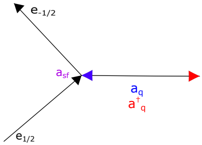


Modelling ultrafast magnetization dynamics in Fe, Ni, Co with the Microscopic Three Temperature model

Theodor Griepe
Freie Universität Berlin

Midterm presentation for Master thesis

Outline

Introduction

The Microscopic Three temperature Model

Experimental Data

Implemented Model

Discussion of parameters

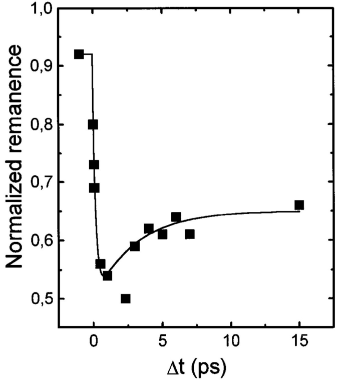
Results

Outline

Introduction

- Beaurepaire et al. 1996: UFD in Nickel
- optically excite sample with fs laser pulse
- measure magnetization by probing at different delays

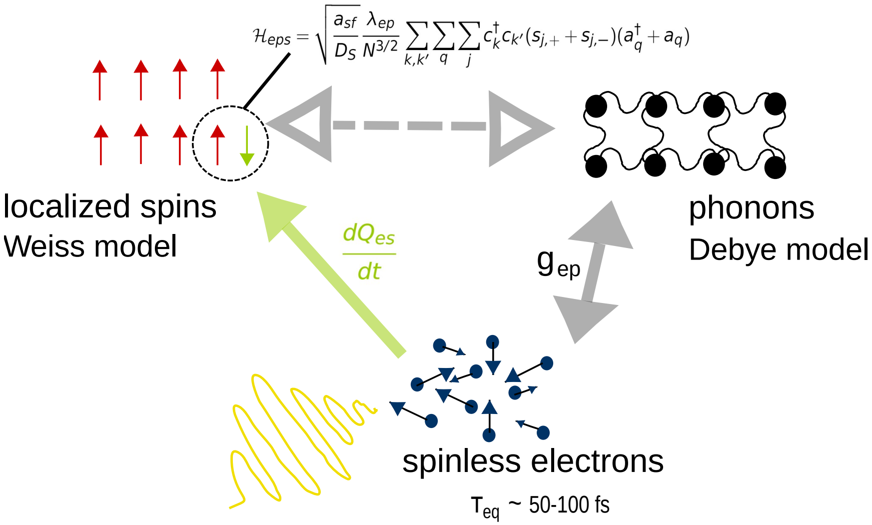
- microscopic processes?



UFD in Nickel, captured by Beaurepaire et al. [1]

[1] Beaurepaire et al., PRL 76, 1996

Sketch of Interactions



Freie Universität Berlin

Dynamics of electronic, lattice and spin subsystems [2]

$$C_{\mathrm{e}}\frac{dT_{\mathrm{e}}}{dt}=g_{\mathrm{e-p}}(T_{\mathrm{p}}-T_{\mathrm{e}})+S(z,t)+\nabla(\kappa\nabla T_{e})$$

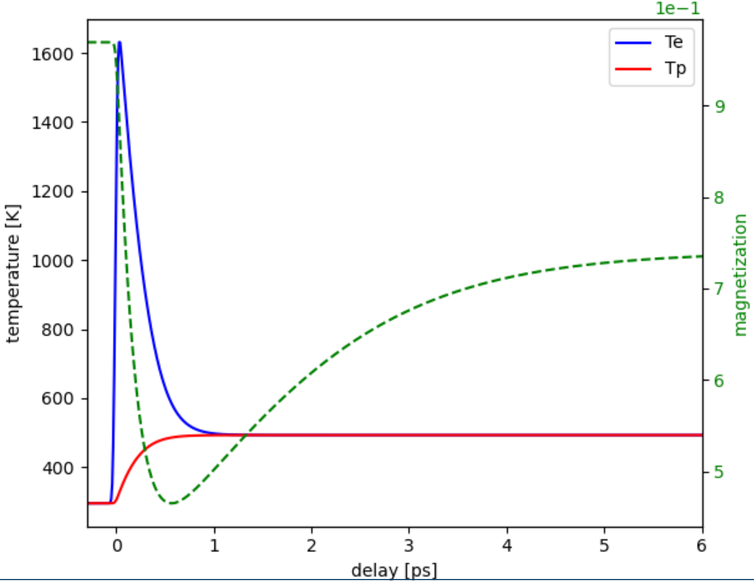
$$C_{\mathrm{p}}\frac{dT_{\mathrm{p}}}{dt}=-g_{\mathrm{e-p}}(T_{\mathrm{p}}-T_{\mathrm{e}})$$

