Modelling 1:
Basic models

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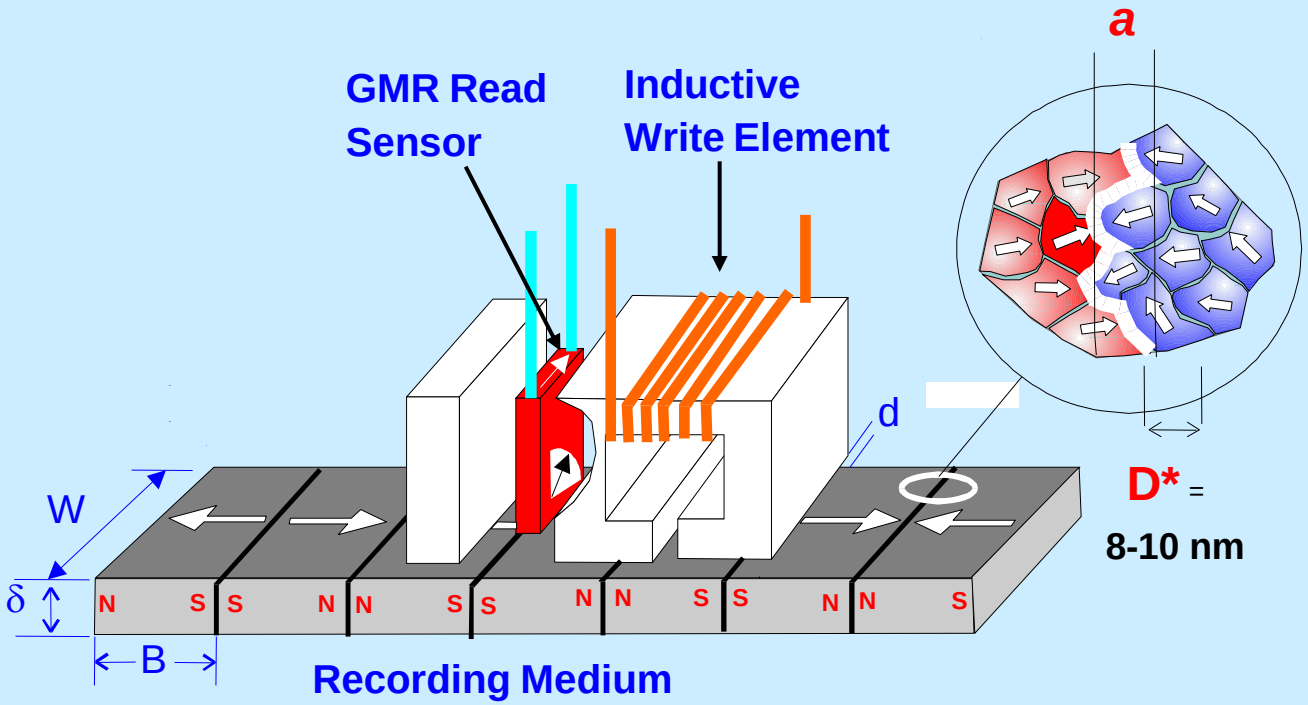
Summary

- Introduction – high anisotropy materials and magnetic recording
- The need for atomistic simulations
- Static properties – Ising model and MC simulations
- Atomistic simulations
  - Model development
  - Langevin Dynamics and Monte Carlo methods
  - Magnetisation reversal
- Applications
  - Pump-Probe processes
  - Opto-magnetic reversal
  - Atomistic model of Heat Assisted Magnetic Recording (HAMR)

Media Noise Limitations in Magnetic Recording

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



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

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	Saturation Magnetization	Anisotropy Field	Minimum stable grain size	
		K_u (10^7erg/cc)	M_s (emu/cc)	H_k (kOe)	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	

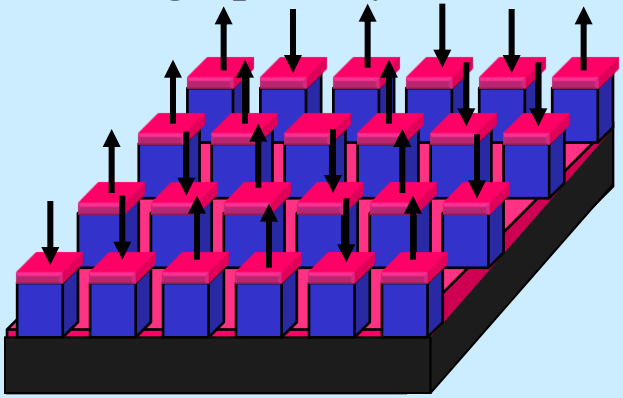
Write Field is limited by B_S (2.4T today!)of Recording Head

$H_0 = \alpha H_K - N M_S$

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

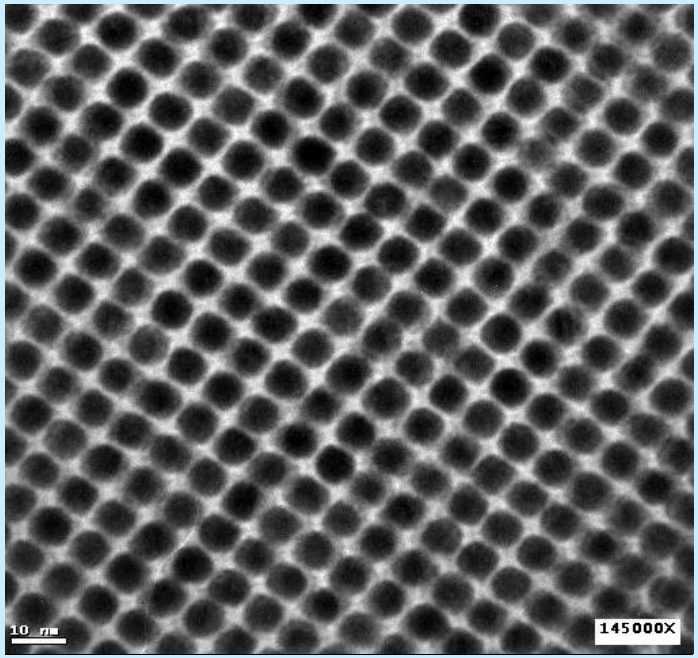
Bit Patterned Media Lithography vs Self Organization

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).

What we have to deal with

- Lengthscales
  - Electronic structure (exchange, anisotropy, etc …)
  - Atomistic – introduces thermodynamics
  - Micromagnetic
- Timescales
  - 100 femtoseconds – ultrafast processes
  - nanoseconds – magnetic recording
  - Seconds (VSM)
  - Years (thermal stability in recording)
  - Geological ages (geomagnetism)
- No single model can be expected to do everything

Overview of models

- '*ab-initio*' calculations
  - Information on electronic structure and intrinsic magnetic properties
  - Restricted to zero K and small numbers of atoms
- Atomistic models
  - Larger number of atoms (10^6 to 10^8)
  - Non-zero temperature and ultrafast dynamics
  - Still relatively small systems
- Micromagnetic models
  - System size up to microns
  - Non-zero temperature and ultrafast dynamics
  - Not good at high temperatures close to T_c
- Macroscopic models (eg Preisach)
  - Very large systems
  - Phenomenological models

Micromagnetics

- Around since the pioneering work of William Fuller Brown in the 1960s
- Used for studying non-uniform magnetisation reversal processes
- Since the mid 1980s, significant advances in modelling techniques
- Micromagnetics is now a very mature theory
- Large scale calculation – cannot introduce atomic lengthscale calculation explicitly
- Essential approach is to make an approximation to the exchange valid for long wavelength magnetisation changes

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.

Dynamic behaviour

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

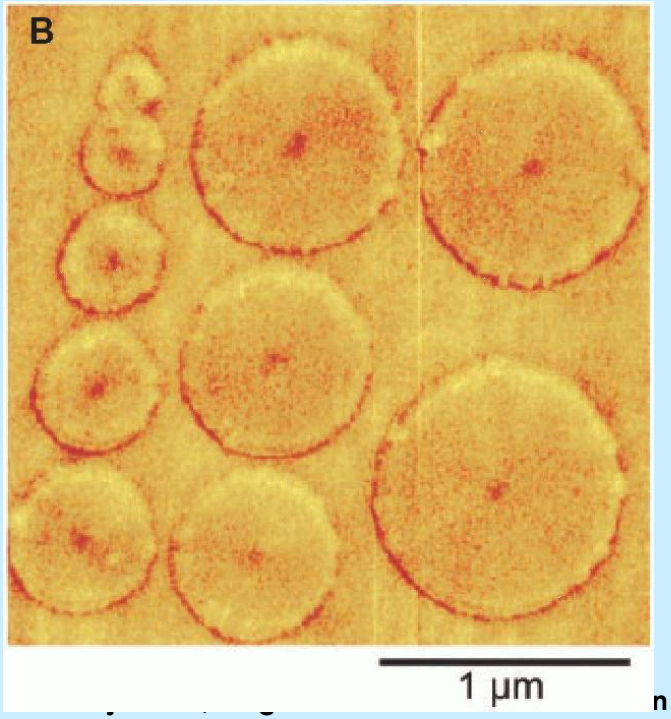
Langevin Dynamics (introduces non-zero temperature)

- 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

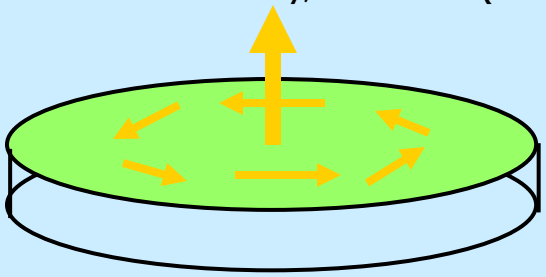
$$< h_j(t) >= 0 \qquad < h_i(0) h_j(t) >= \delta(t) \delta_{ij} 2\alpha k_b T / \gamma$$

