Spin-lattice dynamics (SLD) within the VAMPIRE software package

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Implementation based on: PRB 103, 024429 (2021)

PHYSICAL REVIEW B **103**, 024429 (2021)

Spin-lattice dynamics model with angular momentum transfer for canonical and microcanonical ensembles

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Outline

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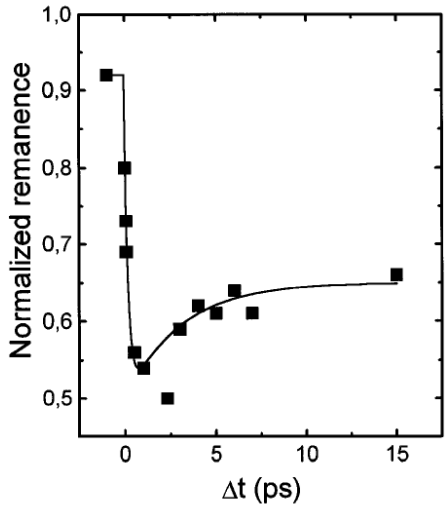
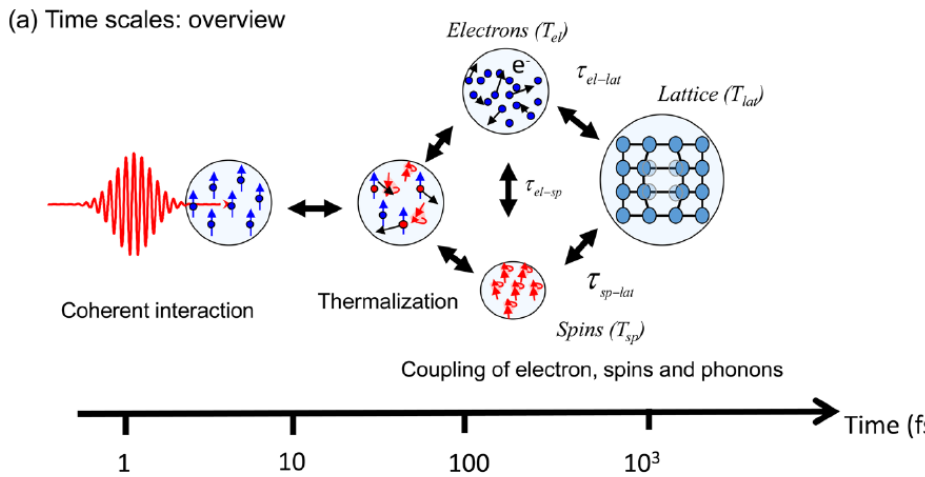
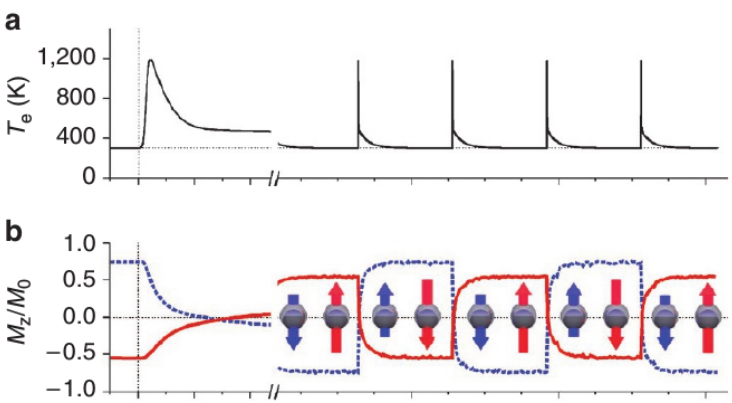
Controlling magnetisation with fs laser pulses