$$\frac{dm}{dt}=Rm\frac{T_{\mathrm{p}}}{T_C}\left(1-\frac{m}{B_{1/2}\left(\frac{Jm}{k_B T_e}\right)}\right)$$

$$\mathrm{R}=a_{sf}8g_{ep}k_B T_C^2 V_{at}/(\mu_{at}E_D^2)$$

[2] Koopmans et al., NMat 2593, 2009

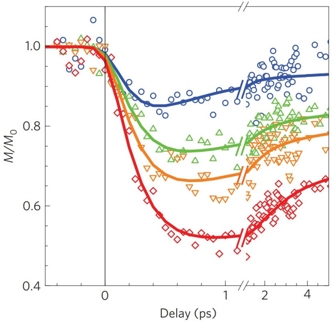
Dynamics of the subsystems in the M3TM



Koopmans' estimation of a_{sf}

- fit parameters $c_e, c_p, g_{ep}, S_0, a_{sf}$
- spin flip probability found by Koopmans very high
- Carva et al.[3] retrieved a_{sf} from DFT calculations

Sample	a_{sf}	Koopmans
Nickel	$0.04 - 0.09$	$0.17 - 0.2$
Cobalt	$0.01 - 0.022$	$0.135 - 0.165$
Iron	$0.04 - 0.07$	

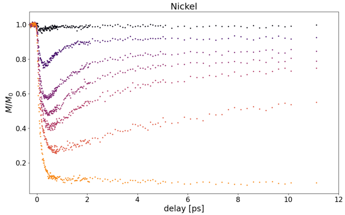


simulation fits for low fluences, reprinted from [3]

[3] Carva et al., PRB 87, 2013
[4] Koopmans et al., NMat 2593, 2009

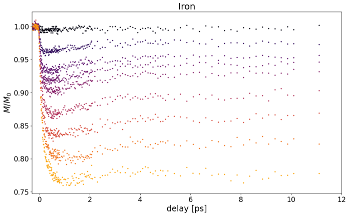
Outline

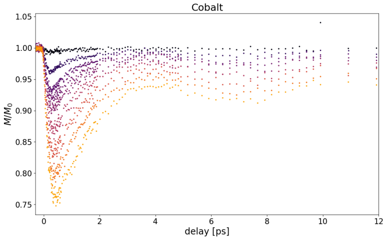
Experimental data



- Ni, Fe, Co thin films ($d = 15$ nm) on glass wafers
- room temperature, fluence $0.5 - 15\,\frac{\mathrm{mJ}}{\mathrm{cm}^2}$
- magnetization measured under same conditions for several pump fluences

Borchert et al., arXiv:2008.12612, 2020





Implemented model

Dynamics of electronic, lattice and spin subsystems[4]

$$C_{\mathrm{e}} \frac{dT_{\mathrm{e}}}{dt} = g_{\mathrm{e-p}}(T_{\mathrm{p}} - T_{\mathrm{e}}) + S(z,t) + \frac{dQ_{se}}{dt}$$

$$C_{\mathrm{p}} \frac{dT_{\mathrm{p}}}{dt} = -g_{\mathrm{e-p}}(T_{\mathrm{p}} - T_{\mathrm{e}})$$

$$\frac{dm}{dt} = Rm \frac{T_{\mathrm{p}}}{T_C} \left(1 - \frac{m}{B_{1/2}\left(\frac{Jm}{k_B T_e}\right)} \right)$$

$$\frac{dQ_{se}}{dt} = Jm \frac{dm}{dt}$$

$$R = a_{sf} 8 g_{ep} k_B T_C^2 V_{at} / (\mu_{at} E_D^2)$$

*Ab initio parameters [5]

