Modeling of magneto-thermo-dynamics

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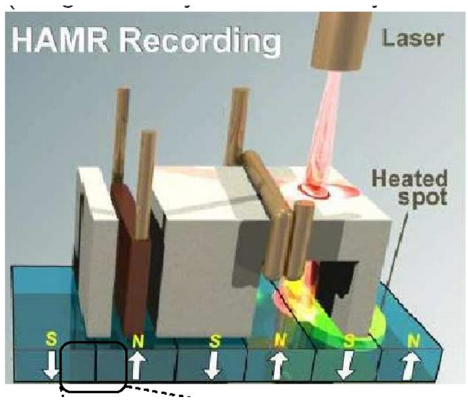
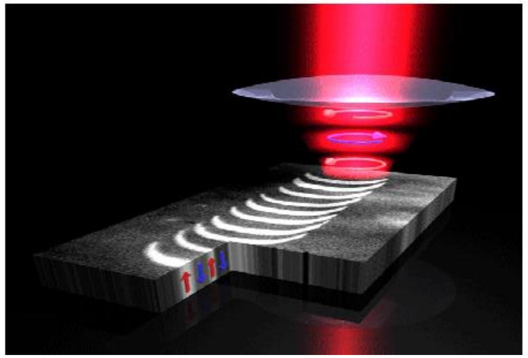
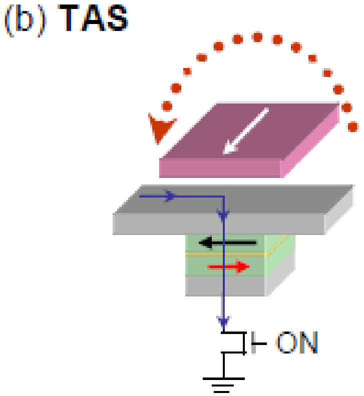
Magneto- thermo- dynamics applications



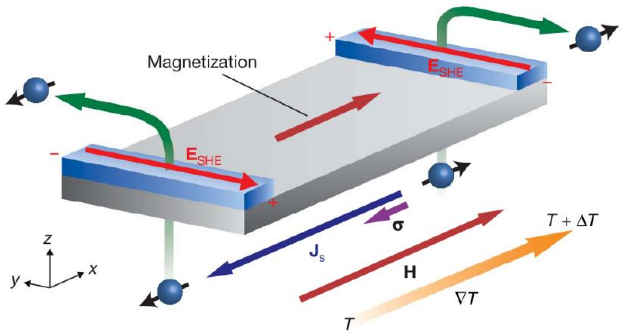
Ultra-fast laser-induced dynamics,
All-optical recording



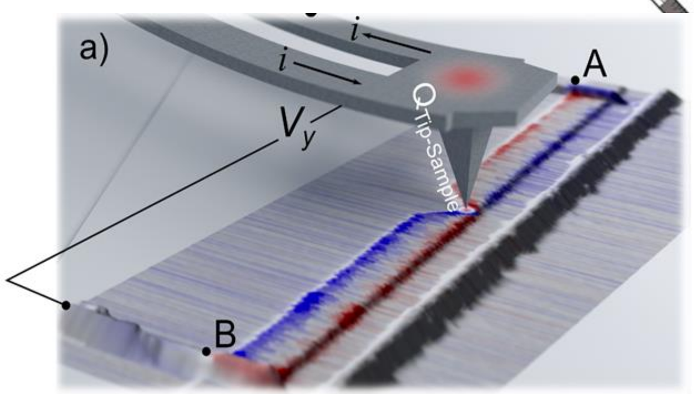
Spintronics:
Thermally-assisted MRAM



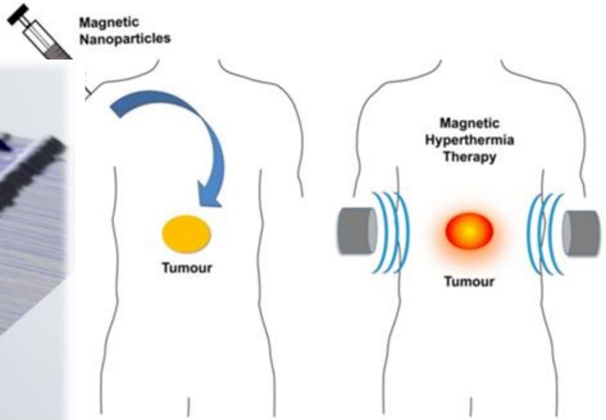
Spin-caloritronics
Motion under thermal gradients



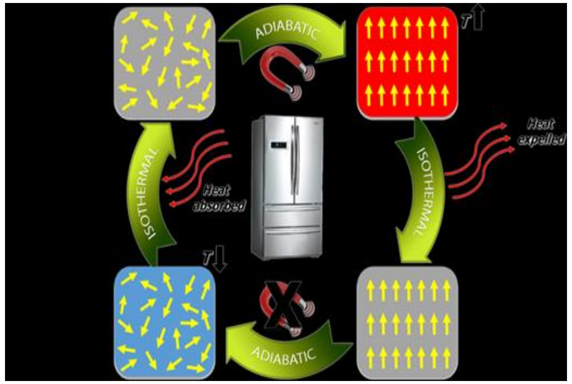
Thermal magnetometry

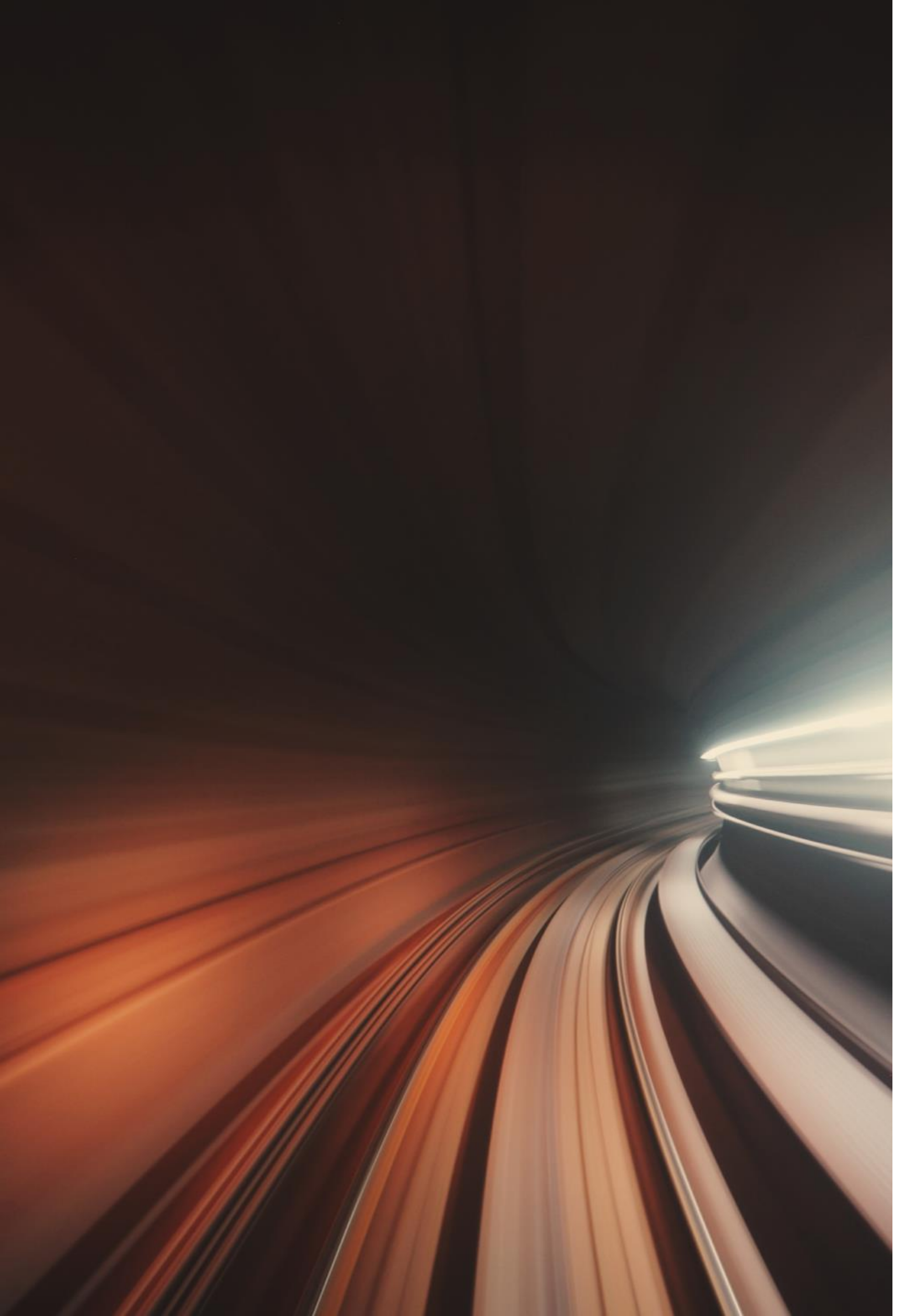


Magnetic fluid hyperthermia



Magnetic refrigiration





OUTLINE

Introduction: some fundamentals for thermal modelling

1. Stochastic atomistic dynamics and Landau-Lifshitz-Bloch (LLB) micromagnetics
2. Scaling of temperature-dependent parameters: Domain wall width and skyrmion radius increase with temperature

Reciprocal magneto-thermodynamics effects:

1. **Spin-Seebeck effect.**

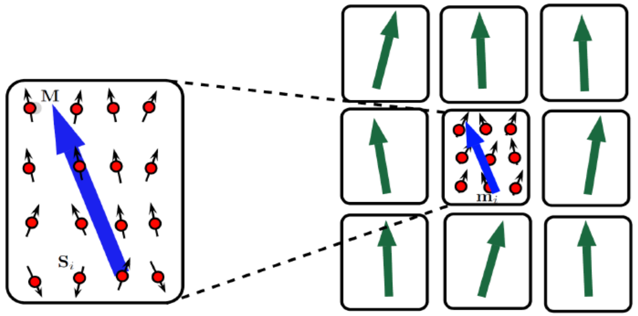
Motion of domain walls and skyrmions in thermal gradients

2. Giant localized **spin-Peltier effect** for ultrafast domain wall motion in antiferromagnets

Introduction: Atomistic/micromagnetic approach:

•Atomistic spins (localized classical magnetic moments μ in the Heisenberg description with J and on-site anisotr. d), $\alpha(\lambda)$ defines coupling to thermal bath

Characteristic timescale is determined by exchange (fs-ps)



•Micromagnetic units (averaged magnetisation, Ms(T)), A(T), K(T)

The temperature in this case is included twice:

- The damping α contains already thermal averaging: $\alpha(T)$
- Langevin dynamics defines different trajectories

Characteristic timescale is determined by applied field /anisotropy (ps-ns)

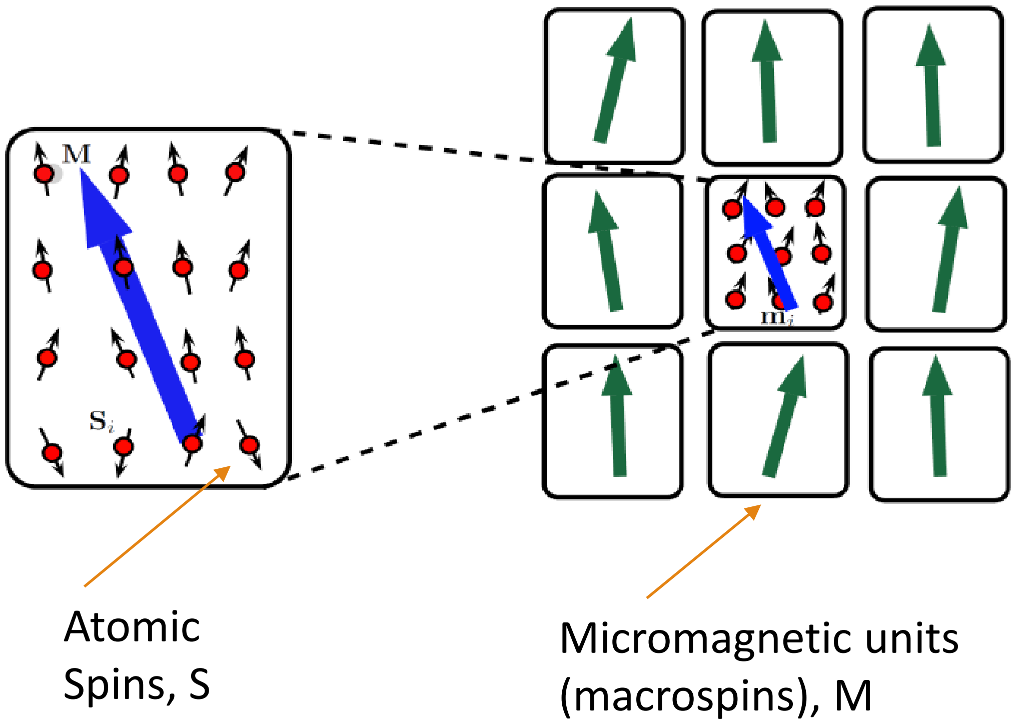
$$\dot{\vec{S}}_i = -\frac{\gamma}{1+\alpha^2}\vec{S}_i \times H_i(t) - \frac{\alpha\gamma}{1+\alpha^2}\vec{S}_i \times (\vec{S}_i \times \vec{H}_i(t))$$

Stochastic fields are added

$$< h_j(t) >= 0 \qquad < h_i(0)h_j(t) >= \delta(t)\delta_{ij}\frac{2\alpha}{1+\alpha^2}k_bT/\gamma$$

Role of thermal fluctuations in magnetism

At the microscopic (atomistic) level:

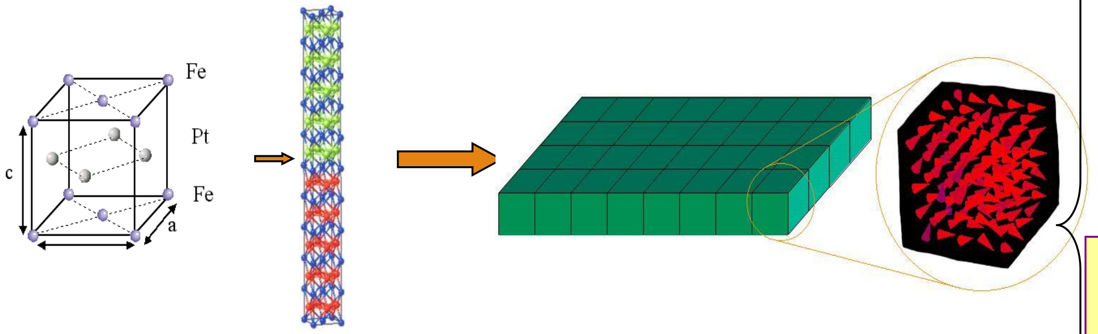


Thermally excited spinwaves are responsible for temperature-dependence of macroscopic properties and for thermal magnetisation reversal via the spinwave instabilities.