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

Typical application of micromagnetics; structure of the vortex state



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



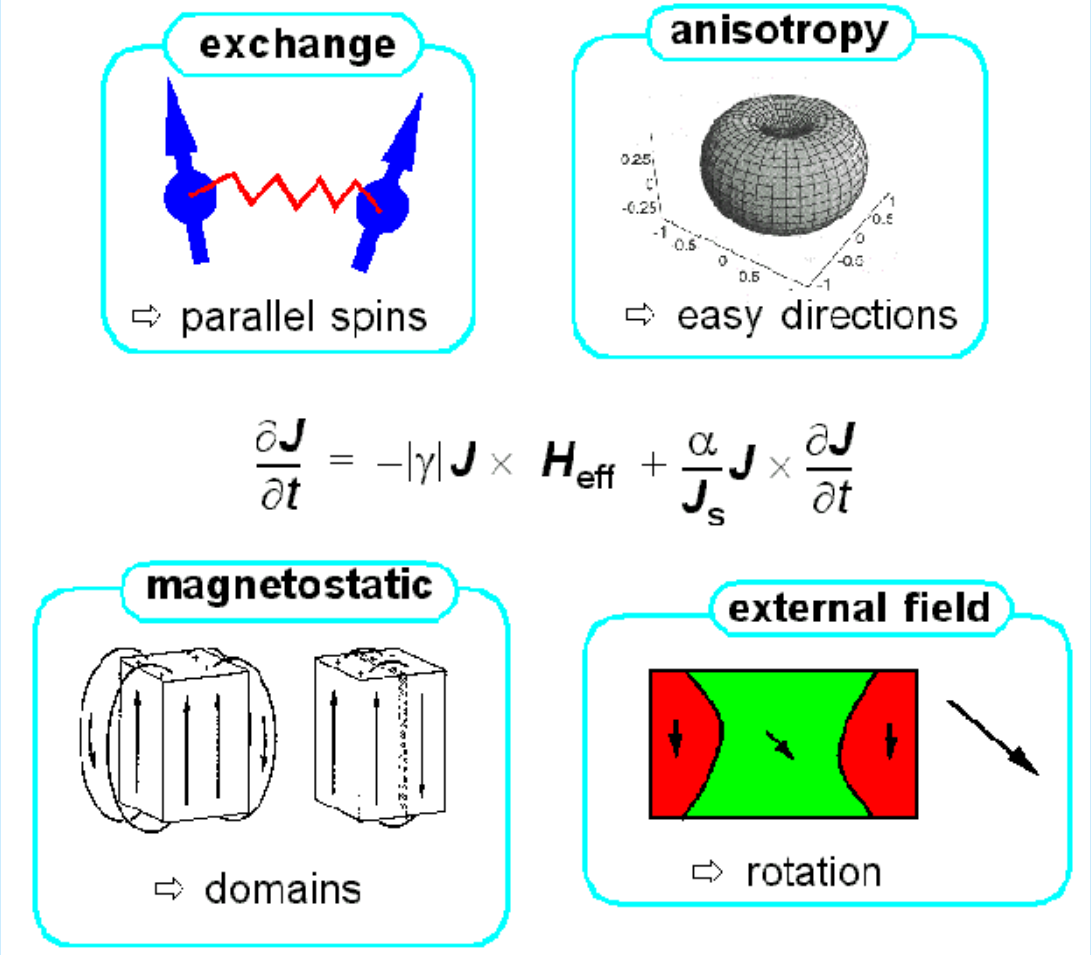
vortex state

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

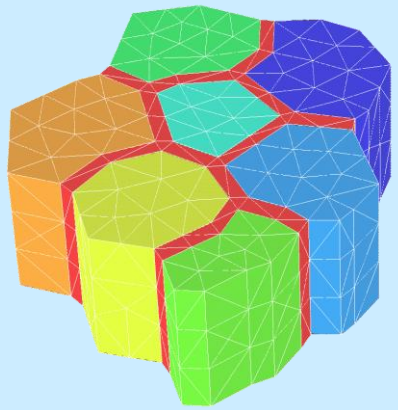
- Saturation magnetization:
  $M_s = 8 \cdot 10^5$ A/m = $8 \cdot 10^2$ G
  $J_s \approx 1$ T
- Exchange constant:
  $A = 13 \cdot 10^{-12}$ J/m = $1.3 \cdot 10^{-6}$ erg/cm
- Anisotropy has been neglected
- Radius of 100 nm, thickness of 20 nm

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**



Finite Element Approach

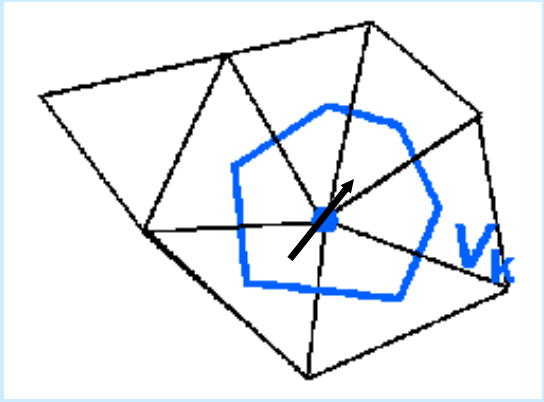


- divide particles into finite elements
  ⇨ triangles, tetrahedrons
- expand J with basis function J_i

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

- energy as a function of J_1, J_2 … J_N

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

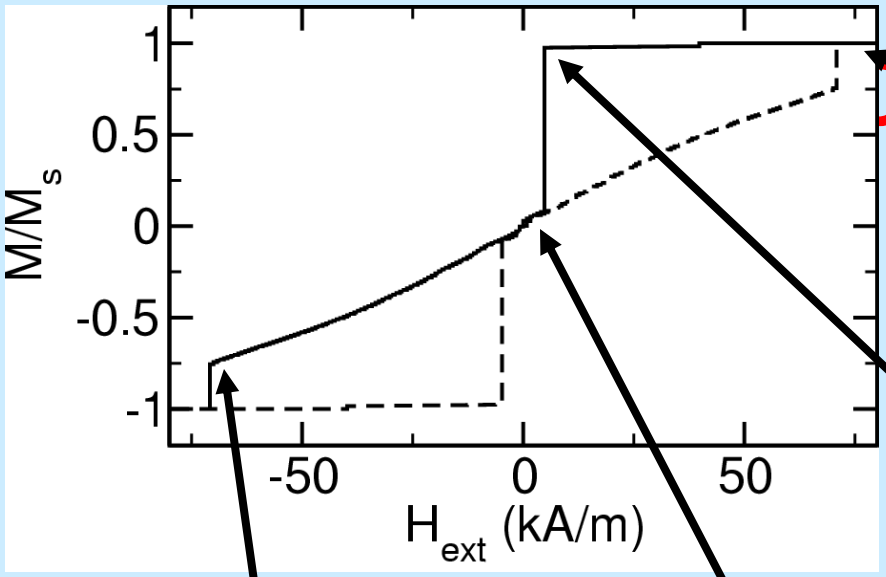


- effective field

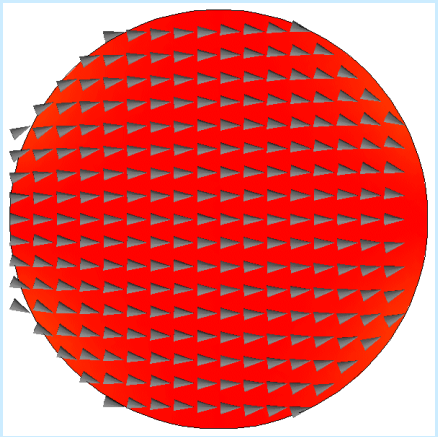
$$\vec{H}_k = -\frac{1}{V_k} \frac{\partial E(\vec{J}_1, \vec{J}_2 .... \vec{J}_N)}{\partial \vec{J}_k}$$

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

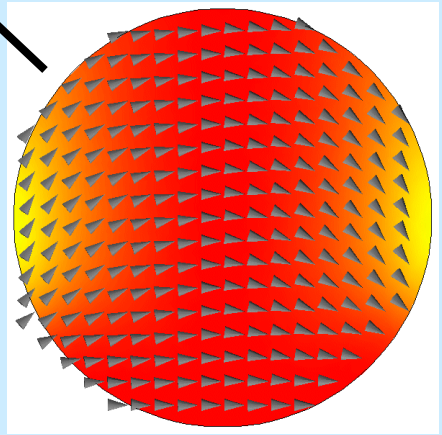
W Scholz et al **J Magn. Magn. Mater., 266, 155-163 (2003)**

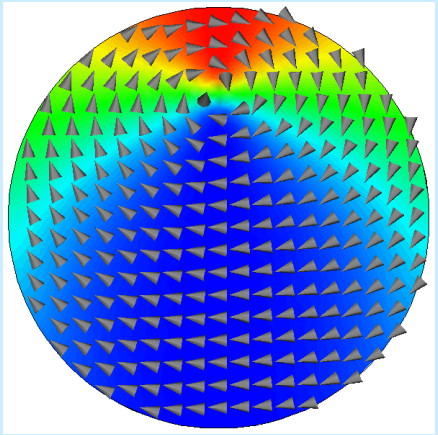


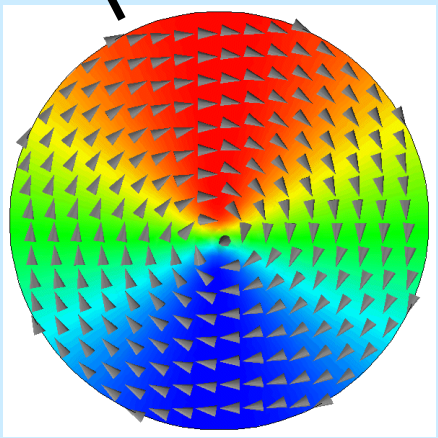
saturated state



"C" state







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

Equilibrium in zero field

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

- Micromagnetics is highly successful with large scale magnetisation structures with long-wavelength magnetisation variations only
- BUT it cannot deal with short wavelength fluctuations and fails to predict the Curie Temperature.

Modelling magnetic properties:The need for atomistic/multiscale approaches

- Standard approach (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.

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.

Relation to ab-initio calculations and micromagnetics

- Ab-initio calculations are carried out at the electronic level.
- Number of atoms is strictly limited, also zero temperature formalism.
- Atomistic calculations take averaged quantities for important parameters (spin, anisotropy, exchange, etc) and allow to work with 10^6 to 10^8 spins. Phase transitions are also allowed.
- Micromagnetics does a further average over hundreds of spins (continuum approximation)
- Atomistic calculations form a bridge
  - Lecture 1: concentrates on the link to ab-intio calculations – development of a classical spin Hamiltonian for FePt from ab-initio calculations and comparison with experiment.
  - Lecture 2: Development of multi-scale calculations- link to micromagnetics via the Landau-Lifshitz-Bloch (LLB equation).

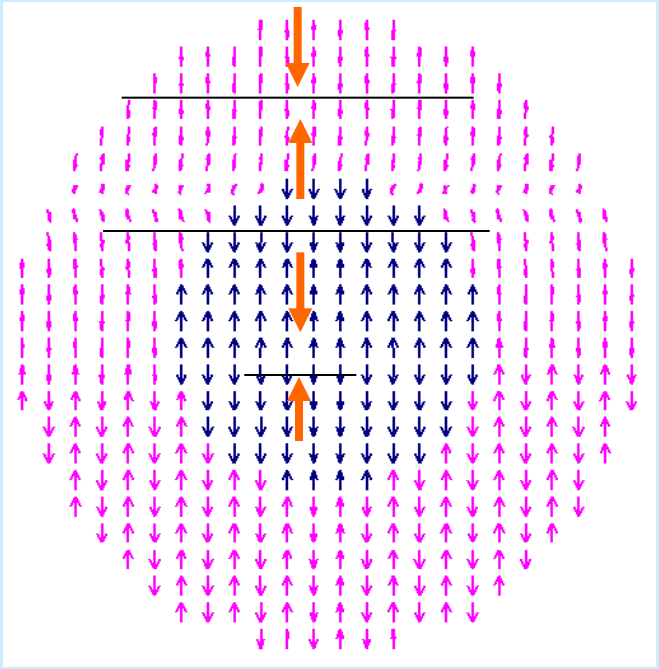
Atomistic models and thermodynamics

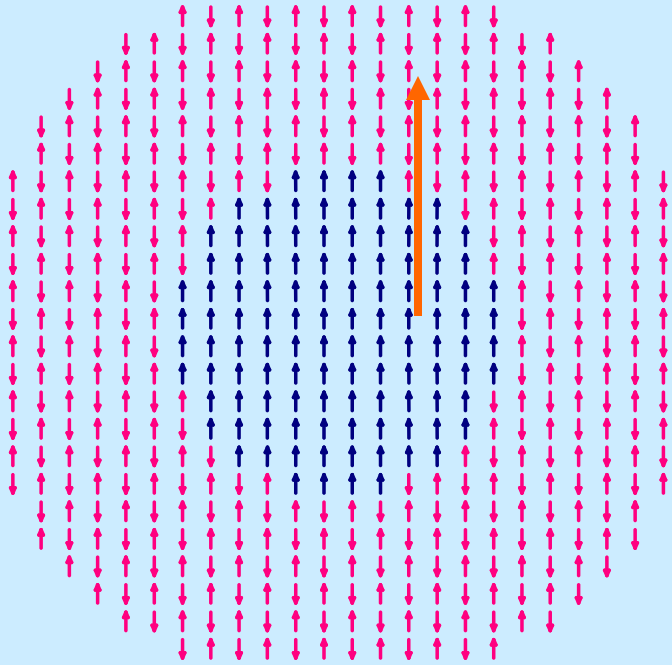
- Ising model – simplest model of magnetic phase transtions
- Can calculate thermodynamic properties analytically
- Introduction of the Monte-Carlo technique
- Check of analytical theory vs numerical calculations
- Important demonstration of the computational physics approach – always test the code!
- Numerical techniques are normally necessary to investigate complex physical systems.