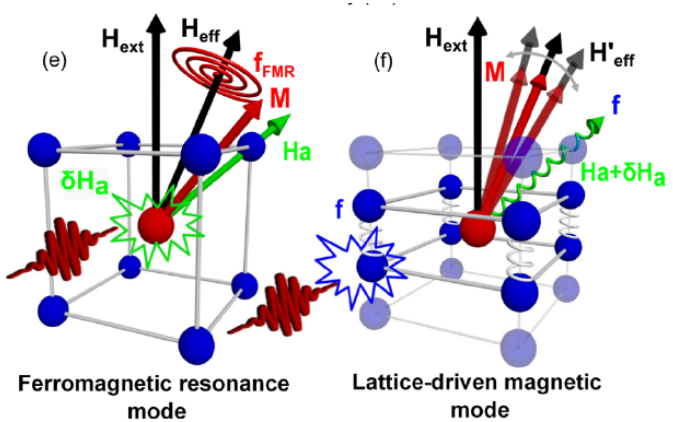
Beaurepaire, E., et al. PRL 76.22 (1996)



Walowski, J., Münzenberg, M. J. of Appl. Phys (2016)



Ostler, T. A. et al, Nature Comm. (2012)

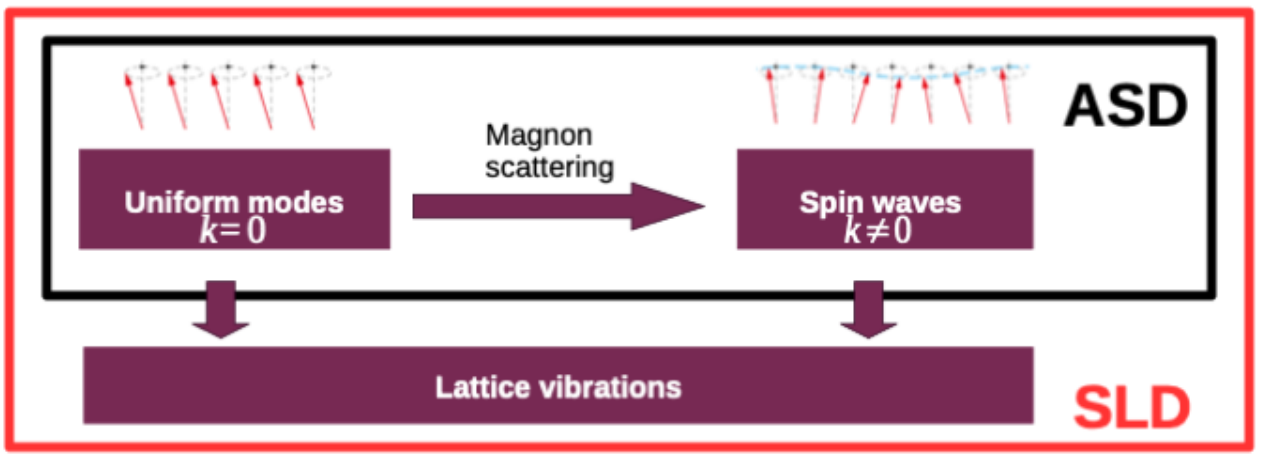


Afanasiev, D. et al, PRL (2014)

Exploring magnon-phonon damping with Spin-Lattice Dynamics Models

- Direct flow of angular momentum between lattice and spins;
- Magnon-phonon contribution to damping;
- Possibility of modelling dissipation in magnetic insulators;

LLG Equation: $$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma}{(1+\alpha^2)}\mathbf{S}_i \times (\mathbf{H}_i + \alpha \mathbf{S}_i \times \mathbf{H}_i)$$



ASD – Atomistic spin dynamics (fixed lattice)
SLD – Spin-lattice dynamics (dynamic lattice)

Applications

Outline

Hamiltonian = Magnetic + Mechanical

$$H_{tot} = -\sum_{i,j} J(r_{ij})(\mathbf{S}_i \cdot \mathbf{S}_j) - \sum_{i,j} f(r_{ij})((\mathbf{S}_i \cdot \hat{\mathbf{r}}_{ij})(\mathbf{S}_j \cdot \hat{\mathbf{r}_{ij}}) - \frac{1}{3}\mathbf{S}_i\mathbf{S}_j) + \sum_i \frac{\mathbf{p}_i^2}{2m_i} + \frac{1}{2}\sum_{i,j} U(r_{ij})$$

$$\frac{\partial \mathbf{r}_i}{\partial t} = \mathbf{v}_i, \qquad \mathbf{H}_i = -\frac{1}{\mu_S \mu_0}\frac{\partial H_{tot}}{\partial \mathbf{S}_i} + \boldsymbol{\xi}_i$$

$$\frac{\partial \mathbf{v}_i}{\partial t} = \frac{\mathbf{F}_i}{m_i}, \qquad \mathbf{F}_i = -\frac{\partial H_{tot}}{\partial \mathbf{r}_i} - \eta m_i \mathbf{v}_i + \boldsymbol{\Gamma}_i$$

$$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma}{(1+\alpha_{\mathrm{G}}^2)}\mathbf{S}_i \times (\mathbf{H}_i + \alpha_{\mathrm{G}}\mathbf{S}_i \times \mathbf{H}_i),$$

