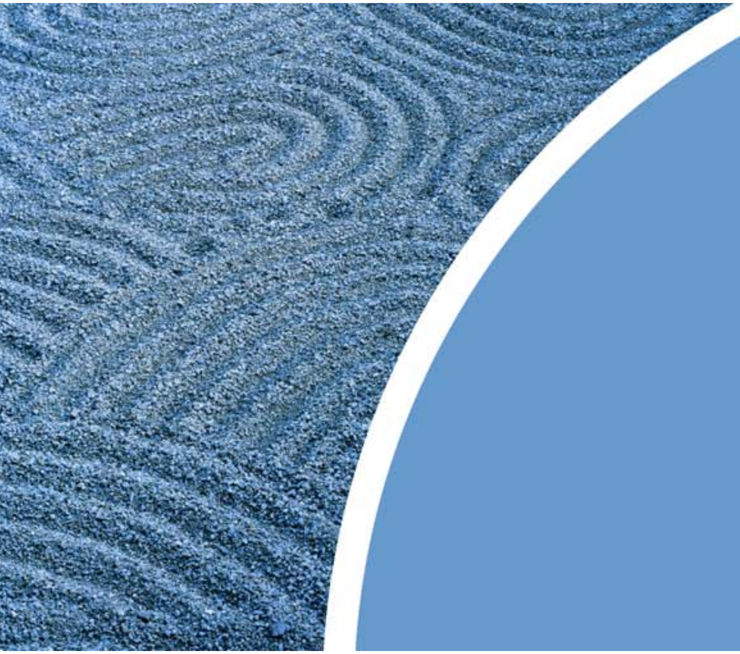


Computational Applied Magnetics

Olle Heinonen
Seagate Technology

Seagate
We turn on ideas

Computational applied magnetics - micromagnetics

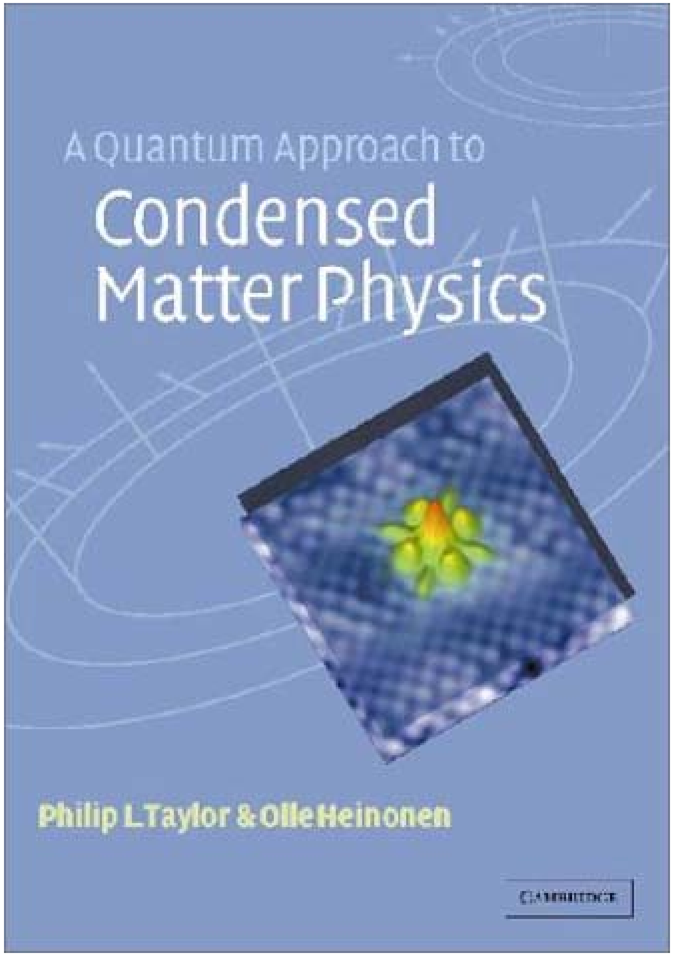
Olle Heinonen, Seagate Technology

Thanks to Jan van Ek, Martin Plumer, Greg Parker

My background, what I do

- Condensed Matter Theory (quantum Hall effect, Fermi liquids, polymer physics, low-dimensional magnets, mesoscopic transport, density functional theory)
- First principle electronic and magnetic structure calculations, semi-classical transport in spin valves,
- Micromagnetic modeling, finite-temperature micromagnetic calculations, thermal magnetic noise; reader and writer design/modeling
- Contact: Olle.G.Heinonen@seagate.com

