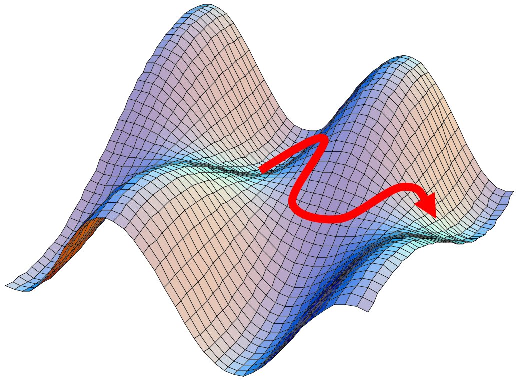
Modelling & Simulation
Thursday 14 August
14:00-15:30
16:00-17:30



Robert Stamps received BS and MS degrees from the University of Colorado, and a PhD in Physics from Colorado State University. He was with the University of Western Australia until 2010, and is currently Professor of Solid State Physics at the University of Glasgow in Scotland. He was an IEEE Magnetics Society Distinguished Lecturer in 2008 (including visits to CBPF and elsewhere in Brazil), and he was the IEEE/IOP Wohlfarth Lecturer in 2004. He is chair of the IRUK IEEE Magnetics Society Chapter, was chair of the 2007 MML Symposium, and will co-chair the Joint European Magnetics Symposia in 2016. This is the fourth time he has lectured at an IEEE Magnetics School.

Aim of lectures:

To provide an introduction to the philosophy and art of modelling of the essential physics at play in magnetic systems.

Examples will be given of how simple models can be constructed and applied to understand and interpret observable phenomena, ranging from magnetisation processes to high frequency spin wave dynamics.

Along the way, an introduction to some general tools will be provided, including Monte Carlo models and micromagnetics.

University of Glasgow

Modelling and Simulation

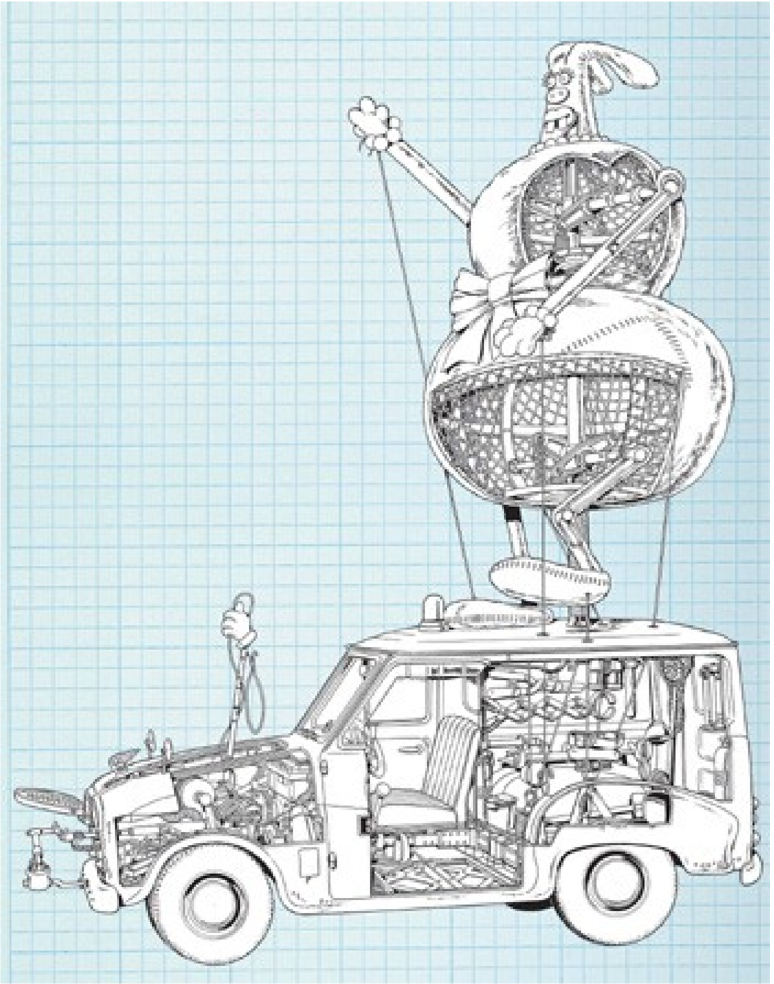
Robert Stamps

IEEE Magnetics Society School 2014

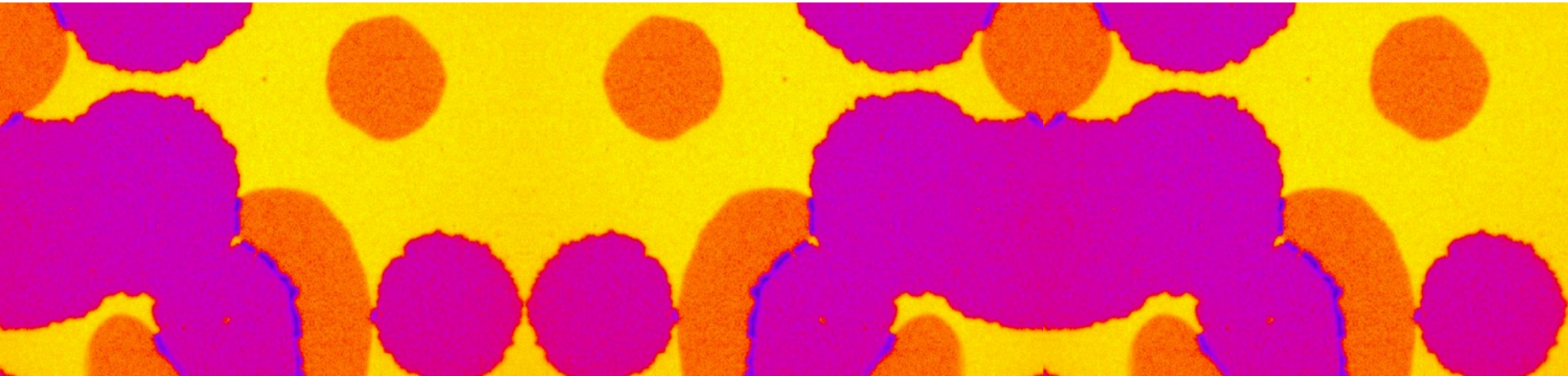
IEEE MAGNETICS 50 YEARS 1964 2014

Outline

- **Modelling: where to start?**
  - Starting points
  - Phenomenology
- **Some generic tools:**
  - Micromagnetics
  - Mean field theory & Monte Carlo
- **Spin dynamics**
  - Torque equations
  - Spinwaves & resonances
- **Domains and domain walls**
  - Stoner-Wohlfarth models
  - Magnetic domains and domain walls



Modelling: where to start?



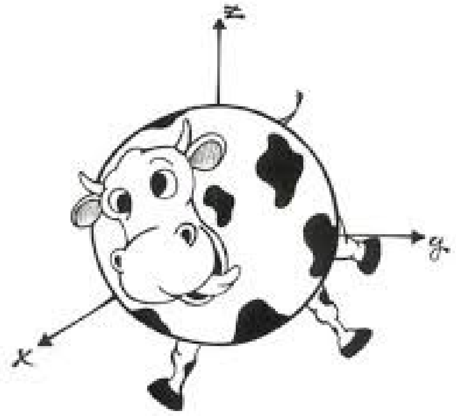
Models for **research & development**: magnetic ordering, dynamics, transport ...

Some starting points for model makers

Tools

1) **Simulations**
do not by themselves provide interpretations or insights

2) **Analytic/conceptutal models**
often go where simulations cannot



The dark arts of simplification: ***phenomenology***

Energies

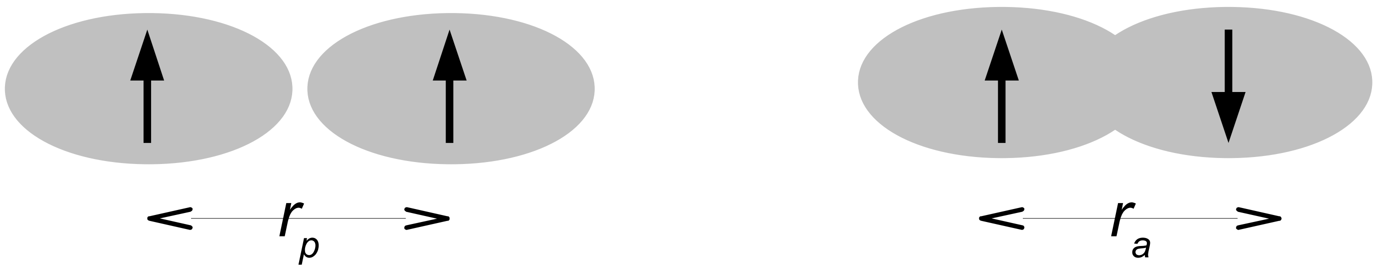
Relevant energy scales (P. W. Anderson, 1953):

1 – 10 eV	Atomic Coulomb integrals Hund's rule exchange energy Electronic band widths Energy/state at ε_f
0.1 – 1.0 eV	Crystal field splitting
10^{-2} – 10^{-1} eV	Spin-orbit coupling $k_B T_C$ or $k_B T_N$
10^{-4} eV	Magnetic spin-spin coupling Interaction of a spin with 10 kG field
10^{-6} – 10^{-5} eV	Hyperfine electron-neuclear coupling

magnon region (bracketing 10^{-4} eV and 10^{-6} – 10^{-5} eV)

Concept: Exchange Energy

Pauli exclusion **separates** like spins:



Can be **energetically favourable**: *suppose* alignment determines average separation. Then *if*:

$$\langle r_a \rangle \sim 0.3\, nm \Rightarrow \frac{e^2}{r_a} \sim 4.8\, eV$$

$$\langle r_p \rangle \sim 0.31\, nm \Rightarrow \frac{e^2}{r_p} \sim 4.75\, eV$$

$$\Big\} \quad E_{\uparrow\uparrow} - E_{\uparrow\downarrow} = 0.05\, eV\, (580\, K)$$

… equivalent field: $\frac{E_{\uparrow\uparrow} - E_{\uparrow\downarrow}}{\mu_B} = 870\, T$

Exchange Interactions

Exchange: electrostatic repulsion + quantum mechanics.

Hamiltonian as **spin functions:** (Dirac & Heisenberg)

Pauli spin matrices

$$\widetilde{H} = -J_{1,2}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

Generalised for multi-electron orbitals (**van Vleck**):

$$H_{ex} = -\sum_{a,b} J(\boldsymbol{r}_a - \boldsymbol{r}_b)\boldsymbol{S}(\boldsymbol{r}_a)\cdot\boldsymbol{S}(\boldsymbol{r}_b)$$

total spin at sites ***r***

Using Symmetry: Exchange

Measurable moment **density** (not an operator):

$$\boldsymbol{m}(\boldsymbol{r}) = Tr\left(\rho\,\hat{\boldsymbol{M}}(\boldsymbol{r})\right)$$

density matrix

Exchange still in Heisenberg form:

$$E_{ex} = \Sigma_{j,\delta}\, J\, \boldsymbol{m}(\boldsymbol{r}_j)\cdot \boldsymbol{m}(\boldsymbol{r}_{j+\delta})$$

neighbours

Atomic to continuum: Expand ***m*** field about $\boldsymbol{r}_j$

$$\boldsymbol{m}(\boldsymbol{r}_{j+\delta}) = \boldsymbol{m}(\boldsymbol{r}_j) + \left[(\delta\cdot\nabla)\,\boldsymbol{m}(\boldsymbol{r}_{j+\delta})\right]_{j=\delta} + \frac{1}{2}\left[(\delta\cdot\nabla)^2\,\boldsymbol{m}(\boldsymbol{r}_{j+\delta})\right]_{j=\delta} + \ldots$$

Using Symmetry: Exchange

When **lattice symmetry** allows:

$$\delta_x \frac{\partial \boldsymbol{m}}{\partial x} + (-\delta_x) \frac{\partial \boldsymbol{m}}{\partial x} = 0$$

Example: **isotropic medium**

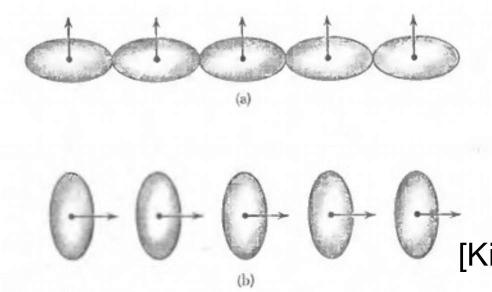
$$\boxed{E_{ex} = m_x(\nabla^2 m_x) + m_y(\nabla^2 m_y) + m_z(\nabla^2 m_z)}$$

Exchange energy must be compatible with symmetry of the crystal

$$E_{ex} = \Sigma_{\alpha k l} C_{kl} \frac{\partial m_\alpha(\boldsymbol{r})}{\partial r_k} \frac{\partial m_\alpha(\boldsymbol{r})}{\partial r_l}$$

Using Symmetry: Anisotropy

Local **atomic environment** affects spin orientation:



[Kittel, Introduction to Solid State]

Spin orbit interaction and crystal field effects

Anisotropies & **symmetries**: (**u** = **m**/M_s)

- Uniaxial: $E_{ani}(u_z) = E_{ani}(-u_z)$

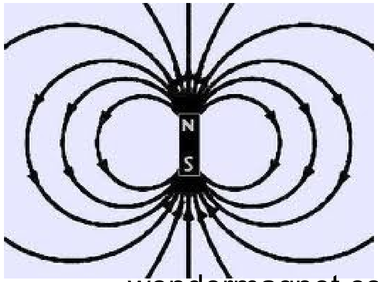
$$E_{ani} = -K_u^{(1)} u_z^2 - K_u^{(2)} u_z^4 + \ldots$$

- Cubic: $E_{ani}(u_x, u_y, u_z) = E_{ani}(-u_x, u_y, u_z)$, etc.

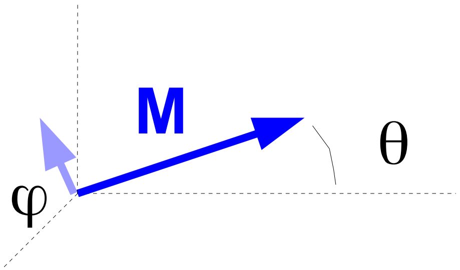
$$E_{ani} = K_4 (u_x^2 u_y^2 + u_x^2 u_z^2 + u_y^2 u_z^2) + \ldots$$

Using Symmetry: Anisotropy

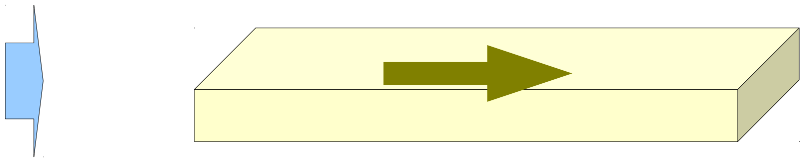
All moments interact throughout sample.
Sample **shape** creates an anisotropy:



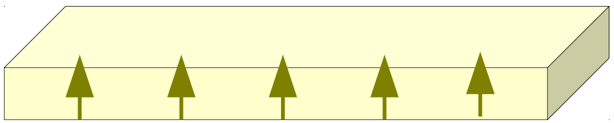
wondermagnet.com



$$E_{ani} = \frac{M^2 V}{2\mu_o}\left(N_x \sin^2\theta \cos^2\varphi + N_y \sin^2\theta \sin^2\varphi + N_z \cos^2\theta\right)$$



Easy direction

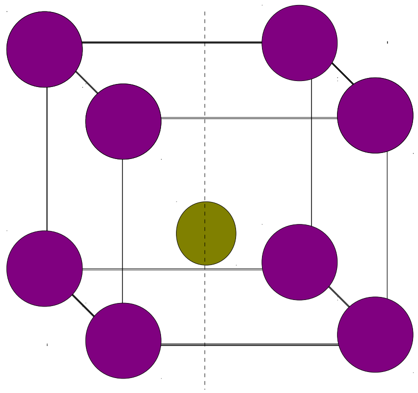


Hard direction

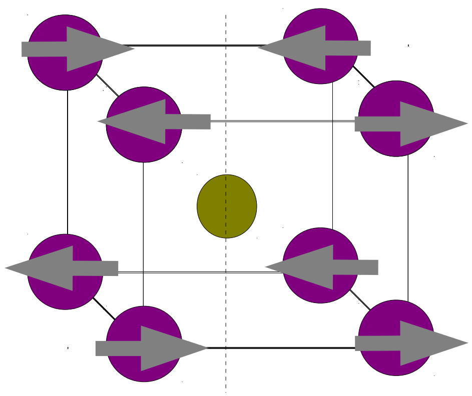
Dzyaloshinski-Moriya Interaction

Asymmetric interaction possible when inversion symmetry absent:

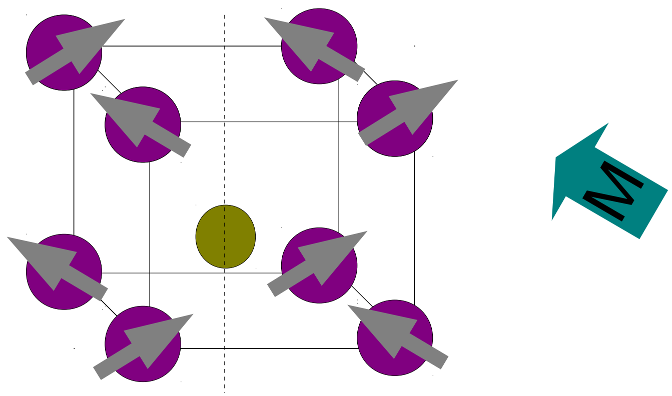
$$H = \sum_{i,j} \left[J\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \boldsymbol{D} \cdot \left(\boldsymbol{S}_i \times \boldsymbol{S}_j \right) \right]$$



Describes weak ferromagnetism of canted antiferromagnets:



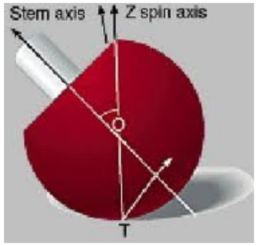
$D = 0$

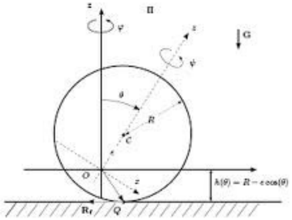


$D \neq 0$

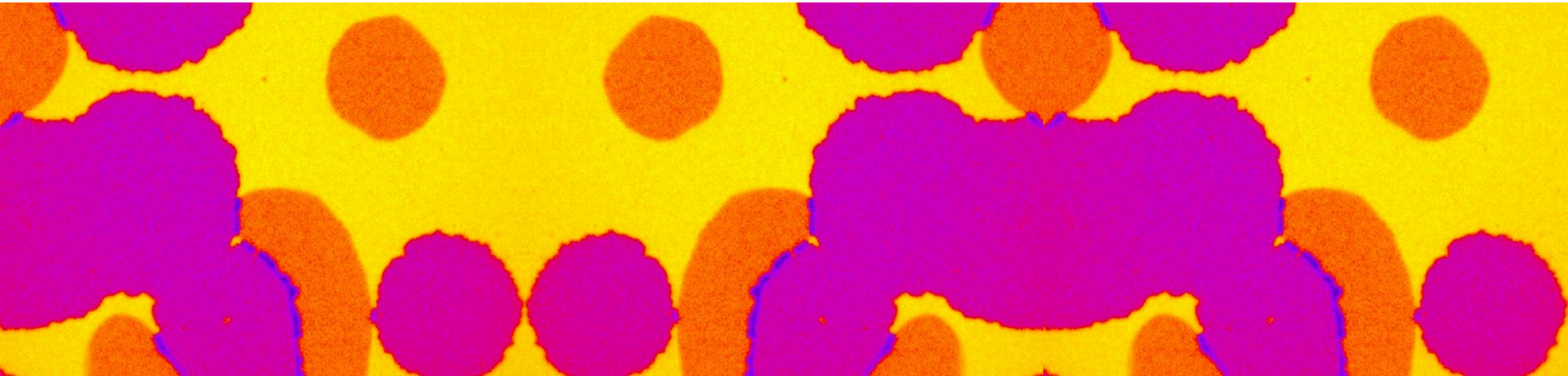
It's Only Angular Momentum

Bohr and Pauli Study Angular Momentum



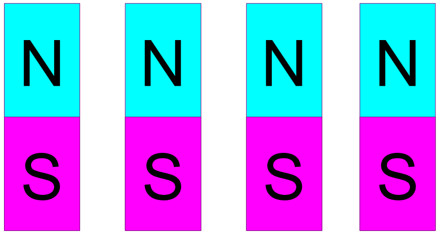


Some generic tools

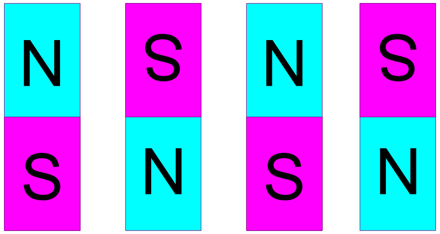


Magnetostatics and Domains

Dipolar fields compete with other local fields:



High magnetostatic energy

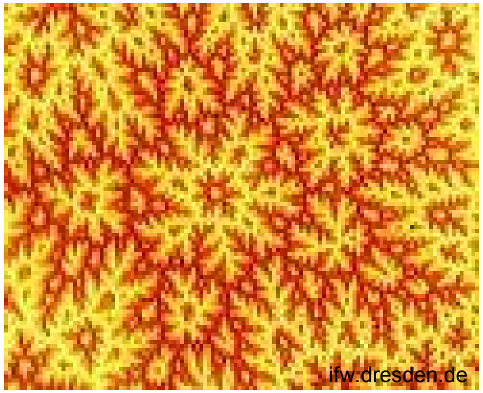


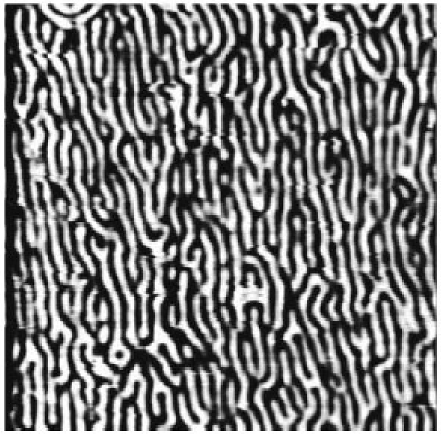
Low magnetostatic energy

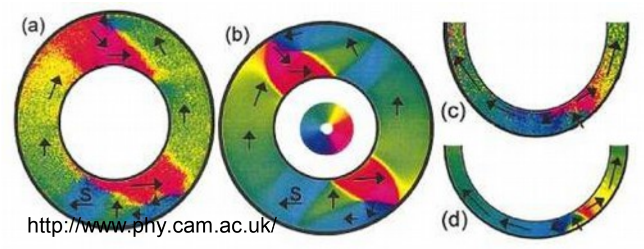
Competition between exchange, anisotropy and magnetostatic energies

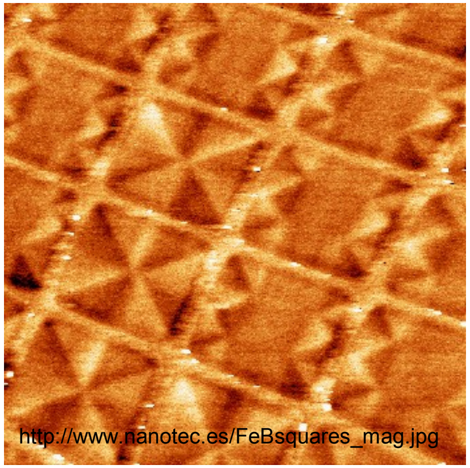
Domain Patterns

Pattern detail depends on magnetization, exchange, anisotropy...





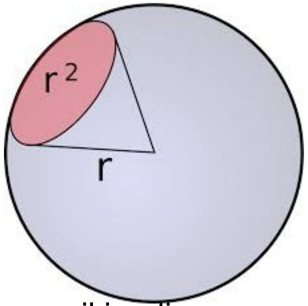




… and geometry!

