Introduction to Atomistic Spin Dynamics Simulations

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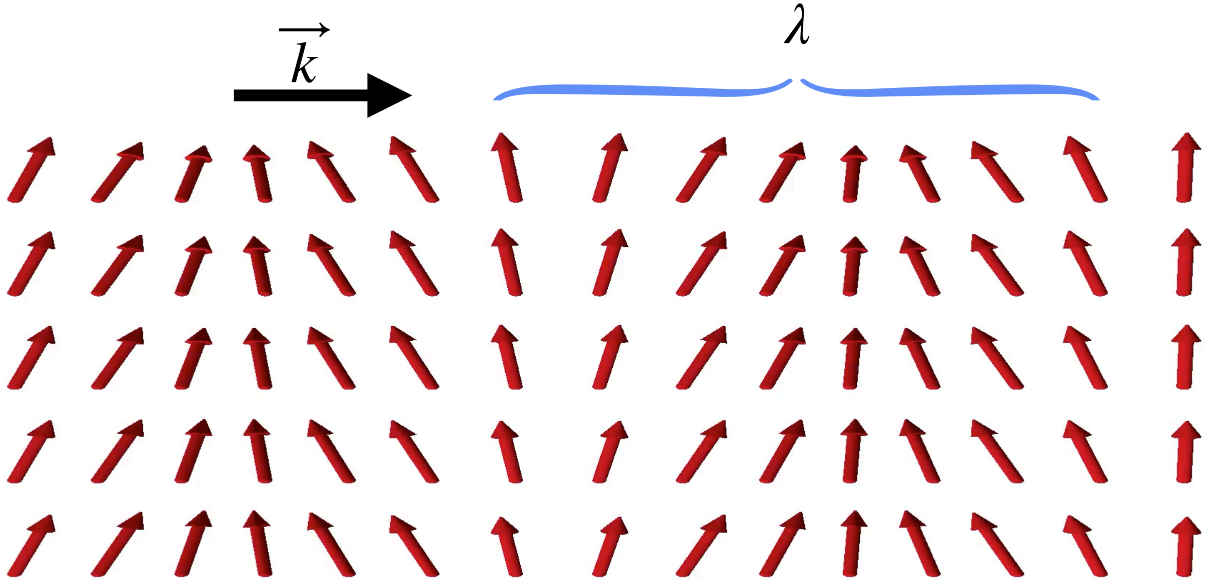
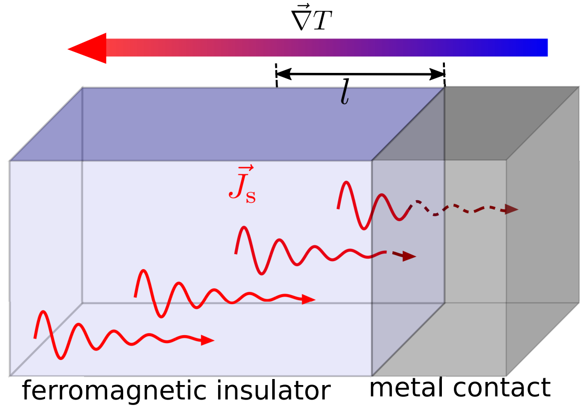
- **Timetable:**
  - **Today (10.00-15.00):** Introduction and compiling the code
  - **Next week:** 3 different tasks you work on in teams
  - **Tuesday (14.00-16.00):** Q&A
  - **Friday (14.00-16.00):** Final evaluation

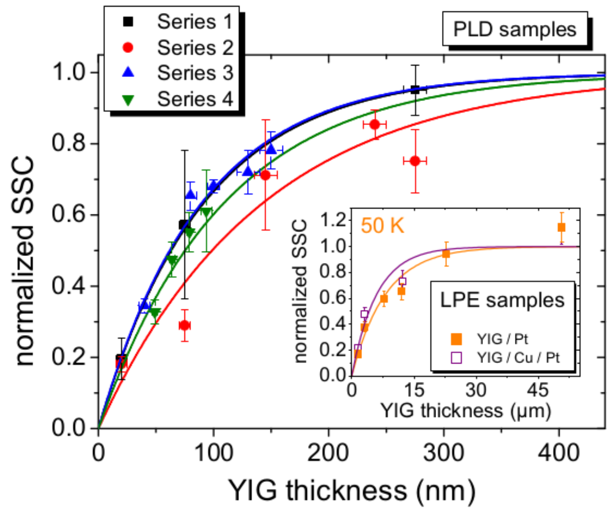
- **Tasks:**
  - Simulate monochromatic spin waves and calculate dispersion curve
  - Simulate magnetization curve
  - Simulate laser-induced demagnetization
  - Your ideas?

