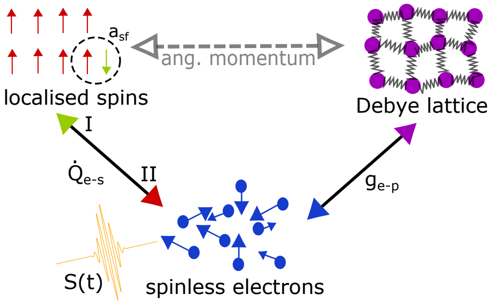
M3TM model concept



- decoupled systems of spinless electrons, phonons and localized spins in Mean field approximation (MFA)
- laser pulse heats electron system
- energy distribution to lattice and spins
  (for FGT: no remagnetization so energy flow $\dot{Q}_{es}$ (see next slide) unidirectional e $\longrightarrow$ s)
- spin flips (/magnon excitations) upon e-p scattering event from Elliott-Yafet spin mixing
- implicit angular momentum exchange between spins and lattice

M3TM equations

Dynamics of electronic, lattice and spin subsystems[6]

$$C_{\mathrm{e}} \frac{dT_{\mathrm{e}}}{dt} = g_{\mathrm{e-p}}(T_{\mathrm{p}} - T_{\mathrm{e}}) + S_0 G(t,z)) + \dot{Q}_{\mathrm{es}}$$

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

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

$C_{e(p)}$ electron (phonon) heat capacity

g_{ep} electron phonon coupling

$\dot{Q}_{es} = Jm\dot{m}/V_{at}$ energy exchange of spin-and electron system

$R = 8 \frac{a_{sf} g_{ep} T_C V_{at}}{\mu_{at} k_B T_{Deb}^2}$ magnetization rate parameter

a_{sf} spin flip probability upon e-p-scattering event

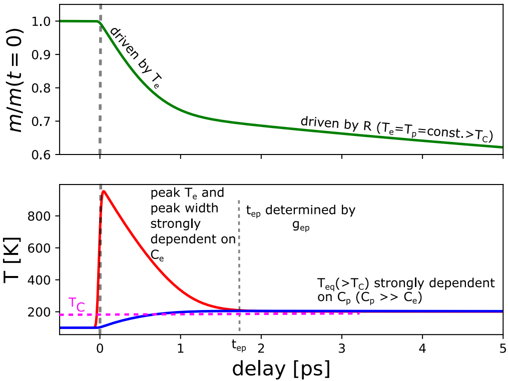
B_S Brillouin function for effective spin S

parameter impact

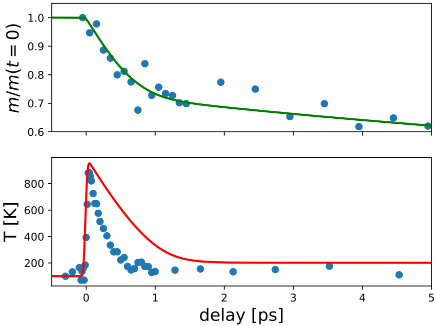
easy first attempt: take parameters used before for a very similar model

Model	symbol	meaning	estimate	unit
M3TM	$\mu_a t$	Atomic magnetic moment [a]	1.47×10^{-23}	Am^2
	γ	Electron heat capacity constant [a]	1561	$Jm^{-3}K^{-2}$
	V_{at}	Atom spin density volume [a]	1.68×10^{-29}	m^3
	T_C	Curie temperature [b]	191	K
	σ	pulse width [b]	85	fs
	g_{ep}	Electron-phonon relaxation rate [c]	1.33×10^6	$Jm^{-3}K^{-1}ps^{-1}$
	C_p	phonon heat capacity [c]	6.28×10^6	$Jm^{-3}K^{-1}$
	E_D	Debeye energy [c]	6.49×10^{-21}	J
	a_{sf}	Spin-flip probability	0.14	unity

Lichtenberg et al., arXiv:2206.01452v1

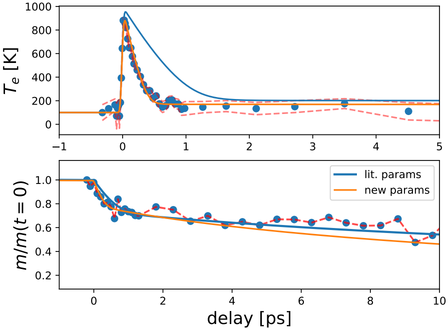


Fitting with literature parameters



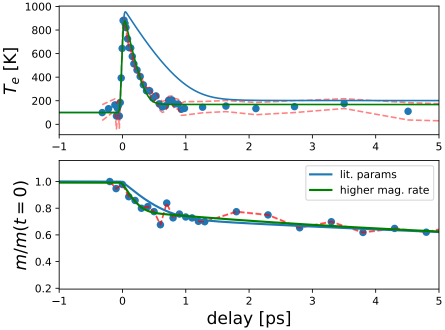
- parameters used to fit magnetization dynamics in paper cited above
- good fit of mag dynamics
- electron dynamics $\approx$ 3 times slower than in experiment
- equilibrium temperature too high in simulations

first try of fit adjustment



- increase c_p by a factor of 1.5 to adjust equilibrium magnetization
- increase g_ep by a factor of 3 to speed up electron dynamics
- decrease spin flip probability by a factor of 3 to stabilize magnetization dynamcis
- $\rightarrow$ **electron dynamics well reproduced**
- **magnetization rate after e-p-equilibration seems to fast**
- **next try: increase a_{sf} at the cost of pump power to match the magnetization behaviour for $t > \tau_{ep}$**

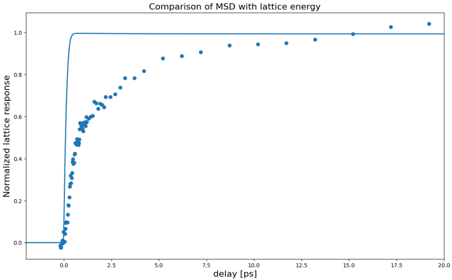
state at the moment



- both T_e and m are nicely reproduced
- lattice dynamics data important to validate use of g_{ep}, c_p
- instead of rate parameter, also c_e can be changed to adapt peak of T_e and magnetization rate
- investigation for multiple fluences important (I'd like to talk again about the initial consitions and repetition rate/effective starting temperature)

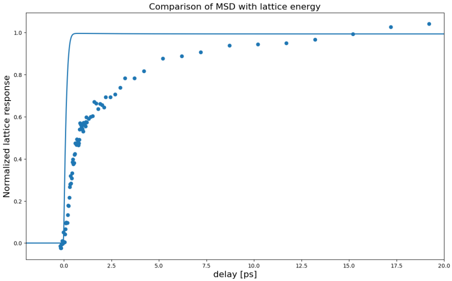
Lattice response

- fitted is norm. $\Delta(C_p T_p)$ to norm. MSD
- above simulation parameters do not fit lattice response



Lattice response

- lattice equilibrates on similar timescale **as electron temperature** ≤ 1 ps
- lattice temperature **descreases** slighty over time due to $\dot{Q}_{\mathrm{es}} < 0$



Layer resolved data

- 50 nm ≈ 33 layers of FGT
- heat transport set to 0
- Lambert-Beer adsorption, 20 nm penetration depth

- constant g_{ep} for all layers

  (temperature independent)
  - last layer equilibrates ≈ 300 % faster than first layer