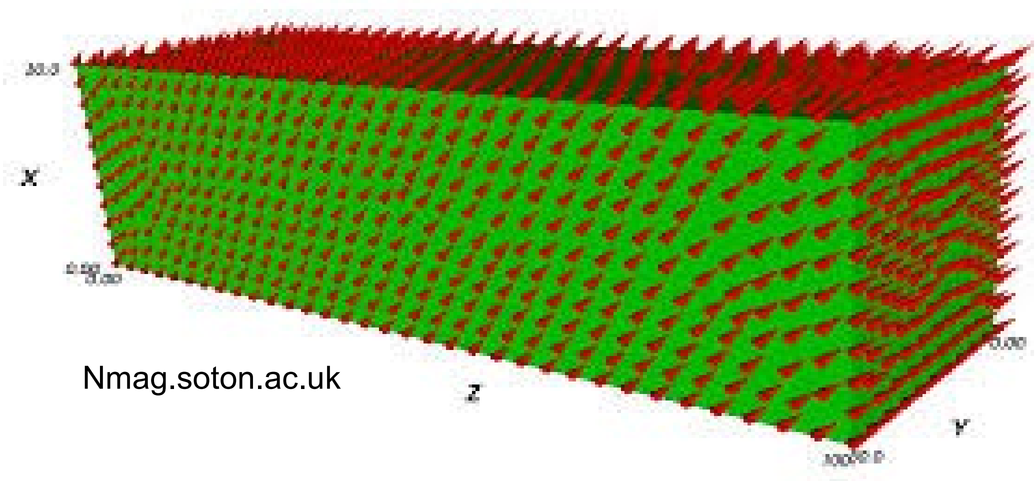
The Problem of Dipolar Interactions

Magnetic fields decrease slowly with distance-- sample shape matters



wikipedia.org

Magnetisation is generally <u>not</u> uniform:



Nmag.soton.ac.uk

Micromagnetics

Minimising the Energy

Goal: find stable (and metastable) configurations that define minima of the total energy *E*

$$E(\vec{u}) = \int \left[A(\nabla \vec{u})^2 - K_n(\hat{n}\cdot\vec{u})^2 - \mu_o M_s\left(\vec{u}\cdot\vec{H}_a + \vec{u}\cdot\vec{h}_d\right)\right] dV$$

exchange — *anisotropy* — *applied field* — *magnetostatic*

$$\vec{u} = \frac{\vec{M}}{M_s}$$

reduced M

Minimisation = vanishing **torques**:

$$\delta E = 0 \quad \Rightarrow \quad \vec{u} \times \left(-\frac{\partial E}{\partial \vec{u}} \right) = 0$$

Finding Zero Torque Solutions

Strategy: Numerically integrate torque equations

$$\frac{\partial \vec{u}}{\partial t} \propto \vec{u} \times \left(-\frac{\partial E}{\partial \vec{u}} \right) + \Gamma_{damping} \rightarrow 0$$

Gilbert damping:

damping parameter

$$\left(\frac{1+\alpha^2}{|\gamma|} \right) \frac{\partial \vec{M}}{\partial t} = -\vec{M} \times \vec{H}_{eff} - \frac{\alpha}{M_s} \vec{M} \times \vec{M} \times \vec{H}_{eff}$$

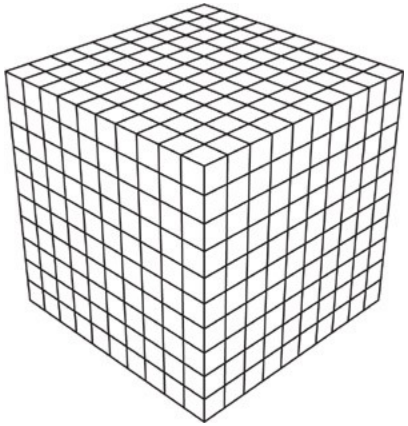
$$\vec{H}_{eff} = -\frac{\partial E(\vec{M})}{\partial \vec{M}}$$

Finite Differences

Convert differential equations to difference equations:

$$u_\beta(x+\Delta x)=u_\beta(x)+\Delta x\frac{\partial}{\partial x}u_\beta(x)+\frac{1}{2}(\Delta)^2\frac{\partial^2}{\partial x^2}u_\beta(x)$$

$$u_\beta(x-\Delta x)=u_\beta(x)-\Delta x\frac{\partial}{\partial x}u_\beta(x)+\frac{1}{2}(\Delta)^2\frac{\partial^2}{\partial x^2}u_\beta(x)$$



Divide **magnetisation** into blocks, replace differentials, construct torque equations for **each** block

Magnetostatic Terms

Maxwell equations define a magnetostatic potential

$$\vec{B} = \mu_o(\vec{H} + \vec{M})$$

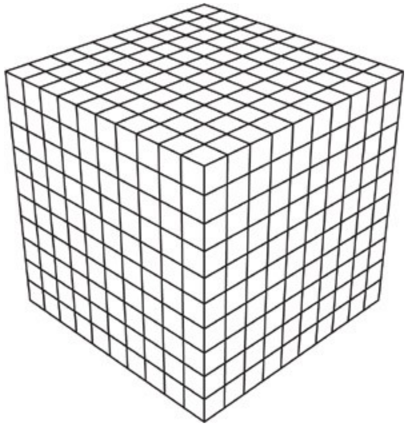
$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} \approx 0$$

$$\vec{H} = -\nabla \Phi$$

$$\nabla^2 \Phi = -\nabla \vec{M}$$

Blocks are ***sources*** *of H field*

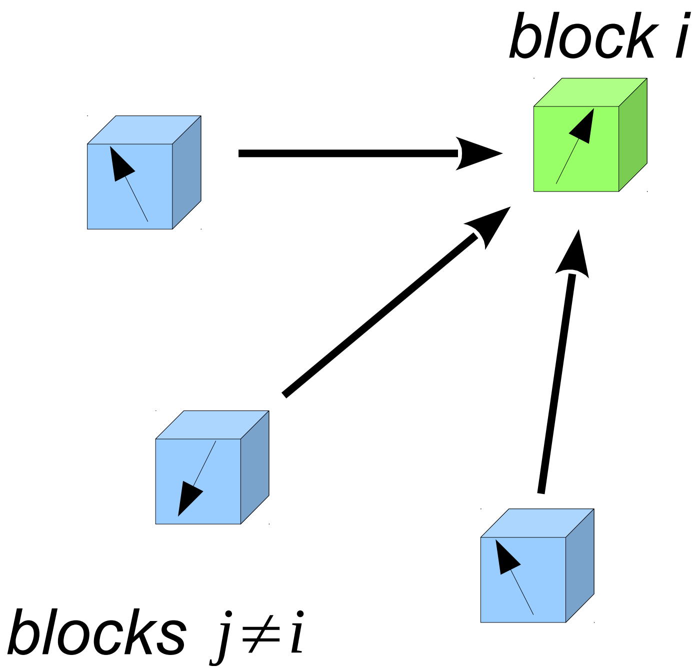


The magnetostatic terms link **all blocks** throughout the sample

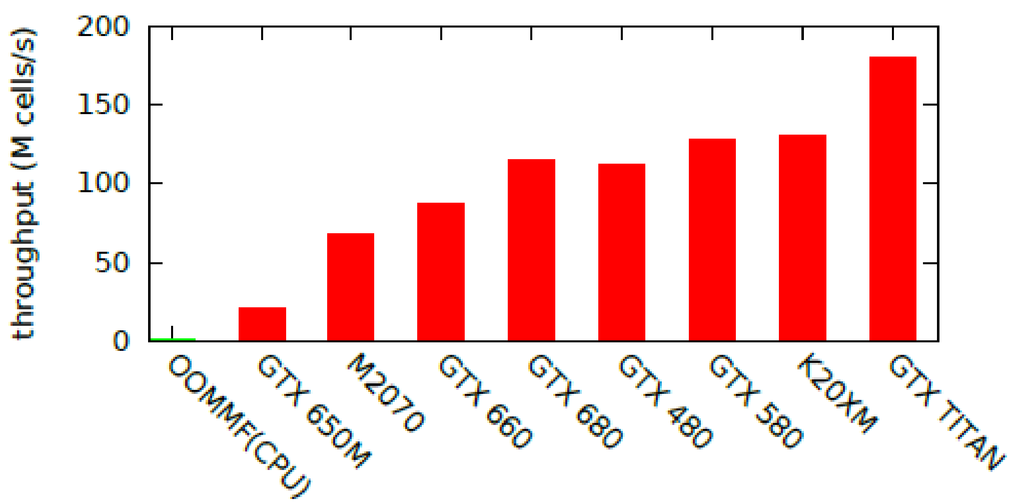
Micromagnetics and GPU's

The magnetostatic calculation involves convolution over all blocks:

$$\vec{H}(i) = \hat{K}(i,j) * \vec{M}(j)$$



Accelerate calculations using
Graphical Processing Units



[Vansteenkiste, et al. arXiv:1406.7635]

Example: Mumax3

// Standard Problem #4

```
SetGridsize(256, 64, 1)
SetCellsize(500e-9/256, 125e-9/64, 3e-9)
```
define grid and sizes (m)

```
Msat  = 800e3
Aex   = 13e-12
alpha = 0.02
```
parameters (SI)

Information & Download:
http://mumax.github.io/index.html

```
m = uniform(1, .1, 0)
relax()
save(m)    // relaxed state
```
initialse M
find zero torque configuration
save configuration

```
autosave(m, 200e-12)
tableautosave(10e-12)
```
save configurations every 0.2 ns
create table of m(t)

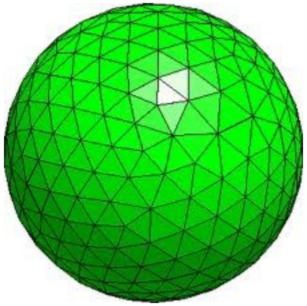
```
B_ext = vector(-24.6E-3, 4.3E-3, 0)
run(1e-9)
```
apply magnetic field
time evolution

Run Standard Problem 4

Approaches (with example codes)

Finite difference: mumax3, OOMMF

Finite element: useful for complex geometries



http://nmag.soton.ac.uk

Nmag
http://nmag.soton.ac.uk/nmag/

MAGPAR
http://magnet.atp.tuwien.ac.at/

Atomistic: model atomic lattice scale variations

VAMPIRE

http://www-users.york.ac.uk/~rfle500/research/vampire/

… and many more !

Limitations!

Lengthscales are limited

Shapes are approximate

Timescales are limited

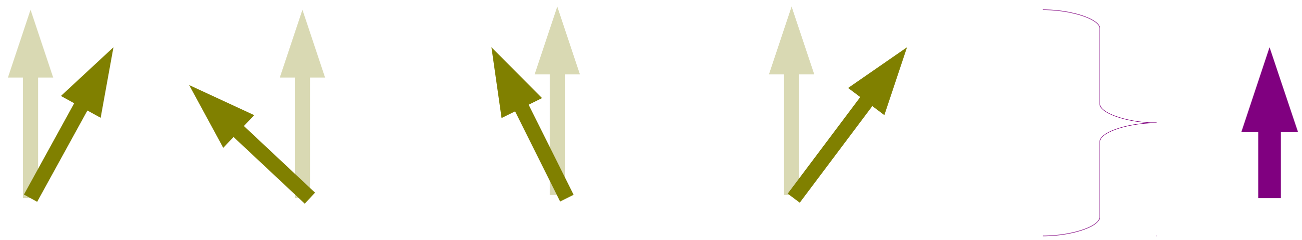
Classical limits: dynamics & thermodynamics

Questions?

Mean field approximation

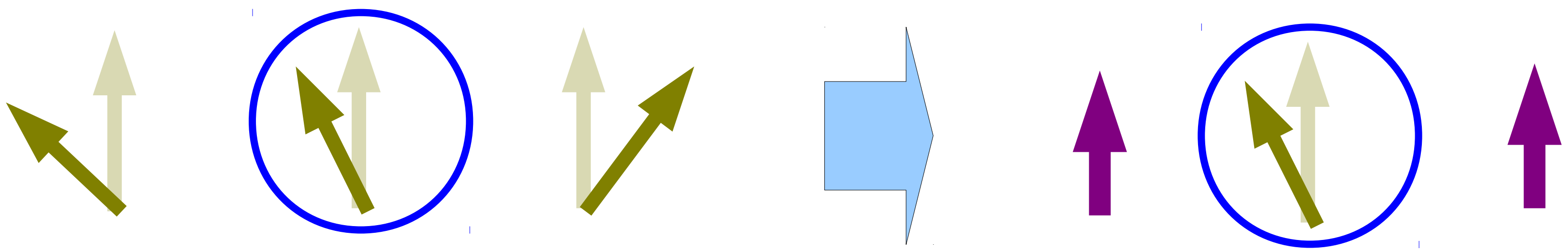
Thermal Fluctuations

Reduction in magnetisation:



$M(T) \sim \langle \boldsymbol{S} \rangle$

Replace local site field with **averaged effective field**:



Dynamic correlations are replaced by a **static field**:

$$H = -2\sum_{i,j} J_{ex}\boldsymbol{S}_i \cdot \boldsymbol{S}_j \approx -2\sum_{i,j} \boldsymbol{S}_i \cdot B_{ex} \qquad B_{ex} = \frac{2ZJ_{ex}}{Ng\mu_B}\langle \boldsymbol{S} \rangle$$

Heisenberg Model and Mean Field

Heisenberg exchange energy:

$$H = -\sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Thermal averaged magnetisation (N moments):

$$\vec{M} = N g \mu_B \langle \vec{S} \rangle$$

Fluctuations:

$$\vec{s}_i = \vec{S}_i - \langle \vec{S} \rangle$$

$$\Rightarrow \quad H = -\sum_{i,j} J_{ij} \left(\vec{s}_i + \langle \vec{S} \rangle \right) \cdot \left(\vec{s}_j + \langle \vec{S} \rangle \right)$$

Heisenberg Model and Mean Field

Z near neighbours:

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j - 2ZJ \sum_i \vec{S}_i \cdot \langle \vec{S} \rangle + ZN |\langle \vec{S} \rangle|^2$$

Second term is the **mean field**:

$$\vec{B}_{ex} = -2ZJ \langle \vec{S} \rangle$$

Mean field approximation: neglect first term **(correlations)**

$$H_{fluctuations} = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

Reminder: Paramagnetism

Probabilities to be antiparallel (down) and parallel (up):

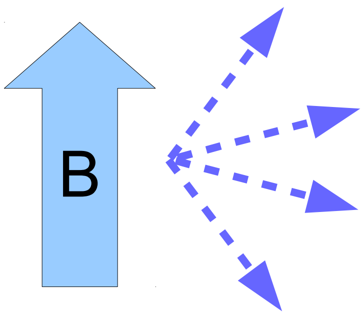
$$\frac{n_\downarrow}{N} \propto \exp\left(\frac{-\mu_B B}{k_B T}\right) \qquad \frac{n_\uparrow}{N} \propto \exp\left(\frac{\mu_B B}{k_B T}\right)$$

Magnetisation = difference:

$$\Rightarrow \quad \langle S \rangle = \left(\frac{N_\uparrow - N_\downarrow}{N}\right) = \tanh\left(\frac{\mu_B B}{k_B T}\right)$$

Generalised Paramagnetism

Angular momentum states
(J = 1/2, 3/2, 5/2, …):



Brillouin function for any J:

$$B_J(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\coth\left(\frac{1}{2J}x\right)$$

$$x = \frac{g J \mu_B B}{k_B T}$$

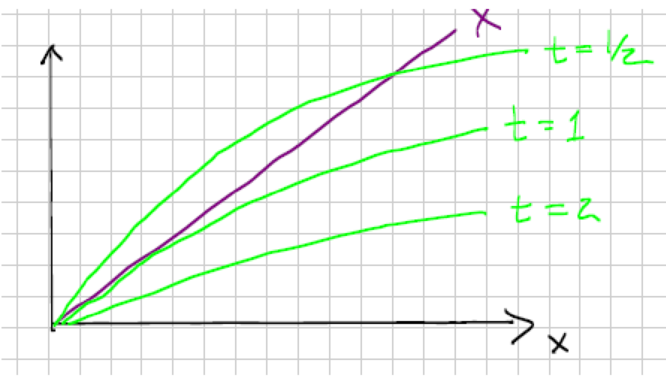
Average magnetisation from: $M \propto \langle S \rangle = B_J(x)$

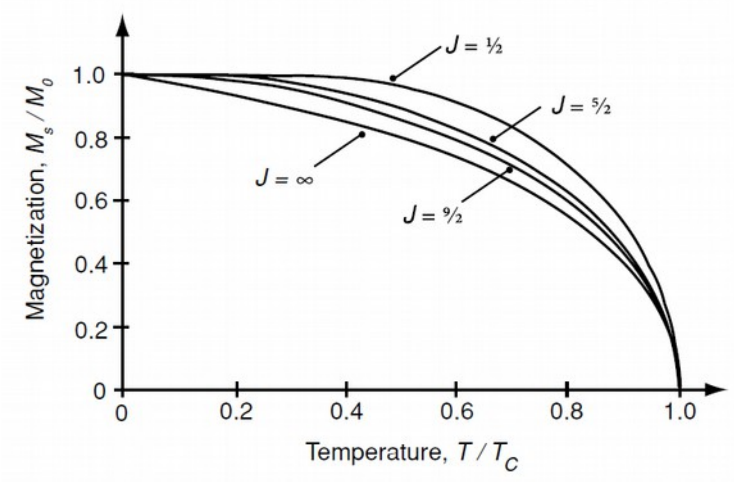
Exchange: Replace B by B_{ex}

Average M with **mean field** B_{ex}:

$$\langle \vec{S} \rangle = B_J \left(\frac{g \mu_B Z J_{ex} \langle \vec{S} \rangle}{k_B T} \right)$$

Plot left and right hand sides to see graphical solution:

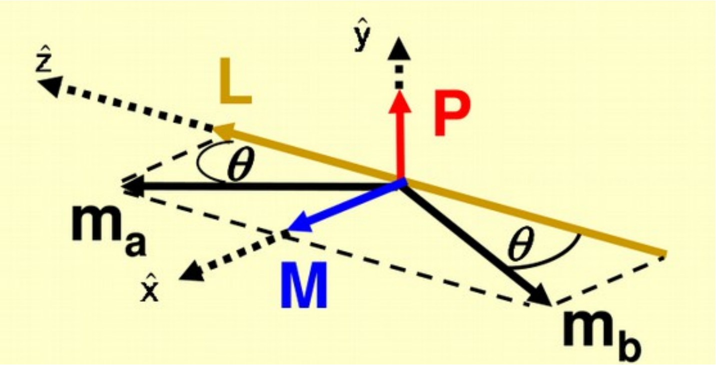




Example: Multiferroics

Coupled order parameters: **M & P**

(M = sum of canted antiferromagnetic sublattices)

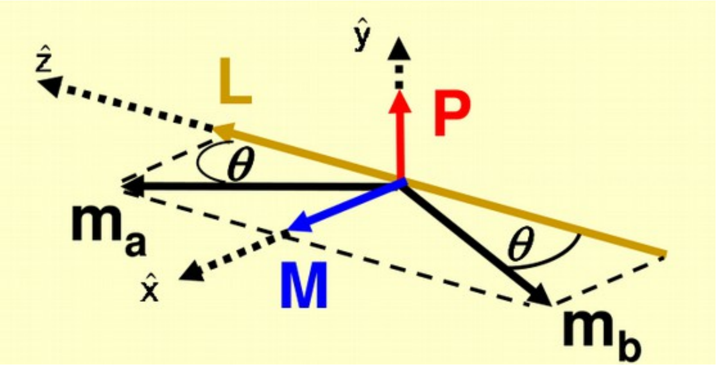


Challenges:

- correlations between spin and charge distributions
- how to describe dynamics?
- how to describe effects of thermal fluctuations?

Example: Multiferroics

Coupled order parameters: **M & P**



Approach:

(Vincinsius Gunawan PhD 2012)

Mean field approximation for **free energy**:

$$F = F_{FE}(P) - \vec{P}\cdot\vec{E} - \lambda\,\vec{m}_a\cdot\vec{m}_b - K\left(m_{az}^2 + m_{bz}^2\right) - \vec{m}\cdot\vec{H} + F_{ME}$$

polarization part — magnetization part — *magneto-electric coupling*

Example: Multiferroics

Brillouin function for components of **m**:

$$m_{s,\alpha} = g \mu_B J B_J (\vec{m}_s \cdot \vec{B}_s)$$

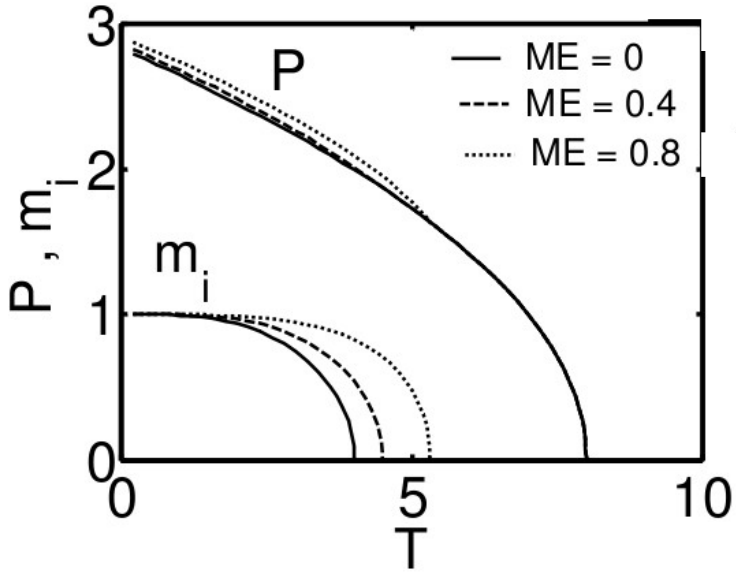
Landau-Ginzburg mean field theory for P:

$$F_{FE}(P) = \alpha_o (T - T_c) P^2 + \beta P^4$$

Minimise free energy for P and θ:

$$\frac{d}{d\theta} F = 0$$

$$\frac{d}{dP} F = 0$$

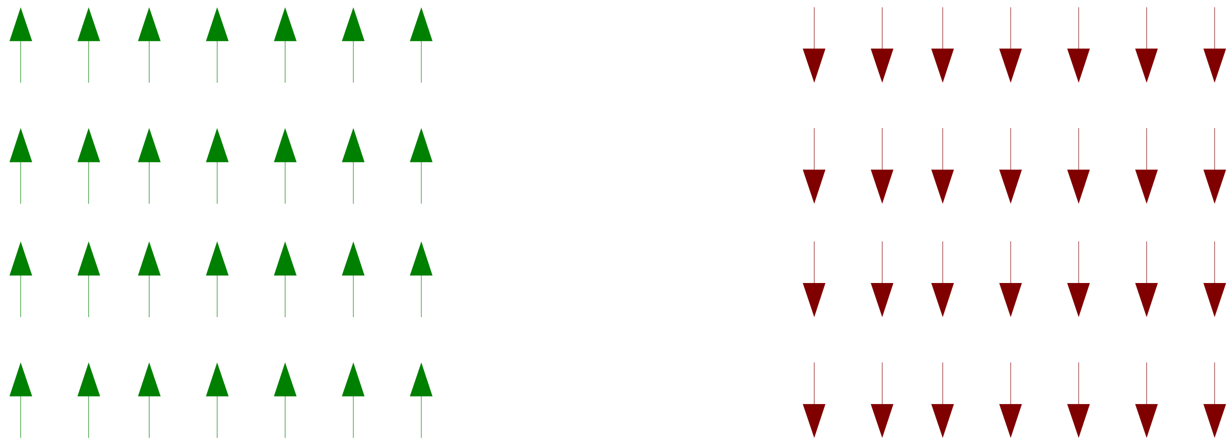


[Gunawan et al., JPCM (2011)]

Monte Carlo methods

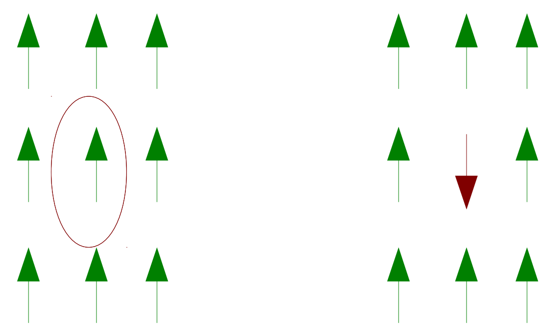
Ising model and Monte Carlo

Suppose two possible states: 'up' and 'down'



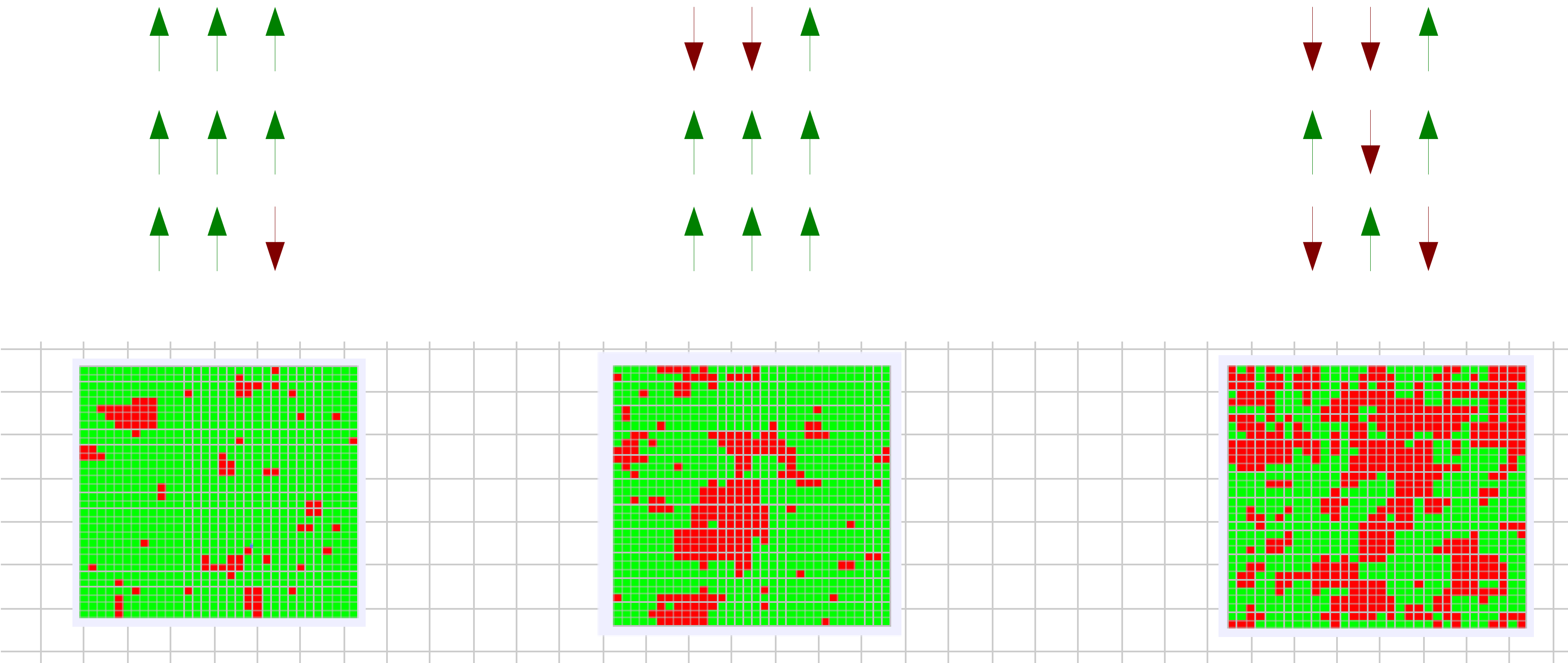
Boltzman probability for individual flips:

$$P(-S_i) \sim \exp\left(\frac{-J\left(\sum_i S_i\right)}{k_B T}\right)$$



Sampling Random Fluctuations

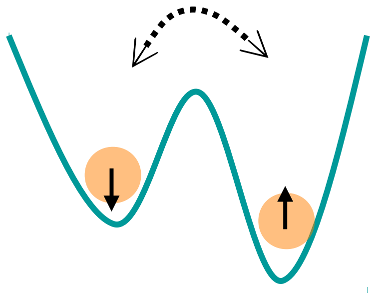
Thermal fluctuations and 2 dimensional Ising model:



Low T — Near T_c — Above T_c

Constructing Averages

Fluctuations drive the system towards thermal **equilibrium**.



$$P_{\uparrow\downarrow} \sim \exp\left(\frac{-\Delta E(\uparrow \Rightarrow \downarrow)}{k_B T}\right)$$

$$P_{\downarrow\uparrow} \sim \exp\left(\frac{-\Delta E(\downarrow \Rightarrow \uparrow)}{k_B T}\right)$$

Sample a **distribution** for averages:

$$\langle A \rangle = \sum_\sigma A(\sigma)\rho(\sigma) \qquad \rho(\sigma) = \frac{1}{Z}\exp\left(-\frac{E(\sigma)}{k_B T}\right)$$

***Key idea**: σ is a configuration from the **ensemble** of **equilibrium** spin configurations*

The Metropolis Algorithm

Sample from {σ}: Start with some ξ, generate a σ' with a single spin flip.