Akhiezer, A. I.et al, 1968; Ma, P.-W.et al PRB 2008; Aßmann, M.et al JMMM 2019

Summary of contributions to damping in SLD models

Model	Lattice	Lattice thermostat	Spin thermostat	Intrinsic Spin damping
SLD	Dynamic	On	Off	Phonon induced
ASD	Fixed	Off	On	Electronic mainly

Summary comparison of the SLD model developed here against other spin dynamics models.

Integration: Suzuki-Trotter decomposition, svrvs

$$\frac{\partial \mathbf{X}}{\partial t} = \hat{L}\mathbf{X(t)} = (\hat{L}_r + \hat{L}_v + \hat{L}_S)\mathbf{X}(t)$$

$$\mathbf{X}(t+\Delta t) = e^{\hat{L}_s(\Delta t/2)} e^{\hat{L}_v(\Delta t/2)} e^{\hat{L}_r(\Delta t)} e^{\hat{L}_v(\Delta t/2)} e^{\hat{L}_s(\Delta t/2)} \mathbf{X}(\Delta t) + O(\Delta t^3)$$

$$e^{\hat{L}_s(\Delta t/2)} = e^{\hat{L}_{s1}(\Delta t/4)} \ldots e^{\hat{L}_{sN}(\Delta t/2)} \ldots e^{\hat{L}_{s1}(\Delta t/4)} + O(\Delta t^3)$$

$$e^{\hat{L}_v \Delta t}\mathbf{v}_i = \mathbf{v}_i + \frac{\Delta t}{m_i}\mathbf{F}_i$$

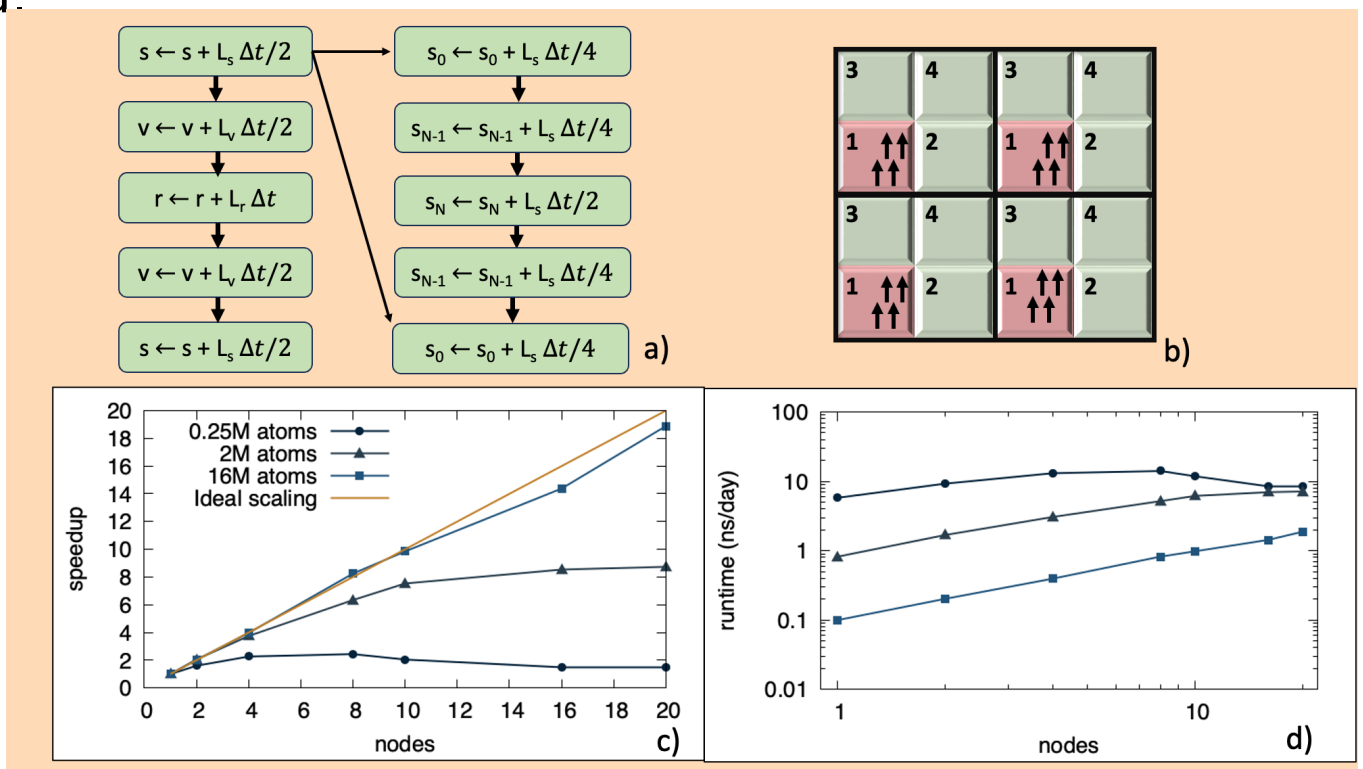
$$e^{\hat{L}_r \Delta t}\mathbf{r}_i = \mathbf{r}_i + \Delta t \mathbf{v}_i$$