At more macroscopic (micromagnetic) level

- Thermal fluctuations are responsible for dispersion of trajectories and a random walk in a complex energy landscape
- Eventually energy barriers could be overcome with the help of thermal fluctuations leading to magnetisation decay.

Hierarchical multi-scale approach



Ab-initio calculations
μ, J, k, d

Parametrised Hamiltonian

Discrete(atomistic)models
Ms(T), K(T), A(T), D(T,)α(T)

Micromagnetic models

atomic cells

$$K(T) \propto m^{\alpha}$$

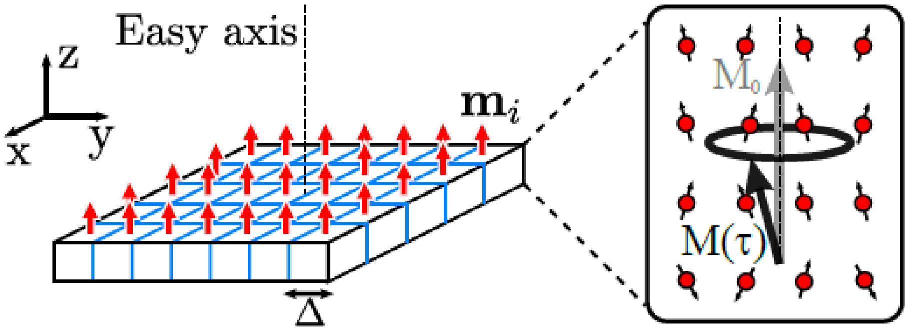
α=3 (uniaxial anisotropy)

α=10 (cubic anisotropy)

DFT → atomistic(Heisenberg) Hamiltonian → micromagnetics (LLB)

N. Kazatseva et al Phys. Rev. B 77 (2008) 184428

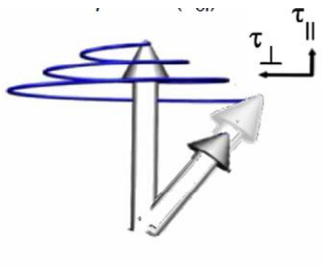
Micromagnetics with the Landau-Lifshitz-Bloch (LLB) equation



For non-constant or high temperatures and though the phase transition

$$T \neq 0 \;\Rightarrow\; |M| \neq \text{const}$$

$$\frac{d\vec{m}}{dt} = \gamma[\vec{m}\times\vec{H}] + \gamma\alpha_{\parallel}\frac{(\vec{m}\vec{H}_{eff})}{m^2} - \gamma\alpha_{\perp}\frac{[\vec{m}\times[\vec{m}\times\vec{H}_{eff}]]}{m^2}$$



$$\mathbf{H}_{\text{eff}} = \mathbf{H} + \mathbf{H}_A + \begin{cases} \frac{1}{2\tilde{\chi}_{\parallel}}\left(1 - \frac{m^2}{m_e^2}\right)\mathbf{m} & T \lesssim T_C \\ -\frac{J_0}{\mu_0}\left(\frac{T}{T_C} - 1 + \frac{3}{5}m^2\right)\mathbf{m} & T \gtrsim T_C \end{cases}$$

$$\alpha_{\perp} = \lambda\left(1 - \frac{T}{3T_C}\right)$$

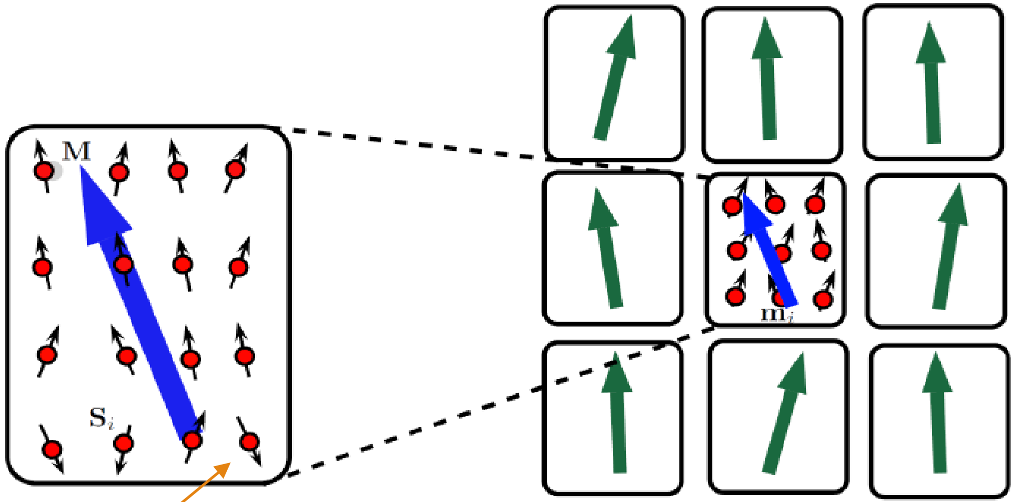
$$\alpha_{\parallel} = \frac{2}{3}\frac{T}{T_C}\lambda$$

Temperature –dependent micromagnetic parameters M(T), K(T), A(T), D(T)

D.Garanin PRB 55 (1997) 3050 classical derivation

D.Garanin Physica A 172 (1991) 470; P.Nieves, …O.C.-F. PRB 90, 104428 (2014) Quantum derivation

From atomistic to micromagnetic approach: exchange stiffness



Atomic Spins, S

Micromagnetic units (macrospins), m

Generalized Heisenberg

Micromagnetic exchange

$$H = -\frac{1}{2}\sum_{ij} J_{ij}^{\alpha\beta} S_i^{\alpha} S_j^{\beta} \rightarrow E = A\int_V \left[\left(\frac{\partial m_x}{\partial x}\right)^2 + \left(\frac{\partial m_y}{\partial y}\right)^2 + \left(\frac{\partial m_z}{\partial x}\right)^2\right] dV$$

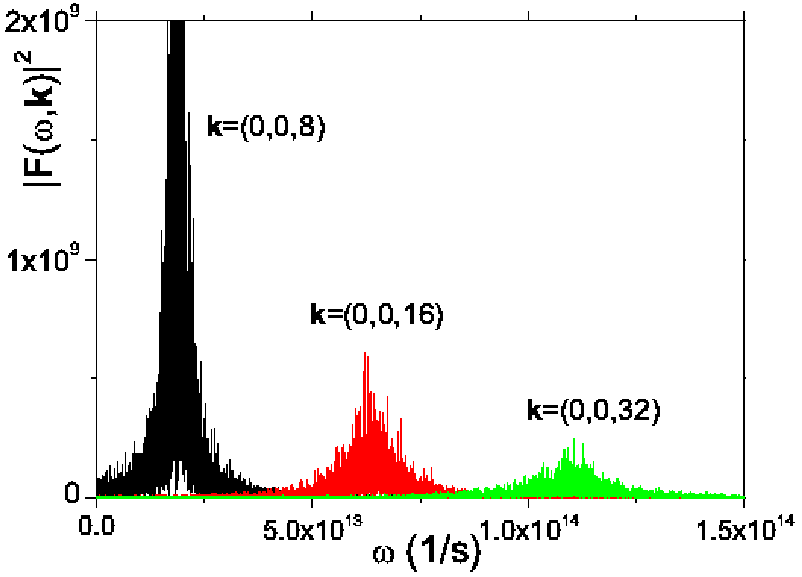
Takes into account crystal structure

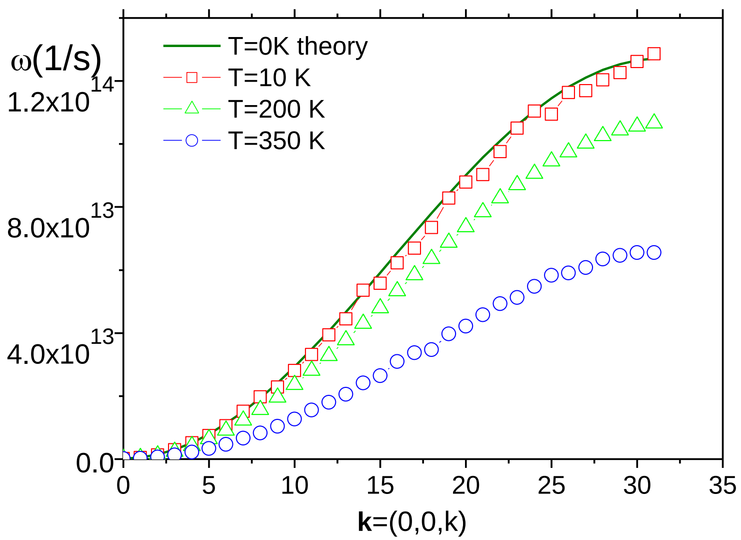
Can be long-range

$$A_{\nu}(0\ K) = \frac{1}{V_{at}}\sum_j J_{0j}^{\nu}\left(a_{0j}^{\nu}\right)^2$$

$$E_{DMI} = -\frac{1}{2}\sum_{i,j} \mathbf{D}_{ij}\left[\mathbf{S}_i \times \mathbf{S}_j\right] \longrightarrow E_{DMI} = 2\hat{D}\int \left[m_z \nabla \mathbf{m} - (\mathbf{m}\cdot\nabla) m_z\right] dS$$

From atomistic to micromagnetic approach: Temperature-dependent spin wave spectrum





Due to the averaging over thermal fluctuations, the longwave length spinwaves are temperature-dependent

$$A(T) = A(0)m^{2-\varepsilon}$$

$$D(T) = D(0)m^{2-\delta}$$

$$\omega(k) = \gamma_0 (H + \frac{D}{M} k\cos(ak) + \frac{2A}{M}\sin^2(ak))$$

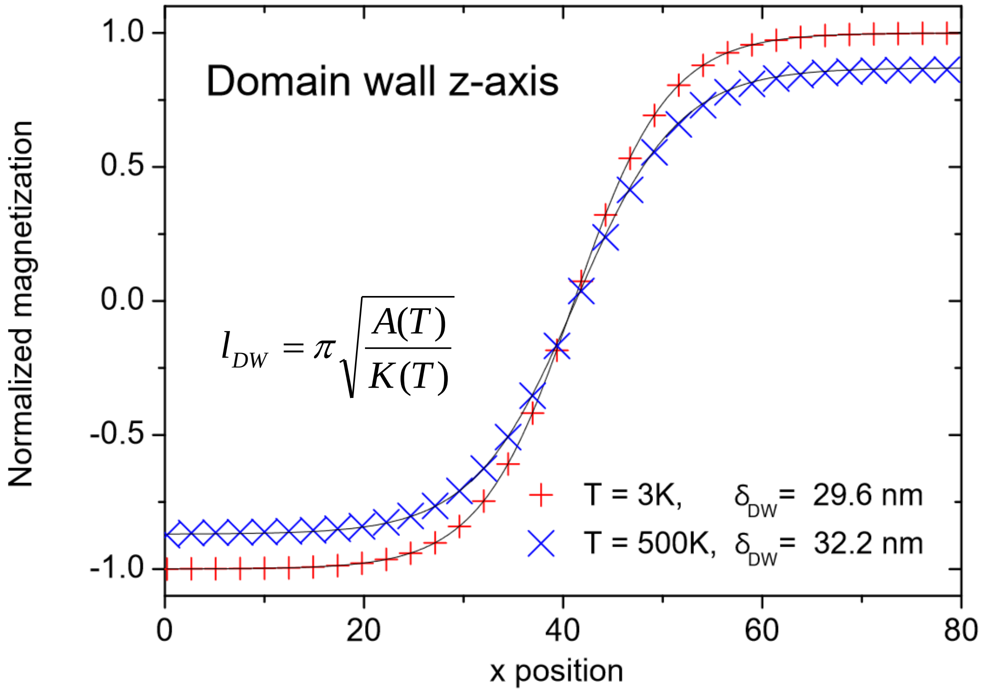
due to spin-spin correlations

U.Atxitia. … O.C.-F… PRB 82 (2010) 054415

Material-specific, depends on number of neighbors, crystal structure etc.