Atomic resolution micromagnetics; do we need a new model?

- Why not use micromagnetics with atomic resolution?
- Micromagnetics is a continuum formalism
- Requirement – exchange MUST reduce to the Heisenberg form.
- Then, micromagnetic model becomes an atomistic simulation. BUT
  - Very limited; sc lattice, nearest neighbour exchange (cf for FePt ≈ 5 lattice spacings + exchange is directional + 2-ion anisotropy leads to complex effects at surfaces.
  - Unnecessarily good calculation of magnetostatic field – dipolar approximation more appropriate + dominance of exchange field and short timestepping means that it is not necessary to update the magnetostatic field at every timestep (Berkov).

Nguyen N. Phuoc et al
Phys. Stat. Sol (b) 244, 4518-21 (2007)





Micromagnetic simulation

Atomistic simulation

z

0 y

Weak exchange coupling: $J_{AF\text{-}FM} = 0.016 \times 10^{-14}$ erg

The Ising model

Consider the case of a magnetic system with infinite anisotropy. Then the spin values can only take values of ± 1. Mathematically this is formalised as follows: For every lattice site $i = 1, ...N$, there is a (spin) variable $\sigma_i \in \{+1, -1\}$ such that the multispin state is identified by $\underline{\sigma} = (\sigma_1, \sigma_2, ...\sigma_N)$. The exchange forces which give rise to the ferromagnetic state are very short ranged and can be taken to involve nearest neighbours only. Consequently the energy of the system consists of a summation over nearest neighbours $(i, j)_{nn}$ as well as over all sites i.

(1)
$$H = -J \sum_i \sum_{(i \neq j)_{nn}} \sigma_i \sigma_j - B \sum_i \sigma_i.$$

The term proportional to B describes the effect of an external magnetic field which has the effect of aligning the spin parallel to B. Note that the Ising model is not limited to magnetic systems; it is an important model in relation, for example, to order/disorder transitions in alloys.

Consider a 2-D square lattice of interacting spins in zero external field ($h = 0$) with N spins and $N \to \infty$. The Hamiltonian then takes the form

(2) $$H = \sum_i \sum_{nn} J\sigma_i\sigma_j,$$

where the sum runs over 4 nearest neighbours. This problem was solved exactly by Onsager in 1944, for which he received the Nobel prize. A number of theoretical approaches have been used, eg graph theory, transfer matrix methods. Here we just quote the solution for the internal energy,

(3) $$\frac{U}{N} = -J\coth\left(\frac{2J}{kT}\right)\left[1 + \frac{2}{\pi}\left(2\tanh^2\left(\frac{2J}{kT}\right) - 1\right)\kappa_1(\mathcal{H})\right],$$

with

(4) $$\mathcal{H} = \left(2\sinh\left(\frac{2J}{kT}\right)\right) / \left(\cosh^2\left(\frac{2J}{kT}\right)\right),$$

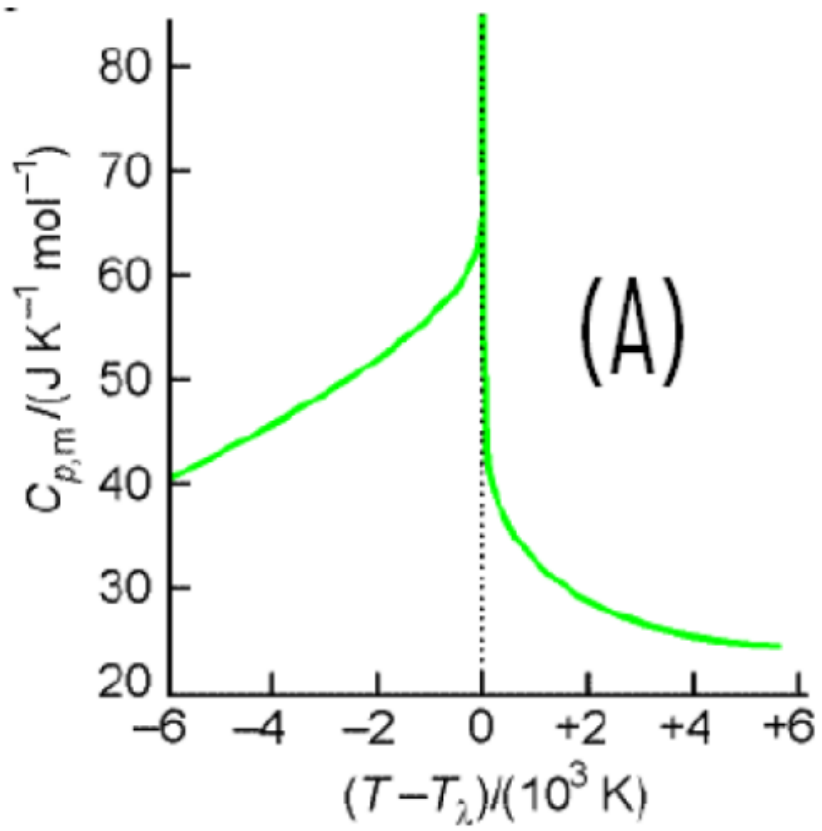
$$\kappa_1(\mathcal{H}) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - \mathcal{H}^2\sin^2\phi}},$$

where κ_1 is the complete elliptic integral of the first kind. U is non-analytic at a critical temperature defined by

(5) $$\sinh\left(\frac{2J}{kT_c}\right) = 1, \qquad \cosh\left(\frac{2J}{kT_c}\right) = \sqrt{2},$$

which gives $kT_c = 2.269J$.

Heat capacity



$\kappa_1(\mathcal{H})$ has a singularity for H $\longrightarrow 1$, in which limit

$$\kappa_1(\mathcal{H}) \sim \ln \frac{4}{\sqrt{1-\mathcal{H}^2}}.$$

As $T \longrightarrow T_c$, from equ. 4 $\mathcal{H} \longrightarrow 1$. In this limit, U remains finite, but *derivatives diverge*. For example, the specific heat,

$$C(T \rightarrow T_c) \sim -ln \mid 1 - \frac{T}{T_c} \mid$$

The divergence is characteristic of a so-called λ transition

Mean field theories

- Statistical Mechanical models are normally not amenable to analytical solution
- hence the invention of numerical techniques such as the Monte-Carlo method.
- The Mean Field Theory (MFT) is one of the most common approximate analytical approaches. A formal derivation of the MFT starts with the Bogoliubov inequality

(6) $$F \leq \Phi = F_0 + < \mathcal{H} - \mathcal{H}_0 >_0,$$

where

- F is the true free energy of the system corresponding to the Hamiltonian $\mathcal{H}$,
- $\mathcal{H}_0$ a trial Hamiltonian dependent on some parameter h_0, F_0 is the corresponding free energy and
- $<>_0$ defines an ensemble average taken in the ensemble defined by $\mathcal{H}_0$.

- $\mathcal{H}$ and F are not known (in closed form).
- We can develop a mean-field approximation to F by minimising Φ with respect to the variational parameter h_0.
- (NB This is directly analogous to the variational principle in Quantum Mechanics).
- This gives $F_{mf} = \min_{h_0}\{\Phi\}$, where F_{mf} is the mean-field approximation to the free energy, from which the important thermodynamic quantities can be calculated.
- Obviously the success of MFT depends on the most appropriate choice of $\mathcal{H}_0$.
- Generally, in order to make the problem tractable we choose for $\mathcal{H}_0$ a Hamiltonian with no interactions, which enables calculation of the RHS of eq 6.

Ising model MF theory

Consider the Ising model in zero external field, with the Hamiltonian $\mathcal{H} = -J\sum_{ji} S_i S_j$, on a lattice of N sites each with z nearest neighbours. Now, take as the trial Hamiltonian

$$\mathcal{H}_0 = -h_0 \sum_i S_i,$$

where h_0 is termed the mean field. This of course is the Hamiltonian for a paramagnet. For which the free energy and magnetisation are

(7) $$F_0 = -NkT\ln(2\cosh\beta h_0), \qquad < S >_0 = \tanh\beta h_0$$

We need to evaluate $< \mathcal{H} - \mathcal{H}_0 >_0$ remembering that this is an ensemble average using probabilities determined by the trial Hamiltonian. This gives

(8) $$< \mathcal{H} - \mathcal{H}_0 >_0 =$$

$$\frac{\sum_S(-J\sum_{ji} S_i S_j + h_0\sum_i S_i)\exp(\beta h_0\sum_i S_i)}{\sum_i \exp(\beta h_0\sum_i S_i)} = -J\sum_{i,j} < S_i >_0 < S_j >_0 + h_0\sum_i < S_i >_0$$

The factorisation of the interaction term is possible because $\mathcal{H}_0$ contains only single-site terms. For a translationally invariant system $< S_i >_0 = < S_j >_0 = < S >_0$., and eq 8 becomes

(9) $$< \mathcal{H} - \mathcal{H}_0 >_0 = -JzN < S >_0^2 /2 + Nh_0 < S >_0,$$

where $zN/2$ is the number of bonds in the lattice (avoiding double counting).

Substituting eq 9 into eq 6 then gives

(10) $$\Phi = -NkT\ln(2\cosh\beta h_0) - JzN < S >_0^2 /2 + Nh_0 < S >_0,$$

and using eq 7

(11) $$\Phi - NkT\ln(2\cosh\beta h_0) - JzN(\tanh\beta h_0)^2/2 + Nh_0\tanh\beta h_0.$$

To minimise we set the derivative to zero, ie

$$\frac{d\Phi}{dh_0} = -N(\tanh\beta h_0) - JzN(\tanh\beta h_0)(1 + (\tanh\beta h_0)^2)$$

$$= N\tanh\beta h_0 + Nh_0\beta(1 + (\tanh\beta h_0)^2) = 0.$$

(12) $$\therefore h_0 = zJ\tanh\beta h_0.$$

Eq 12 must be solved self-consistently for h_0. We can also determine the magnetisation given that $< S >_o = \tanh\beta h_0$ (eq 7) which gives $h_0 = zJ < S_0 >_0$,

$$\therefore < S_0 >_0 = \tanh\beta zJ < S_0 >_0,$$

Graphical solution

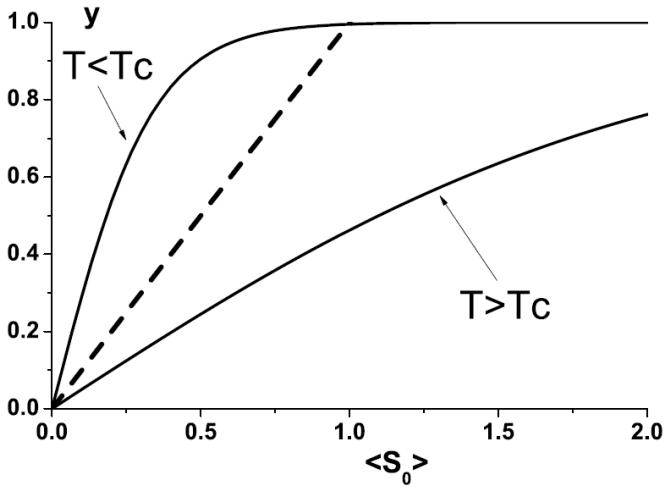


Illustration of the method of graphical solution. The solid lines are the function $y = \tanh \beta z J < S_0 >_0$ and the dotted line represents $y =< S_0 >_0$.