Applications

Example 1: Magnonic Spin Currents

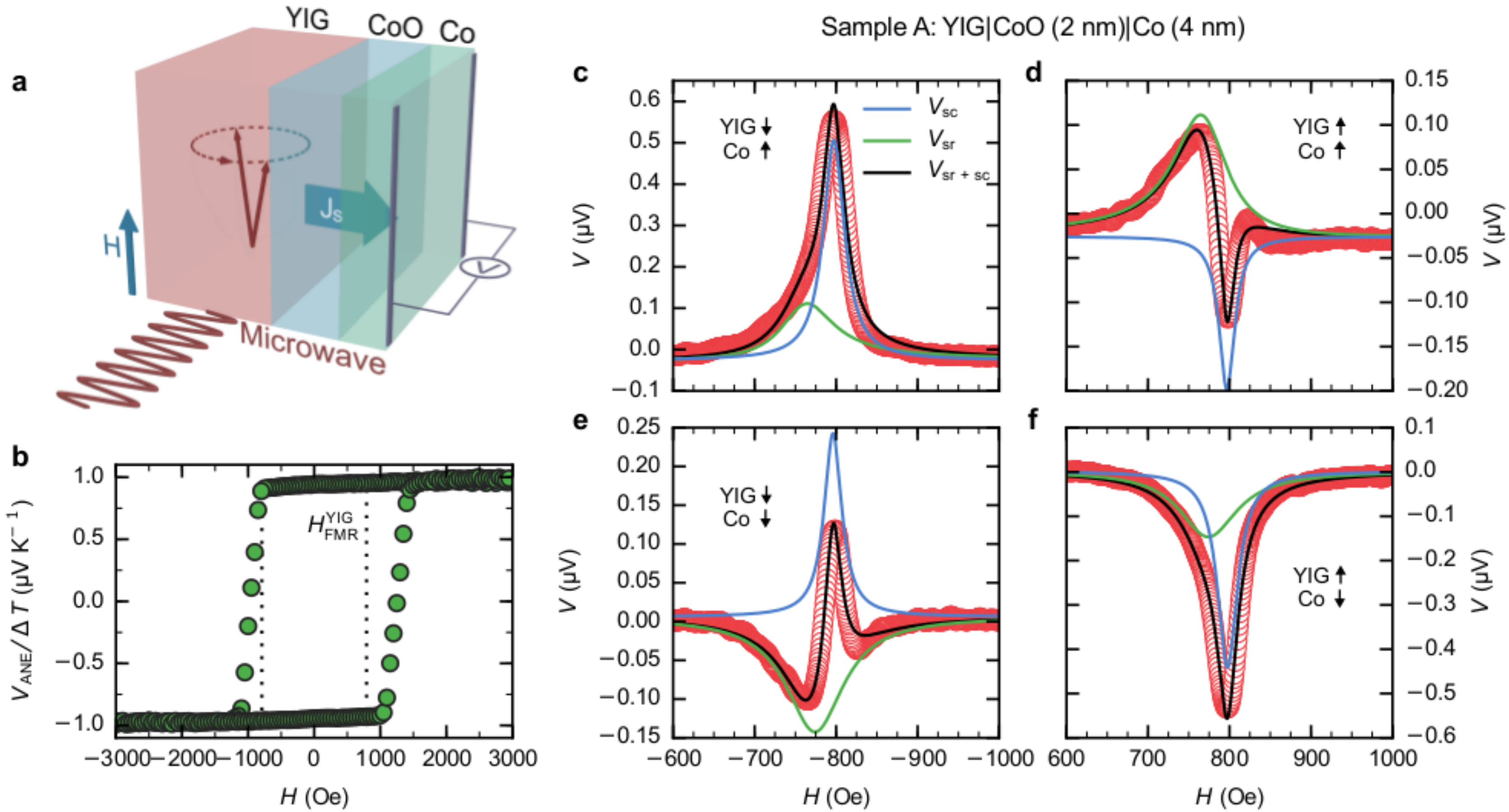






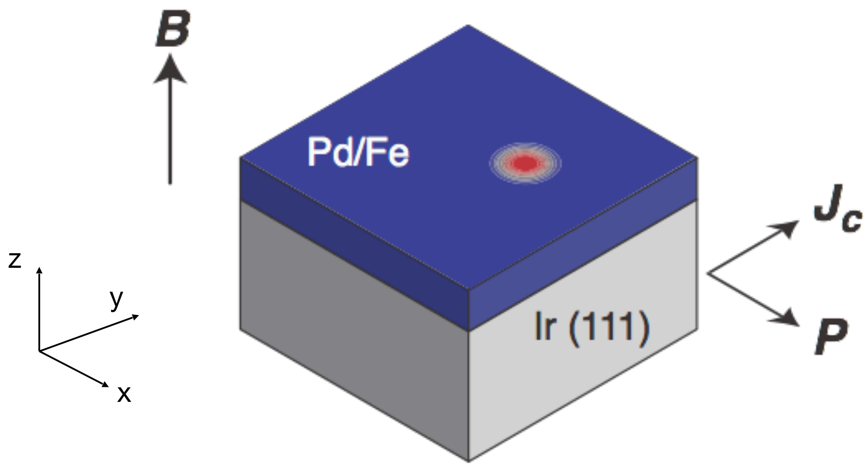
Kehlberger et al., PRL **115**, 096602 (2015)

Example 1: Magnonic Spin Currents



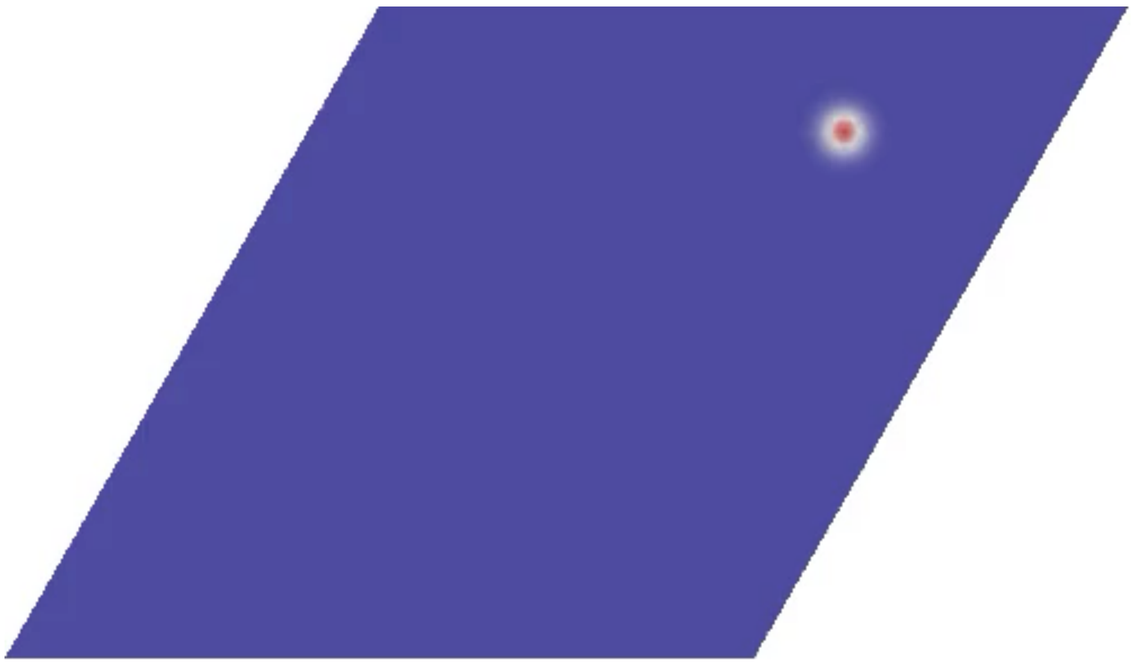
Cramer *et al.*, Nat. Commun. **9**, 1089 (2018)

Example 2: Current driven skyrmion motion



Dynamics described by Thiele equation:

$$\boxed{q\,\mathbf{G} \times \frac{\partial \mathbf{X}}{\partial t} + \alpha D \frac{\partial \mathbf{X}}{\partial t} = \mathbf{F}}$$



U. Ritzmann et al., Nat. Electron. **1**, 451 (2018)

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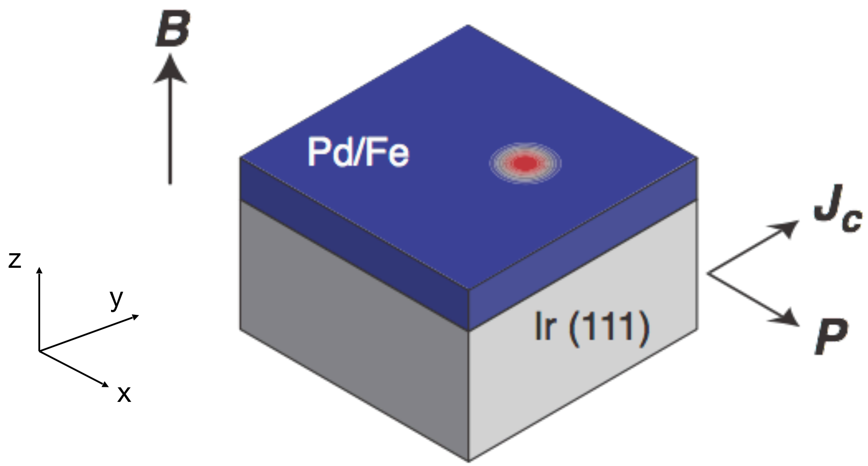
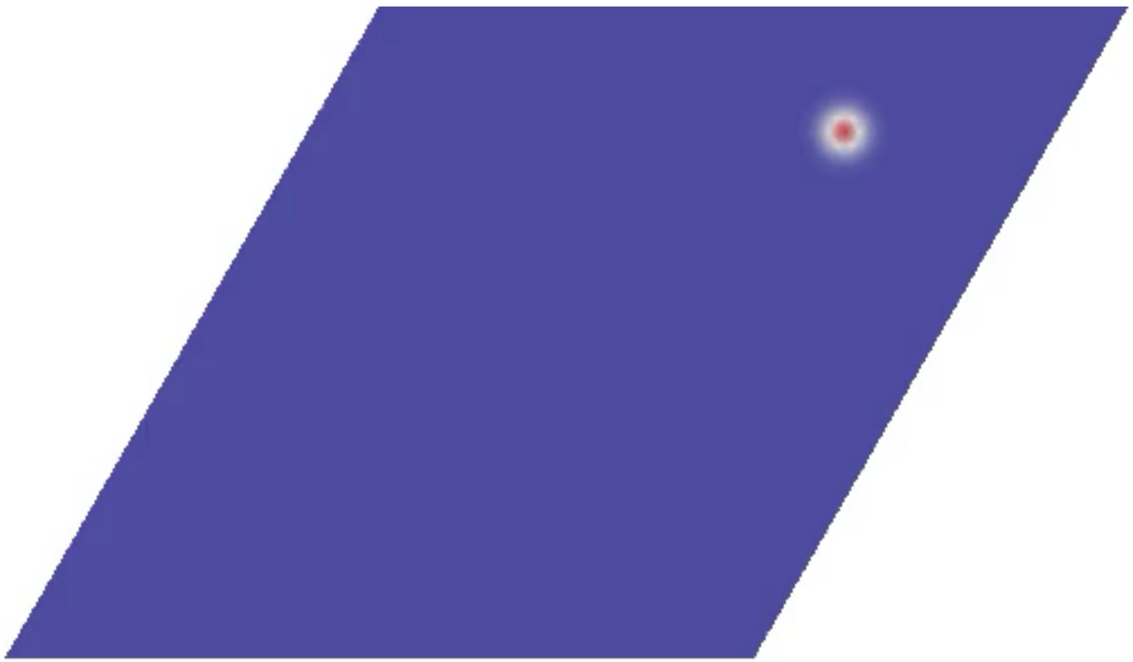




Dynamics described by Thiele equation:

$$q\,\mathbf{G} \times \frac{\partial \mathbf{X}}{\partial t} + \alpha D \frac{\partial \mathbf{X}}{\partial t} = \mathbf{F}$$

