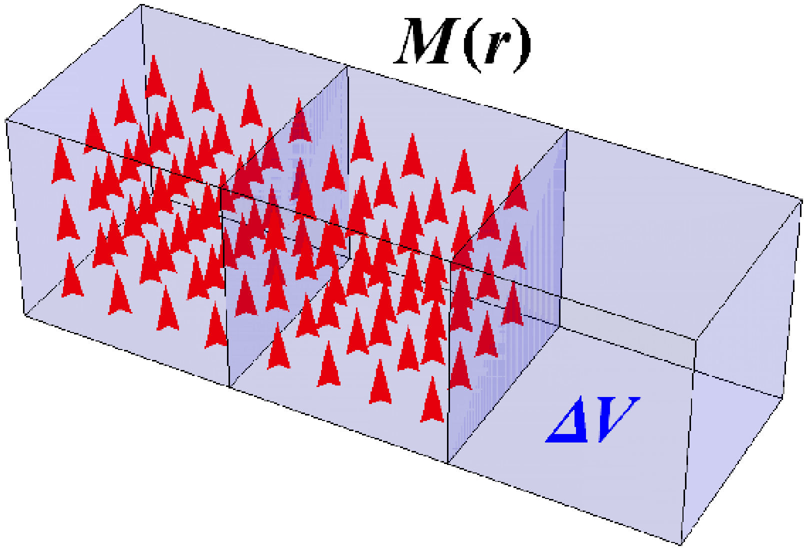
Micromagnetism and magnetization processes

Gianfranco Durin

Istituto Nazionale di Ricerca Metrologica (INRIM), Torino, Italy

lecture@ESM2021 - September 9-10, 2021

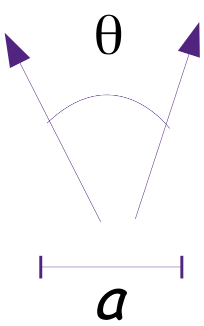
Free energy in the continuum approximation



- $M(r)$ is an average over the elementary volume ΔV
- The internal free energy $G(r)$ is no longer a function of a single moment, but a *functional* $G[M(r)]$ of $M(r)$
- The ground state is given by the energy minimum $\delta G[\delta M(r)] = 0$

The exchange in the continuum limit

$$\boxed{H_{ex} = -2\sum_{i>j} J_{ij}\vec{S}_i \cdot \vec{S}_j}$$



$$E_{ex} = -2\sum_{i>j} J_{ij}S^2\cos\theta_{ij} \cong JS^2\sum_{i>j}\theta_{ij}^2 + const$$

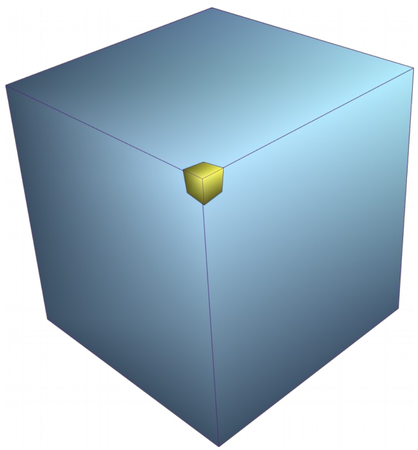
$$\boxed{\frac{E_{ex}}{V} = u_{ex} = A\left(\frac{\nabla M}{M}\right)^2}$$

Exchange stiffness $A = \frac{S^2a^2JN_v}{2} = 1 \div 2\ 10^{-11} J/m$

Energy terms

ENERGY TERM	Coeff.	Definition	Value	Units
Exchange	A	Mater. const.	10^{-11}	[J/m]
Anisotropy	K_u, K_1	Mater. const.	10^{2}-10^{7}	[J/m^3]
Stray field	K_d	$1/2\mu_o M_s^2$	0-3 10^{6}	[J/m^3]
External stress	$\lambda_s\sigma$	-	10^{2}-10^{5}	[J/m^3]
External field	$\mu_o M_s H$	-	1 - 10^{8}	[J/m^3]

Why materials are so different?



Let us introduce a <u>space-dependent</u> free energy G_L in the continuum limit:

(I) The static case

$$G_L[\vec{M};\vec{H}_a] = \int_V \underbrace{[A(|\nabla M_x|^2 + |\nabla M_y|^2 + |\nabla M_z|^2)+}_{\text{Exchange}}$$

$$+\underbrace{u_a(\vec{M})}_{\text{Anisotropy}} - \underbrace{\frac{\mu_o}{2}\vec{H}_d\cdot\vec{M}}_{\text{Magnetostatics}} - \underbrace{\mu_o\vec{H}_a\cdot\vec{M}]}_{\text{External field}}\, d^3r$$

It is always a good idea to NORMALIZE!

$$\boxed{\vec{m} = \vec{M}/M_s}$$

$$\boxed{f(\vec{m}) = \frac{1}{2K_1} u_a(\vec{M}/M_s)}$$

$$\vec{h}_d = \frac{\vec{H}_d}{M_s} \qquad \vec{h}_a = \frac{\vec{H}_a}{M_s} \qquad g_L = \frac{G_L}{\mu_o M_s^2 V}$$

$$\boxed{g_L[\vec{m}; \vec{h}_a] = \frac{1}{V} \int_V \left[\frac{l_{ex}^2}{2} (\nabla \vec{m})^2 + \kappa f(\vec{m}) - \frac{1}{2} \vec{h}_d \cdot \vec{m} - \vec{h}_a \cdot \vec{m} \right] d^3 r}$$

$$= g_{ex} + g_{an} + g_d + g_H$$

$$\boxed{l_{ex} = \sqrt{\frac{A}{K_d}} = \sqrt{\frac{2A}{\mu_o M_s^2}}}$$

$$\boxed{\kappa = \frac{K_1}{K_d} = \frac{2K_1}{\mu_o M_s^2} = \frac{H_{an}}{M_s}}$$

Classification of materials (I)

Soft and hard materials

$$\kappa = \frac{K_1}{K_d} = \frac{2K_1}{\mu_o M_s^2} = \frac{H_{an}}{M_s}$$

<< 1 SOFT

~ 1 HARD

TABLE D.1 Micromagnetic parameters

Material	T_c [K]	$\mu_0 M_s$ [T]	A [10^{-11} J m^{-1}]	K_1 [10^5 J m^{-3}]	κ	H_{AN} [10^5 Am^{-1}]	$(A\|K_1\|)^{1/2}$ [10^{-3} J m^{-2}]	l_{EX} [nm]	l_W [nm]	l_D [nm]
Fe	1044	2.16	~1.5	0.48	0.026	0.44	0.85	2.8	18	0.46
Co	1398	1.82	~1.5	5	0.38	5.5	2.7	3.4	5.5	2.05
Ni	627	0.62	~1.5	−0.057	0.037	0.18	0.29	9.9	51	1.9
γ-Fe_2O_3		0.52	~0.1	−0.046	0.043	0.18	0.068	3.05	15	0.63
CrO_2		0.5	~0.1	0.22	0.22	0.88	0.15	3.2	6.7	1.5
$BaFe_{12}O_{19}$	723	0.48	0.6	2.5	2.7	10	1.2	8.1	4.9	13
$Nd_2Fe_{14}B$	585	1.61	0.9	50	4.8	30	6.7	2.95	1.3	6.5
Sm_2Co_{17}	1100	1.29	2.5	33	5	51	9.1	6.1	2.75	14
$SmCo_5$	993	1.05	2.4	170	39	320	20	7.4	1.2	46

Classification of materials (II)

Large and small bodies: the exchange length

$$l_{ex} = \sqrt{\frac{A}{K_d}} = \sqrt{\frac{2A}{\mu_o M_s^2}}$$

> L SMALL (uniform M)

< L LARGE (non-uniform M)