From atomistic to micromagnetic approach: temperature-dependent domain wall width, skyrmion size etc.

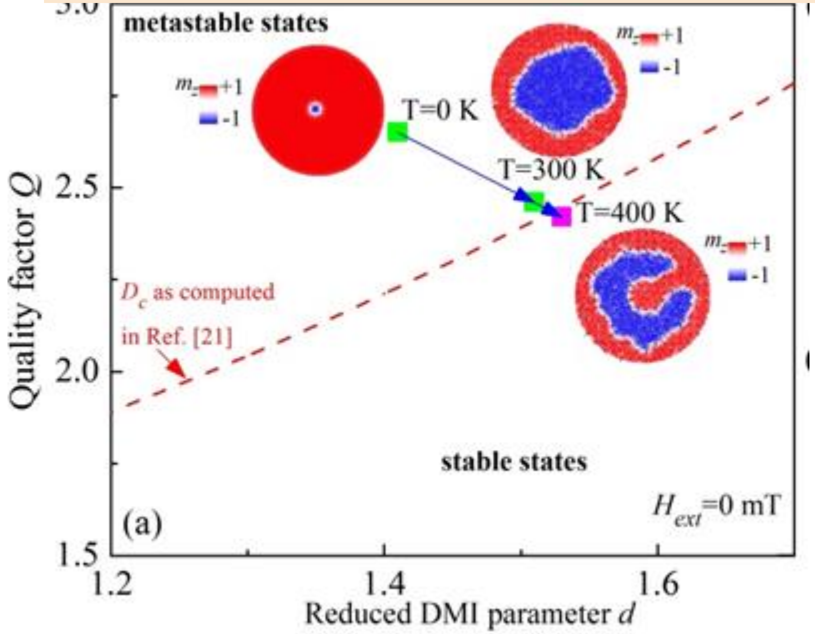
$A(T) \propto m^{1.8}, K(T) \propto m^3$



DW width increases with temperature

R. Moreno, ..O.C.-F. et al PRB 94 (2016) 104433

$K \propto m^3$, A $\propto m^{1.5}$, D $\propto m^{1.5}$



Temperature-dependent skyrmion radius

R.Tomasello, --O.C.F. et al PRB 97 (2018) 0604402

Motion in thermal gradient
(spin-Seebeck effect)

- Energy minimization due to scaling of magnetic parameters:

(Exchange and anisotropy energies are minimized in the hot region, magnetostatic and DMI energy –typically in the cold region

e.g. $E_{DW} = 4\sqrt{AK} - \pi D \quad K_{eff} = K - \frac{1}{2}\mu_0 M_s^2$

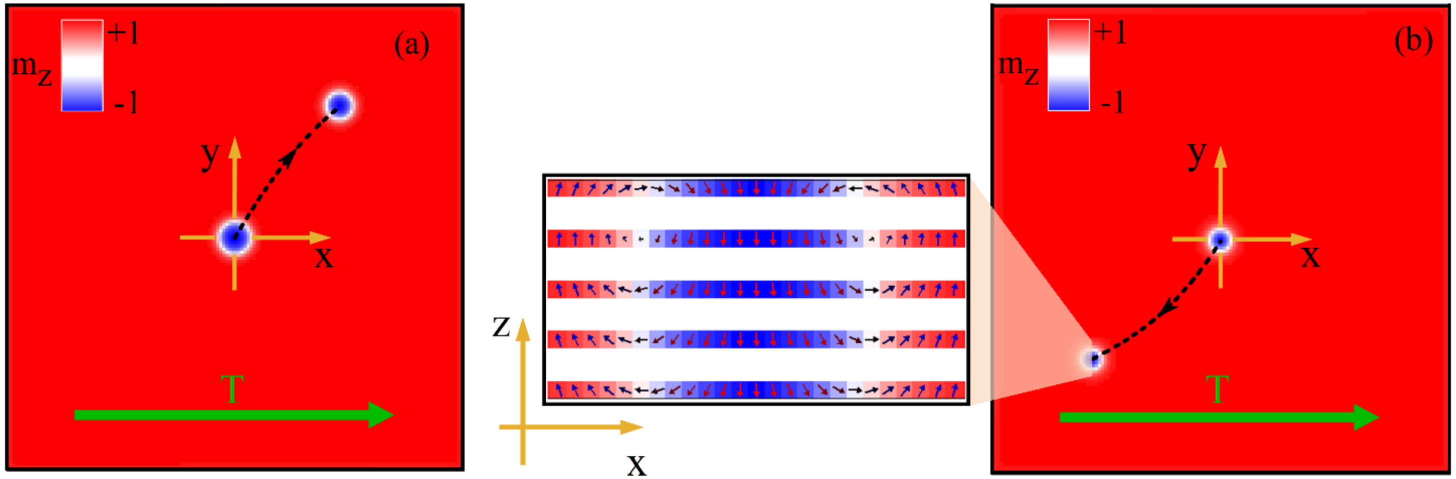
- Entropy (free energy) S is maximum in the hot region

- Spin currents move from hot to cold

- Other effects: (spinwave emision by DW and interaction,

changing of DW character (Bloch->Neel), going from in-plane to out-of plane etc.)

Skyrmions in thermal gradients



HM/single-layer FM

Multilayer

Pt/FeCo/Ir
Multilayeres
(5 repetitions)

$K \propto m^3$
$\mathrm{A} \propto m^{1.5}$
$\mathrm{D} \propto m^{1.5}$

$K \propto m^{2.5}$
$\mathrm{A} \propto m^{1.7}$
$\mathrm{D} \propto m^2$

Competition between magnetostatic energy and all other energies

Neél domain wall in thermal gradient

(Entropic motion, FeCoB parameters, perpend anisotropy)

$A(T) \propto m^{1.75}$

50-5K

150-5K

Neél domain wall in thermal gradient

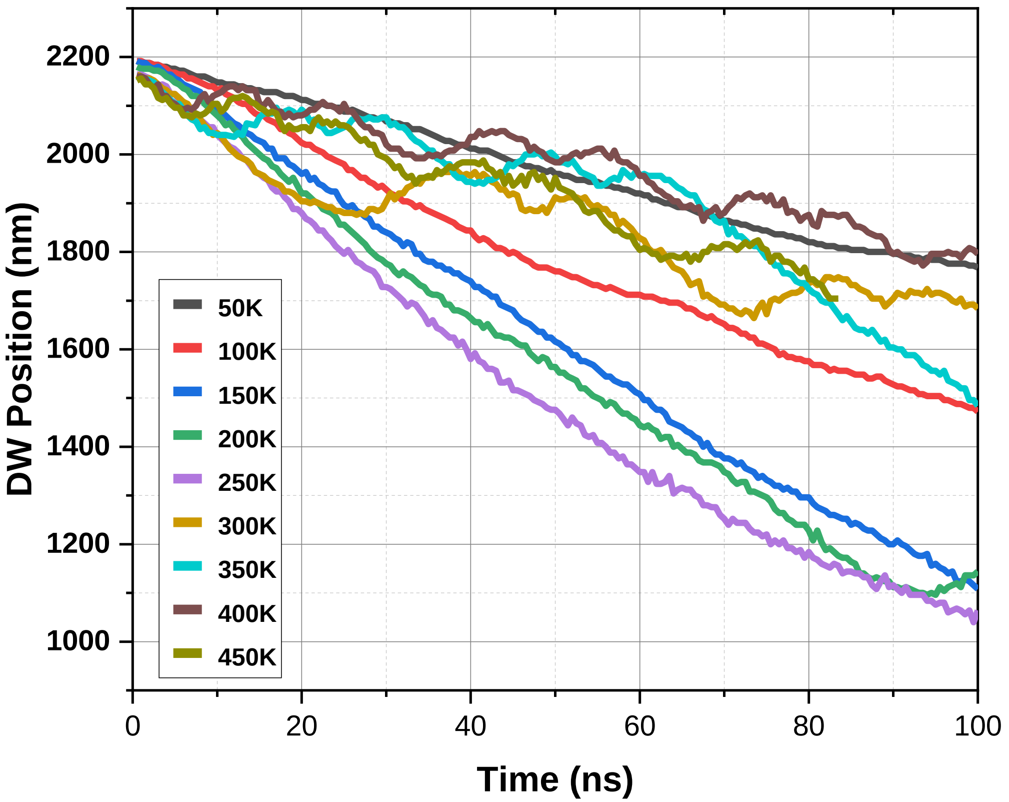
(Magnonic motion)

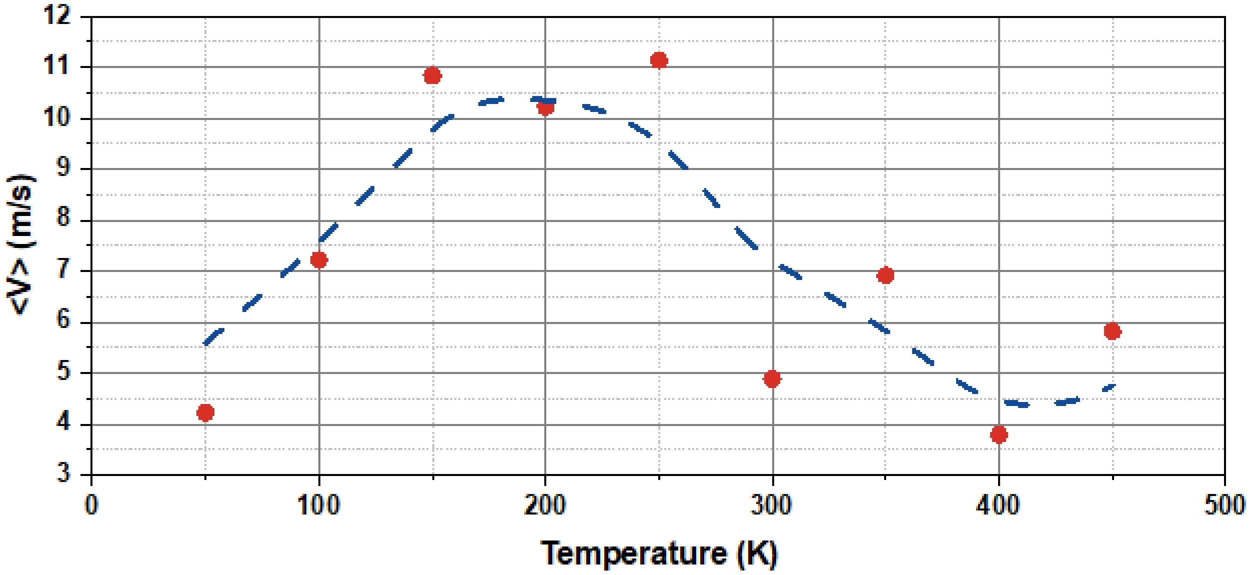
50-5K

300-5K

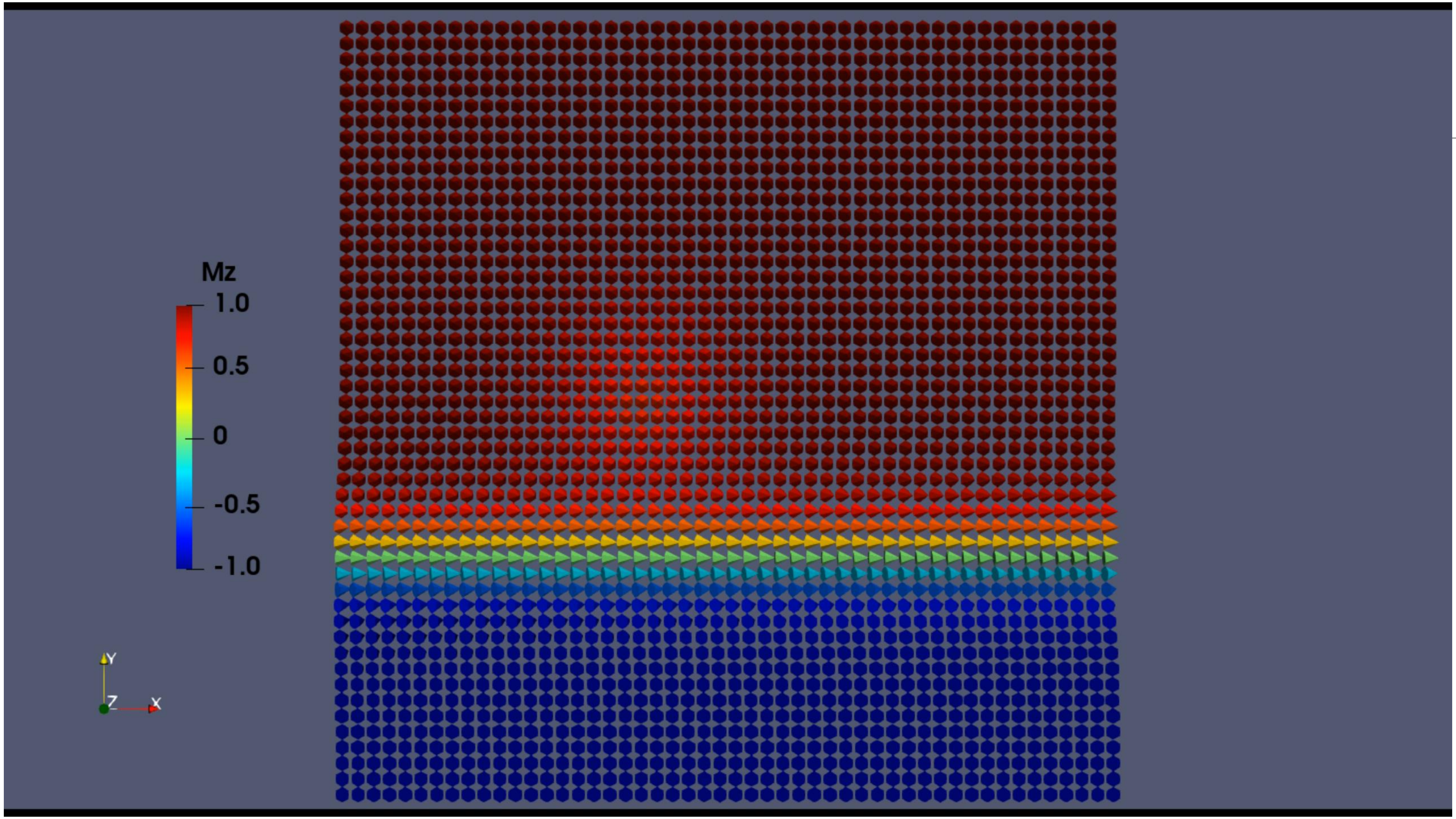
Neél domain wall in thermal gradient

(Full calculations)





