Stochastic processes in magnetism; basic approaches

Roy Chantrell, Physics Department, York University

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Co-workers

Richard Evans, Natalia Kazantseva, Tom Ostler, Joe Barker, Yvette Hancock, Fleur Burrows, Claire Parker

Physics Department, The University of York

Denise Hinzke, Uli Nowak,

Universitaet Konstanz

Oksana Chubykalo-Fesenko, Unai Atxitia,

ICMM, Madrid

K Vahaplar, A Kalashnikova, Th Rasing, A Kirilyuk, A Kimel,

IMM, Radboud University Nijmegen, NL

(Opto-magnetic reversal experiments)

C Bunce, J Wu

Physics Department, The University of York

(HAMR experiments)

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Summary

- Lecture 1:
  - The timescale and lengthscale problem
  - Stocastic single spin models
  - Multispin models; micromagnetics and atomistic theories
  - Spin excitations in ferromagnets and antiferromagnets

- Lecture 2:
  - Introduction to pulsed laser processes
  - New (linear) magnetisation reversal mechanism
  - Linear reversal is calculated to give reversal times as fast as 300fs !
  - Dynamics and the Landau-Lifshitz- Bloch (LLB) equation of motion
  - LLB-micromagnetics and dynamic properties for large-scale simulations at elevated temperatures
  - Heat Assisted Magnetic Recording (HAMR); experiments and LLB-micromagnetic model
  - Opto-magnetic reversal – the ultimate speed record?

Magnetism; characteristic timescales

- Femtoseconds; pulsed laser processes
- Picoseconds; fastest reversal with pulsed field
- Nanoseconds; magnetic recording process
- Seconds; quasi-static magnetic measurements
- 10^3 - 10^4 s; slow dynamic processes
- 1-10 years; requirement for stored information stability
- Geological ages; Geophysical processes (core reversal, ageing of deposits ...)

And lengthscales

- Electronic; ab-initio calculations of spin moments, exchange, anisotropy
- Atomistic; many interacting spins, non-zero temperatures.
- Mesoscopic; continuum formalism (micromagnetics)
- Linking these lengthscales is currently an important problem

Anisotropy

- The term ANISOTROPY refers to the fact that the properties of a magnetic material are dependent on the directions in which they are measured.
- Anisotropy makes an important contribution to Hysteresis in magnetic materials and is therefore of considerable practical importance.
- The anisotropy has a number of possible origins.
  - Magnetocrystalline
  - Shape
  - Stress

SINGLE DOMAIN PARTICLES

- A crystal will spontaneously break up into domains in order to lower the magnetostatic energy. However, what happens as the size of the sample is reduced?
- We know that the magnetostatic energy α Volume, i.e. to L^3 for a cubic sample of side L. The wall energy will vary with cross-sectional area, i.e. with L^2.
- Because of this there comes a point at which it is energetically unfavourable to form domains.
- The critial size for single domain (SD) behaviour is about 10-50 nm for Fe, or approximately equal to the domain wall width.

Single domain particles

- Recording media
- Ferrofluids (magnetic colloids)
- Biophysics
  - Drug targetting
  - Hyperthermia
- Nanoparticles can be considered as a single 'macrospin' comprised of many (up to 10^6 coupled atomic spins)
- First application of stochastic methods in magnetism was to the study of the escape over energy barriers.

Dynamic behaviour; isolated spin

- Dynamic behaviour of the magnetisation is based on the Landau-Lifshitz-Gilbert equation

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

- Where γ_0 is the gyromagnetic ratio and α is a damping constant

Langevin Dynamics

- Based on the Landau-Lifshitz-Gilbert equations with an additional stochastic field term h(t).
- From the Fluctuation-Dissipation theorem, the thermal field must must have the statistical properties

$$< h_j(t) >= 0 \qquad < h_i(0) h_j(t) >= \delta(t) \delta_{ij} 2\alpha k_b T / \gamma$$

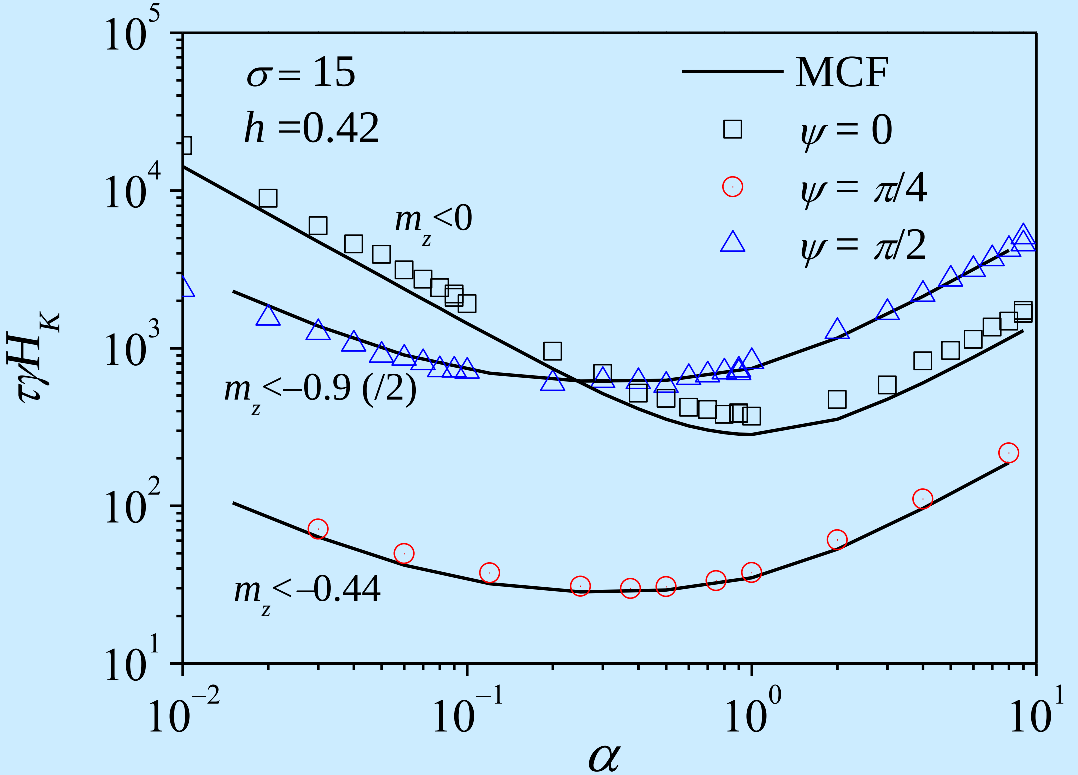
- From which the random term at each timestep can be determined.
- In numerical simulations h(t) is added to the local field at each timestep.

Analytic approach (Brown)

Construct the relevant Fokker-Planck equation for the time evolution of the magnetisation probability density

$$2\tau_N \frac{\partial W}{\partial t} = \frac{\beta}{\alpha}\mathbf{n}\cdot\left(\nabla V \times \nabla W\right) + \nabla\cdot\left(\nabla W + \beta W \nabla V\right)$$

Determine the smallest non-vanishing eigenvalue; related to the inverse relaxation time



- Good agreement between analytical and numerical calculations

Brown theory; axially symmetric case

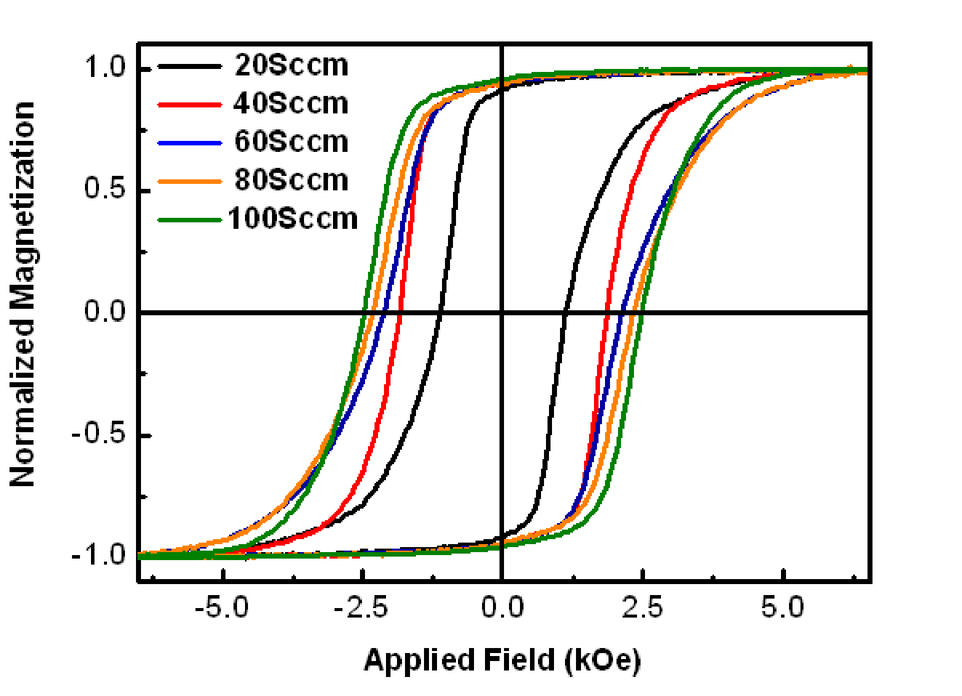
$$\tau \sim \tau_0(\alpha + \alpha^{-1}) \frac{\sigma^{-3/2}\sqrt{\pi}}{1-h^2} \left[(1-h) e^{-\sigma(1-h)^2} + (1+h) e^{-\sigma(1+h)^2} \right]^{-1}$$

- With τ_0 = VM_s /(2kTγ), σ=KV/kT, h=H/H_K with =2K/M_s the ‘anisotropy field’.
- K is the anisotropy constant and V the particle volume.

Superparamagnetism

- If the escape time<‘measurement time’ spin can move freely between energy minina
- Reversible (super) paramagnetic behaviour

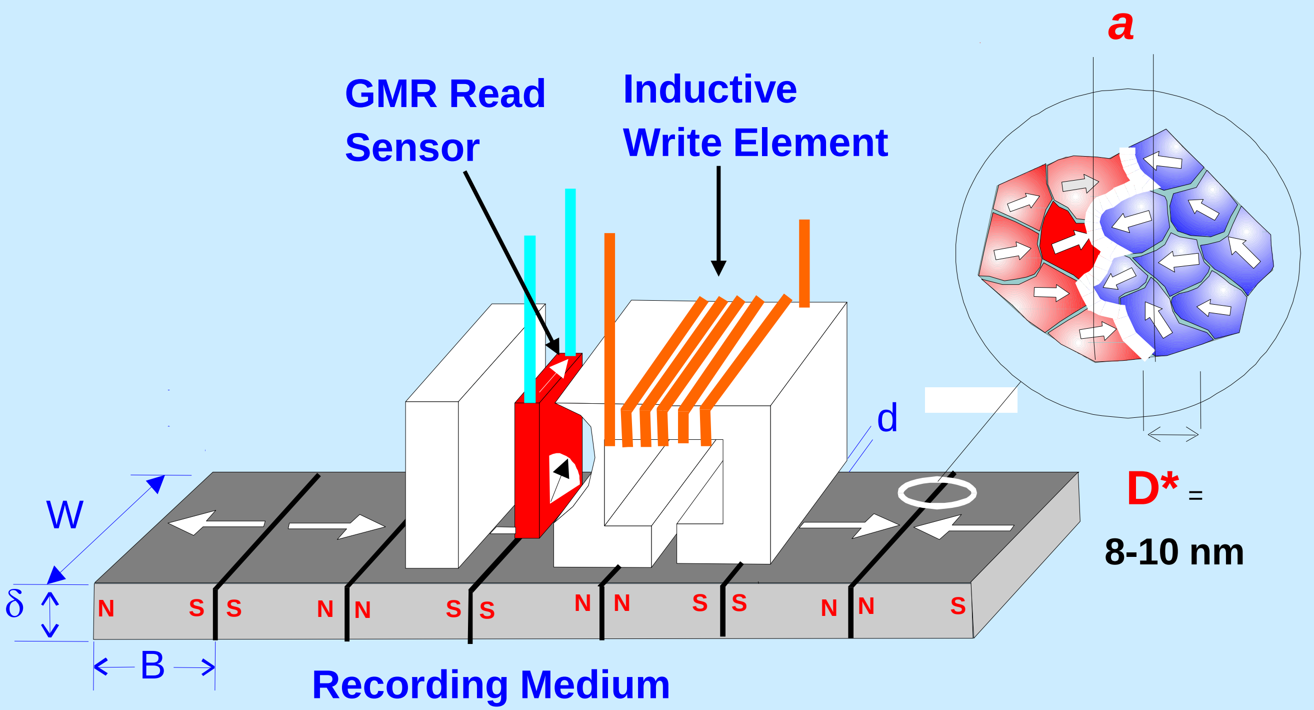
Magnetisation of recording medium



- Bistable behaviour required for information storage.
- This vanishes at the onset of superparamagnetic behaviour

Media Noise Limitations in Magnetic Recording

$$SNR \sim 10\times\log(\mathbf{B}/\sigma_j)$$



$$\sigma_j \propto a\sqrt{\frac{D^*}{W}}$$

Need $\sigma_j/B<10\%$

1. Transition position jitter σ_j limits media noise performance!
2. Key factors are cluster size D* and transition width a.
3. Reducing the grain size runs into the so-called superparamagnetic limit – information becomes thermally unstable

Superparamagnetism

- The relaxation time of a grain is given by the Arrhenius-Neel law

$$\tau_{\pm}^{-1} = f_0 \exp(-\Delta E_{\pm} / kT)$$

- where $f_0 = 10^9 s^{-1}$. and ΔE is the energy barrier
- This leads to a critical energy barrier for superparamagnetic (SPM) behaviour

$$\Delta E_c = KV_c = k_B T ln(t_m f_0)$$

- where t_m is the 'measurement time'
  - Grains with $\Delta E < \Delta E_c$ exhibit thermal equilibrium (SPM) behaviour - no hysteresis

Minimal Stable Grain Size (cubic grains)

$$\frac{K_u V}{k_B T} = r_K(\ln(\tau \cdot f_0), \sigma, H_D) \approx 60$$

1. Time
2. Temperature
3. Anisotropy

Alloy System	Material	Anisotropy K_u (10^7 erg/cc)	Saturation Magnetization M_s (emu/cc)	Anisotropy Field H_k (kOe)	Minimum stable grain size D_p (nm)	
	CoCrPtX	**0.20**	**200-300**	**15-20**	**8-10**	today
Co-alloy	Co	0.45	1400	6.4	8.0	
	Co_3Pt	2.00	1100	36	4.8	
	FePd	1.8	1100	33	5.0	
$L1_0$-phase	FePt	6.6-10	1140	116-175	2.8-3.3	future
	CoPt	4.9	800	123	3.6	
	MnAl	1.7	560	69	5.1	
RE-TM	$Nd_2Fe_{14}B$	4.6	1270	73	3.7	
	$SmCo_5$	11-20	910	240-400	2.2-2.7	

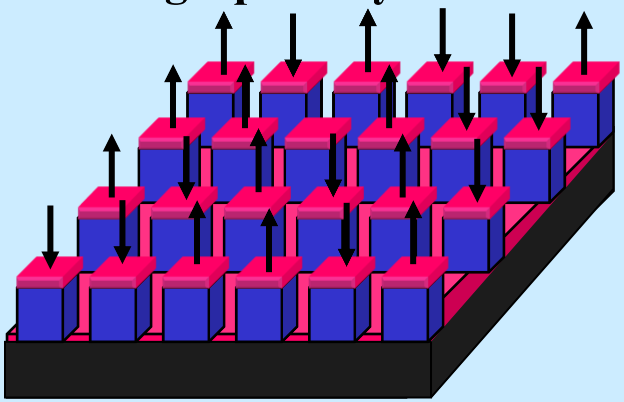
Write Field is limited by B_S (2.4T today!)of Recording Head

$H_0 = \alpha H_K - N M_S$

D. Weller and A. Moser, IEEE Trans. Magn.35, 4423(1999)

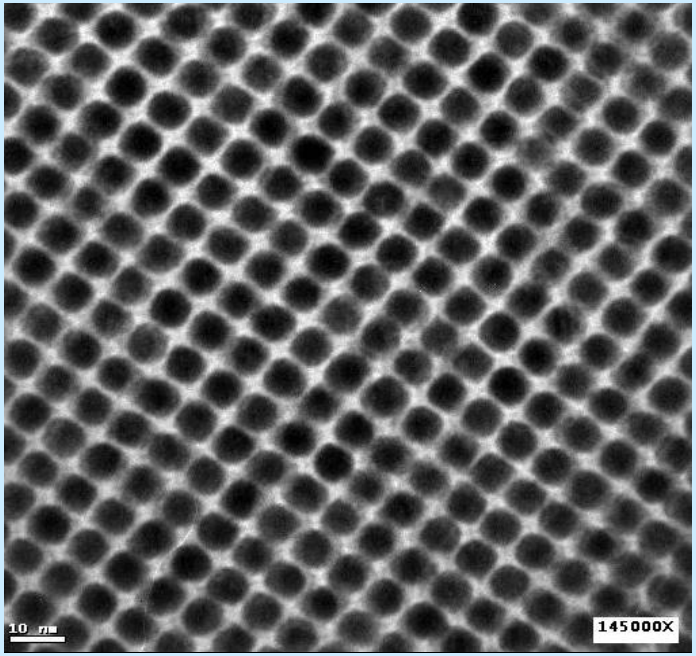
Bit Patterned Media
Lithography vs Self Organization

Lithographically Defined



- **Major obstacle is finding low cost means of making media.**
  - **At 1 Tbpsi, assuming a square bit cell and equal lines and spaces, 12.5 nm lithography would be required.**
  - **Semiconductor Industry Association roadmap does not provide such linewidths within the next decade.**

FePt SOMA media



•6.3+/-0.3 nm FePt particles
□$\sigma_{Diameter} \cong 0.05$

S. Sun, Ch. Murray, D. Weller, L. Folks, A. Moser, Science 287, 1989 (2000).

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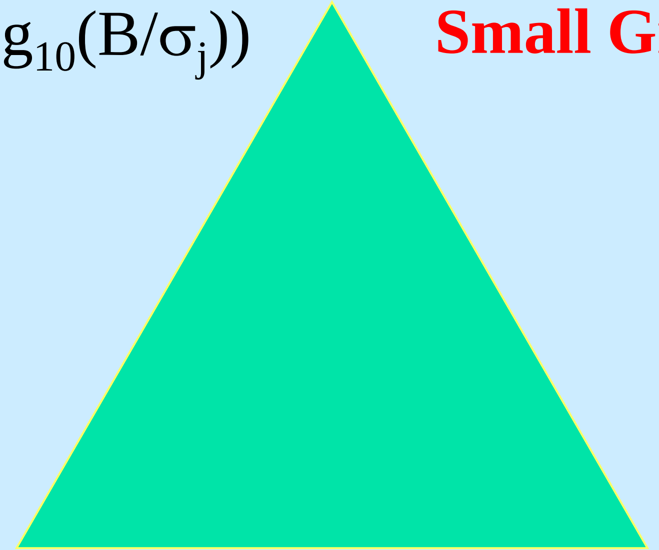
Media Design Constraints - "Trilemma"

Media SNR

SNR~10×log$_{10}$(B/σ_j))

Small Grains (V)



Thermal Stability

$$E_B \cong K_u V \cdot \left[1 - \frac{|H_d|}{H_0}\right]^{3/2}$$

$K_u V = r_k(T, t, \sigma, H_d) \times k_B T$

Writability

$$H_0 = \alpha \cdot \frac{2 \cdot K_u}{M_S} - N_{eff} \cdot M_S$$

H_0 < Head Field

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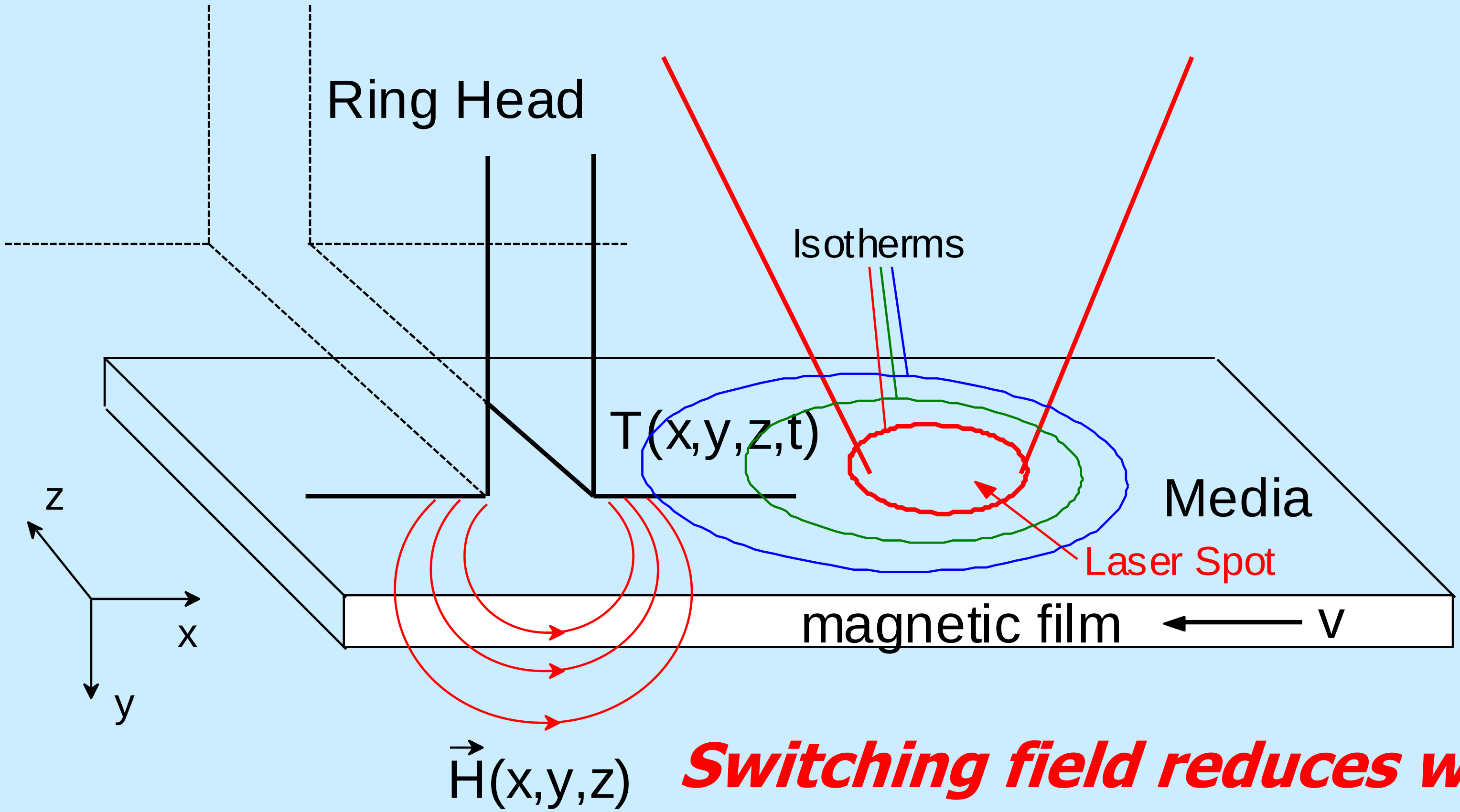
Heat-Assisted Magnetic Recording