[4] Koopmans et al., Nmat 2593, 2009
[5] Zahn et al., PRR 3, 2020

M-Dynamics for arbitrary spin

material	S_{eff} [6]
Nickel	0.5
Iron	2
Cobalt	1.5

Arbitrary Spin Rate Equations [7]

$$\frac{dm}{dt} = -\frac{1}{S} \sum_{ms=-S}^{ms=+S} m_s \frac{df_{m_s}}{dt}$$

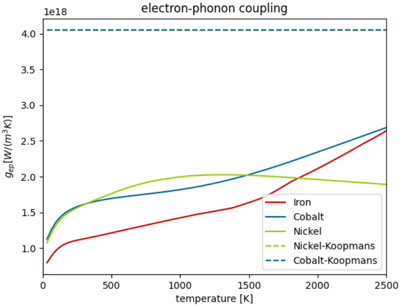
$$\frac{df_{m_s}}{dt} = -(W_{m_s}^{+} + W_{m_s}^{-}) f_{m_s} + W_{m_{s-1}}^{+} f_{m_{s-1}} + W_{m_{s+1}}^{-} f_{m_{s+1}}$$

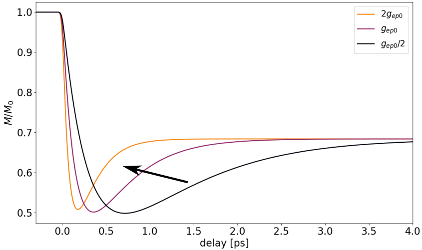
$$W_{m_s}^{\pm} = R \frac{Jm}{4Sk_B T_c} \frac{T_p}{T_c} \frac{e^{\mp \frac{Jm}{2Sk_B T_e}}}{\sinh(\frac{Jm}{2Sk_B T_e})} (S(S+1) - m_s(m_s \pm 1))$$