Domain wall is bent and is attracted by the heat spot



Self-consistent magnetisation and temperature dynamics

$\Delta T \Rightarrow d\mathbf{M}/dt$ (e.g. magnetisation dynamics under spin-Seebeck)

Reciprocity? self-consistent treatment?

$d\mathbf{M}/dt \Rightarrow \Delta T$ –(e.g.hysteresis heating)

Self-consistent magnetisation and temperature dynamics

$\Delta T \Rightarrow d\mathbf{M}/dt$ (e.g. magnetisation dynamics under spin-Seebeck)

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$d\mathbf{M}/dt \Rightarrow \Delta T$ –(e.g.hysteresis heating)

Self-consistent magnetisation and temperature dynamics

$\Delta T \Rightarrow$ **dM/dt** (e.g. magnetisation dynamics under spin-Seebeck)

Reciprocity? self-consistent treatment?

dM/dt $\Rightarrow \Delta T$ –(e.g.hysteresis heating, magnetocalorics)

LLB+ $$\frac{dT}{dt} = \tilde{\alpha}_{||}(\mathbf{m}\cdot\mathbf{H}_{\mathrm{eff}}) + \tilde{\alpha}_{\perp}\frac{\mathbf{m}\times(\mathbf{m}\times\mathbf{H}_{\mathrm{eff}})}{\mathbf{m}^2}$$

$$\tilde{\alpha}_{||} = \frac{\gamma\alpha_{||}M_s J_0}{C\mu}, \qquad \tilde{\alpha}_{\perp} = \frac{\gamma\alpha_{\perp}M_s}{C}$$

Two derivations: quantum (denstity matrix) or repciprocity principle
Electron (Metals) or phonon (insulators) bath

P. Nieves,.. O.C.-F. PRB 94 (2016) 04409

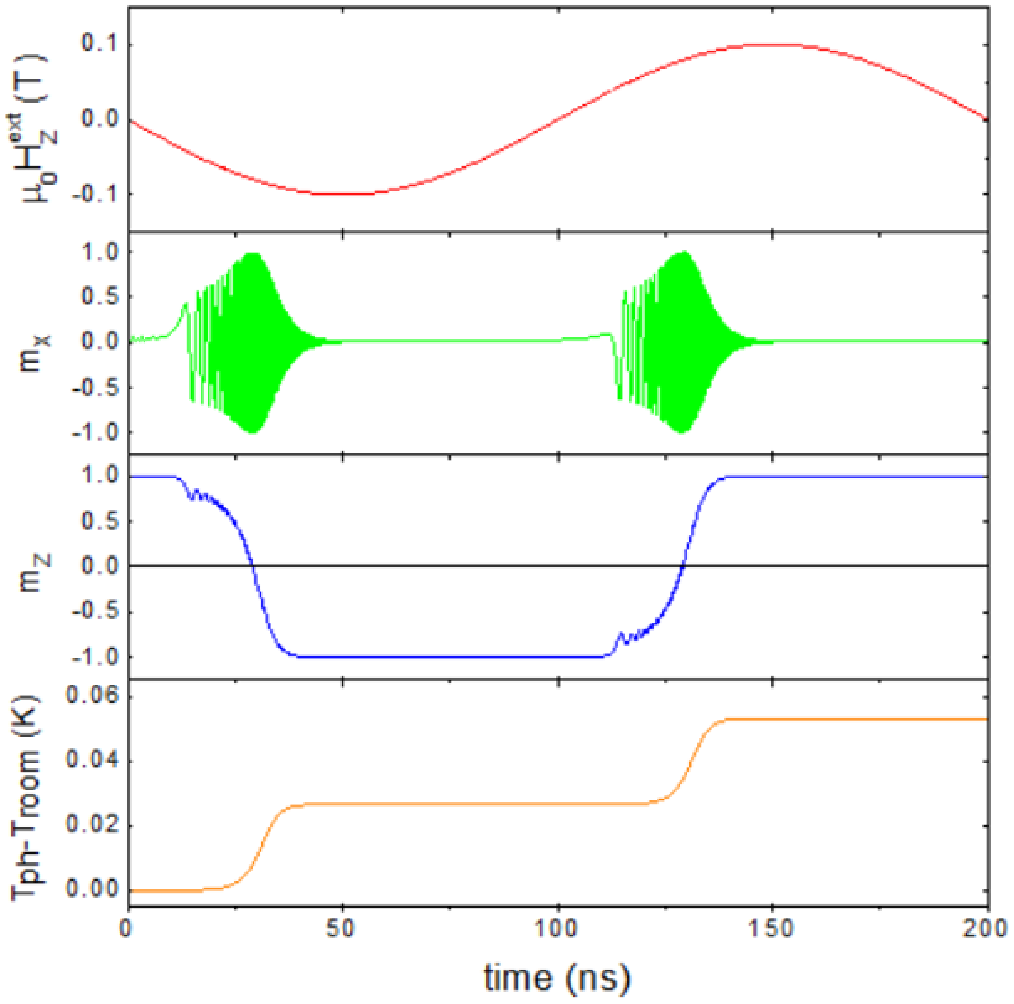
The heat (Q) dynamics occurs in the same timescale as the magnetisation dynamics fs-ps for longitudinal changes and ps-ns for transverse changes

The change of the temperature occurs for:

- Irreversible processes
- Ultra-fast processes

20 nm Magnetite nanoparticle under ac-field-

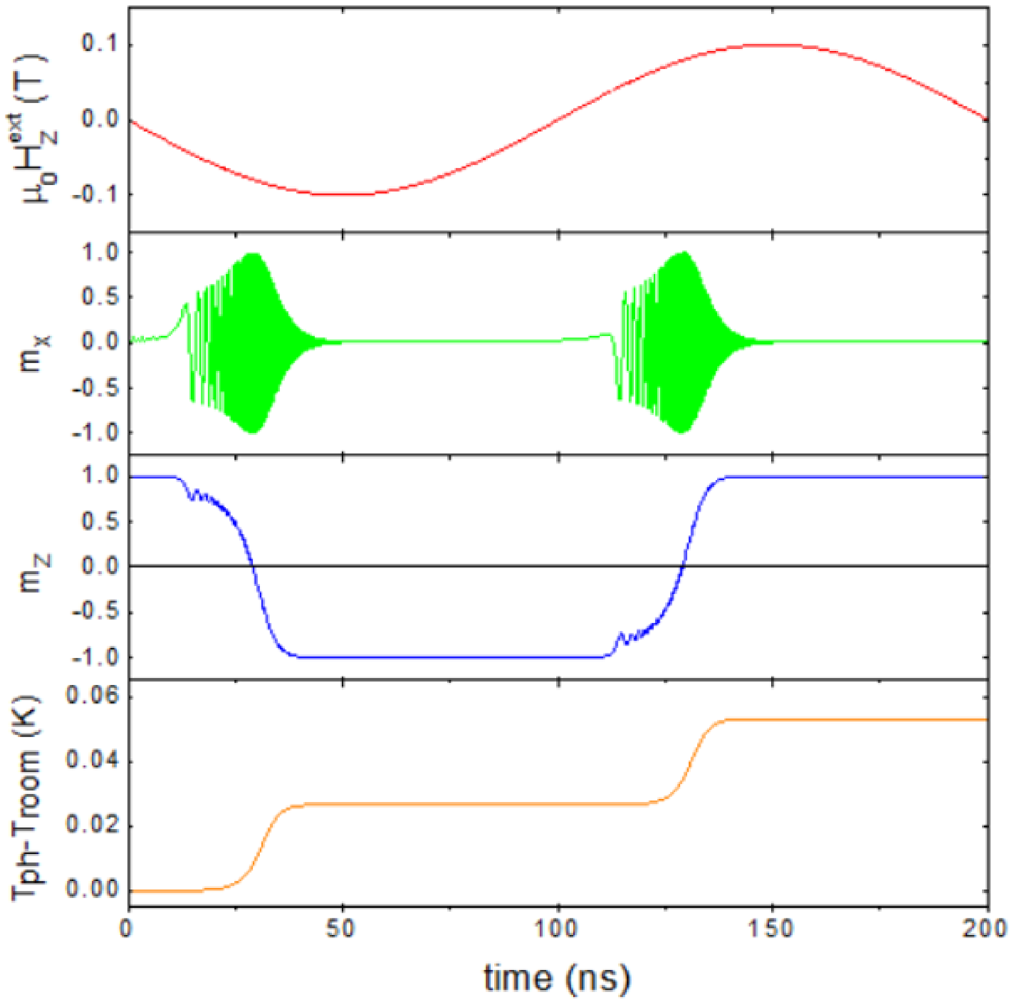
around 10 mK heat per switch



'Self-consistent description of spin-phonon dynamics in ferromagnets', P. Nieves, D. Serantes, O. Chubykalo-Fesenko, Phys. Rev. B, 2016, 94, 014409

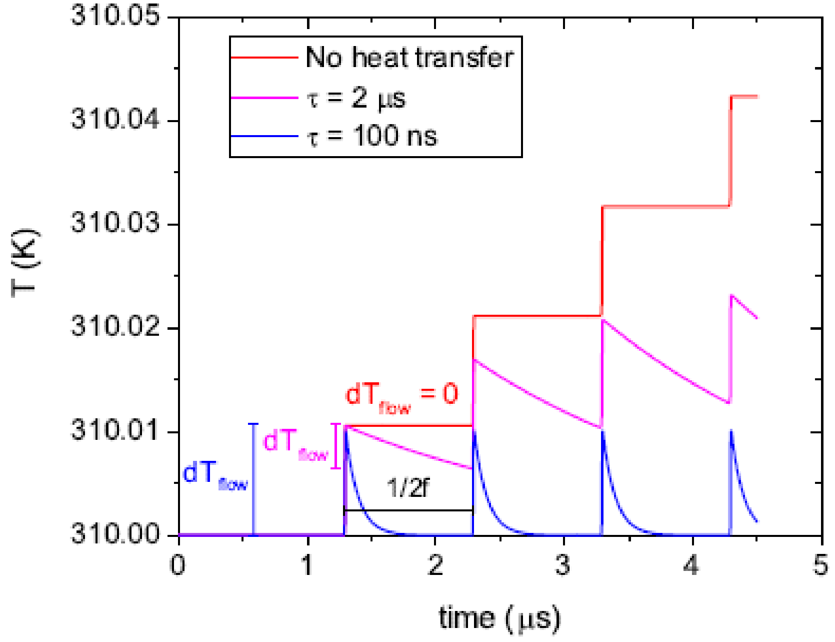
20 nm Magnetite nanoparticle under ac-field-

around 20 mK heat per switch



- Diffusion (or conduction)

