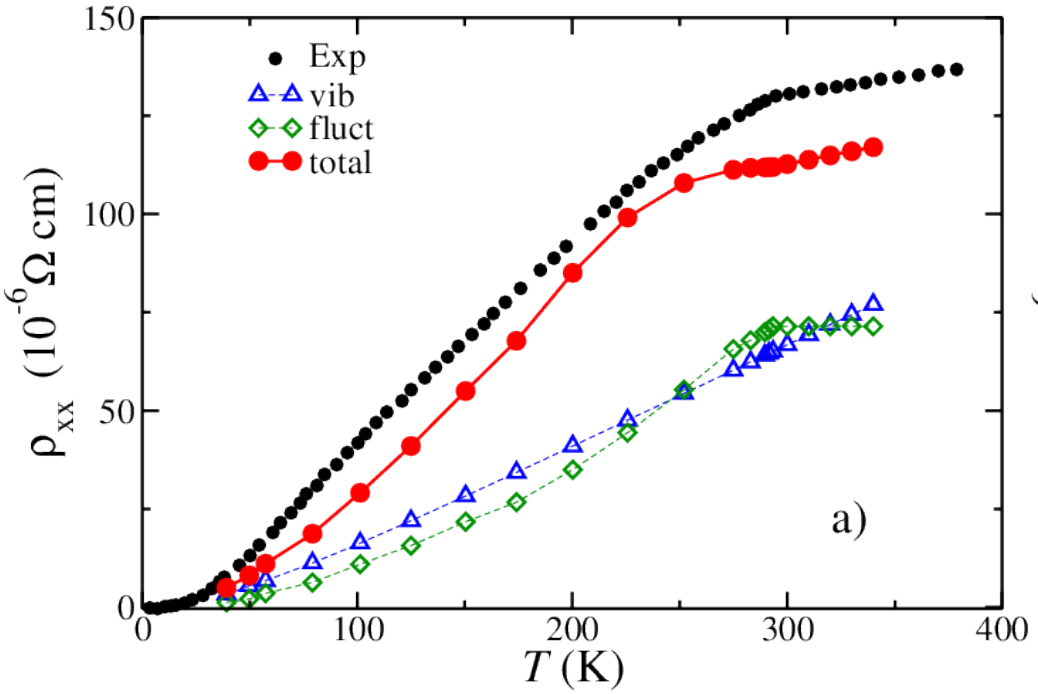


- Resistivity: Longitudinal fluctuations should be taken into account near T_C
- Gilbert damping: main contribution – from lattice vibrations

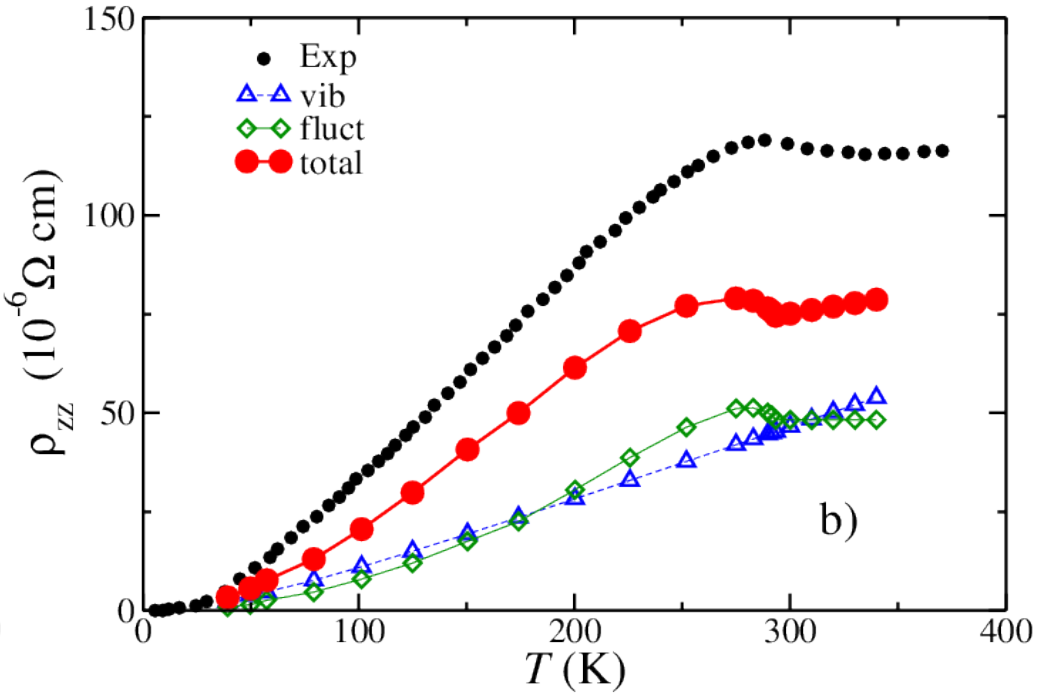
H. Ebert, S. Mankovsky, K. Chadova, S. Polesya, J. Minár, and D. Ködderitzsch, PRB **91**, 165132 (2015)

Gd: Resistivity contributions, M||(001)