Interesting reading



A Quantum Approach to

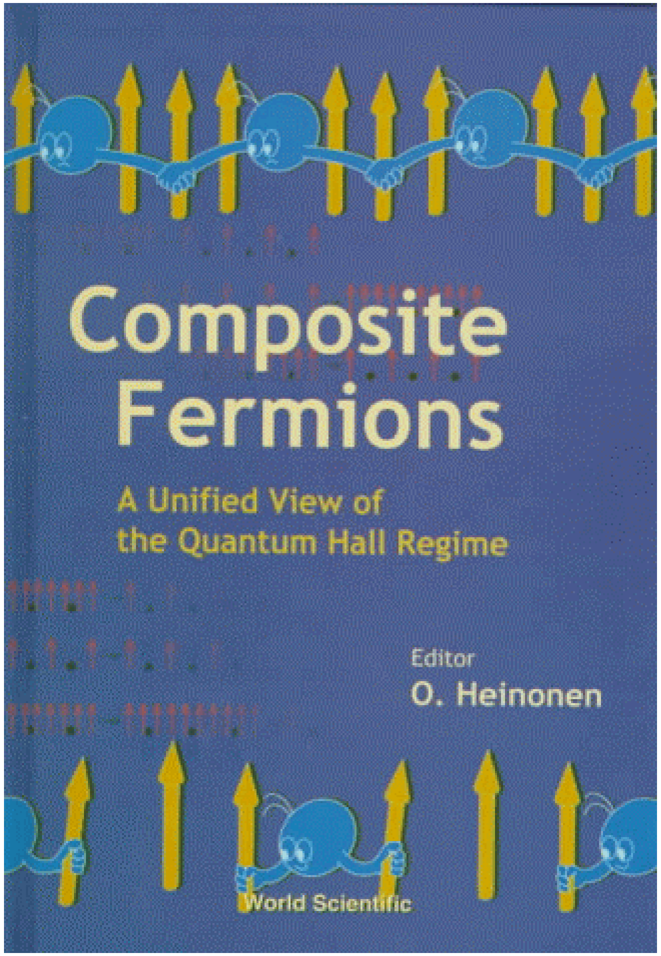
Condensed Matter Physics

Philip L Taylor & Olle Heinonen

CAMBRIDGE

Many Particle Theory

by E.K.U. Gross, E. Runge, O. Heinonen



Composite Fermions

A Unified View of the Quantum Hall Regime

Editor

O. Heinonen

World Scientific

Course Objectives

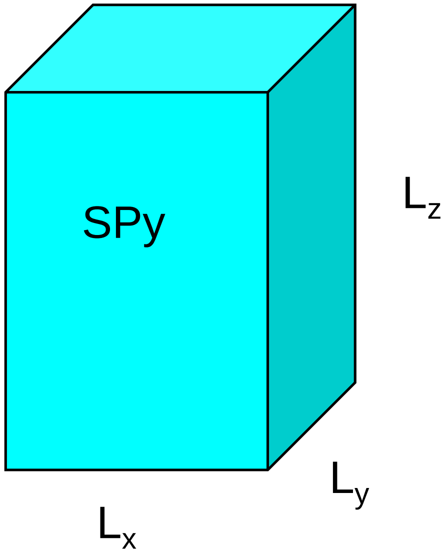
- Provide intuition for the physical behavior of micron-and sub-micron size magnetism
- Contrast traditional macroscopic approaches and concepts with those of micromagnetic approaches
- Provide an understanding for the basics of micromagnetics, its applicability and limitations
- Provide background so you can bang together and run a micromagnetic code