$$e^{\hat{L}_S \Delta t}\mathbf{S}_i = \frac{\mathbf{S}_i + \Delta t \mathbf{H}_i \times \mathbf{S}_i + \frac{\Delta t^2}{2}((\mathbf{H}_i \cdot \mathbf{S}_i)\mathbf{H}_i - \frac{1}{2}\mathbf{H}_i^2 \mathbf{S}_i)}{1 + \frac{1}{4}\Delta t^2 \mathbf{H}_i^2}$$

Parallel implementation and scalability;

For the parallel update the sectoring method (illustration panel b) is used.

[htb!]



a)

Illustration of Suzuki-Trotter decomposition update; b) Illustration of sectoring for a 2x2 CPUs for 2D system. c-d) Scalability tests performed on ARCHER2.

BCC Fe parameters

Quantity	Symbol	Value	Units
Exchange[1]	J_0	0.904	
	r_c	3.75	
Harmonic potential[2]	V_0	0.15	eV
	r_c	7.8	
Magnetic moment	μ_s	2.22	μ_B
Coupling constant	C	0.5	
Mass	m	55.845	u
Lattice constant	a	2.8635	
Lattice damping	η	0.6	s^{-1}

$$J(r_{ij}) = J_0(1 - \frac{r_{ij}}{r_c})^3\Theta(r_c - r_{ij})$$

[1] *Ma, P.W.et al. PRB*(2008)

$$\mathrm{f}(r_{ij}) = CJ_0/{r_{ij}}^4$$

[2] *Aßmann, M.et al. JMMM*(2019)

Choices of Mechanical Potential

Harmonic potential:

$$U(r_{ij}) = V_0(r_{ij} - r_{ij}^0)^2$$

Morse potential:

$$U(r_{ij}) = D[exp(-2\alpha(r_{ij} - r_0) - 2exp(-\alpha(r_{ij} - r_0))]$$

Outline

Tutorial 1 - equilibration of the spin and lattice subsystems

- **Change integrator to Suzuki-Trotter decomposition**
  - Use the flag `sim:integrator = spin-lattice` in your input.
- **Set BCC iron crystal structure.**
  - Use `create:crystal-structure=bcc`.
  - Enable periodic boundaries in all directions: `create:periodic-boundaries-x/y/z`.
  - Define the unit cell size: `dimensions:unit-cell-size = 2.87 !A`.
  - Define the system dimensions in nm: `dimensions:system-size-x/y/z = 2.87 !nm`.
  - Sanity check: confirm the resulting number of atoms is reasonable for equilibration tests.
- **Load material parameters.**
  - In the material file: `material:file = fe.mat` add parameters for both spin and lattice dynamics needed by the spin-lattice integrator.