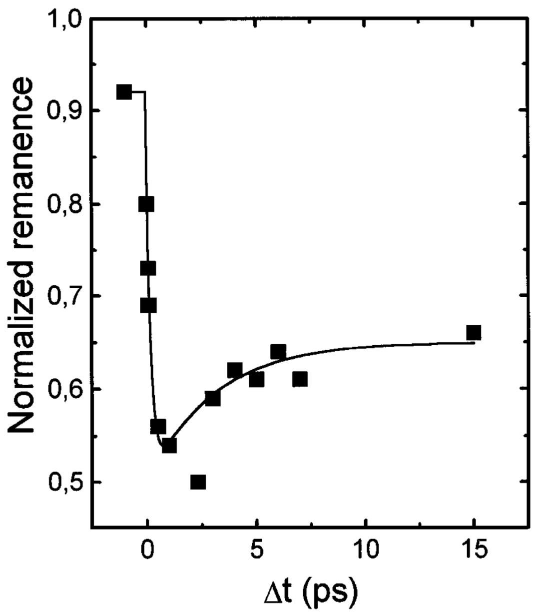
Time-dependent forces by helicity dynamics:

$$D_\psi \frac{\partial \psi}{\partial t} = \sigma_\psi\ \hbar \beta_{DL}\ \eta\ cos\left(\phi_p - \phi_t\right) - \frac{\partial U}{\partial \psi}$$

U. Ritzmann et al., Nat. Electron. **1**, 451 (2018)

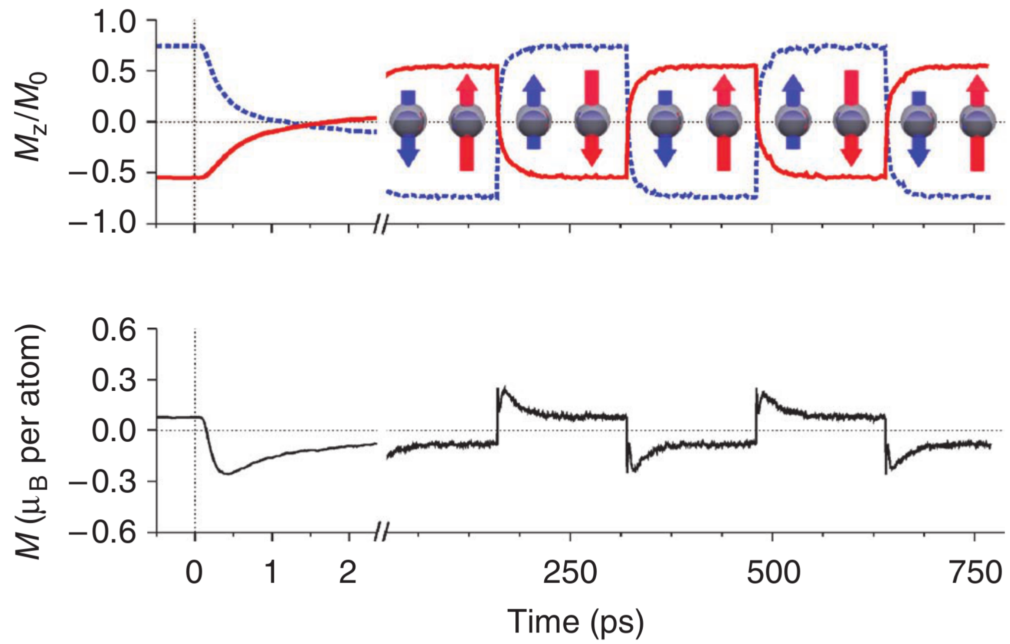
Example 3: Ultrafast Demagnetization and Switching

Laser-induced demagnetization in nickel:



Beaurepaire *et al.*, PRL **76**, 4250 (1996)

Deterministic switching in GdFeCo:



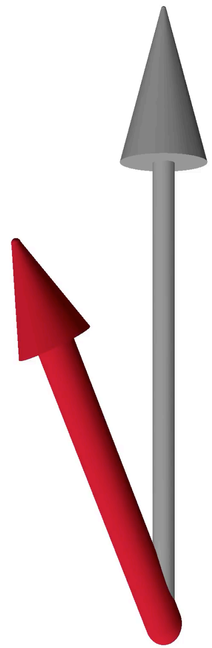
Ostler *et al.*, Nat. Commun. **3**, 666 (2012)

Basics

Atomistic Spin Dynamics Simulations

Numerical integration of stochastic Landau-Lifshitz-Gilbert equation:

$$\frac{\mathrm{d}\mathbf{m}_i}{\mathrm{d}t} = -\frac{\gamma}{\mu_\mathrm{s}(1+\alpha^2)} \times \left(-\frac{\partial\mathcal{H}}{\partial\mathbf{m}_i} + \zeta_i\right) - \frac{\alpha\gamma}{\mu_\mathrm{s}(1+\alpha^2)}\mathbf{m}_i \times \left(\mathbf{m}_i \times \left(-\frac{\partial\mathcal{H}}{\partial\mathbf{m}_i} + \zeta_i\right)\right)$$



Hamiltonian:

$$\mathcal{H} = -\underbrace{\sum_{ij} J_{ij}\mathbf{m}_i \cdot \mathbf{m}_j}_{\text{exchange interaction}} - \underbrace{\sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{m}_i \times \mathbf{m}_j)}_{\substack{\text{Dzyaloshinskii-Moriya}\\ \text{interaction}}} - \underbrace{\sum_i d\,(\mathbf{m}_i^x)^2}_{\text{anisotropy}} - \underbrace{\sum_i \mathbf{B} \cdot \mathbf{m}_i}_{\text{magnetic field}}$$

Thermal noise: $\langle \zeta_i(t) \rangle = 0 \qquad \zeta_{i\eta}(0)\zeta_{j\theta}(t) = \delta_{ij}\delta_{\eta\theta}\delta(t)2\alpha k_\mathrm{B}T\mu_\mathrm{s}/\gamma$

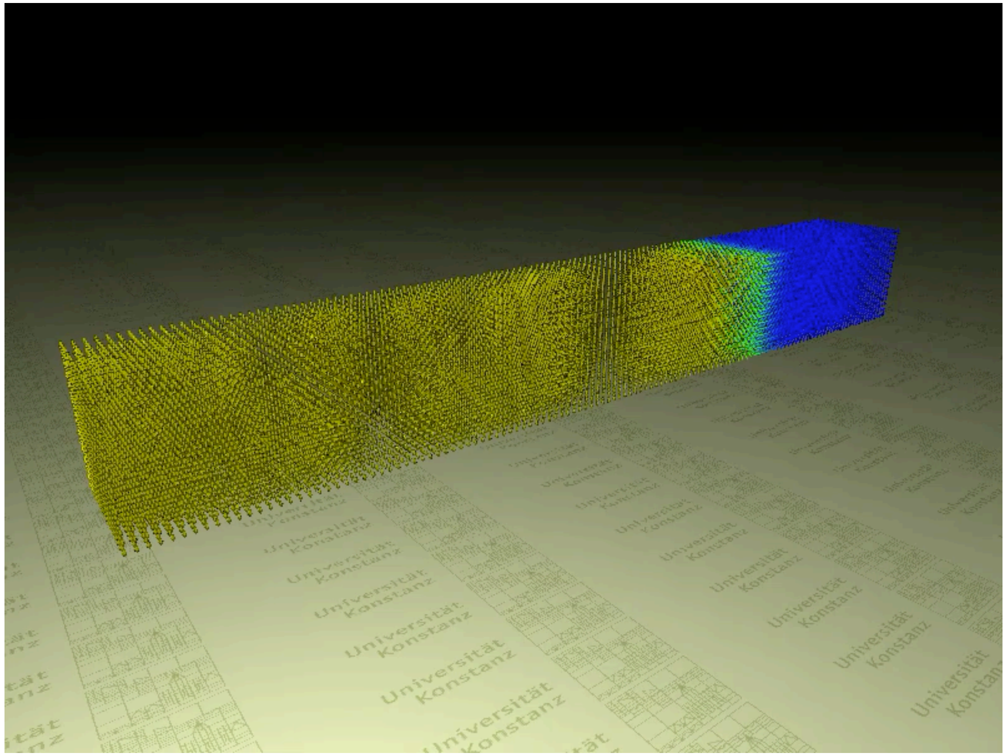
and further dissipative contributions as ***STT, SOT*** *…*

Key features:

- Atomic resolution
- Complex magnetic structures and interactions
- Ultrafast dynamics and non-equilibrium effects