$\rho_{xx}(T)$



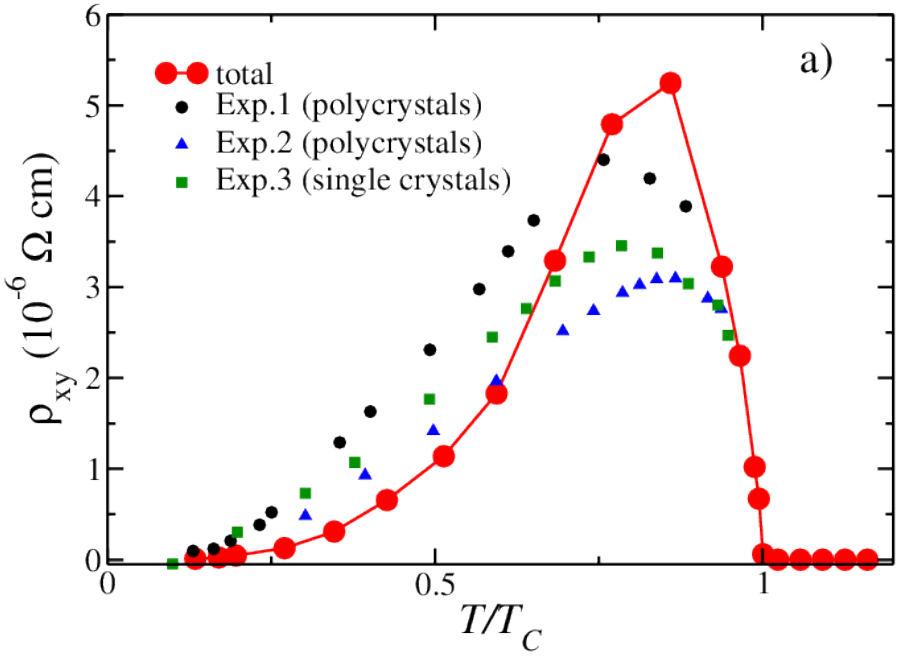
$\rho_{zz}(T)$



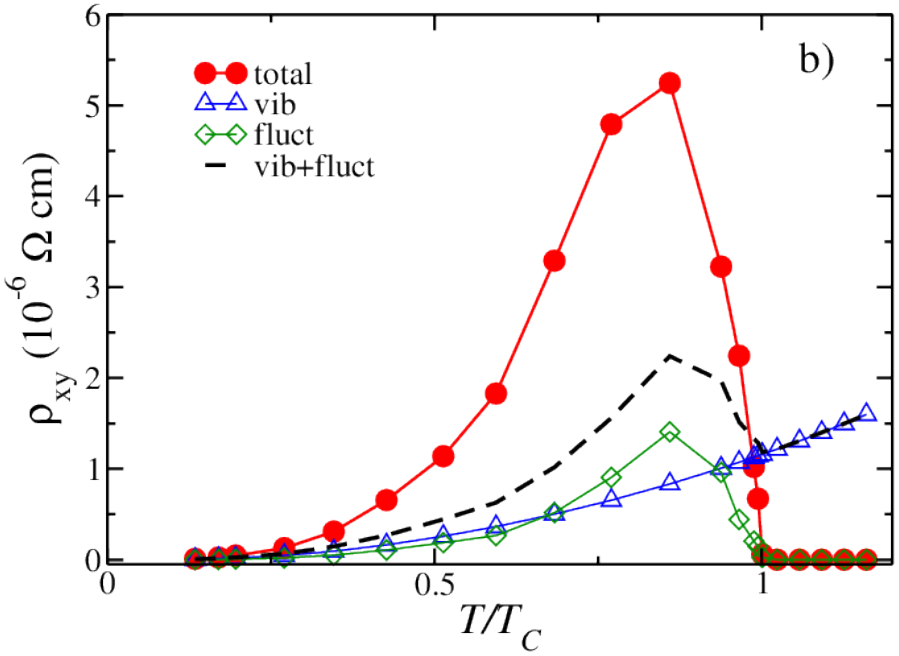
- LDA+U calculations, U = 6 eV, J = 0.9 eV
- Strong anisotropy of electrical resistivity
- Non-additive contributions from lattice vibrations and spin fluctuations
- Comparable contributions from lattice vibrations and spin fluctuations
- Resistivity kink at Curie temperature

Gd: Off-diagonal resistivity, M||(001)

$\rho_{xy}(T)$: Theory vs experiment



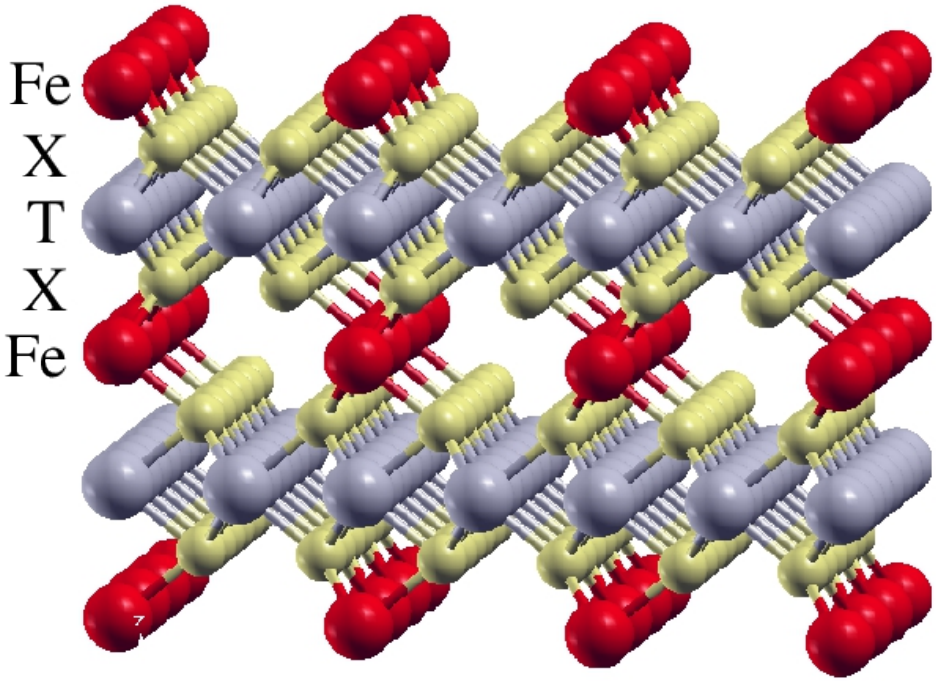
$\rho_{xy}(T)$: Contributions



- Non-additive contributions from lattice vibrations and spin fluctuations
- Comparable contributions from lattice vibrations and spin fluctuations
- Crucial effect of spin fluctuations at Curie temperature

Fe intercalated 2H-TaS_2

Structure



Fe_xTaS_2

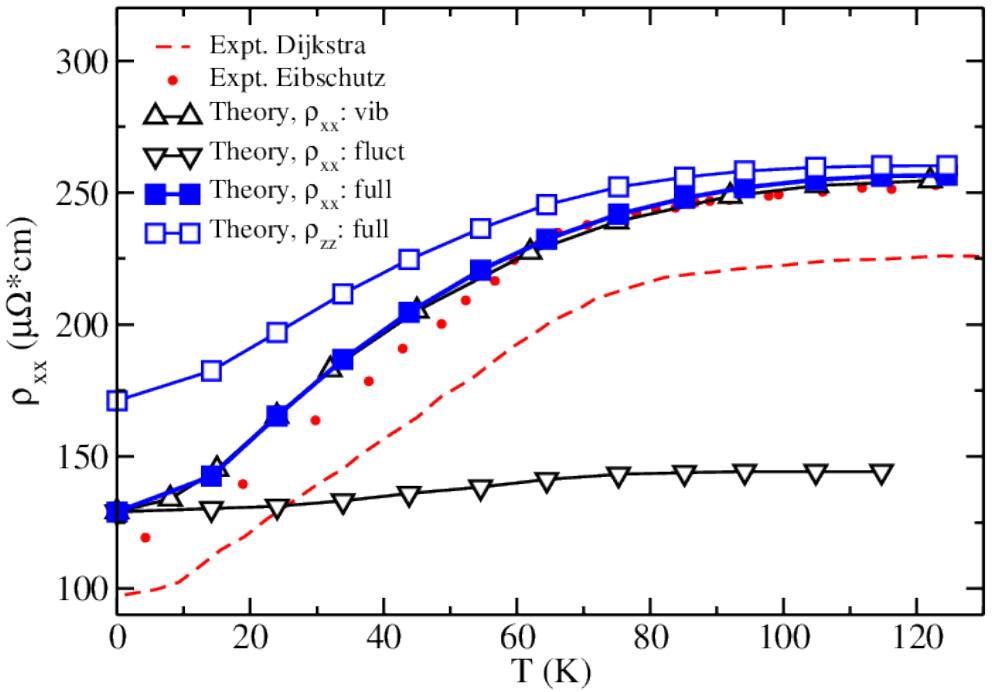
x	T_C (K)
0.20	90
0.26	163
0.28	90
0.34	55