Rules: Calculate $\Delta E = E(\xi) - E(\sigma')$

1) If $\Delta E < 0$, accept σ' as an equilibrium fluctuation
2) If $\Delta E > 0$, accept σ' if $P(\Delta E) < 1$

For **equilibrium** fluctuations, $P(\Delta E)$ must satisfy **detailed balance**:

$$P(\sigma')W(\uparrow \Rightarrow \downarrow) = P(\xi)W(\downarrow \Rightarrow \uparrow)$$

$$\frac{W(\uparrow \Rightarrow \downarrow)}{W(\downarrow \Rightarrow \uparrow)} = \frac{P(\xi)}{P(\sigma')} = P(\Delta E) = \exp\left(-\frac{E(\xi) - E(\sigma')}{k_B T}\right)$$

Run Monte Carlo

Example: Interacting magnetic particles

Challenges:

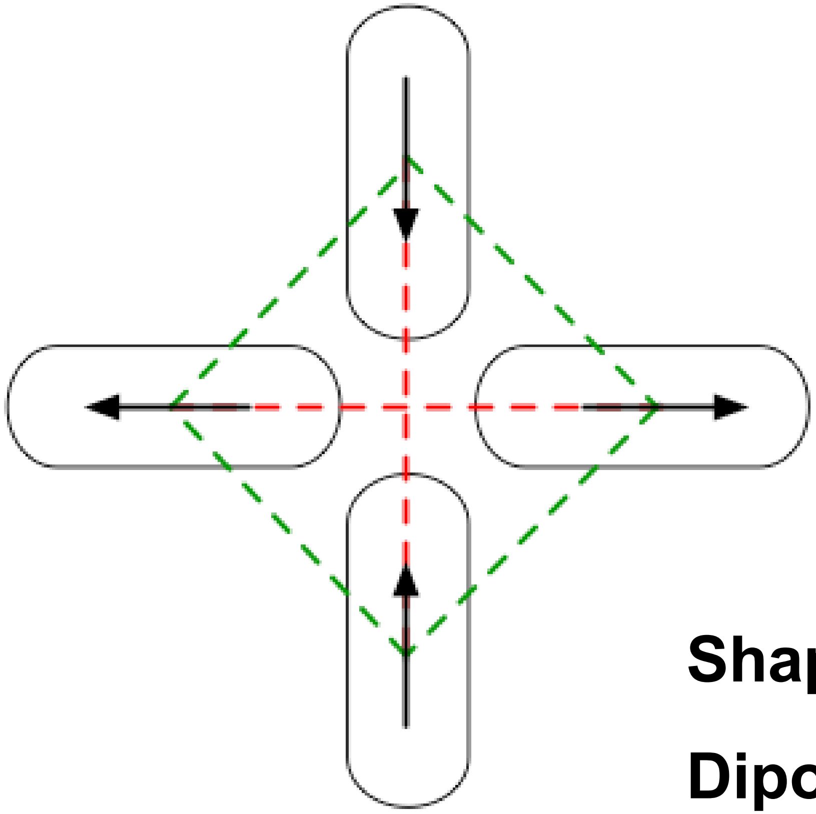
- large arrays of submicron elements
- super-paramagnetic
- long range interactions

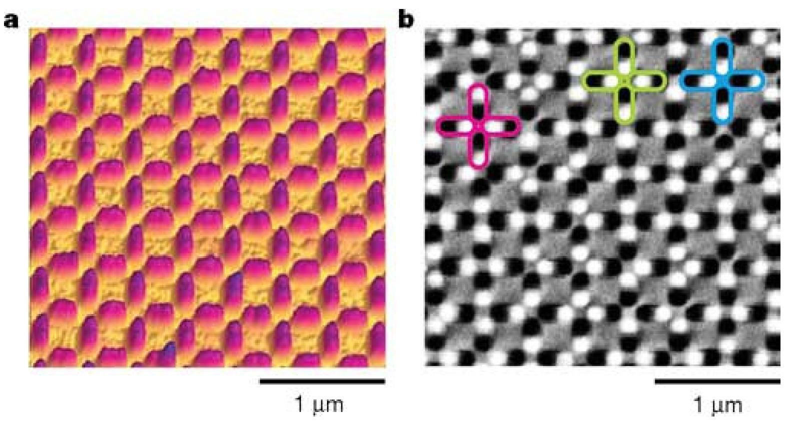
Approach:

(Zoe Budrikis, PhD 2012)

Combine Mean Field & Monte Carlo

Example: Artificial Antiferromagnet (artificial square spin ice)





Wang et al., Nature (2006)

Shape anisotropy: Ising spins

Dipolar interactions

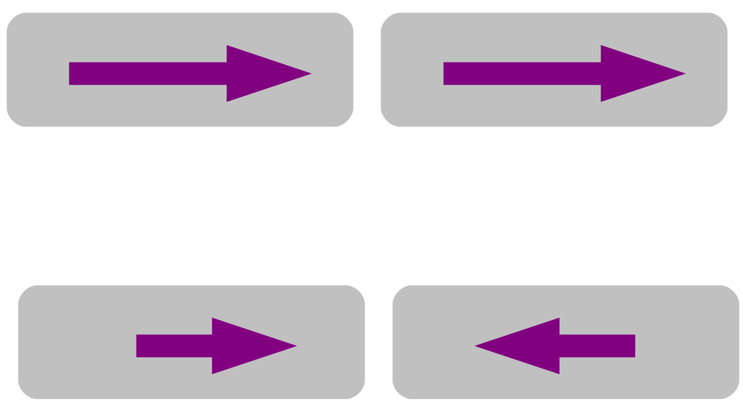
6 interactions but can only **minimise** 4

Thermal evolution of domains

Thermal fluctuations on 2 timescales:

- small volumes (reversal) $$\frac{KV}{k_B T} \sim 1$$

- thermal reduction of element M



enhancement

suppression

Configuration dependent local M

Mean field model: thermal dynamics

Mean field model for ***element*** magnetisations:

$$\langle m_j \rangle = B_{1/2}\left[\beta m_j \cdot \left(h_c + \sum_{k \neq j} J_{j,k} \langle m_k \rangle\right)\right] \qquad h_c = K \langle m_j \rangle$$

Algorithm:

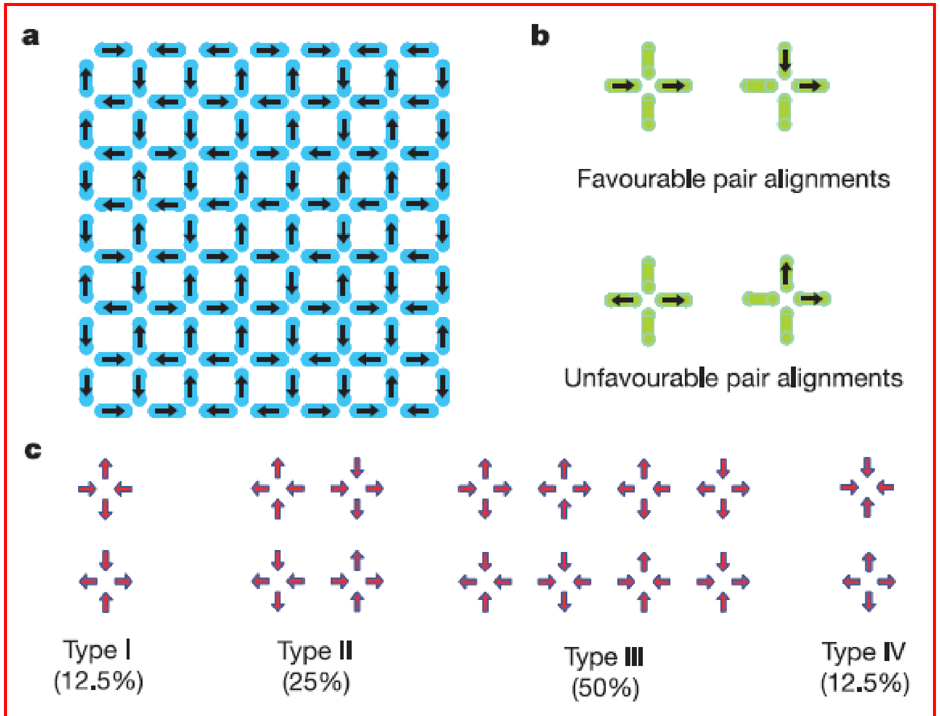
- self consistent iteration for $<m_j>$
- stochastic reversal (**Monte Carlo**)

Disorder: uniform distribution for *K* centred on K_o

$$K = K_o\left(1 + \frac{r}{2}\right) \qquad r \in [-\Delta, \Delta]$$

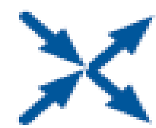
Configurations

Local spin configurations:



Nisoli et al., Nature Physics (2010)

Type I
(ground)

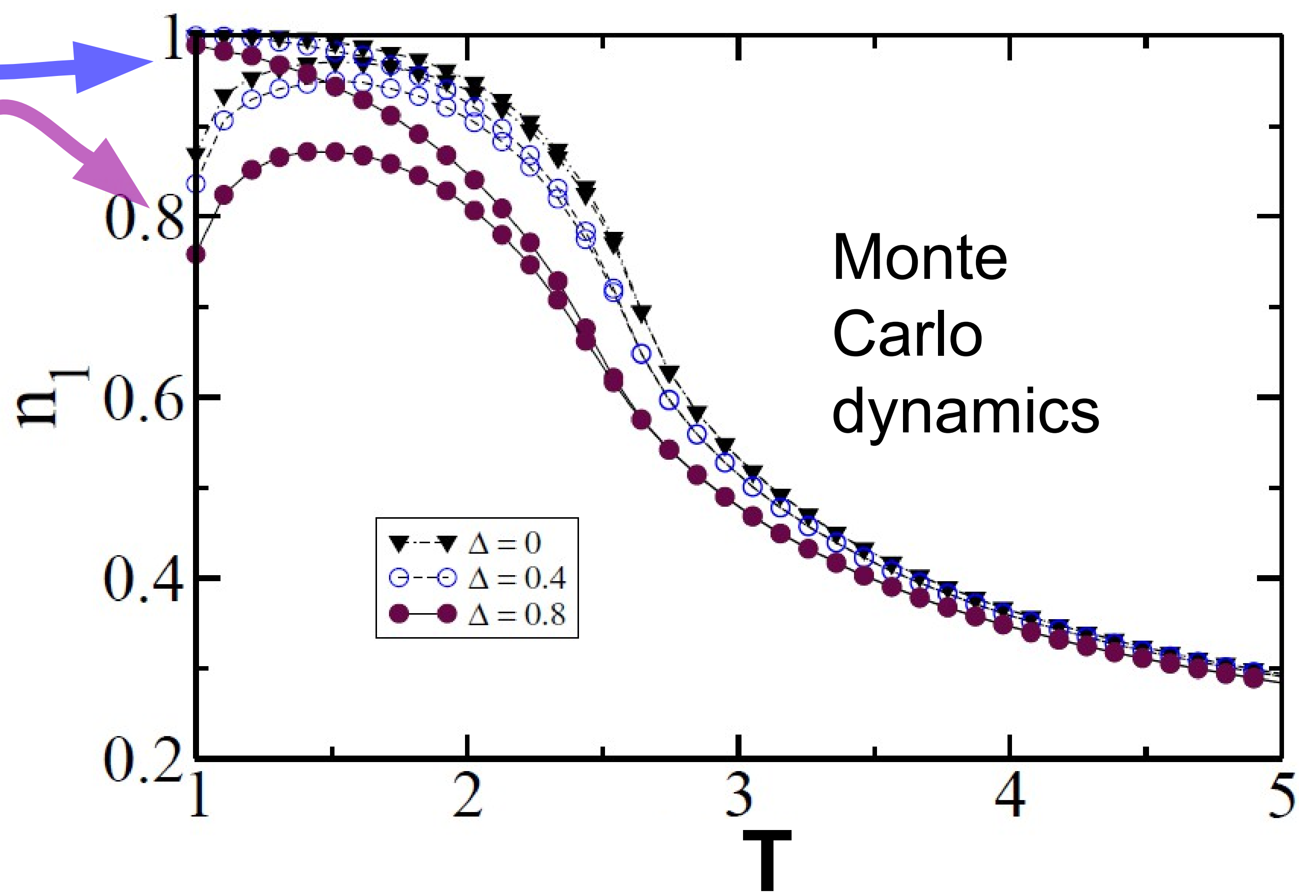


Type II
(wall)

Type III
(defect)

Approach to Ground State

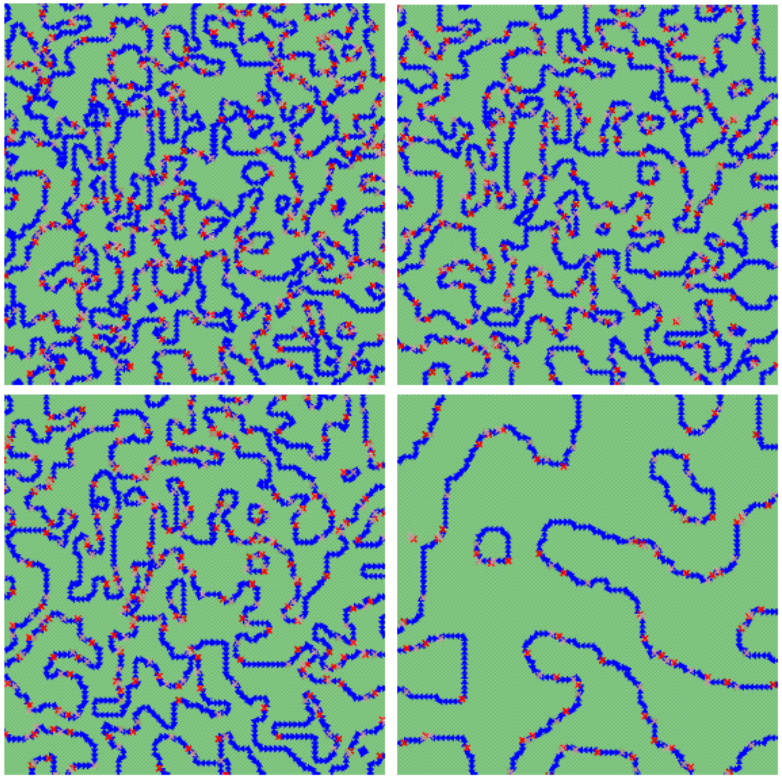
Initial T=0 Type I state (~ "FC"): thermal decay



Initial T=0 quenched random state (~ "ZFC"):

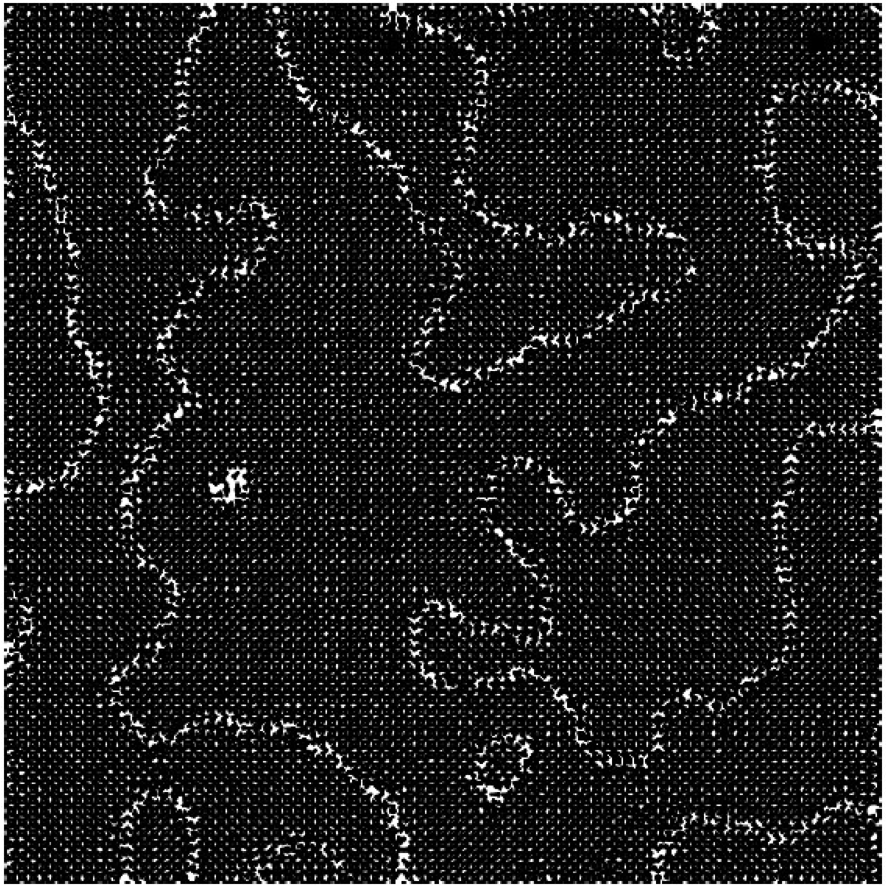
Growth of Domains and Wall Motion

Type I domains separated by Type II walls:



Type III 'charge' production during wall motion

Thermal fluctuations at walls



- M = 1
- M = 0.1

*Thermal **fluctuations** largest on domain walls*

Challenge: modelling kinetics in real time with Monte Carlo

Continuous Time Monte Carlo

Probability for **acceptance** of a single flip (out of N spins):

$$Q = \frac{1}{N} \sum_{\Delta E} n(\Delta E) P(\Delta E)$$

number of spins with ΔE

Probability that a spin **will flip** in time Δ*t*:

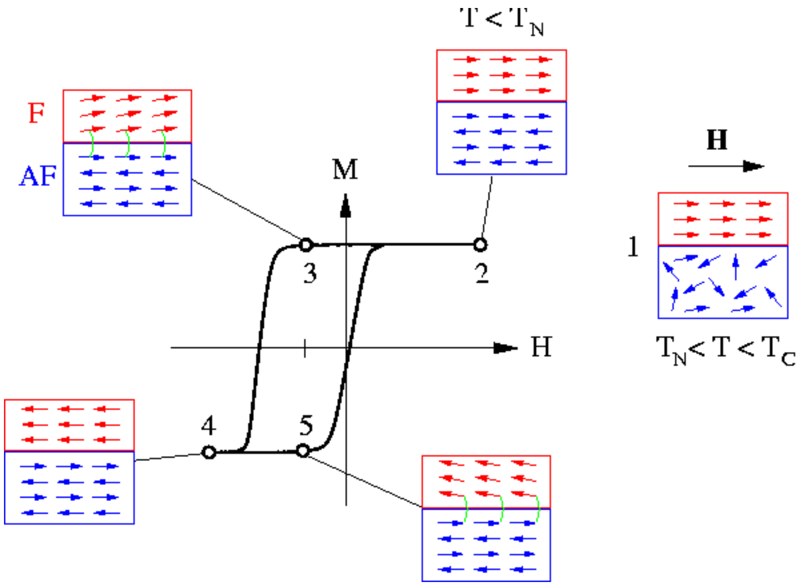
$$P_{flip}(\Delta t) = \exp\left(-\frac{\Delta t}{\tau} Q\right)$$

Rejection free algorithm:

1) track **all** possible transitions
2) accept **one** according to random *R*
3) update **time** according to $\Delta t = -\frac{\tau}{Q} \ln R$

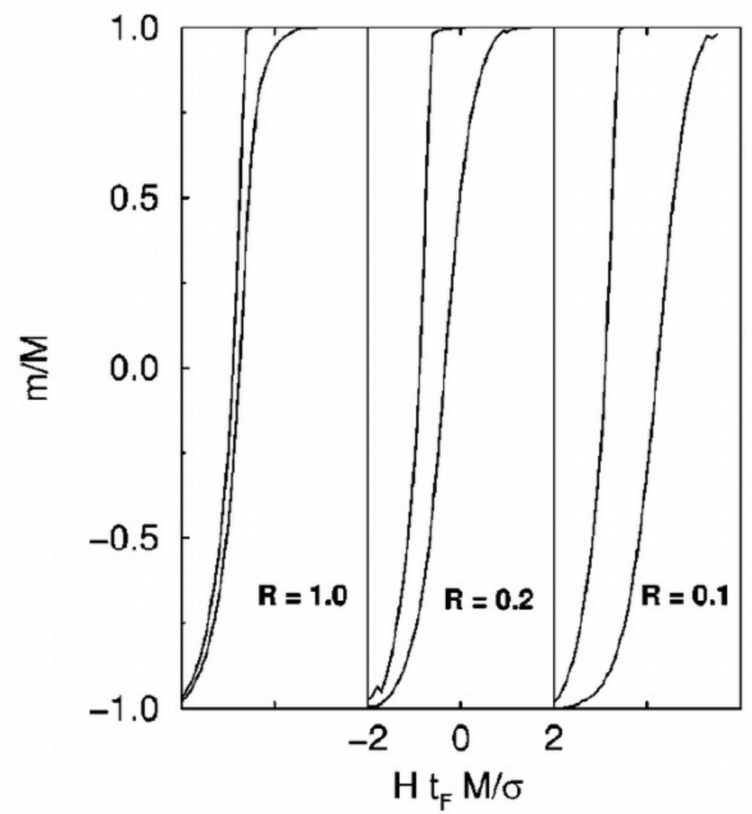
Example: Exchange Bias

Thermal setting of bias:



M Kirschner http://magnet.atp.tuwien.ac.at

Time dependent coercivity:
Field sweep rates

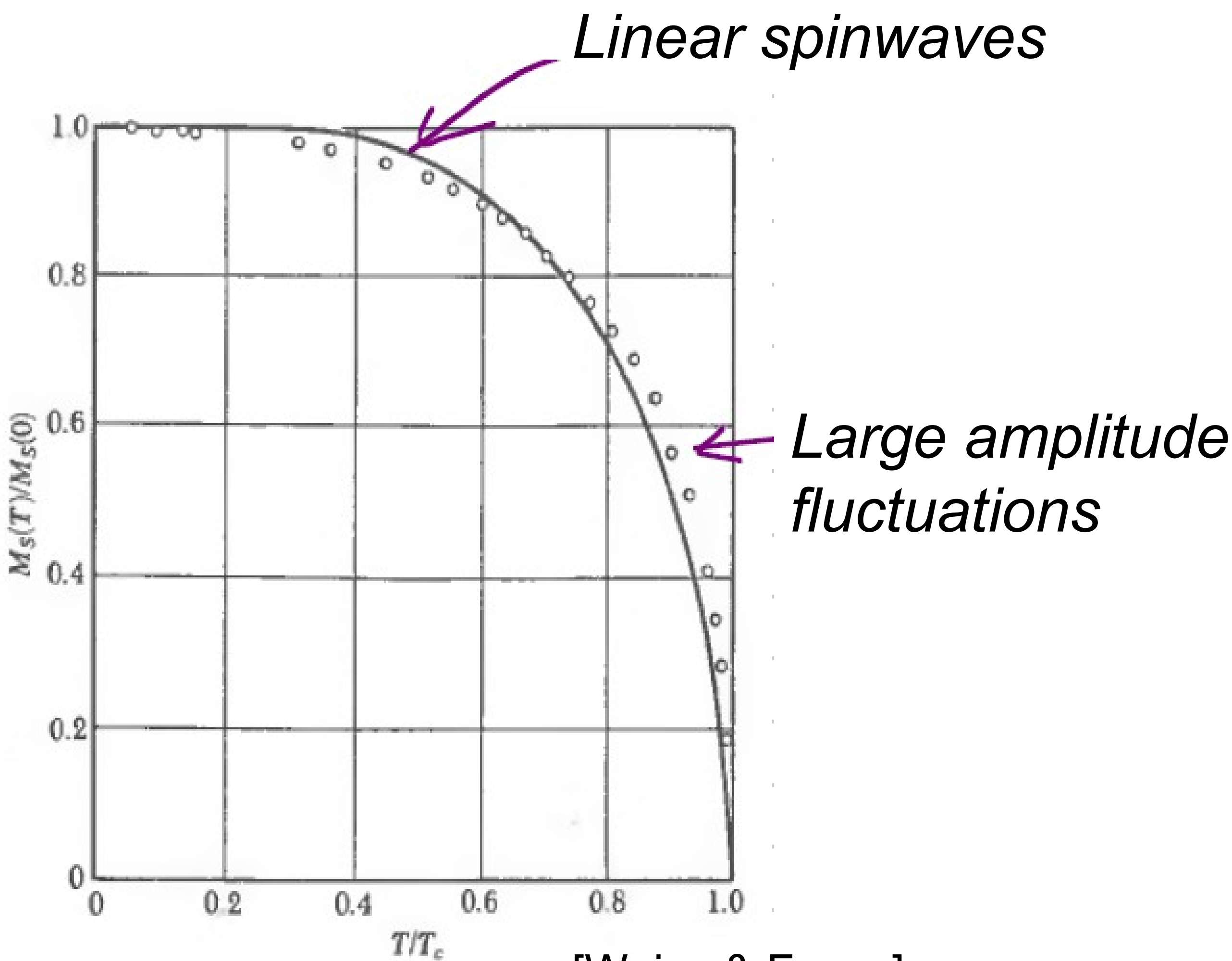


Stamps, PRB 2000

Note on phase transitions:

Scaling near *critical points*

Schematic of the Transition (2nd order)



[Weiss & Forrer]

Scaling

Mean field theory: $M(T) \sim (T - T_C)^{1/2}$

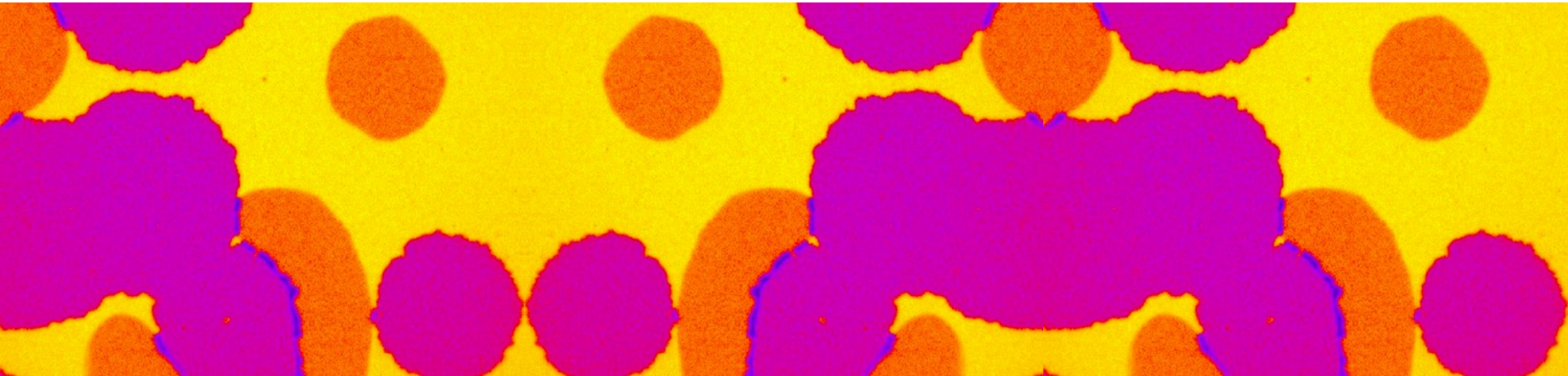
Reality includes correlations: $M(T) \sim (T - T_C)^{\beta}$ $\beta \approx 0.34$

Note on dimensionality:
- Ultra thin films ~ two dimensional systems
- fluctuations destroy long range order
- nano-thermodynamics for small elements (~ 0 D!)