Course Outline

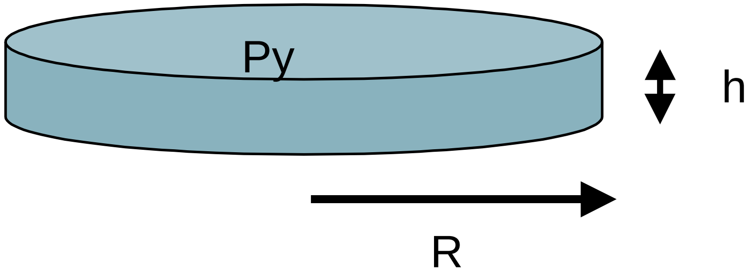
- Susceptibility - introduction
- Maxwell’s equations and constitutive relations - quick review
- Linear response
- Poles and demagnetizing fields
- More demagnetizing fields and the Pole Avoidance Principle
- (Paramagnets, diamagnets and ferromagnets)
- (Transition metals)
- Heisenberg model of exchange and ferromagnets
- Basic ingredients in micromagnetics: exchange, Zeeman, and magnetostatic energy, and approximations
- Domain walls and anisotropy, exchange length
- (Stoner-Wohlfart model)
- Micromagnetic energy minimization, torque equations
- Landau-Lifshitz-Gilbert (LLG) equation
- Micromagnetics at finite temperatures
- Thermal magnetic noise

Introduction

Question: What are the susceptibilities of the systems below?



a	b
L_x=15 mm	L_x=0.15 μm
L_y=0.5 mm	L_y=0.005 μm
L_z=30 mm	L_z=0.3 μm



a	b
R=8 mm	R=400 nm
h=1.0 mm	h=50 nm

How is susceptibility measured? What is it?

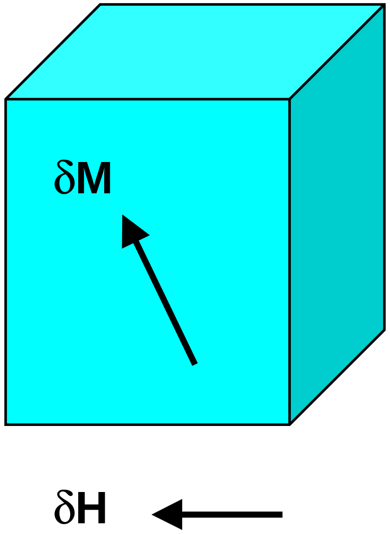
1. Prepare system in a specific magnetic state $\mathbf{M}_0$ (usually, *but not always*, $\mathbf{M}_0$=0). Note: $\mathbf{M}_0$ is in general not a uniform magnetization density

2. Apply a *small* magnetic field δ**H** in a specific direction

3. Measure the resulting *change* in magnetization δ**M**

4. Susceptibility χ is defined as

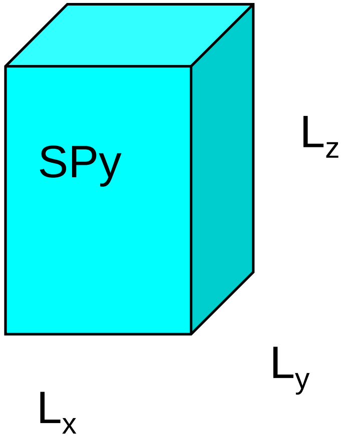
$$\boxed{\overleftrightarrow{\chi} = \frac{\delta\vec{M}}{\delta\vec{H}}}$$



Note:

- The susceptibility depends on the initial state $\mathbf{M}_0$
- δ**M** is magnetization density *averaged* over the system. This is OK if the magnetization density is uniform on a macroscopic scale. What if it's not?
- δ**M** and δ**H** need not be in the same direction, in which case χ is a tensor.
- The susceptibility is closely related to the permeability μ