Atomistic spin dynamics simulations

- Lattice in simulations corresponds to real magnetic lattice structure (in contrast to micromagnetics)
- Simulations with up to **10 000 000 lattice points** and **timesteps of 0.1-1 fs**
- Input parameters can be obtained by *ab initio* calculations or can be fitted from experiments



source: Uli Nowak, Konstanz

Atomistic spin dynamics simulations

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Advantages:

- **Includes lattice effects**
  - Correct dispersion curve
  - Exchange interaction beyond NN
- **Complex magnetic structures**
  - Antiferromagnets, ferrimagnets
  - Non-collinear states and magnetic textures
- **Non-equilibrium effects**

Disadvantages:

- Limited to small system sizes and short timescales
- Thermal noise and phenomenlogical damping is a pure phenomenological model
- Classical spin model

Stochastic equation of motion:

$$\dot{x}_i(t) = f(x_i(t), t) + g(x(t), t)\zeta(t)$$

Heun-method:

Predictor-step (Euler):

$$\bar{x}_{n+1} = x_n + f\left(x_n, t_n\right)\Delta t + g\left(x_n, t_n\right)\zeta(t_n)$$

Heun-step:

$$x_{n+1} = x_n + \frac{1}{2}\left(f\left(x_n, t_n\right) + f\left(\bar{x}_{n+1}, t_{n+1}\right)\right)\Delta t$$

$$+ \frac{1}{2}\left(g\left(x_n, t_n\right) + g\left(\bar{x}_{n+1}, t_{n+1}\right)\right)\zeta(t_n)$$

Random numbers:

Gaussion distribution: $p\left(\zeta\right) \propto \exp\left(-\frac{\zeta^2}{2\sigma^2}\right)$

Variance: $\sigma^2 = 2\alpha k_{\mathrm{B}} T \frac{\mu_{\mathrm{s}}}{\gamma} \Delta t$

I use a Zigggurat algorithm provided by gsl-library: *gsl_ran_gaussian_ziggurat*

Why are we using Heun-method?

Euler algorithm: $$\bar{x}_{n+1} = x_n + f\left(x_n, t_n\right) \Delta t + g\left(x_n, t_n\right) \zeta(t_n)$$

Converges towards wrong solution with stochastic noise: **Itô-Stratonovich dilemma**

→ Heun-method is lowest possible order (2nd order)

Higher-order Runge-Kutta are used (typically for simulations without temperature):
- advantages: adaptive step sizes possible, better stability enabling larger step size

Semi-implicit solver:
- possible larger timesteps

Mentink *et al.*, *J. Phys.: Condens. Matter* ***22****, 176001 (2010)*

Simple examples

Examples that you can explore with more details:

- Magnon dispersion

- Magnetization curve

- Demagnetization of a ferromagnet

Spin wave dispersion in ferromagnets

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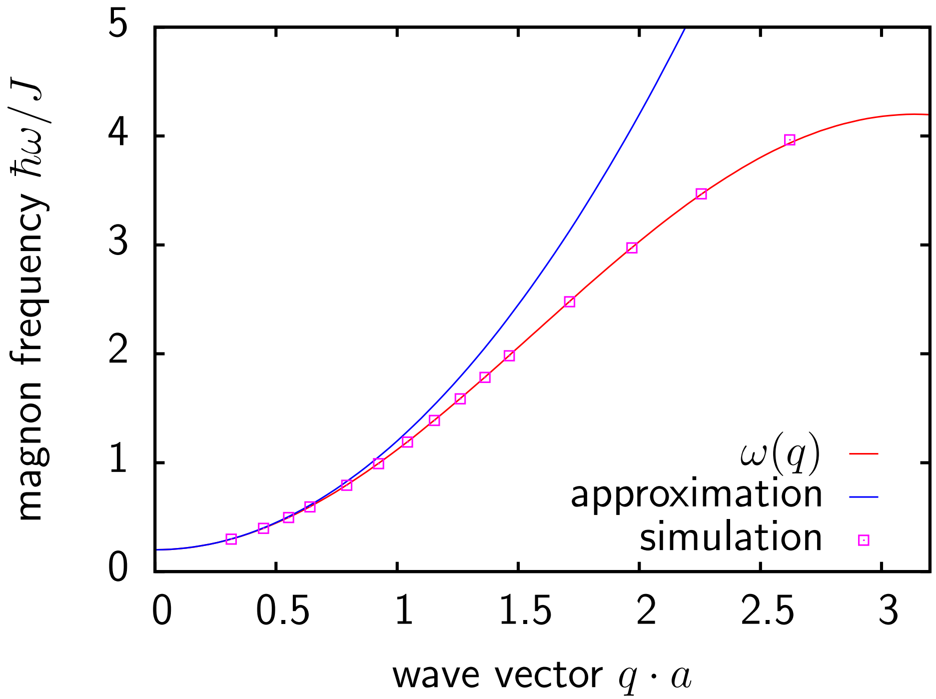
Linear spin wave theory:

- Linear LLG equation:

$$\frac{\partial S_i^x}{\partial t} = -\frac{\gamma}{\mu_\mathrm{s}}\Big(2d_z S_i^y + J\sum_j \left(S_i^y - S_j^y\right)\Big)$$

$$\frac{\partial S_i^y}{\partial t} = \frac{\gamma}{\mu_\mathrm{s}}\Big(2d_z S_i^x + J\sum_j \left(S_i^x - S_j^x\right)\Big)$$

$$\frac{\partial S_i^z}{\partial t} = 0$$



- Dispersion relation:

$$\hbar\omega_\mathbf{q} = 2d_z + J\sum_\theta \left(1 - \cos(q_\theta a)\right)$$

- Lifetime of a magnon: $\tau = \dfrac{1}{\alpha\omega_\mathbf{q}}$

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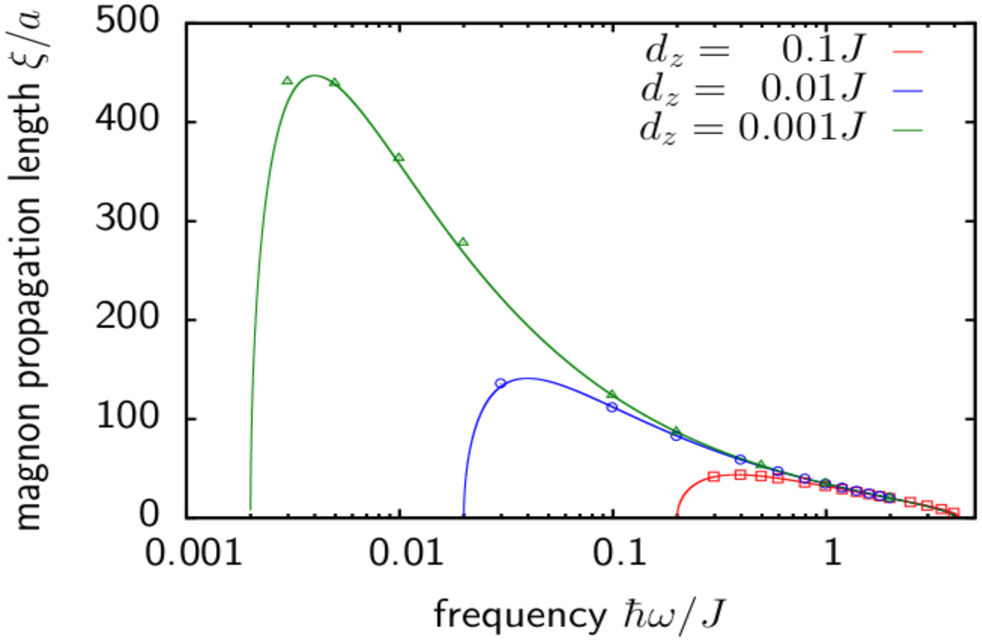

- Magnon propagation length:

$$\xi_{\mathbf{q}} = (\mathbf{v}_{\mathbf{q}}\mathbf{e}_z)\cdot\tau(\omega) = \frac{\partial\omega_{\mathbf{q}}}{\partial q_z}\cdot\frac{1}{\alpha\omega}$$