- The interface heat transfer $dT/dt = (T-T0)/\tau$



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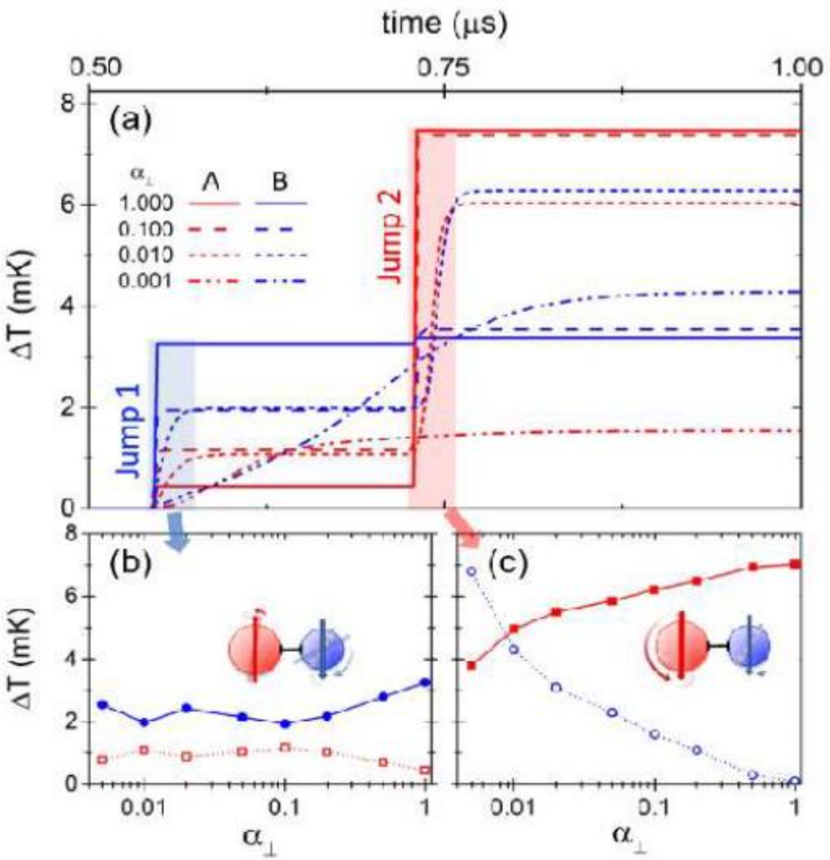
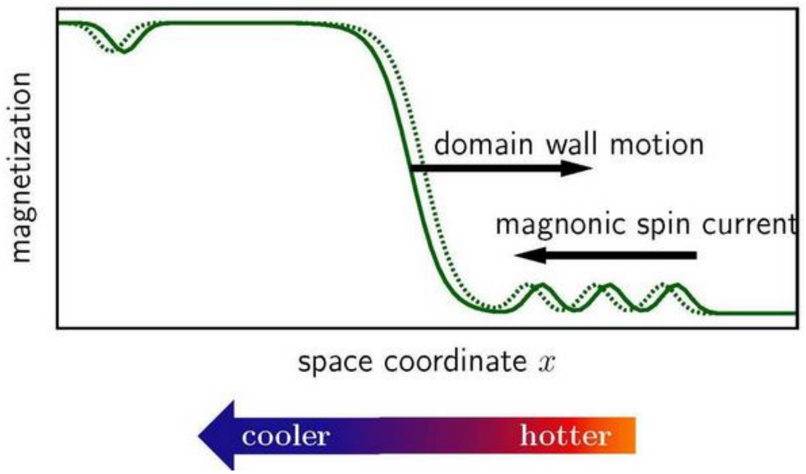
Two interacting nanoparticles



- Nanoparticles release heat in intrawell and interwell processes
- The intrawell heat release may be even higher
- Importance of dynamics and precession

C. Muñoz-Mendez, …O.C.-F. PRB **102**, 214412 (2020)

Domain wall motion by spin-Seebeck effect



D. Hinzke and U. Nowak

Phys. Rev. Lett. 107, 027205 (2011)

The opposite effect:
moving domain wall (vortex, skyrmion etc.) produces heat dynamics?

The answer is YES!   How much?

The effect is GIANT, ULTRAFAST and LOCALIZED in AFM

Spin-Peltier effect for moving magnetic structures

The approach is equivalent to Rayleigh function for m(t)

$$\frac{dQ}{dt} \approx \int \frac{\alpha M_S}{\gamma} \left(\frac{dm}{dt}\right)^2 dV$$

Spin-Peltier effect for moving magnetic structures

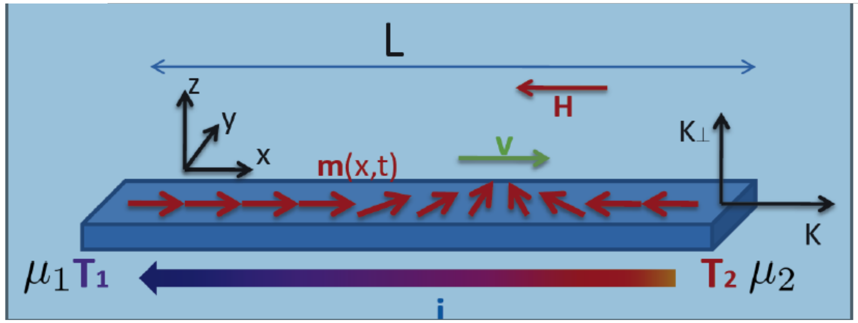
The approach is equivalent to Rayleigh function for m(t)

$$\frac{dQ}{dt} \approx \int \frac{\alpha M_s}{\gamma}\left(\frac{dm}{dt}\right)^2 dV$$

- Any moving object should produce a change of temperature

- The effect is cuadratic in magnetisation (AFM)

1D stationary moving domain wall



$$\theta(x,t) = 2\tan^{-1}\left(exp\left[\frac{x+vt}{\Delta}\right]\right)$$

Temperature (energy) profile accompanying moving domain wall

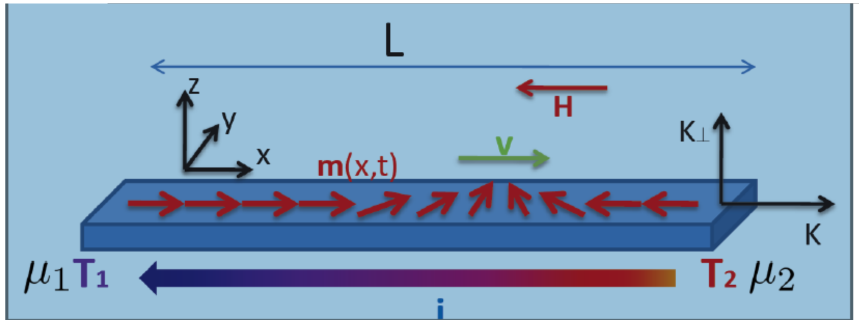
$$T(x,t) = T_0 + \frac{\alpha M_s v}{\gamma C \Delta}\tanh\left(\frac{x+vt}{\Delta}\right)$$

Estimations:
Permalloy
Ms=1T
C =10^6J/Km^3
V=500 m/s
Δ=50nm
α=0.01

ΔT =0.4 mK

R.Otxoa, ...O.C.-F.
Comm.Phys. 3, 31 (2020)

1D stationary moving domain wall



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With thermal diffusion:

$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2} + \frac{\alpha M_s v^2}{\gamma C \Delta^2}\frac{1}{cosh^2\left[\frac{x+vt}{\Delta}\right]}$$

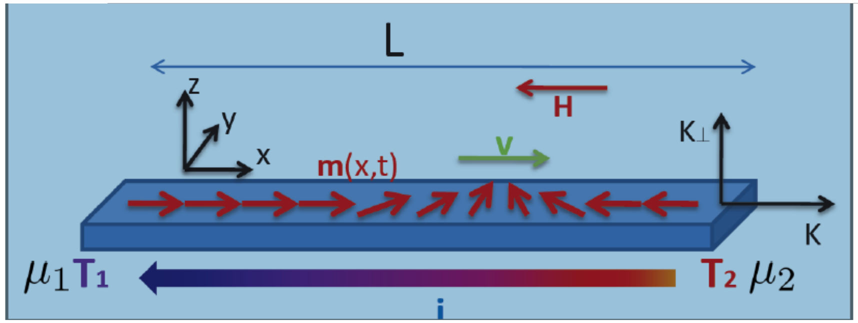
$$T(x,t) = \frac{2\alpha M_s v^2}{C\gamma D \Delta}(x+vt)$$

D=10^{-4} m^2/s
η=0.01 <<1 diffusion-dominated motion, heat is
Is rapidlly delocalized.

$$\eta = \frac{v\Delta}{D}$$

R.Otxoa, ...O.C.-F.
Comm.Phys. 3, 31 (2020)

1D stationary moving domain wall



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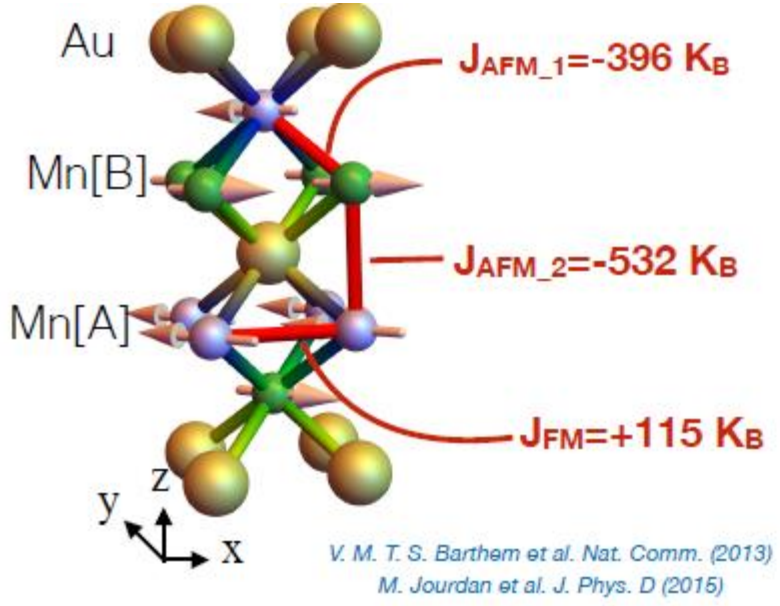
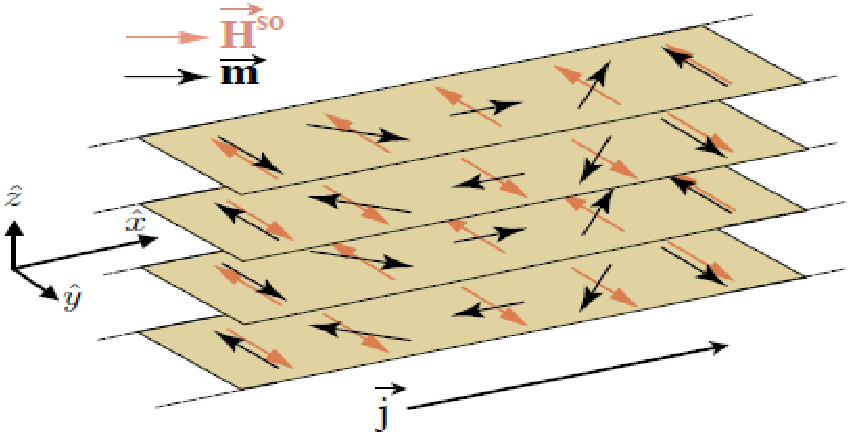
R.Otxoa, ...O.C.-F.
Comm.Phys. 3, 31 (2020)

Atomistic model of Mn_2Au antiferromagnet



180 Neel domain wall moved by current (SOT field)



One biaxial (basal plane) Anisotropy

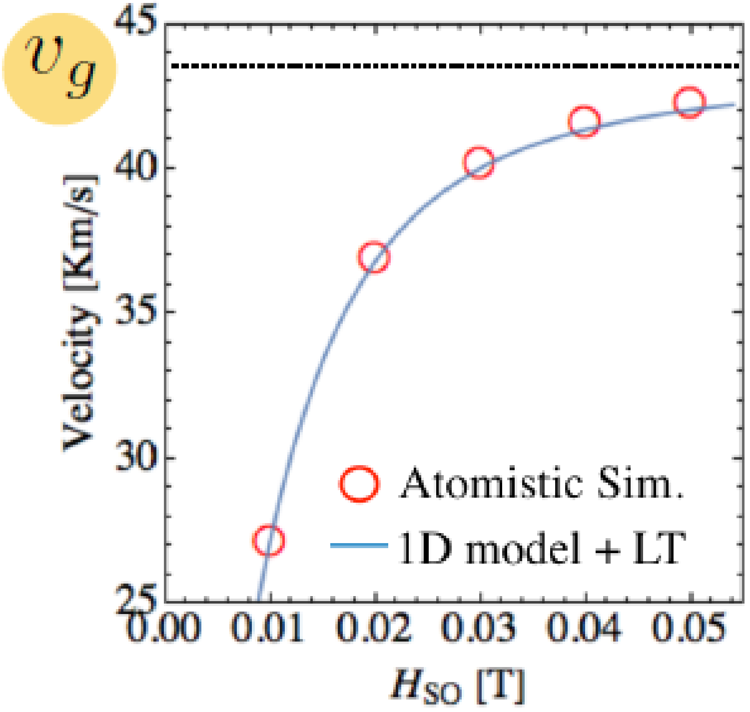
Two perpendicular anisotropies
(uniaxial and cubic)
The uniaxial anisotropy >>others