A solution for non-zero $< S_0 >_0$ exists if the function $y = \tanh \beta z J < S_0 >_0$ is intersected by the line $y =< S_0 >_0$, which occurs for $T < T_c$. At the critical temperature T_c the gradients at $< S_0 >_0 = 0$ are equal, ie

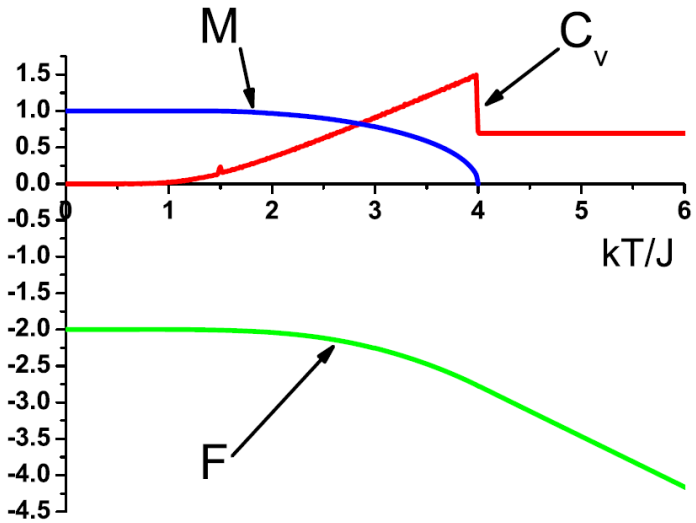
$$1 = \frac{\partial}{\partial < S_0 >_0} \tanh \beta z J < S_0 >_0$$

$$= \beta z J (1 - \tanh^2 \beta z J < S_0 >_0).$$

We are in the limit $< S_0 >_0 \rightarrow 0$, ie $\tanh \beta z J < S_0 >_0 \rightarrow 0$.

$$\therefore 1 = \frac{zJ}{kT_c}, \qquad T_c = zJ/k$$

Thermodynamic quantities



The figure shows plots of the calculated free energy, heat capacity and magnetisation in the Mean-Field theory. It can be seen that the free energy is continuous, but the heat capacity shows a discontinuity at a critical value of $kT/J = 4$, consistent with a continuous phase transition. The plot is calculated for the 2-D case with $z = 4$, and the critical temperature is consistent with the earlier expression $T_c = zJ/k$.

Calculation of equilibrium properties

- Description of the properties of a system in thermal equilibrium is based on the calculation of the partition function Z given by

$$Z = \sum_{\underline{S}} \exp(-H(\underline{S}))/k_B T.$$

where S is representative of the spin system

- If we can calculate Z it is easy to calculate thermal average properties of some quantity A(S) as follows

$$< A >= \sum_{\underline{S}} p(\underline{S}) A(\underline{S})$$

$$p(\underline{S}) = Z^{-1} \exp(-H(\underline{S})/k_B T).$$

Where p(S) is the probability of a given spin-state

Monte-Carlo method

- It would be possible in principle to do a numerical integration to calculate <A>.
- However, this is very inefficient since p(S) is strongly peaked close to equilibrium.
- A better way is to use 'importance sampling', invented by Metropolis et al

N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E Teller, J. Chem. Phys. **21**, 1087 (1953).

Importance sampling

- We define a transition probability between states such that the 'detailed balance condition is' obeyed

$$W(\underline{S} \rightarrow \underline{S'}) \exp(-H(\underline{S})/k_B T) = W(\underline{S'} \rightarrow \underline{S}) \exp(-H(\underline{S'})/k_B T).$$

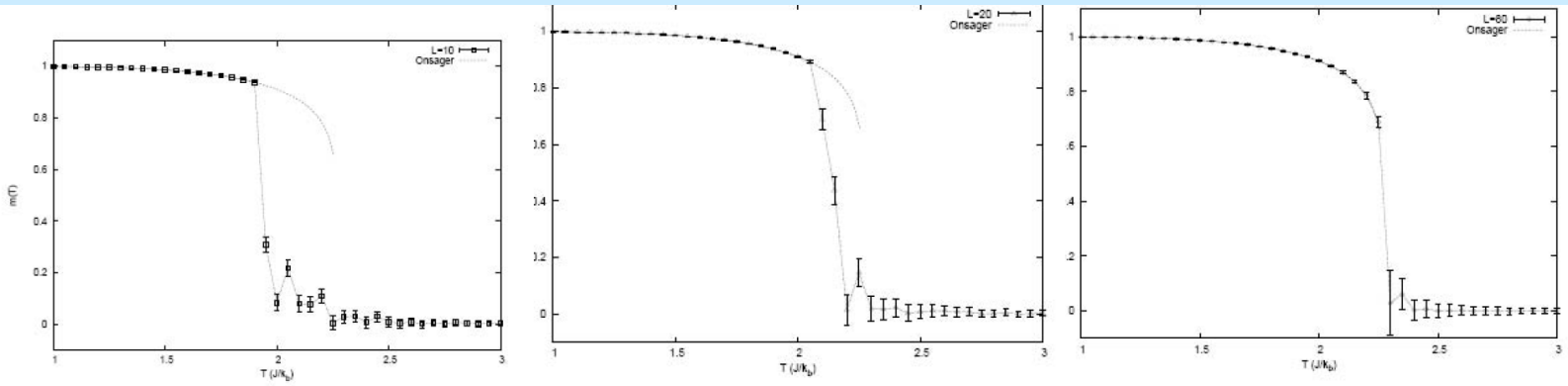
- The physics can be understood given that $p(S)=Z^{-1}\exp(-H(S)/k_BT)$, ie p(S) does not change with time at equilibrium.

Metropolis algorithm

1. For a given state choose a spin *i* (randomly or sequentially), change the direction of the spin, and calculate the energy change ΔE.
2. If $\Delta E < 0$, allow the spin to remain in the new state. If $\Delta E > 0$, choose a uniformly distributed random number $r \in [0; 1]$. if $r < \exp(-\Delta E/k_B T)$ allow the spin to remain in the new state, otherwise the spin reverts to its original state.
3. Iterate to equilibrium
4. Thermal averages reduce to an unweighted summation over a number (N) of MC moves, eg for the magnetisation

$$< M >= N^{-1} \sum_{i=1}^{N} M_i$$

M vs T for 2-D Ising model (MC calculations of Joe Barker)



(a) L=10 (b) L=20 (d) L=80

M vs T for the 2-D Ising model for systems of different sizes. The results are compared with the Onsager expression for the magnetisation.

For the case of the $2-D$ Ising model there is an analytical expression (due to Onsager) for the magnetisation.

(13)
$$M = \left\{ 1 - \left[\sinh\left(\ln(1+\sqrt{2}) \frac{T_c}{T} \right) \right]^{-4} \right\}^{1/8}$$

Fig. 10 shows the variation of magnetisation with temperature for a number of system sizes with the Onsager equation shown for comparison. The finite size effects lead to a reduction of the ordering temperature and decreased criticality. For the large system size there is good agreement between the numerical results and the Onsager equation.

Summary

- Thermodynamic properties of magnetic materials studied using Ising model
  - Analytical and mean-field model
  - MC approach for atomistic calculations agrees well with analytical mode (Onsager)
- In the following we introduce a dynamic approach and apply this to ultrafast laser processes
- We also investigate the link between ab-initio and atomistic models.

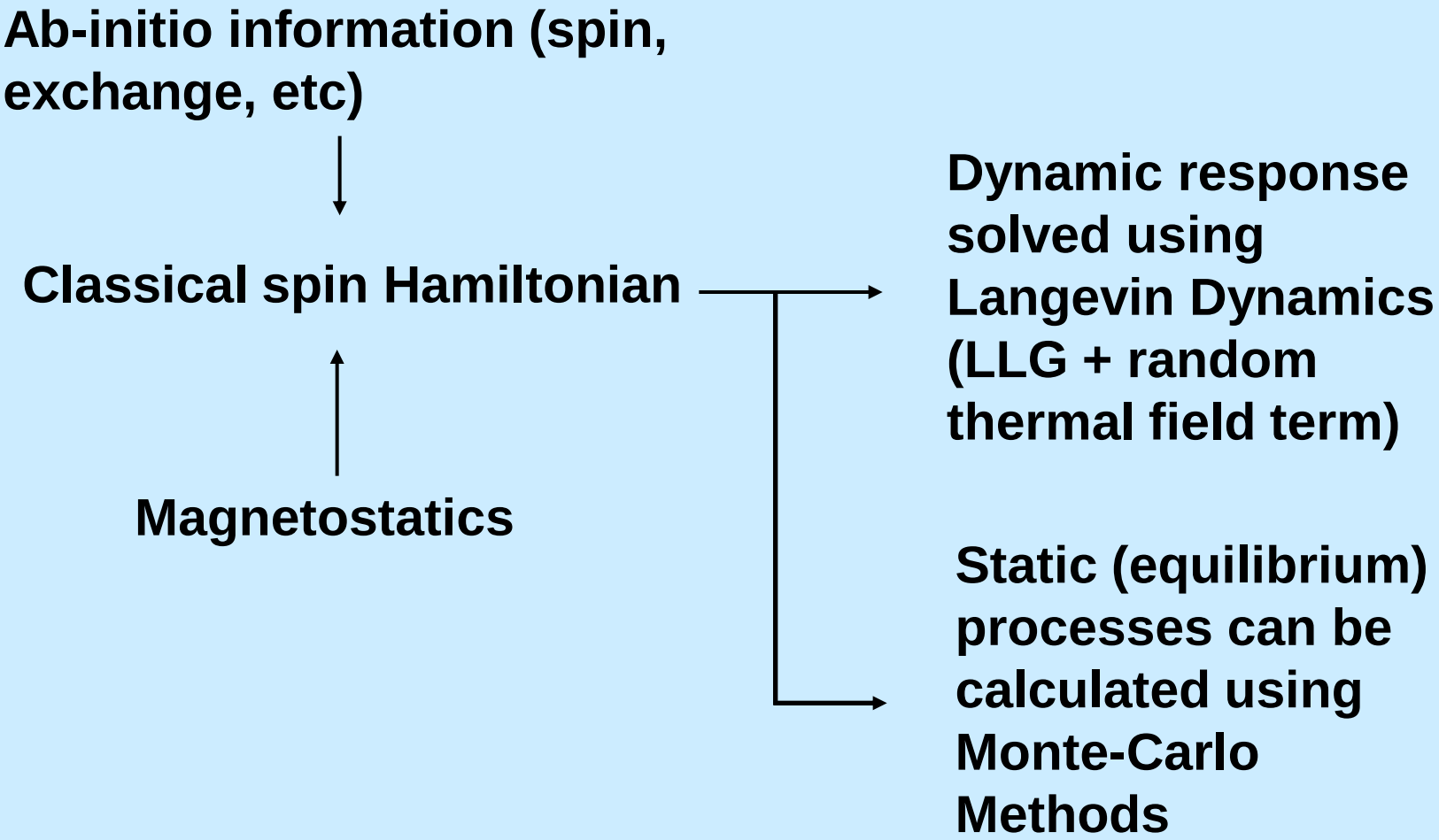
Atomistic model of dynamic properties

- Uses the Heisenberg form of exchange

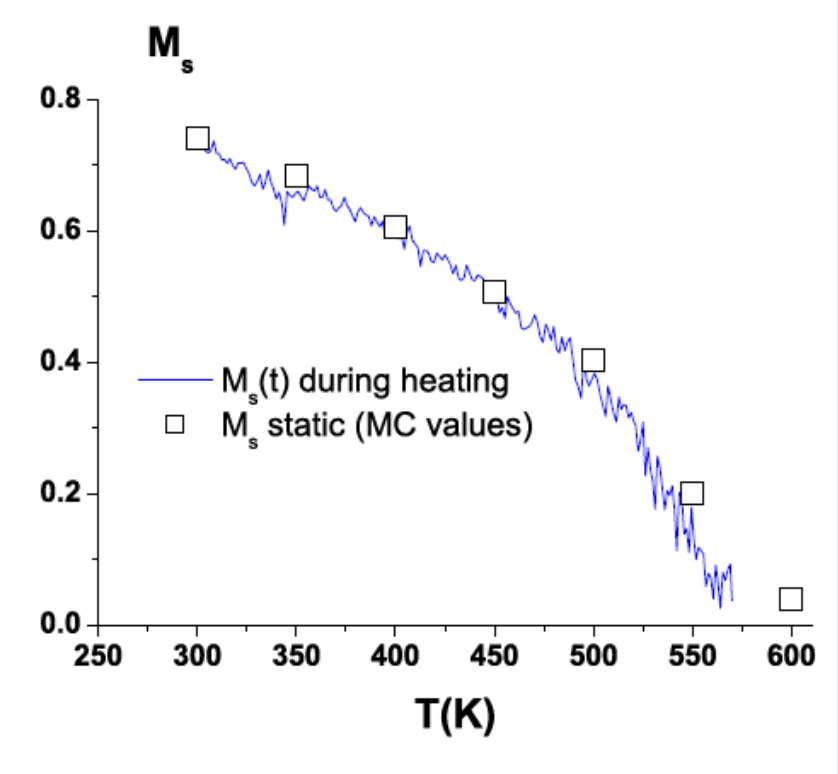
$$E_i^{exch} = \sum_{j \neq i} J_{ij} \vec{S}_i . \vec{S}_j$$

- 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



M vs T; static (MC) and dynamic calculations



- Dynamic values are calculated using Langevin Dynamics for a heating rate of 300K/ns.
- Essentially the same as MC values.
- ❶ Fast relaxation of the magnetisation (see later)

How to link atomistic and ab-initio calculations?