Hybrid Recording Using Light

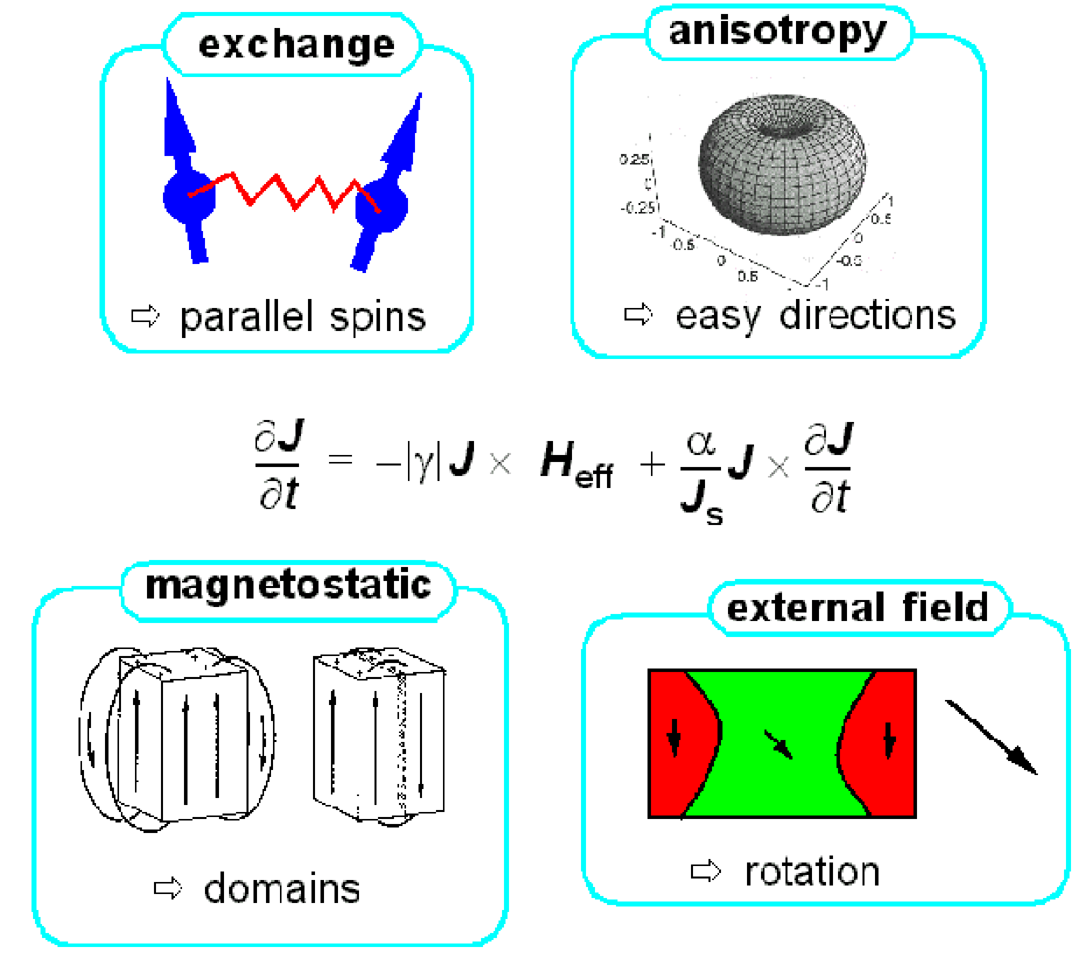


M. Kryder , et al. TMRC 2002

Switching field reduces with increasing temperature

Micromagnetics (thanks to Werner Scholz, Seagate)

- Effective field H_{eff} :
  - exchange
  - anisotropy
  - magnetostatic
  - external field
- Find energy minima by integration of the Gilbert equation of motion or direct energy minimization



$$\frac{\partial \boldsymbol{J}}{\partial t} = -|\gamma| \boldsymbol{J} \times \boldsymbol{H}_{eff} + \frac{\alpha}{J_s} \boldsymbol{J} \times \frac{\partial \boldsymbol{J}}{\partial t}$$

Micromagnetic exchange

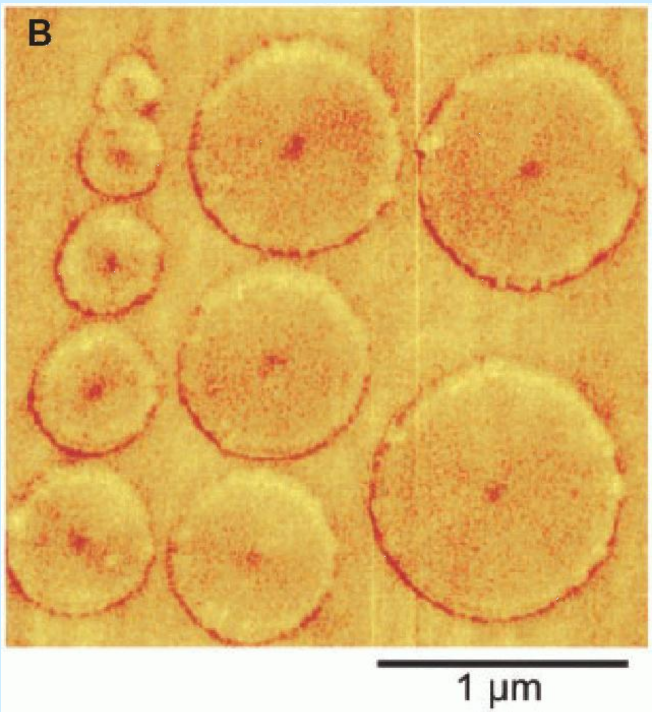
- The exchange energy is essentially short ranged and involves a summation of the nearest neighbours. Assuming a slowly spatially varying magnetisation the exchange energy can be written

$$E_{exch} = \int W_e dv, \text{ with } W_e = A(\nabla \mathbf{m})^2$$

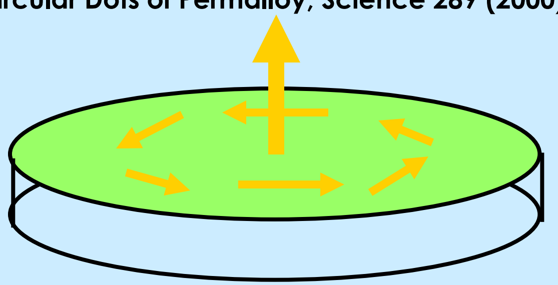
$$(\nabla \mathbf{m})^2 = (\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2$$

- The material constant $A = JS^2/a$ for a simple cubic lattice with lattice constant a. A includes all the atomic level interactions within the micromagnetic formalism.

Typical application of micromagnetics; structure of the vortex state



n in Circular Dots of Permalloy, Science 289 (2000) 930

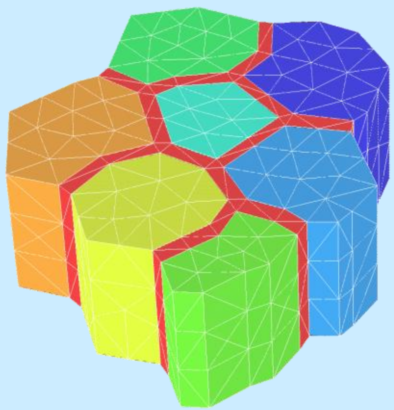


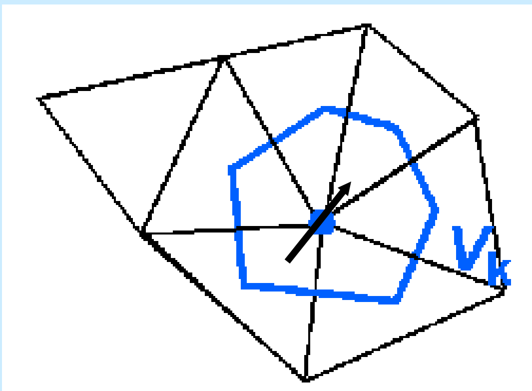
vortex state

Permalloy ($Ni_{80}Fe_{20}$) nanodots

- Saturation magnetization:
  $M_s = 8 \cdot 10^5$ A/m $= 8 \cdot 10^2$ G
  $J_s \approx 1$ T
- Exchange constant:
  $A = 13 \cdot 10^{-12}$ J/m $= 1.3 \cdot 10^{-6}$ erg/cm
- Anisotropy has been neglected
- Radius of 100 nm, thickness of 20 nm

Finite Element Approach





- divide particles into finite elements
  ⇨ triangles, tetrahedrons
- expand *J* with basis function J_i

$$\vec{J}(\vec{x}) = \sum_{i=1}^{nodes} \vec{J}_i \varphi_i(\vec{x})$$

- energy as a function of J_1, J_2 … J_N

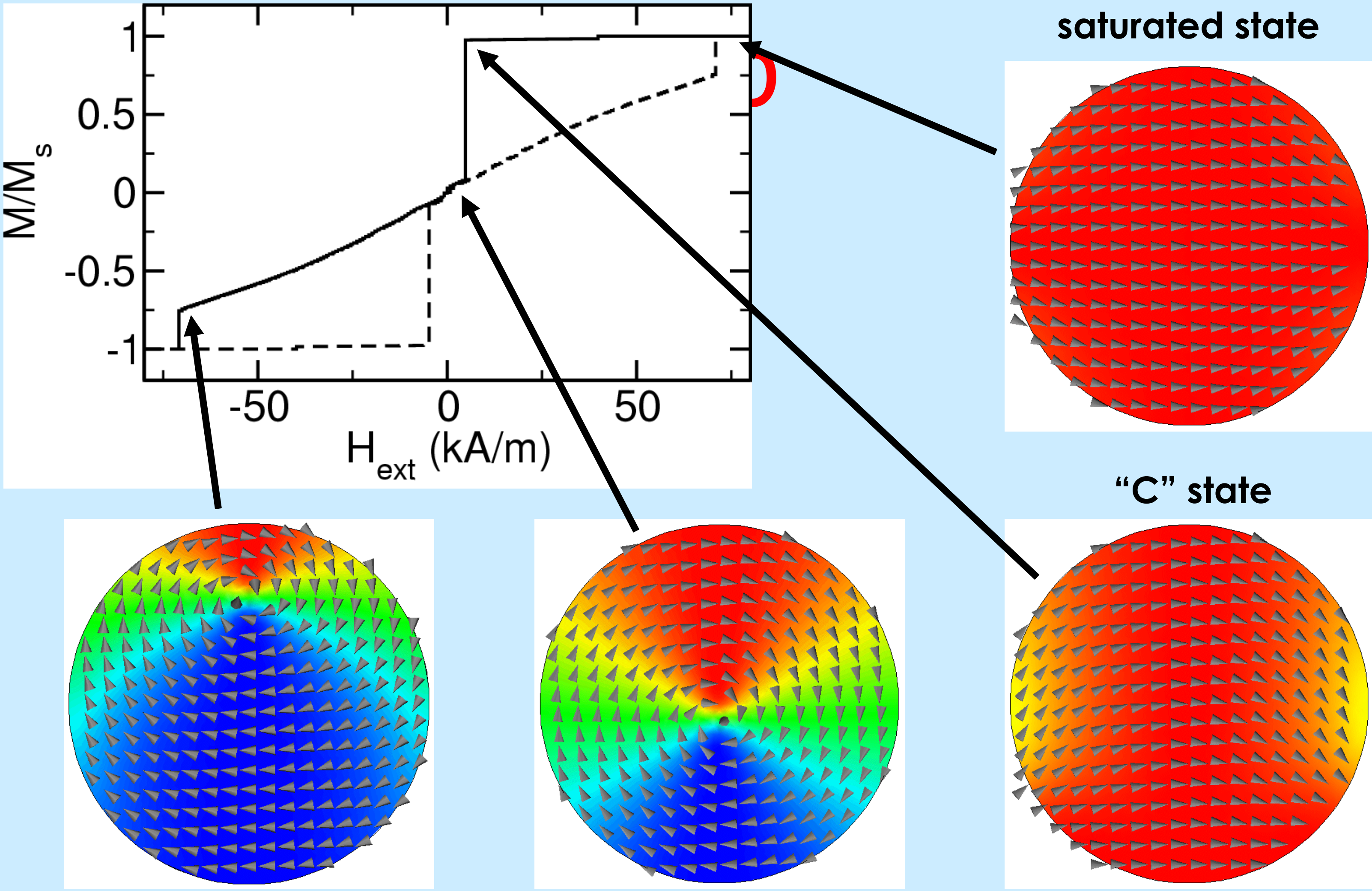
$$E(\vec{J}_1, \vec{J}_2 .... \vec{J}_N)$$

- effective field

$$\vec{H}_k = -\frac{1}{V_k} \frac{\partial E(\vec{J}_1, \vec{J}_2 .... \vec{J}_N)}{\partial \vec{J}_k}$$

⇨ effective field on irregular grids
⇨ rigid magnetic moment at the nodes

W Scholz et al **J Magn. Magn. Mater., 266, 155-163 (2003)**

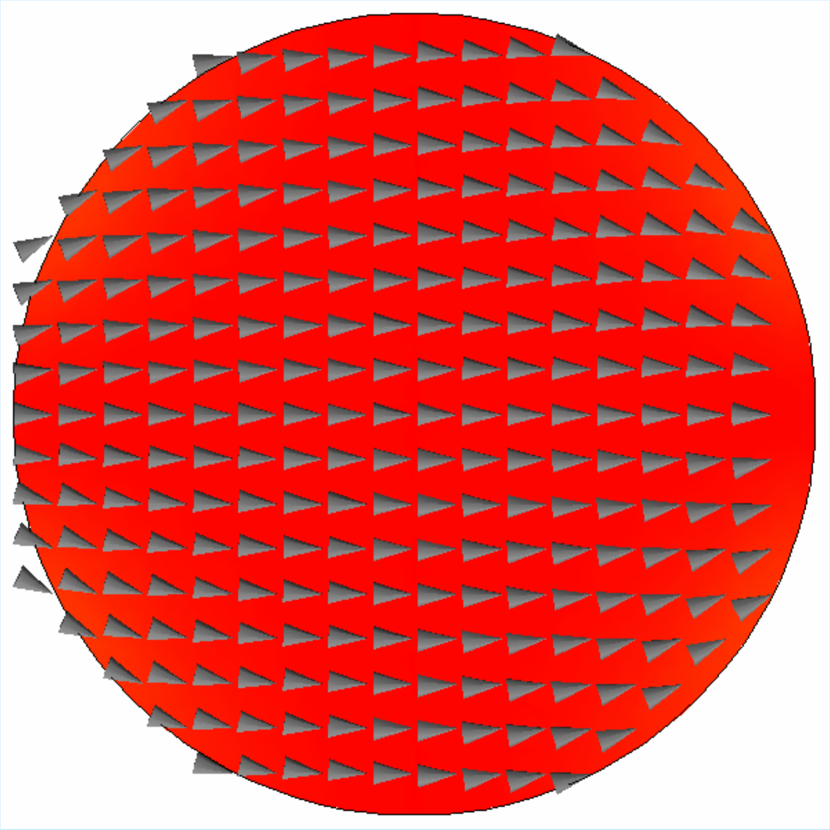


annihilation field:
70 kA/m = 880 Oe = 88 mT

Equilibrium in zero field

nucleation field:
5 kA/m = 62 Oe = 6.2 mT

Hysteresis movie



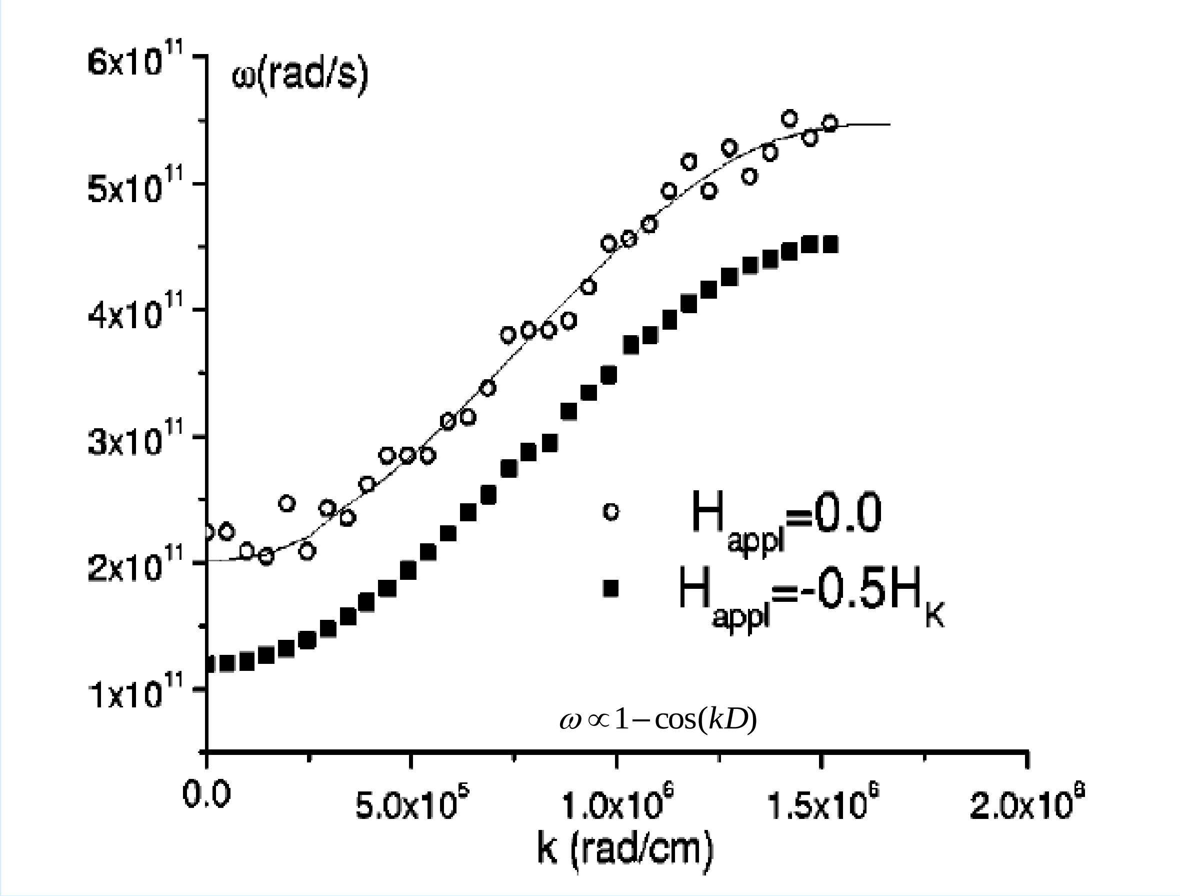
- L/R=20/100 nm
- Nucleation field: 5 kA/m
- Annihilation field: 70 kA/m

Excitations and magnetisation reversal (O. Chubykalo, et al Phys. Rev B 65, 184428 (2002))

- Zero temperature reversal proceeds via well defined eigenmodes according to (athermal) micromagnetics
- Non-zero temperature first studied by Chubykalo et al
- Model used the micromagnetic approach with Langevin Dynamics
- Studied excitations and reversal in a spin-chain

Computational approach

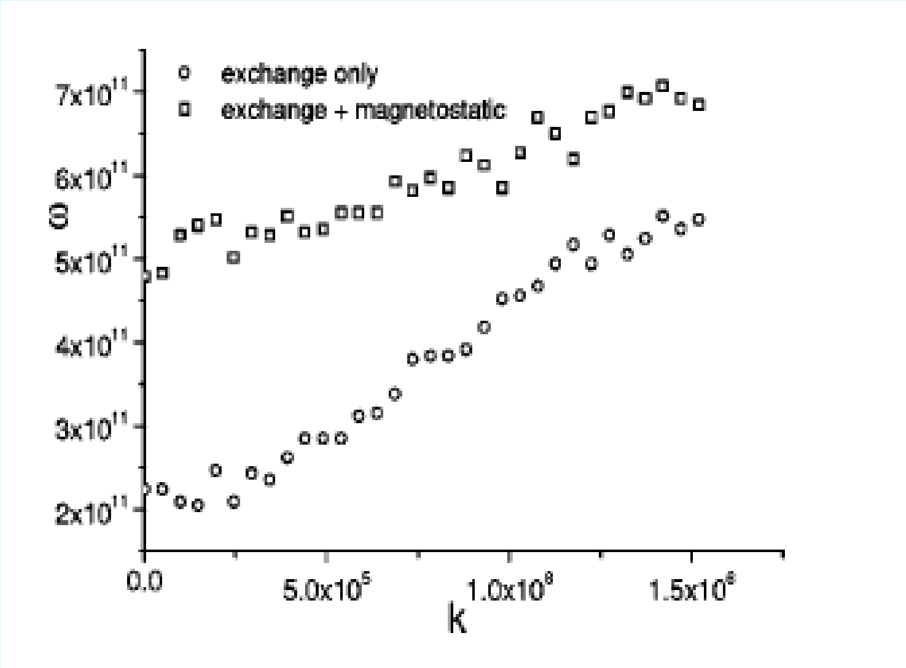
- Allow the system to attain thermal equlibrium
- Spatial correlations are then studied by Fourier transformation of the off-axis components of the magnetizationgiving a wavelength amplitude spectrum that demonstrates the preferential excitation of long-wavelength fluctuations.
- Further, the variation of amplitude with time at each value of the wave vector *k* leads to a time series, Fourier analysis of which leads to a frequency spectrum for each value of *k.*
- These spectra are analyzed in order to give the dispersion relation.