Atomistic dynamics

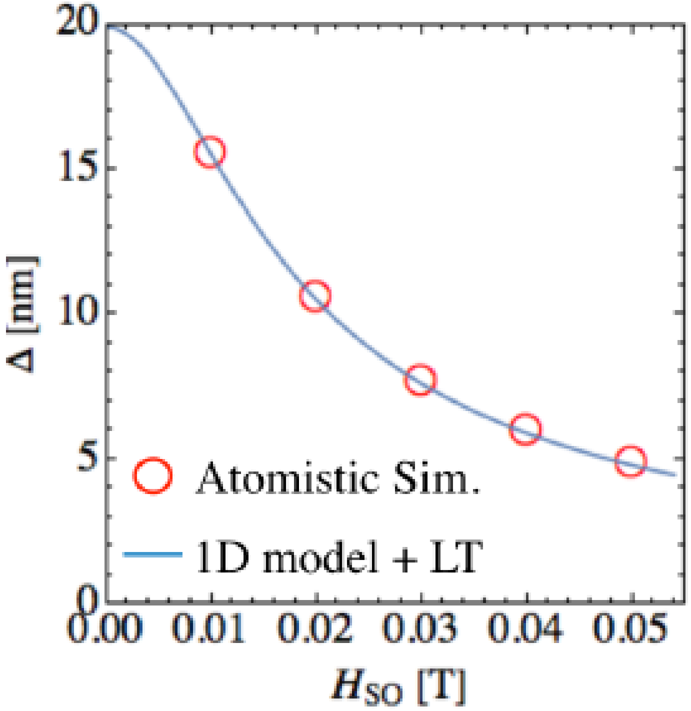
$$\dot{\vec{S}}_i = -\frac{\gamma}{1+\alpha^2}\vec{S}_i \times H_i(t) - \frac{\alpha\gamma}{1+\alpha^2}\vec{S}_i \times (\vec{S}_i \times \vec{H}_i(t))$$

Domain wall velocity and width in MnAu

$$\dot{q}(t) = \frac{\gamma}{\alpha} H_{SO} \Delta$$



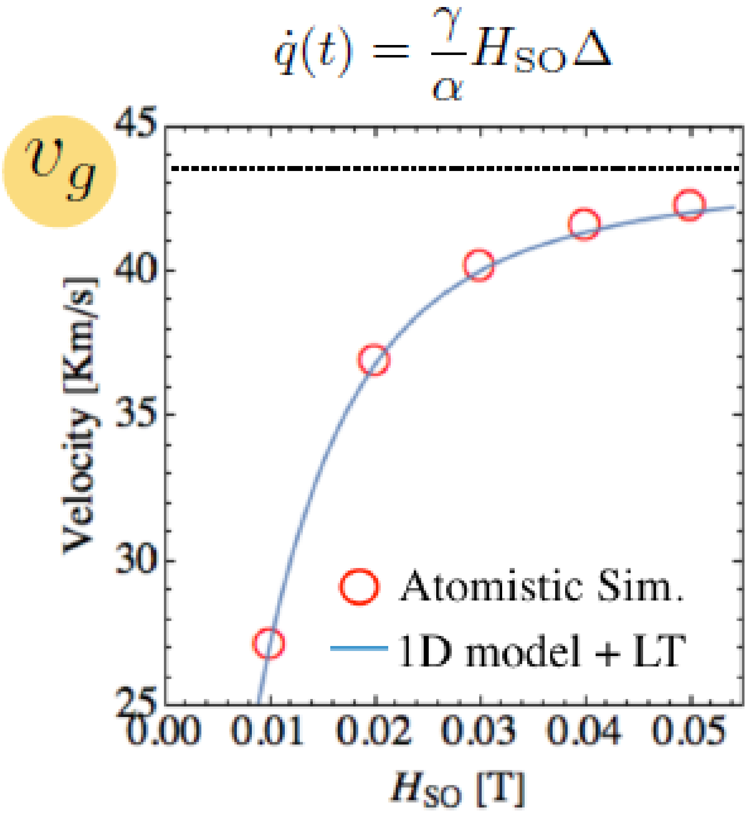
$$\Delta = \Delta_0 \left(1 - \dot{q}(t)^2 / v_g^2\right)^{1/2}$$

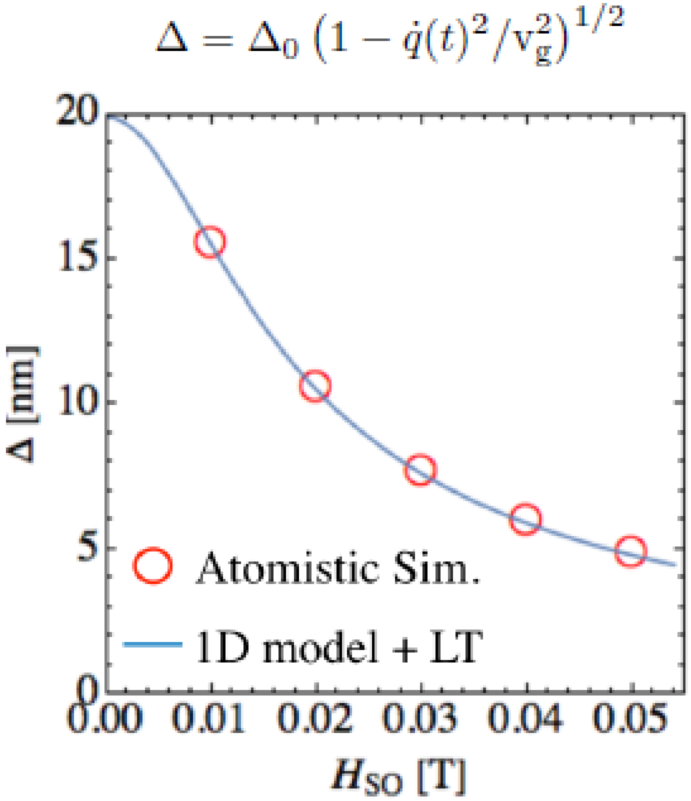


- ✓ Velocity increases up to 40 km/s (limited by spinwave emission)
- ✓ Domain width decreases down to 4 nm (relativistic effect)

R.Otxoa, …O.C.-F.
Comm.Phys. 3, 31 (2020)

Domain wall velocity and width in MnAu





Mn_2Au

V≈40 km/s

Δ=5nm

α=0.001

$$\eta = \frac{v\Delta}{D} \approx 4$$ Localized heat wave

ΔT =0.7 K

Huge effect!
2 order of magnitude larger than in nanoparticle with coherent rotation
3 orders of magnitude larger than for FM DW

- ✓ Velocity increases up to 40 km/s (limited by spinwave emission)
- ✓ Domain width decreases down to 4 nm (relativistic effect)

40 nm/ps (ultrafast timescale)

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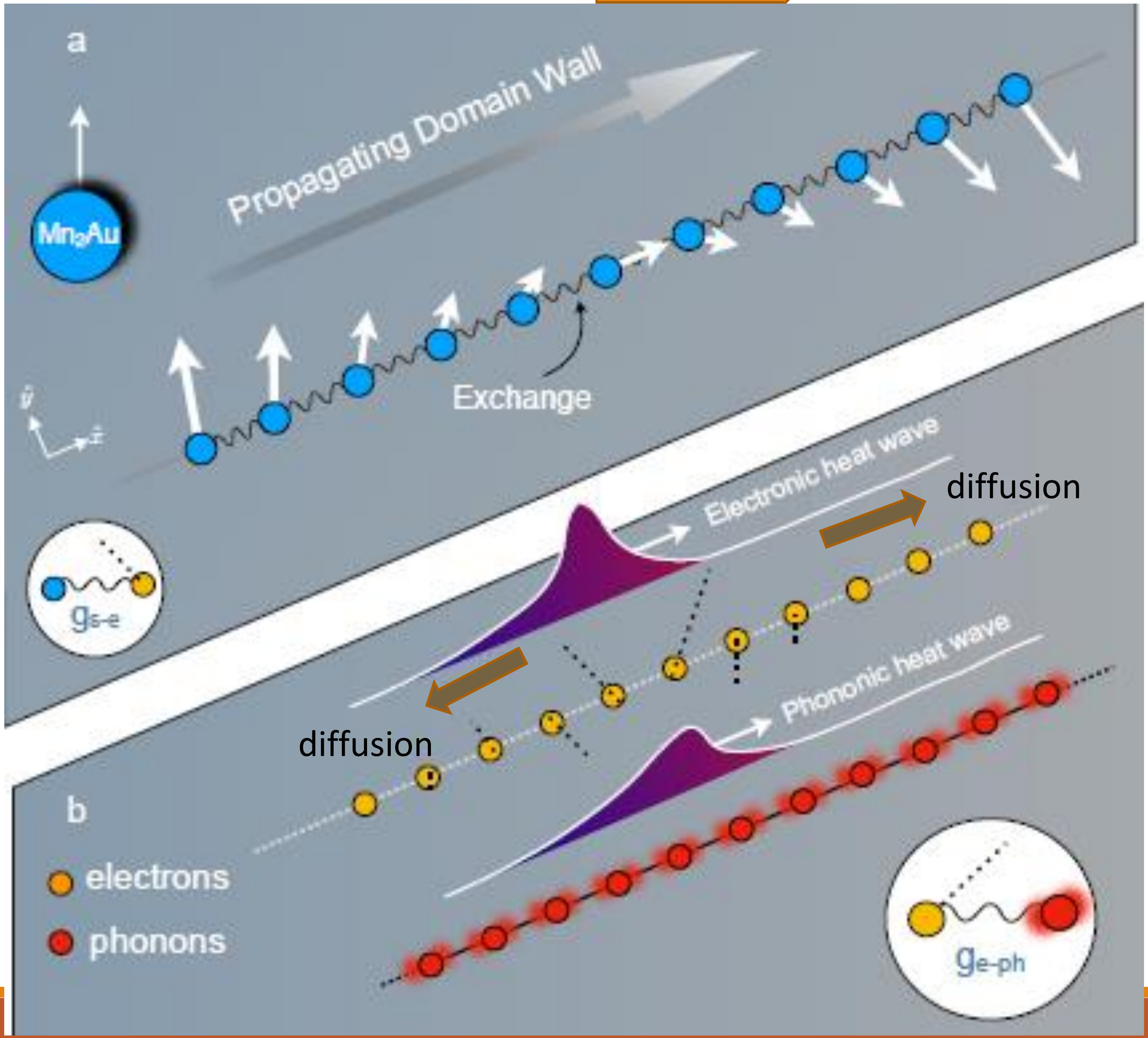
Comm.Phys. 3, 31 (2020)

Current I



Two temperature model

$$C_e \frac{dT_e}{dt} = g_{e-ph}(T_e - T_{ph}) + k_e \frac{\partial^2 T}{\partial x^2} + \dot{Q}_{s-e}(x,t)$$

$$C_{ph} \frac{dT_{ph}}{dt} = -g_{e-ph}(T_e - T_{ph}) + \frac{T_{ph} - T_0}{\tau_d}$$