- Needs to be done on a case-by-case basis
- In the following we consider the case of FePt, which is especially interesting.
- First we consider the ab-initio calculations and their representation in terms of a classical spin Hamiltonian.
- The model is then applied to calculations of the static and dynamic properties of FePt.

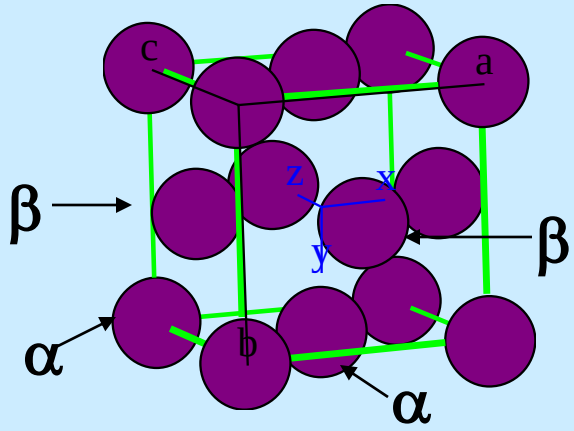
Ab-initio/atomistic model of FePt

- Anisotropy on Pt sites
- Pt moment induced by the Fe
- Treating Pt moment as independent degrees of freedom gives incorrect result (Low T_c and 'soft' Pt layers)
- New Hamiltonian replaces Pt moment with moment proportional to exchange field. Exchange values from ab-initio calcuations.
- Long-ranged exchange fields included in a FFT calculation of magnetostatic effects
- Langevin Dynamics used to look at dynamic magnetisation reversal
- Calculations of
    - Relaxation times
    - Magnetisation vs T

Disorder to Order Transformation

50% Fe/50% Pt

As Deposited



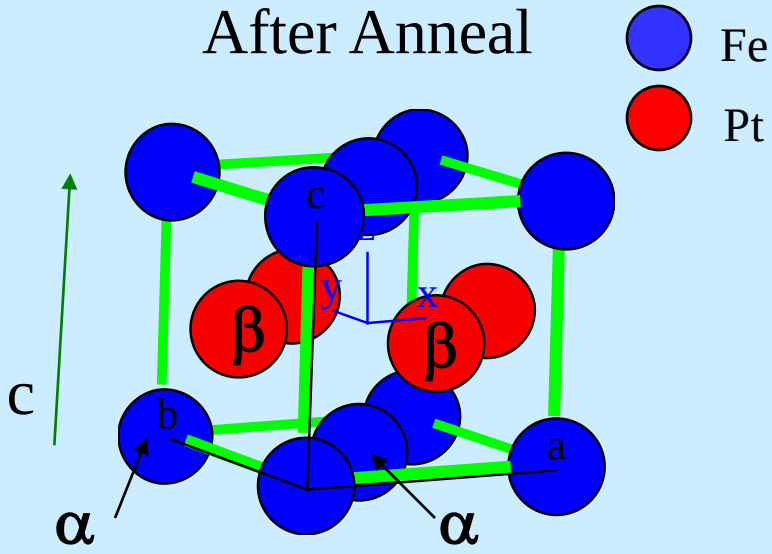
FCC disordered alloy

$$a = b = c$$

Small cubic Anisotropy

Anneal

After Anneal



Ordered $L1_0$ (ex. FePt)

$$a = b = 3.853A \neq c = 3.713A$$

$$K_{1\,partial} \approx K_{1ordered} S^2$$

Degree of Chemical Order = S $\equiv \dfrac{r_\alpha - x_A}{y_\beta}$

r_α=fraction of a sites occupied by correct atom

x_A=atom fraction of A

y_β=fraction of β sites

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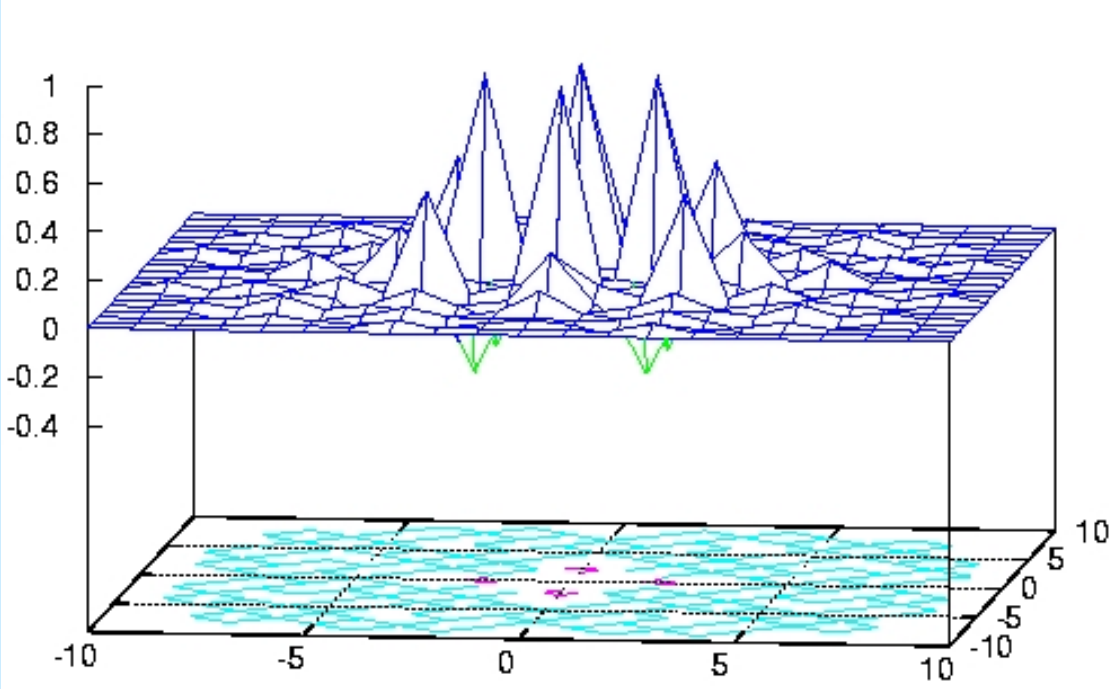
FePt exchange



- Exchange coupling is long ranged in FePt

FePt Hamiltonian

Exchange: Fe/Fe Fe/Pt Pt/Pt

$$H = -\sum_{i,j}\frac{J_{ij}}{2}\vec{S}_i.\vec{S}_j - \sum_{i,k}\frac{J_{ik}}{2}\vec{S}_i.\vec{S}_k - \sum_{k,l}\frac{J_{kl}}{2}\vec{S}_k.\vec{S}_l$$

$$- d_{Fe}\sum_i (S_i^z)^2 - d_{Pt}\sum_k (S_k^z)^2$$

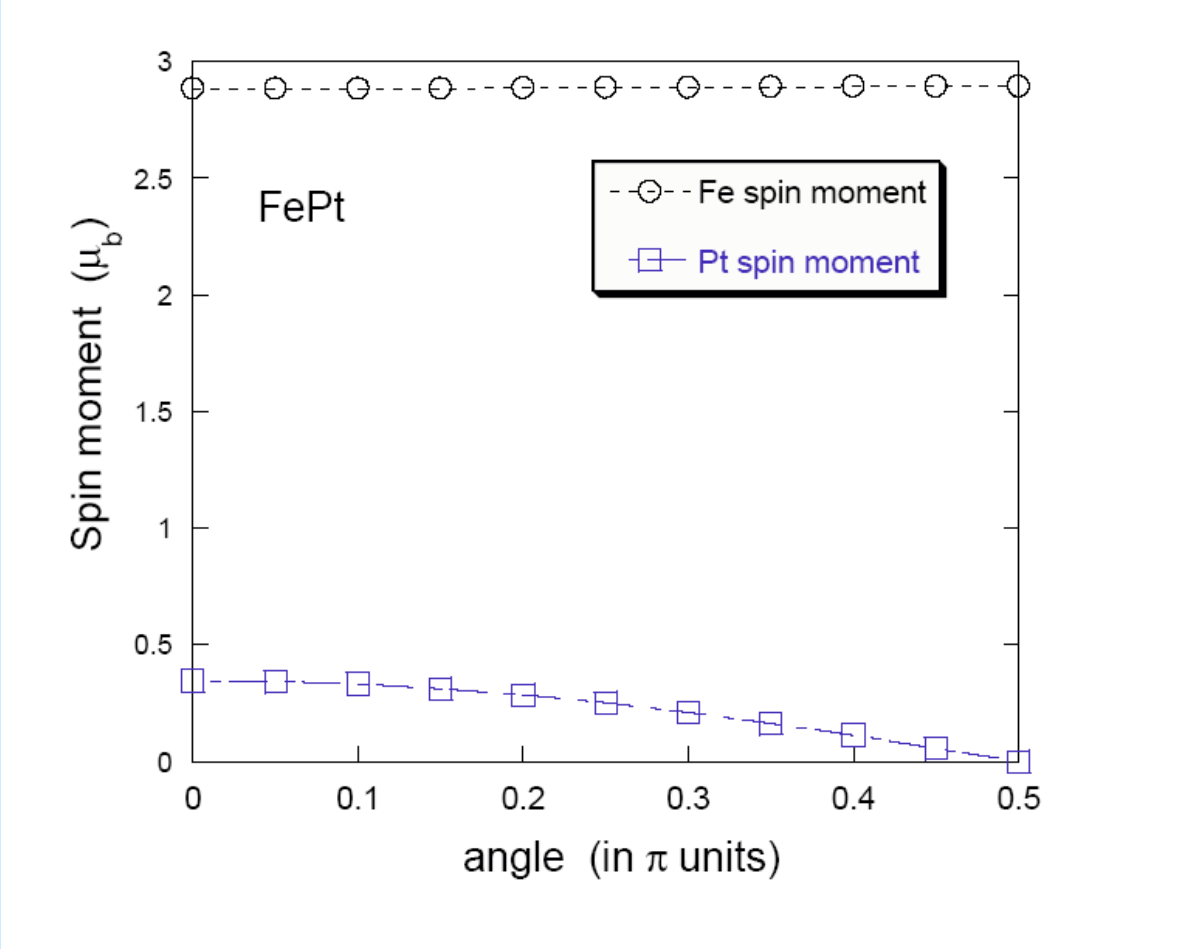
Anisotropy

$$- \mu_{Fe}\vec{B}.\sum_i \vec{S}_i - \mu_{Pt}\vec{B}.\sum_k \vec{S}_k$$

Zeeman

Convention: Fe sites i,j Pt sites k,l

Localisation (ab-initio calculations)