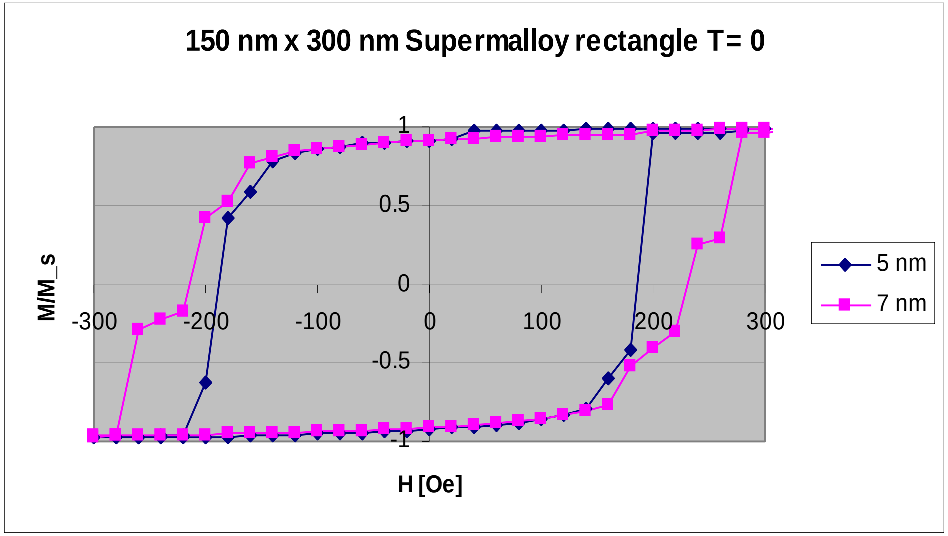
Susceptibility of Supermalloy rectangles



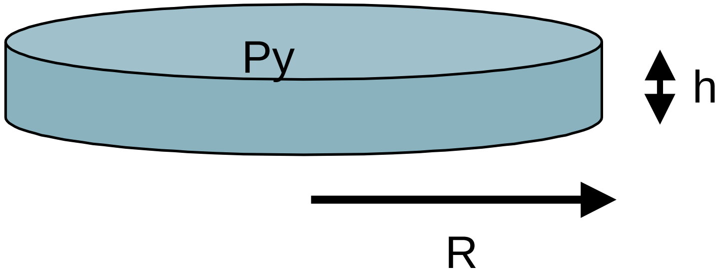
a	b
L_x=15 mm	L_x=0.15 μm
L_y=0.5 mm	L_y=0.005 μm
L_z=30 mm	L_z=0.3 μm

For macroscopic system, no coercivity and large susceptibility and permeability.

For microscopic system, large coercivity and small initial susceptibility and permeability.