TABLE D.1 Micromagnetic parameters

Material	T_c [K]	$\mu_0 M_s$ [T]	A [10^{-11} J m^{-1}]	K_1 [10^5 J m^{-3}]	κ	H_{AN} [10^5 Am^{-1}]	$(A\|K_1\|)^{1/2}$ [10^{-3} J m^{-2}]	l_{EX} [nm]	l_W [nm]	l_D [nm]
Fe	1044	2.16	~1.5	0.48	0.026	0.44	0.85	2.8	18	0.46
Co	1398	1.82	~1.5	5	0.38	5.5	2.7	3.4	5.5	2.05
Ni	627	0.62	~1.5	−0.057	0.037	0.18	0.29	9.9	51	1.9
γ-Fe_2O_3		0.52	~0.1	−0.046	0.043	0.18	0.068	3.05	15	0.63
CrO_2		0.5	~0.1	0.22	0.22	0.88	0.15	3.2	6.7	1.5
$BaFe_{12}O_{19}$	723	0.48	0.6	2.5	2.7	10	1.2	8.1	4.9	13
$Nd_2Fe_{14}B$	585	1.61	0.9	50	4.8	30	6.7	2.95	1.3	6.5
Sm_2Co_{17}	1100	1.29	2.5	33	5	51	9.1	6.1	2.75	14
$SmCo_5$	993	1.05	2.4	170	39	320	20	7.4	1.2	46

Classification of materials (III)

The exchange vs. anisotropy ratio

$$l_w = \sqrt{\frac{A}{K_1}} = \frac{l_{ex}}{\sqrt{\kappa}}$$

Domain formation

$$l_D = \frac{\sqrt{2AK_1}}{\mu_o M_s^2} = l_{ex}\sqrt{\kappa}$$

TABLE D.1 Micromagnetic parameters

Material	T_c [K]	$\mu_0 M_s$ [T]	A [10^{-11} J m^{-1}]	K_1 [10^5 J m^{-3}]	κ	H_{AN} [10^5 Am^{-1}]	$(A\|K_1\|)^{1/2}$ [10^{-3} J m^{-2}]	l_{EX} [nm]	l_W [nm]	l_D [nm]
Fe	1044	2.16	~1.5	0.48	0.026	0.44	0.85	2.8	18	0.46
Co	1398	1.82	~1.5	5	0.38	5.5	2.7	3.4	5.5	2.05
Ni	627	0.62	~1.5	−0.057	0.037	0.18	0.29	9.9	51	1.9
γ-Fe_2O_3		0.52	~0.1	−0.046	0.043	0.18	0.068	3.05	15	0.63
CrO_2		0.5	~0.1	0.22	0.22	0.88	0.15	3.2	6.7	1.5
$BaFe_{12}O_{19}$	723	0.48	0.6	2.5	2.7	10	1.2	8.1	4.9	13
$Nd_2Fe_{14}B$	585	1.61	0.9	50	4.8	30	6.7	2.95	1.3	6.5
Sm_2Co_{17}	1100	1.29	2.5	33	5	51	9.1	6.1	2.75	14
$SmCo_5$	993	1.05	2.4	170	39	320	20	7.4	1.2	46

Energy minimization

$$g_L[\vec{m};\vec{h}_a] = \frac{1}{V}\int_V \left[\frac{l_{ex}^2}{2}(\nabla\vec{m})^2 + \kappa f(\vec{m}) - \frac{1}{2}\vec{h}_d\cdot\vec{m} - \vec{h}_a\cdot\vec{m}\right] d^3r$$

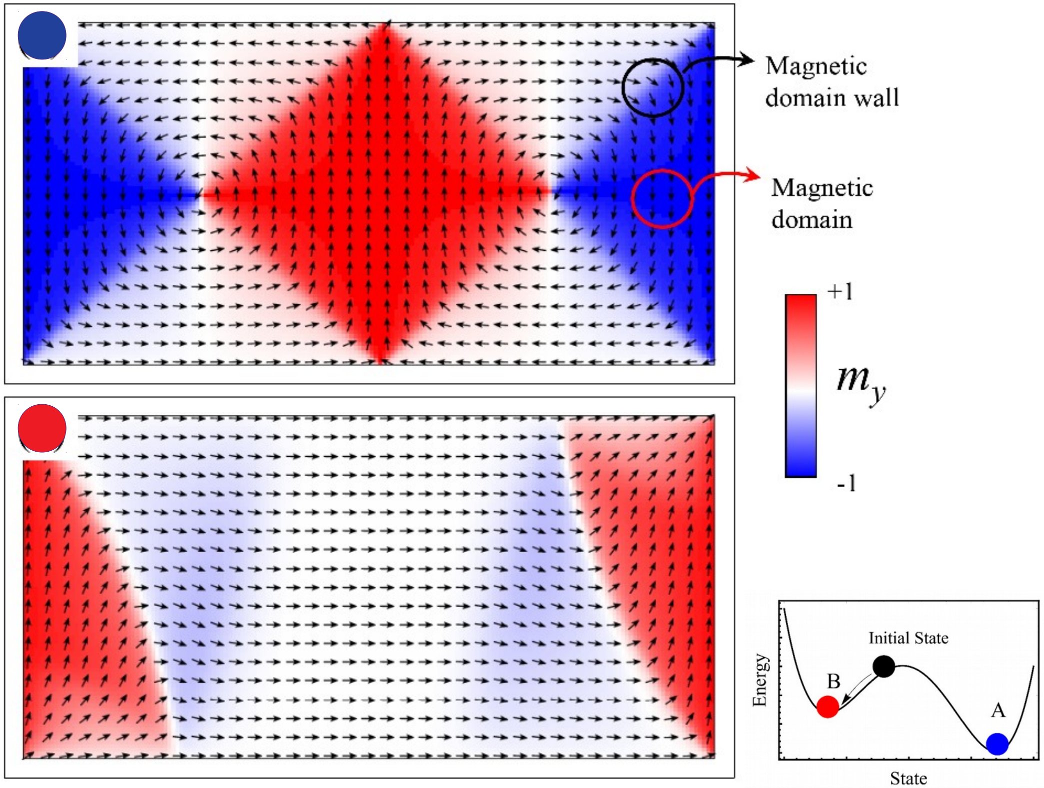
$$\boxed{\delta g_L[\delta\vec{m}] = 0}$$

... skipping ...