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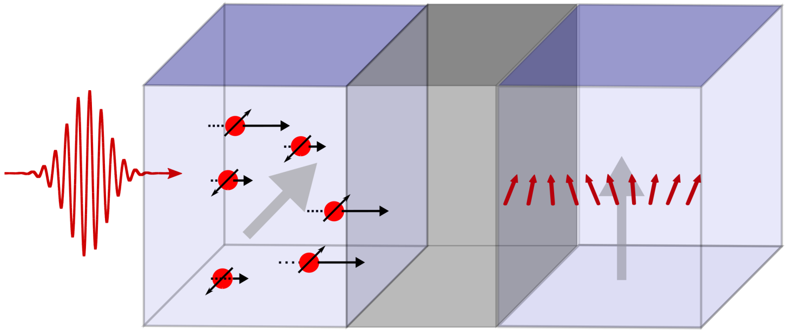
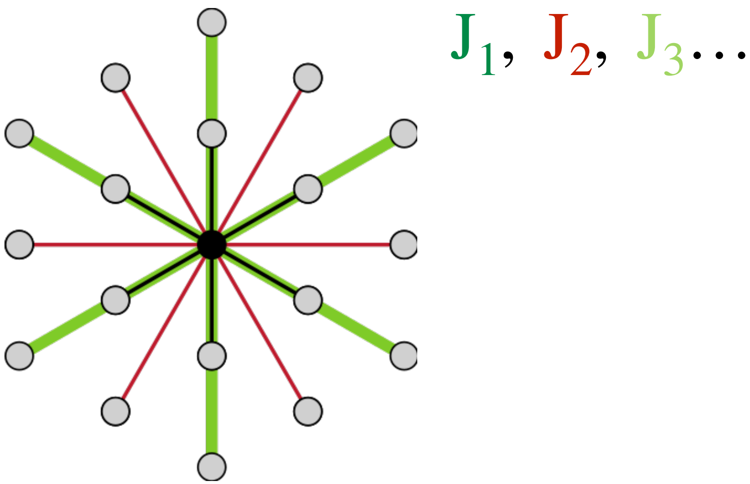
FeICuIFe layer:

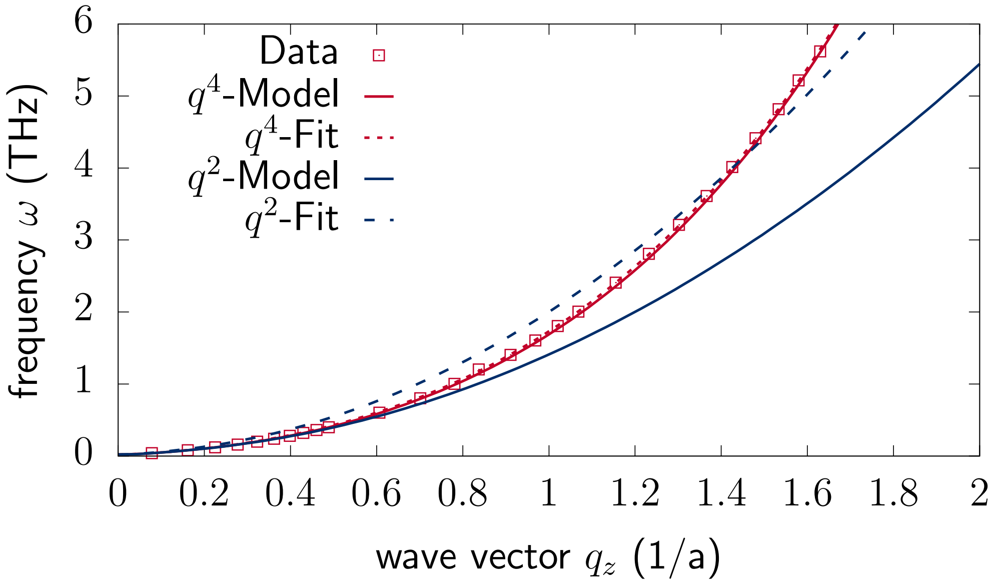




- Exchange interactions up to 6th neighbor:

$$\hbar\omega = \sqrt{(2k_x + J_{\text{eff}}(\mathbf{q})) \cdot (2k_x - 2k_z + J_{\text{eff}}(\mathbf{q}))}$$

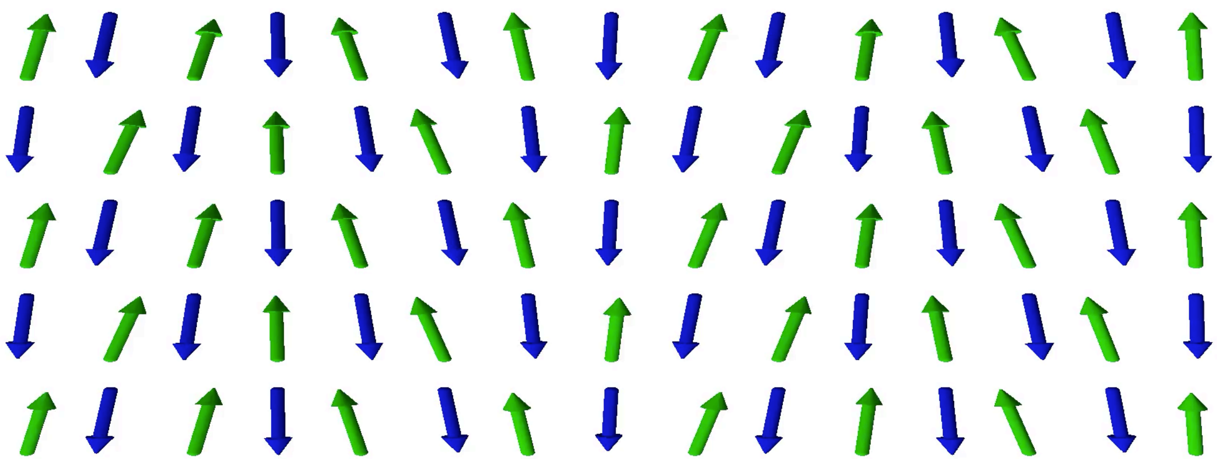
$$J_{\text{eff}}(\mathbf{q}) = \sum_{k=1}^{6} J_k \cdot \left(N_k - \sum_{\theta_k} 2 \cdot \cos(\mathbf{q} \cdot \boldsymbol{\theta}_k) \right)$$

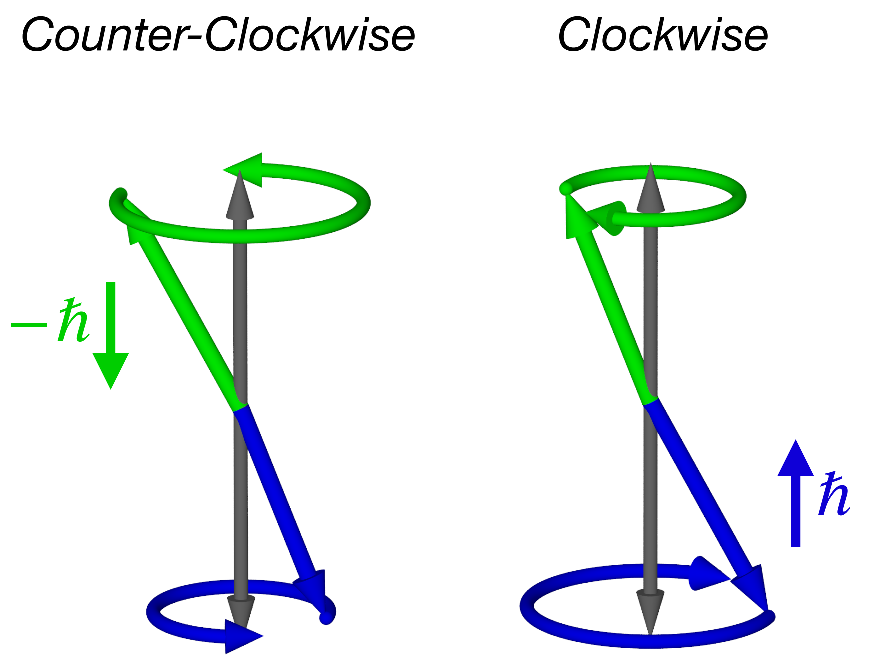


Spin waves in antiferromagnets

Dispersion relation:

$$\omega = \pm\left(\frac{\gamma}{\mu_{\rm s}}\right)\sqrt{\left(\left(2d_z + 6|J|\right)^2 - 4J^2\left(\sum_{\theta}\cos(qa)\right)^2\right)}$$