- Ordering within Fe layers:

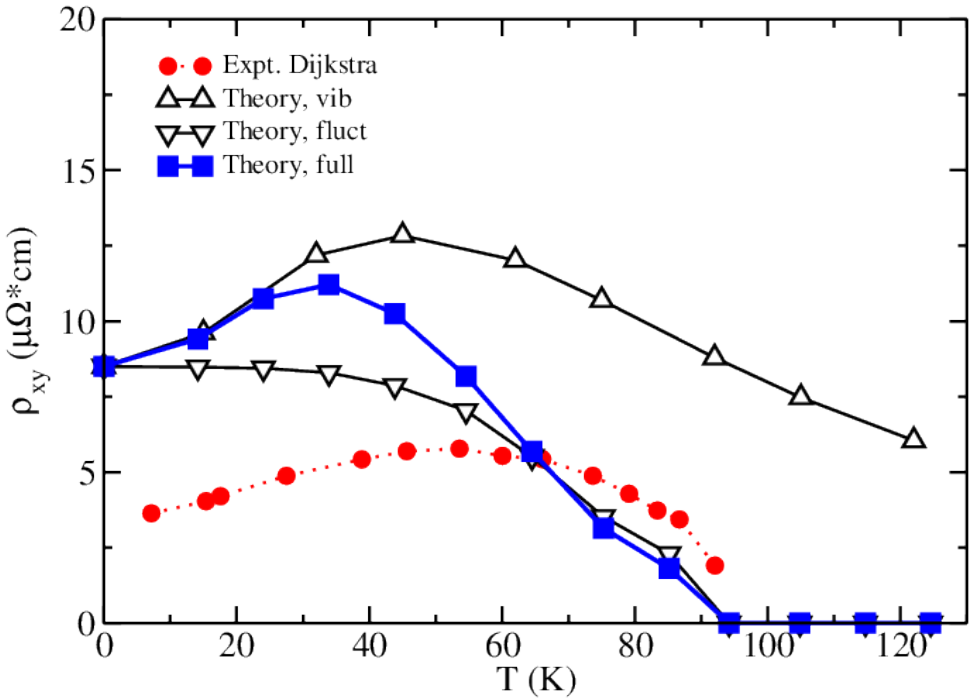
  2×2 at $x = 0.25$ and $\sqrt{3} \times \sqrt{3}$ at $x \approx 0.34$

Fe intercalated 2H-TaS_2 resistivity, M||(001)

$\rho_{xx}(T), \rho_{zz}(T)$



$\rho_{xy}(T)$

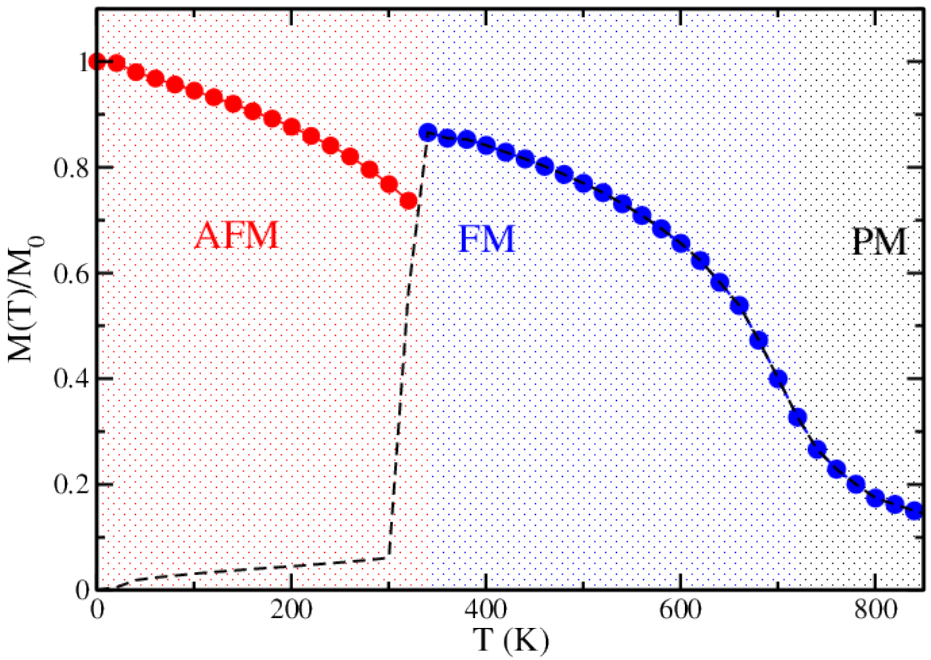


- Longitudinal resistivity: anisotropic at low temperature
- AHE: important role of spin fluctuatuions