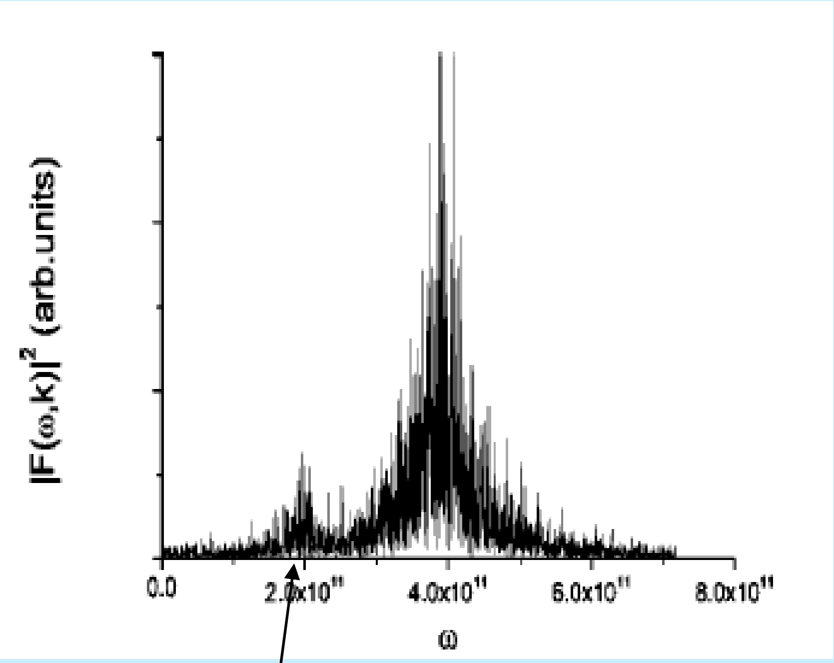


- Dispersion relation for exchange coupling only
- Follows the expected relation (with D the discretisation size)

$$\omega \propto 1 - \cos(kD)$$

Exchange and magnetostatic interactions





Magnetostatic mode

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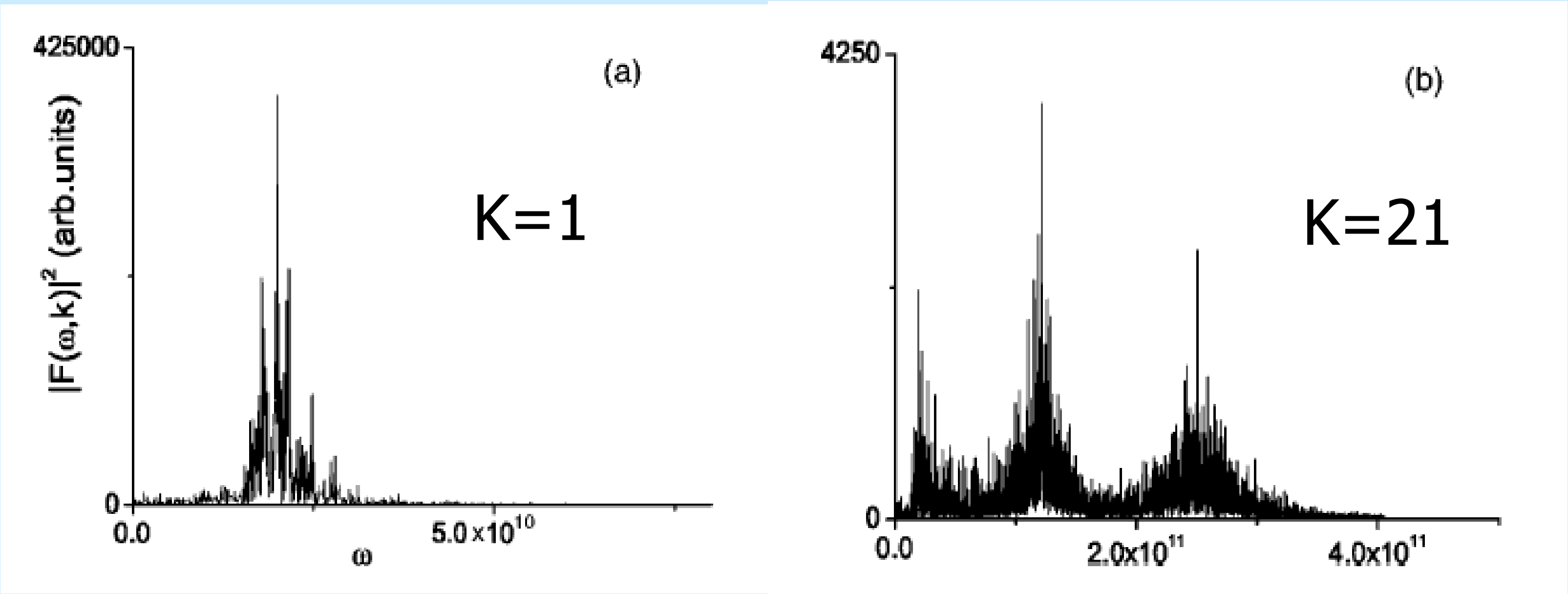
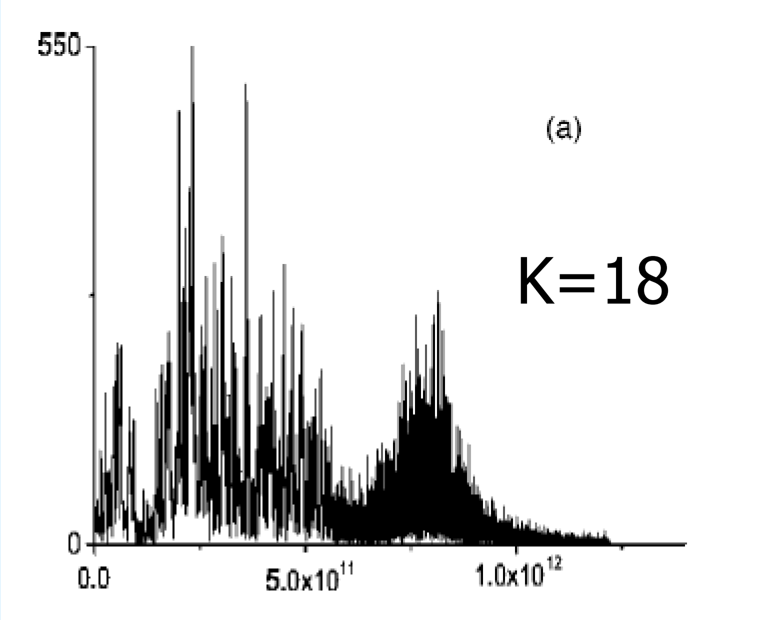
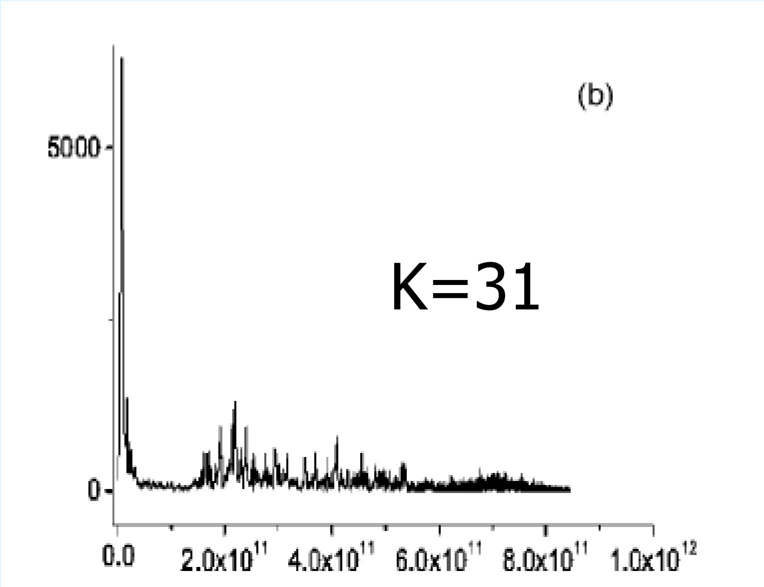
Reversal; exchange coupled system



- Long wavelength mode excited
- Consistent with coherent rotation (all spins parallel)
- Peaks in higher k mode indicative of complex non-linear dynamics

Magnetostatic interactions

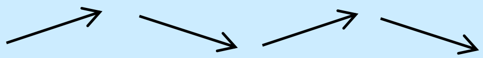




- Long wavelength excitations established

Modes

Coherent (exchange dominated)



Fanning (magnetostatically dominated)

- Thermal excitation preferentially establishes the eigenmode for reversal.

Long timescales

- Cannot use the spin dynamic approach (restricted to 10^3 ns)
- Use kinetic MC approach
- First, local field approximation
- Secondly; collective reversal model

The model

- Allows time and temperature dependence - superparamagnetic effects
- Dynamic behaviour is studied via the Arrhenius-Neel law
- Local field approach introduces both exchange and magnetostatic interactions

Thermally activated dynamics

- The relaxation time of a grain is given by the Arrhenius-Neel law

$$\tau_{\pm}^{-1} = f_0 \exp(-\Delta E_{\pm} / kT)$$

where $f_0 = 10^9 s^{-1}$. and ΔE is the energy barrier

- This leads to a critical energy barrier for superparamagnetic (SPM) behaviour

$$\Delta E_c = KV_c = k_B T ln(t_m f_0)$$

where t_m is the 'measurement time'

- Grains with $\Delta E < \Delta E_c$ exhibit thermal equilibrium (SPM) behaviour - no hysteresis

Thermally stable grains ($\Delta E > \Delta E_c$)

- Reversals are governed by a transition probability

$$P_r = 1 - e^{-t_m/\tau}$$

- In general

$$\tau^{-1}(H_T, T, \psi) = f_{H_T} e^{-[\Delta E(H_T,\psi)/k_B T]}$$

where the easy axis is oriented at some angle ψ to the local field

- Numerical approximation to ΔE is used

$$\Delta E(H_T, \psi) = \Delta E_0 \left[1 - h_T / g(\psi)\right]^{\kappa(\psi)}$$

where $g(\psi) = \left[\cos^{2/3}\psi + \sin^{2/3}\psi\right]^{-3/2}$ $\kappa(\psi) = 0.86 + 1.14 g(\psi)$

Field calculation

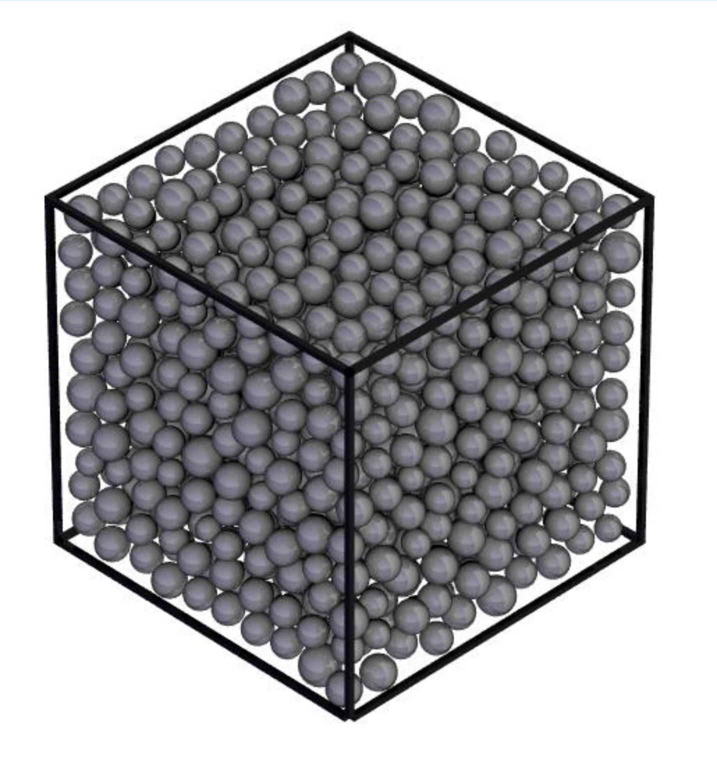
- Direct summation over nearest neighbours

$$\vec{\mathbf{H}}_T = H_a \hat{z} + \sum_{i \neq j} \left[\frac{3\left(\vec{\mu}_j \cdot \vec{\mathbf{r}}_{ij}\right)\vec{\mathbf{r}}_{ij}}{d_{ij}^5} - \frac{\vec{\mu}_j}{d_{ij}^3} \right] + c^* \sum_{i \neq j} \vec{\mu}_j$$

Truncation range of 5 grain diameters

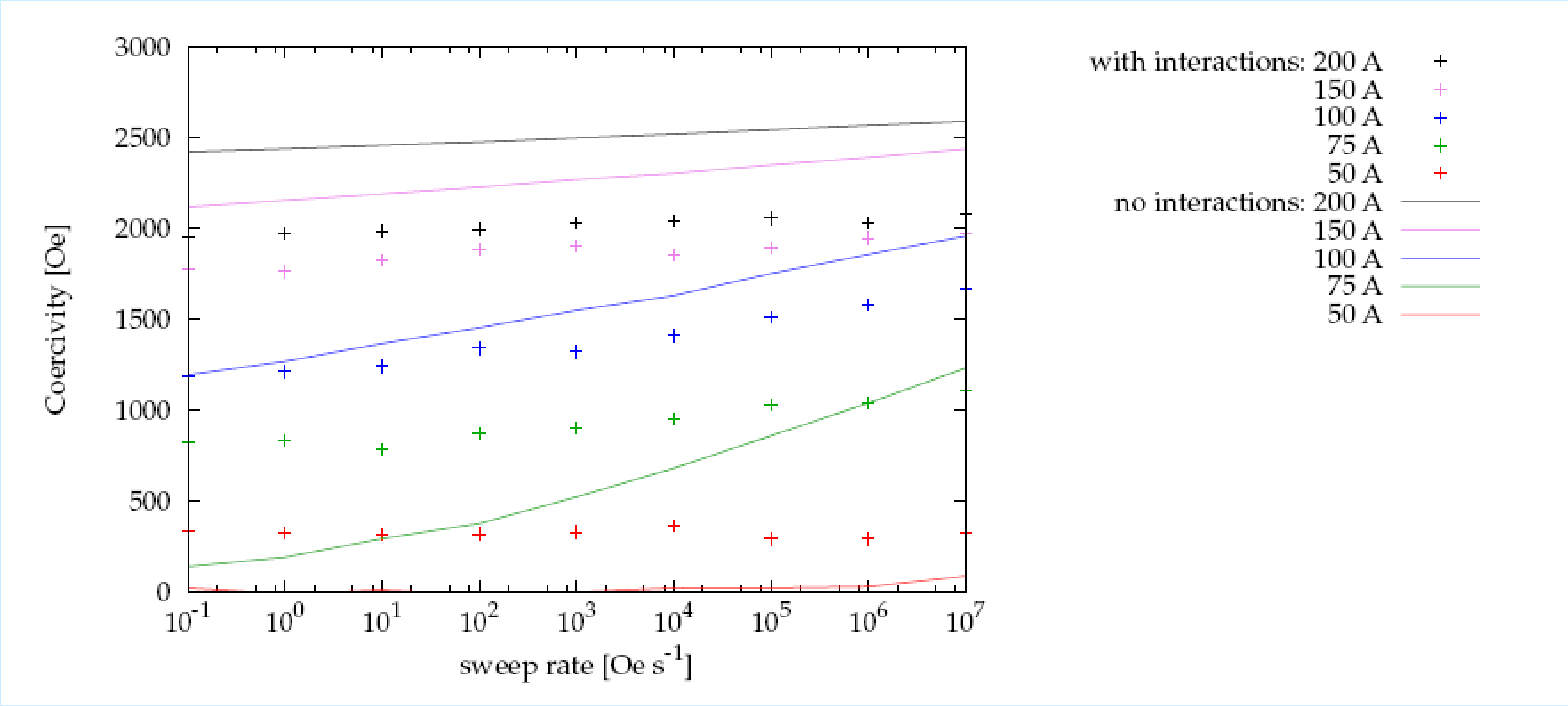
- Includes exchange field contributions. C^* is H_{exch}/H_k
- long-range field term included via a mean-field approach

Magnetic hyperthermia



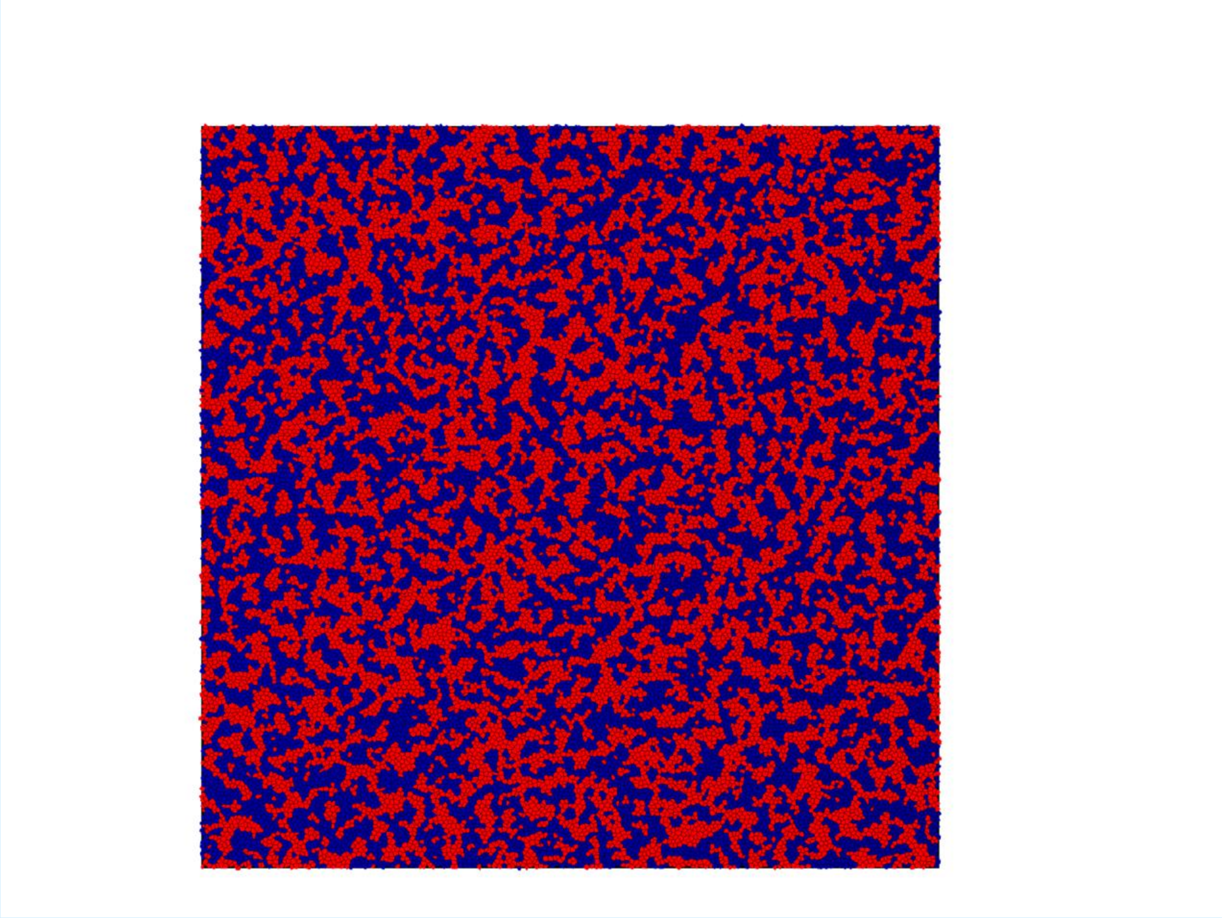
- Hysteresis heating can be used to kill tumours
- Effect of interactions, dynamics?

Fe particles



- Strong effect of interactions
- Effect of reduction in max field with sweep rate?

Correlated reversal – recording media

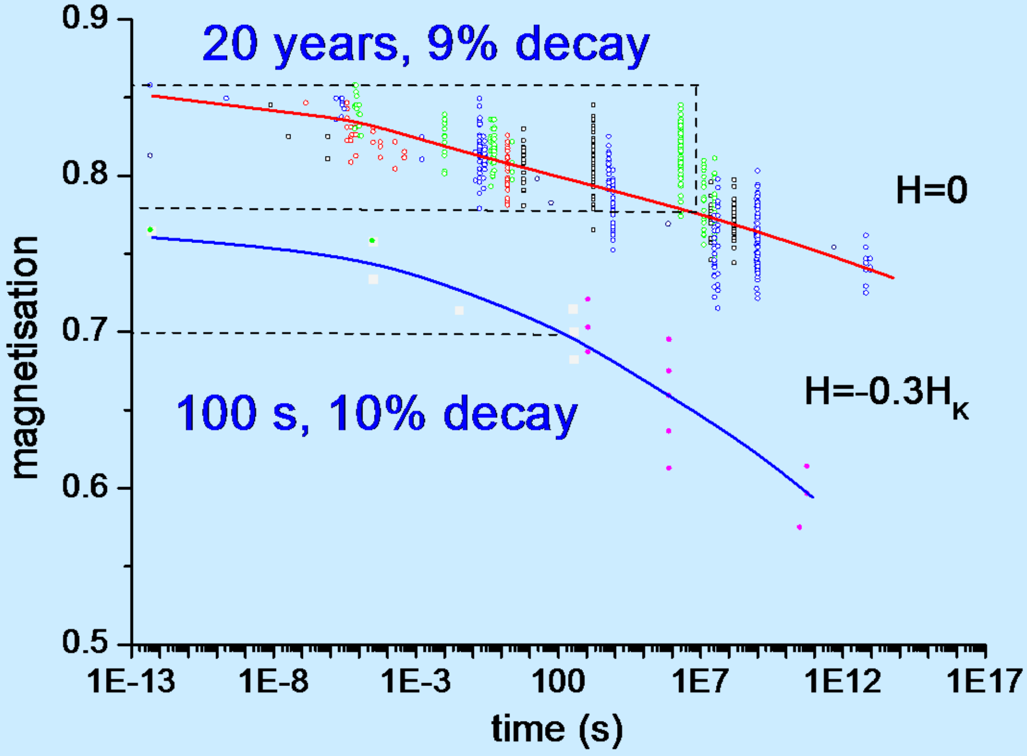


- Erased state of recording medium with perpendicular anisotropy

Computational approach

- Determine energy barriers and saddle points by ridge method
- Use Arrhenius-Neel law to determine the relaxation time and reversal probability
- pre-exponential factor determined using transition state theory

Time decay of recorded signal



The need for atomistic/multiscale approaches

- Micromagnetics is based on a continuum formalism which calculates the magnetostatic field exactly but which is forced to introduce an approximation to the exchange valid only for long-wavelength magnetisation fluctuations.
- Thermal effects can be introduced, but the limitation of long-wavelength fluctuations means that micromagnetics cannot reproduce phase transitions.
- The atomistic approach developed here is based on the construction of a physically reasonable classical spin Hamiltonian based on ab-initio information.