Remember *this for later when we talk about domain wall creep*

Break!

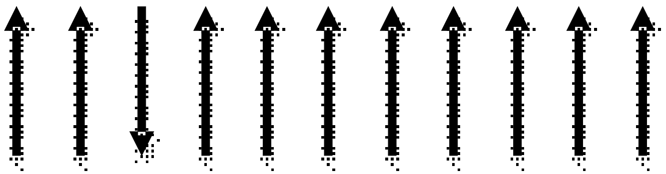
Spin Dynamics



Low Temperature Fluctuations

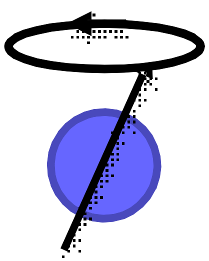
Energy to reverse one spin: *2 J*

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$



Superposition of ways to flip one spin:

$$|n = 1\rangle = |\uparrow\downarrow\uparrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\uparrow\downarrow\uparrow\rangle + \ldots$$

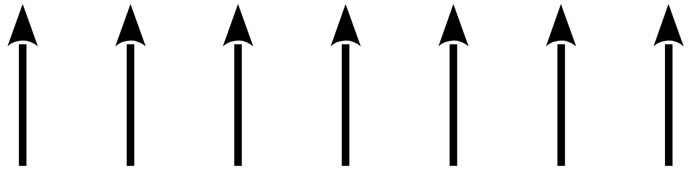


Spinwave excitation

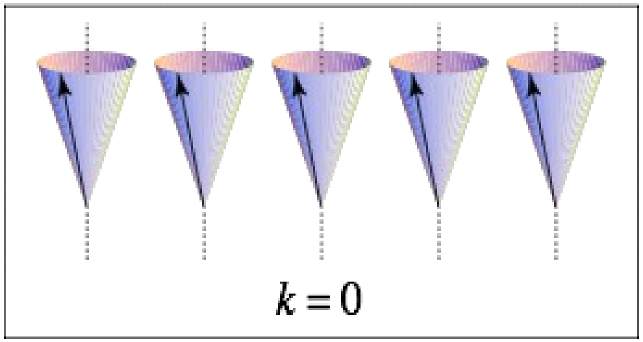
Torque equations

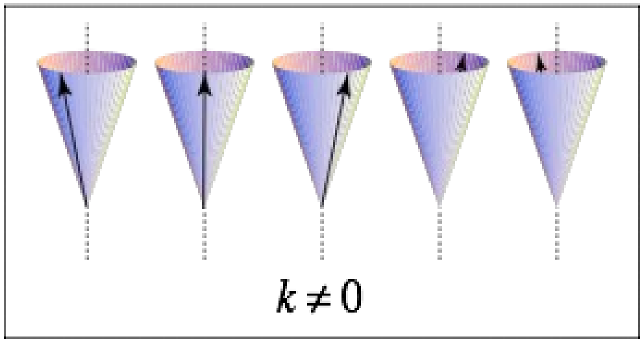
Excitations: Spin Waves

Ground state magnetic orderings:



Excitations: Precessional dynamics





slide courtesy J-V Kim

***Note**: The excitations are bosons!*

Spin Waves and Micromagnetics

Procedure:

1) **Relax** to steady state
2) Use **broadband** pulse to excite spin waves
3) Record **time** evolution (for spectral analysis)

Example: exciting precession in mumax3 script

```
defregion(1,rect(10e-9,125e-9))
save(regions)
```

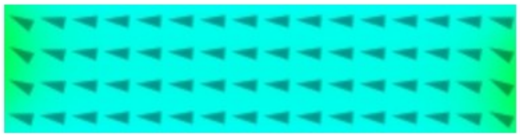
define antenna region

```
driv := 0.001          // amplitude driving field
f    := 1.0e9          // frequency units
fdel := 20.*f*2.*pi    // frequency window
time := 1000./fdel     // evolve time
toff := 3./f           // offset

B_ext = vector(-24.6E-3, 4.3E-3,driv*sin( (t-toff)*fdel )/(2*pi*(t-toff)*fdel))
run(time)
```

sinc function pulse

Results

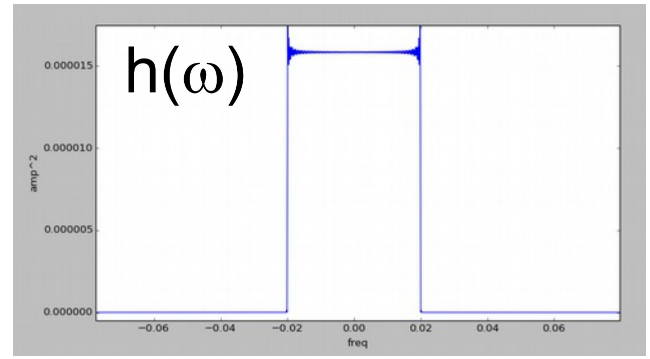
Ground state:

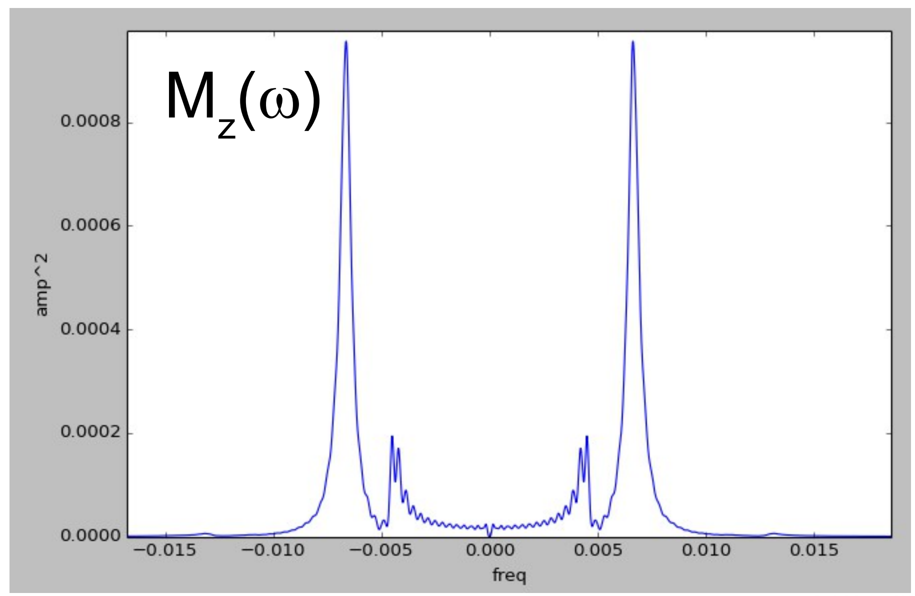


Antenna:

Note: *Spectral analysis performed separately on mumax generated data.*

Spectra:





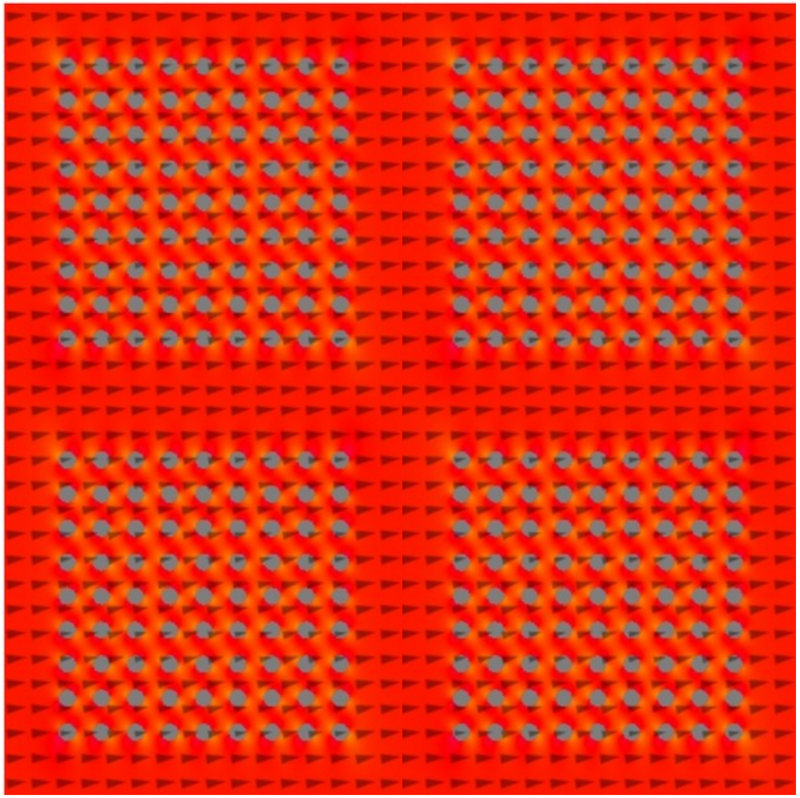
Geometry Example: Antidot Array

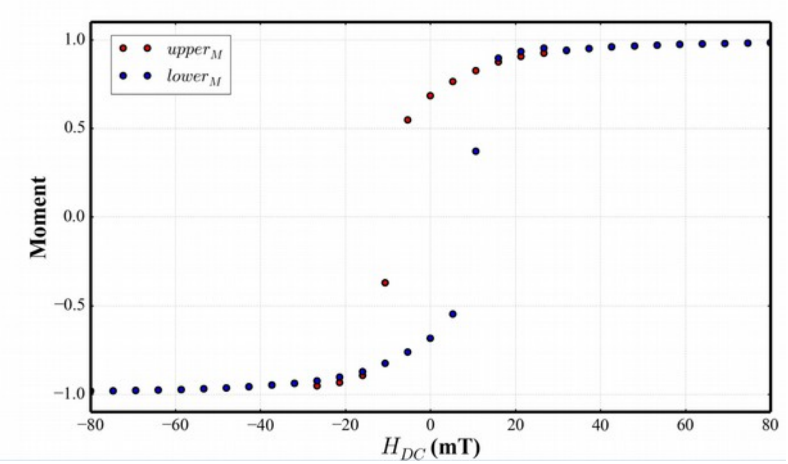
```
// array of holes set in repeating frame

SetPBC(3, 3, 0)   // for periodic bc

ndots := 9        // number of dots in each frame
r := 100e-9       // period of lattice
b := ndots * r
c := b * 1.3      // frame size

h  := 55e-9
hole := cylinder(h, h)
EdgeSmooth = 8  // use small blocks to smooth dots

setgeom( rect(c,c).sub(rect(b,b)).add( rect(b,b).sub(hole.repeat(r,r,0))) )
```

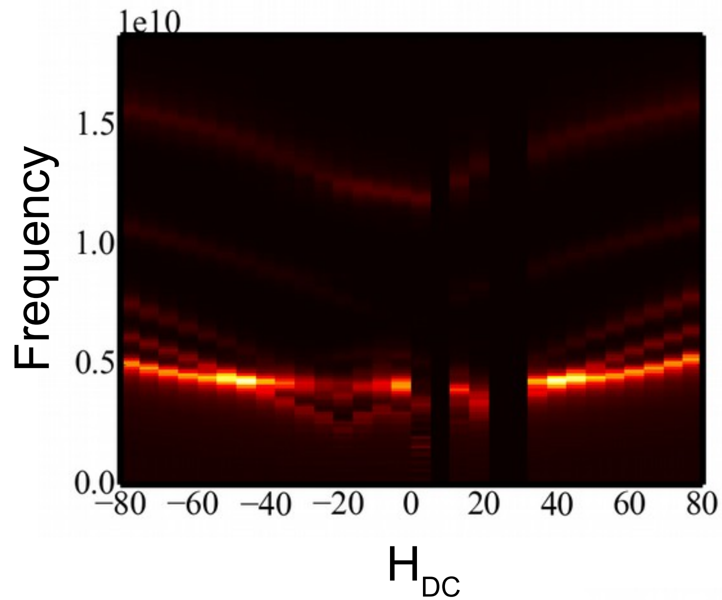
surround by copies, depth 3

combine basic elements to construct geometry

Results *(Francisco Trinidade PhD ~2015)*







IEEE MAGNETICS 50 YEARS 1964 2014

University of Glasgow

Example:

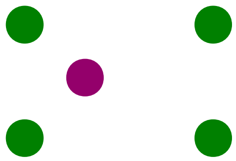
(Pablo Boyrs, PhD ~2015)

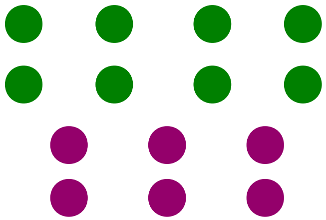
Dyzaloshinskii-Moriya Interaction (DMI) and Spin Waves

Spin Waves and DMI

Low symmetry allowed exchange terms

$$E_{DM} = D\,\vec{m}\cdot\nabla\times\vec{m}$$

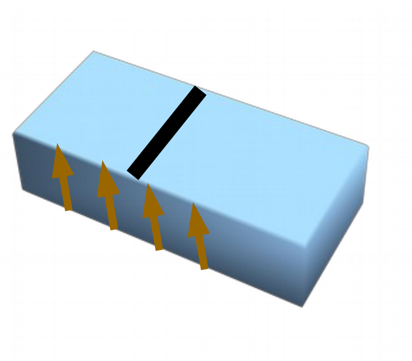




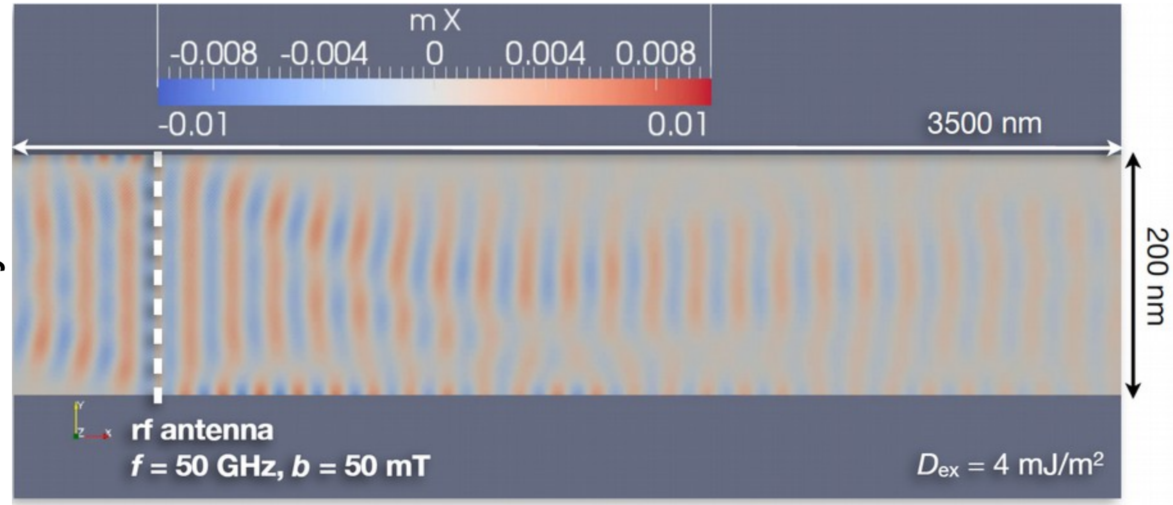
Phenomena:

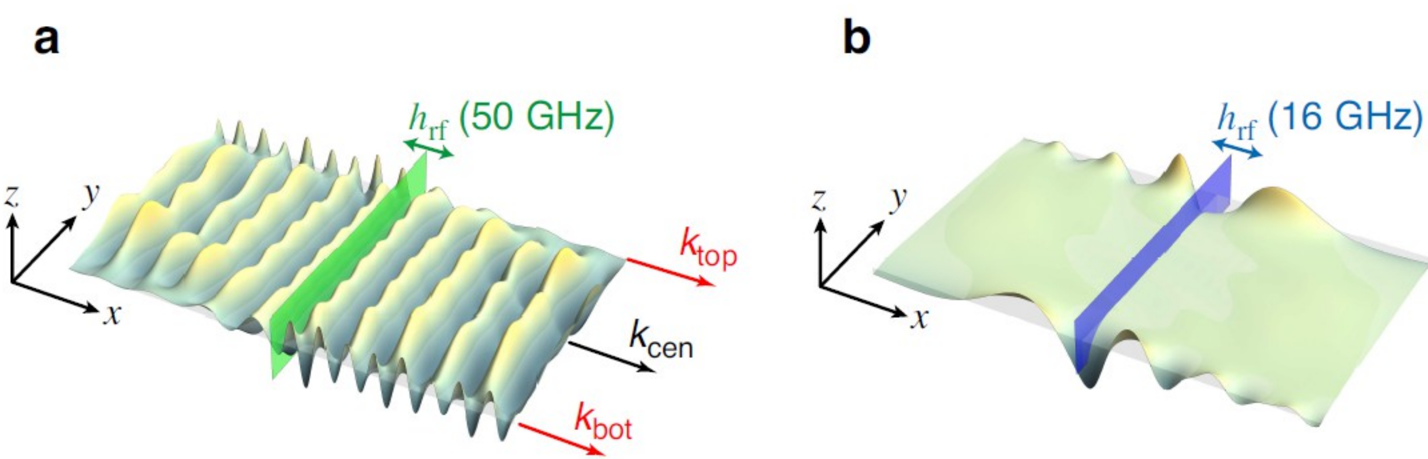
- **weak ferromagnetism** and multiferroics
- **helicoidal** and **skyrmionic** spin textures
- **exchange bias** (Dong et al. PRL 2009, Yanes et al. ArXiv 2013)
- **metal** films (Fert & Levy, PRL 1980; Bodanov et al. PRL 2001)
- **domain wall** structures (Thiaville et al. EPL 2012; K-J Lee)

Asymmetry of Spin Wave Profiles



Courtesy J-V Kim





Spin Waves & DMI: Domain Walls

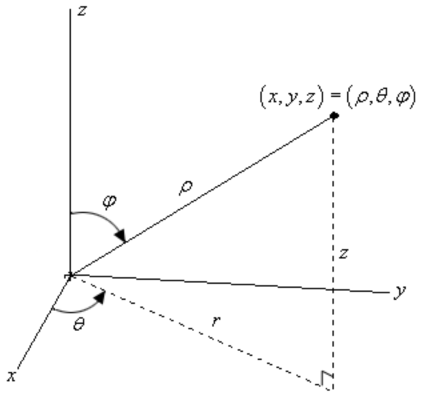
Profile determined by exchange + anisotropy

$$E = \int \left[\left[A\left(\frac{\partial \theta}{\partial x}\right)^2 + \sin^2\theta \left(\frac{\partial \varphi}{\partial x}\right)^2 \right] + D\sin^2\theta \frac{\partial \varphi}{\partial x} - k_u \cos^2\varphi \sin^2\theta + k_p \cos^2\theta \right] dx$$

Heisenberg

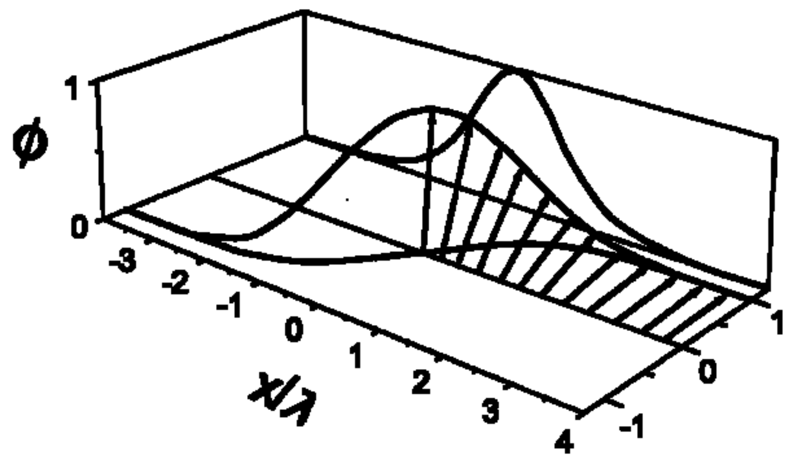
DM exchange

Anisotropies

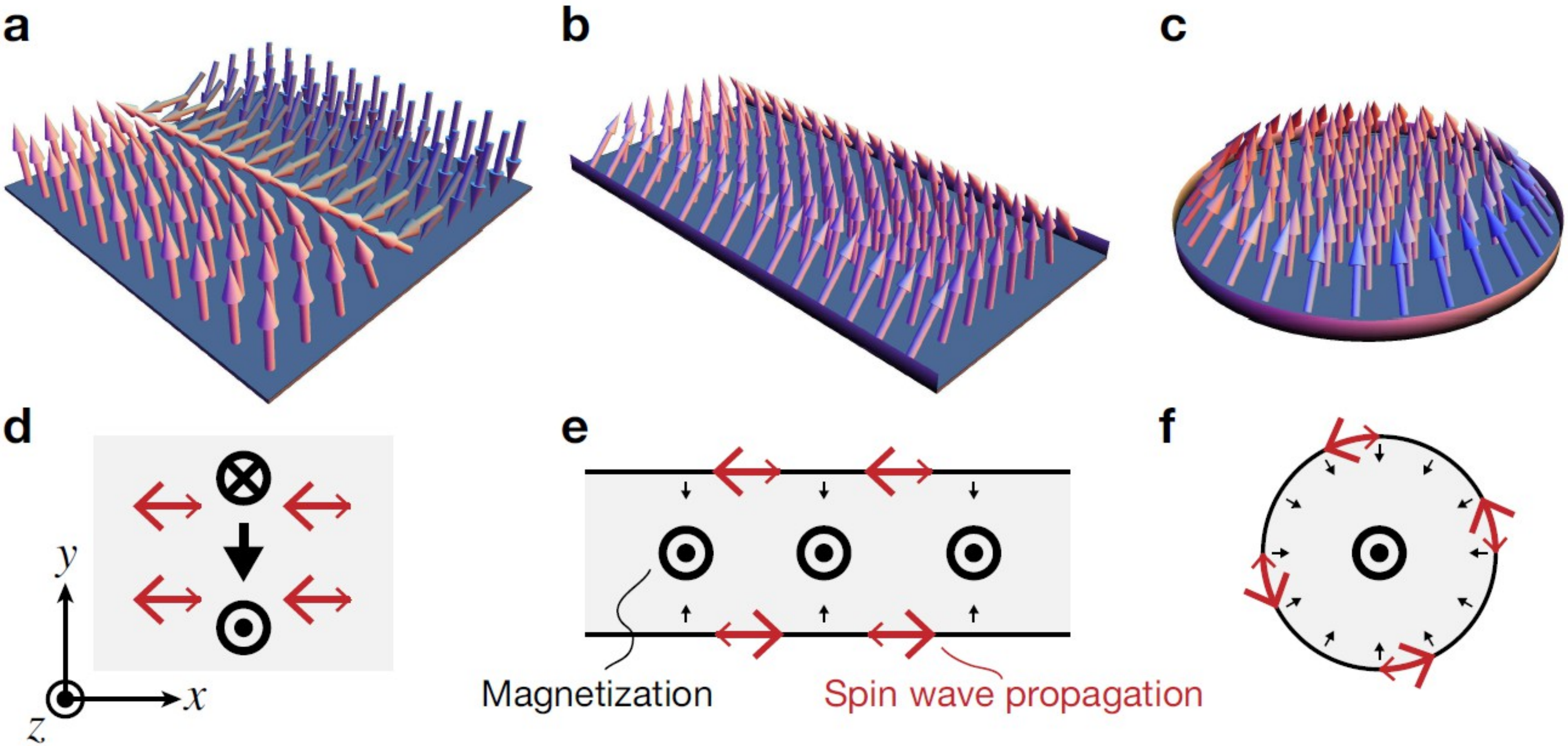


Example: Bloch-Neél wall

[Thiaville, et al ELP 2013]



DMI Edge States & Nonreciprocity

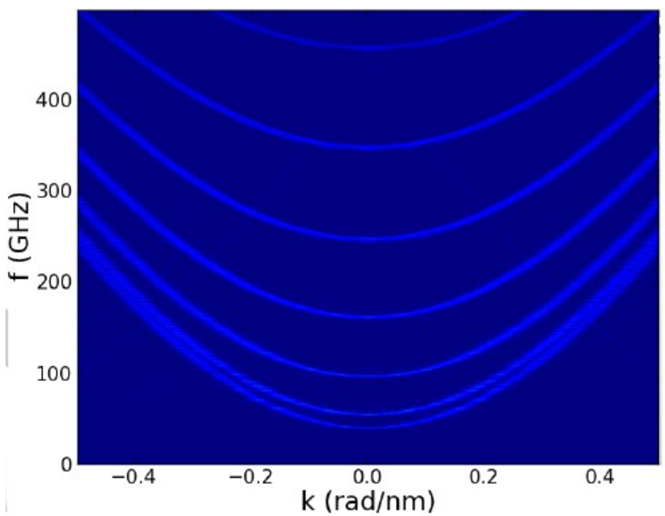


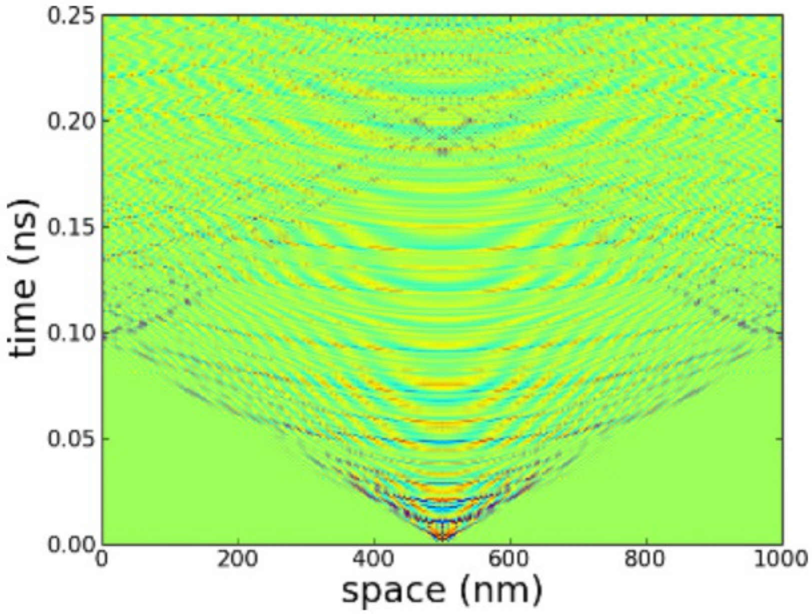
PRB 2014

Note: Spin Wave Dispersions

Spin wave $\omega(\mathbf{k})$ from micromagnetics:

$$h(x,y,t)=sinc((x-x')k_x)\,sinc((y-y')k_y)\,sinc((t-t')\omega)$$





Venkat, Fangohr, et al., IEEE Trans. Magn. 49 (2013)

Don't forget analytic models!