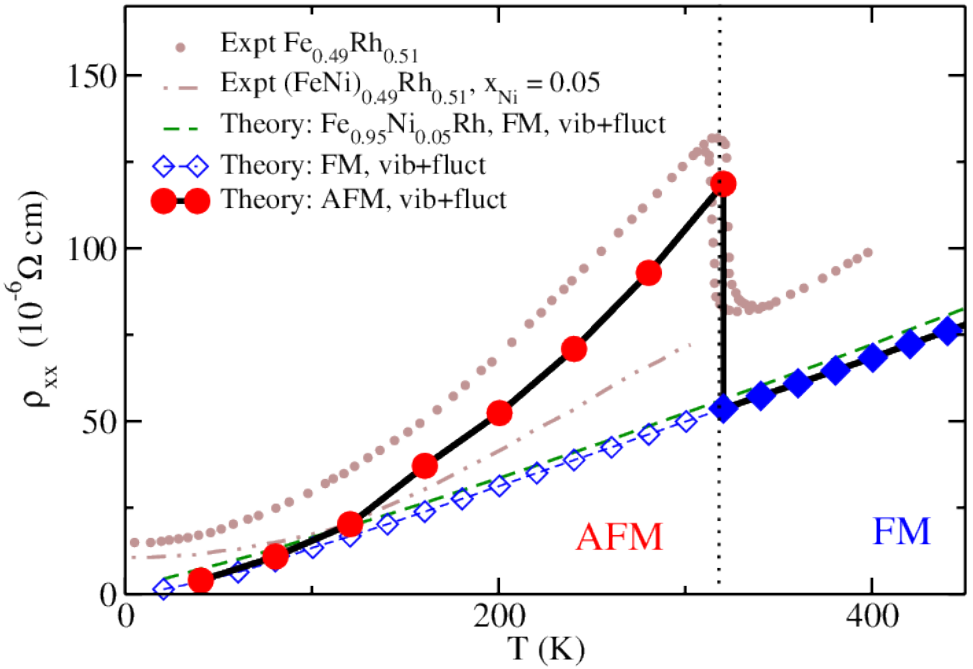
S. Mankovsky, K. Chadova, D. Ködderitzsch, W. Bensch, H. Ebert, accepted PRB, arXiv:1509.03581 (2015)

FeRh electrical resistivity

MC: M(T) for **one Fe sublattice**



Expt vs theory: resistivity vs T

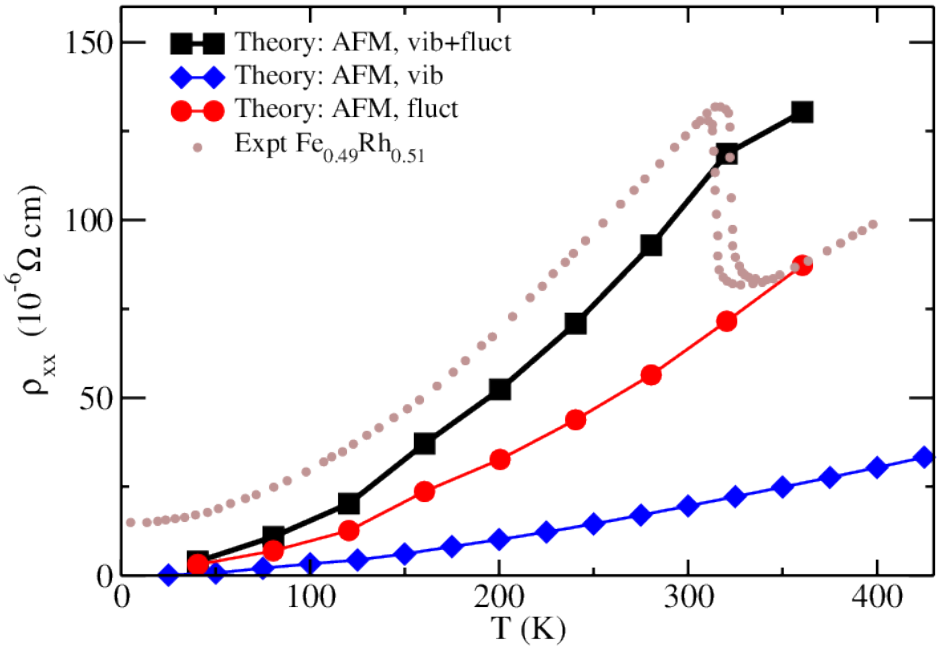


- Monte Carlo simulations: Temperature dependent **magnetization** of AFM-aligned **sublattices** of Fe
- **AFM** state: Faster decrease of Fe sublattice magnetization (**stronger spin fluctuations**) → **more steep increase of resistivity**

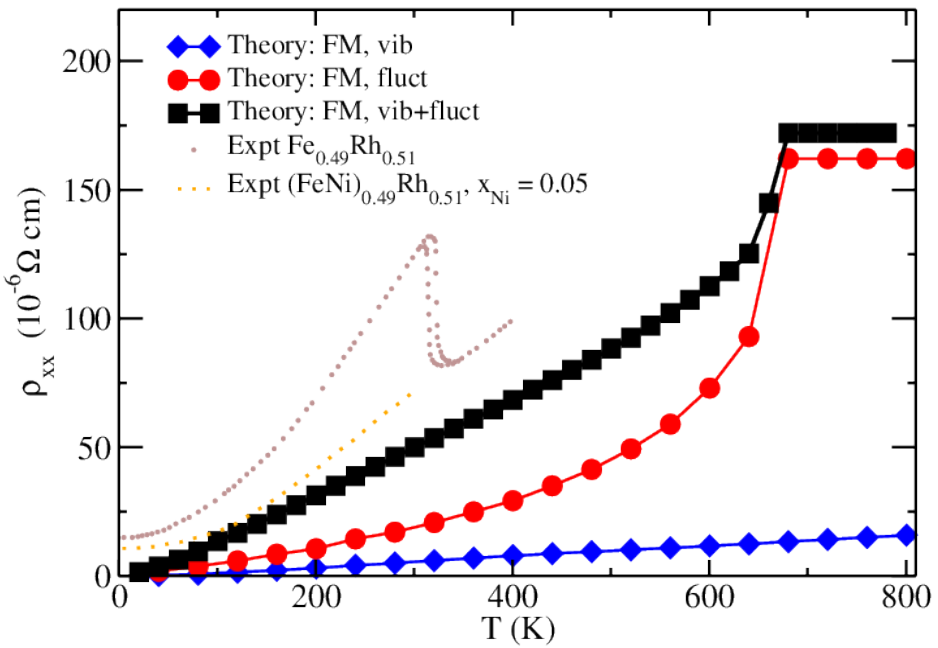
S. Polesya, S. Mankovsky, D. Ködderitzsch, J. Minár, H. Ebert, arXiv:1509.03581 (2015)