$$\vec{h}_{eff} = \frac{\partial g_L(\vec{m})}{\partial \vec{m}}$$

$$\vec{m}\times\vec{h}_{eff} = 0 \qquad \forall r \in V$$

$$\vec{m}\times\frac{\partial\vec{m}}{\partial n} = 0 \qquad \forall r \in S$$

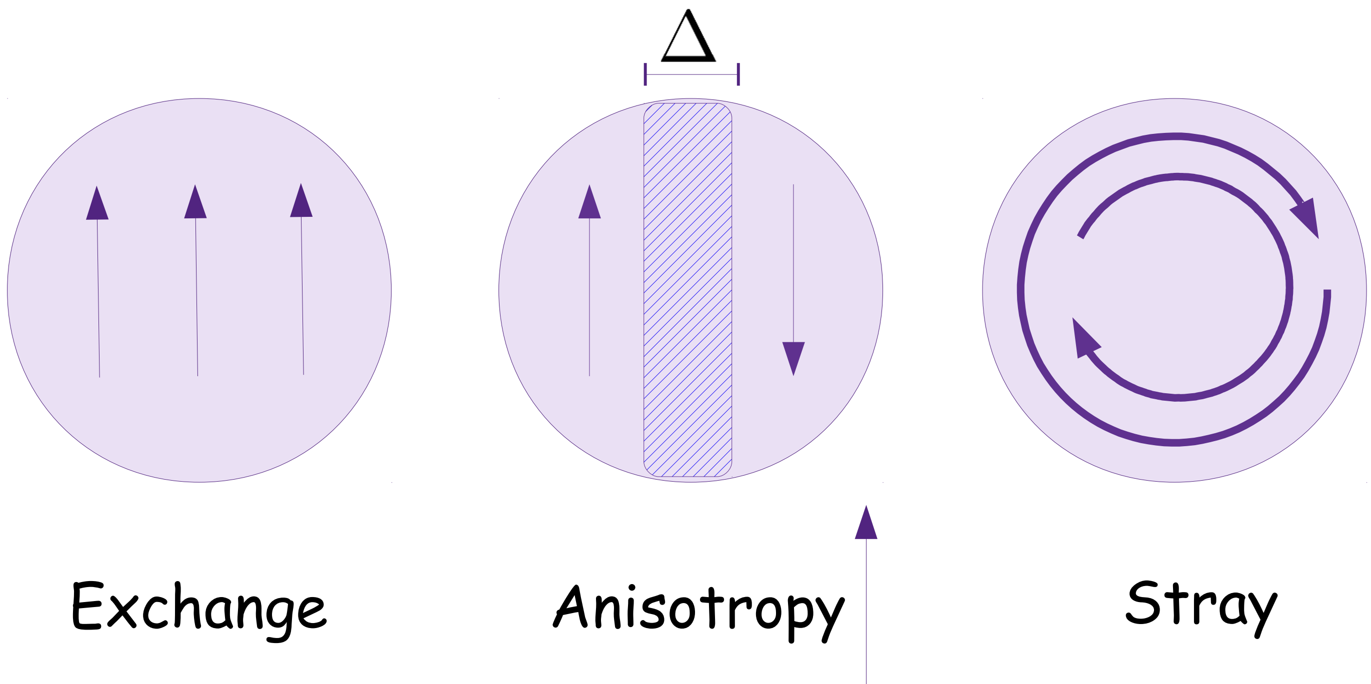


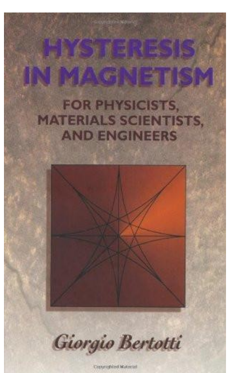
Competing energies

What is the magnetization configuration in a body?

Minimize the free energy above! (ps. difficult)

Sphere of radius R



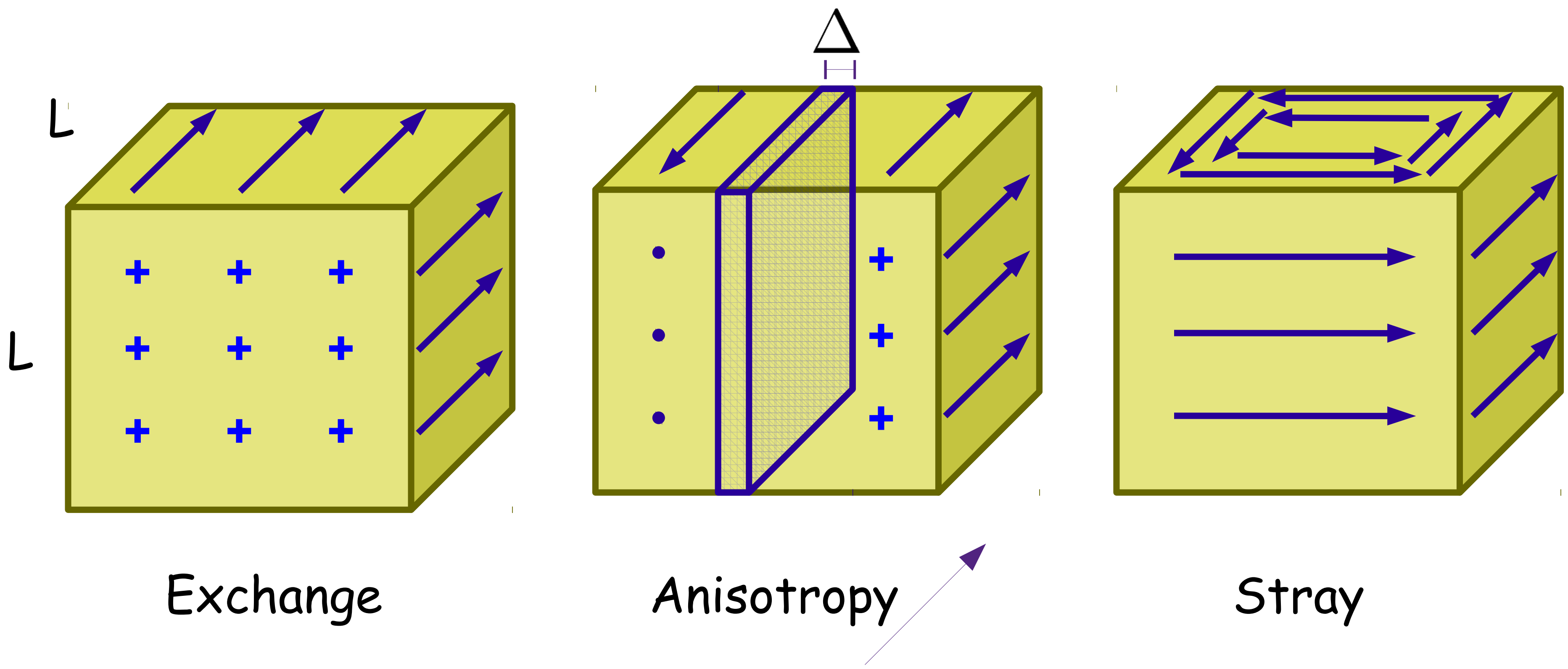


(Thanks to G. Bertotti)

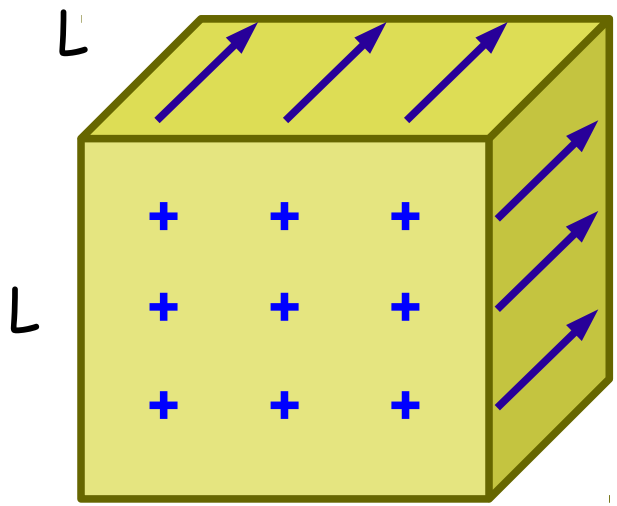
Competing energies

What is the magnetization configuration in a body?

Minimize the free energy above! (ps. difficult)



Competing energies (case I)



Exchange

Not only exchange but also anisotropy energies are minimized

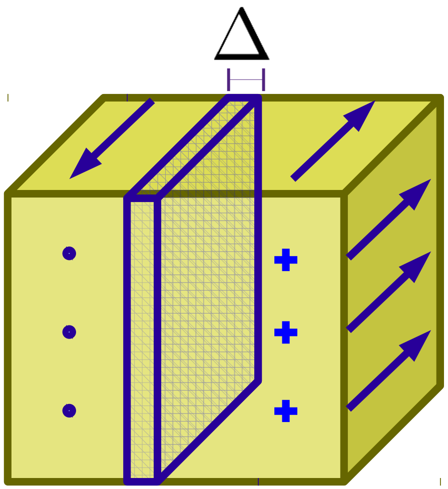
$$g_{ex} = g_{an} = 0$$

Demagnetizing factor of a cube ~ 1/3

$$g_I = g_d = \frac{1}{6}$$

This is independent of the body size!