Atomistic model

- Uses the Heisenberg form of exchange

$$E_i^{exch} = \sum_{j \neq i} J_{ij} \vec{S}_i . \vec{S}_j$$

- Spin magnitudes and J values can be obtained from ab-initio calculations.
- We also have to deal with the magnetostatic term.
- 3 lengthscales – electronic, atomic and micromagnetic – Multiscale modelling.

Model outline

Ab-initio information (spin, exchange, etc)

↓

Classical spin Hamiltonian → **Dynamic response solved using Langevin Dynamics (LLG + random thermal field term)**

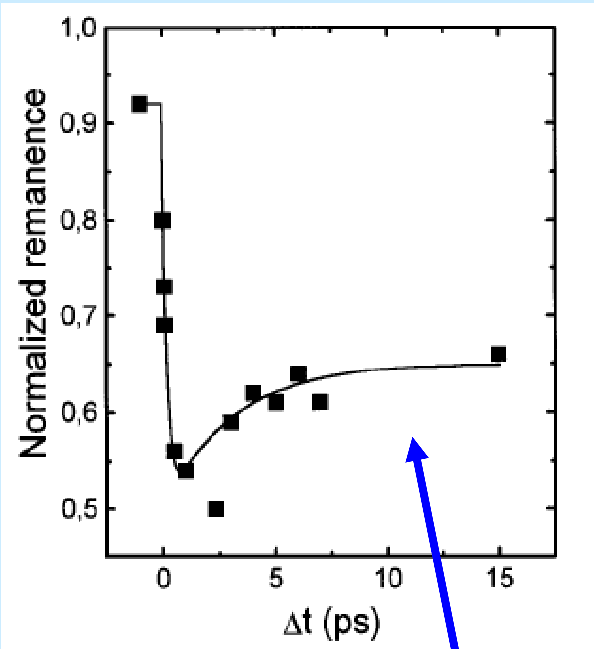
↑

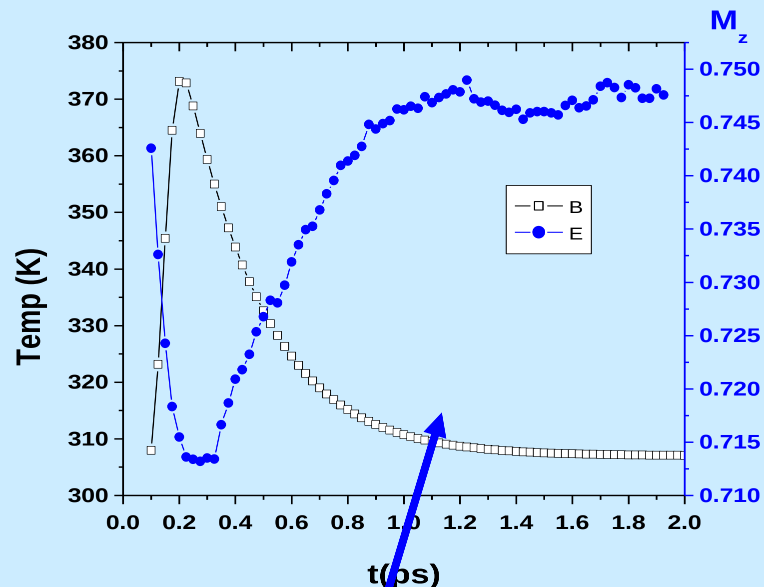
Magnetostatics

Laser Pump-probe experiments

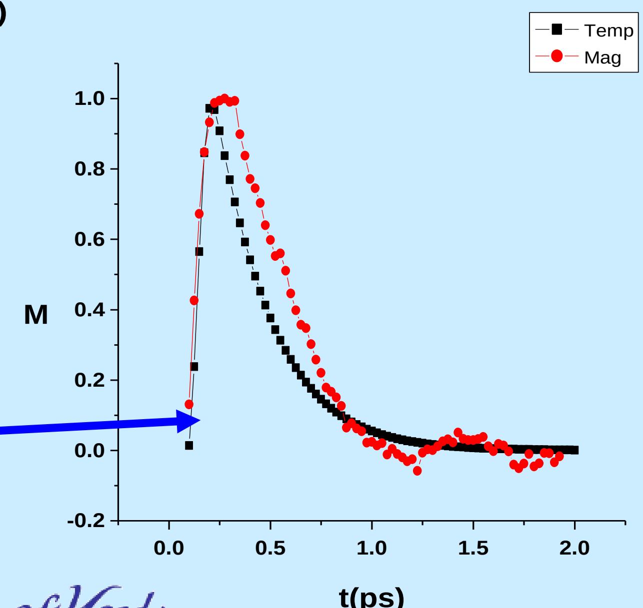
- High energy laser beam (pump) causes rapid heating of a magnetic film
- Part of the beam is split off and used to measure the magnetisation of the film using the Magneto-Optic Kerr Effect (MOKE)
- Magnetisation changes on the sub-picosecond timescale can be demonstrated experimentally
- Very important physics
- Also, potentially important because of the possible use of Heat Assisted Magnetic Recording (HAMR)

Ultrafast demagnetisation





- Experiments on Ni (Beaurepaire et al PRL <u>76</u> 4250 (1996)
- Calculations for peak temperature of 375K
- Normalised M and T. During demagnetisation M essentially follows T



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Excitation modes during ultrafast heating

- Same approach as before:
  - Spatial and temporal Fourier transforms
  - Gives the dispersion relation
  - Can also calculate a ‘mode occupancy’ from the power/mode normalised by the total power
- We have studied the excitations in both ferromagnets and antiferromagnets

Analytical dispersion relations

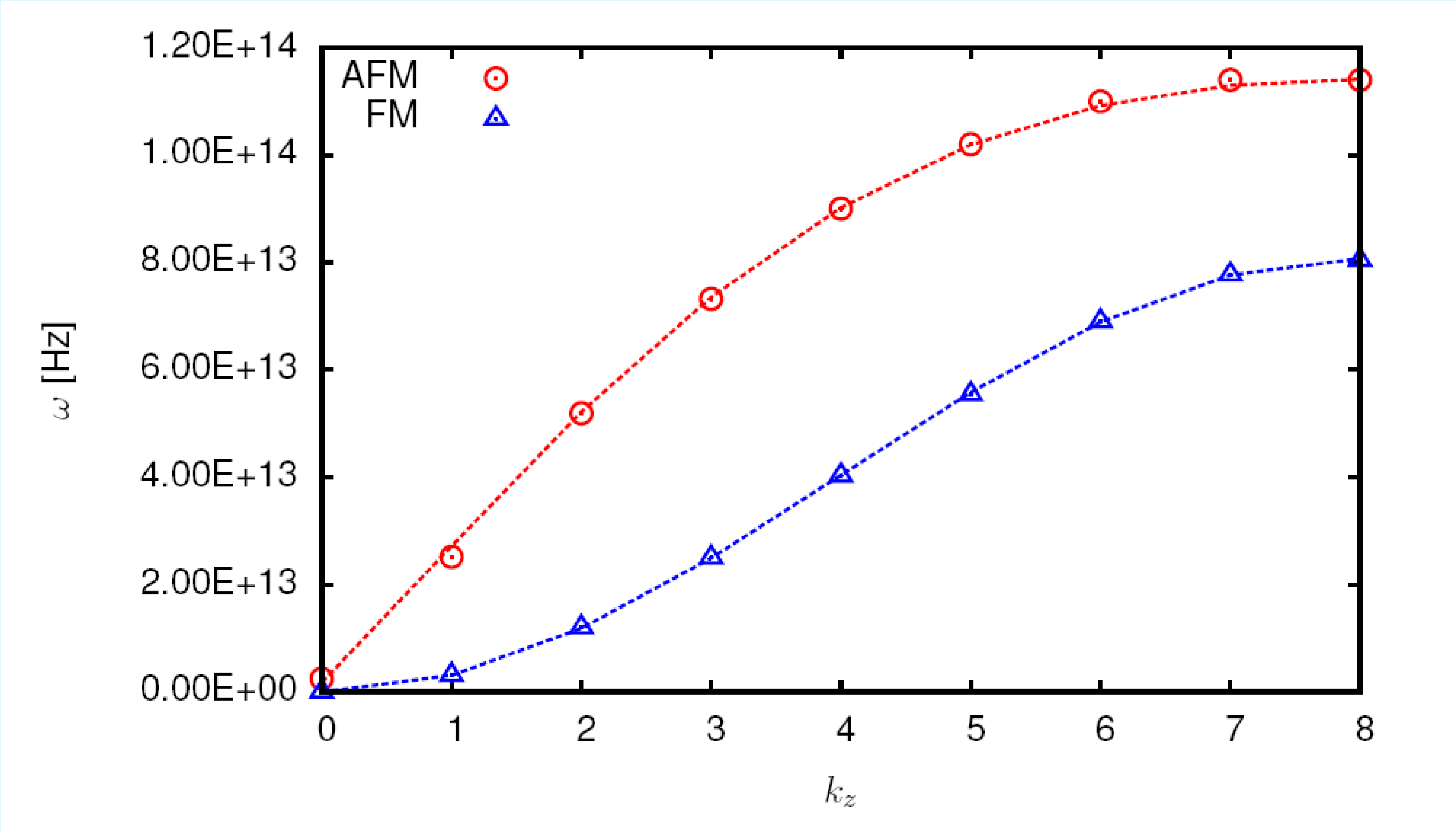
Ferromagnet

$$\omega(k_z) = \gamma \left[B_{ani} + B_{app} + 2SJ(1 - \cos k_z a)\right]$$

Antiferromagnet

$$\omega(k_z) = \gamma \left[B_{app} \pm \sqrt{(B_{ani} + 6SJ)^2 - (2SJ(1 \cos k_z a + 2))^2}\right]$$

Analytical vs numerical



- Solid lines; analytical, symbols; numerical

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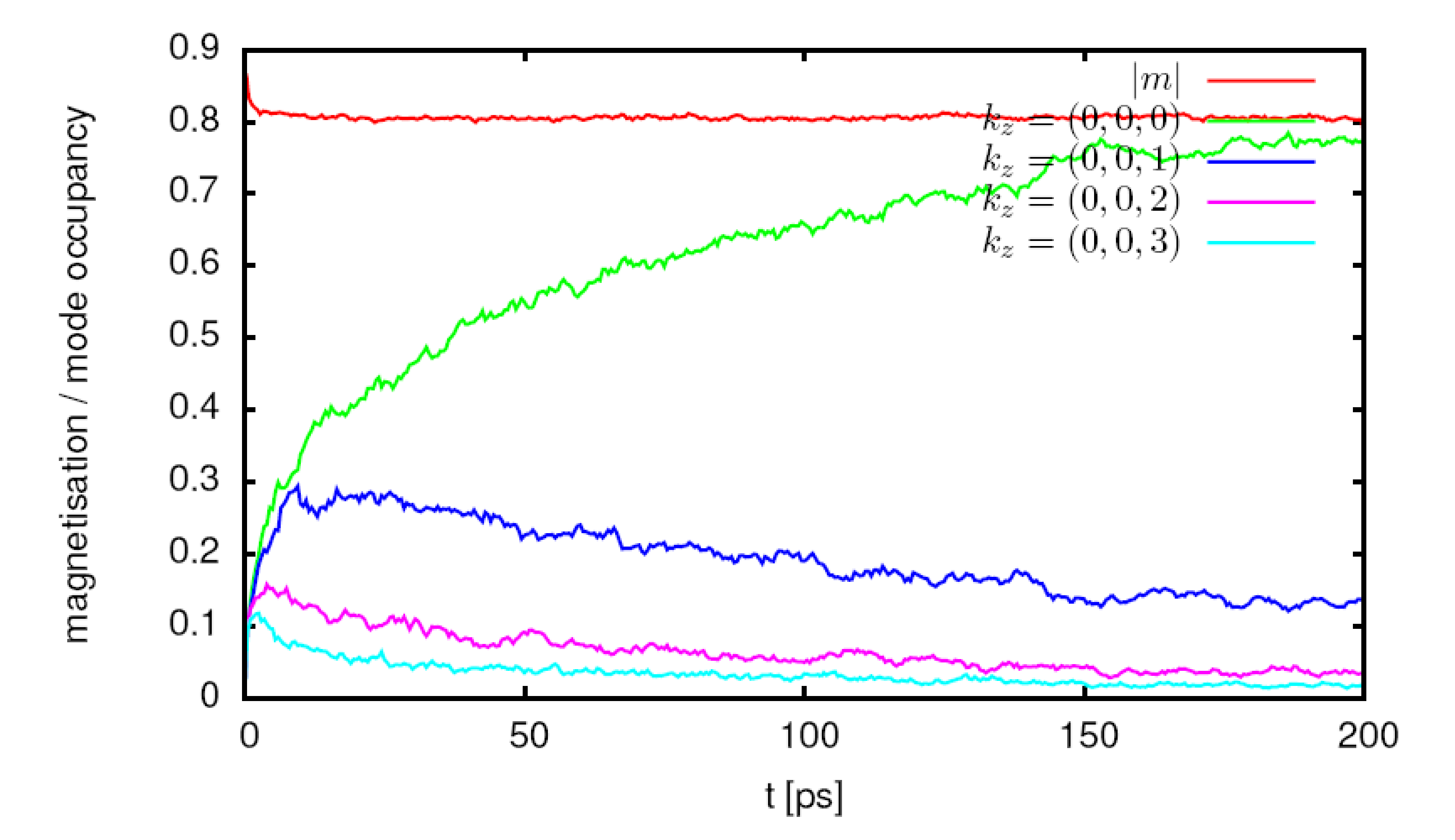
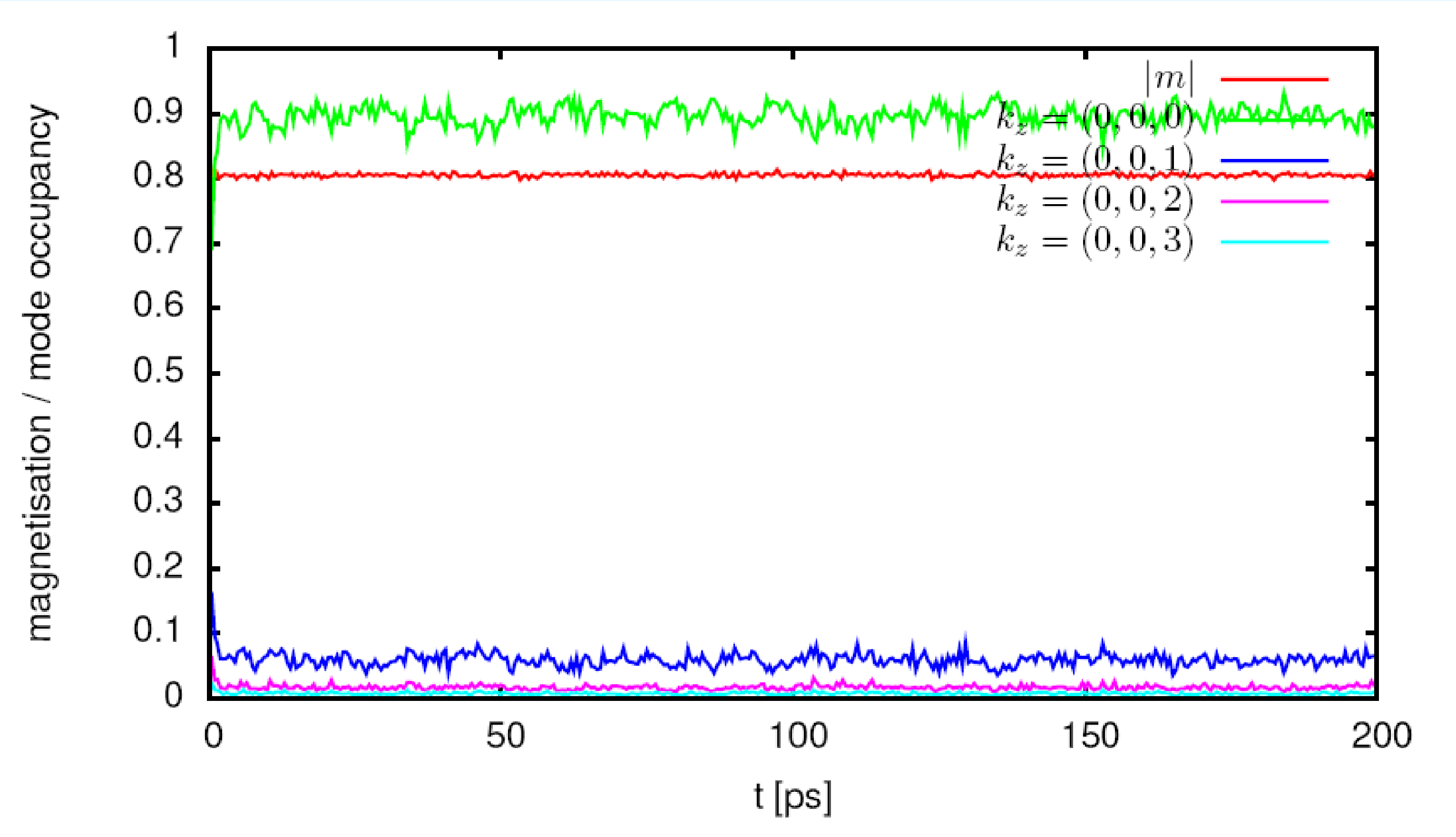
Response to step temperature change: ferromagnet