FeRh electrical resistivity

FeRh, AFM: contributions



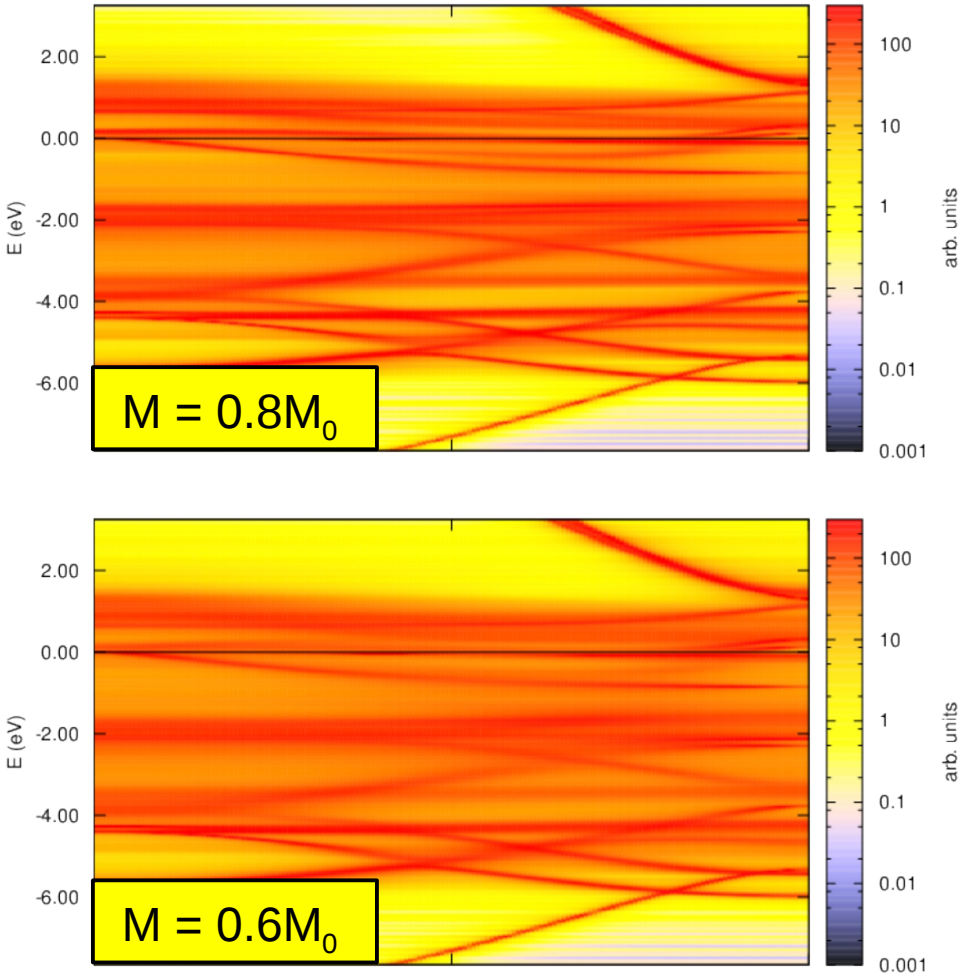
FeRh, FM: contributions



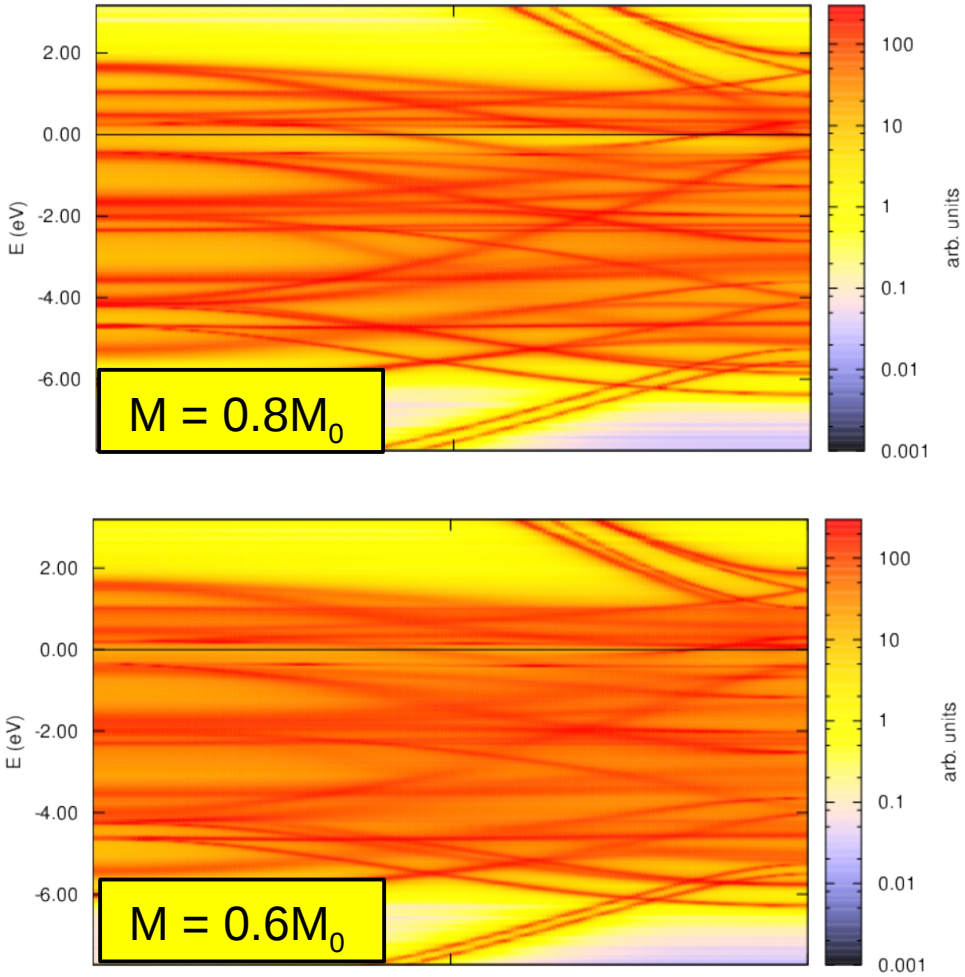
- **FM** state: **Small** contribution to the resistivity from the scattering on **lattice vibrations**.
- **AFM** state: **higher vibration-determined resistivity** than for **FM** state
- **AFM** state: **stronger spin fluctuations → more steep increase of resistivity**