Competing energies (case II)



Exchange and anisotropy relevant the transition region

$$g_L \cong \frac{1}{V}\int_V \left[\frac{l_{ex}^2}{2}(\nabla\vec{m})^2 + \kappa f(\vec{m})\right] d^3r$$

$g_d \approx 0$, and m rotates out of plane (for inst.)

2 components of m change by ~ 1 over Δ/2;
the region occupies ~ ΔL²/L³ of the volume

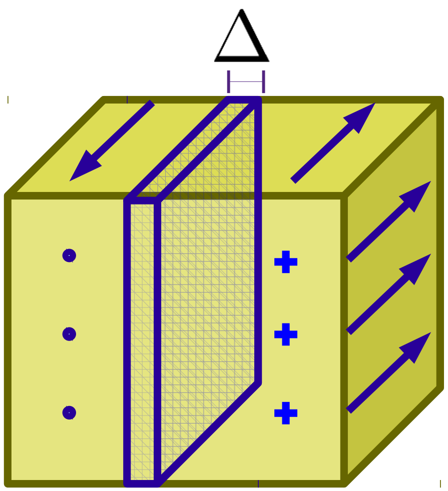
$$g_{ex} \sim \frac{l_{ex}^2}{2}\frac{8}{\Delta^2}\frac{\Delta}{L} = \frac{4l_{ex}^2}{\Delta L}$$

assuming Uniaxial anisotropy f(m) = sin²θ / 2
averaged over the Δ/L

$$g_{an} \sim \frac{\kappa}{4}\frac{\Delta}{L}$$

$$g_{II} = g_{ex} + g_{an} + g_d \cong \frac{1}{L}\left[\frac{4l_{ex}^2}{\Delta} + \frac{\kappa\Delta}{4}\right]$$

Competing energies (case II)



Anisotropy

$$g_{II} = g_{ex} + g_{an} + g_d \cong \frac{1}{L}\left[\frac{4l_{ex}^2}{\Delta} + \frac{\kappa\Delta}{4}\right]$$

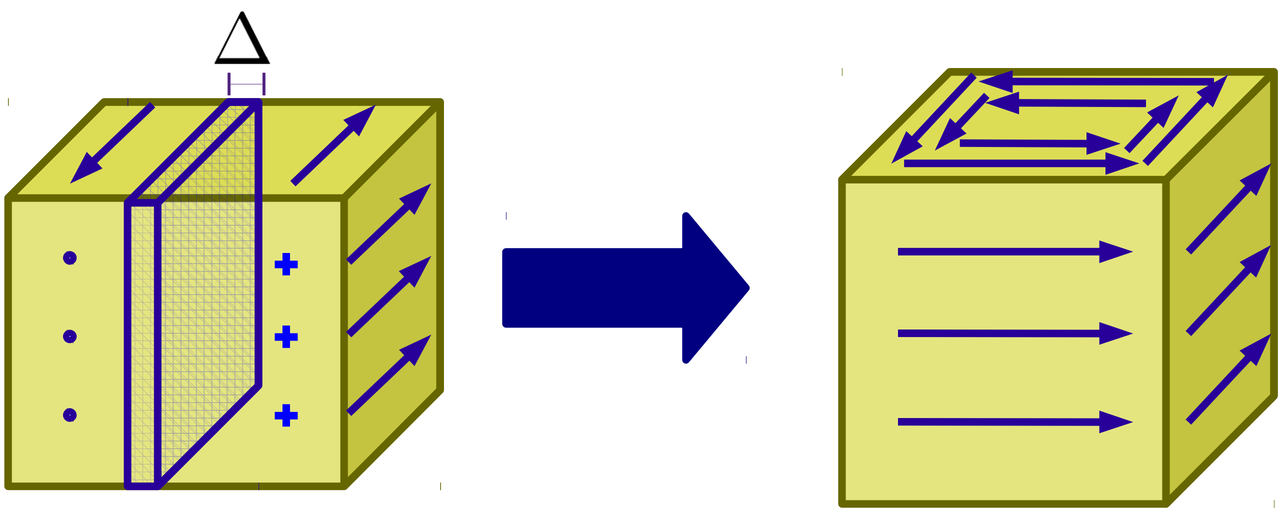
$$\boxed{\frac{4l_{ex}^2}{\Delta} = \frac{\kappa\Delta}{4}}$$

Domain wall width

$$\Delta = 4\,\frac{l_{ex}}{\sqrt{\kappa}} = 4\,l_w$$

$$\boxed{g_{II} \cong \frac{2l_{ex}\sqrt{\kappa}}{L} = \frac{2l_D}{L}}$$

Competing energies (case III)



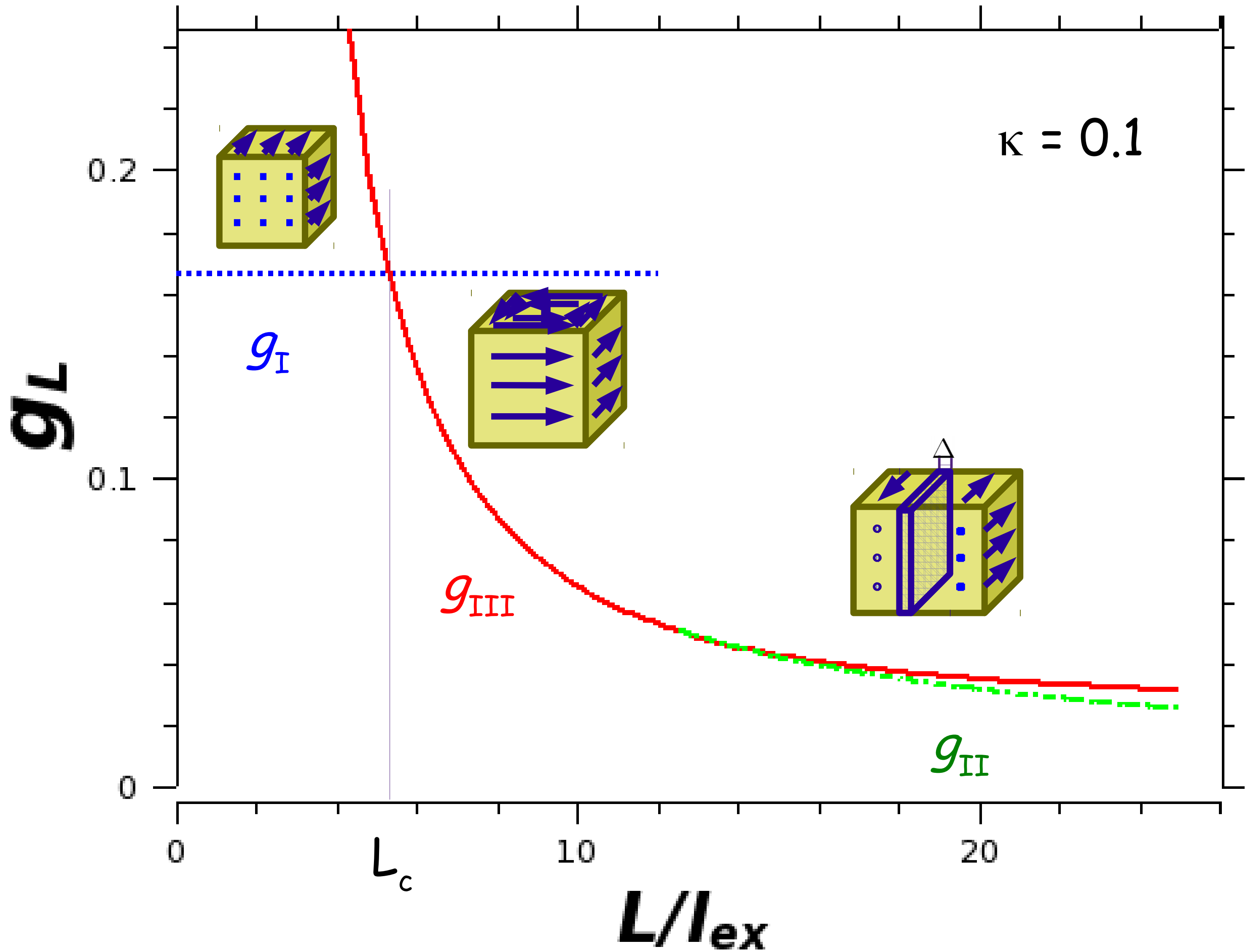
when Δ => L

$$g_{III} = g_{ex} + g_{an} + g_d \cong \frac{4l_{ex}^2}{L^2} + \frac{\kappa}{4}$$