[6] Köbler et al., Condensed matter, 2003
[7] Beens et al., Phys. Rev. B, 2019

Outline

Electron phonon coupling g_{ep}

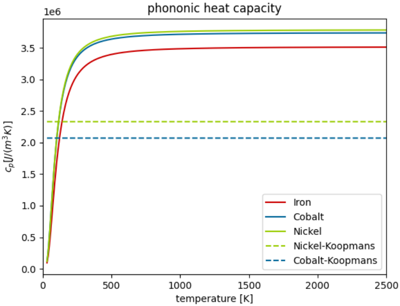


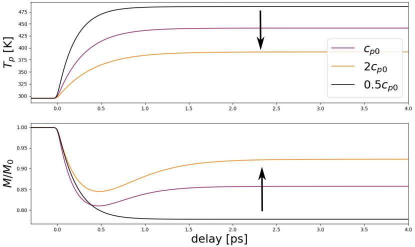


fixed $\frac{R}{g_{ep}}, c_e, c_p$

vary g_{ep}

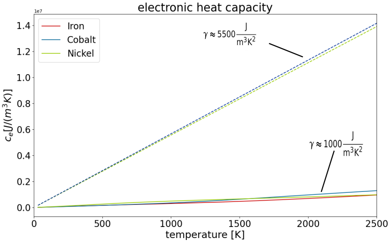
Phonic specific heat c_p



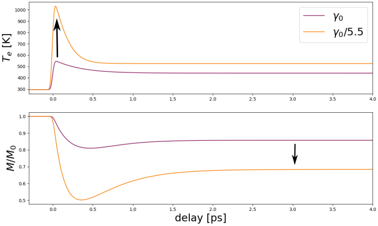


fixed R, c_e, g_{ep},
vary c_p

Electronic specific heat c_e

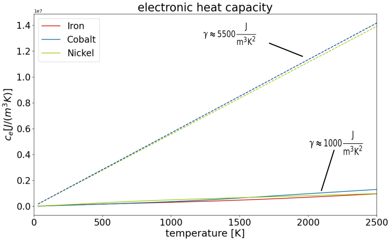


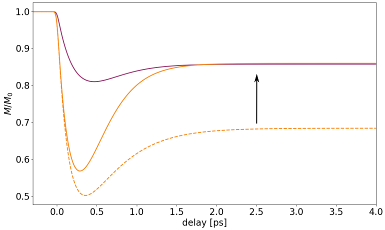
$$c_e = \gamma T_e$$



fixed R, c_p, g_{ep},
decrease c_e

Electronic specific heat c_e



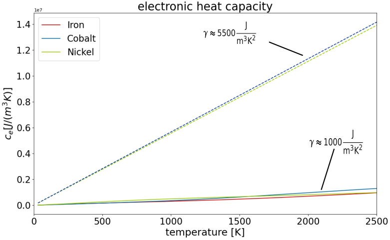


$$c_e = \gamma T_e$$

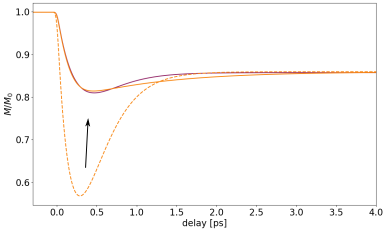
fixed R, g_{ep}

$\approx 2c_p$

Electronic specific heat c_e

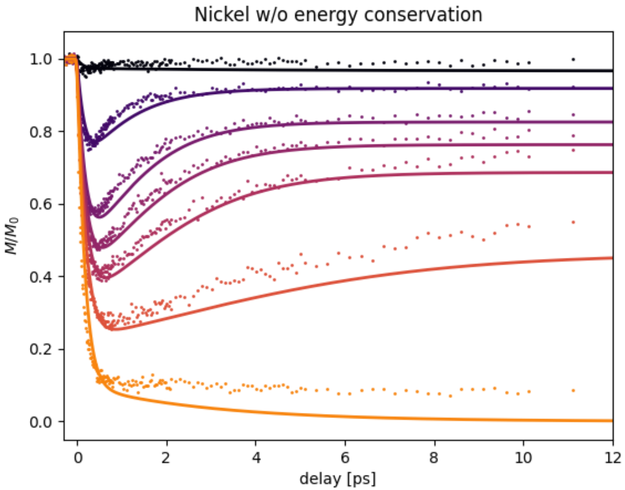


$$c_e = \gamma T_e$$



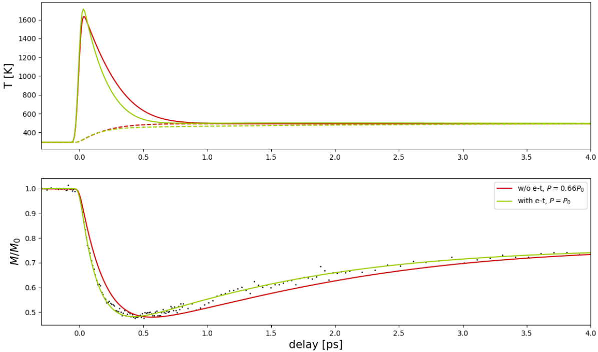