150 nm x 300 nm Supermalloy rectangle T= 0

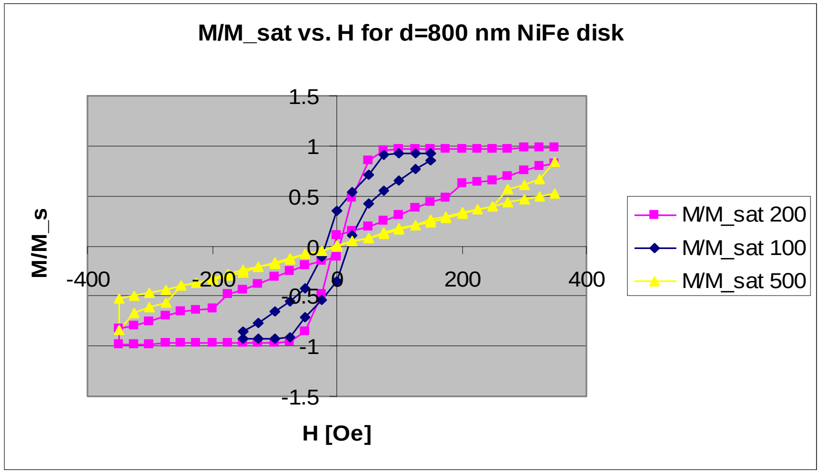
Susceptibility of disks

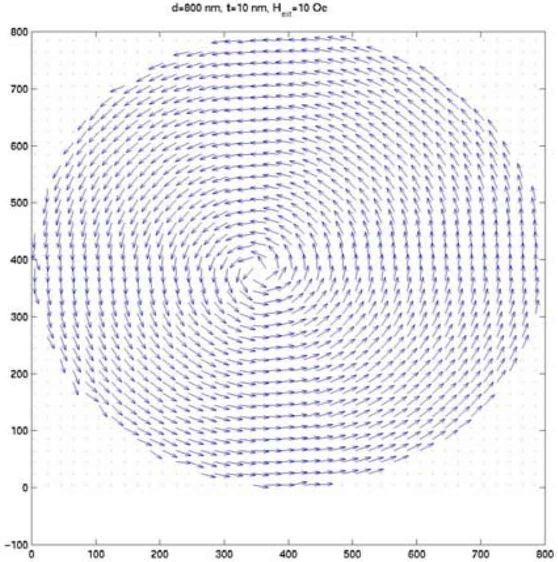


a	b
R=8 mm	R=400 nm
h=1.0 mm	h=50 nm

For case a, system is macroscopic and the susceptibility and permeability can be looked up (*e.g.*, Bozorth), μ=10,000 for $Ni_{80}Fe_{20}$ initial permeability

For case b, one obtains μ=25 with **H** in plane of disk





Conclusion

When the system under consideration is so small that the magnetization density cannot be considered uniform, the magnetic behavior of the system cannot be obtained from that of a larger system simply by scaling,

e.g., **μ(large system) is not equal to μ(small system).**

Permeability and susceptibility are not useful concepts for micron- and sub-micron size magnetic systems.

The relevant length scale is set by the size of the exchange length (about 1000 A in Py), which characterizes over what distance the magnetization can change.

Electromagnetism (cgs units)

Electromagnetism is completely described by Maxwell’s equations:

$$\nabla \bullet \vec{E} = 4\pi\rho(\vec{r})$$

Gauss’ law: $\rho(r)$ is charge density

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

There are no magnetic monopoles

$$\nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$$

Faraday’s law of induction

$$\nabla \times \vec{B} = \frac{1}{c}\frac{\partial \vec{E}}{\partial t} + \frac{4\pi}{c}\vec{j}$$

Ampere’s law

These equations are exact. In them, **E** and **B** are *total* electric and magnetic fields, respectively. This is OK for vacuum. In materials, however, bound charges and currents give rise to polarization density **P** and magnetization density **M.** These act as sources of induced fields, which add to the external fields and alter the total fields:

$$\mathbf{E}=\mathbf{E}_{\text{applied}}+\mathbf{E}_{\text{ind}}$$

$$\mathbf{B}=\mathbf{B}_{\text{applied}}+\mathbf{B}_{\text{ind}}$$

Constitutive relations

It is convenient to formally define fields **D** and **H** which are due only to free charges and free currents and to separate out these from the total fields:

$$\boxed{\begin{aligned} \nabla \bullet \vec{D} &= 4\pi\rho_{free} \\ \nabla \times \vec{H} &= \frac{4\pi}{c}\vec{j} + \frac{1}{c}\frac{\partial \vec{D}}{\partial t} \end{aligned}}$$

For our applications, we can drop the displacement current contribution (relativistic effect) and take **H** to be the externally applied field. This means that we can consider this field to be generated by external currents **j**. Extra *internal* currents (*e.g.,* bias currents in spin valves) generate additional fields which have to be added to the total magnetic field **B**. This choice is one of convenience and one which we are free to make. But once we make it we have to be consistent and careful with our book-keeping, that is, keep track of what is externally applied and what is not.

Note that E and B are the physical fields to which charges respond.

The response of the material is buried in the relations between **D** and **E**, and between **H** and **B**. These relations are all the tricky parts of electricity and magnetism in materials.

Constitutive relations

For *macroscopic* media, one writes the constitutive relations

$$\boxed{\begin{aligned} &\vec{D} = \overleftrightarrow{\varepsilon} \bullet \vec{E} \\ &\vec{B} = \overleftrightarrow{\mu} \bullet \vec{H} = \vec{H} + 4\pi \vec{M} \end{aligned}}$$

From now on, let's focus only on magnetic fields and forget about the dielectric constant ε.