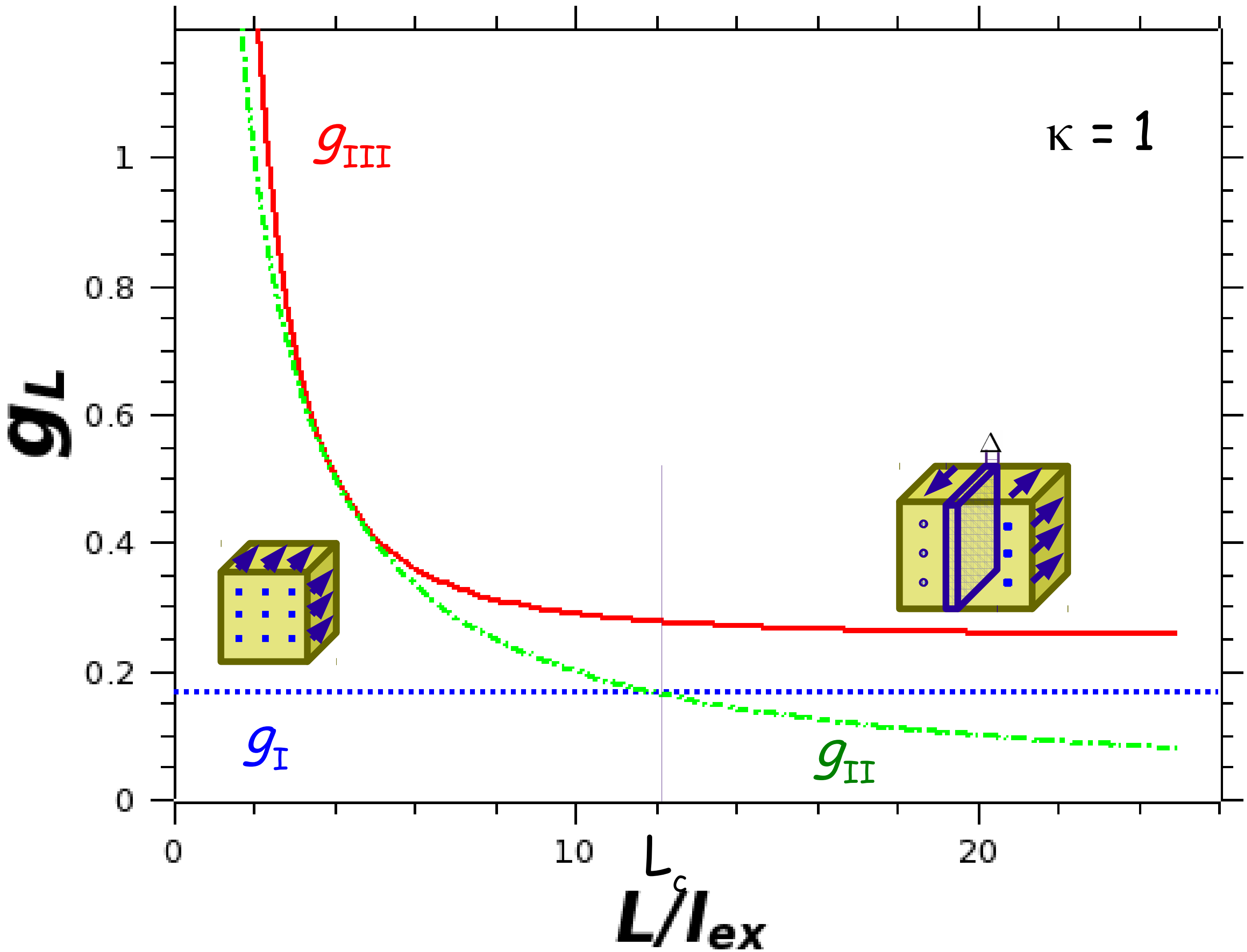
vs.

$$g_I = g_d = \frac{1}{6}$$

Competing energies: soft material (low κ)



Competing energies: hard material (high κ)



Competing energies (comments)

Small particles: uniform magnetization along an easy axis (depend on the field history)

Large bodies: much more complicated magnetization configuration (vortex, domains)

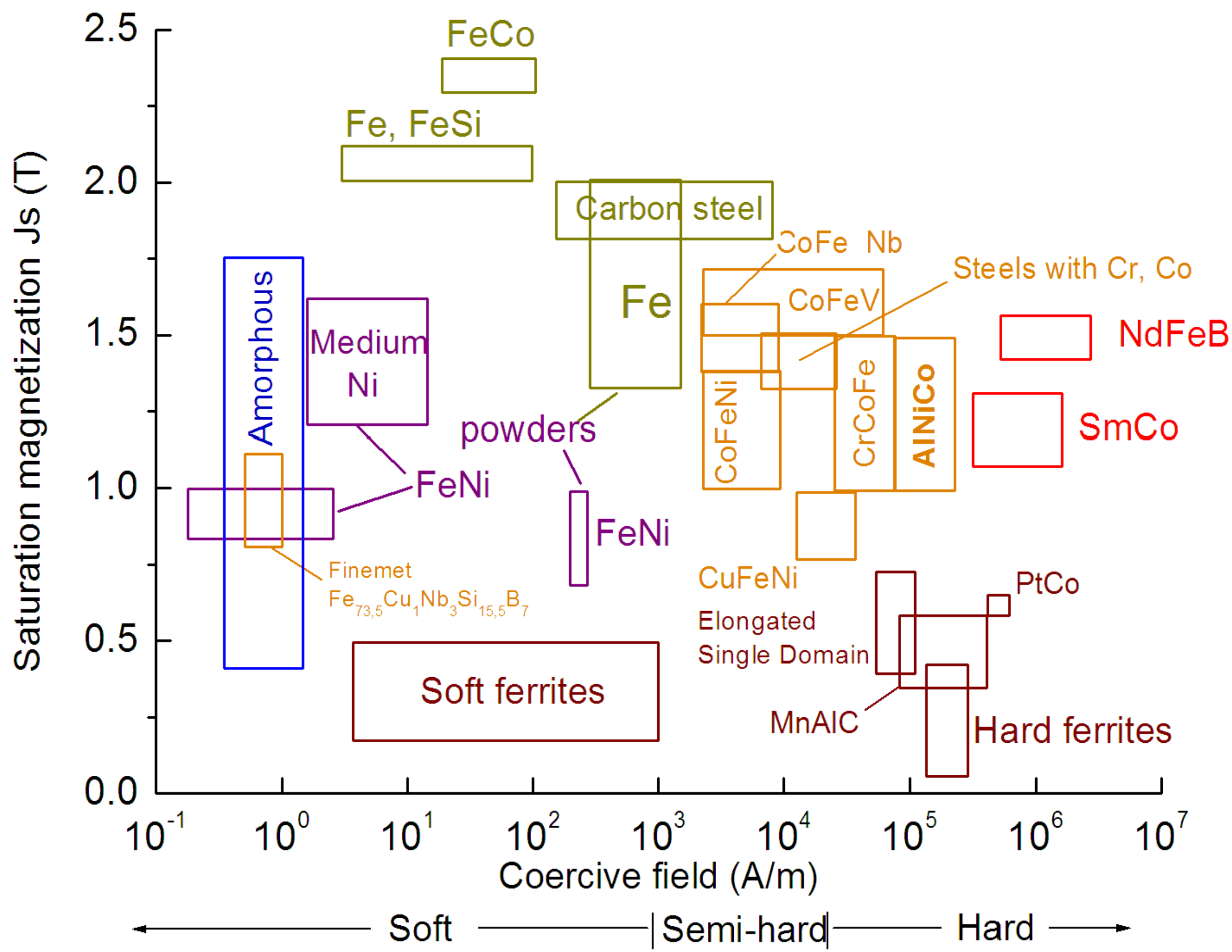
Hysteresis: there are metastable states, separated by energy barriers (strongly depend on the field history)