fixed g_{ep}
$\approx 0.4R$

Implementation of ab-initio parameters in Nickel



$$a_{sf} \approx 0.05$$

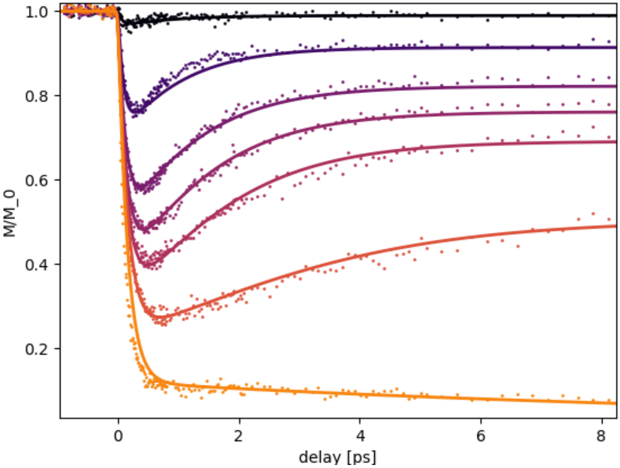
Influence of e-s energy flow



$$\frac{dQ_{es}}{dt} = Jm\frac{dm}{dt} \qquad (1)$$

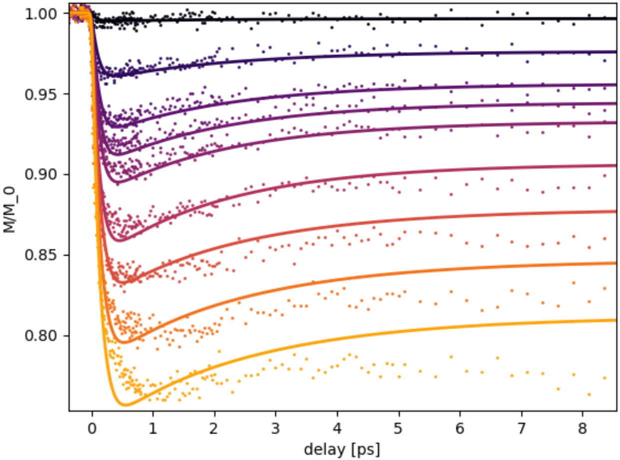
Outline

Nickel



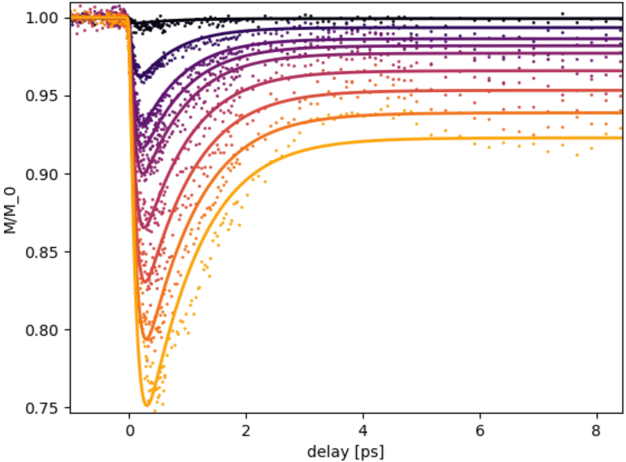
P_s	Koopmans	simulated
$0.04 - 0.09$	$0.17 - 0.2$	$0.05 - 0.06$

Iron



P_s	Koopmans	simulated
$0.04 - 0.07$		$0.03 - 0.035$

Cobalt



P_s	Koopmans	simulated
$0.01 - 0.022$	$0.135 - 0.165$	$0.04 - 0.05$

Thanks

Thank you for your attention

fluence [$\frac{mJ}{cm^2}$]	P_0 [$10^{21}\frac{W}{m^3}$] Nickel	P_0 [$10^{21}\frac{W}{m^3}$] Iron	P_0 [$10^{21}\frac{W}{m^3}$] Cobalt
0.5	1.68	1.33	1.33
3	10.08	8	8
5	16.8	13.3	13.3
6	20.3	16	16
7	23.7	18.6	18.6
9	30.5	23.9	23.9
11	38.5	29	29
13		34.2	34.2
15		39.4	39.4