Tutorial 1 - equilibration of the spin and lattice subsystems (continuation

- **Choose simulation program.** Use the benchmark `sim:program = benchmark`.
- **Define program parameters.**
  - Set target temperature: `sim:temperature = 10`.
  - Set timestep and total steps: `sim:time-step = 0.5 !fs`, `sim:total-time-steps = ----`.
- **Configure spin–lattice (SLD) model.**
  - Set the interatomic potential and cutoffs: `spin-lattice:potential=harmonic`, `spin-lattice:potential-cutoff-range=7.8 !A`.
  - Set field cutoff and coupling: `spin-lattice:fields-cutoff-range=3.75 !A`, `spin-lattice:coupling=pseudodipolar`.
  - Set exchange range: `exchange:interaction-range = 3`.

Tutorial 1 - equilibration of the spin and lattice subsystems

- **Enable configurations.**
  - Write atomic configuration snapshots: `config:atoms`.
  - Choose snapshot frequency: `config:atoms-output-rate=10000`.
  - Enable SLD output: `config:sld`.
- **Select observables for lattice and spin equilibration.**
  - File output: `output:real-time`, `output:magnetisation`, `output:spin-temperature`, `output:lattice-temperature`.
  - Screen output (quick monitoring): `screen:real-time`, `screen:magnetisation`, `screen:spin-temperature`, `screen:lattice-temperature`.

Tutorial 1 - equilibration of the spin and lattice subsystems

- **Run and check equilibration criteria.**
  - Confirm `spin-temperature` and `lattice-temperature` approach the target (10 K) and fluctuate around steady means.
- **Additional exercises**
  - Increase `sim:total-time-steps` if either subsystem equilibrates slowly.
  - Investigate the effect of different parameters, such as target temperature.

Solutions tutorial 1: BCC Fe.mat file

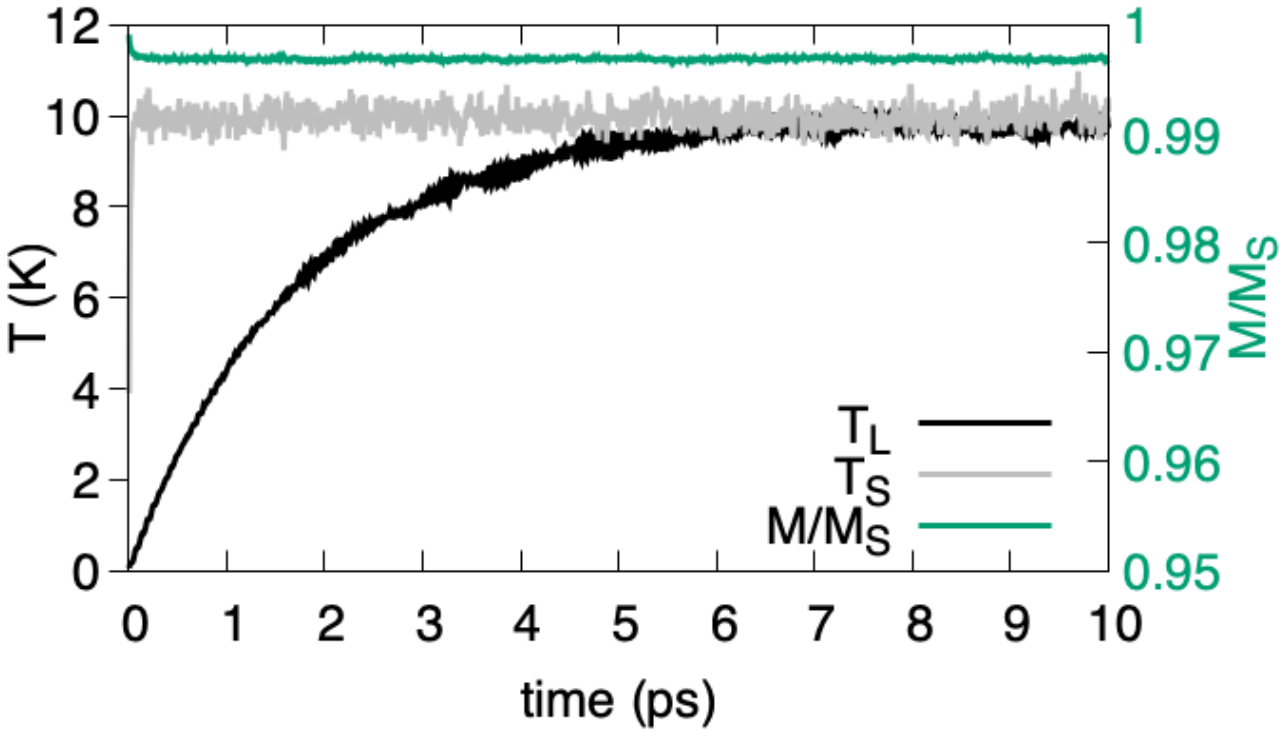
```
#=====================================================
# Sample vampire material SLD
#=====================================================

#-----------------------------------------------------
# Number of Materials
#-----------------------------------------------------
material:num-materials=1
#-----------------------------------------------------
# Material 1 BCC Fe
#-----------------------------------------------------
material[1]:material-name=Co
material[1]:damping-constant=0.1
material[1]:atomic-spin-moment=2.22 !muB
material[1]:initial-spin-direction=0,0,1
#material[1]:uniaxial-anisotropy-constant=1.0e-24

# SLD Parameters
#-----------------------------------------------------
material[1]:mass=5.7915e-3
material[1]:damping-constant-lattice=0.6
material[1]:exchange-J0=0.904 !eV
material[1]:harmonic-potential-V0=0.15 !eV
material[1]:coupling-C0=0.5
```