Magnetization configurations: in general are much more complicated --> micromagnetism, domain theory

Magnetostatic effects: shape is important (as you know)

Disorder: real materials are more or less disordered

Real magnetic materials



Dynamics of magnetization

Let us consider the temporal evolution of the magnetization toward the equilibrium state

(II) The dynamic case:
Landau-Lifshitz (LL) and
Landau-Lifshitz-Gilbert (LLG) equation

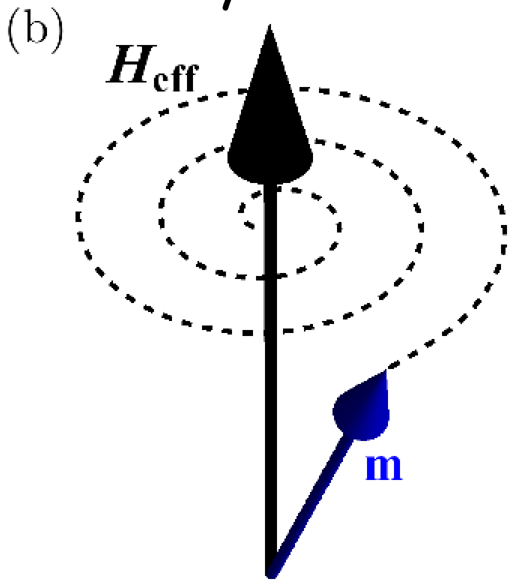
statics

$$\vec{h}_{eff} = \frac{\partial g_L(\vec{m})}{\partial \vec{m}}$$

$$\vec{m} \times \vec{h}_{eff} = 0 \qquad \forall r \in V$$

$$\vec{m} \times \frac{\partial \vec{m}}{\partial n} = 0 \qquad \forall r \in S$$

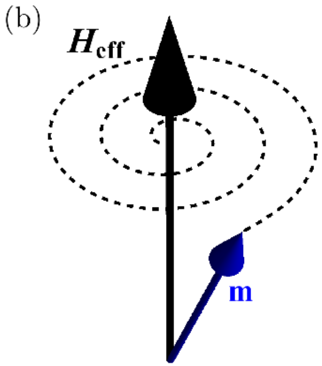
dynamics



The LL and LLG equations

$$\frac{d\vec{m}}{dt} = precession + dissipation$$

$$\frac{d\vec{m}}{dt} = -\gamma_0(\vec{m} \times \vec{H}_{eff}) + dissipation$$

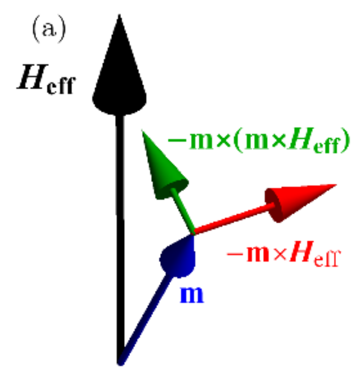


$$\boxed{\frac{d\vec{m}}{dt} = -\gamma_0'(\vec{m} \times \vec{H}_{eff}) - \alpha_{LL}\vec{m} \times (\vec{m} \times \vec{H}_{eff})}$$

LL

$$\boxed{\frac{d\vec{m}}{dt} = -\gamma_0(\vec{m} \times \vec{H}_{eff}) + \alpha(\vec{m} \times \frac{d\vec{m}}{dt})}$$

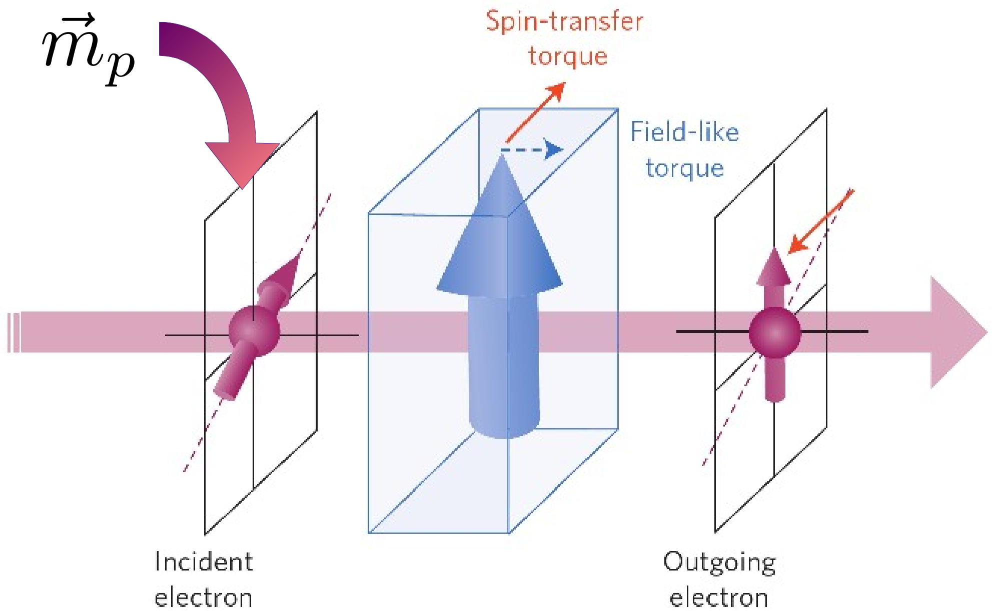
LLG

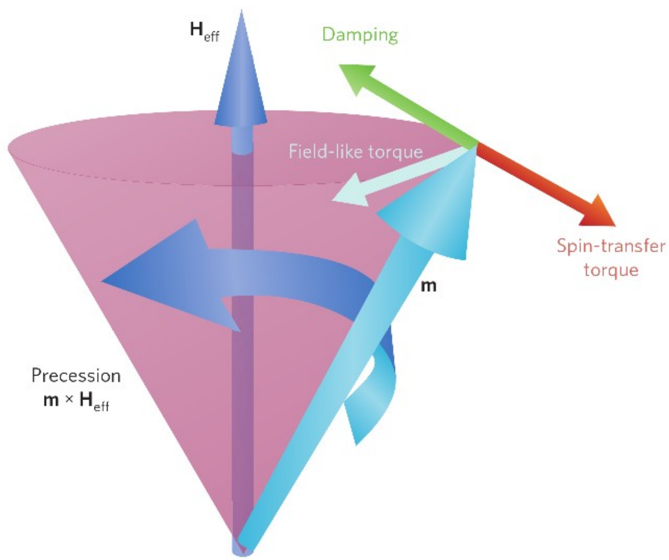


$$\alpha_{LL} = \gamma_0\alpha/(1+\alpha^2) \quad ; \quad \gamma_0' = \gamma_0/(1+\alpha^2)$$

$$\alpha = 10^{-3}(Py) \div 0.3(PMA) \qquad \gamma_0 = |\gamma\mu_0| = 2.21 \times 10^5 rad \cdot m \cdot A^{-1} \cdot s^{-1}$$