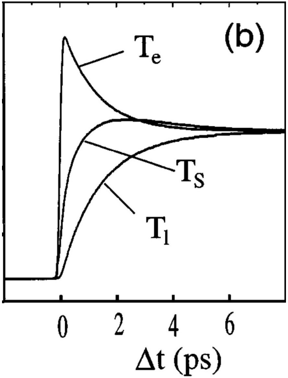
Three temperature model

$$
\begin{aligned}
C_e\ \partial_t T_e &= -g_{ep}(T_e - T_p) - g_{es}(T_e - T_s) + S(t) \\
C_p\ \partial_t T_p &= g_{ep}(T_e - T_p) - g_{ps}(T_p - T_s) \\
C_s\ \partial_t T_s &= g_{es}(T_e - T_s) + g_{ps}(T_p - T_s)
\end{aligned} \tag{2}
$$

- C_i heat capacity of subsystem i
- g_{ij} coupling constant of systems i,j

- $g_{ps} \ll g_{es}$
- $C_s \ll C_p$
- spin system not in internal equilibrium [8]

- energy redistribution within sample
- microscopic processes behind spin flip events?



[8] Kazantseva et al., EPL 81, 2007

Landau-Lifshitz-Bloch description

$$\partial_t \boldsymbol{n} = \gamma[\boldsymbol{n} \times \boldsymbol{H}_{\mathbf{eff}}] - \frac{\gamma\alpha_\perp}{n^2}[\boldsymbol{n} \times [\boldsymbol{n} \times \boldsymbol{H}_{\mathbf{eff}}]] + \frac{\gamma\alpha_\parallel}{n^2}[\boldsymbol{n} \cdot \boldsymbol{H}_{\mathbf{eff}}]\boldsymbol{n} \quad (3)$$

[9]

γ gyromagnetic ratio

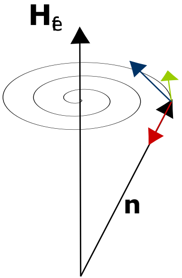
$$\boldsymbol{n} = \frac{\langle \boldsymbol{S} \rangle}{m_e(T_e)}$$

$$\alpha_\perp = \frac{\lambda}{m_e}\left[\frac{\tanh(q_s)}{q_s} - \frac{T}{3T_C}\right]$$

$$\alpha_\parallel = \frac{2\lambda T}{3 m_e T_C} \frac{2q_s}{\sinh(2q_s)}$$

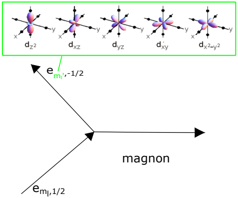
λ dissipation constant

$$\boldsymbol{H}_{\mathrm{eff}} = \boldsymbol{H}_{\mathbf{int}} + \frac{m_e(T)}{2\chi_\parallel}(1 - n^2)\boldsymbol{n}$$



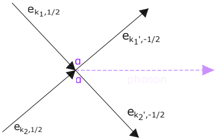
[9] Atxitia et al., PRB 84, 2011

Proposed Elliott-Yafet like spin flip interactions



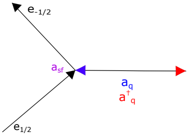
e-m scattering,
Carpene et al., PRB 78, 2008

- low energy magnon excitations



Coulomb-scattering,
Krauß et al., PRB 80, 2009

- inelastic scattering leads to Stoner excitations
- angular momentum not explicitly considered



e-p scattering,
Koopmans et al., Nmat 2593, 2009

- lattice = sink for angular momentum

Elliott-Yafet spin flips

- SOC couples majority and minority bands, thus [10]

$$\left|\Psi^{\uparrow}_{k,n}\right\rangle = a^{\uparrow}_{k,n}\left|\uparrow\right\rangle + b^{\uparrow}_{k,n}\left|\downarrow\right\rangle$$

- spin transitions upon spin-diagonal interactions yield finite

$$\left\langle \Psi^{\uparrow}_{k,n} \middle| \mathcal{H}_{\text{int}} \middle| \Psi^{\downarrow}_{k',n} \right\rangle$$

Proposed mechanisms include

- electron-magnon-scattering
- Coulomb scattering
- electron phonon-scattering

[10] Elliott†, PR 96, 1954