FeRh electronic structure

$A(\vec{k}, E)$ for AFM FeRh



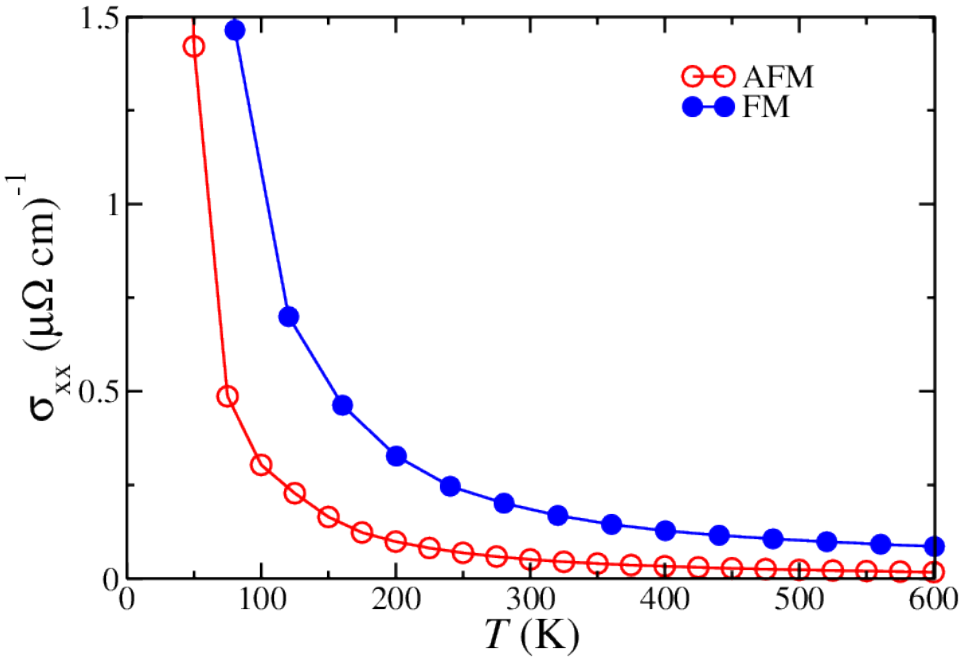
$A(\vec{k}, E)$ for FM FeRh



- **No significant difference between FM and AFM** states due to magnetic disorder

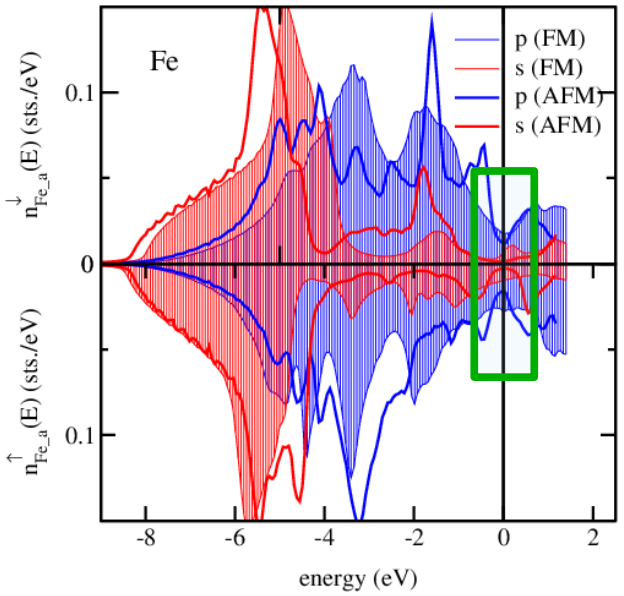
FeRh electrical conductivity

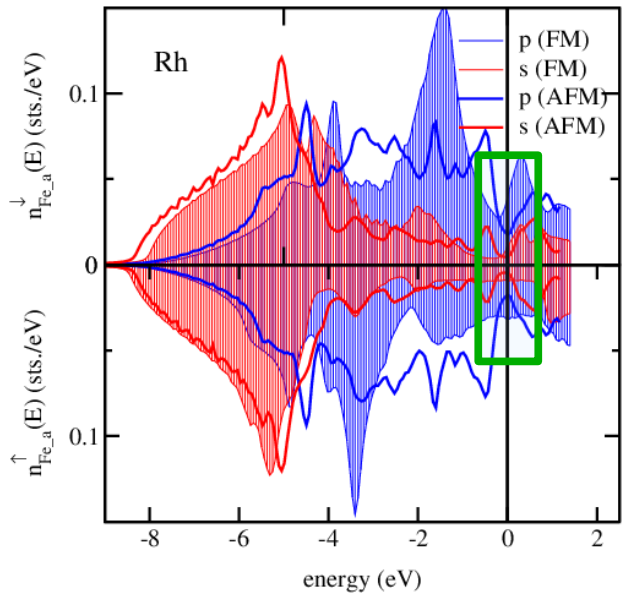
Conductivity: AFM vs FM



- **FM** state: **higher conductivity** when compared to the **AFM** state
- **FM** state: **higher s,p-DOS(E_F)** when compared to the **AFM** state