The Spin Transfer Torque





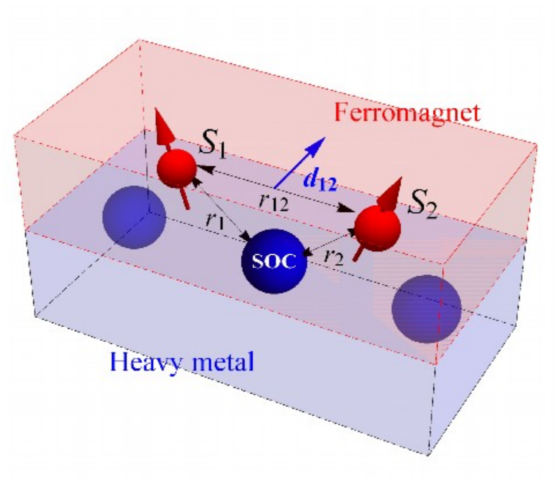
$$\tau_{SLT} = \frac{|g|}{2}\frac{\mu_B J P}{M_s|e|d}[\vec{m} \times (\vec{m} \times \vec{m}_p)]$$

Adiabatic SST or Slonczewski-like STT

$$\tau_{SLT} = -\frac{|g|}{2}\frac{\mu_B P \xi}{M_s|e|(1+\xi^2)}\left[\vec{m} \times (\vec{J} \cdot \vec{\nabla})\vec{m}\right]$$

Non-adiabatic SST, field-like STT or Zhang-Li STT

The Dzyaloshinskii-Moriya interaction



Super-exchange interaction mediated
by an high Spin-Orbit Coupling metal

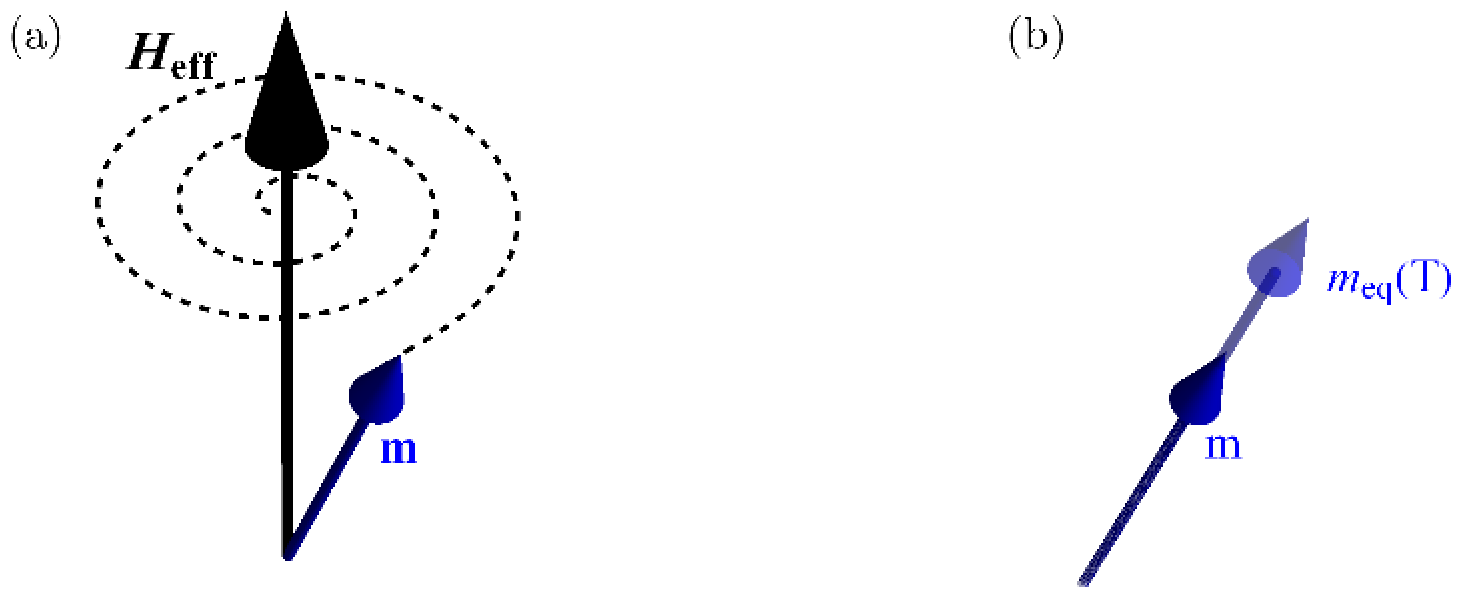
$$E_{DMI} = \sum_{ij} \vec{D}_{ij} \cdot (\vec{S}_i \times \vec{S}_j)$$

$$\vec{H}_{DMI} = \frac{2D}{\mu_0 M_s} \left[\nabla m_z - (\vec{\nabla} \cdot \vec{m}) \vec{u}_z \right]$$

$$= \frac{2D}{\mu_0 M_s} \left[\frac{\partial m_z}{\partial x} \widehat{\mathbf{x}} + \frac{\partial m_z}{\partial y} \widehat{\mathbf{y}} + \left(\frac{\partial m_z}{\partial x} + \frac{\partial m_z}{\partial x} \right) \widehat{\mathbf{z}} \right]$$

$$\frac{\partial \vec{m}}{\partial n} = \frac{D}{2A} \left[\vec{m} \times (\widehat{\mathbf{z}} \times \widehat{\mathbf{n}}) \right]$$

Thermal effects: the LL-Bloch eq.



- Needed when close to T_c
- Add a longitudinal damping parameter
- The effective field changes with the temperature
- The material's parameters change as well
- Thermal field is introduced using fluctuation-dissipation theorem

Available codes

Language: C++
Method: finite differences
Licence: Open-source

OOMMF is a project in the Applied and Computational Mathematics Division (ACMD) of ITL/NIST, in close cooperation with μMAG, aimed at developing portable, extensible public domain programs and tools for micromagnetics. This code forms a completely functional micromagnetics package, with the additional capability to be extended by other programmers so that people developing new code can build on the OOMMF foundation. (math.nist.gov/oommf/)

Language: Go
Method: finite differences
Licence: Open-source

mumax3 is a GPU-accelerated micromagnetic simulation program developed at the DyNaMat group of Prof. Van Waeyenberge at Ghent University. The code is written and maintained by Arne Vansteenkiste. A speed-up of the order of 100x compared to CPU-based simulations can easily be reached, even with relatively inexpensive gaming GPUs. Additionally, the software is optimized for low memory use and can handle about 16 million FD cells with 2GB of GPU RAM. (mumax.github.io/)

Language: C++, Cuda
Method: multi-mesh finite elements
Licence: Open-source

Boris Computational Spintronics is a multi-physics software designed to solve three-dimensional magnetisation dynamics problems, coupled with a self-consistent charge and spin transport solver, heat flow solver with temperature-dependent material parameters, and mechanical stress-strain solver in arbitrary multi-layered structures and shapes.
The software is intended for research and design of spintronics devices, as well as analysis and modelling of experimental results. (www.boris-spintronics.uk/)

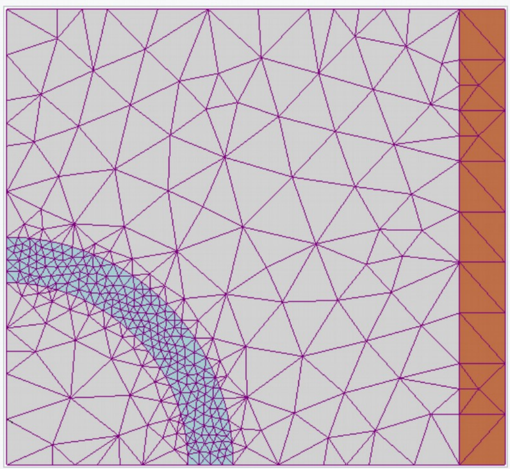
Language: Python
Method: finite elements
Licence: Open-source