Solution tutorial 1: Basic input SLD

```
#----------------------------------------
# Sample vampire input file to perform
# benchmark calculation for v4.0
#
#----------------------------------------
create:crystal-structure=bcc
create:periodic-boundaries-x
create:periodic-boundaries-y
create:periodic-boundaries-z


#----------------------------------------
# Creation attributes:
#----------------------------------------
dimensions:unit-cell-size = 2.87 !A
dimensions:system-size-x = 2.87 !nm
dimensions:system-size-y = 2.87 !nm
dimensions:system-size-z = 2.87 !nm


#----------------------------------------
# Material Files:
#----------------------------------------
material:file = fe.mat
```

```
#----------------------------------------
# Simulation attributes:
#----------------------------------------
sim:temperature = 10
sim:time-steps-increment = 1
sim:total-time-steps = 20000
sim:time-step = 0.5 !fs

#----------------------------------------
# Program and integrator details
#----------------------------------------
sim:program = benchmark
sim:integrator = spin-lattice

spin-lattice:potential-cutoff-range=7.8 !A
spin-lattice:fields-cutoff-range=3.75 !A
spin-lattice:coupling=pseudodipolar
spin-lattice:potential=harmonic

exchange:interaction-range = 3

config:atoms
config:atoms-output-rate=10000
config:sld

output:real-time
output:magnetisation
output:spin-temperature
output:lattice-temperature
```

Solution tutorial 1: Benchmark T=10K



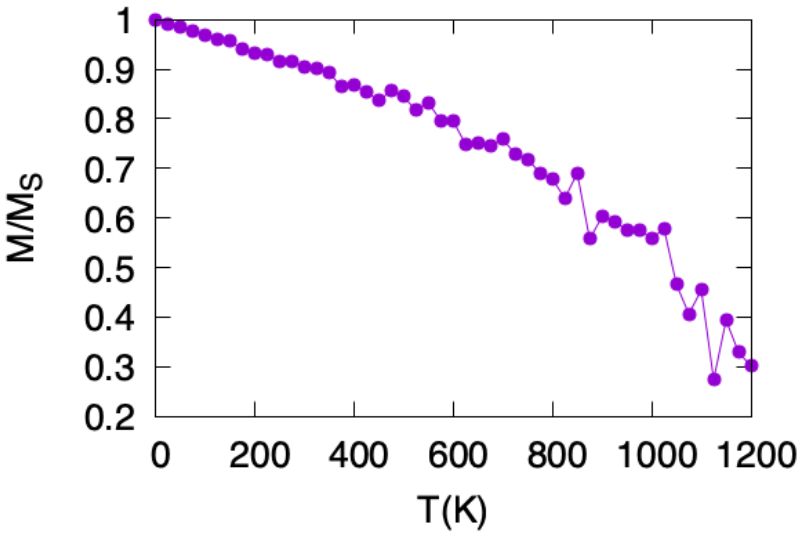
Tutorial 3 - Calculation of Curie Temperature