To good approximation the Pt moment is found numerically to be ✪ Exchange field from the Fe

Thus we take the FePt moment to be given by

$$\vec{S}_k = \frac{1}{S_{FePt}} \sum_i J_{ik} \vec{S}_i$$

With $S_{FePt} = \sum_i J_{ik}$

Substitution for the Pt moments leads to a Hamiltonian dependent only on the Fe moments;

$$H = -\sum_{i,j} \frac{\tilde{J}_{ij}}{2} \vec{S}_i . \vec{S}_j - d^0 \sum_i (S_i^z)^2 - \sum_{ij} d_{ij}^2 S_i^z S_k^z - \tilde{\mu}\ \vec{B} . \sum_i \vec{S}_i$$

With new effective interactions $\tilde{J}_{ij} = J_{ij} + S_{FePt} \sum_k J_{ik} J_{jk}$

Single ion anisotropy $d^0 = d_{Fe} + d_{Pt} S_{FePt}^2 \sum_k J_{ik}^2$

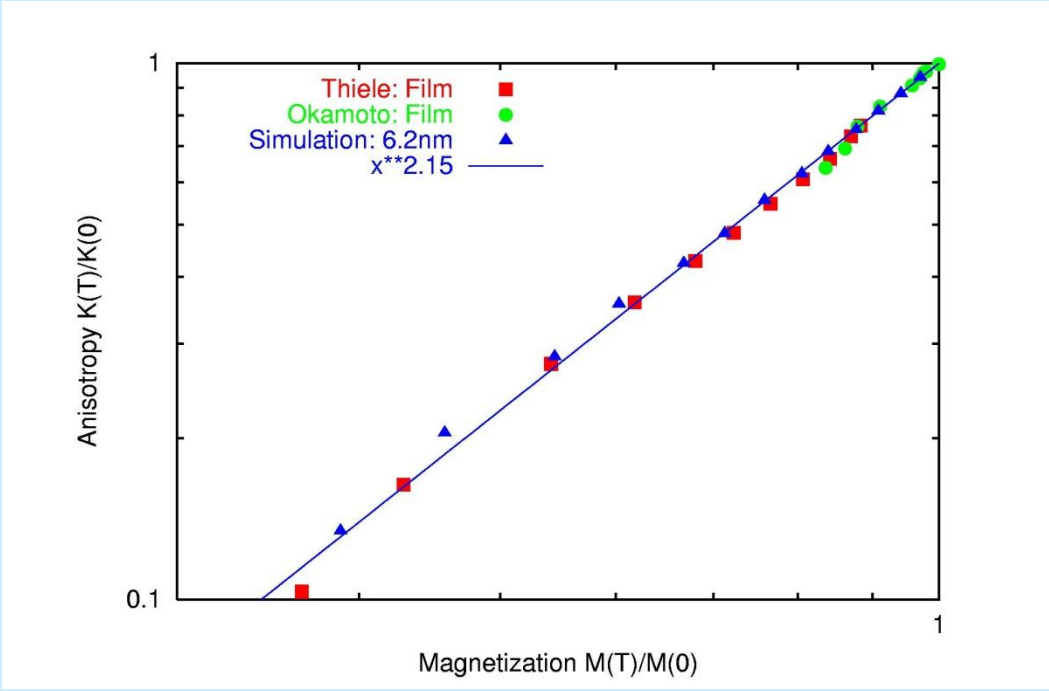
2-ion anisotropy (new term) $d_{ij}^2 = 2 d_{Pt} S_{FePt}^2 \sum_k J_{ik} J_{jk}$

And moment $\tilde{\mu} = \mu_{Fe} + \mu_{Pt}$. $S_{FePt} = \sum_i J_{ik}$

- All quantities can be determined from ab-initio calculations
- 2-ion term (resulting from the delocalised Pt degrees of freedom) is dominant

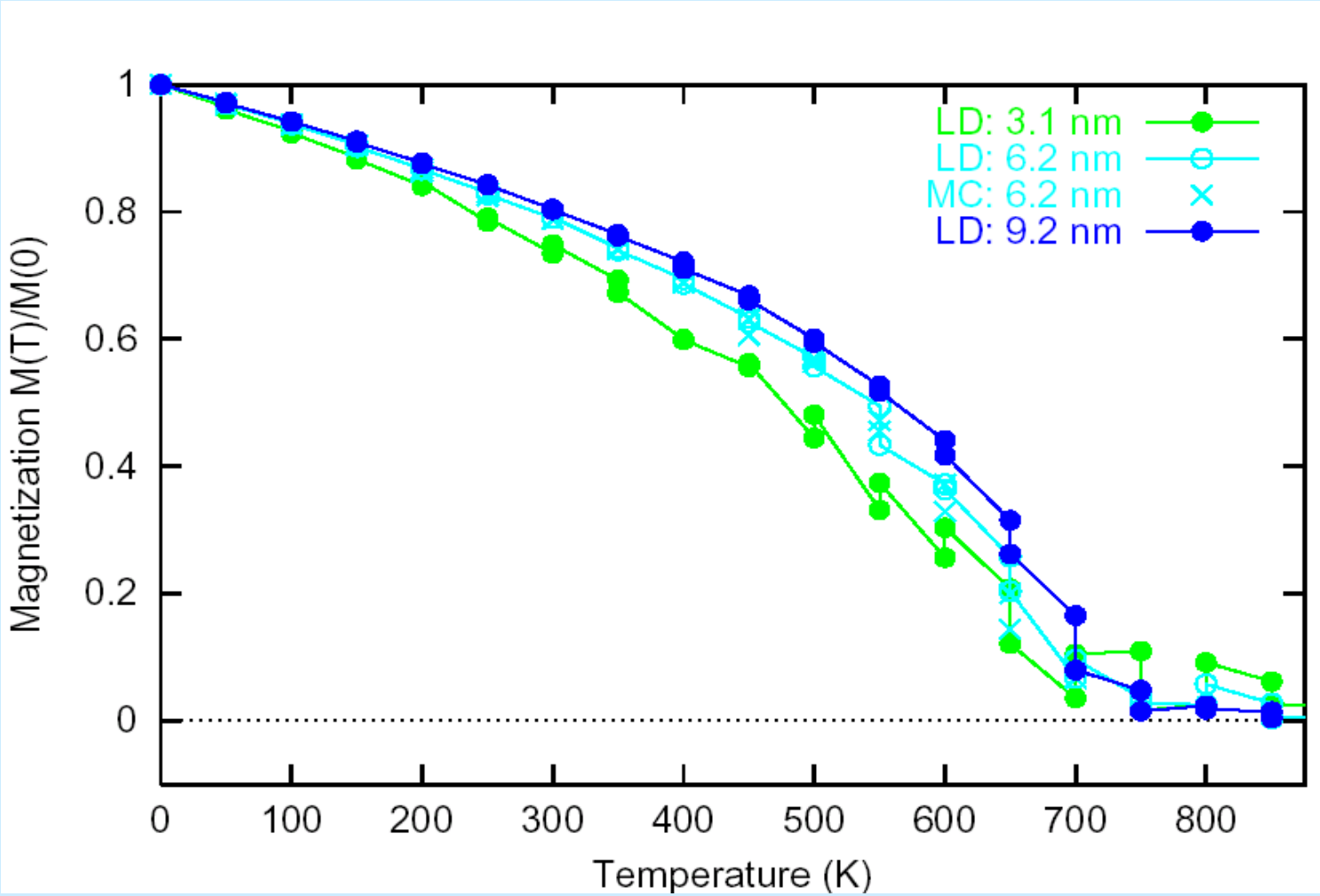
Anisotropy of FePt nanoparticles

- New Hamiltonian replaces Pt moment with moment proportional to exchange field from Fe. Gives a 2 ion contribution to anisotropy
- Exchange and K(T=0) values from ab-initio calculations.
- Long-ranged exchange fields included in a FFT calculation of magnetostatic effects
- Langevin Dynamics or Monte-Carlo approaches
- Can calculate
  - M vs T
  - K vs T
  - Dynamic properties



- Good fit to experimental data (Theile and Okamoto)
- First explanation of origin of experimental power law – results from 2 ion anisotropy

Model of magnetic interactions for ordered 3d-5d alloys: Temp. dependence of equilibrium properties.



Reasonable estimate of T_c (no fitting parameters)

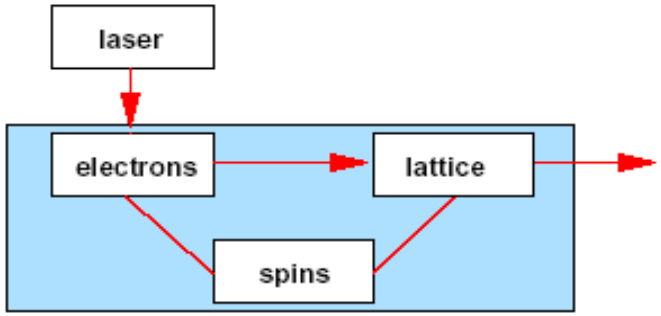
Ultrafast Laser induced magnetisation dynamics

- The response of the magnetisation to femtosecond laser pulses is an important current area of solid state physics
- Also important for applications such as Heat Assisted Magnetic Recording (HAMR)
- Here we show that ultrafast processes cannot be simulated with micromagnetics.
- An atomistic model is used to investigate the physics of ultrafast reversal.

Pump-probe experiment

- Apply a heat pulse to the material using a high energy fs laser.
- Response of the magnetisation is measured using MOKE
- Low pump fluence – all optical FMR
- High pump fluence – material can be demagnetised.
- In our model we assume that the laser heats the conduction electrons, which then transfer energy into the spin system and lattice.
- Leads to a '2-temperature' model for the temperature of the conduction electron and lattice

2 temperature model



1. photon energy is transferred to electrons

2. energy is exchanged between electrons and phonons

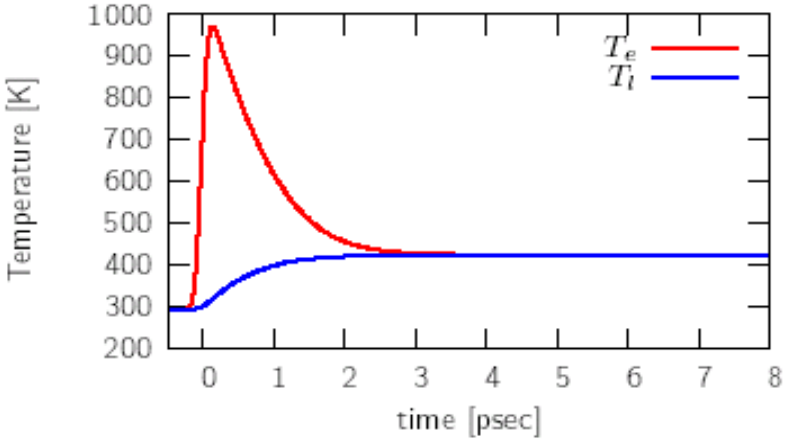
3. energy dissipates into environment

Two temperature model:

$$\text{electrons:} \quad C_e \frac{\mathrm{d}T_e}{\mathrm{d}t} = -G_{el}(T_e - T_l) + P(t)$$

$$\text{lattice:} \quad C_l \frac{\mathrm{d}T_l}{\mathrm{d}t} = G_{el}(T_e - T_l)$$

(M. I. Kaganov et al., Sov. Phys. JETP **4**, 173 (1957))