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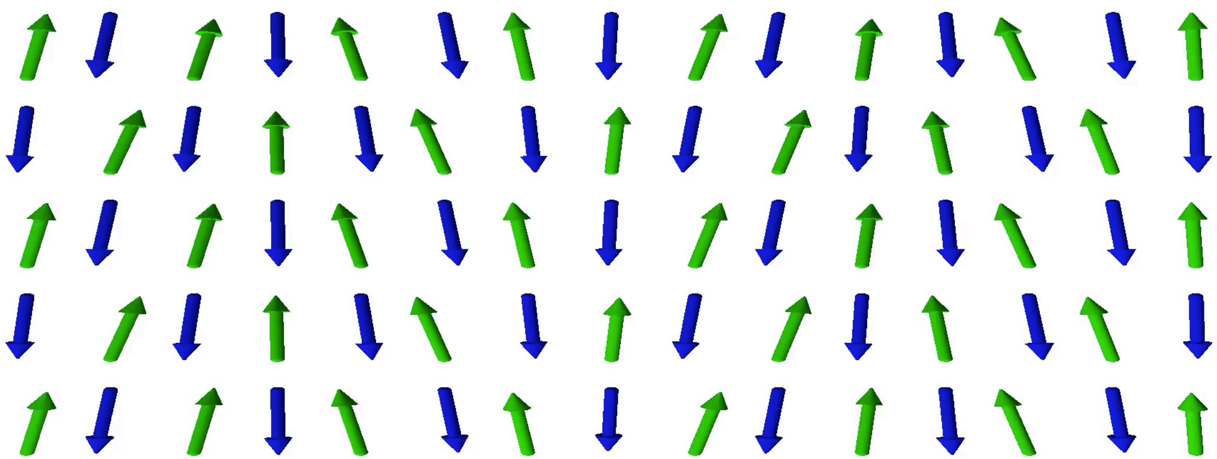

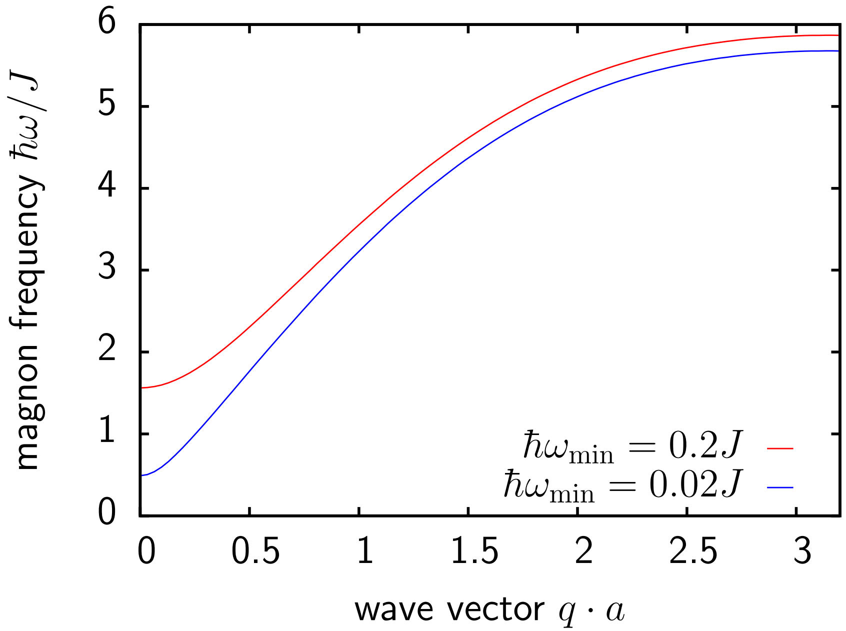

Magnetization curve

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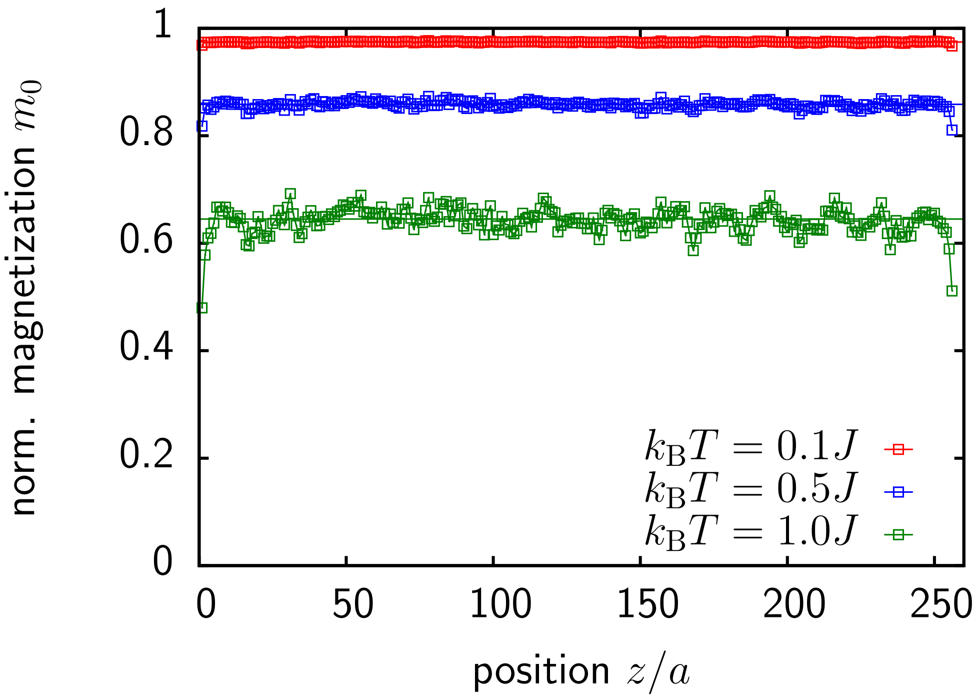
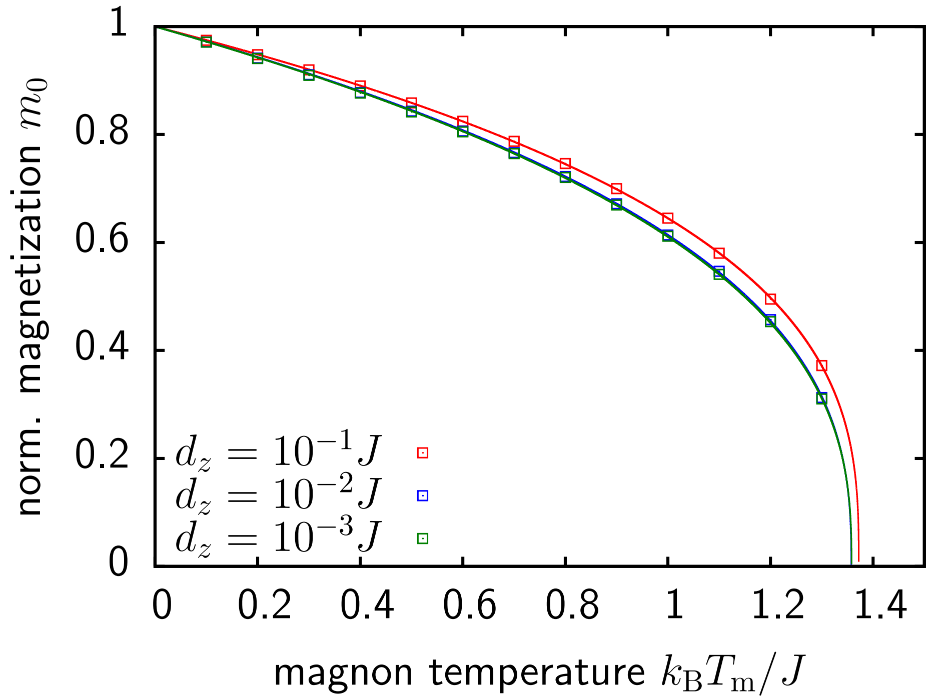