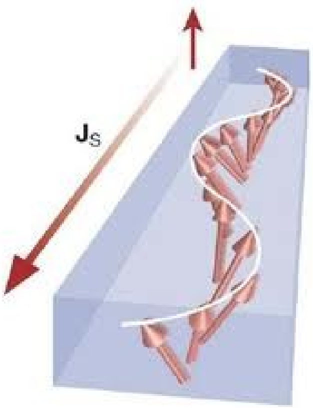
Example:

(Rhet Magaraggia, PhD 2011)

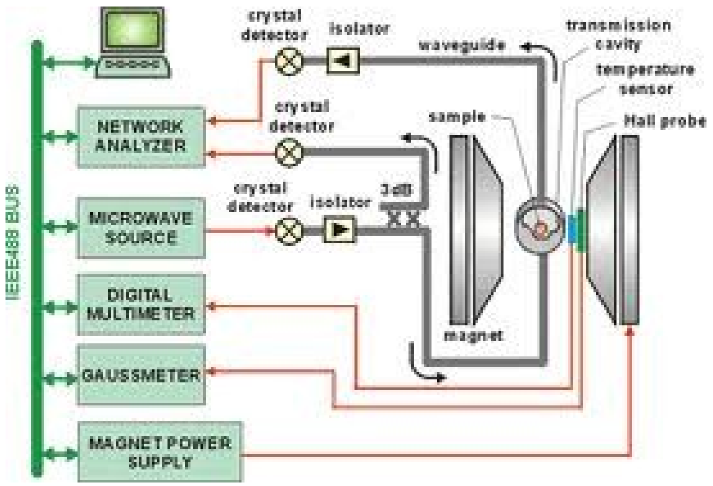
Microwave spectroscopy of thin films

Microwave Spectroscopy

- Resonant absorption and standing spinwaves
- Energies (~ μ eV): fine scale electronic states and processes
- ***Buried interfaces and surfaces***



nanotechweb.org

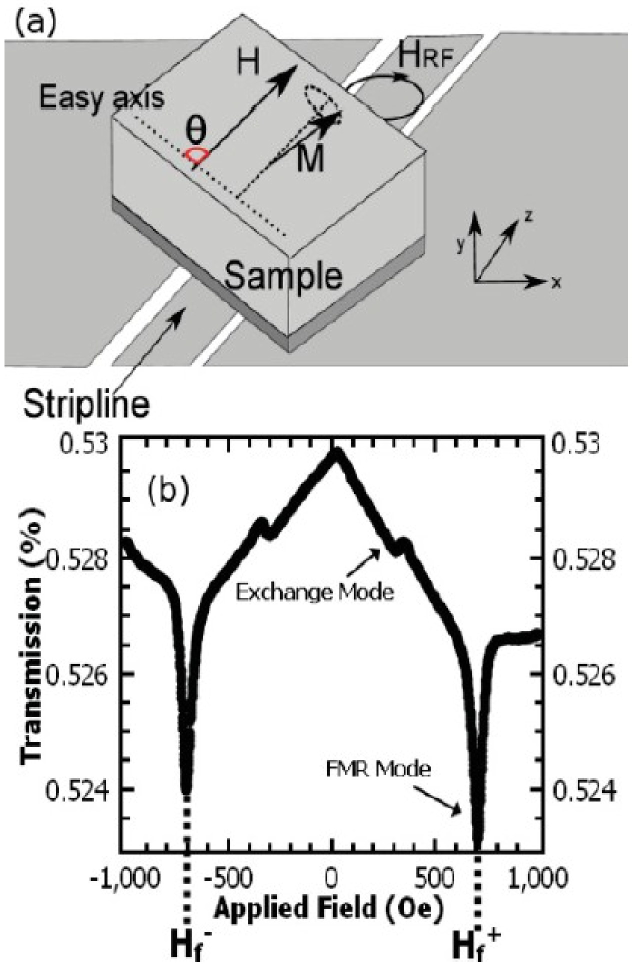


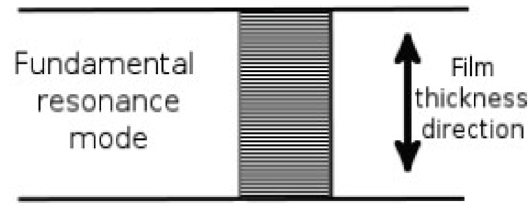
physics.colostate.edu

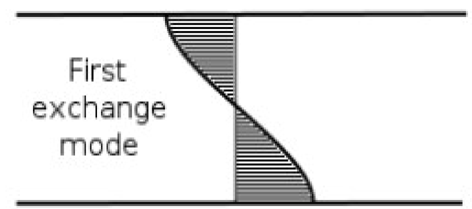
- 1-20 (40) GHz range
- Sensitivity to ~ 3 nm thick Py
- Parameter extraction: vary field magnitude and orientation

FMR Spectra

Broadband FMR with 60 nm FeNi:





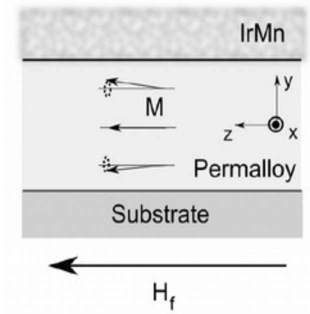


Magaraggia, et al., PRB 83, 054405 (2011)

Exchange Anisotropy

'Kittel' formula for FMR:

$$\left(\frac{\omega}{\gamma}\right)^2 = [H_f(\theta) + D k_y^2(\theta)] \times [H_f(\theta) + D k_y^2(\theta) + \mu_o M_S]$$

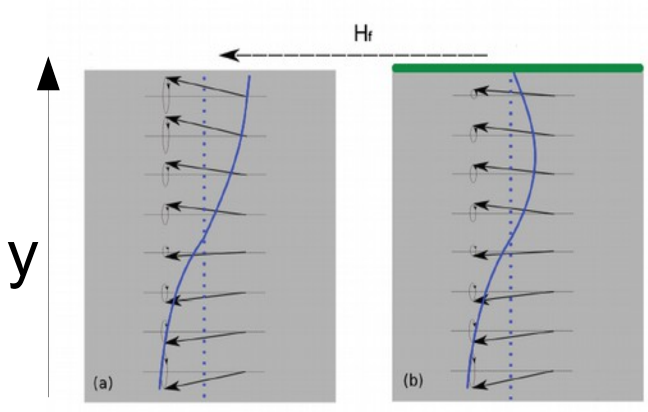


Pinning changes k_y:

$$\vec{T}_{surf} = -\vec{M} \times \nabla_M E_{SA} = -\vec{M} \times \vec{p}$$

$$\Rightarrow \quad p(\theta) = \left(\frac{2A}{M_s}\right)\left[\frac{-k_y(\theta)}{\cot(k_y(\theta) t_{eff})}\right]$$

Simplify: assume single uniform thin film



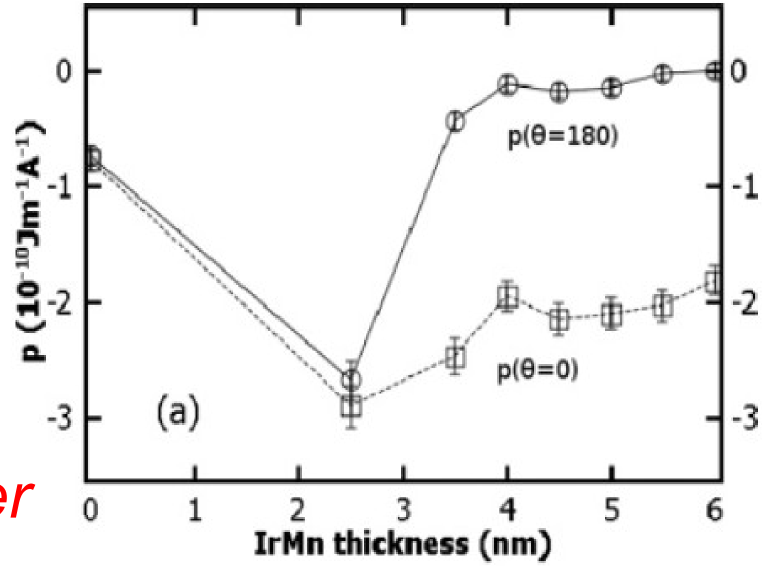
Require: p(FMR) = p(FEX)

Pinning & Effective Thickness

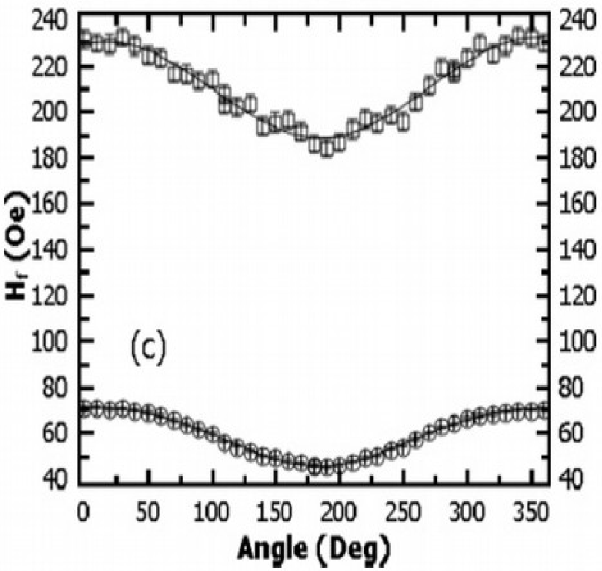
Pinning parameter:

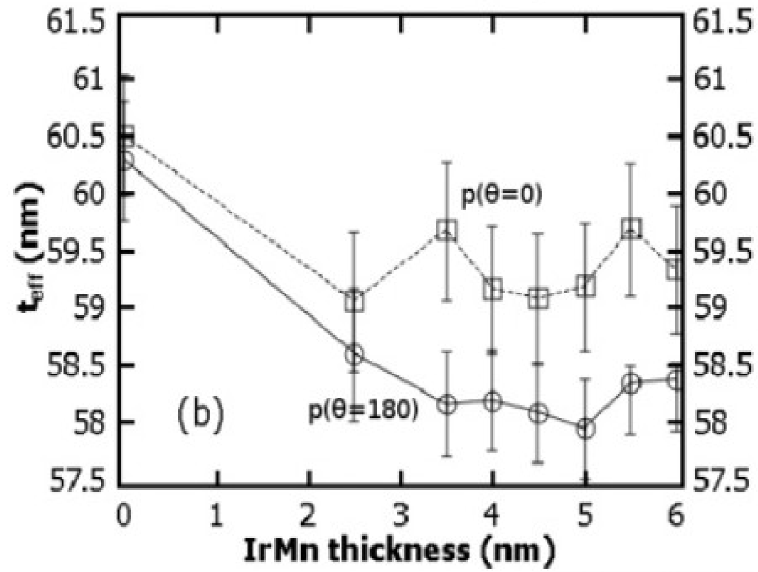
$$p(\theta)=\left(\frac{2A}{M_s}\right)\left[\frac{-k_y(\theta)}{\cot\left(k_y(\theta)t_{eff}\right)}\right]$$

fit parameter



Angular dependence:





Don't forget analytic models!

Example:

(Karen Livesey, PhD 2009)

Nonlinear spin waves

Spinwave Interactions

Beyond linearisation: spin wave interactions

$$M_z = M_s\left[1-\frac{(m_x^2+m_y^2)}{M_s^2}\right]^{1/2} = M_s\left[1-\frac{m_+^2+m_-^2}{M_s^2}\right]^{1/2}$$

$$m_{\pm} = m_x \pm i\, m_y$$

Expand in **spin wave** amplitudes:

$$m_+ = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} c_{\boldsymbol{k}}^+ \qquad m_- = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} c_{\boldsymbol{k}}$$

Energy now includes **interactions**:

Example three wave processes:

$$g(\boldsymbol{k})\, c_{\boldsymbol{k}} c_{-\boldsymbol{k}} c_0^+ + g^*(\boldsymbol{k})\, c_{\boldsymbol{k}}^+ c_{-\boldsymbol{k}}^+ c_0^+$$

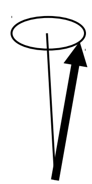
Reversal & Spin Waves

$$\mathscr{H} = \sum_{n\boldsymbol{k}} \omega_{n\boldsymbol{k}} c^*_{n\boldsymbol{k}} c_{n\boldsymbol{k}} + \frac{1}{2} \sum_{1,2,3,4} \widetilde{V}^{(2)}_{1234} c^*_1 c^*_2 c_3 c_4 + \cdots$$

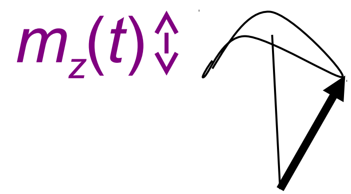
Instability for growth of mode amplitudes:

$$\frac{\partial c_{0\boldsymbol{k}}}{\partial t} + i(\omega_{0\boldsymbol{k}} + i\eta_{\boldsymbol{k}})c_{0\boldsymbol{k}} \approx \widetilde{V}^{(2)}_{0,0,\boldsymbol{k},-\boldsymbol{k}} c_{00} c_{00} c^*_{0-\boldsymbol{k}}$$

Apparent **reduction** of M with onset of instability:



small angle precession



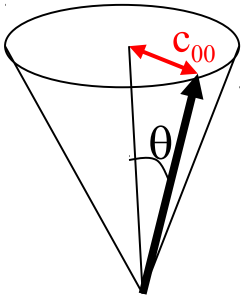
large angle precession

[Livesey et al, Phys. Rev. B (2007)]

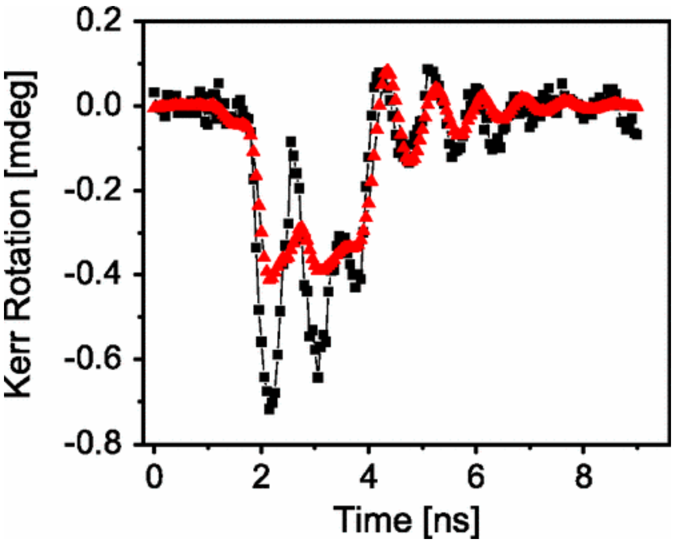
Reversal & Spin Waves

Onset of 4-wave processes:

- **threshold angle**
- **depends on spin wave ω(k)**
- **ω(k) depends on bias direction**

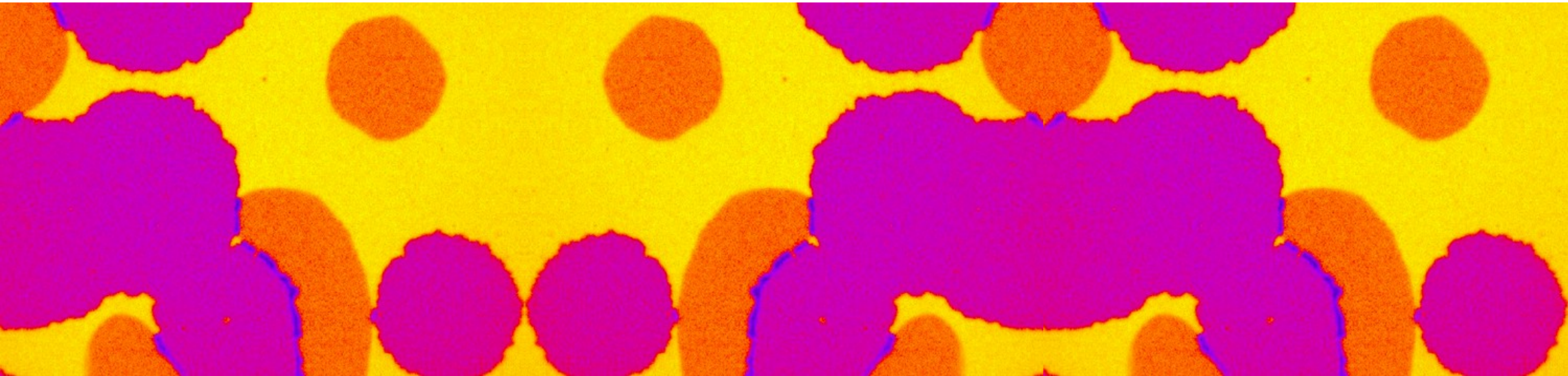


Apparent **reduction of M** because of **spinwave turbulence**

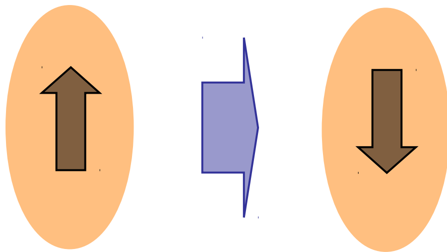


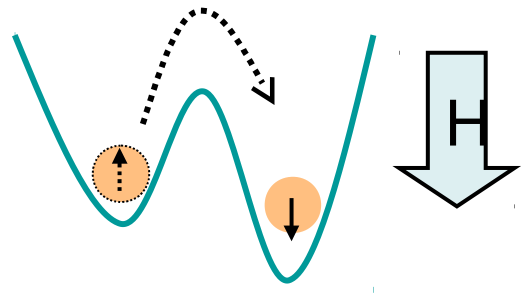
Nembach et al., Phys. Rev. B 84, 184413 (2011)

Domains and Domain Walls

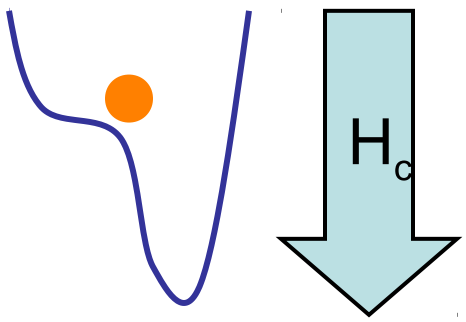


Switching of Single Domain Particles



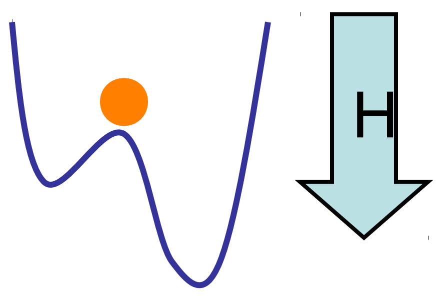


$H \geq H_c$



Dynamics: Precessional reversal

$H < H_c$



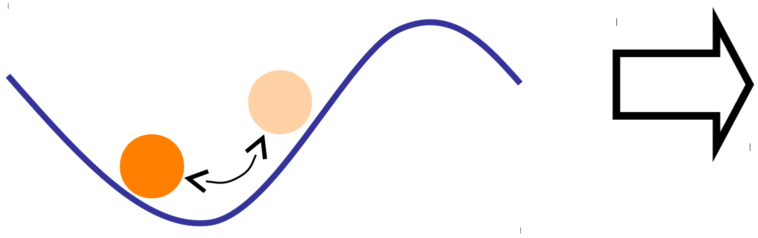
Stability: Thermal activation

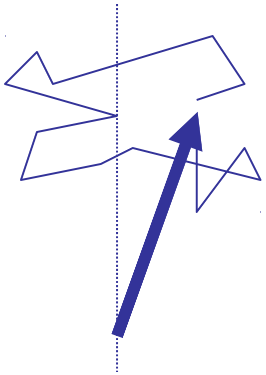
Challenge: fluctuations over long time scales

Approach: Stoner-Wohlfarth models

Independent Particles: H<H$_c$

Climbing to the top: fluctuations





Energy transfer between spin system and heat bath

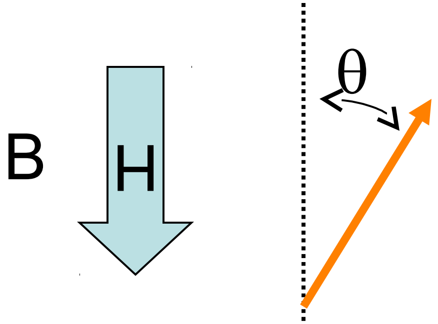
Torque equation of motion: thermal fluctuation 'field'

$$\frac{d}{dt}\vec{m} = -\gamma\,\vec{m}\times\left(\frac{dE}{d\vec{m}} + \vec{h}_f\right)$$

random thermal 'driving torque'

Single Domain Rotation

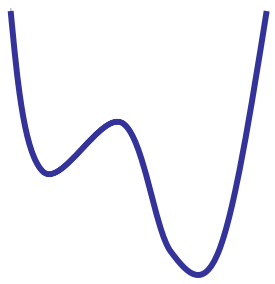
Approximate reversal as pure **relaxation**:



$$E = V\left(-B\,M\cos\theta + K\sin^2\theta\right)$$

$$\epsilon = V\,K\left[1+\left(\frac{B\,M}{2K}\right)^2\right]$$

ε



Stoner-Wohlfarth Model

Rate depends on activation energy and attempt frequency

$$\Gamma = \frac{1}{\tau} = f_o \exp\left(-\epsilon / k_B T\right)$$

Reversal of a Particle Ensemble

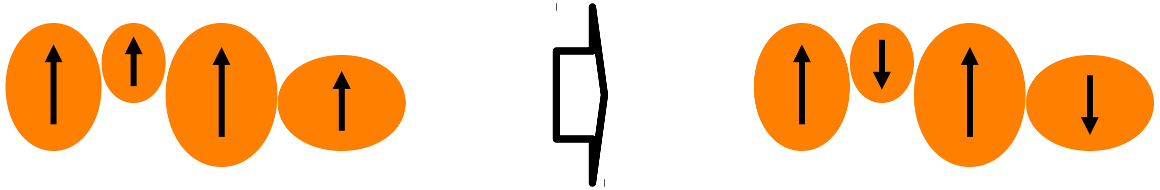
Ensemble of particles: B=0, thermal fluctuations reduce M

Approach to equilibrium: Chemical rate problem

$$\left.\begin{aligned}\frac{dn_\uparrow}{dt} &= W_{\downarrow\uparrow} n_\downarrow - W_{\uparrow\downarrow} n_\uparrow \\ \frac{dn_\downarrow}{dt} &= W_{\uparrow\downarrow} n_\uparrow - W_{\downarrow\uparrow} n_\downarrow\end{aligned}\right\} \quad m(t) = n_\uparrow - n_\downarrow = A\,e^{-\Gamma t}$$

Reversal of a Particle Ensemble

Ensemble of particles: H=0, dipolar fields drive m to 0

m =1  m =0

Approach to equilibrium: Distribution of rates

$$m(t) = A \int P(\Gamma) e^{-\Gamma t} d\Gamma$$

Can one measure the distribution of rates P(Γ)?