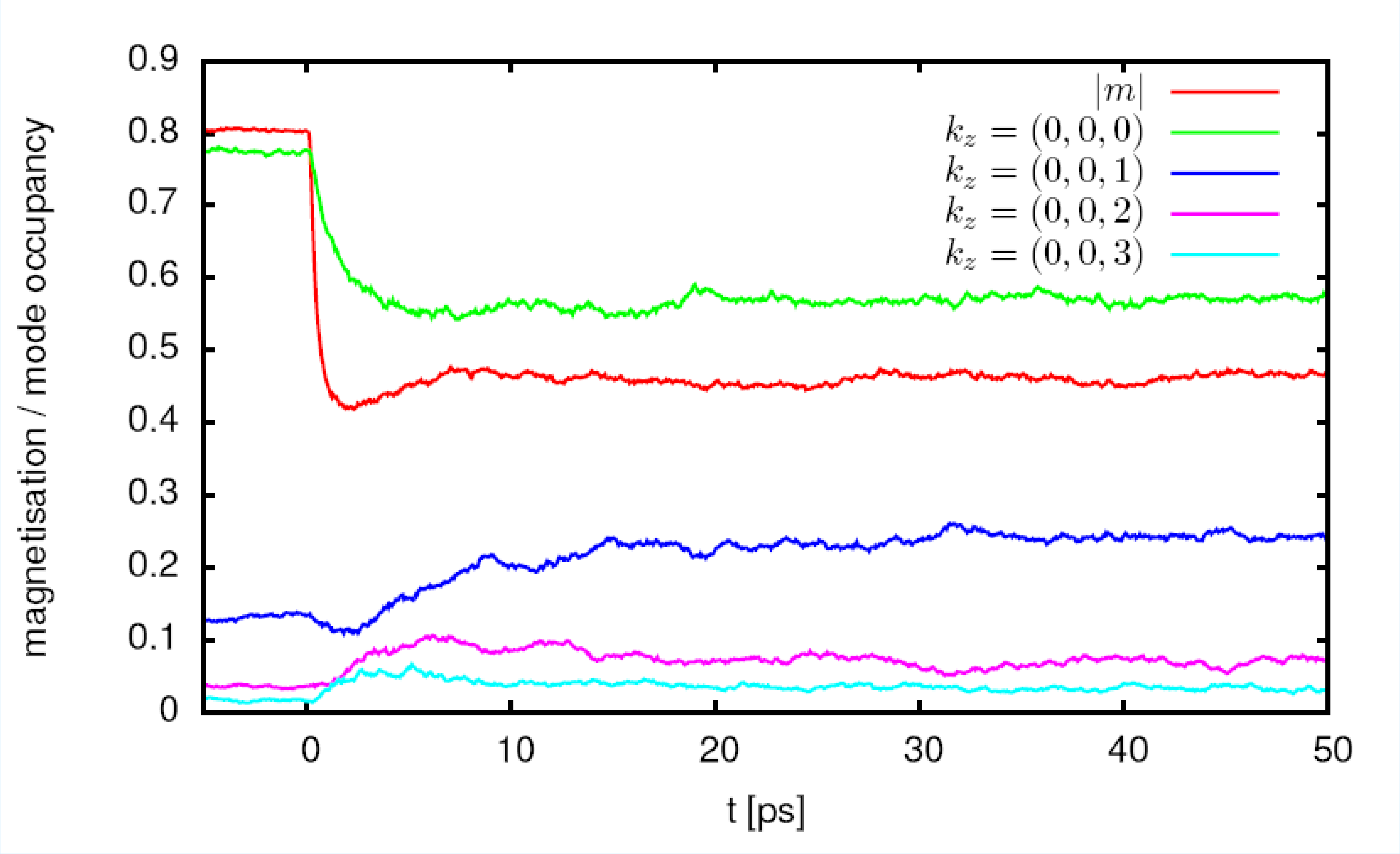


Antiferromagnet

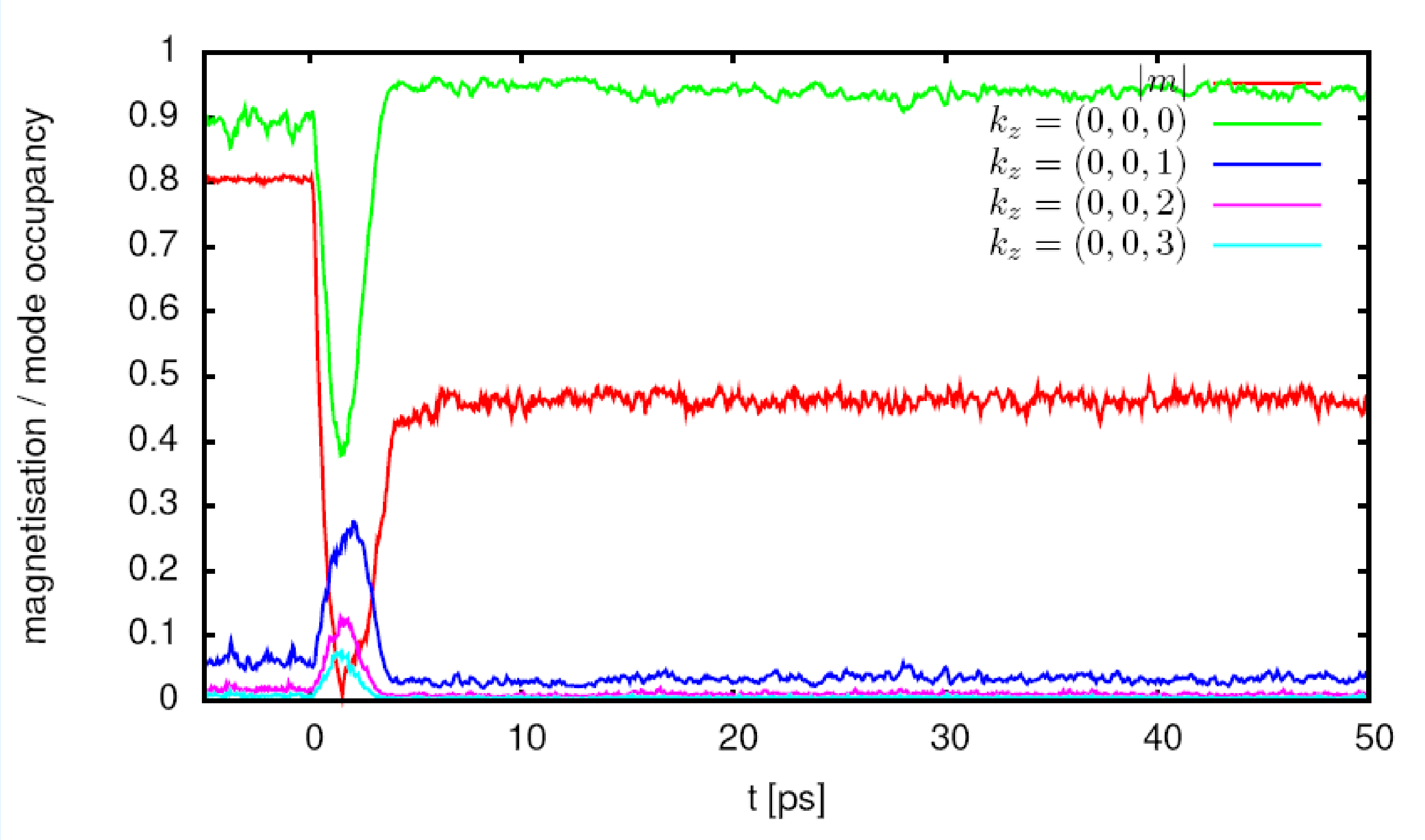


- (Staggered) magnetisation equilibrates more rapidly than FM

Response to pulse temperature change: ferromagnet



Antiferromagnet



- Much faster response
- Consistent with faster demagnetisation of the AF

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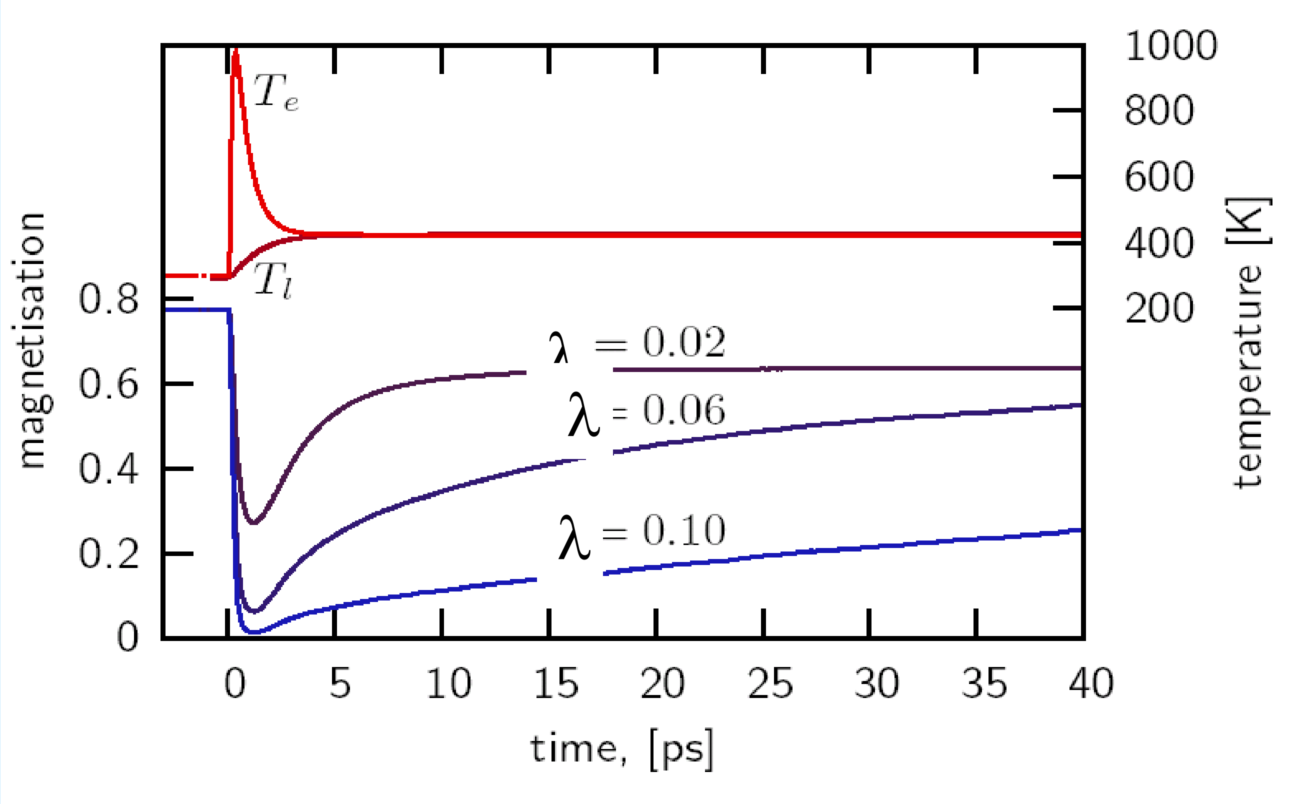
Summary

- Stochastic processes are important for magnetisation reversal
- Dominant eigenmodes for reversal are established by thermal excitation
- Long timescale calculations are still problematic
- Atomistic approaches are important for ultrafast timescales and elevated temperatures
- Even the type of magnetic order affects the dynamics
- Can we link the mesoscopic and atomistic lengthscales?

Pump-probe simulations – continuous thin film



- Rapid disappearance of the magnetisation
- Reduction depends on λ

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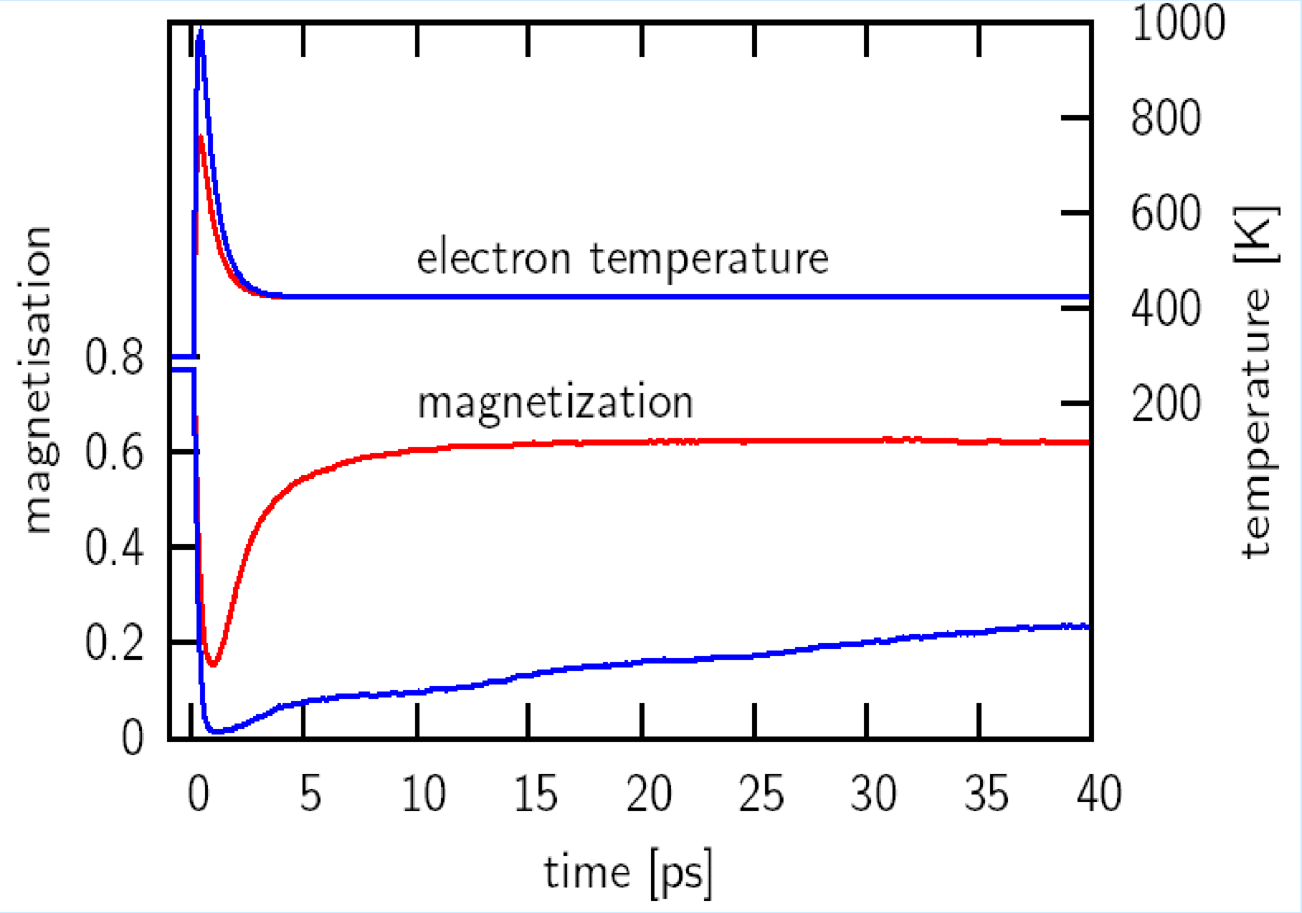
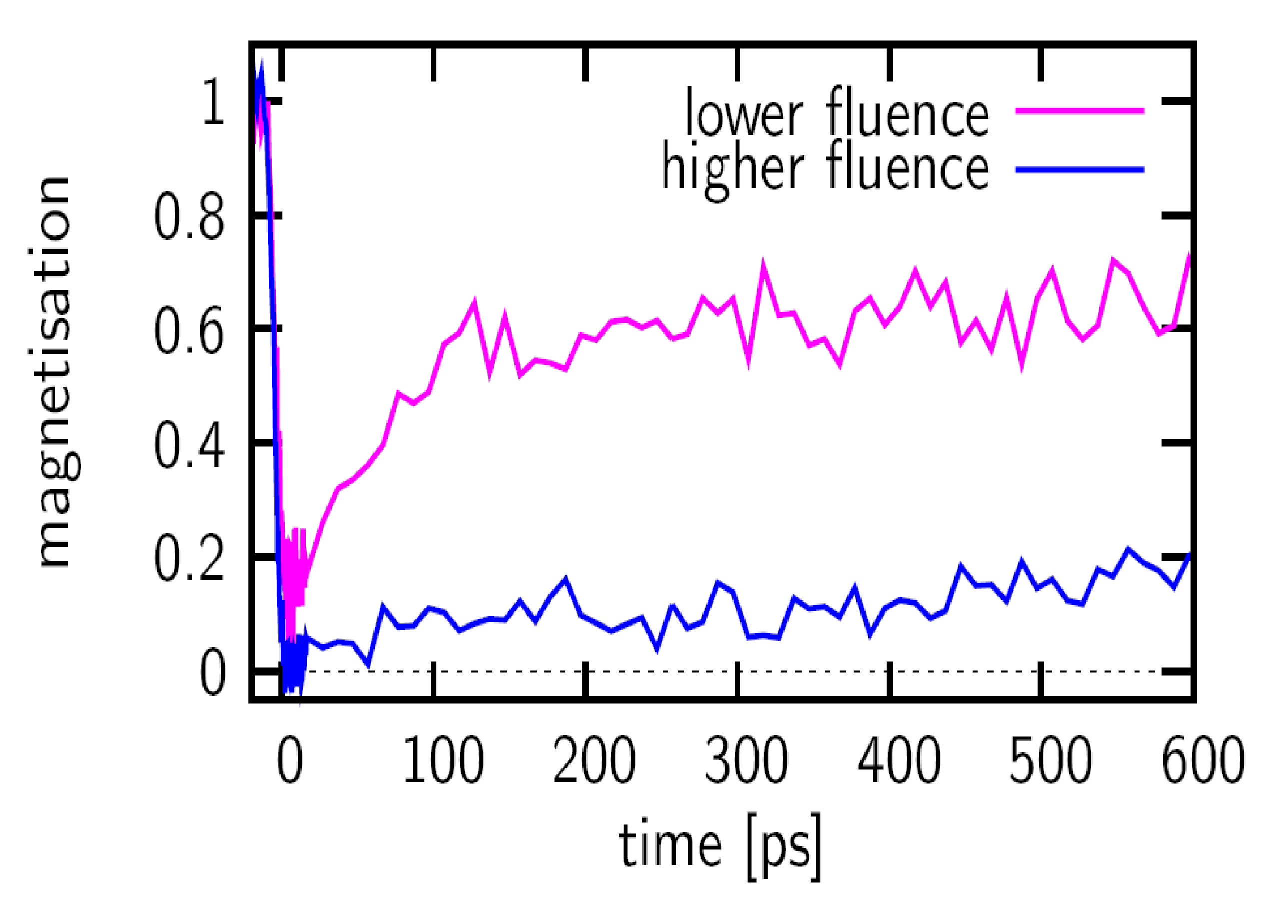
Dependence on the pump fluence

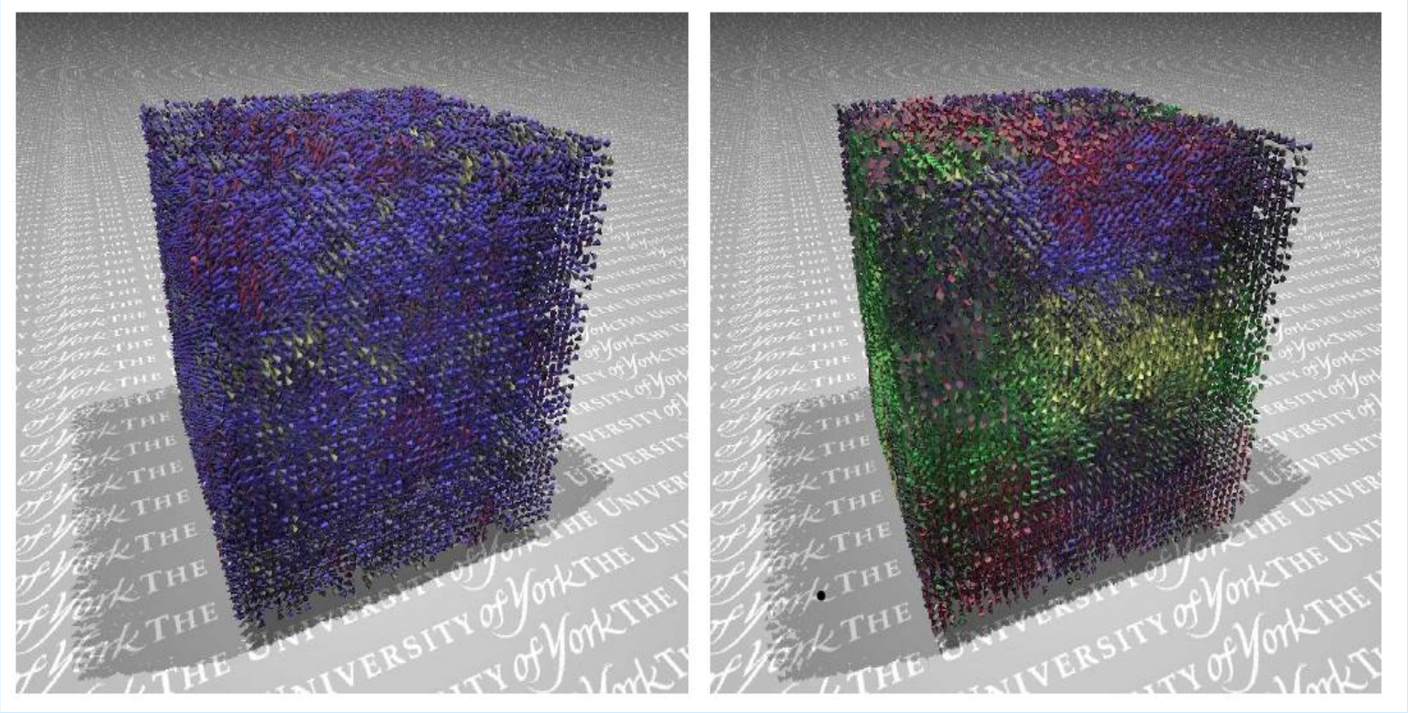


- Note the slow recovery of the magnetisation for the higher pump fluence

Experiment (J. Hohlfeld)



Slow recovery due to disordered magnetic state



- Snapshots of the magnetisation distribution after 19ps for λ = 0:02 (left) and λ = 0:2 (right).
- Fast recovery if there is some ‘memory’ of the initial magnetic state.
- For the fully demagnetised state the recovery is frustrated by many nuclei having random magnetisation directions.

Comment on the use of the LLG equation and Langevin Dynamics

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

Spin system ⇔ **Conduction electrons** ⇔ **Lattice** ⇔ **Heat bath**

- What is α? Transfer of energy via complicated channels
- Very challenging. But interesting physics and important applications
- Are thermal fluctuations really uncorrelated? Next we look at the effects of correlated noise

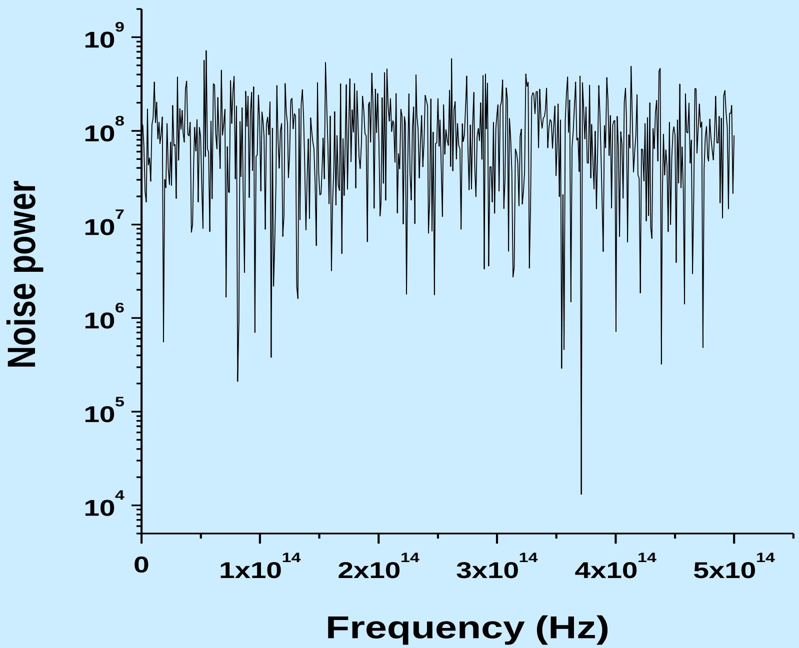
Coloured noise

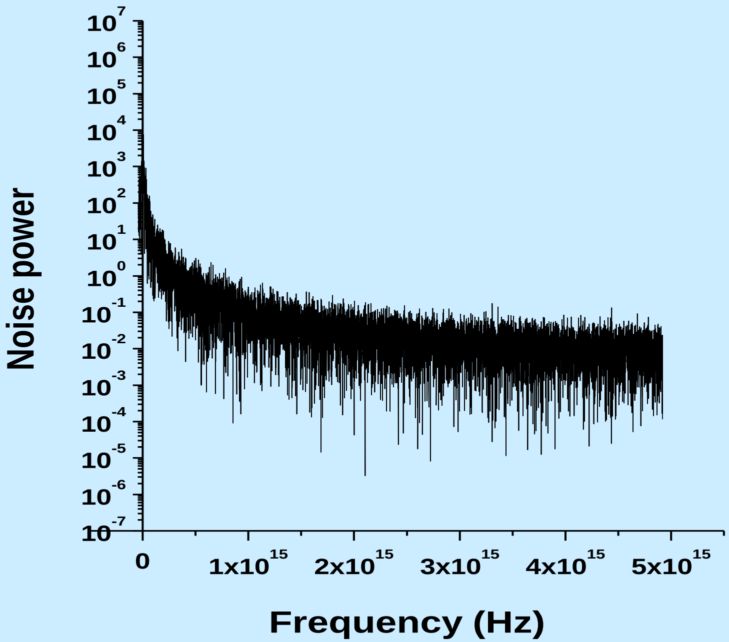
- Simulations so far used white noise
- Assumes uncorrelated noise source
- Here we introduce exponentially correlated noise and investigate the effect on the relaxation time of the magnetisation.