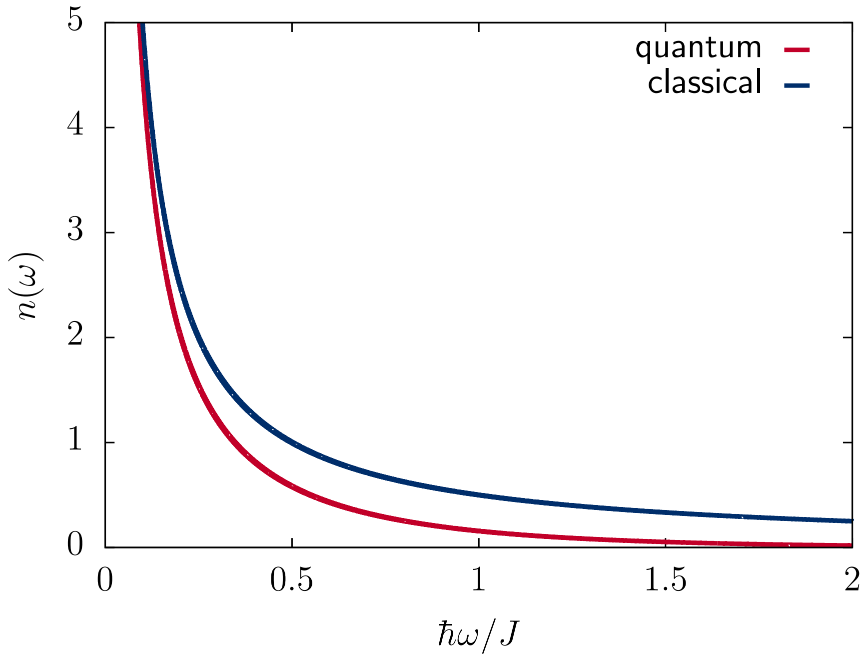


- Classical magnetization curve: linear scaling at low temperatures
- Increasing fluctuations with increasing temperature; finite size effects

Magnon distributions

- Magnons are bosons following Bose-Einstein statistics: $$n(\omega) = \frac{1}{\exp\left(\frac{\hbar\omega}{k_\mathrm{B}T}\right) - 1}$$

- Classical spin models lead to Rayleigh-Jeans distributions: $$n(\omega) = \frac{k_\mathrm{B}T}{\hbar\omega}$$



- numerical simulations include classical spin wave distributions

- High frequency with larger populations than in BE-statistics

- Different temperature-dependence of the magnetisation at low temperature

Magnetization curves in ferrimagnets

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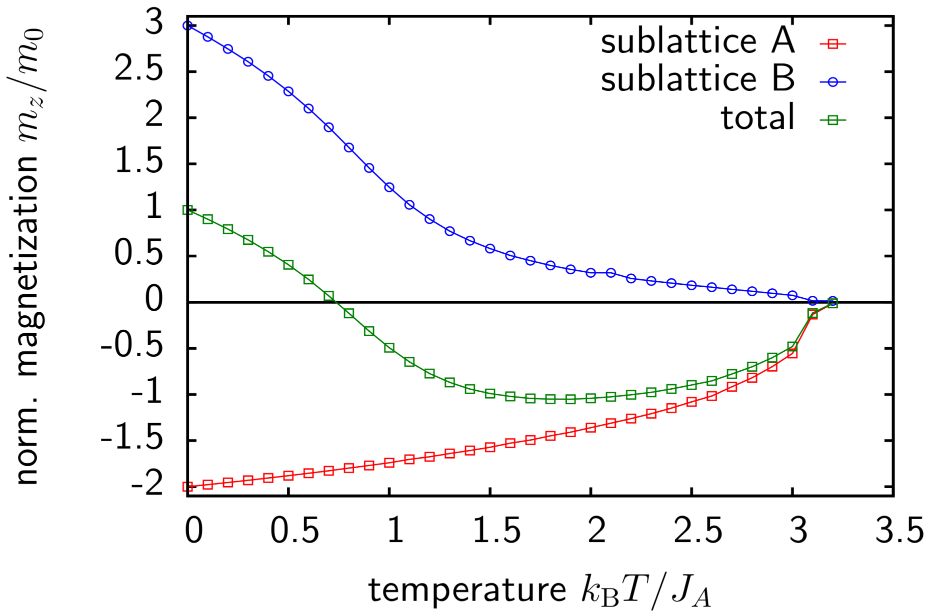
- Simulations in two-sublattice ferrimagnets
- Hamiltonian including next-nearest neighbor interaction

$$\mathcal{H} = \sum_{NN} J_{AB} \mathbf{S}_i \mathbf{S}_j + \sum_{NNN} (J_A \mathbf{S}_{i_A} \mathbf{S}_{j_A} + J_B \mathbf{S}_{i_B} \mathbf{S}_{j_B}) + \sum_i d_z S_{i,z}^2$$



$$J_B = 0.2 J_A; \quad J = -0.1 J_A \qquad \mu_{\mathrm{B}} = 1.5 \mu_{\mathrm{A}}$$

- sublattice B has higher magnetic moment, but demagnetizes at lower temperatures
- **Compensation point around:**

$$k_{\mathrm{B}} T_{\mathrm{comp}} \approx 0.7 J_A$$

Laser-induced Demagnetization and Switching

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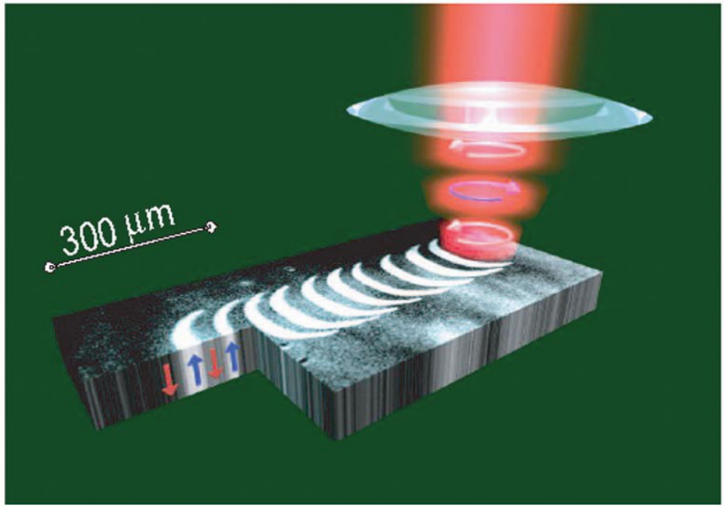


Stanciu *et al.*, *PRL* ***99***, 047601 (2007)

Simulations:

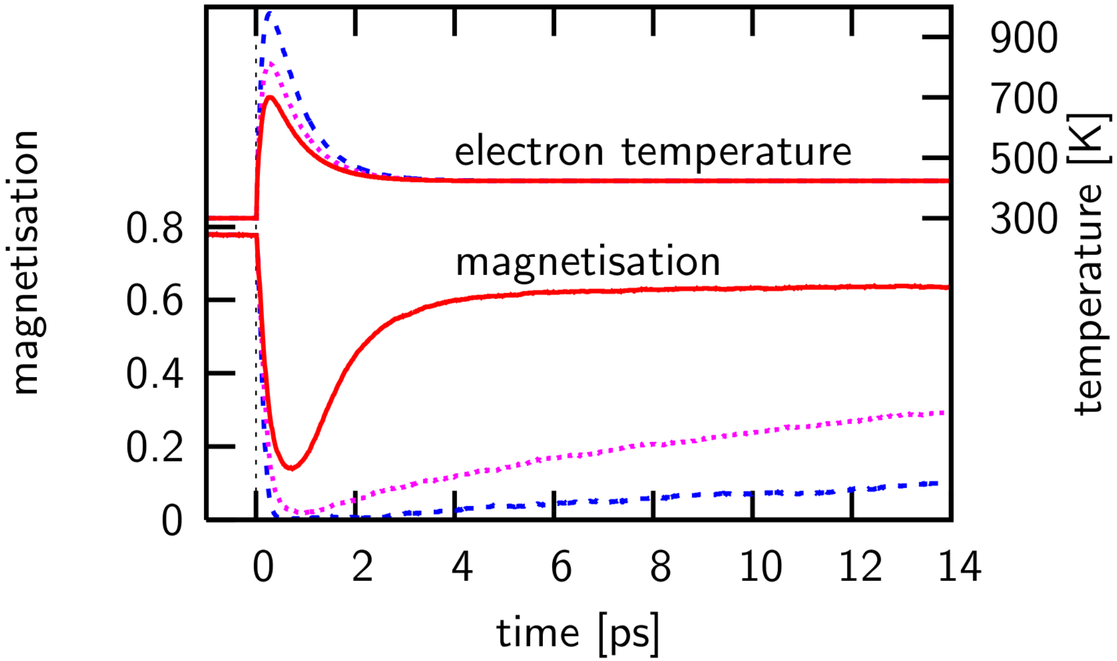
- laser-induced electron-phonon dynamics calculated by the two-temperature model:

$$C_{\mathrm{e}}\frac{\partial T_{\mathrm{e}}}{\partial t} = G_{\mathrm{ep}}(T_{\mathrm{p}}-T_{\mathrm{e}}) + P(z,t) + \frac{\partial}{\partial z}\kappa\frac{\partial T_{\mathrm{e}}}{\partial z} - \frac{\partial(E_{\mathrm{d}}+0.5E_{\mathrm{int}})}{\partial t},$$
$$C_{\mathrm{p}}\frac{\partial T_{\mathrm{p}}}{\partial t} = G_{\mathrm{ep}}(T_{\mathrm{e}}-T_{\mathrm{p}}) - 0.5\frac{\partial E_{\mathrm{int}}}{\partial t}.$$