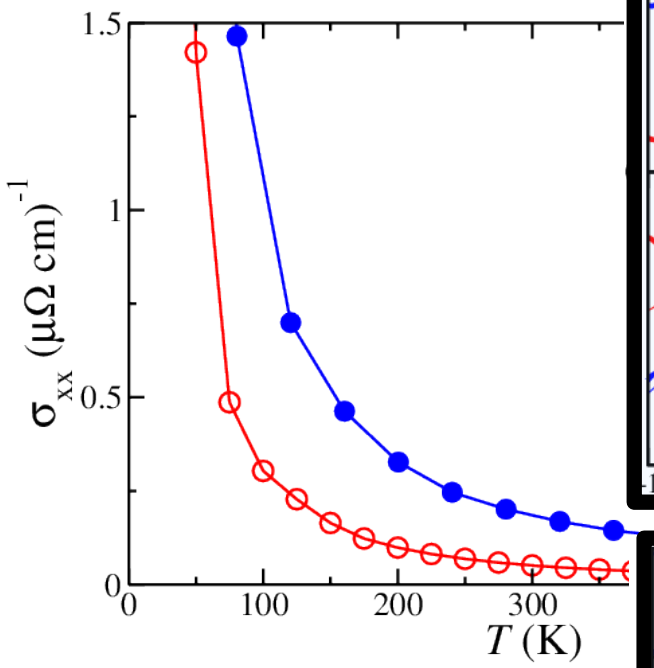
FeRh: sp-DOS

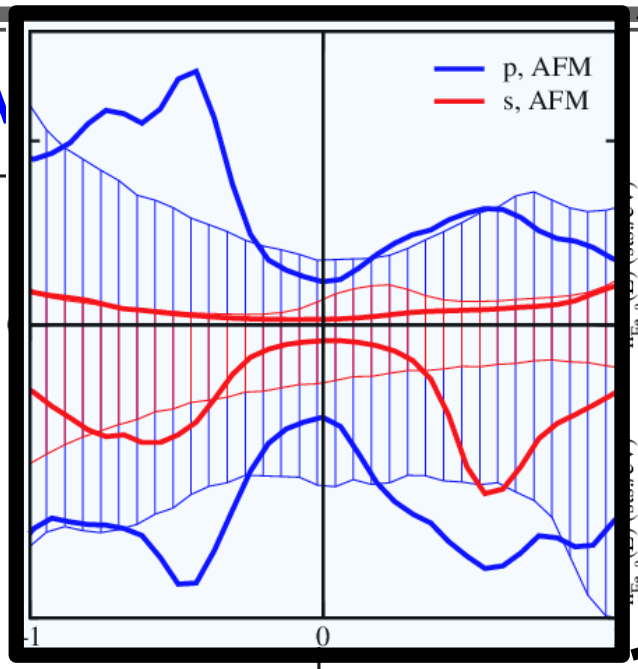


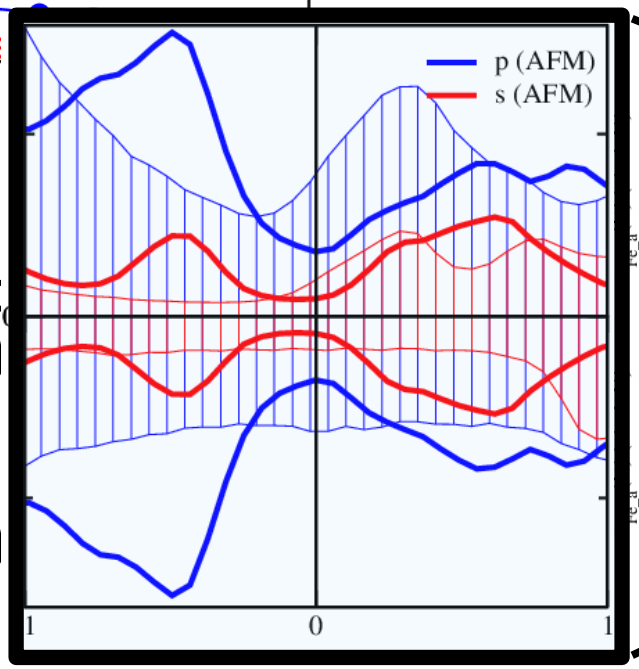


FeRh electrical conductivity

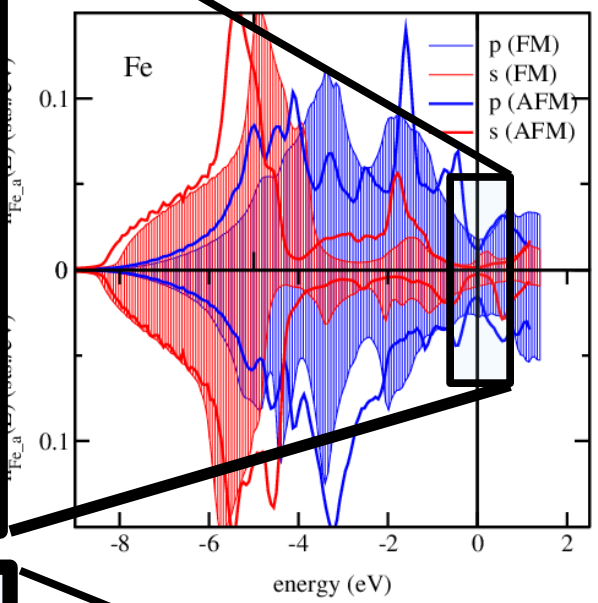
Conductivity: A

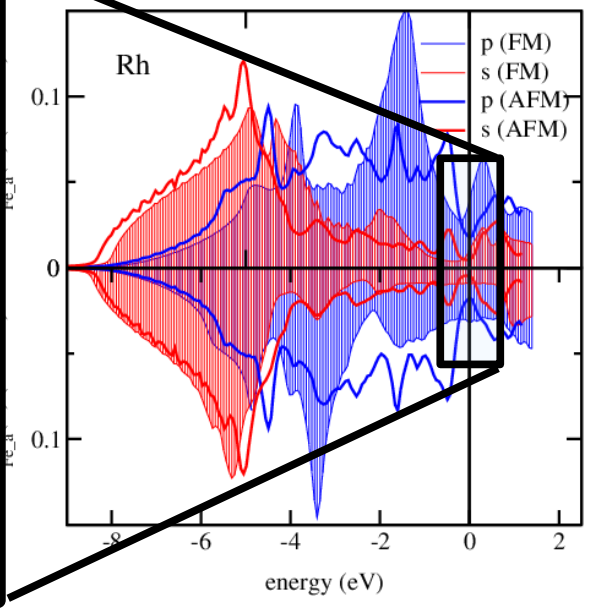






FeRh: sp-DOS

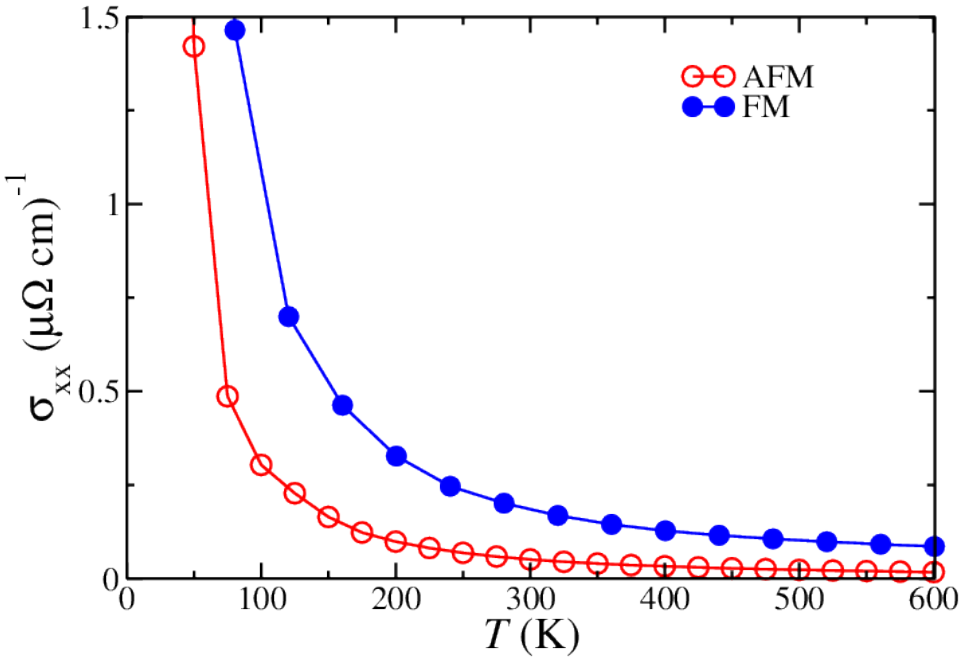




- **FM** state: **higher co**
  when compared to
- **FM** state: **higher s,**
  when compared to