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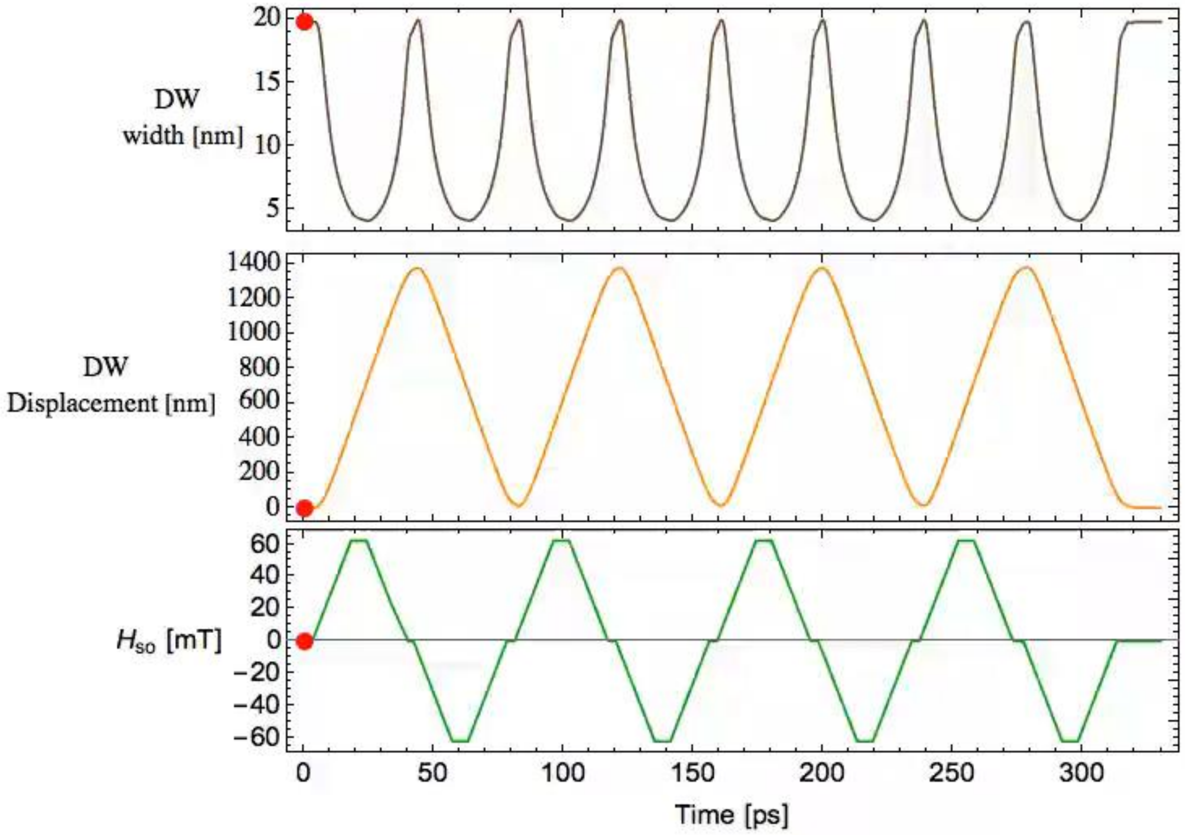
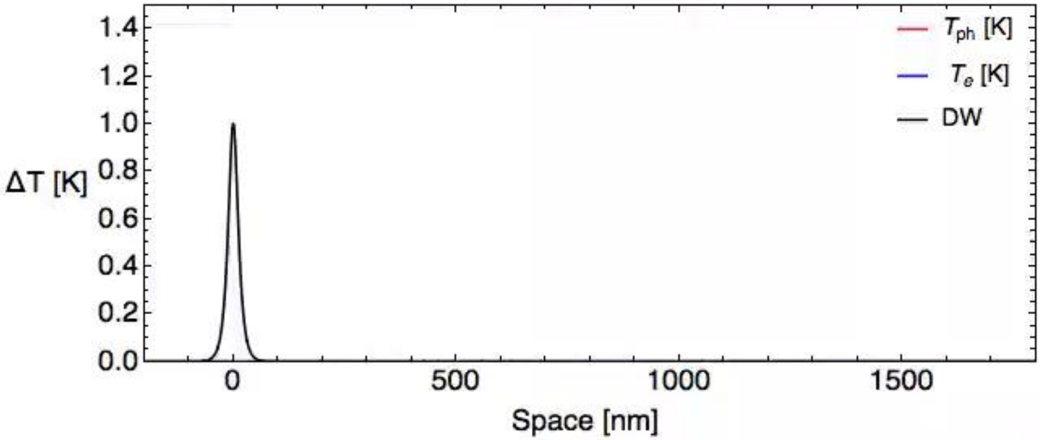
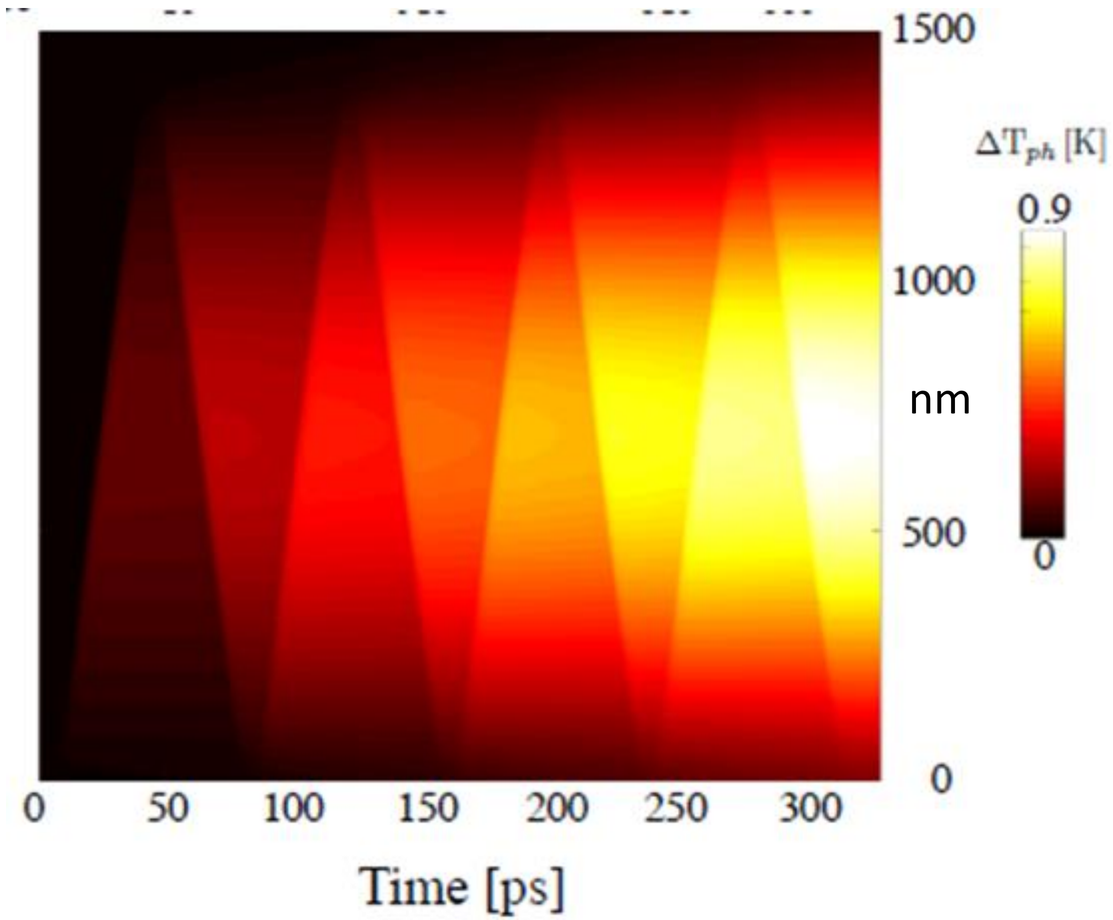
Comm.Phys. 3, 31 (2020)


DW width [nm]
DW Displacement [nm]
H_{so} [mT]
Time [ps]

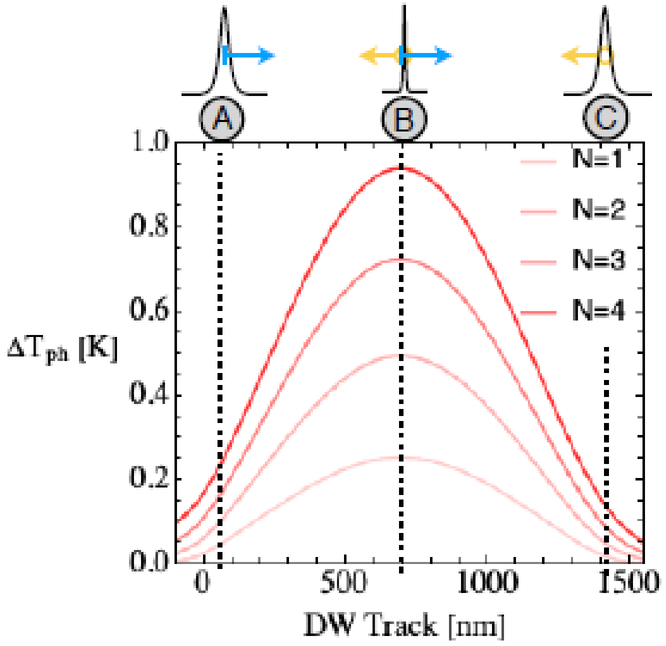

T_{ph} [K]
T_e [K]
DW
ΔT [K]
Space [nm]

Distribution of heat along the track



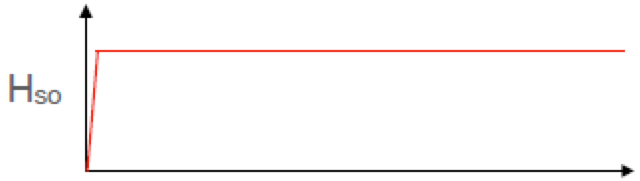
Heat is accumulated in the Center of the track (where H_{SOT} is maximum

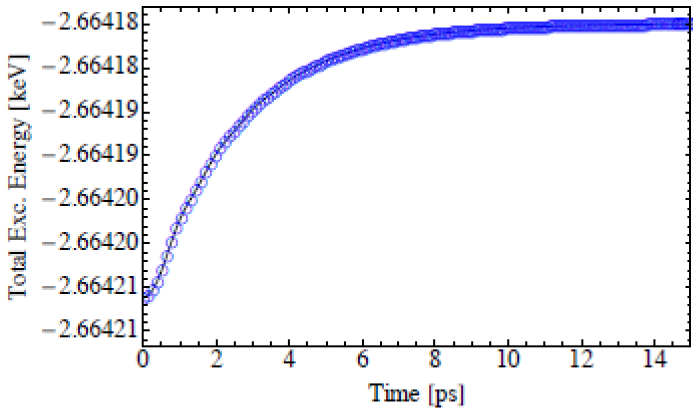
With 4 cycles only phonon temperature has reached 1 K

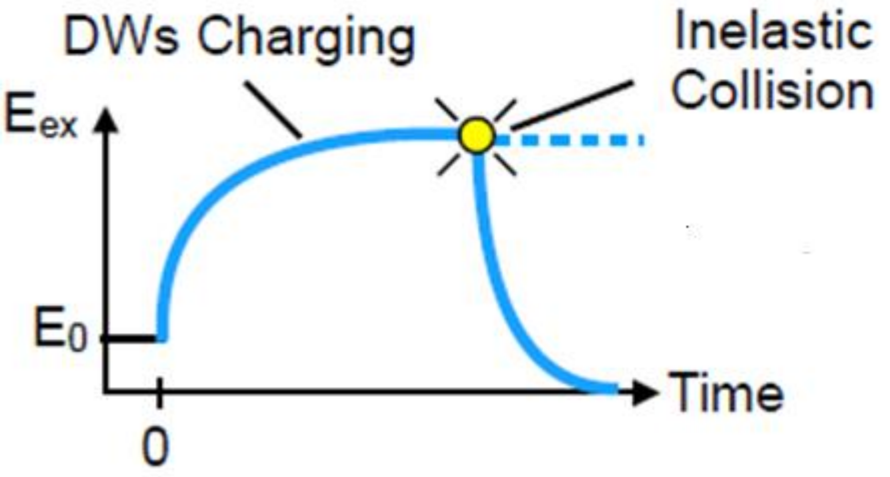


AFM DWs “charge” and “discharge” during the collision

$$E(v_s) = \frac{E_0}{\sqrt{1-(v_s/c)^2}},$$







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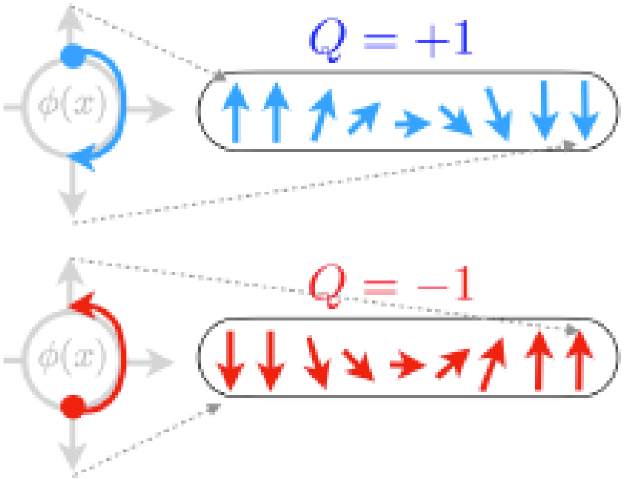
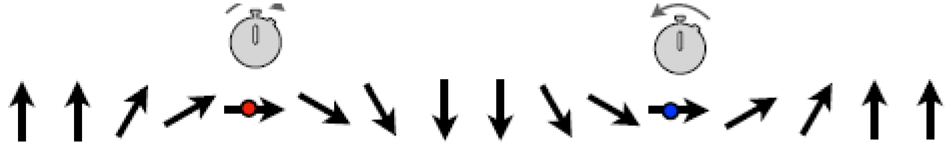
Comm.Phys. 3, 31 (2020)

Topology-selected AFM domain walls annihilation

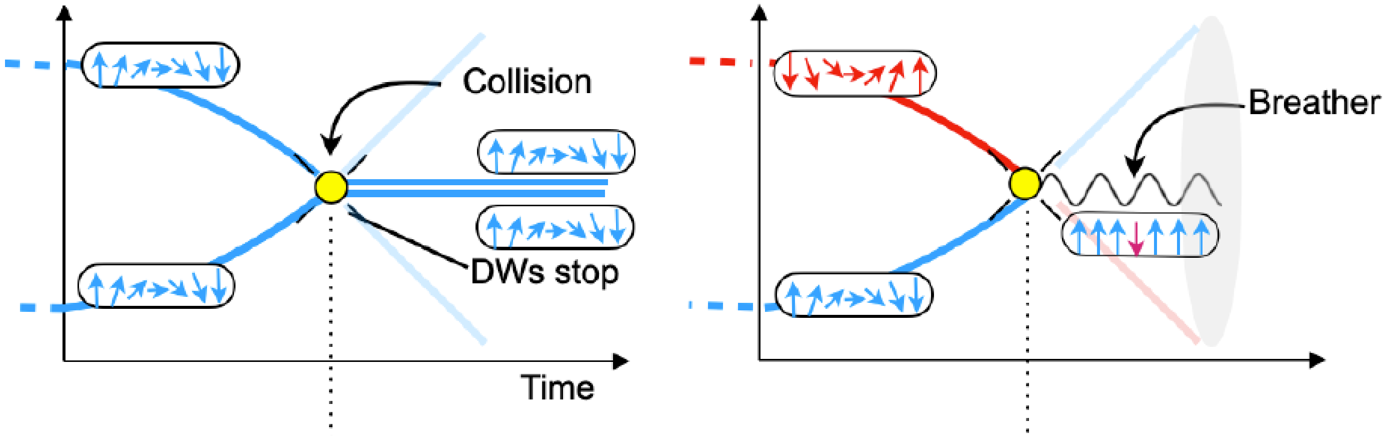
$Q = -\nabla_x \theta$ Topological charge