$\Rightarrow$ perform Langevin dynamics simulation with T_e as temperature of the heat bath

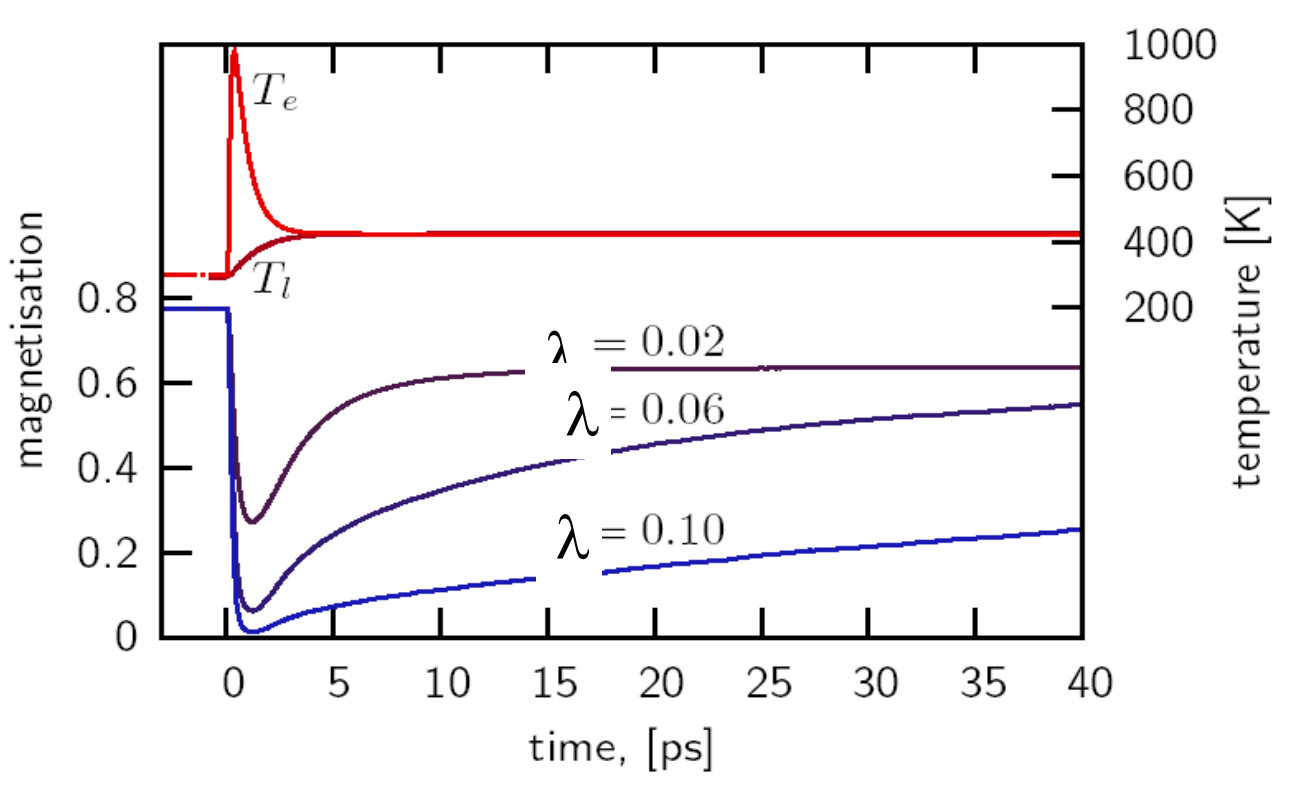
Atomistic model

- Uses the Heisenberg form of exchange

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

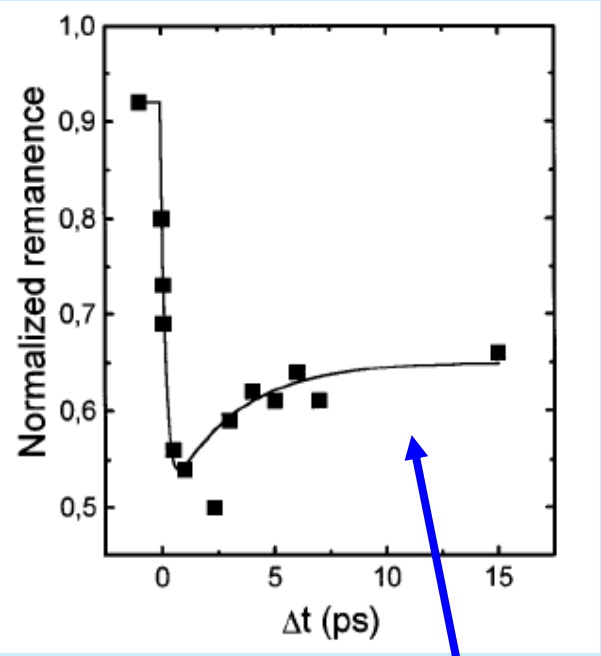
- Dynamics governed by the Landau-Lifshitz-Gilbert (LLG) equation.
- Random field term introduces the temperature (Langevin Dynamics).
- Variance of the random field determined by the electron temperature T_{el}.

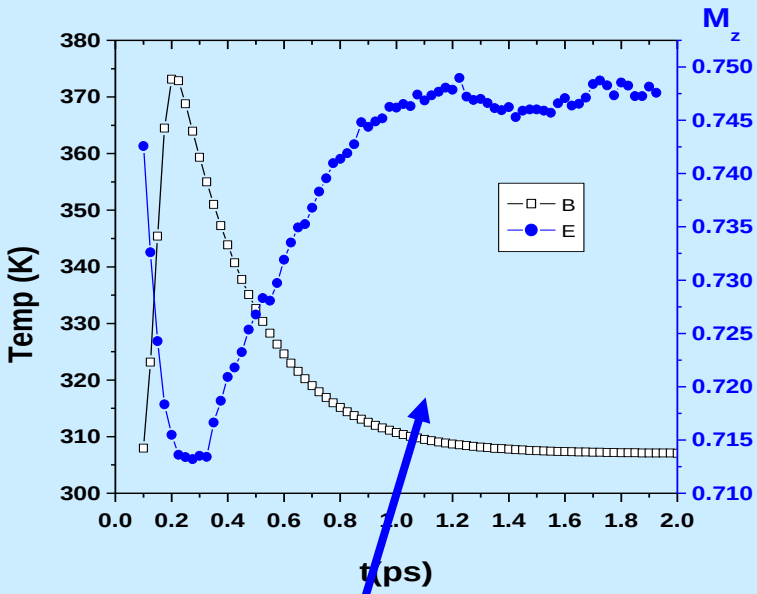
Pump-probe simulations – continuous thin film



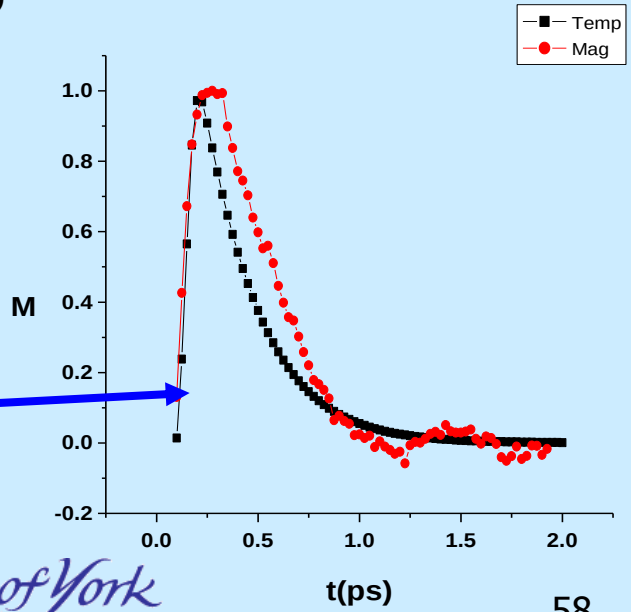
- Rapid disappearance of the magnetisation
- Reduction depends on λ

Ultrafast demagnetisation





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



Opto-magnetic reversal

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

All-Optical Magnetic Recording with Circularly Polarized Light

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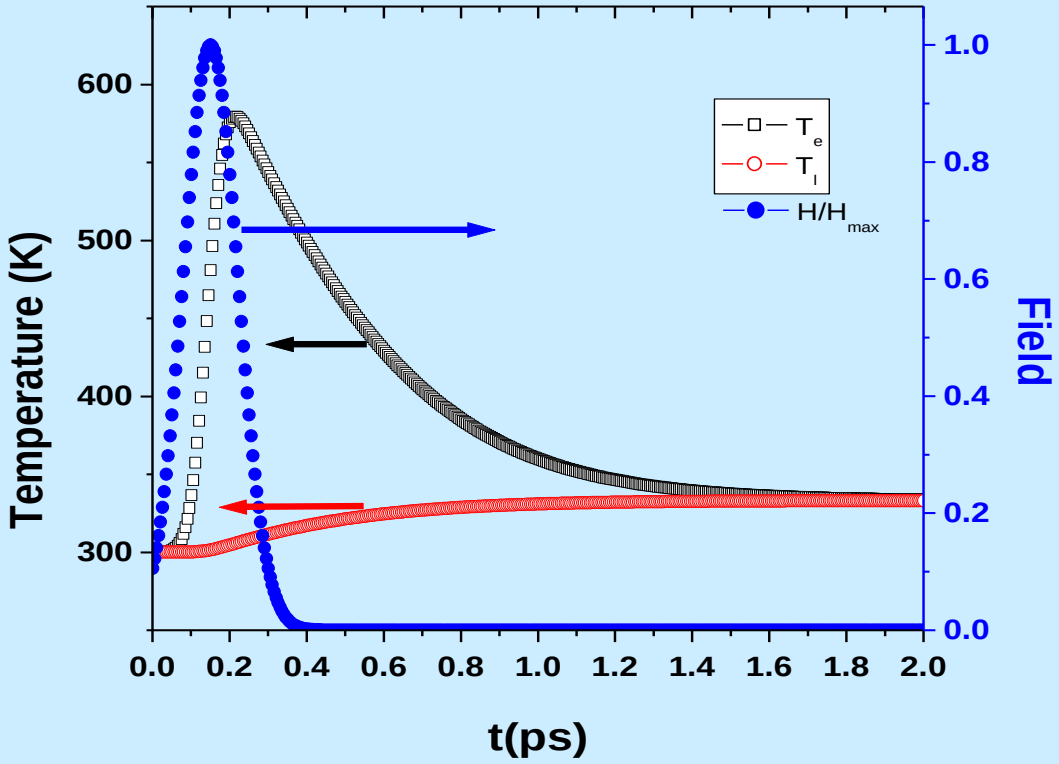
We experimentally demonstrate that the magnetization can be reversed in a reproducible manner by a single 40 femtosecond circularly polarized laser pulse, without any applied magnetic field. This optically induced ultrafast magnetization reversal previously believed impossible is the combined result 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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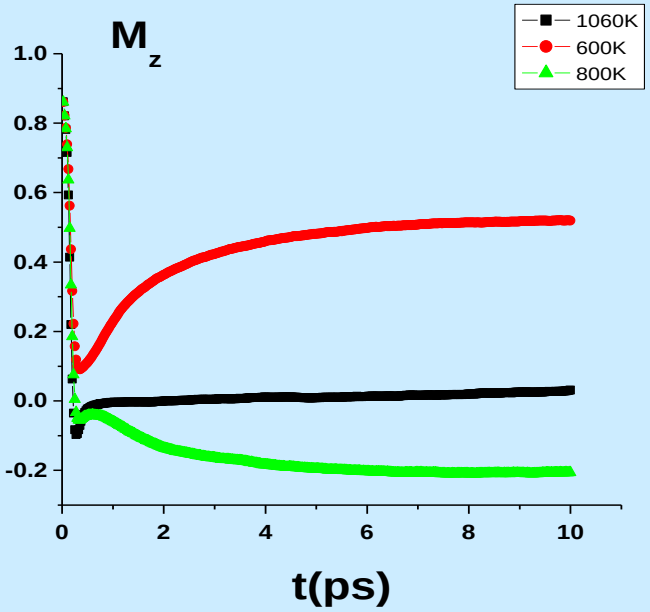
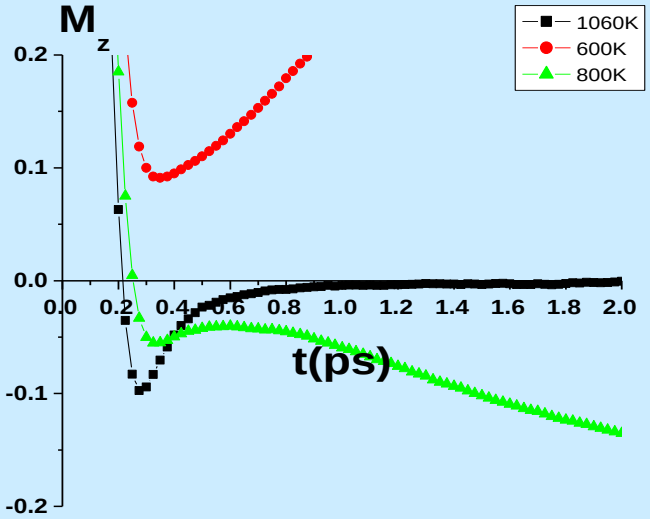
Magnetisation dynamics