(Rebecca Fuller, PhD 2010)

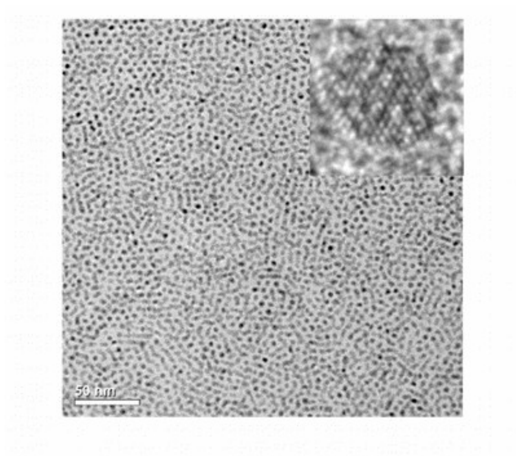
Relaxation: Distributions

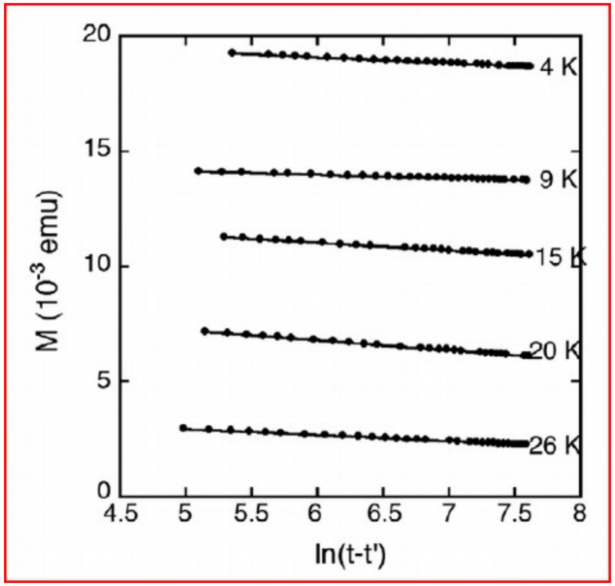
Distribution of energy barriers: $\Gamma = f_o \exp(-\epsilon / k_B T)$

$$m(t) = m(\infty) + A \int_0^\infty P(\epsilon) e^{-t\Gamma(\epsilon)} d\epsilon$$

Magnetic viscosity: ln(t) for broad distributions

$$m(t) = C - S(H) \ln(t \Gamma_o)$$



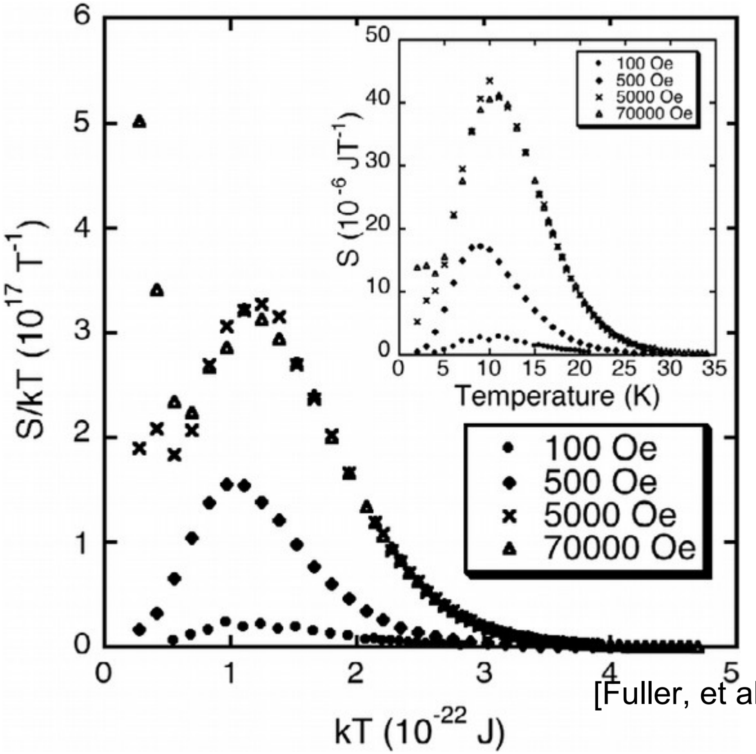


[Fuller, et al., JPCM 2009]

Relaxation: Energy Barriers

Useful measure: study dm/dt at different T

$$P\left(\epsilon = k_B T \ln\left(t/\tau_o\right)\right) \approx \frac{1}{A k_B T}\left(-t \frac{dm}{dt}\right) = \frac{S}{A k_B T}$$



[Fuller, et al., JPCM (2009)]

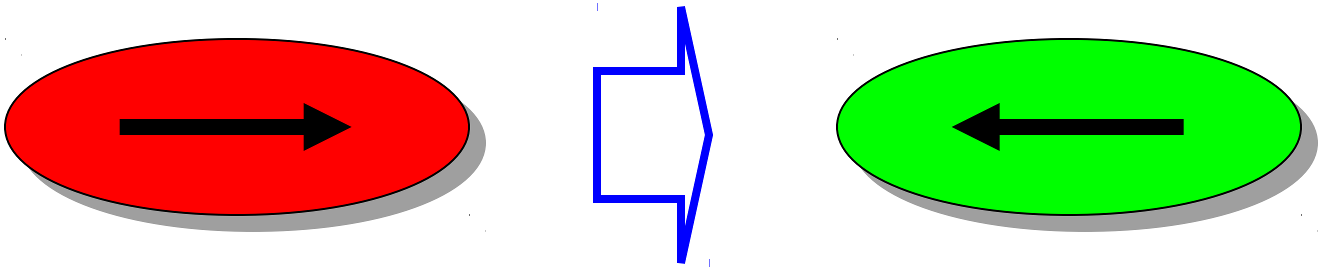
Viscosity at different ***temperatures*** *and* ***fields*** *provides estimates for energy barrier distribution*

Questions?

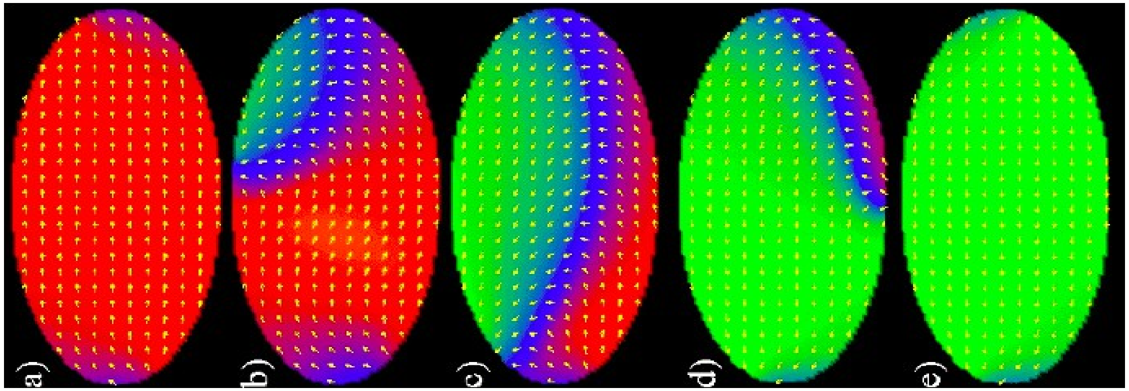

Ultimate Poker Challenge
CHALLENGE
$75,000
$50,000
$25,000
$10,000
$5,000
$2,500
$1,000
$0
BANK

Magnetic domains and domain walls

Routes to Reversal

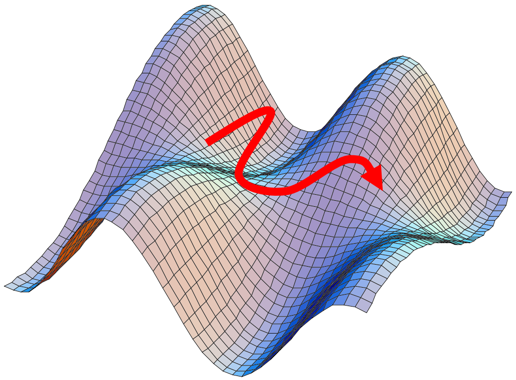


Nucleation of domains and domain walls



[Slaughter, 2000]

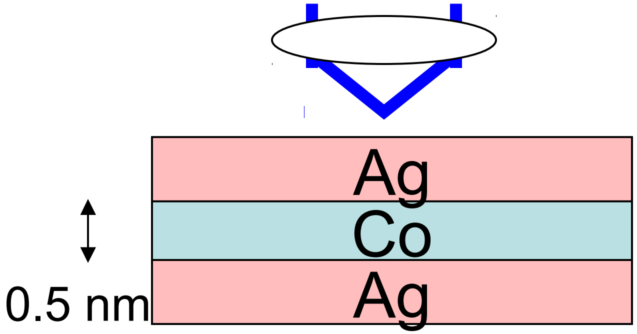
Challenge: fluctuations over long times **and** large lengthscales

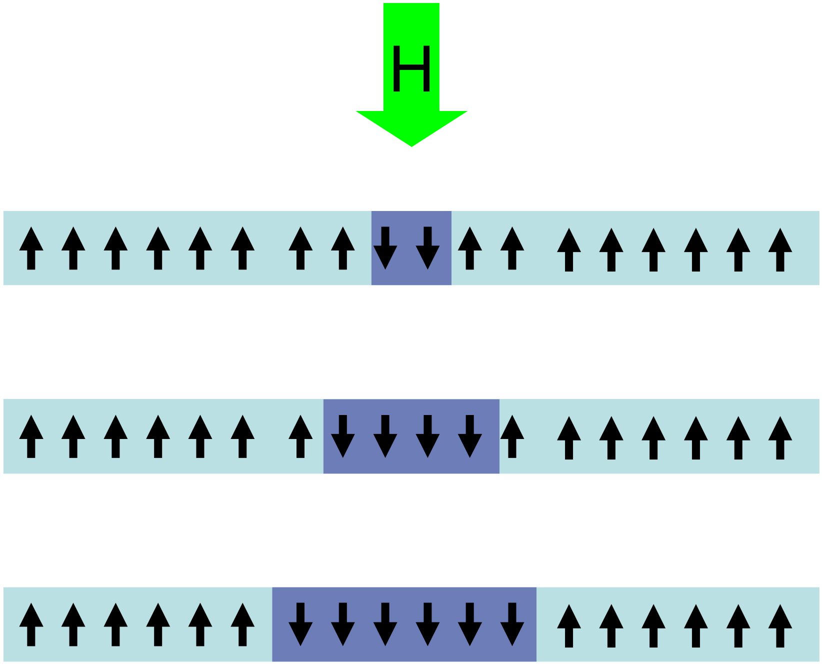


Approach: a Stoner-Wohlfarth model for fluctuating lines

Domain & Wall Dynamics

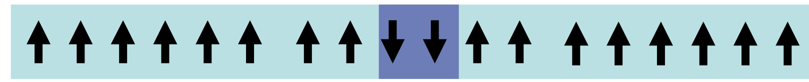
- **Example**: MOKE study
- Perpendicular M in Co
- Method:
  - saturate
  - apply field pulse
  - image & repeat



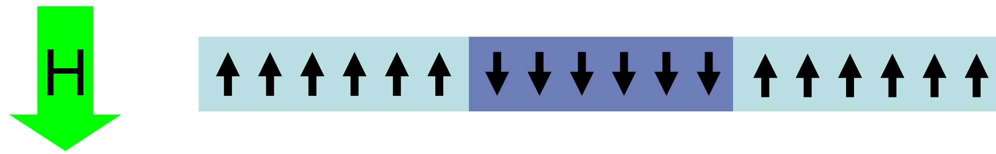


Magnetization Processes & Domains

Nucleation processes:



Growth of a critical domain volume



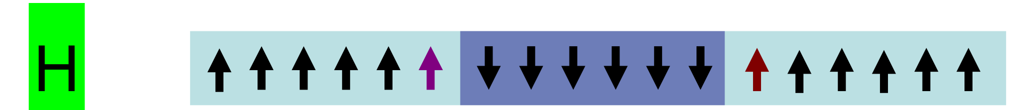
$$E_{Zeeman} = -\mu M V H \qquad E_{DW} = \sigma A$$

Surface energy

$$\Rightarrow \quad \left(\frac{V}{A}\right)_c = \frac{\sigma}{(\mu M H)}$$

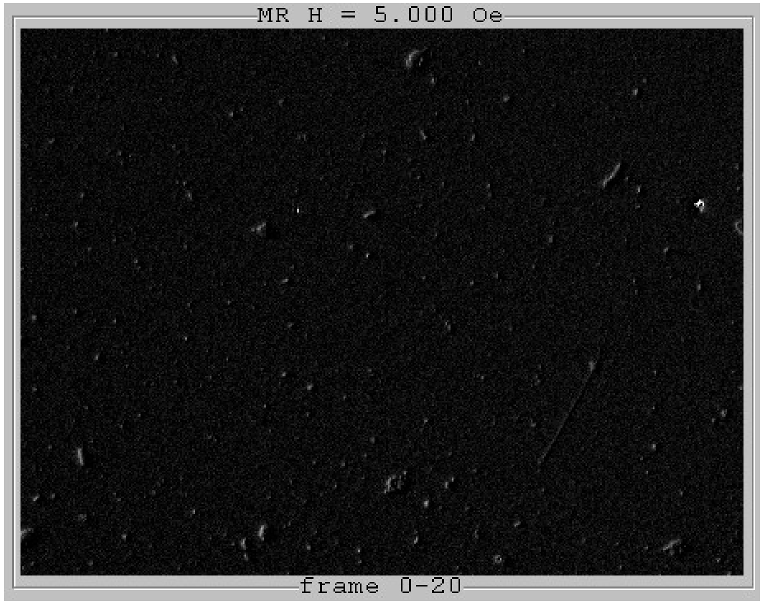
Magnetisation Processes & Domains

Growth stops at local field gradients (pinning 'pressure')



$$pressure \sim -\nabla E_{local}$$

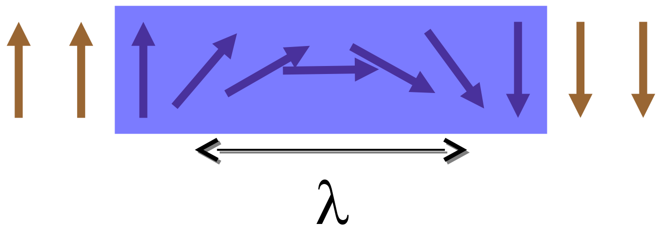
Stroboscopic 'movie' of domain growth



Magnetization Processes & DW's

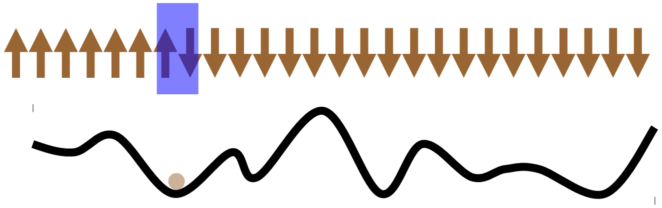
Wall structure:

- Topological excitation
- Surface tension
- Characteristic width



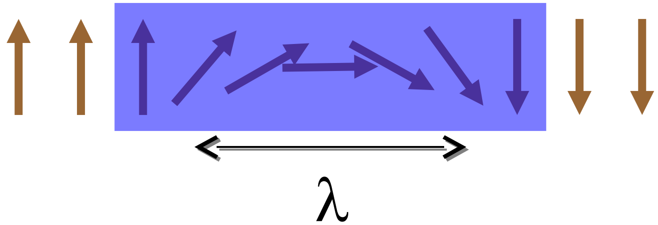
Dynamics:

- **Translation** & fluctuations
- **Pinning & 'creep'**
- Internal modes



Magnetization Processes & DW's

Domain walls define spin reorientation:



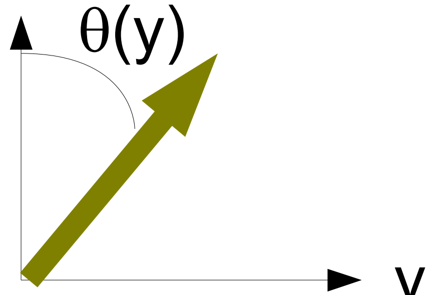
Energy: exchange + anisotropy

$$E = \int \left(\frac{A}{M_s^2} \left[(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2 \right] - \frac{K}{M_s^2} m_z^2 \right) d\,\boldsymbol{r}$$

Allowed spin configurations minimise E

Domain Walls

Suppose wall along y direction:



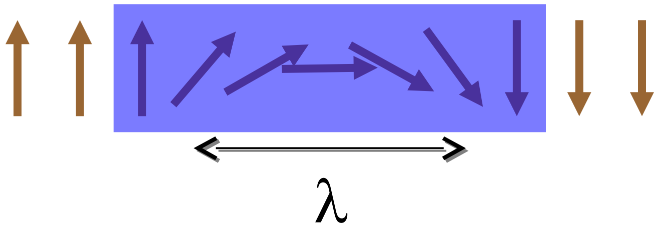
$$m_z = M_s \cos\theta(y) \qquad m_y = M_s \sin\theta(y)$$

$$E = \int \left[\frac{A}{M_s^2} \left(\frac{\partial m_z(y)}{\partial y} \right)^2 - \frac{K}{M_s^2} m_z^2 \right] dx$$

Minimum energy requires $A \frac{\partial^2}{\partial y^2} \theta + K \sin^2\theta = 0$

Solution:

$$\cos\theta = \tanh\left[\frac{y - y_o}{\sqrt{A/K}} \right] \qquad \sigma = \sqrt{4AK}$$

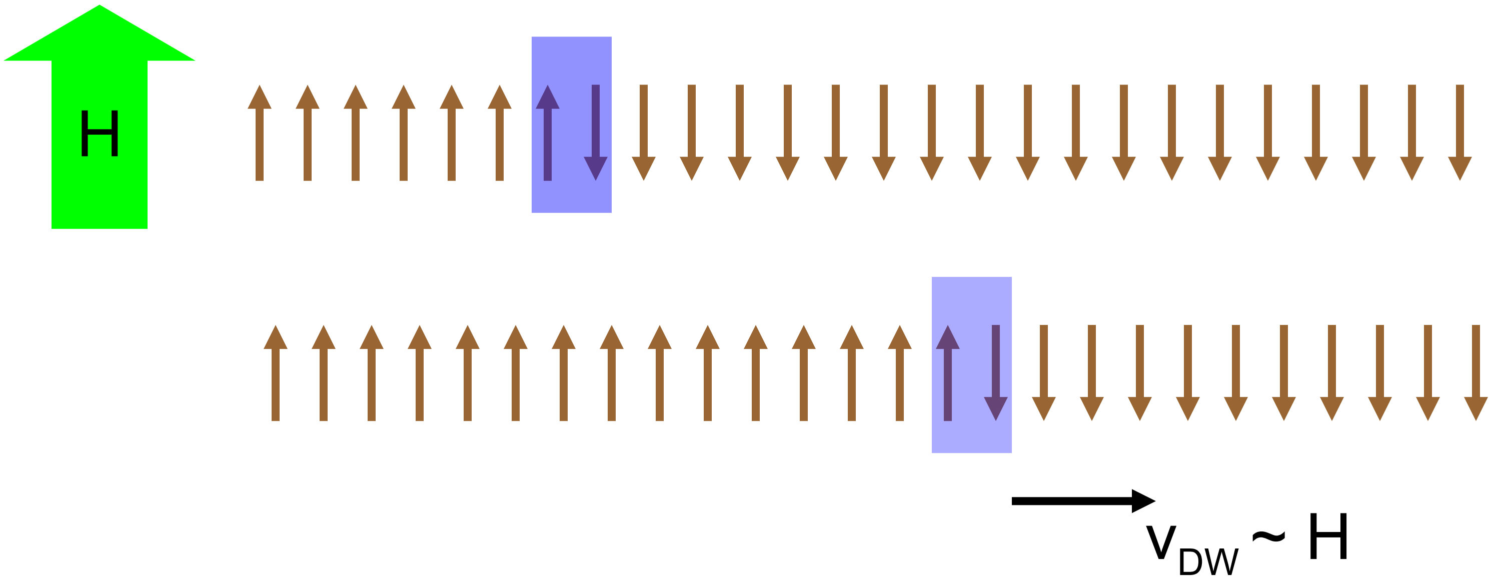


width = λ

energy

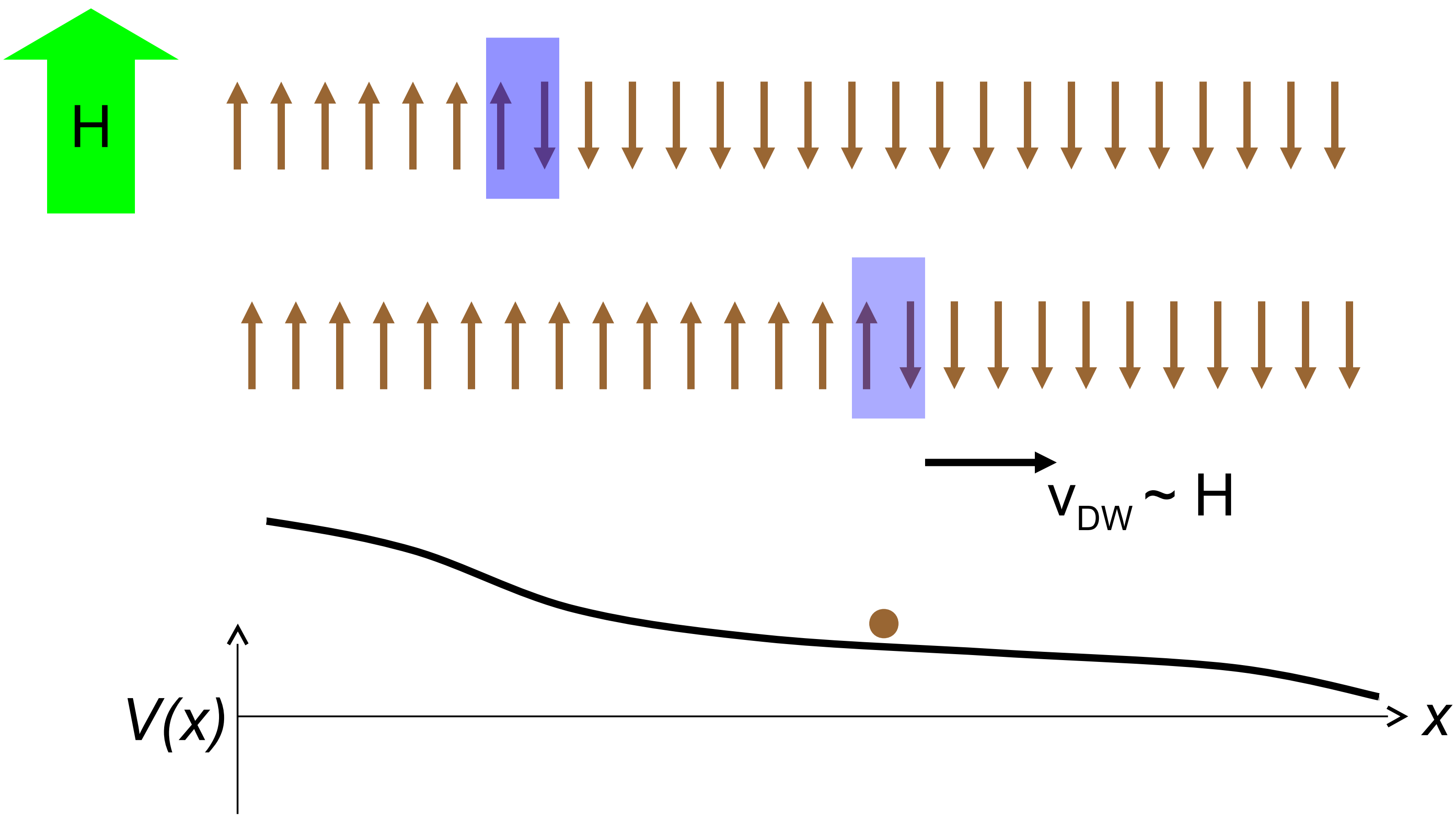
DW Mobility: High Field Flow

Viscous Flow: High field driven dynamics



DW Mobility: High Field Flow

Viscous Flow: High field driven dynamics



DW Mobility Theory: Flow

Torque equations of motion:

$$\frac{\partial \boldsymbol{m}}{\partial t} = -\gamma\, \boldsymbol{m} \times \boldsymbol{H} + \frac{\alpha}{M_s} \boldsymbol{m} \times \frac{\partial \boldsymbol{m}}{\partial t}$$

precessional torque

Gilbert damping

Effective local field: (exchange, anisotropy, dipolar)

$$H = H_{applied} - \frac{\partial E}{\partial \boldsymbol{m}}$$

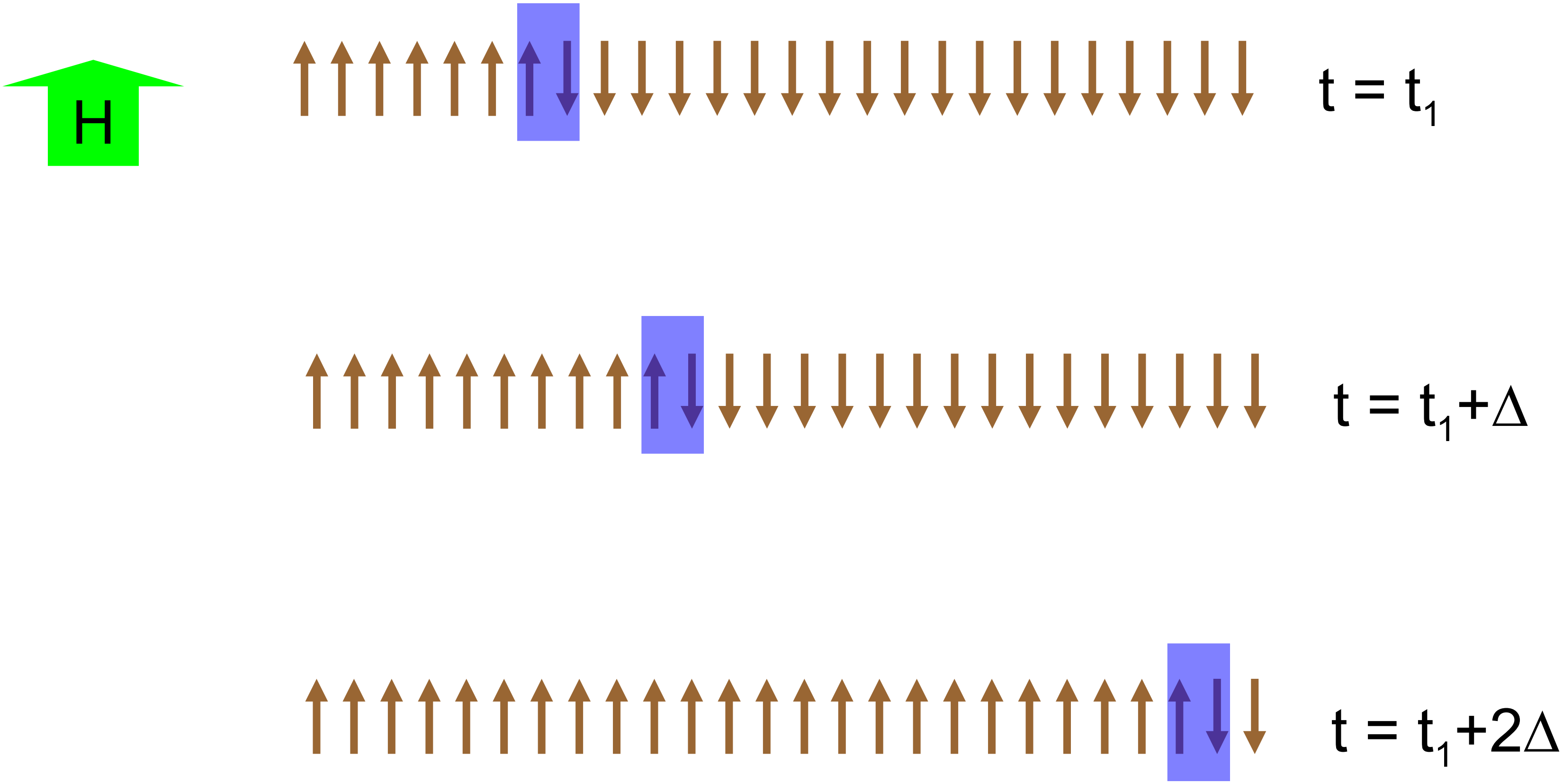
Time averaged velocity (in Flow regime):

$$v \propto \int \overline{|\boldsymbol{m} \times \boldsymbol{H}|^2}\, d^3 x$$

[X Wiang, P Yan, J Lu]