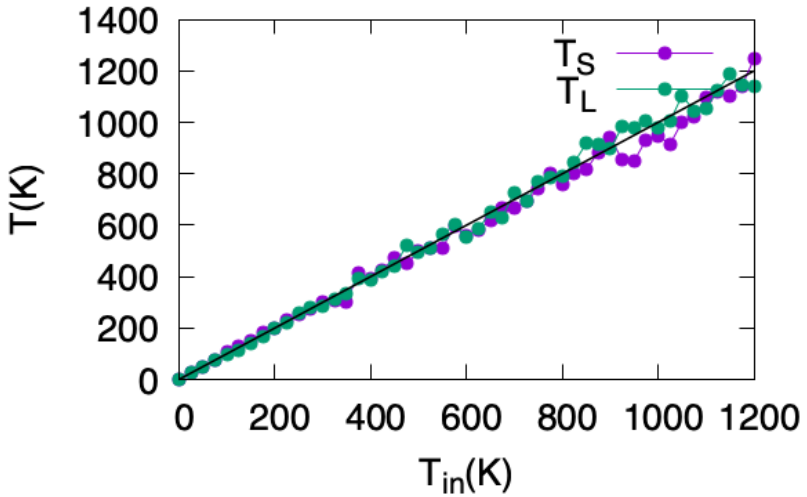
- For this exercise, you can use the previous system defined in `fe.mat`.
- A temperature sweep from 0 K to 1200 K is performed using the `curie-temperature` program, with equilibration at each temperature.
- Spin-lattice dynamics integrator is used.
- The Curie temperature is identified from the temperature dependence of the magnetisation.
- The spin and lattice temperature can be plotted to check for equilibration

Tutorial 3 Solution: Curie temperature

```
dimensions:unit-cell-size = 2.87 !A
dimensions:system-size-x = 1.435 !nm
dimensions:system-size-y = 1.435 !nm
dimensions:system-size-z = 1.455 !nm


#---------------------------------------
# Material Files:
#---------------------------------------
material:file = fe.mat


# Simulation attributes:
#---------------------------------------
sim:equilibration-time-steps = 5000
sim:loop-time-steps = 5000
sim:time-steps-increment = 1

sim:minimum-temperature = 0
sim:maximum-temperature = 1200
sim:temperature-increment = 25
sim:time-steps-increment = 1

sim:time-step = 0.5 !fs

#---------------------------------------
# Program and integrator details
#---------------------------------------
sim:program =curie-temperature
```

Tutorial 3 Solution: Curie temperature





Tutorial 4: THz phonon excitation

PHYSICAL REVIEW B **109**, 224412 (2024)

Route to minimally dissipative switching in magnets via terahertz phonon pumping

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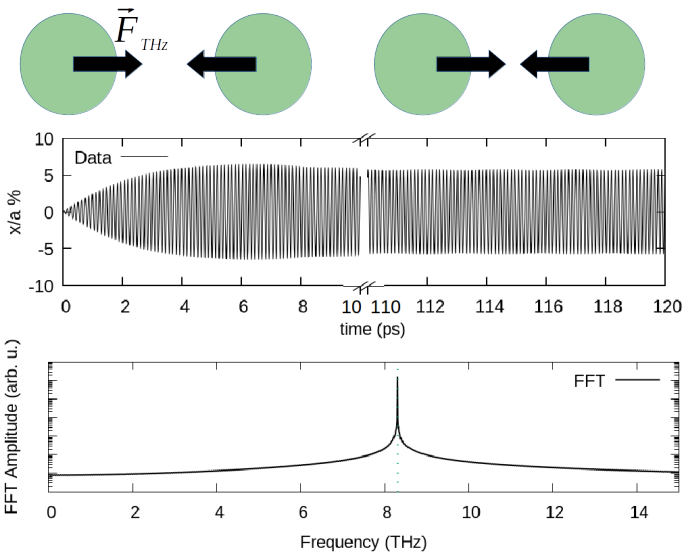
Ultrafast switching of magnetic materials has been shown to be predominantly thermally driven, but excess heating limits the energy efficiency of this process. By employing atomistic spin-lattice dynamics simulations, we show that efficient coherent magnetization switching of an insulating magnet can be triggered by a THz excitation of phonons. We find that switching is driven by excitation near the P point of the phonon spectrum in conditions where spins typically cannot be excited and when manifold k phonon modes are accessible at the same frequency. Our model determines the necessary ingredients for low-dissipative switching and provides insight into THz-excited spin dynamics with a route to energy efficient ultrafast devices.