- ***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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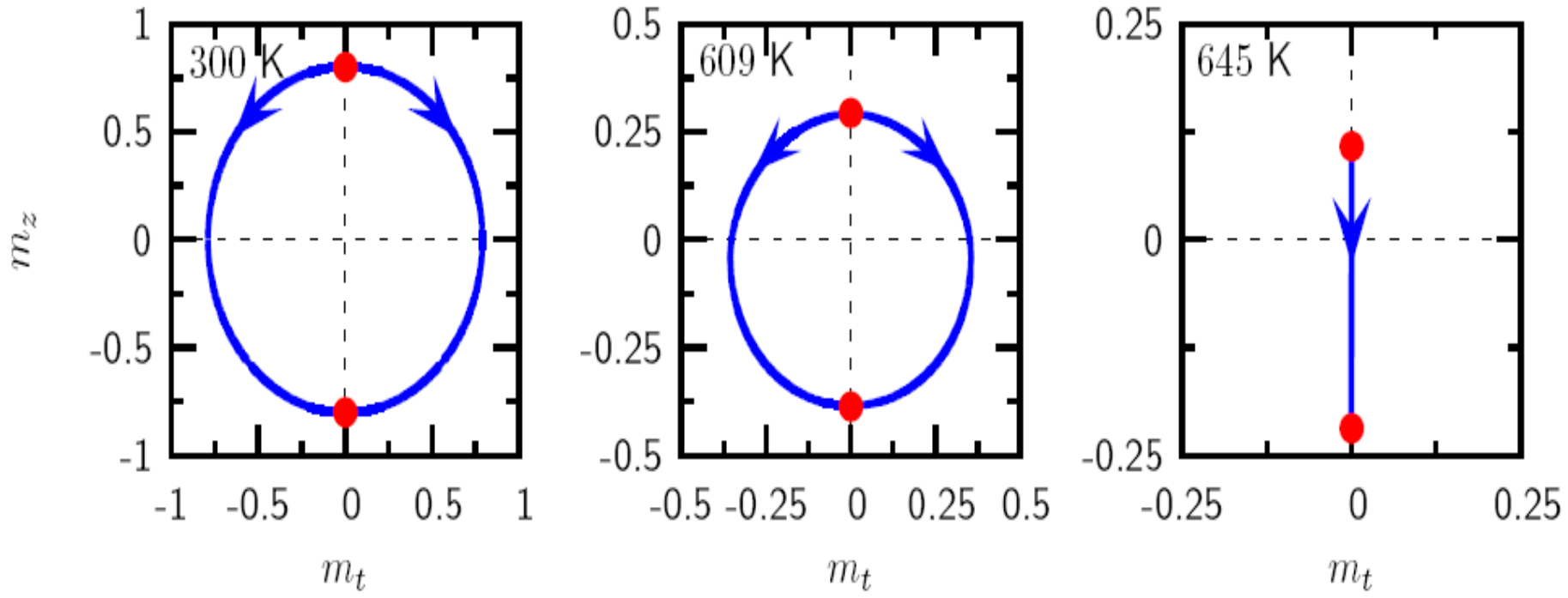
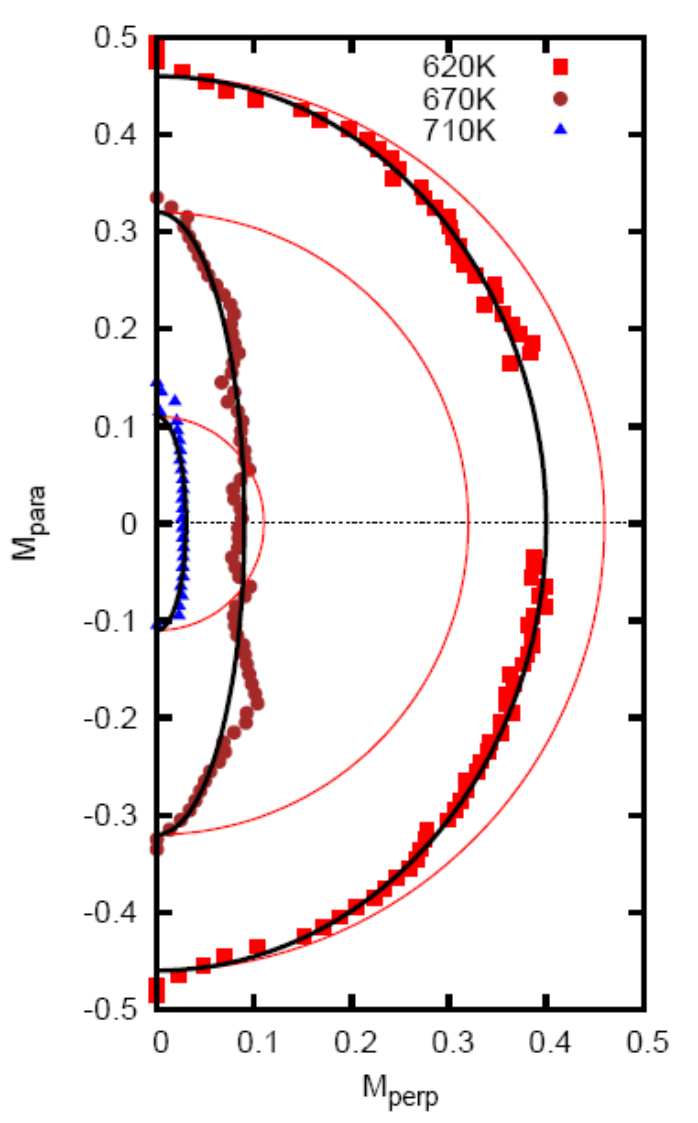
Linear reversal

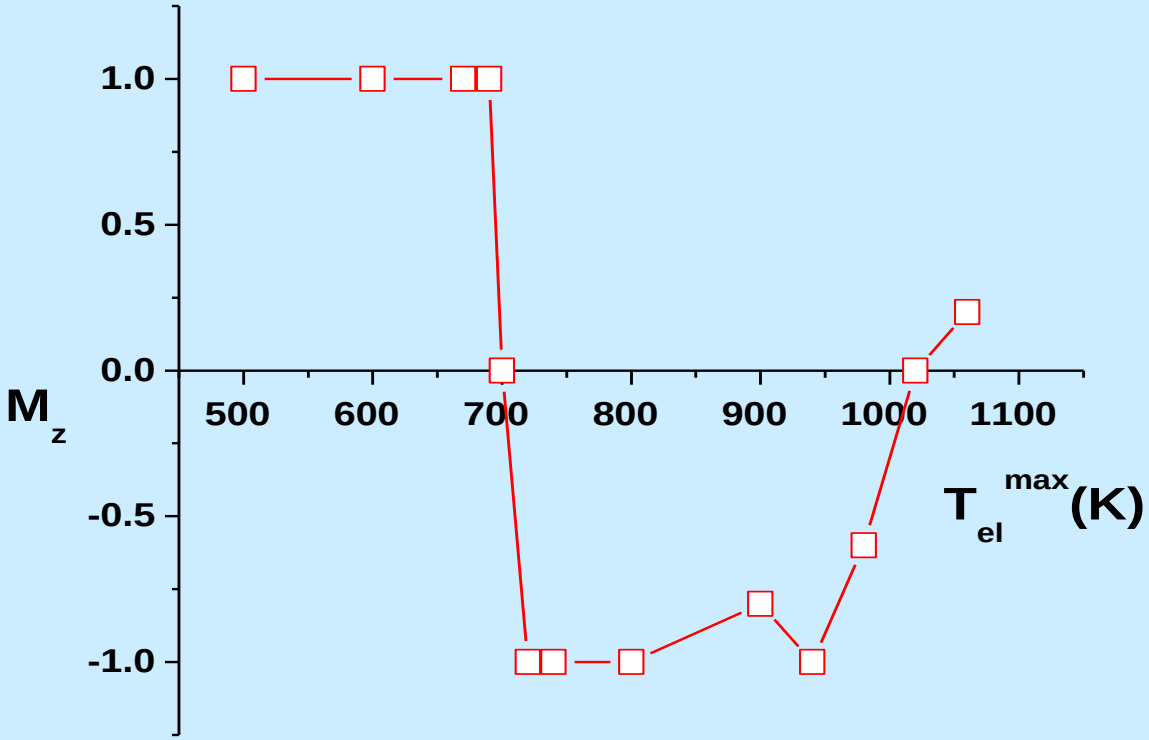


Transition from circular to linear reversal (Joe Barker and Richard Evans)



- At 620K KV/kT=80 – no reversal
- NB, timescale of calculation is 1 ns – KV/kT needs to be around 2 for reversal!
- Reversal occurs at 670K.
- Effective energy barrier for linear reversal much lower than for coherent rotation.

‘Reversal window’



- Well defined temperature range for reversal
- This leads to a ‘phase diagram’ for optomagnetic reversal
- Studied using the Landau-Lifshitz-Bloch equation (lecture 2)

Multiscale magnetism

- Need is for links between ab-initio and atomistic models
- BUT comparison with experiments involves simulations of large systems.
- Typically magnetic materials are 'nanostructured', ie designed with grain sizes around 5-10nm.
- Permalloy for example consists of very strongly exchange coupled grains.
- Such a 'continuous' thin film cannot be simulated atomistically
- Is it possible to 'import' atomistic level information into micromagnetics? This is the subject of Lecture 2!

Summary

- An atomistic approach to the simulation of static and dynamic magnetic properties using ab-initio information was described
- An atomistic model of the magnetic properties of FePt has been developed
- The model predicts the Curie temperature and anisotropy well using ab-initio parameters
- In particular the experimental dependence $K=M^n$ with $n = 2.1$ is explained by a dominant 2-ion anisotropy term introduced by the delocalised Pt moments.
- Atomistic model was used to explore the physics of ultrafast magnetisation processes
- New (linear) magnetisation reversal mechanism operates at temperatures close to T_c – seems to be important for opto-magnetic reversal

- Atomistic model applied to pump-probe experiments shows
  - Fast disappearance of M on application of the laser pulse
  - Slow recovery of the magnetisation after application of the laser pulse (consistent with recent experiments). Origin?
- Experiments and theory are converging on the nm / sub ps scales. Exciting possibilities for understanding the laser/spin/electron/phonon interaction at a very fundamental level.