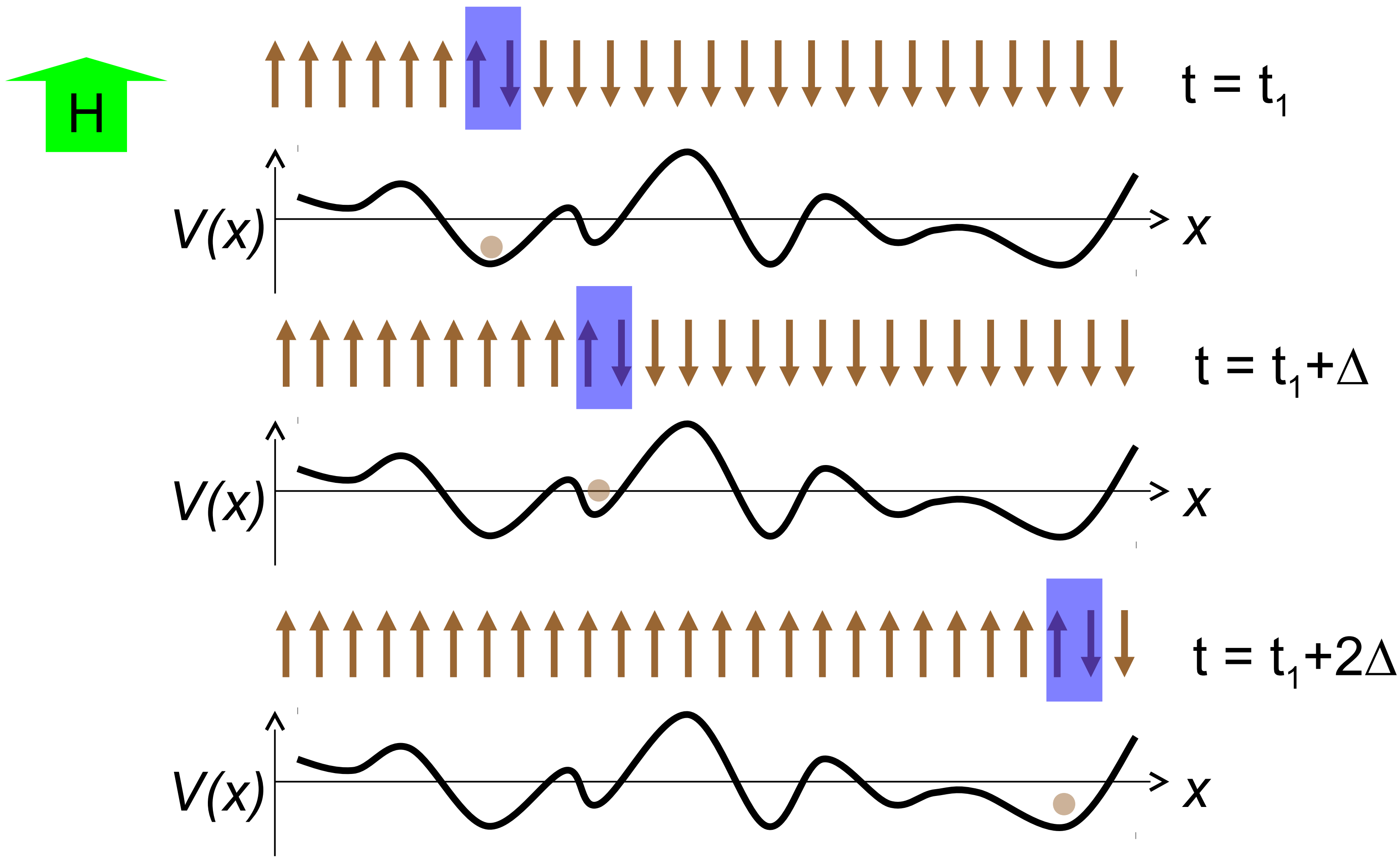
DW Mobility: Low Field Creep

Creep: low field thermally activated dynamics



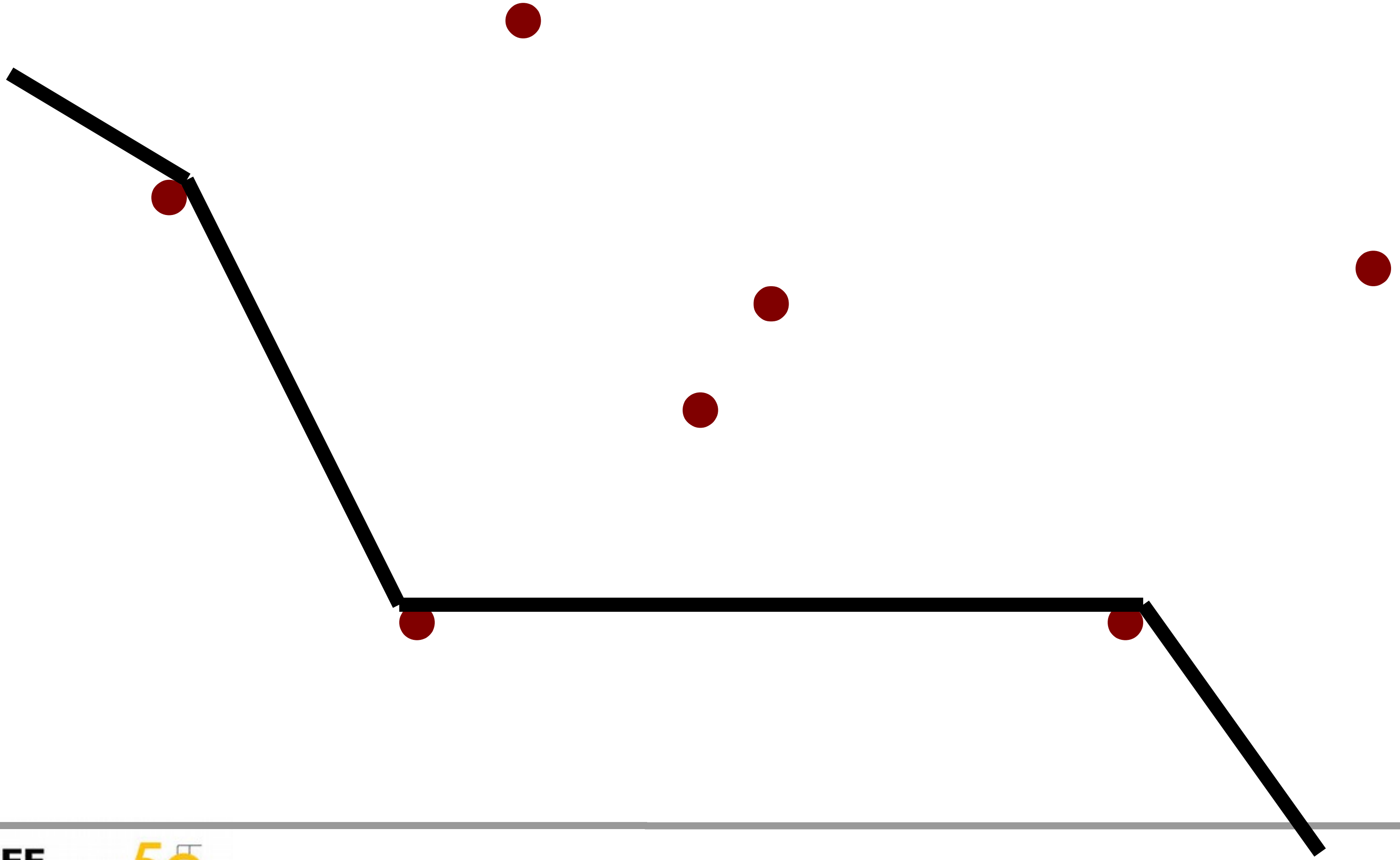
DW Mobility: Low Field Creep

Creep: low field thermally activated dynamics



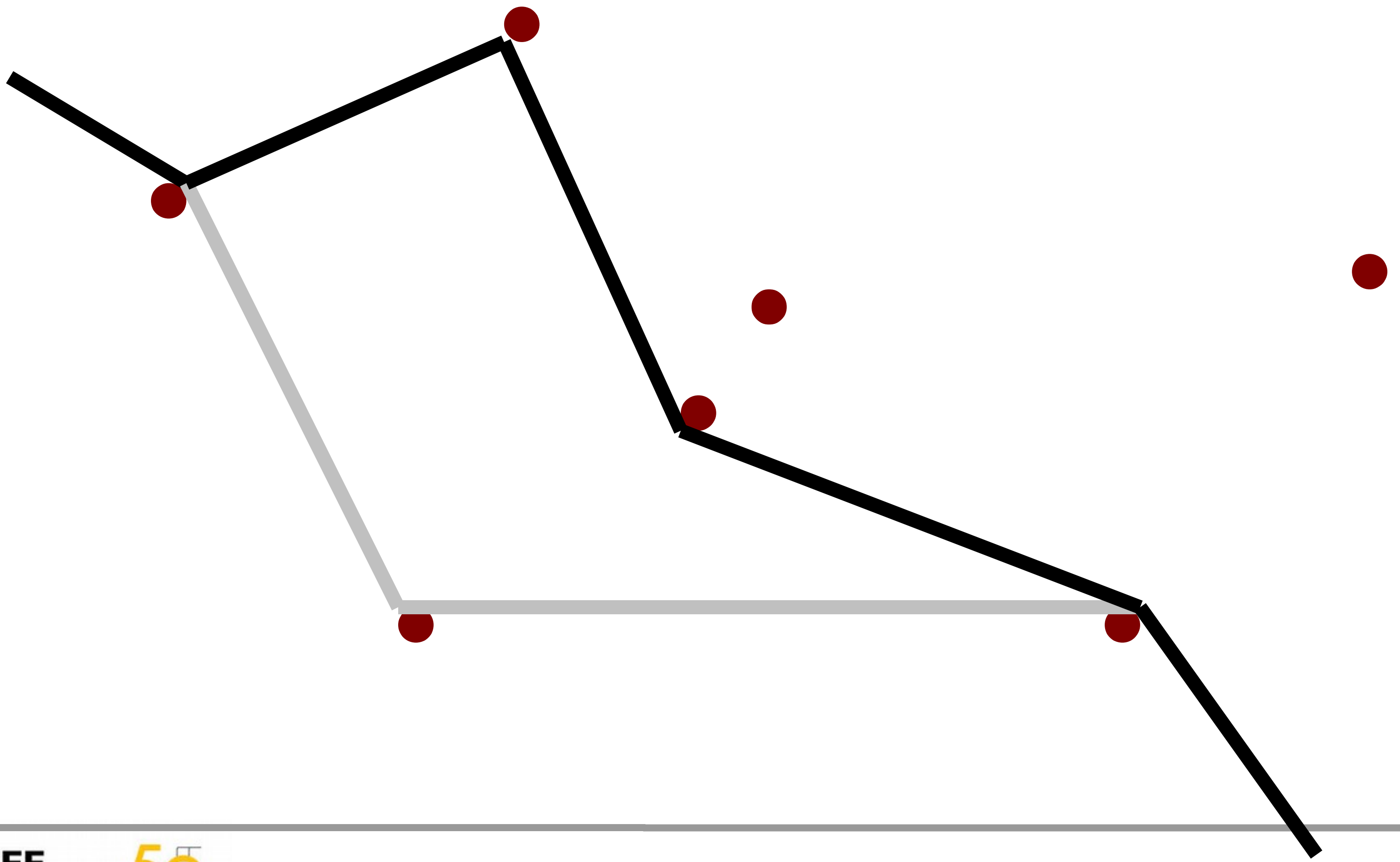
DW Mobility Theory: Creep

Pinning sites oppose wall motion:



DW Mobility Theory: Creep

Pinning sites oppose wall motion:

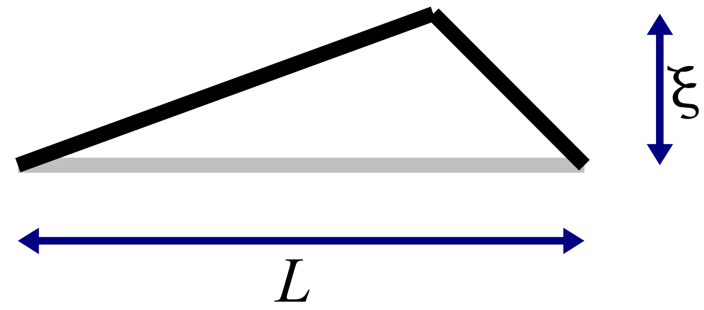


DW Mobility Theory: Creep

Number of pinning sites:

$$E_p = \sqrt{f_{pin}^2 N_p}\,\xi$$

pin force



Macroscopic wall motion through **avalanche**:

Scaling: **critical field** for avalanche onset

$$[E_{elastic} - E_{Zeeman}] = E_B \approx U_C \left(\frac{H_{dep}}{H_{applied}} \right)^{\frac{2\zeta - 2 + D}{2 - \zeta}}$$

DW Mobility Theory: Creep

Depinning rate:

$$\frac{1}{\tau(L)} = \frac{1}{\tau_0}\exp\left[\frac{-E_B(L)}{k_B T}\right]$$

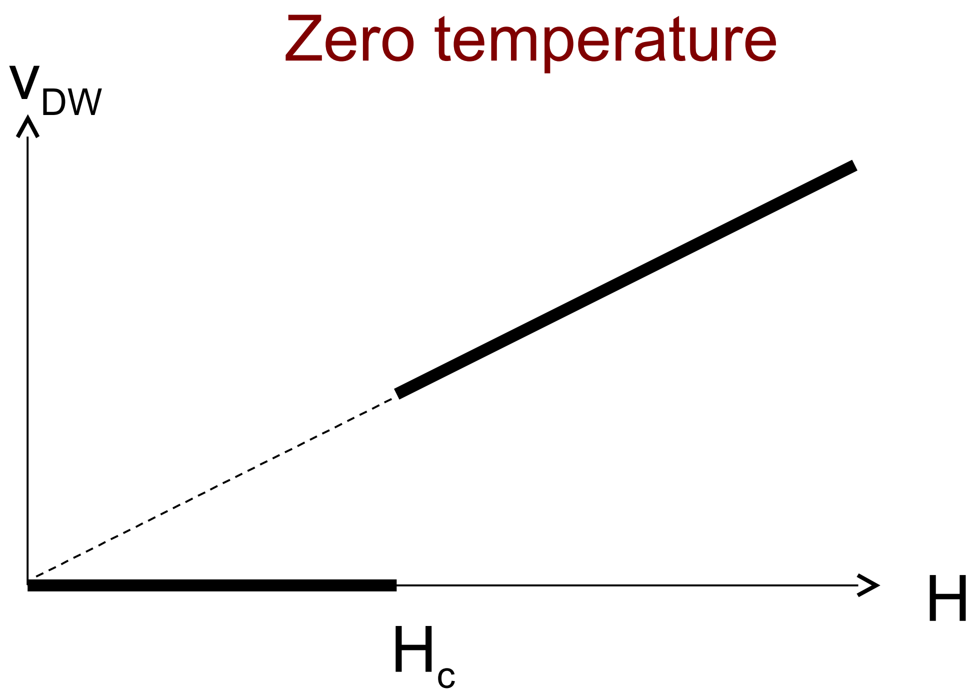
Multiply by distance travelled to give velocity:

$$v = \frac{w(L)}{\tau(L)} \approx \frac{\xi}{\tau_0}\exp\left[\frac{-U_C}{k_B T}\left(\frac{H_{dep}}{H_{applied}}\right)^{\mu}\right]$$

Expect $\mu = 1/4$ for ultra thin films.

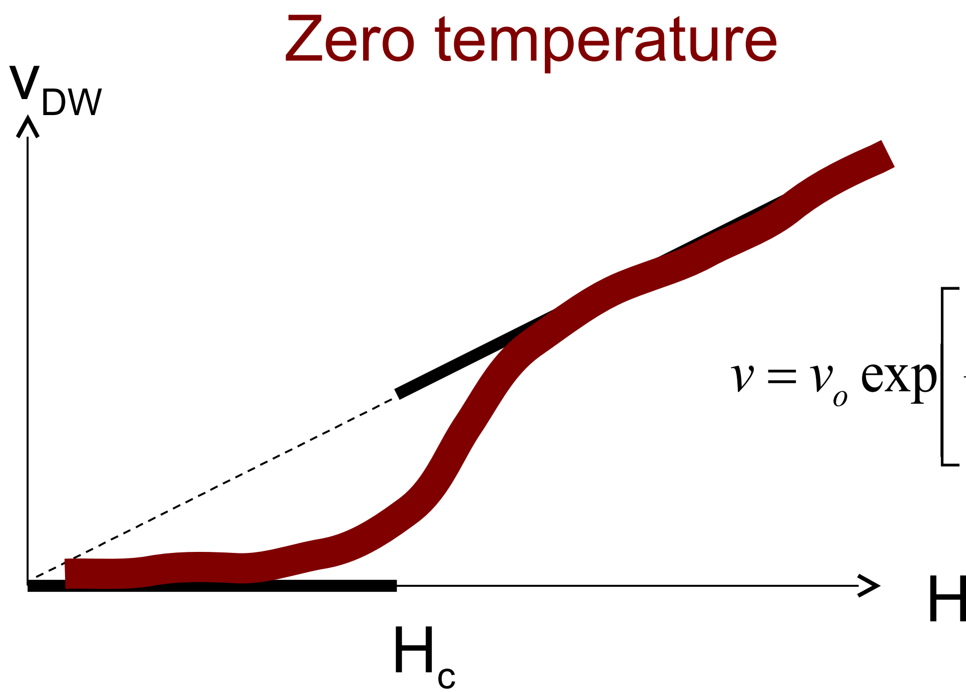
DW Motion: Transition

Threshold: transition from creep to viscous flow



DW Motion: Transition

Threshold: transition from creep to viscous flow

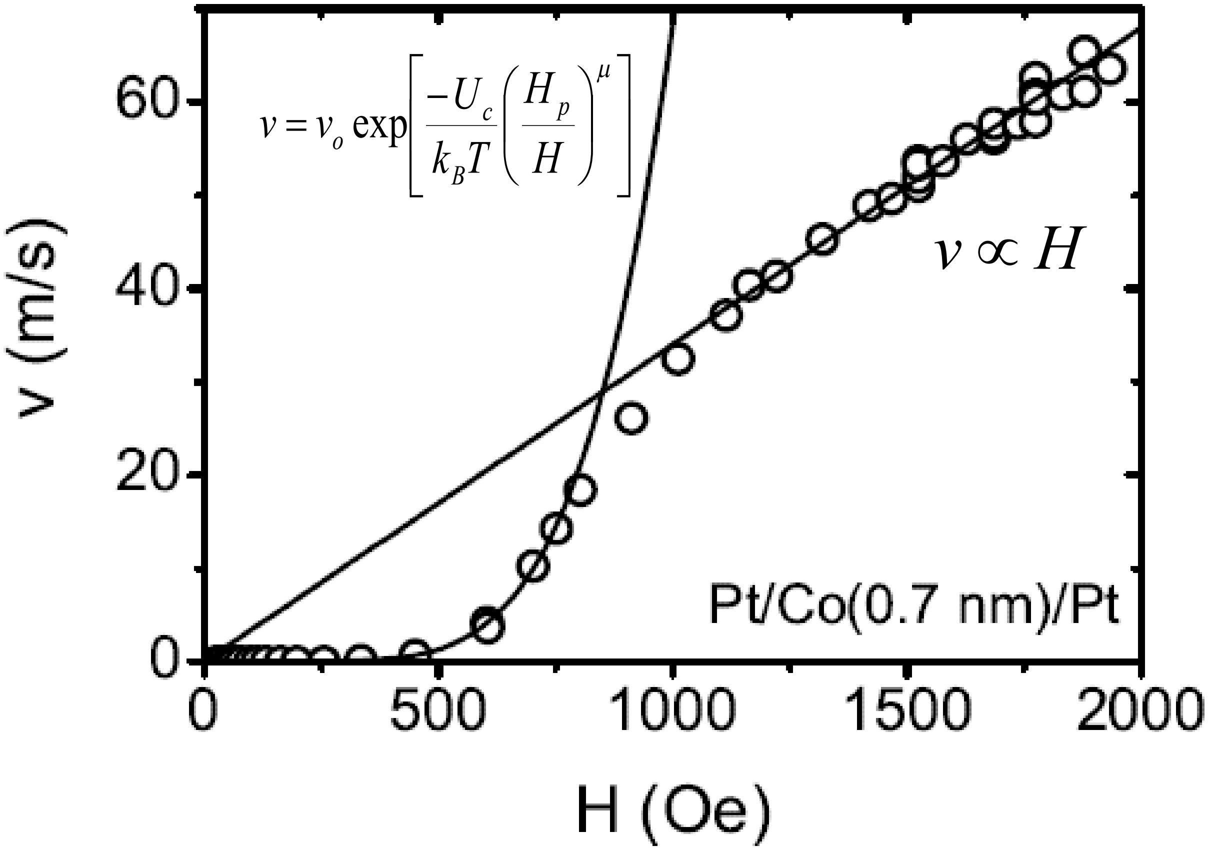


$$v = v_o \exp\left[\frac{-U_c}{k_B T}\left(\frac{H_p}{H}\right)^{\mu}\right]$$

DW Motion: Transition

Observed transition from creep to viscous flow:

(Peter Metaxas, PhD 2009)



[Metaxas, et al., Phys. Rev. Lett., 2007]

Challenge: What are magnetisation processes in chiral spin systems?