Nmag is a micromagnetic simulation package. It has been developed at the University of Southampton with substantial contributions from Hans Fangohr, Thomas Fischbacher, Matteo Franchin. It is released under the GNU GPL. (nmag.soton.ac.uk/nmag/)

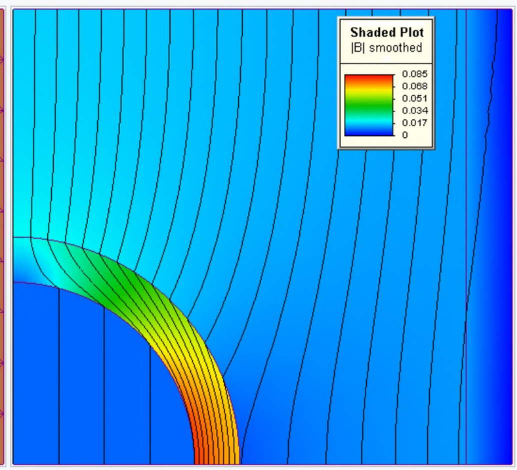
Currently, there is no significant amount of funding or man power available to support Nmag users or develop it further. The software should thus be seen to be provided as is.

Finite differences vs finite elements

The FEM is a general numerical method for solving partial differential equations in two or three space variables (i.e., some boundary value problems). To solve a problem, the FEM subdivides a large system into smaller, simpler parts that are called **finite elements**. This is achieved by a particular space discretization in the space dimensions, which is implemented by the construction of a mesh of the object: the numerical domain for the solution, which has a finite number of points. The finite element method formulation of a boundary value problem finally results in a system of algebraic equations. The method approximates the unknown function over the domain.

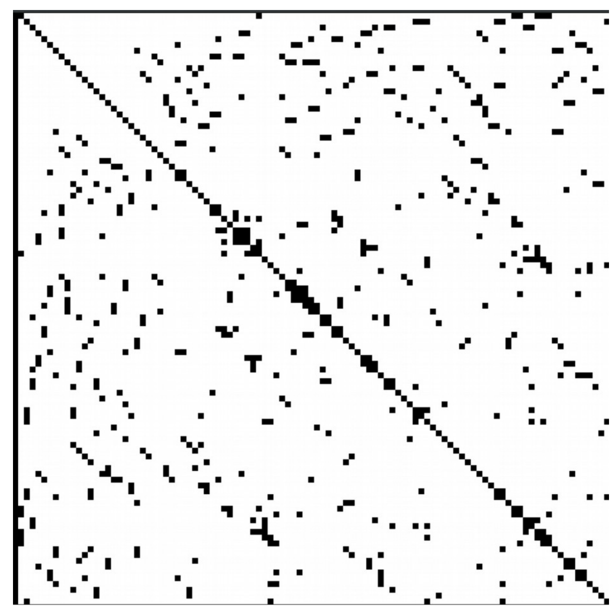


FEM mesh created by an analyst prior to finding a solution to a magnetic problem using FEM software. Colors indicate that the analyst has set material properties for each zone, in this case, a conducting wire coil in orange; a ferromagnetic component (perhaps iron) in light blue; and air in grey. Although the geometry may seem simple, it would be very challenging to calculate the magnetic field for this setup without FEM software, using equations alone.



FEM solution to the problem at left, involving a cylindrically shaped magnetic shield. The ferromagnetic cylindrical part is shielding the area inside the cylinder by diverting the magnetic field created by the coil (rectangular area on the right). The color represents the amplitude of the magnetic flux density, as indicated by the scale in the inset legend, red being high amplitude. The area inside the cylinder is the low amplitude (dark blue, with widely spaced lines of magnetic flux), which suggests that the shield is performing as it was designed to.

Sparse matrix



Voronoi tessellation

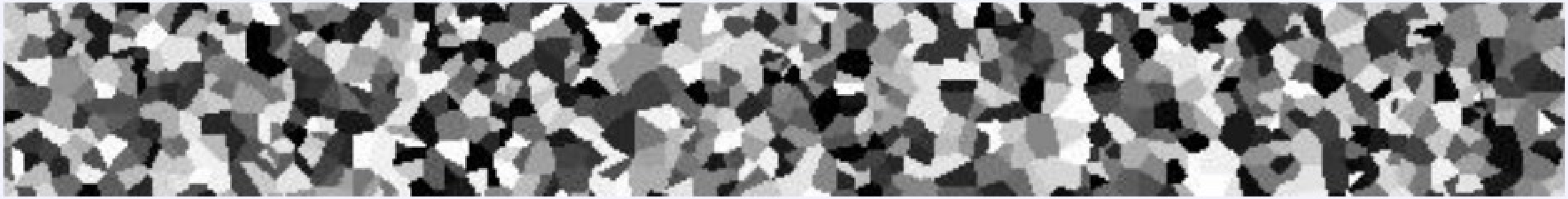
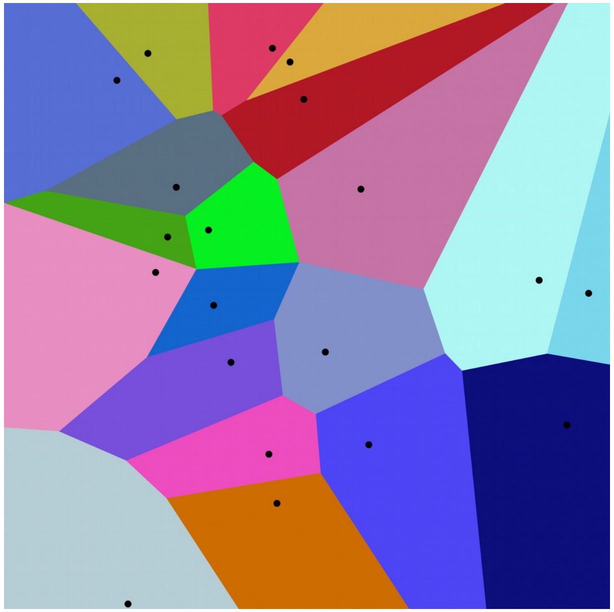
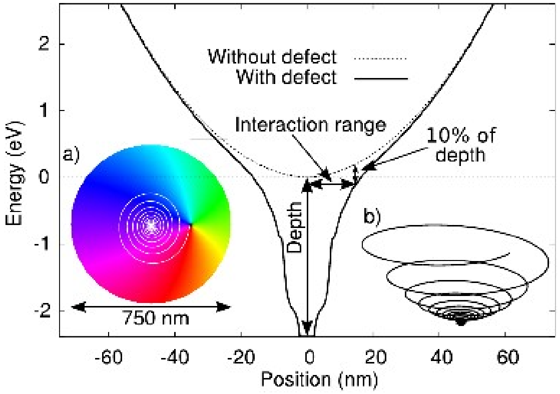


Figure 2.32: An example of a nanowire with a surface of $1600 \times 200\,\mathrm{nm}^2$ subdivided into Voronoi cells (gray scale) with an average diameter of 20 nm.



Realistic defects in simulations

- Reduce by 30% the exchange at the boundaries
- M_s in the cells reduced down to 50%



A couple of good 'references'

Universidad de Salamanca
Departamento de Fisica Aplicada

VNiVERSiDAD D SALAMANCA
CAMPUS OF INTERNATIONAL EXCELLENCE

Doctoral Thesis

Micromagnetic study of magnetic domain wall motion: thermal effects and spin torques

A thesis submitted in fulfilment of the requirements for the degree of doctor of philosophy (Ph.D.) in Applied Physics and Technology at the University of Salamanca

Candidate
Simone Moretti

Supervisor
Dr. Eduardo Martinez

UNIVERSITEIT GENT
FACULTY OF SCIENCES

Magnetic disorder and thermal fluctuations in domain wall motion and nanoparticle dynamics

Jonathan Leliaert