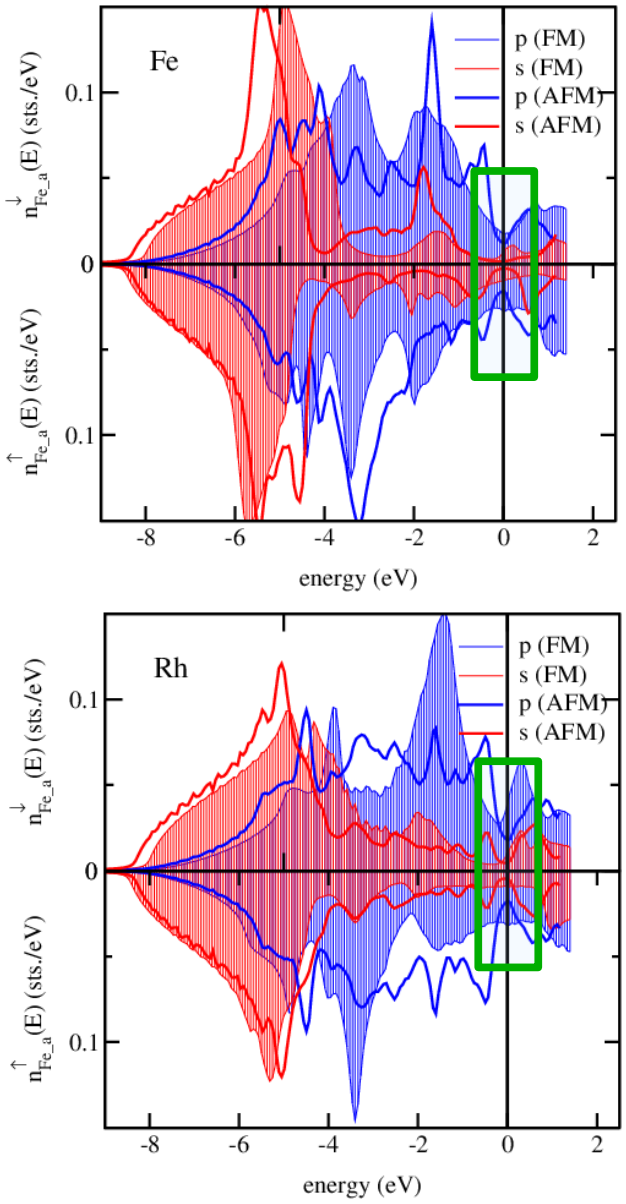
FeRh electrical conductivity

Conductivity: AFM vs FM



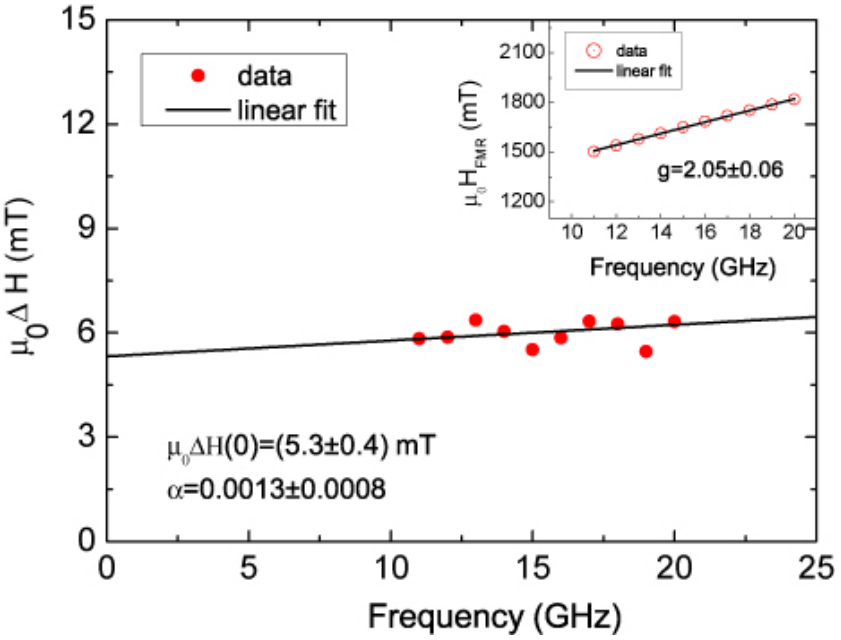
- **FM** state: **higher conductivity** when compared to the **AFM** state
- **FM** state: **higher s,p-DOS(E_F)** when compared to the **AFM** state

FeRh: sp-DOS

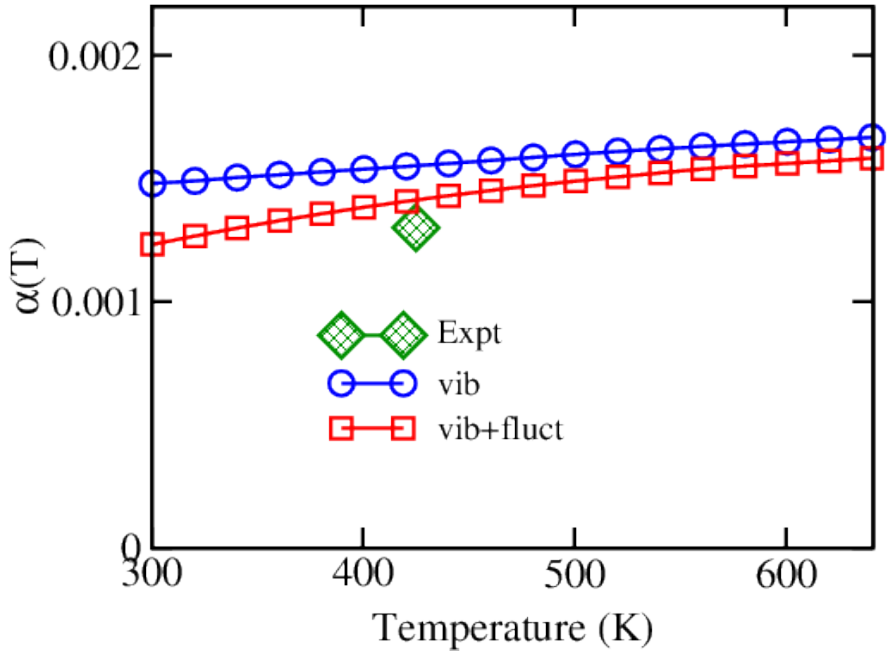


FeRh Gilbert damping

Experiment, T = 425 K



Theory: FM FeRh



Expt: E Mancini, et al., C H Back, J. Phys. D: Appl. Phys. 46 (2013) 245302

- Small contribution from spin fluctuations
- Good agreement with experiment

Summary

- Finite temperature response function using alloy analogy model: reasonable results on resistivity and Gilbert damping, in agreement with experiment
- Strong effect of spin fluctuations for electrical resistivity
- Crucial role of $M(T)$ behaviour related to angular distribution of magnetic moments at given temperature T
- Strong effect of vertex corrections for Gilbert damping
- Deviations from Matthissen rule for resistivity
- Ni: Important effect of longitudinal fluctuations

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