Exponentially correlated (Ornstein-Uhlenbeck) noise

$$\langle \varepsilon(t) \rangle = 0 \qquad \text{and} \qquad \langle \varepsilon(t)\varepsilon(t') \rangle = \frac{D}{\tau} \exp\left(-\frac{|t-t'|}{\tau} \right)$$

- Gaussian noise with zero mean and exponential correlation function.
- Correlation time τ
- Variance $\sigma^2 = \langle \varepsilon^2 \rangle = D/\tau$





Correlations shift the noise to low frequencies (right)

Basis of the simulation – Miyazaki- Seki equation
Atxitia et al Phys. Rev. Lett. 102, 057203 (2009)

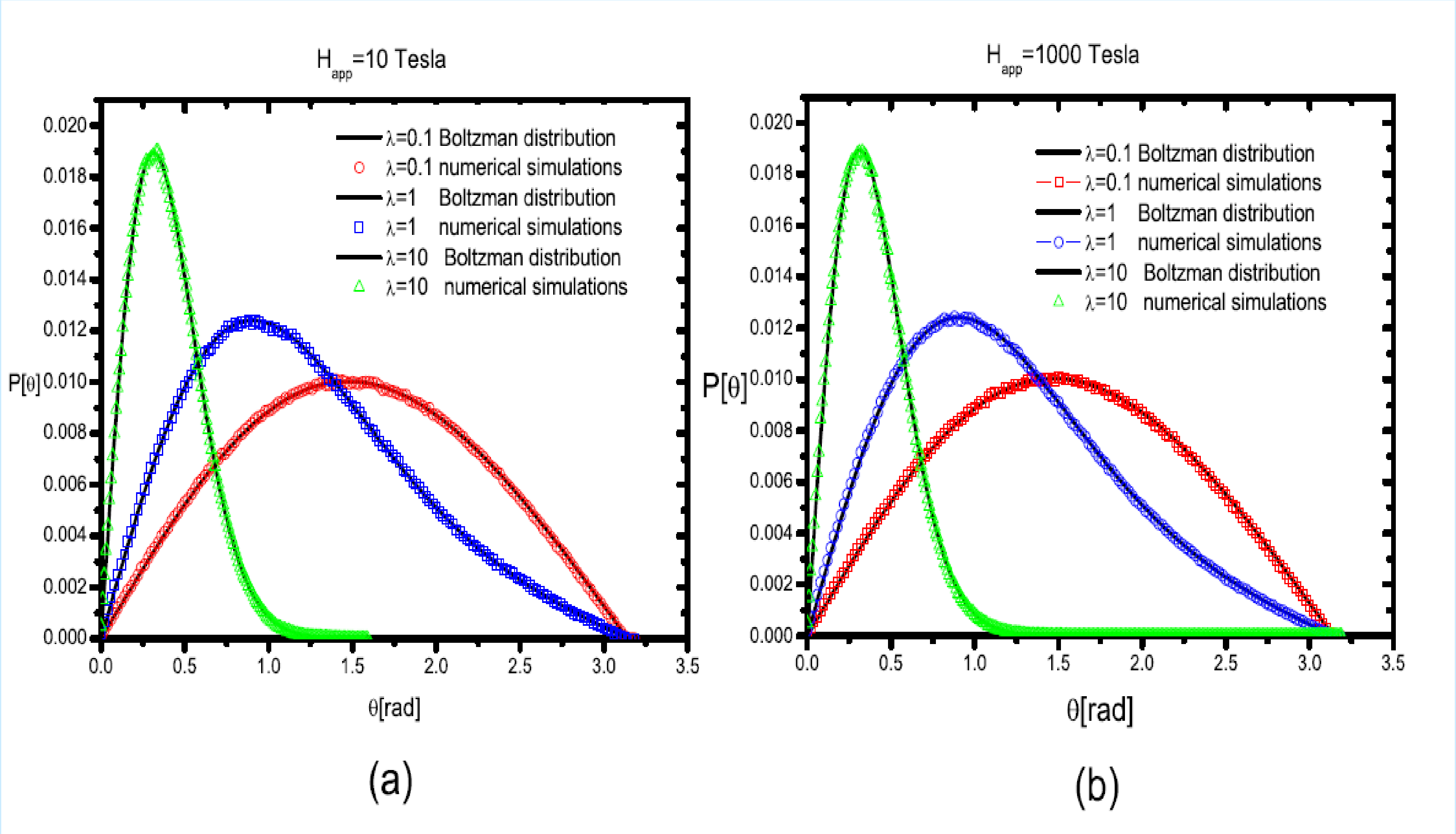
$$\frac{d\mathbf{M}}{dt} = \gamma \mathbf{M} \times (\mathbf{H}_0 + \mathbf{H}_{th})$$
$$\frac{d\mathbf{H}_{th}}{dt} = -\frac{1}{\tau_c}(\mathbf{H}_{th} - \chi \mathbf{M}) + \mathbf{R}$$

$$\langle R_i(t) R_j(t') \rangle = \frac{2}{\tau_c} \chi k_B T \delta_{ij} \delta(t - t')$$

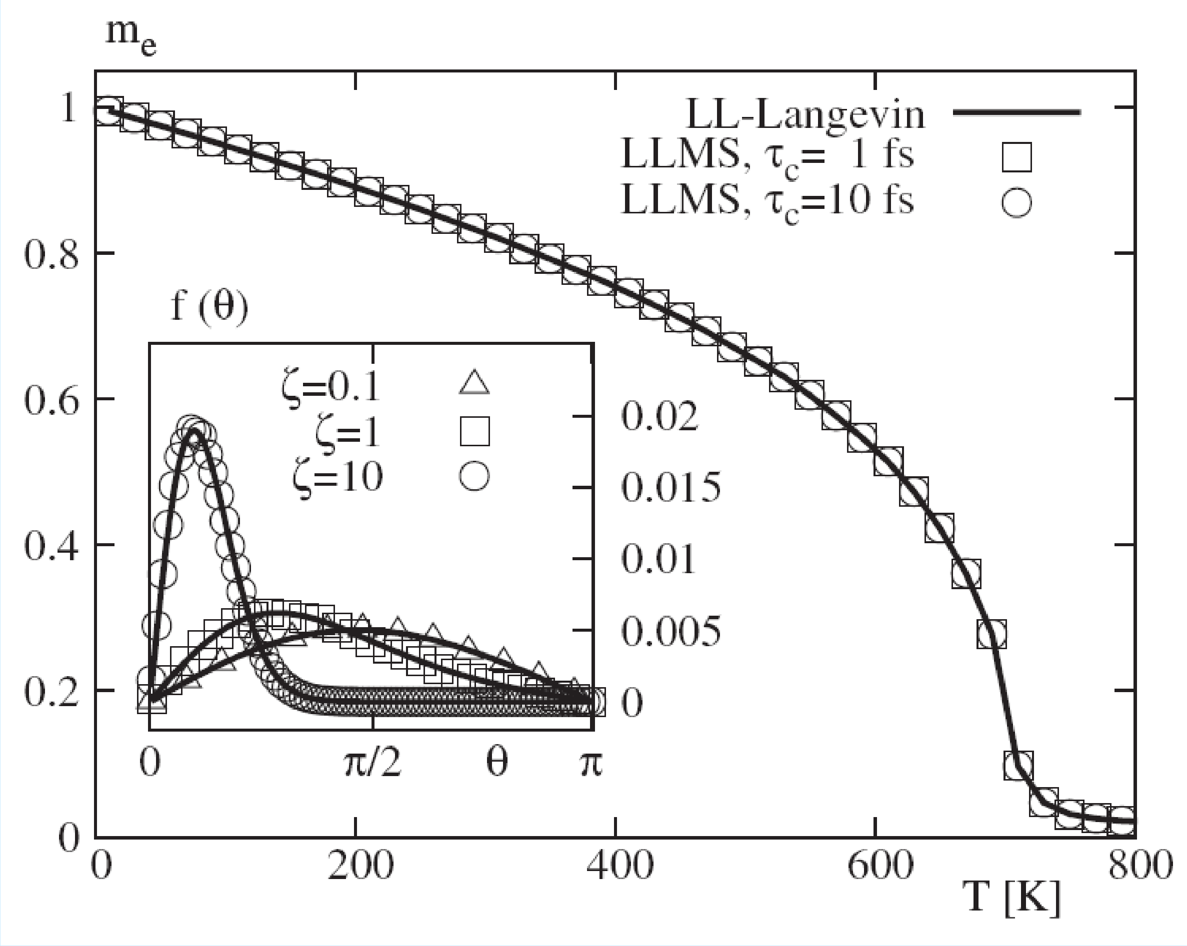
$$\chi = \alpha / (2\gamma\tau_\chi \mu)$$

NB (very crude) direct simulation of the heat bath properties.

Single-spin calculations – probability distributions



Multispin calculations – equilibrium properties



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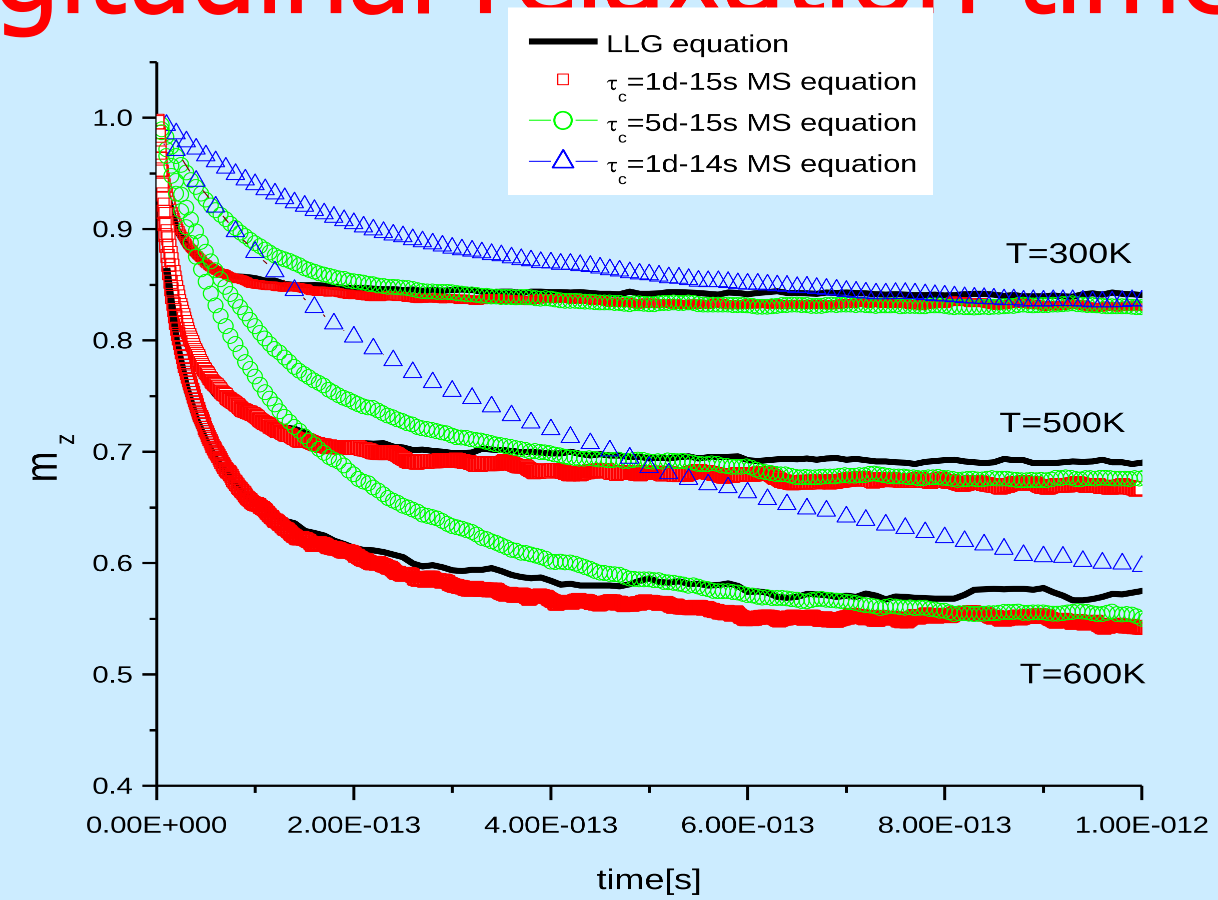
Correlations increase the longitudinal relaxation time



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Multiscale calculations and the LLB equation

- Large scale (micromagnetic) simulations essentially work with one spin/computational cell
- Single spin LLG equation cannot reproduce ultrafast reversal mechanisms at elevated temperature (conserves |M|)
- Pump- probe and HAMR simulations require an alternative approach
- Landau-Lifshitz-Bloch (LLB) equation?

LLB equation

Transverse (LLG) term

Longitudinal term introduces fluctuations of M

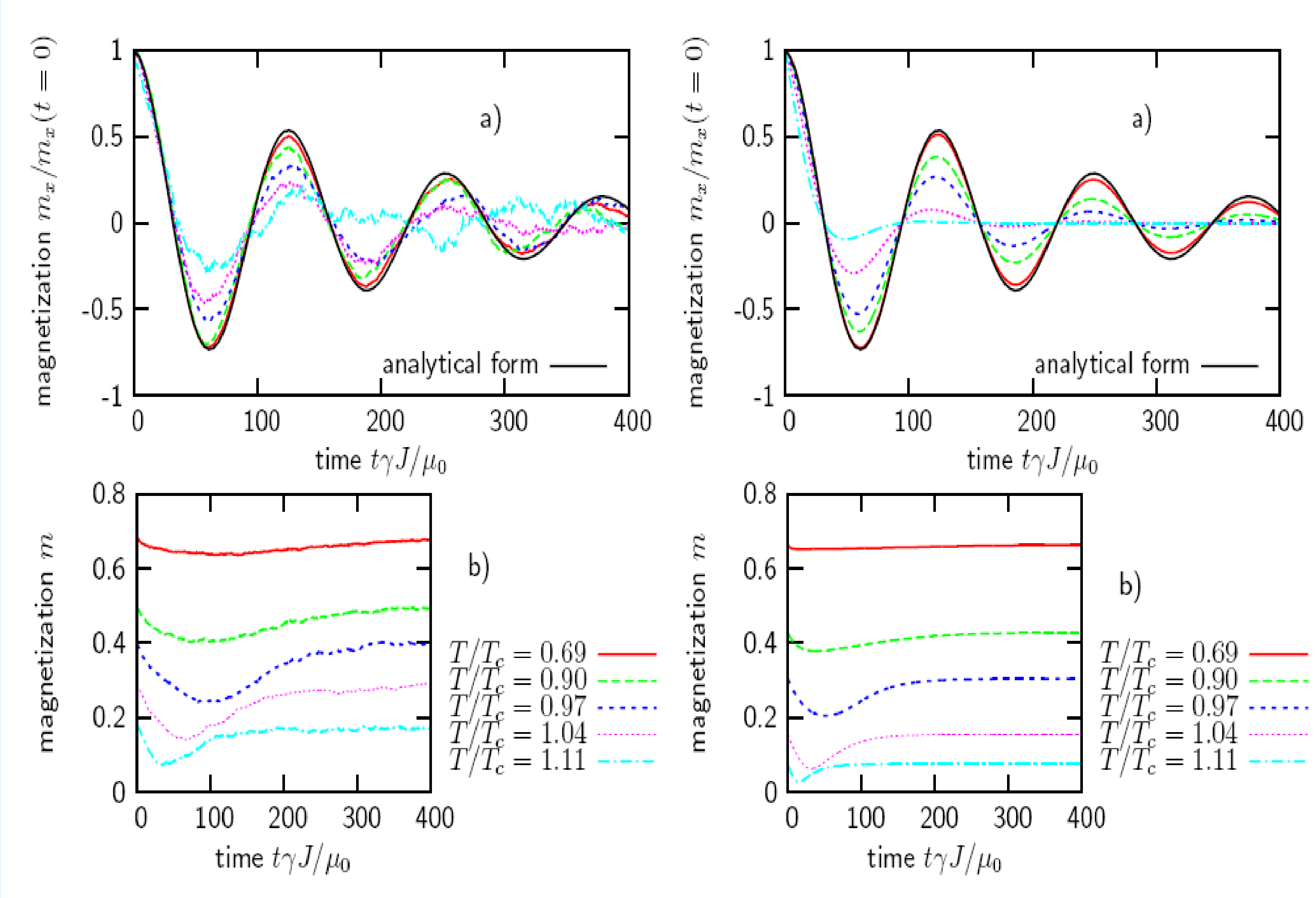
$$\dot{\mathbf{m}} = -\gamma[\mathbf{m}\times\mathbf{H}_{\text{eff}}] + \gamma\alpha_{\parallel}\frac{(\mathbf{m}\cdot\mathbf{H}_{\text{eff}})\mathbf{m}}{m^2} - \gamma\alpha_{\perp}\frac{[\mathbf{m}\times[\mathbf{m}\times\mathbf{H}_{\text{eff}}]]}{m^2}$$

- macro-spin polarization is $\mathbf{m} = \langle \mathbf{S} \rangle$
- longitudinal ($\alpha_{\parallel}$) and transverse ($\alpha_{\perp}$) damping parameters are given by $\alpha_{\parallel} = \alpha\frac{2T}{3T_c}, \quad \alpha_{\perp} = \alpha\left[1 - \frac{T}{3T_c}\right]$
- effective field:

$$\mathbf{H}_{\text{eff}} = \mathbf{H} - \frac{m_x\mathbf{e}_x + m_y\mathbf{e}_y}{\tilde{\chi}_{\perp}} + \begin{cases} \frac{1}{2\tilde{\chi}_{\parallel}}\left(1 - \frac{m^2}{m_e^2}\right)\mathbf{m}, & T \lesssim T_c \\ \frac{J_0}{\mu_s}\left(\epsilon - \frac{3}{5}m^2\right)\mathbf{m}, & T \gtrsim T_c \end{cases}.$$

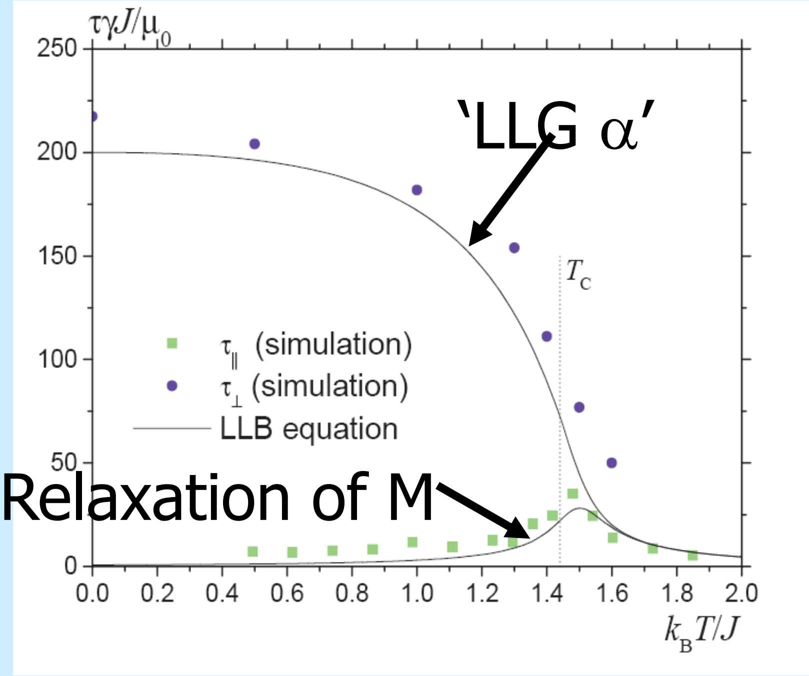
here $\mathbf{H}$ is applied field and m_e is zero-field equilibrium spin polarization

the second term is an expression for the anisotropy field



- Precessional dynamics for atomistic model (left) and (single spin) LLB equation (right)

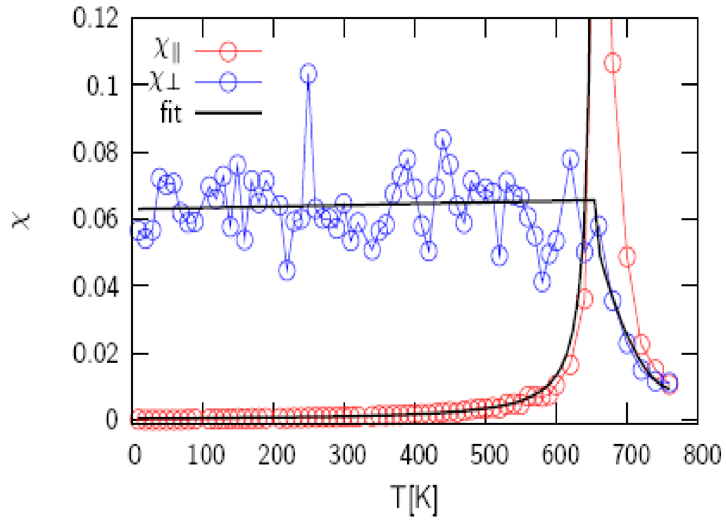
Relaxation times



- Effective α increases with T (observed in FMR experiments)
- Critical slowing down at T_c
- Longitudinal relaxation is in the ps regime except very close to T_c
- Atomistic calculations remarkably well reproduced by the LLB equation
- Makes LLB equation a good candidate to replace LLG equation in micromagnetics.

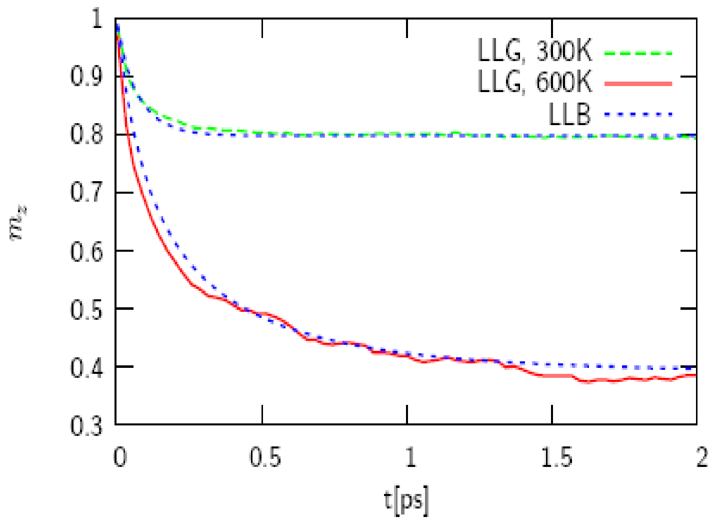
LLB parameters

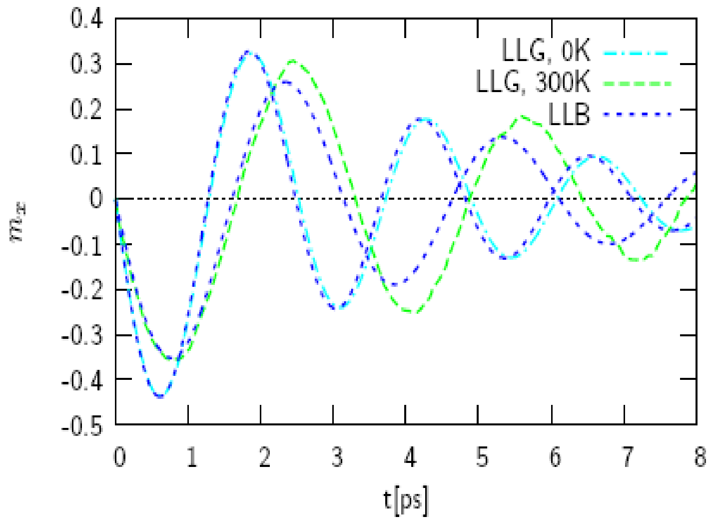
- Important parameters are;
  - Longitudinal and transverse susceptibility
  - K(T), M(T)
- These can be determined from Mean Field theory.
- Also possible to determine the parameters numerically by comparison with the Atomistic model.
- In the following we use numerically determined parameters in the LLB equation and compare the dynamics behaviour with calculations from the atomistic model.