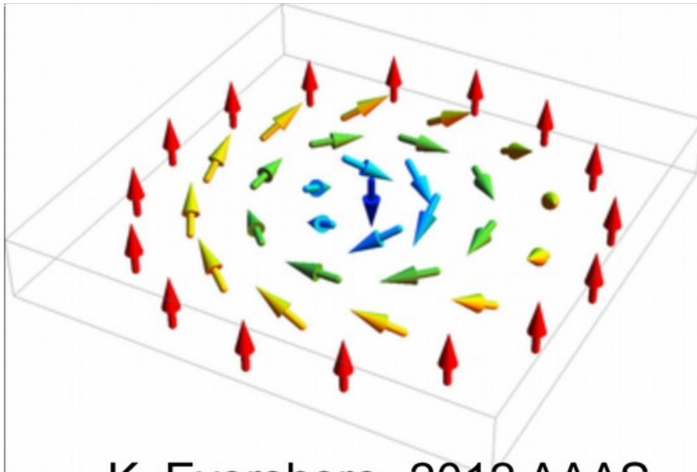
Approach:

(Pablo Boyrs, PhD ~2015)

Visualising 1 D spin textures

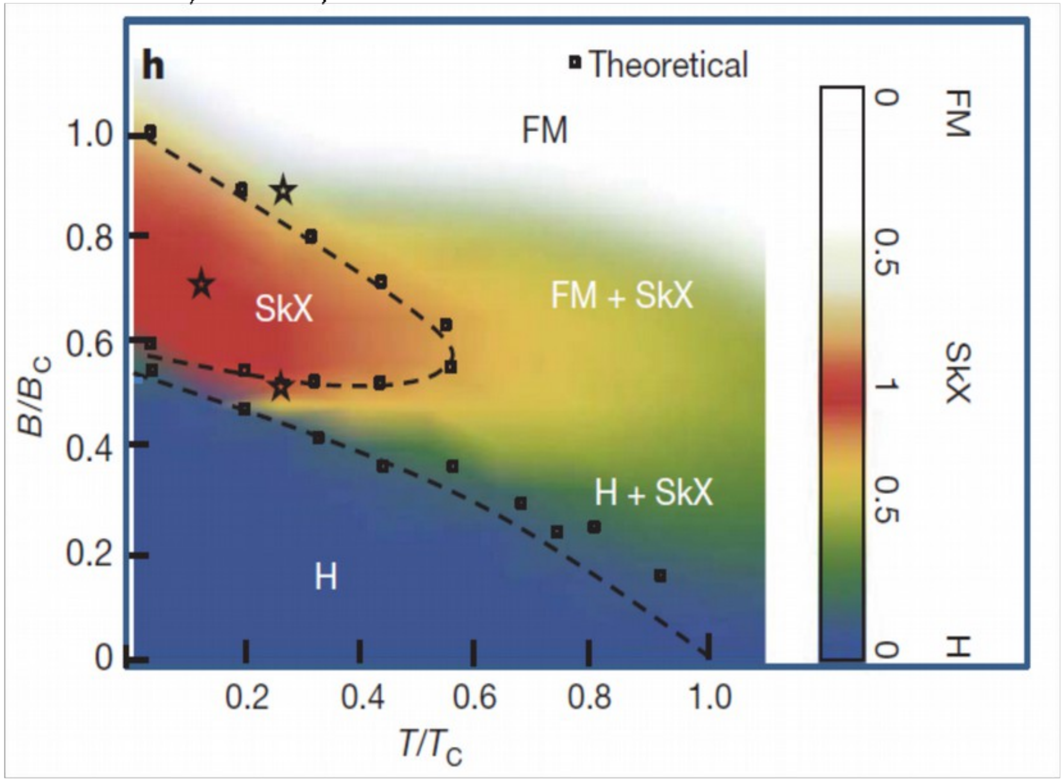
Chiral Spin Textures

Skyrmion:

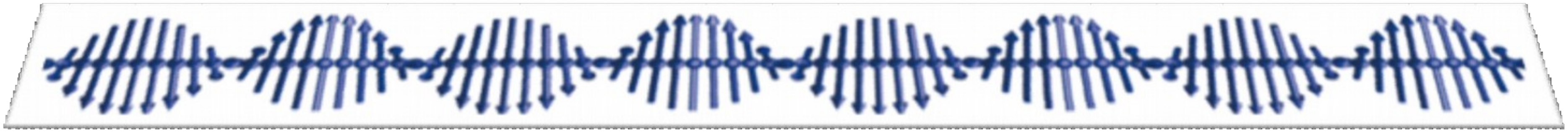


K. Evershore, 2012 AAAS

Yu, et al., Nature 2010



Chiral helicoid:



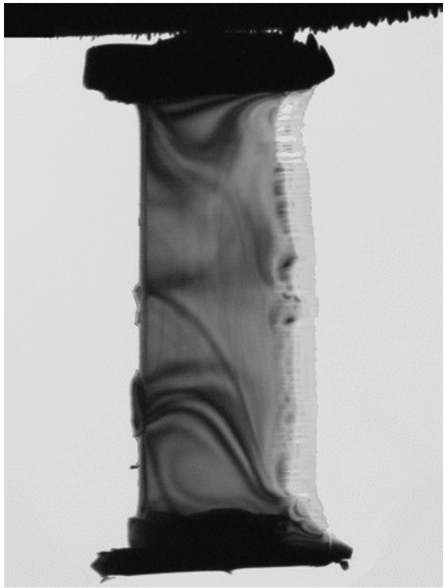
Y Togawa

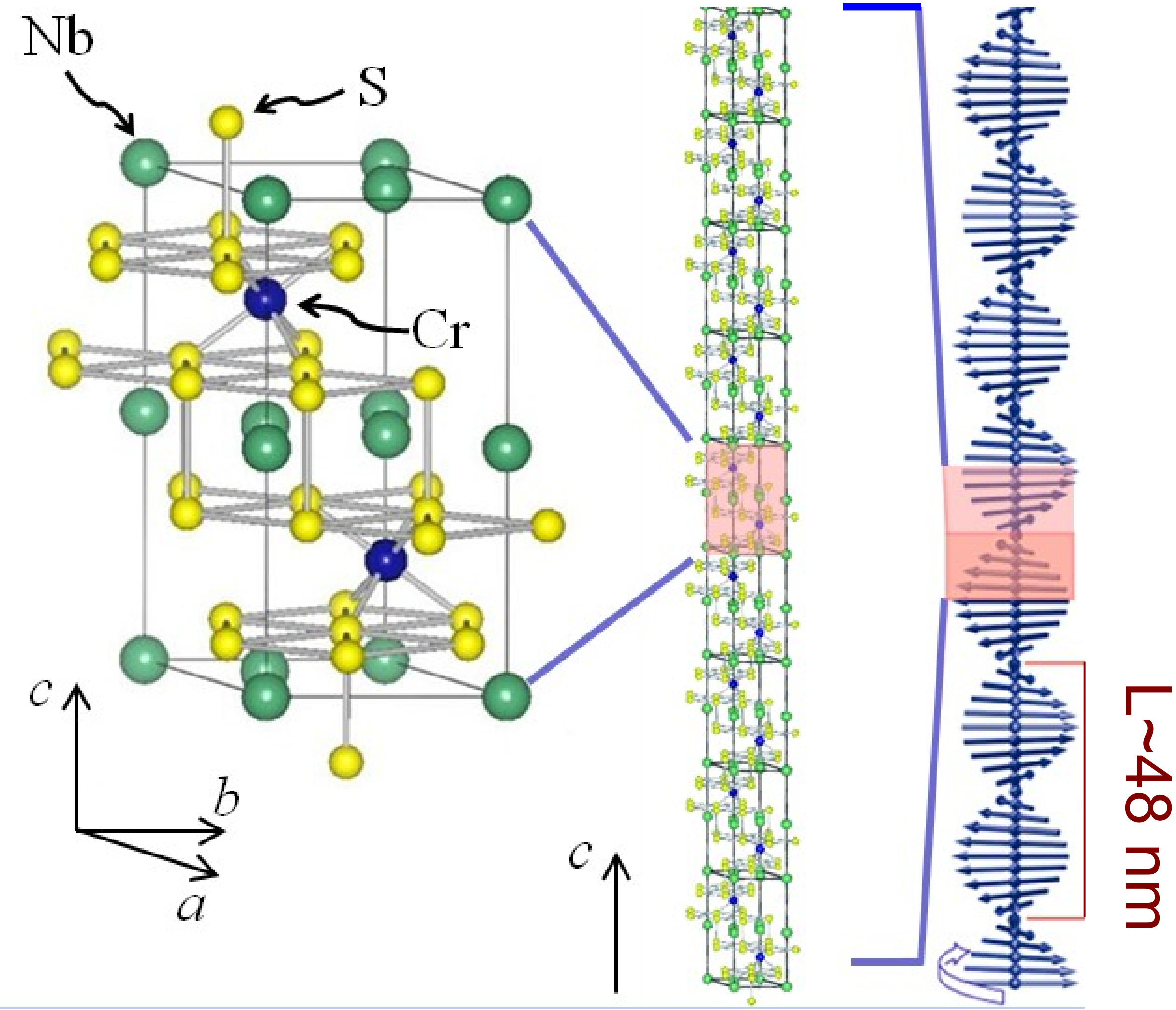
Experimental System

Cr Nb_3S_6: *$P6_322$*

T_c = 130 K

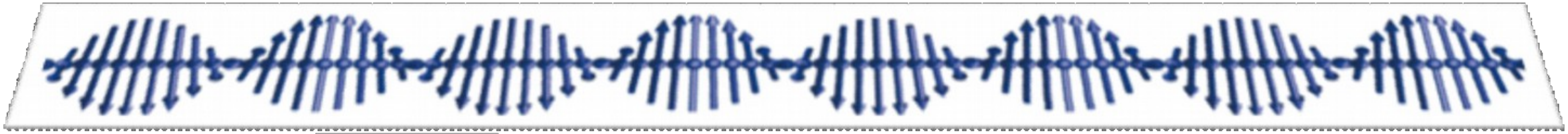
Conductor



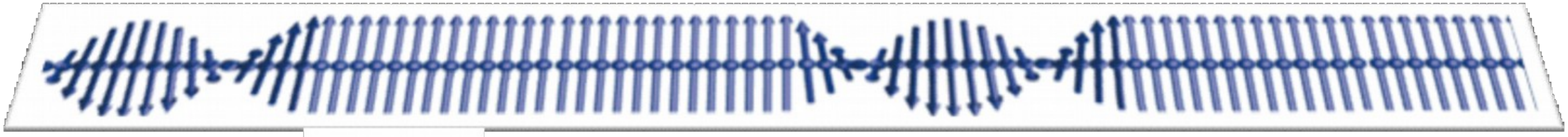


Chiral Soliton Lattice

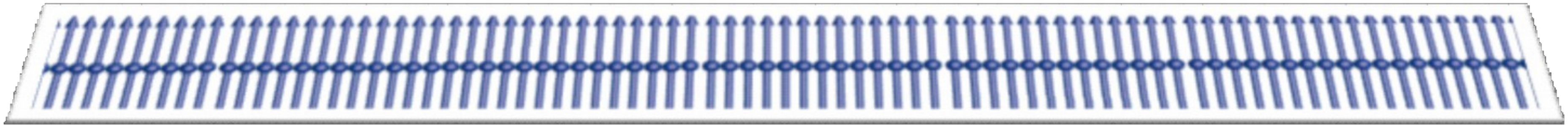
Response to a magnetic field:



H = 0



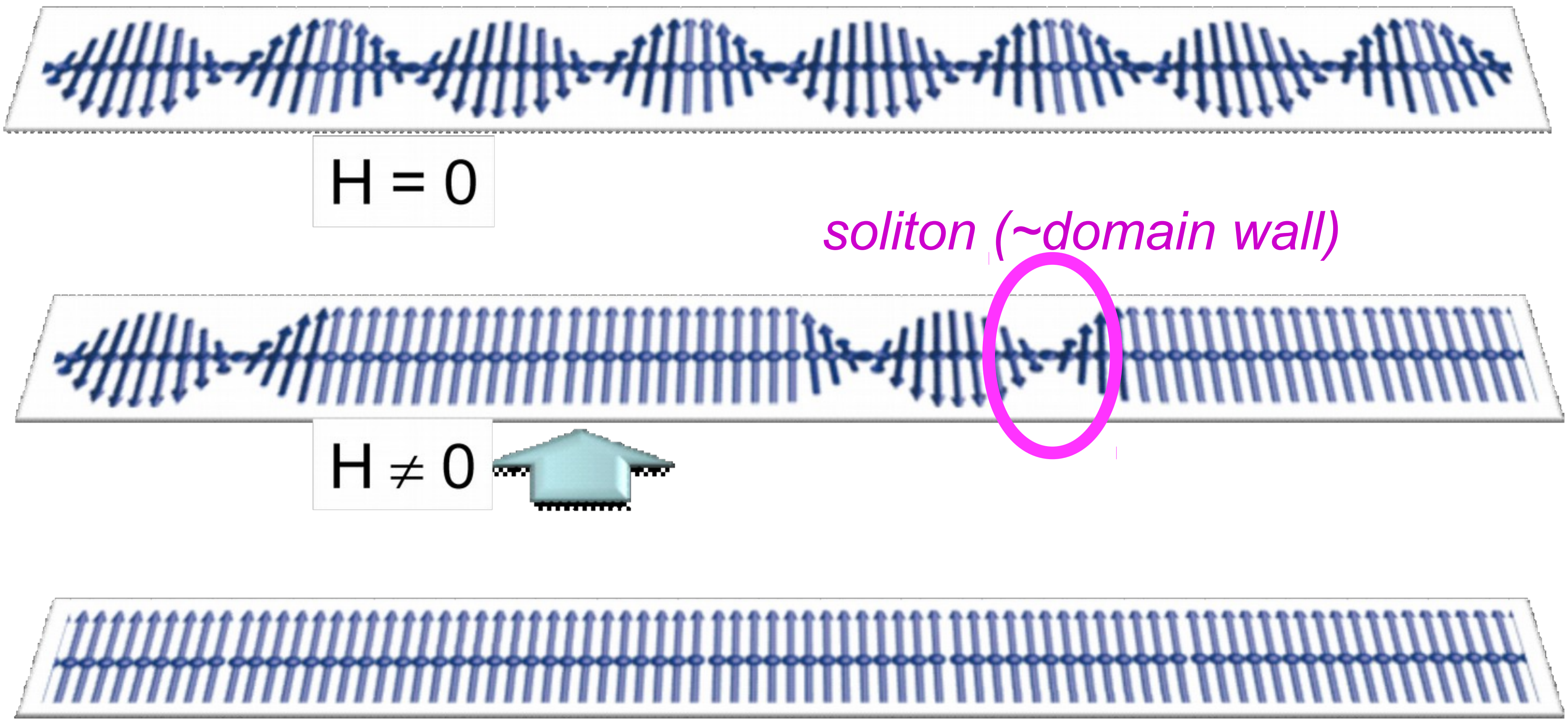
$H \neq 0$



$H > H_C$ Forced ferromagnet

Chiral Soliton Lattice

Response to a magnetic field:

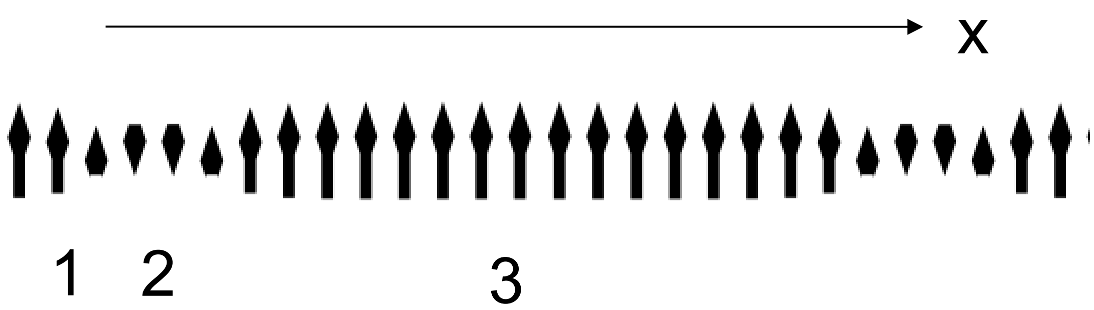


$H > H_C$ Forced ferromagnet

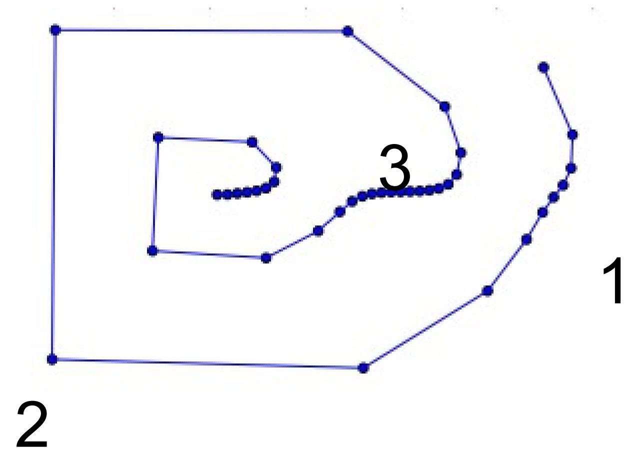
Useful Visualisation

In order to follow rotations, map the spin tips along the chiral axis (x):

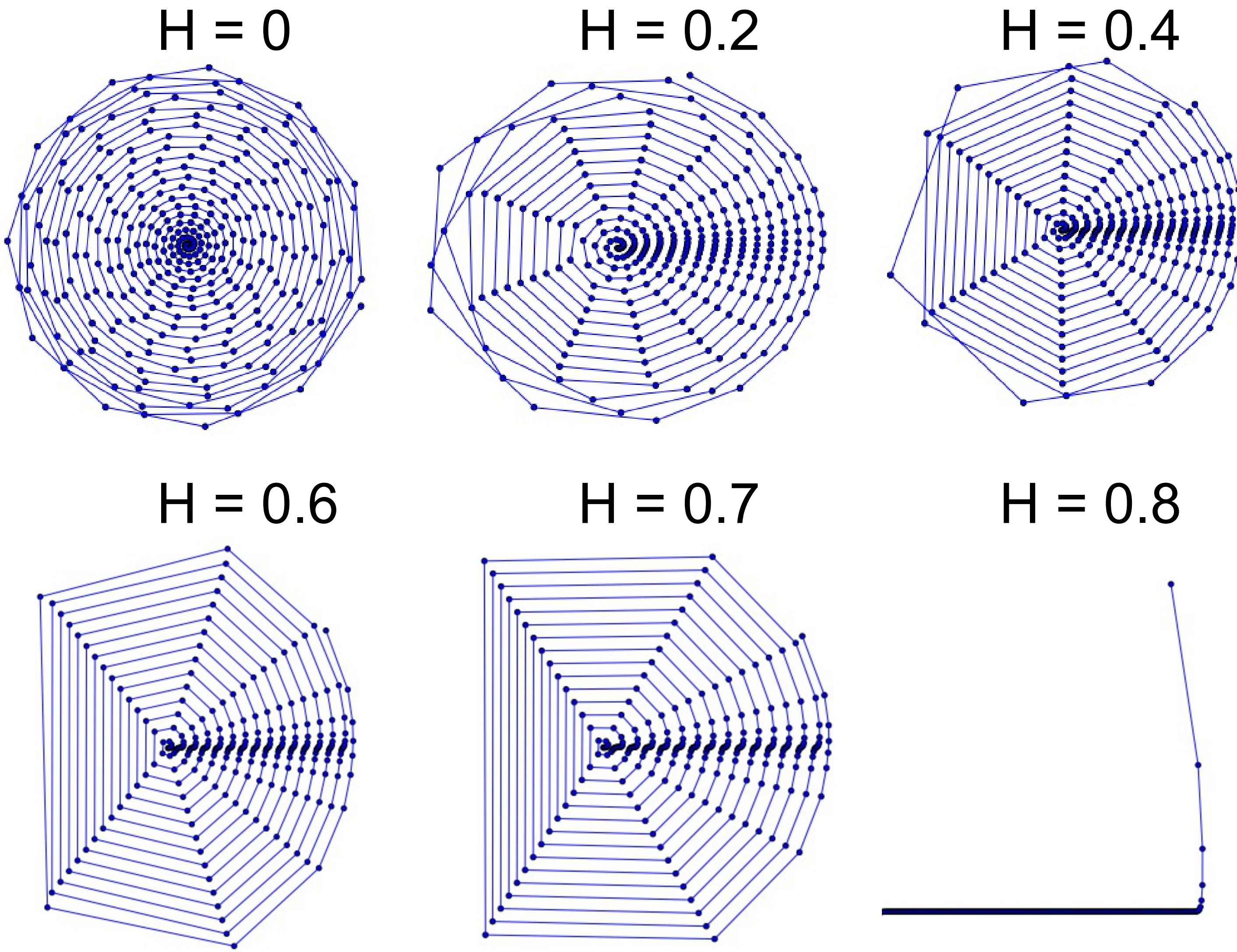
<u>Along the axis view</u>



<u>Down the axis view</u>



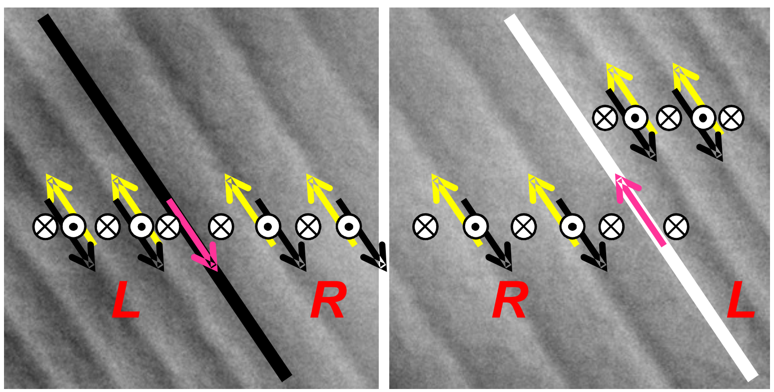
Soliton Formation

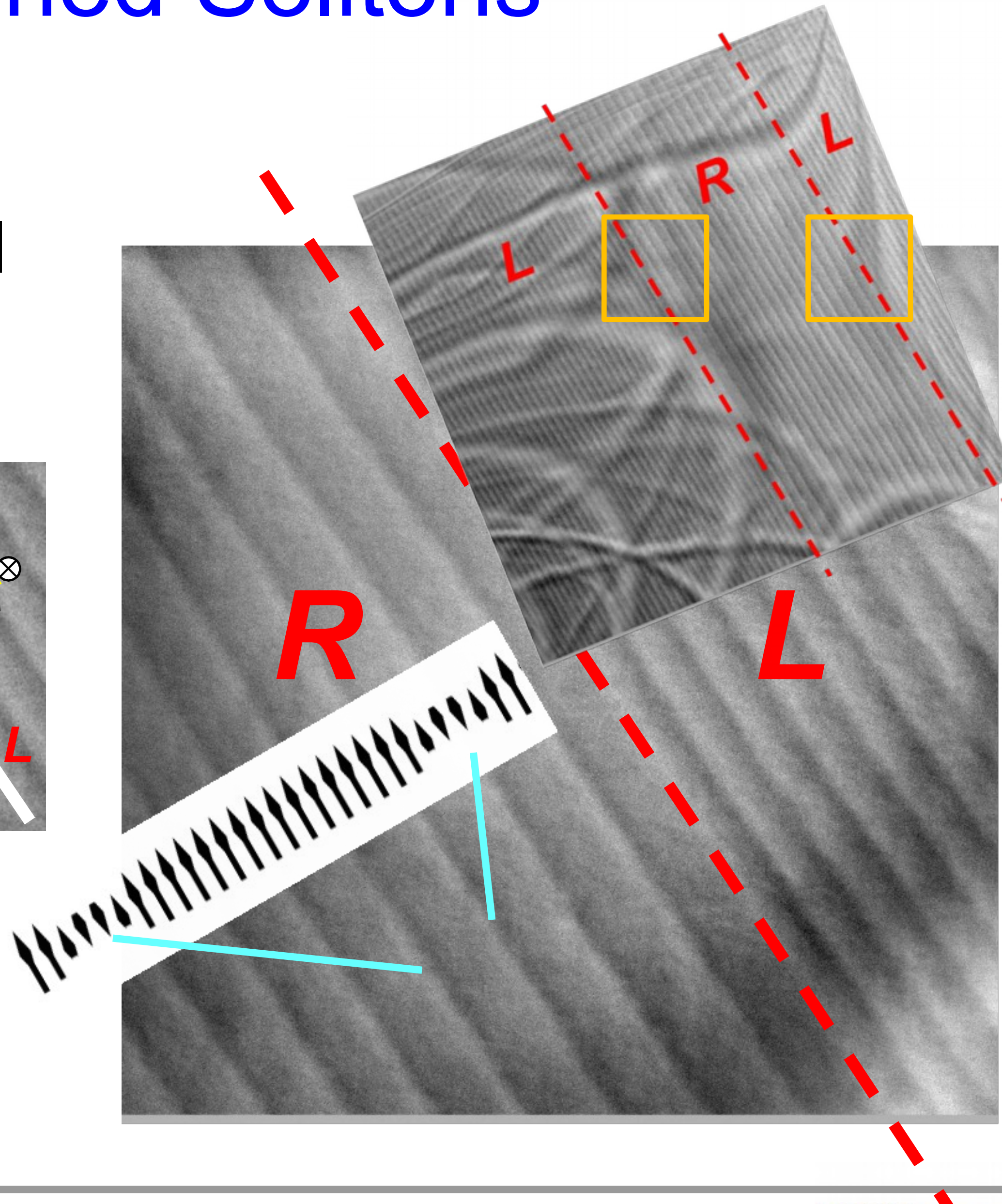


***note**: curl at end is amplified by this method of plotting*

Confined Solitons

Pinning & confinement by chiral **boundaries**





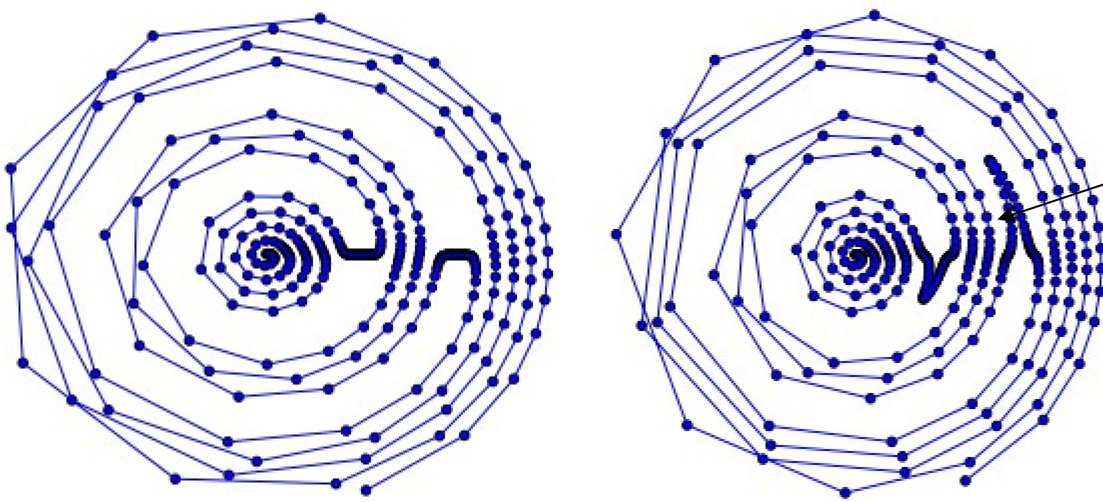
Lorentz TEM
(Y Togawa & S McVitie)

Confined Solitons

Chiral boundaries define twist direction reversal: creates soliton pinning sites

H = 0.2

H =0.2267



Nucleation occurs at chiral boundaries-- deformation of kinks produce solitons

Summary

- **Approximations**: Heisenberg exchange, anisotropy, mean field theory
- **Simulations**: Micromagnetic, Monte Carlo
- **Analytic models**: spin waves, domain walls, thermal activation

The End