- Spin-system coupled to the electron-phonon system

Frietsch *et al.*, *Nat. Commun.* ***6***, 9262 (2015)

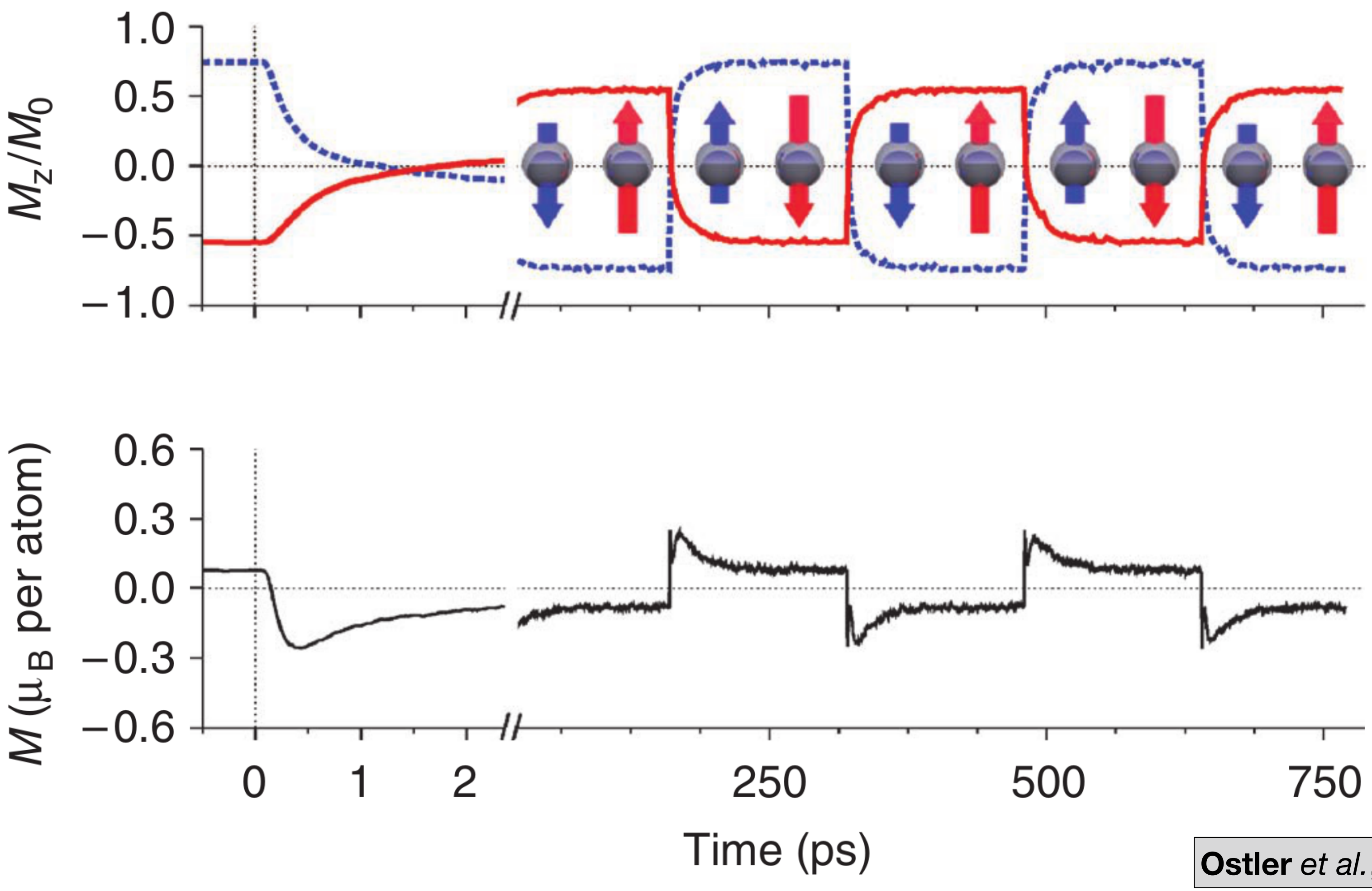
Demagnetization in FePt:



- Ultrafast demagnetization within a few ps
- Slow remagnetization times (formation of several domains)
- Final Magnetization direction not defined
- Further effects: induced moments via IFE

Kazantseva *et al.*, *PRB* ***77***, 184428 (2008)

Laser-induced Demagnetization and Switching



Ostler *et al.*, Nat. Commun. **3**, 666 (2012)

Introduction to the code

Most important parameters

- **System Size:**
  - *LX, LY, LZ* - number of lattice positions
  - *RAND_PLUS* - number of extra lattice positions at the boundaries
- **Flags for structure and boundary conditions:**
  - *KUBUS_SC* - to initialize sc ferromagnet
  - *PBC_X, PBC_Y* - periodic boundary conditions in x, y direction (if not set: open boundaries)
  - *MONO_Z* - to initialise monochromatic spin wave excitation at 0-th layer in z-direction
- **Simulation parameters**:
  - *DT, NMAX* - timestep and number of timesteps
  - *HX, DX, …* - external magnetic field and anisotropy (in units of J_1)
  - *TEMP* - constant temperature
  - *ALPH* - damping constant
  - *OMEGA, AMP* - frequency and amplitude of the oscillating boundary conditions

Most relevant functions of the code

- *Kubus(sx, sy, sz, find_index)* - initialize magnetic moments
- *gsl_ran_gaussian_ziggurat(rng, temp)* - random number generator
- *heun(spin, n, find_index, sx,sy,sz, ceta_x, ceta_y, ceta_z)* - *i*ntegration of 1 timestep
- *ex_sc(sx, i,j,k)* - calculate exchange interaction
- *fx(sx[i][j][k], sy[i][j][k], sz[i][j][k],hx[l], hy[l], hz[l])* - calculate deterministic part of equation of motion
- *cx(sx[i][j][k], sy[i][j][k], sz[i][j][k],hx[l], hy[l], hz[l])* - calculate stochastic part of equation of motion

Suggested tasks of the ATM

Dispersion curve

- **Simulation of a monochromatic wave in a (sc) ferromagnet:**
  - Excitation via oscillating boundary conditions in z-direction
  - Choose correct boundary conditions and excitation parameter (OMEGA, AMP)
  - Use 256x1x1 magnetic moments, ALPH=0.05, TEMP=0, D_X=0.01J, NMAX=10^6
  - Plot spatial magnetization profile and calculate wave vector and propagation length:

$$m_y = A \cdot \cos(q \cdot z + \phi) \cdot \exp(-z/\xi)$$

- **Questions:**
  - How is the dispersion curve defined?
  - What is the frequency range? What are the minimum and maximum value?
  - How is the rescaled frequency defined in the parameter set?
  - What is the order of the timestep?

Magnetization curve

- **Simulation of a monochromatic wave in a ferromagnet:**
  - Choose correct boundary conditions and vary the temperature
  - Use 32x32x32 magnetic moments, ALPH=1, D_X=0.01J, NMAX=10^5, DT=1.76x10^(-3)
  - Plot total magnetization as function of time and determine the equilibrium magnetization as function of the temperature.

- **Questions:**
  - What is the unit of the temperature? What is the critical temperature?
  - What are errors in the current fitting? How can it be improved?
  - How does magnetization and temperature scale for low temperatures? What scaling would you expect in reality?
  - Why are we using ALPH=1.0? What is the influence of the size?

Demagnetization

- **Simulation of demagnetization of a ferromagnet:**
  - Implement the temperature profile: TEMP=2.0 for 10^5<n<1.15 * 10^5, TEMP=0.5 else
  - Use 32x32x32 magnetic moments, ALPH=1, D_X=0.01J, NMAX=5*10^5
  - Plot total magnetization as function of time and vary the maximum temperature and the seed of the random number generator (example: change to 572235)

- **Questions:**
  - For which parameter do you obtain total demagnetization?
  - Why can’t you realize deterministic switching? What is the probability to obtain switching?