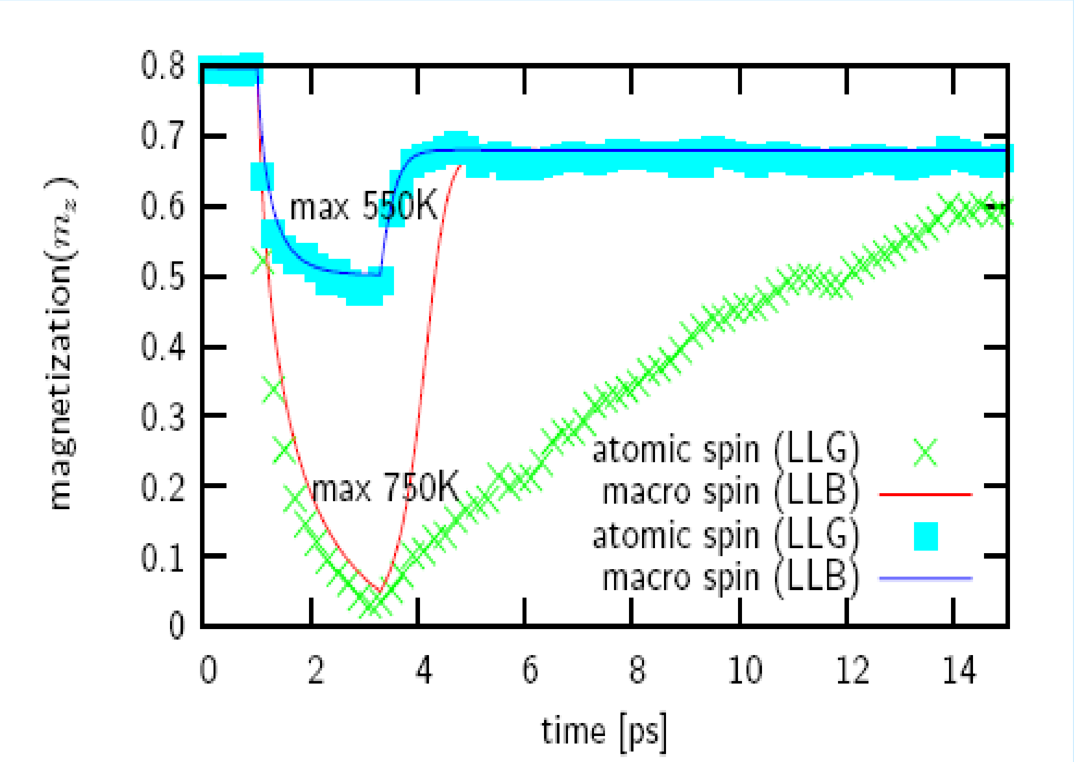
- spin model for FePt [4]
- LLG calculations for a grain of size $32 \times 32 \times 48$ spins
- $\tilde{\chi}_\perp$ (left fig.), $\tilde{\chi}_\parallel$ and m_e were evaluated and used for LLB calculations

longitudinal relaxation (left) and transverse relaxation after 30° exitation (right) for atomistic LLG and macro-spin LLB modeling





Comparison with (macrospin) LLB equation



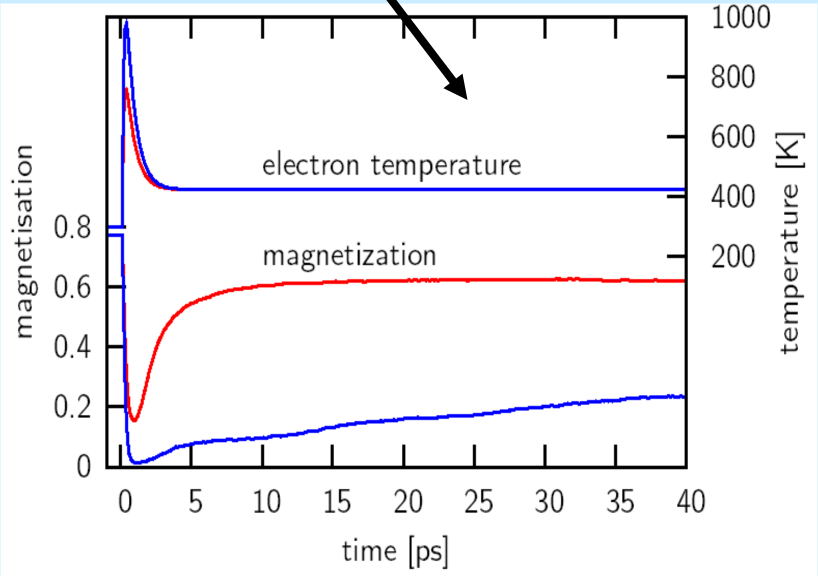
- Single LLB spin cannot reproduce the slow recovery with a single longitudinal relaxation time.
- State dependent relaxation time?
- Big advantage in terms of computational efficiency.
- LLB equation is an excellent candidate approach to complete the multiscale formalism

Slow recovery – multispin LLB

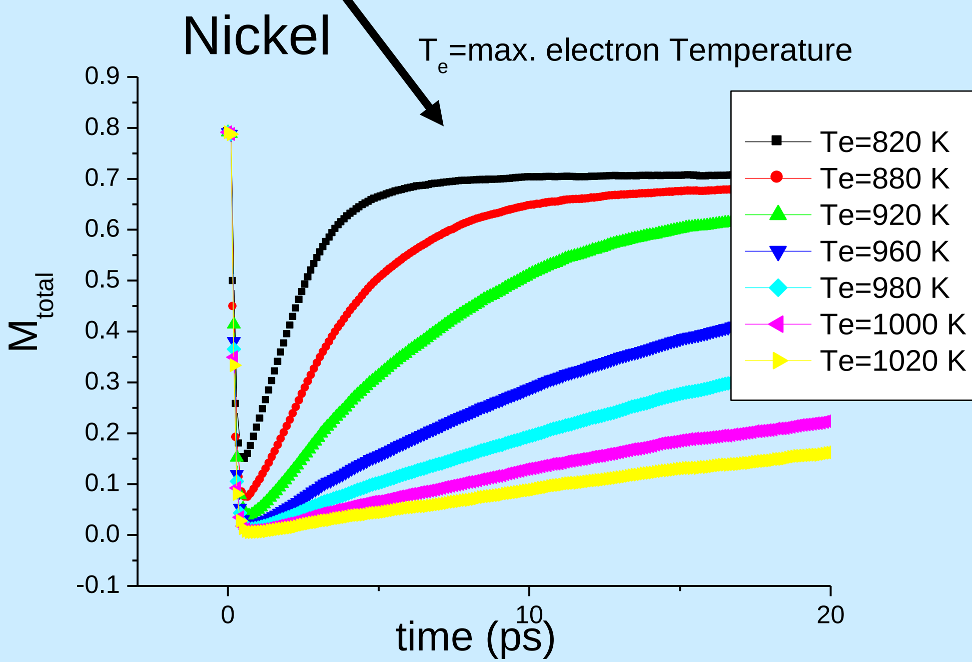
- Essentially micromagnetics with LLG replaced by LLB to simulate the dynamics.
- Exchange between cells taken as $\propto M^2$ (mean-field result)
- Capable of simulating the uncorrelated state after demagnetisation.

Comparison of atomistic and LLB-μmag model

Atomistic model



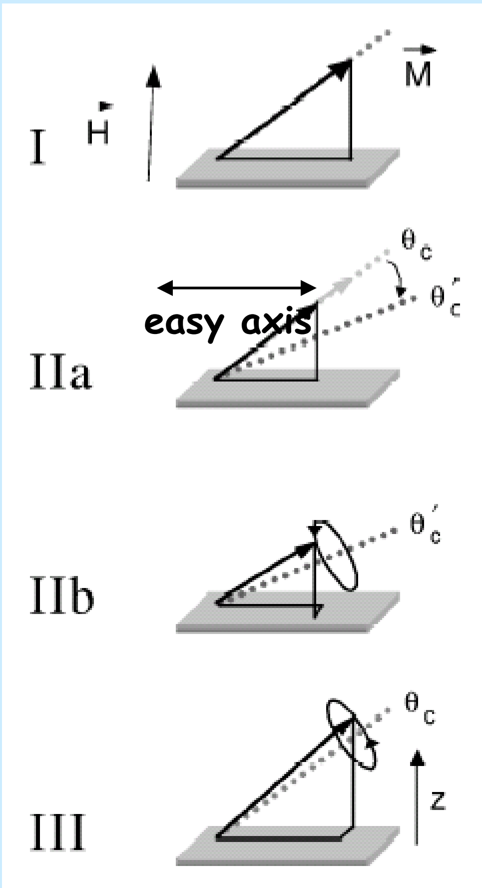
LLB-μmag

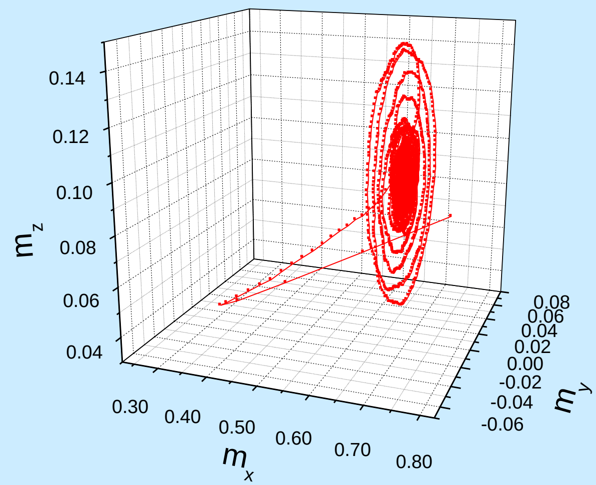


- Calculations with the LLB-μmag model agree well with atomistic calculations, *including the slow recovery*

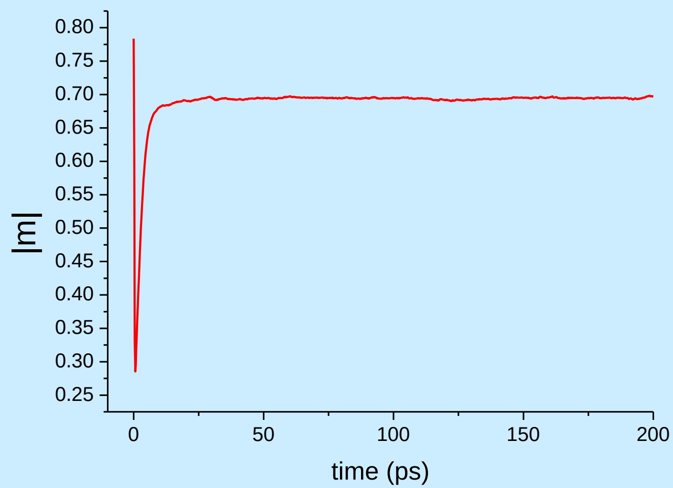
Magnetisation precession during all-optical FMR

Our simulation results





$K(T=0)=5.3\ 10^6\ erg/cm^3$
$M_s(T=0)= 480\ emu/cm^3$
$T_c=630\ K$
$H_{ext}=0.2\ T$



M.van Kampen et al PRL 88 (2002) 227201

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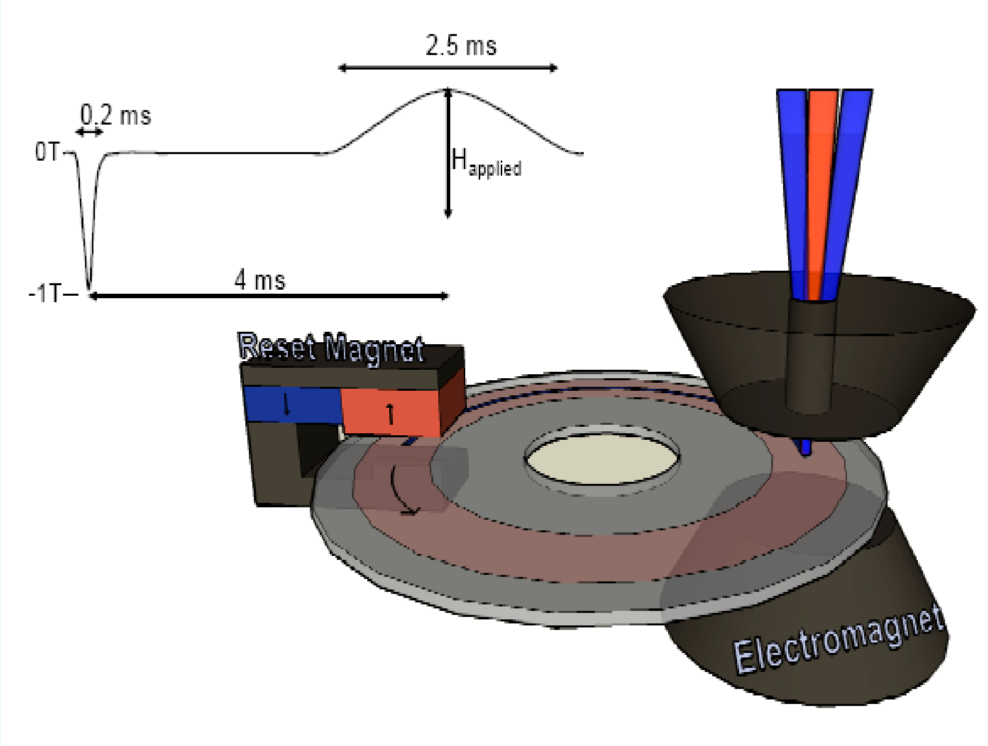
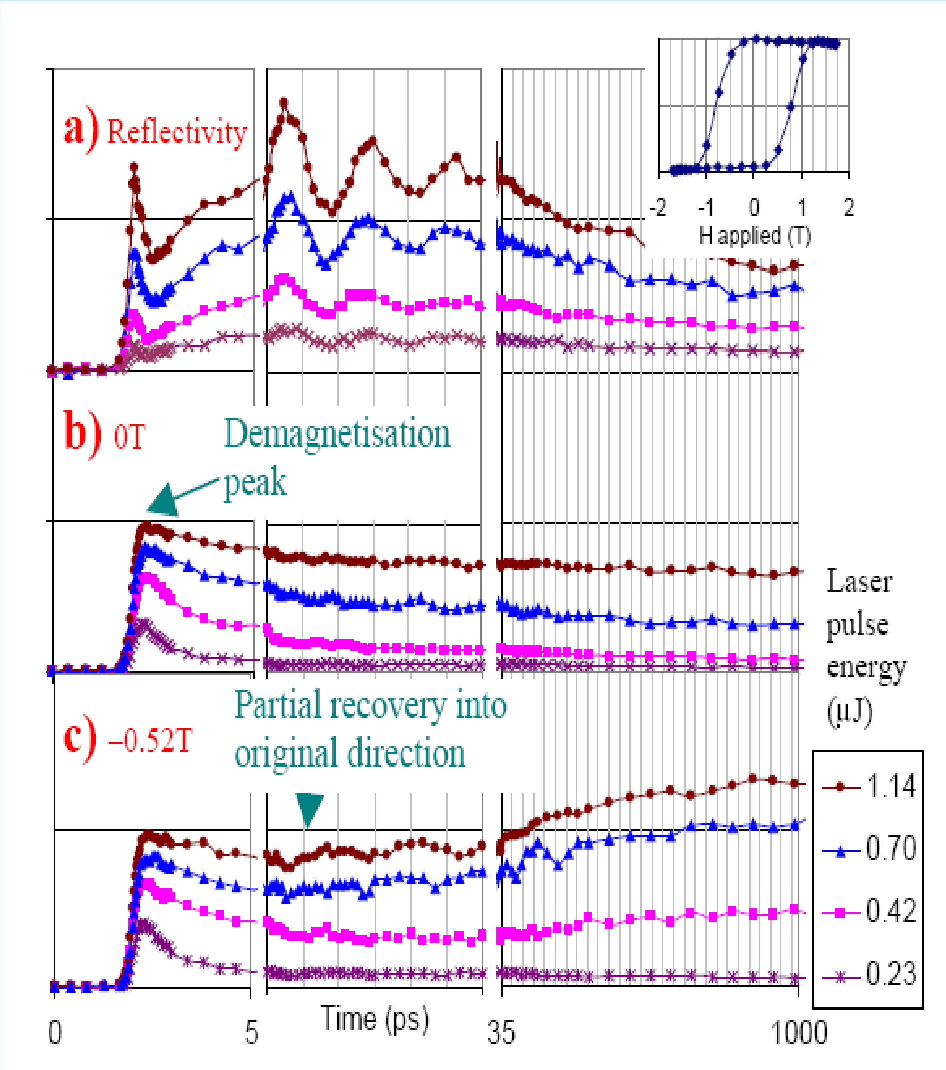
Experimental studies of Heat Assisted Reversal and comparison with LLB-micromagnetic model



- Experimental set-up (Chris Bunce, York)
- Uses hard drive as a spin-stand to alternate between reset field and reversal field
- Sample used – specially prepared CoPt multilayer (G Ju, Seagate)

Results



- Reversal occurs in a field of 0.52T (<< intrinsic coercivity of 1.4T
- Note 2 timescales. Associated with Longitudinal (initial fast reduction of M) and transverse (long timescale reversal over particle energy barriers) relaxation

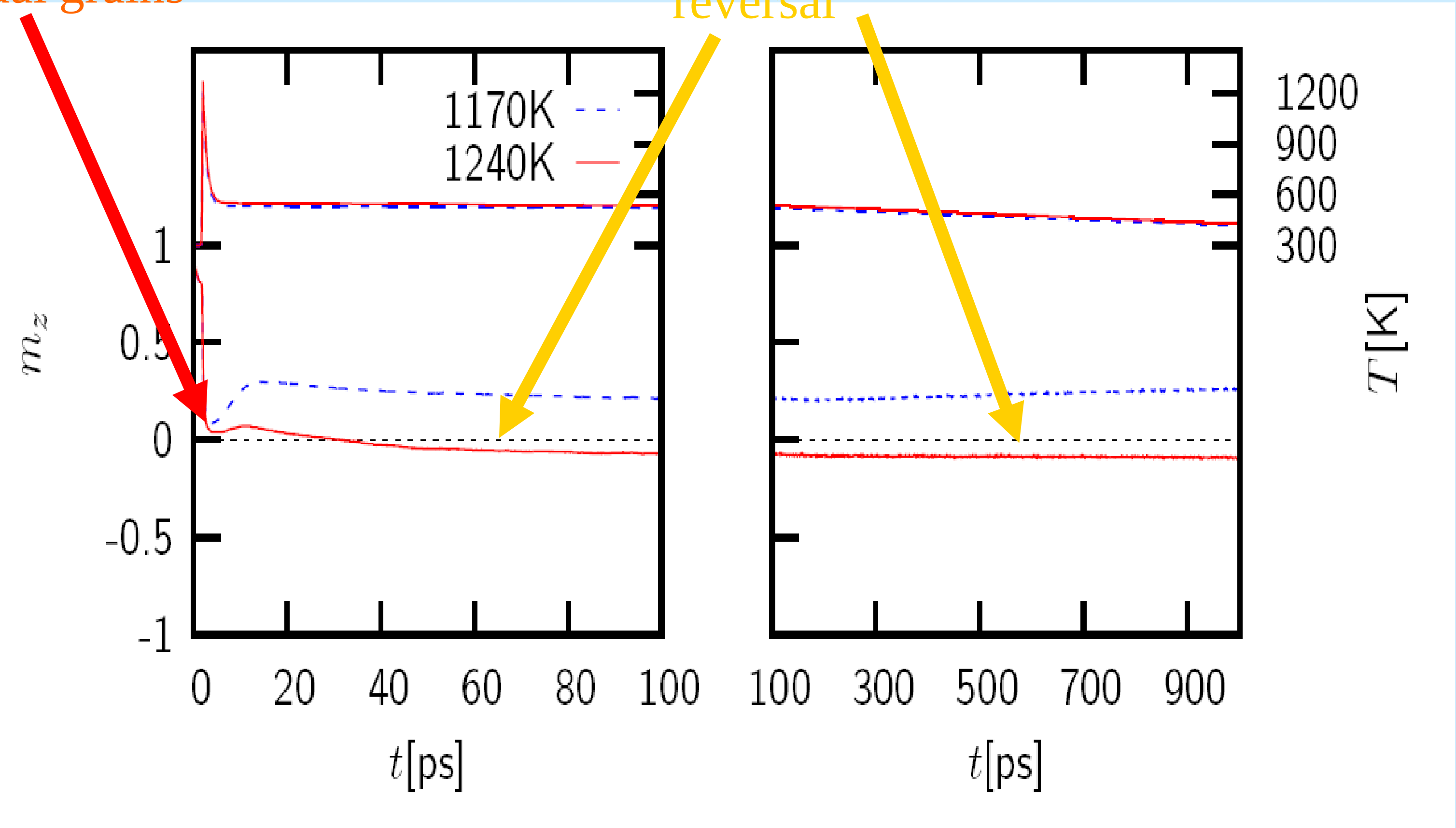
The computational model

- Film is modelled as a set of grains coupled by exchange and magnetostatic interactions.
- The dynamic behaviour of the grains is modelled using the Landau-Lifshitz-Bloch (LLB) equation.
- The LLB equation allows fluctuations in the magnitude of M. This is necessary in calculations close to or beyond T_c.
- The LLB equation can respond on timescales of picoseconds via the longitudinal relaxation time (rapid changes in the magnitude of M) and hundreds of ps - transverse relaxation over energy barriers.
- LLG equation cannot reproduce the longitudinal relaxation
- The film is subjected to a time varying temperature from the laser pulse calculated using a two-temperature model.