DOI: 10.1103/PhysRevB.109.224412

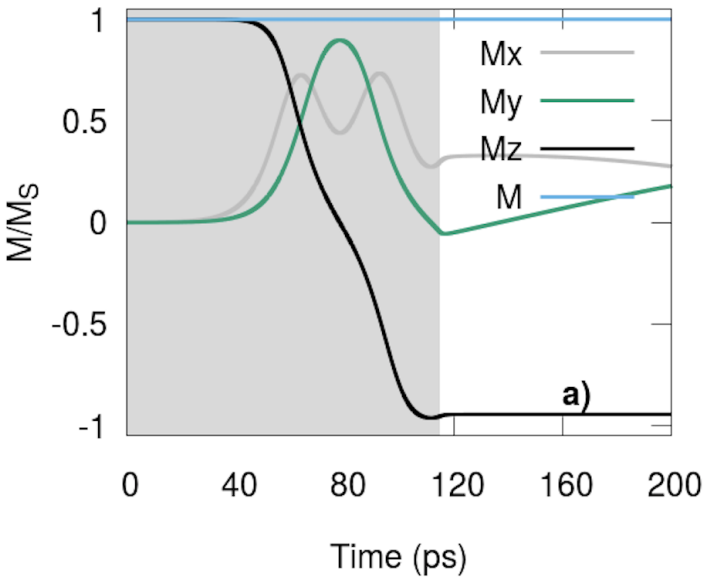
Thz excitation of the lattice

$$Fi^{\alpha}_{Thz} = f^{\alpha}_{0} cos(2\pi\nu t + \vec{k}\cdot\vec{r_i})$$

$$\alpha = x, y, z; k = (2\pi/\lambda, 0, 0).$$



Normalised position and Fourier Transform during the application of a THz force of 8.3 THz.



Magnetisation switching via a THz pulse of 115 ps.

Acknowledgment

The implementation in VAMPIRE of the THz phonons has been done by Muhammad Asim (Hamza) as part of SOE internship at University of Manchester. Implementation is available in vampire-develop.

Tutorial 4: Thz excitation of the lattice

- Use the same system, a bcc Fe supercell. This is a long simulation, with switching being observed after 40ps.
- Spin-lattice dynamics integrator with a harmonic interatomic potential.
- A coherent THz lattice excitation is applied via a linear phonon force, switched on between 5 ps and 400 ps to drive the system out of equilibrium.
- The excitation frequency is set to 8.3 THz,
- The phonon force amplitude is defined along the Cartesian directions.
- The phonon wavevector is specified by its wavelength and direction, corresponding to the P-point of the Brillouin zone, allowing selective excitation of a well-defined **k**-mode.

Tutorial 4 Solution: THz excitation of phonons

```
phonon:linear-pump = true
phonon:frequency = 8.3 ! THz
phonon:pulse-start-time = 5 ! ps
phonon:pulse-end-time = 400 ! ps

#Set the y/z component to the same amplitude as x for chiral simulation
phonon:force-amplitude-x = 0.05 ! A
phonon:force-amplitude-y = 0.0 ! A
phonon:force-amplitude-z = 0.0

#Sets the k wavevector components to P point from the Brillouin zone
phonon:wave-lambda-x = 5.75
phonon:wave-lambda-y = 5.75
phonon:wave-lambda-z = 5.75

phonon:wave-direction-x = 1
phonon:wave-direction-y = 1
phonon:wave-direction-z = 1
```