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

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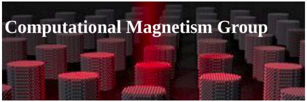

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Spin-lattice dynamics model with angular momentum transfer for canonical and microcanonical ensembles

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Outline

1. Introduction
2. Spin-Lattice Dynamics Framework
3. VAMPIRE tests

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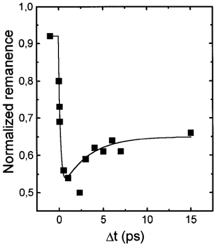
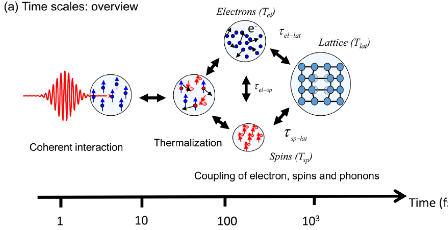
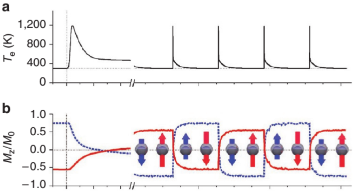
Controlling magnetisation with fs laser pulses



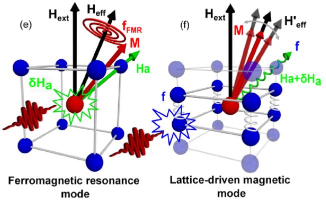
Beaurepaire, E., et al. PRL 76.22 (1996)



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



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



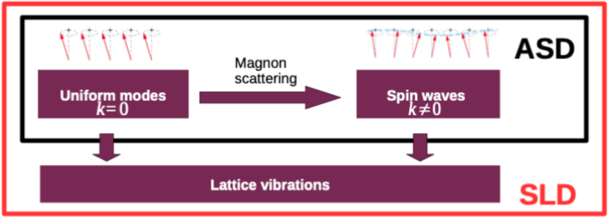
Afanasiev, D. et al, PRL (2014)

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)

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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

Integration: Suzuki-Trotter decomposition, svrvs

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

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

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

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

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

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

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)

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

[2] *Aßmann, M. et al. JMMM* (2019)

Outline

BCC Fe .mat file

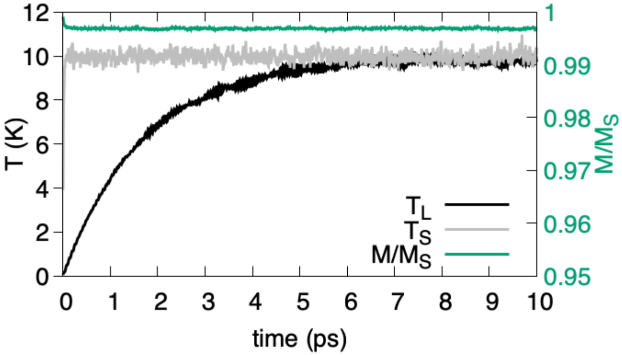
```
#=====================================================
# Sample vampire material SLD
#=====================================================

#-----------------------------------------------------
# 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
```

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
```

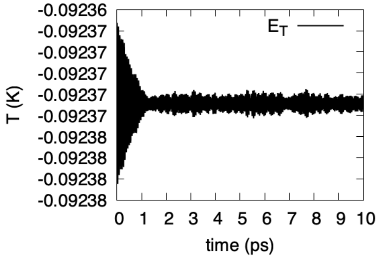
```
#------------------------------------------
# Simulation attributes:
#------------------------------------------
sim:temperature = 10
sim:time-steps-increment = 1
sim:total-time-steps = 20000
sim:time-step = 0.5 !fs

#------------------------------------------
# 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
```

Benchmark T=10K

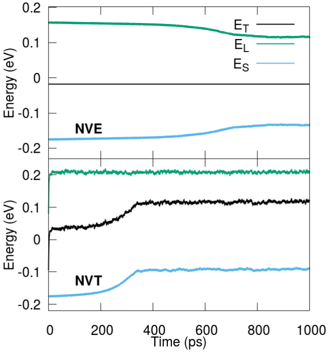


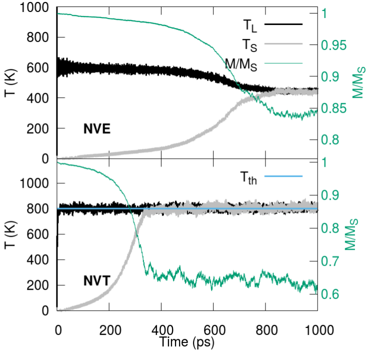
NVE - conservation of energy test

```
#######################################
#fe.mat
material[1]:damping-constant=0.0
material[1]:damping-constant-lattice=0

#######################################
#input
sim:temperature = 0

#some initial energy to go into the system
sim:equilibration-temperature=600
spin-lattice:initial-random-displacement=0.1
spin-lattice:initial-thermal-velocity=600

#output the energies
output:kinetic-energy
output:potential-energy
output:sld-exchange-energy
output:sld-coupling-energy
output:output-rate=1
```



Equilibrium properties NVE/NVT long timescales





NVE (top) and NVT (bottom) simulations for a $10 \times 10 \times 10$ unit cell BCC Fe system and a coupling constant of $C = 0.5$;

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
```

Curie temperature