Calculated results

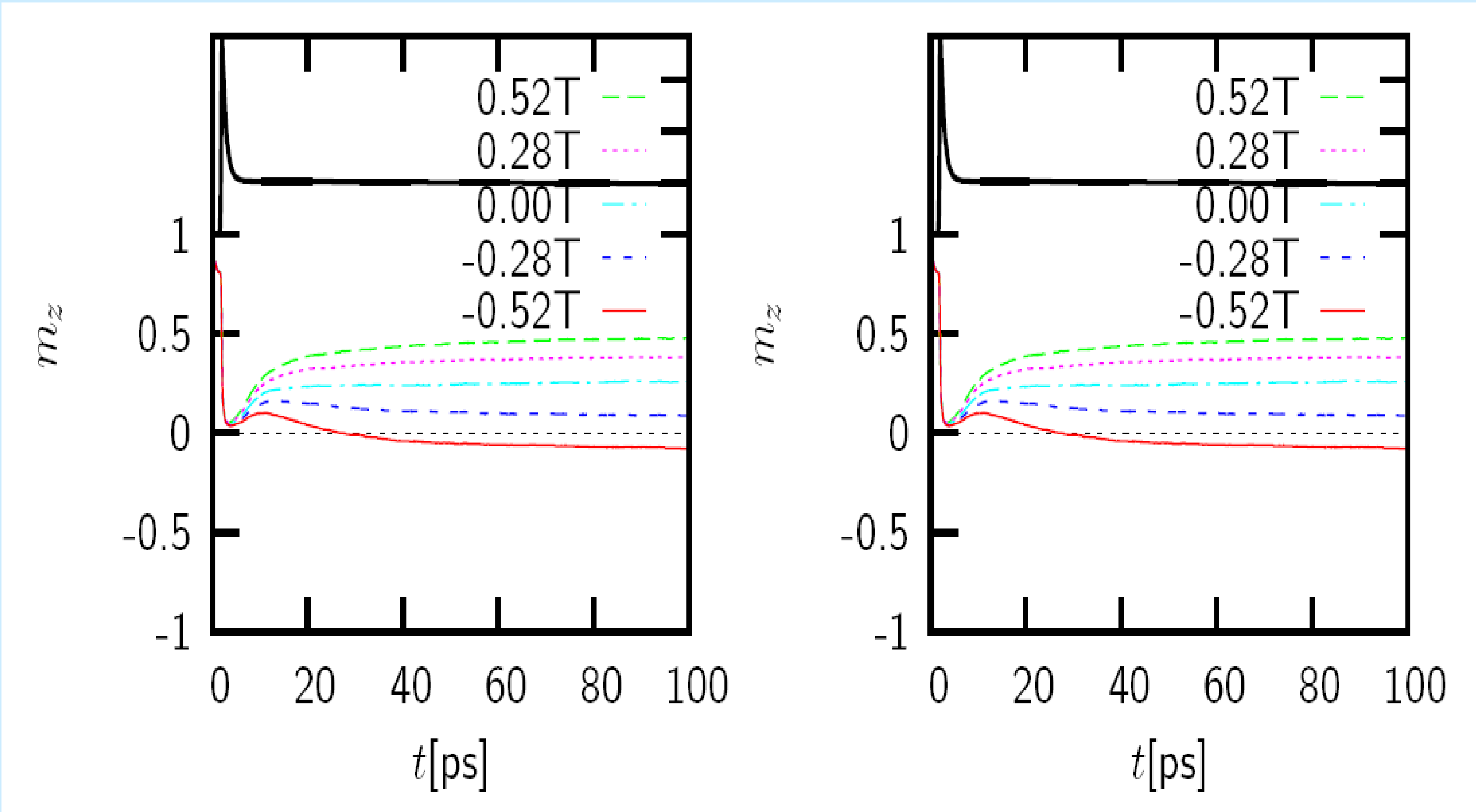
Demagnetisation/recovery of the magnetisation of individual grains

Superparamagnetic reversal



- Simulations show rapid demagnetisation followed by recovery on the short timescale. Over longer times the magnetisastion rotates into the field direction due to thermally activated transitions over energy barriers.
- This is consistent with experimental results

Effect of the magnetic field



- Also qualitatively in agreement with experiments
- LLB equation is very successful in describing high temperature dynamics

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Opto-magnetic reversal

PRL 99, 047601 (2007) PHYSICAL REVIEW LETTERS week ending 27 JULY 2007

All-Optical Magnetic Recording with Circularly Polarized Light

C. D. Stanciu,[1,*] F. Hansteen,[1] A. V. Kimel,[1] A. Kirilyuk,[1] A. Tsukamoto,[2] A. Itoh,[2] and Th. Rasing[1]

[1]*Institute for Molecules and Materials, Radboud University Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands*

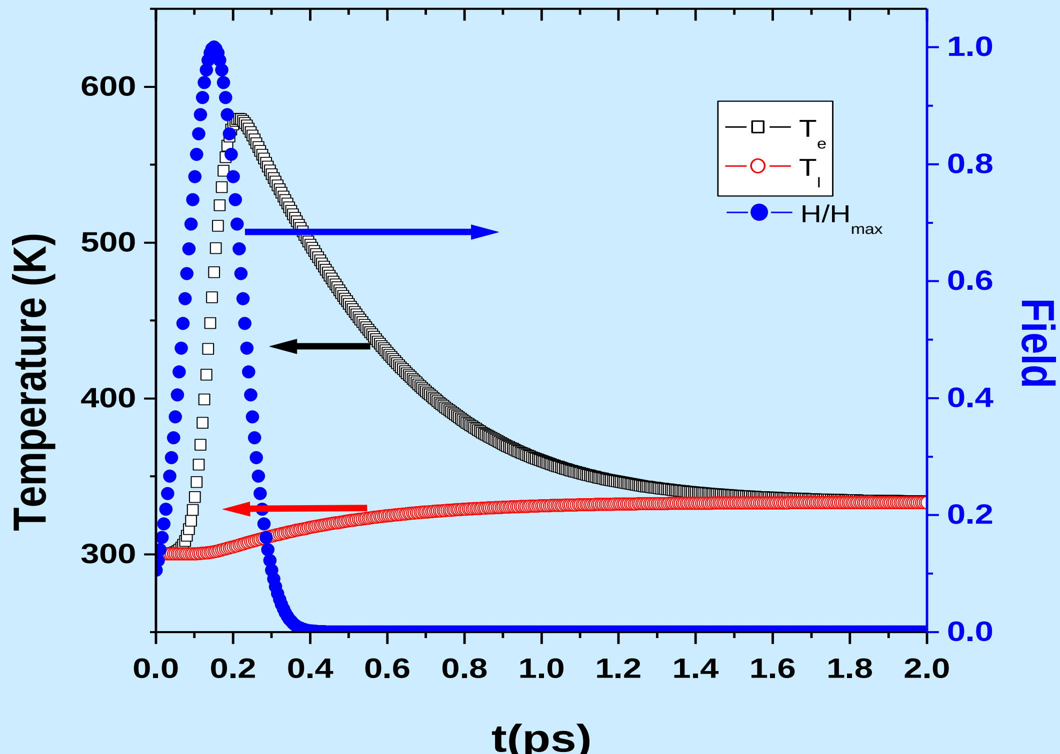
[2]*College of Science and Technology, Nihon University, 7-24-1 Funabashi, Chiba, Japan*

(Received 2 March 2007; published 25 July 2007)

We experimentally demonstrate that the magnetization can be reversed in a reproducible manner by a single 40 femtosecond circularly polarized laser pulse, without any applied magnetic field. This optically induced ultrafast magnetization reversal previously believed impossible is the combined result of femtosecond laser heating of the magnetic system to just below the Curie point and circularly polarized light simultaneously acting as a magnetic field. The direction of this opto-magnetic switching is determined only by the helicity of light. This finding reveals an ultrafast and efficient pathway for writing magnetic bits at record-breaking speeds.

- What is the reversal mechanism?
- Is it possible to represent it with a spin model?

Fields and temperatures



- Simple '2-temperature' model
- Problem – energy associated with the laser pulse (here expressed as an effective temperature) persists much longer than the magnetic field.
- Equlibrium temperature much lower than T_c

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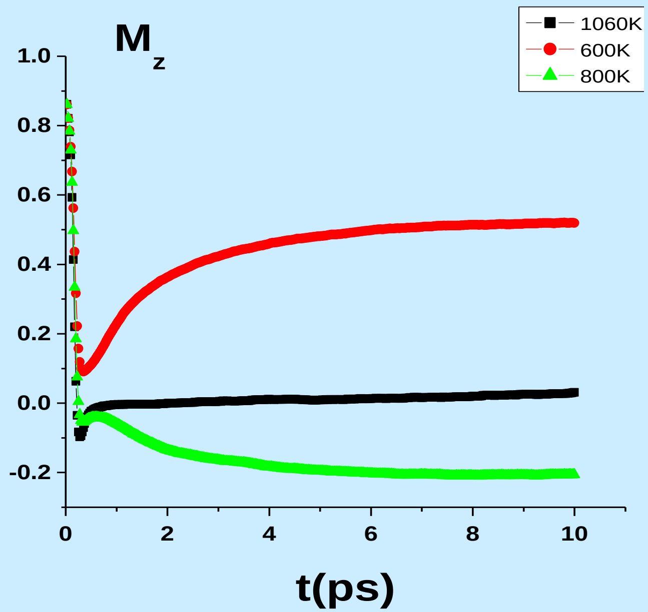
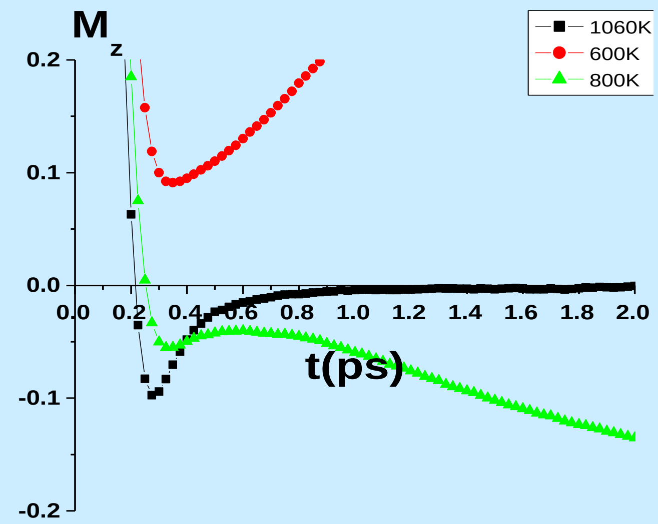
Magnetisation dynamics (atomistic model)





- ***Reversal is non-precessional*** – m_x and m_y remain zero. ***Linear reversal mechanism***
- Associated with increased magnetic susceptibility at high temperatures
- Too much laser power and the magnetisation is destroyed after reversal
- Narrow window for reversal

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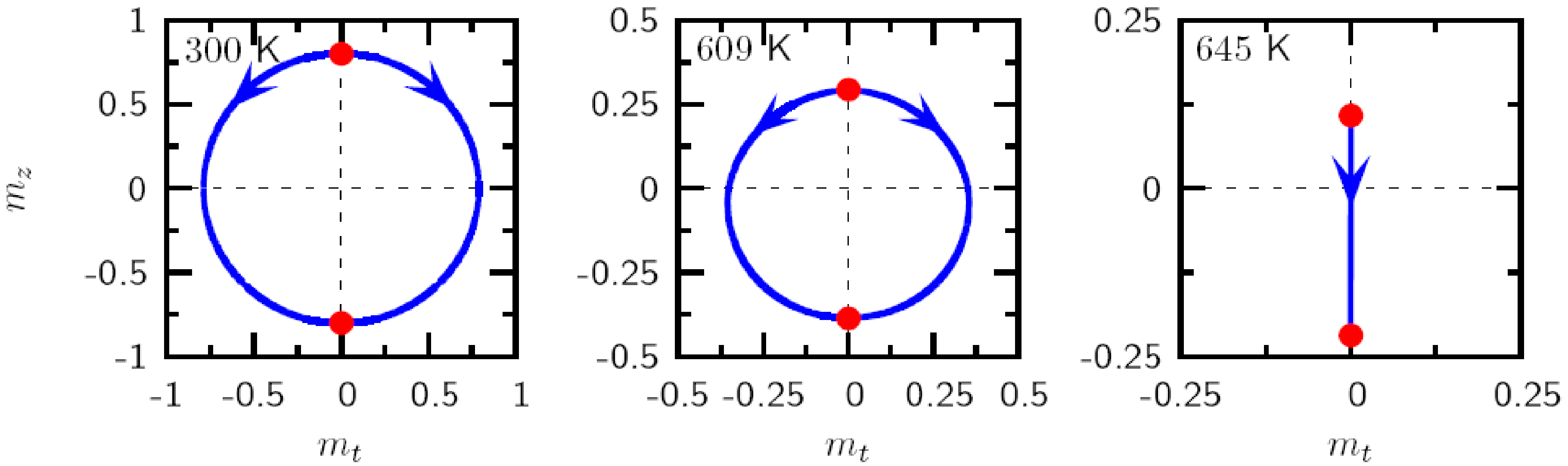
Linear reversal

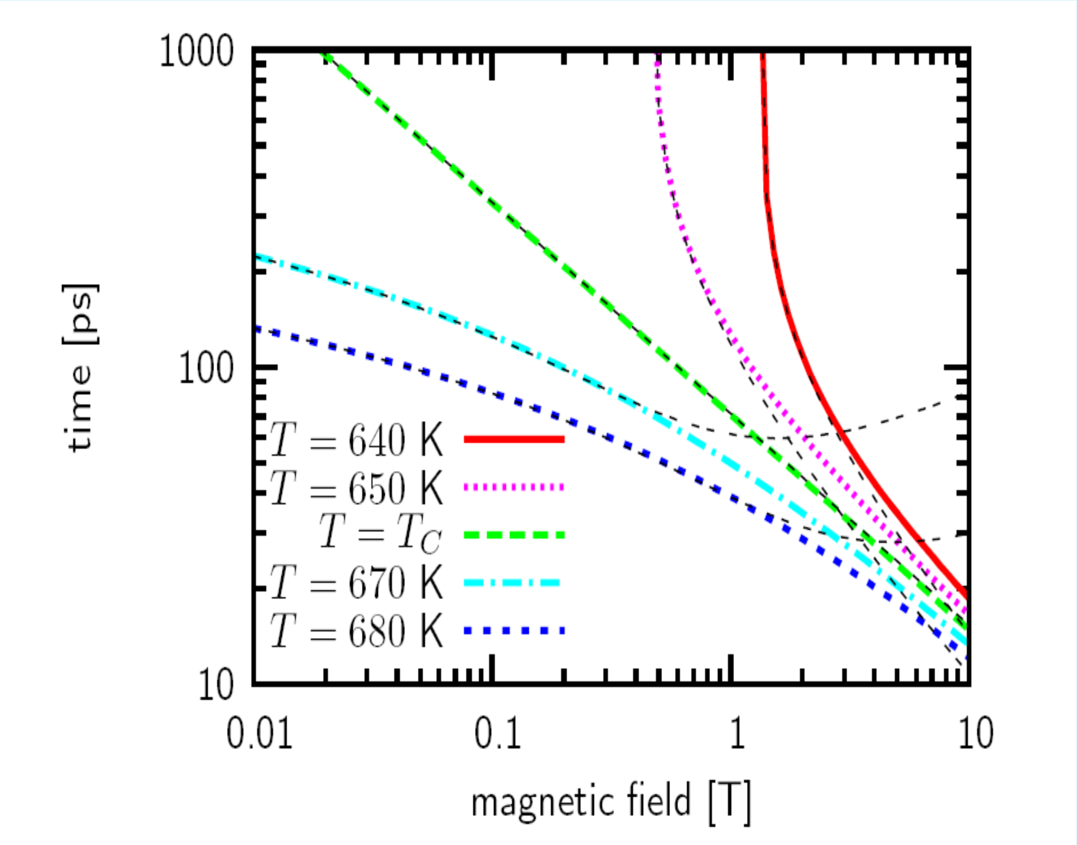


New reversal mechanism via a strongly non-uniform (demagnetised) state.

VERY fast (timescale of longitudinal relaxation)

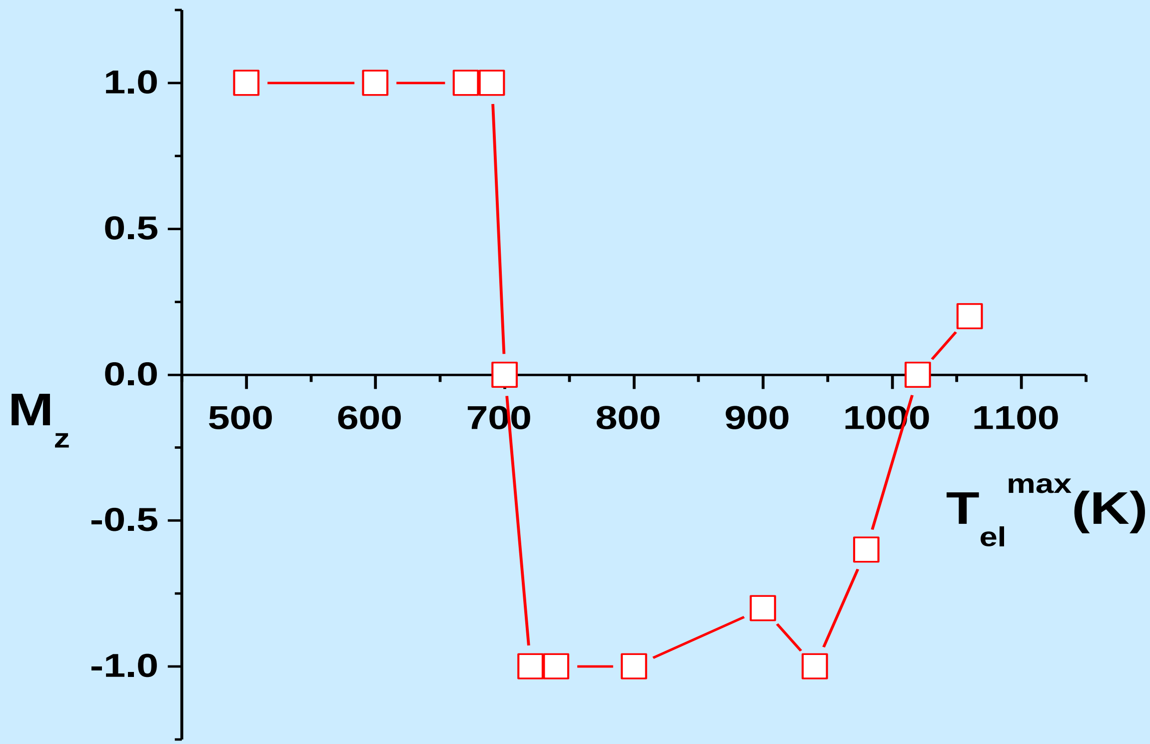
Micromagnetics with LLG equation cannot reproduce behaviour

Analytical calculations of relaxation times using LLB equation



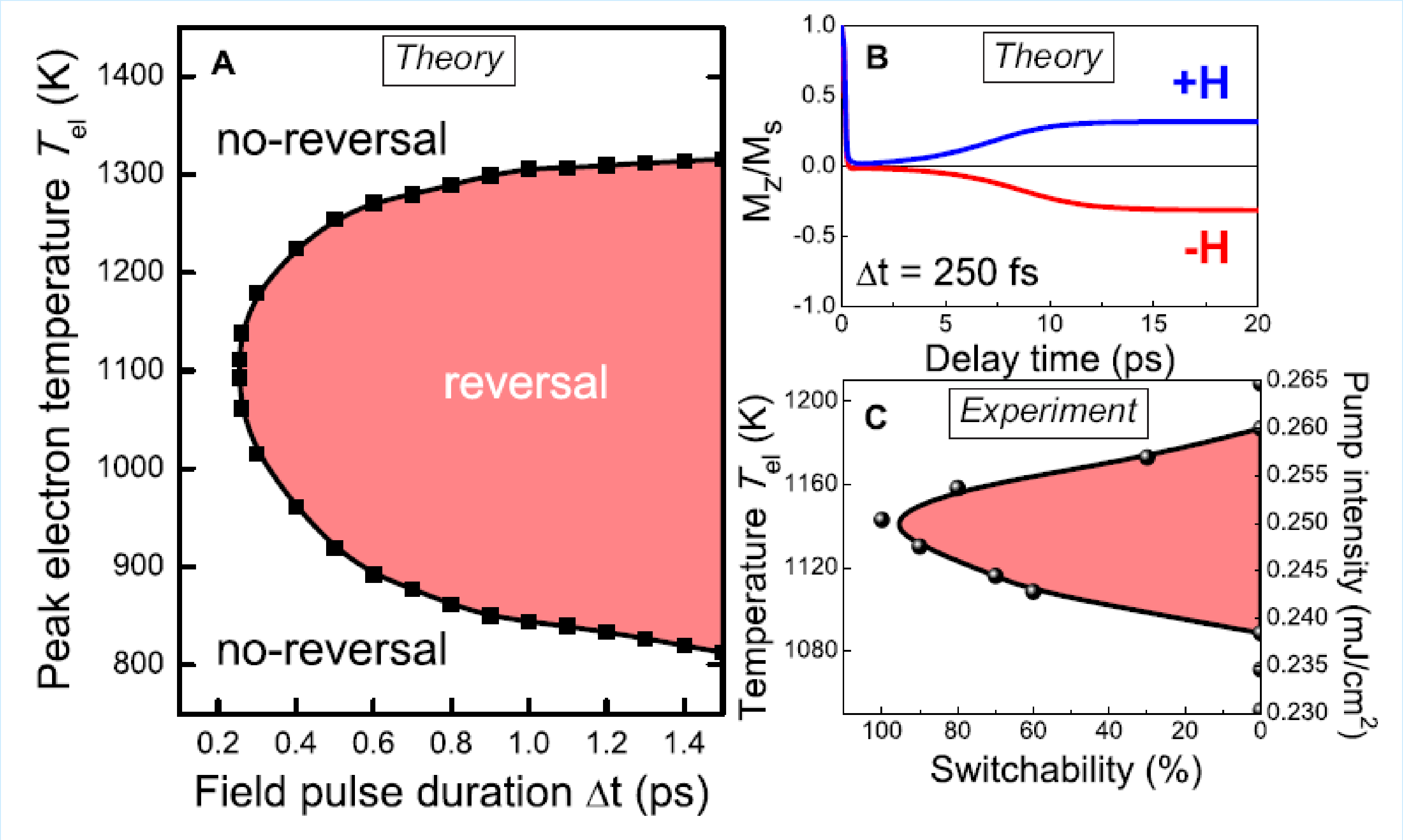
Large fields required for ps reversal (Kazantseva et al, EPL, in press)

‘Reversal window’



- Well defined temperature range for reversal
- Critical temperature for the onset of linear reversal
- BUT atomistic calculations are very CPU intensive
- LLB micromagnetic model used for large scale calculations

Reversal 'phase diagram' Vahaplar et al (submitted)



- Note the criticality of the experimental results
- Characteristic of linear reversal

Conclusions

- Atomistic model has been developed using Heisenberg exchange.
- The Landau-Lifshitz-Bloch (LLB) equation incorporates much of the physics of the atomistic calculations
- LLB-micromagnetics is proposed, essentially using the LLB equation in a micromagnetic formalism.
- LLB-micromagnetics is shown to be successful in simulating ultrafast dynamics at elevated temperatures. Important for pump-probe simulations and models of HAMR. Also thermally assisted MRAM?
- New (linear) reversal demonstrated with sub-picosecond reversal times
- Demonstrates the probable thermodynamic origin of Opto-Magnetic reversal.

Acknowledgements

- Seagate Technology
- EU Seventh Framework Programme (FP7/2007-2013) under grants agreements NMP3-SL-2008-214469 (UltraMagnetron) and N 214810 (FANTOMAS).

Future developments

- Micromagnetics will continue as the formalism of choice for large scale simulations
- However, multiscale calculations will become increasingly necessary as magnetic materials become more nanostructured
- Challenges
  - Picosecond dynamics
  - Damping mechanisms
  - Introduction of spin torque
  - Link between magnetic and transport models
  - Models of atomic level microstructure are necessary. (The ultimate problem of magnetism vs microstructure?)