Q1=Q2

Q1=-Q2



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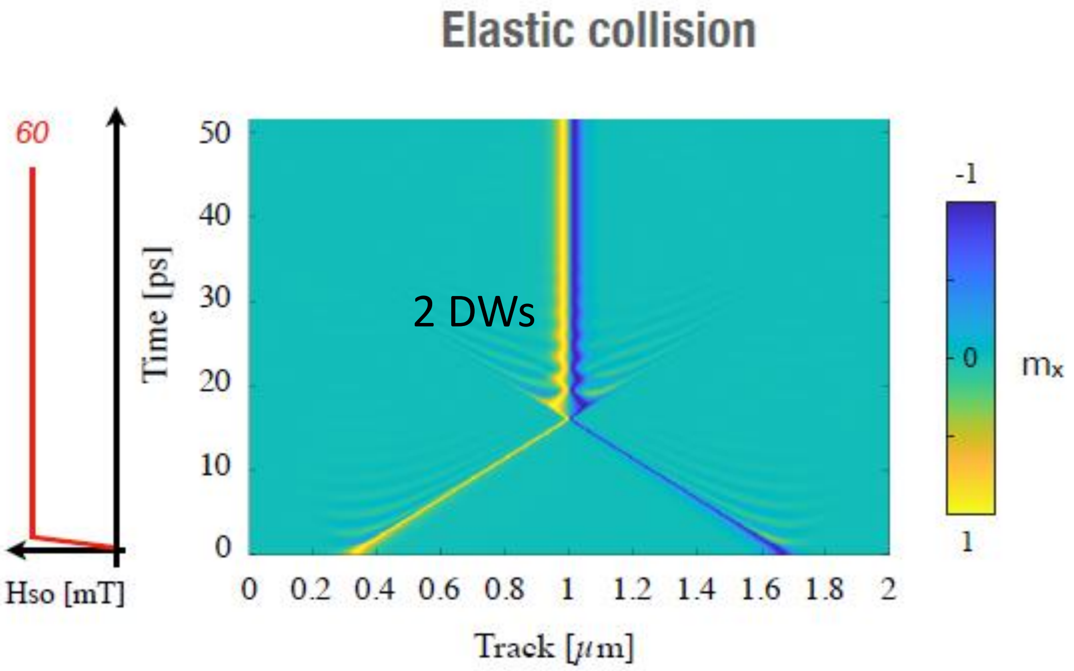
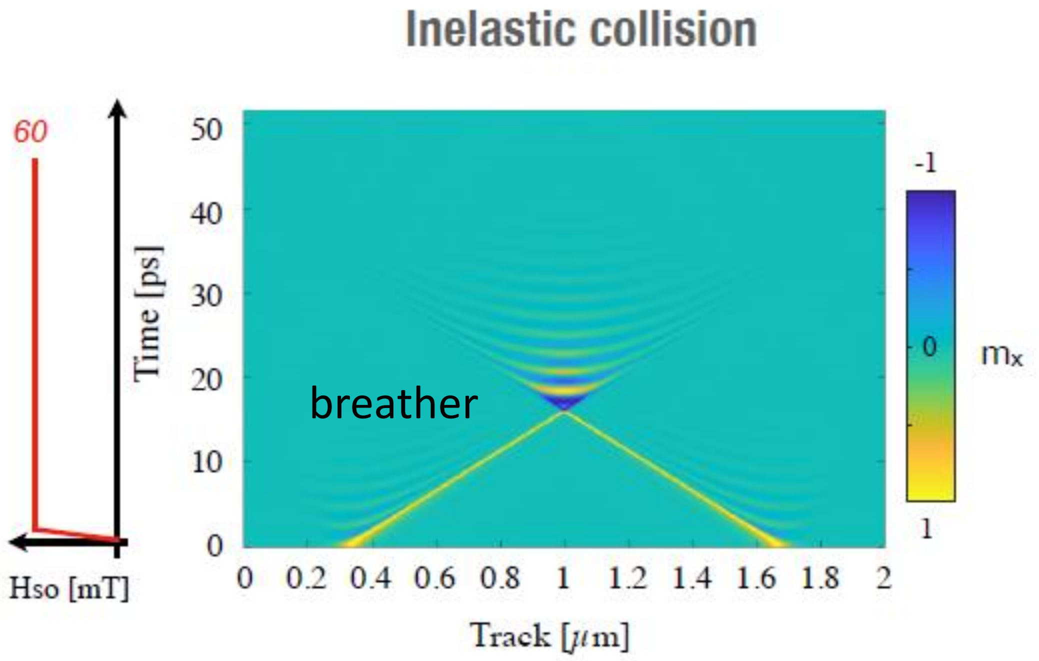
Only if Q1+Q2=0 domain walls can annihilate

AFM domain walls collision

Q1=Q2



Q1=-Q2



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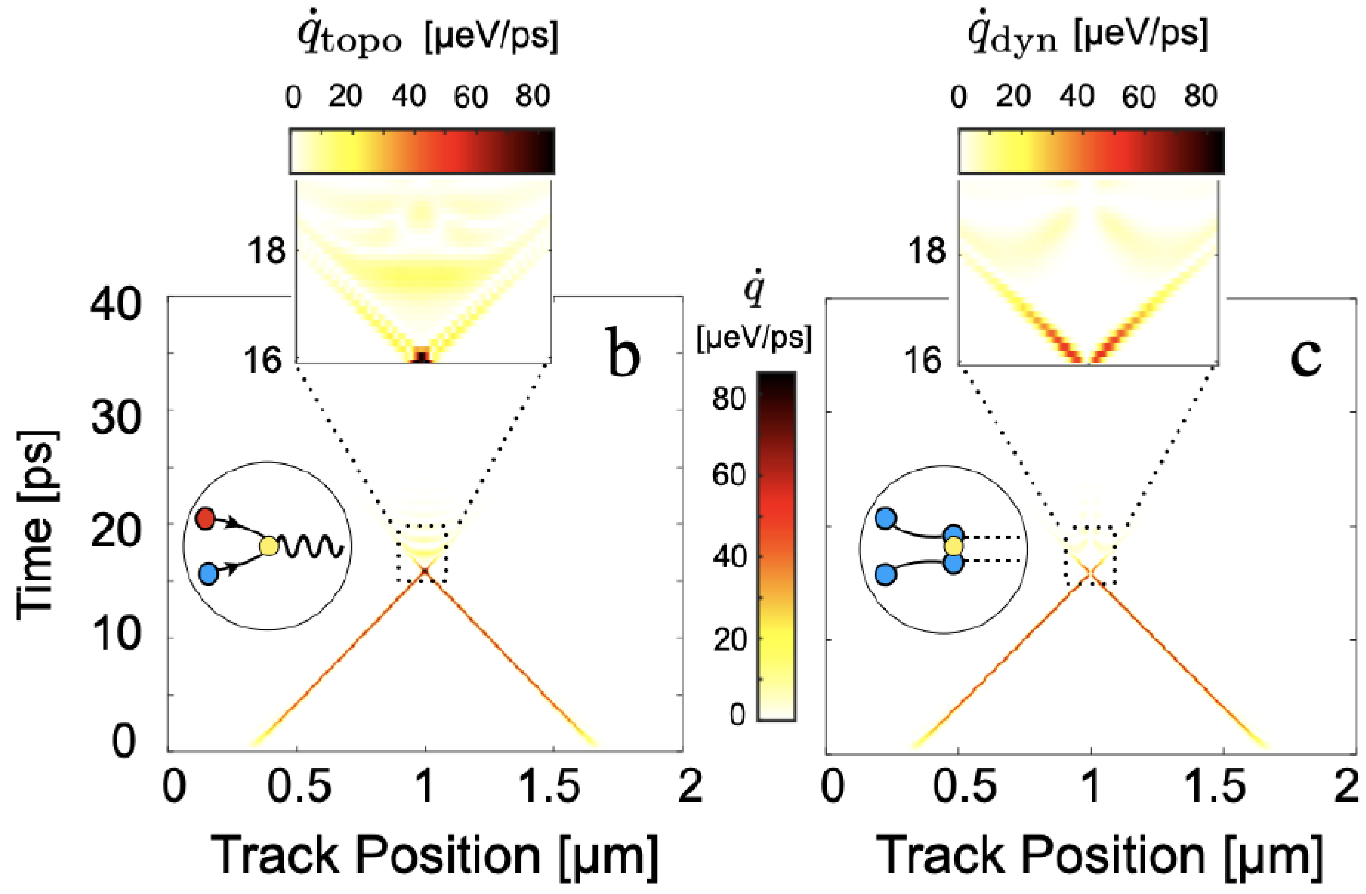
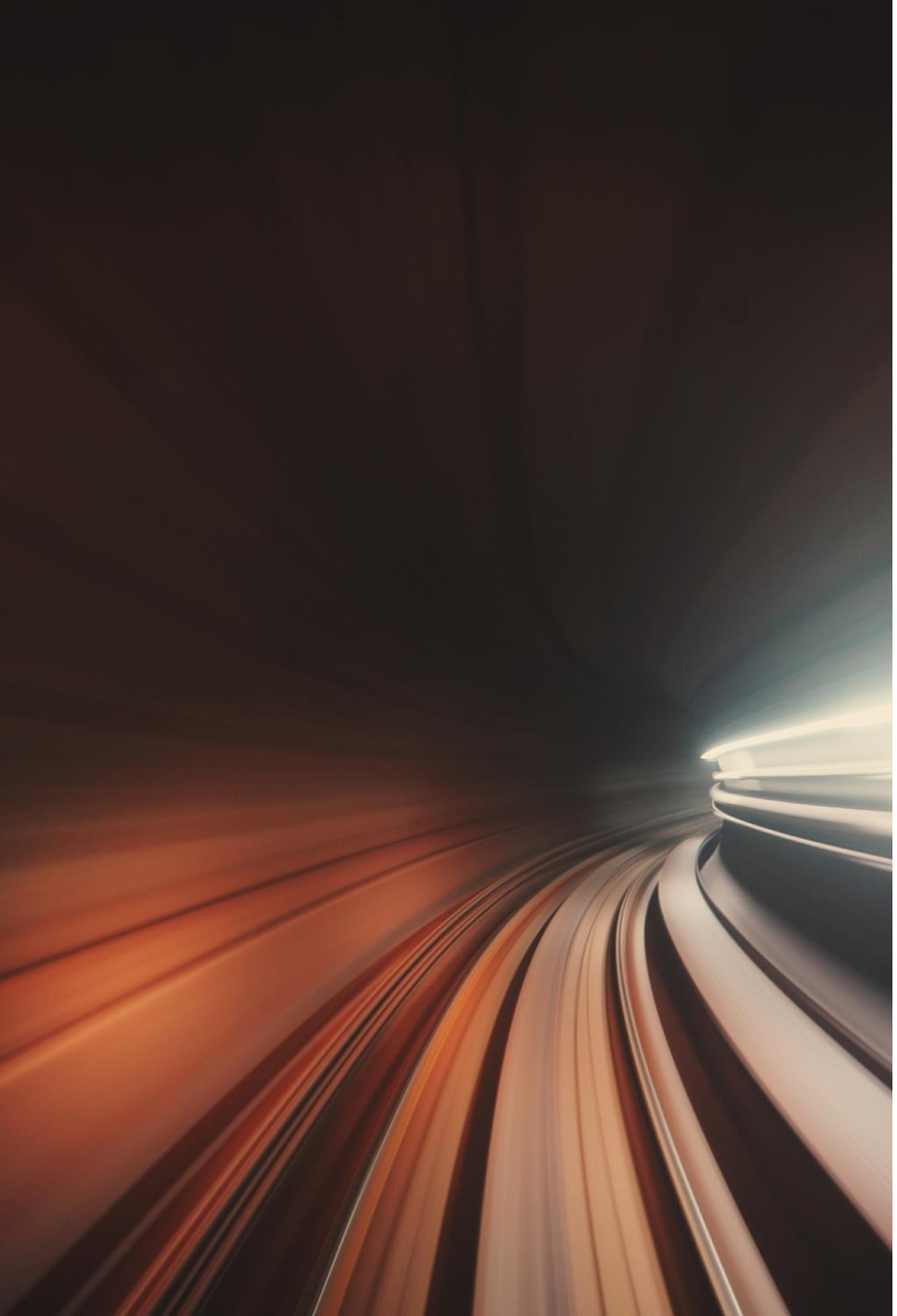
Energy release during AFM DWs collision





Messages

Magneto-thermo-dynamics: reciprocal phenomena

Change of temperature -> magnetization dynamics
Change of magnetization -> temperature dynamics

This manifests in many magneto-thermo-dynamical phenomena: which use one or the other part
(spincaloritronics vs. magnetocalorics etc)

Spin Seebeck effect: domain wall is moved towards hot region, Skyrmions –it depends.

Spin Peltier effect: ultrafast ultrathin domain wall dynamics is accompanied by a localized heat wave

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