The definition of the permeability is general. For *linear* media, the magnetization density is related to the external field through the susceptibility χ:

$$\vec{M} = \overleftrightarrow{\chi} \bullet \vec{H} \Rightarrow$$

$$\vec{B} = \vec{H} + 4\pi \overleftrightarrow{\chi} \bullet \vec{H} = (\overleftrightarrow{1} + 4\pi \overleftrightarrow{\chi}) \bullet \vec{H} \Rightarrow$$

$$\overleftrightarrow{\mu} = (\overleftrightarrow{1} + 4\pi \overleftrightarrow{\chi})$$

Digression: units

Quantity	**Symbol**	**Gaussian, cgs**	**Conversion factor**	**SI**
Magnetic flux density, magnetic field	**B**	gauss (G)	10^{-4}	tesla (T)
Magnetic flux	Φ	maxwell (Mx), G cm^2	10^{-8}	weber (Wb)
Magnetic field strength	H	oerstedt (Oe)	$10^3/4\pi$	A/m
Magnetization density	M	emu/cm^3	10^3	A/m
Susceptibility	χ	dimensionless	4π	dimensionles
vacuum permeability	μ_0	N/A	4π x 10^{-7}	H/m
(relative) permeability	μ	dimensionless		dimensionless

Digression: Maxwell's equations

cgs units

$$\nabla \bullet \vec{E} = 4\pi\rho\,(\vec{r}\,)$$

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

$$\nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{B} = \frac{1}{c}\frac{\partial \vec{E}}{\partial t} + \frac{4\pi}{c}\vec{j}$$

$$\vec{B} = \vec{H} + 4\pi\vec{M}$$

SI units

$$\nabla \bullet \vec{E} = \rho / \varepsilon_0$$

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

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{B} = \mu_0 \vec{j} + \mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t}$$

$$\vec{B} = \mu_0\left(\vec{H} + \vec{M}\right)$$

Constitutive relations

Questions:

- When is it safe to assume that the magnetization density is proportional to the local field **H**, $\vec{M}(\vec{r}) \propto \vec{H}(\vec{r})$?
- Is the constant of proportionality the same at all points in the medium?

Perhaps it is better to assume that the permeability depends on position $\overleftrightarrow{\mu} = \overleftrightarrow{\mu}(\vec{r})$?

Maybe better yet to allow for the susceptibility to be non-local and position-dependent

$$\overleftrightarrow{\chi}(\vec{r}) = \overleftrightarrow{\chi}(\vec{r},\vec{r}\,') \Rightarrow$$

$$\vec{M}(\vec{r}) = \int d^3r \overleftrightarrow{\chi}(\vec{r},\vec{r}\,') \bullet \vec{H}(\vec{r}\,')$$

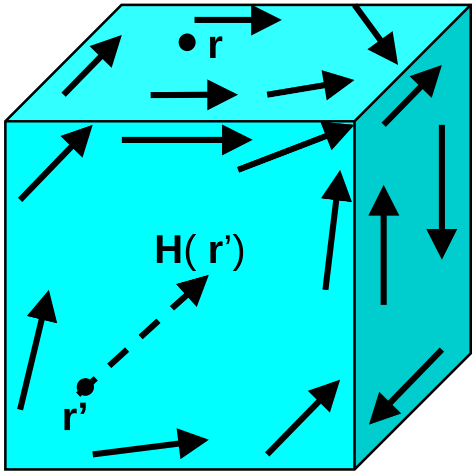
But this is still an assumption of *linear response*, that is, the induced change in magnetization density is proportional to the external field **H**

Constitutive relations

$$\overleftrightarrow{\chi}(\vec{r}) = \overleftrightarrow{\chi}(\vec{r},\vec{r}\,') \Rightarrow$$

$$\vec{M}(\vec{r}) = \int d^3r\, \overleftrightarrow{\chi}(\vec{r},\vec{r}\,') \bullet \vec{H}(\vec{r}\,')$$

For an inhomogeneously magnetized body, the response is in general non-local:

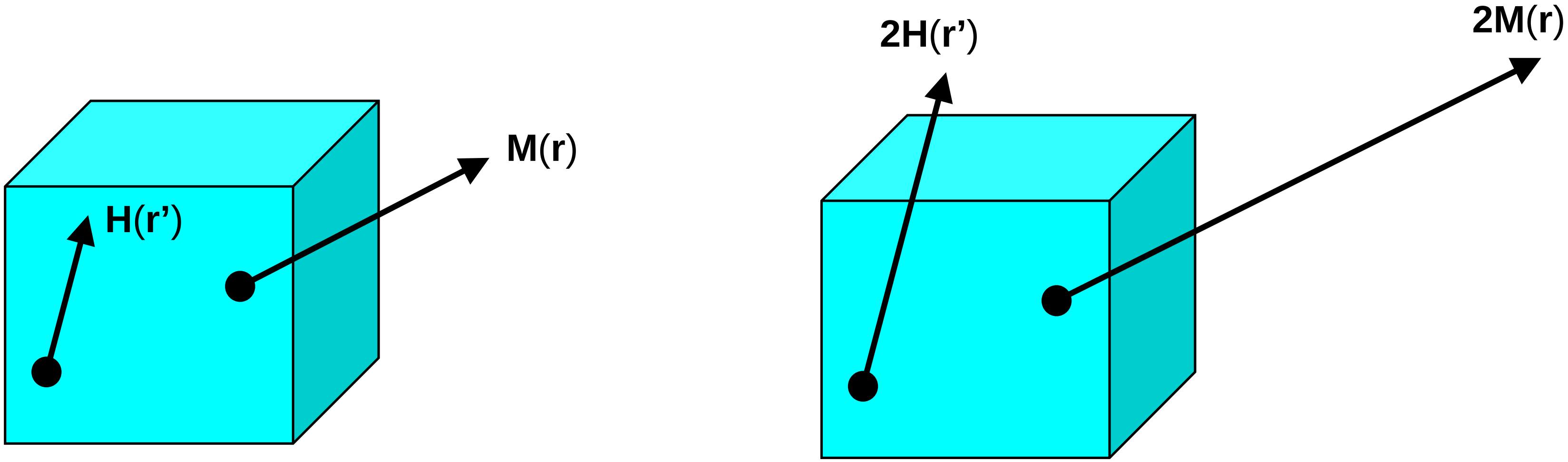


Applying a field **H** to **r**' will change the magnetization at **r**'. Due to long-range magnetostatic interactions and to exchange coupling, this will induce changes in the magnetization at **r**.

Linear Response

$$\vec{M}(\vec{r}) = \int d^3 r \overleftrightarrow{\chi}(\vec{r},\vec{r}\,') \bullet \vec{H}(\vec{r}\,')$$

Increase external field **H** everywhere by a factor α and the induced magnetization density increase everywhere by a factor α.



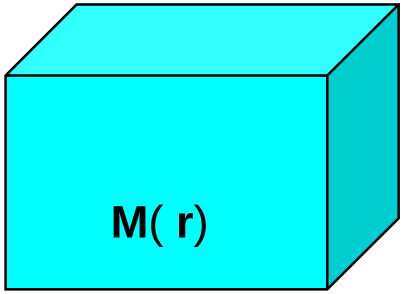
Comes from expanding **M** in powers of **H** about some initial state **M**$_0$(**r)** and keeping only first (linear) term.

$$\overleftrightarrow{\chi}(\vec{r},\vec{r}\,') \equiv \left. \frac{\delta \vec{M}(\vec{r}\,')}{\delta \vec{H}(\vec{r}\,')} \right|_{\vec{M}_0(\vec{r})}$$

(functional derivative)

Poles and demagnetizing fields

Consider a magnetized body. Sort out the contributions to total field **B**(**r**) from magnetization density



Start with time-independent Maxwell's equations for magnetic field

$$\nabla \bullet \vec{B}(\vec{r}) = 0$$

$$\nabla \times \vec{B}(\vec{r}) = \frac{4\pi}{c}\vec{j}(\vec{r})$$

$$\vec{B}(\vec{r}) = \vec{H}(\vec{r}) + 4\pi\vec{M}(\vec{r})$$

Combine first and third of these:

$$\nabla \bullet \vec{B}(\vec{r}) = \nabla \bullet [\vec{H}(\vec{r}) + 4\pi\vec{M}(\vec{r})] = 0 \Rightarrow$$

$$\nabla \bullet \vec{H}(\vec{r}) = -4\pi\nabla \bullet \vec{M}(\vec{r}) \equiv 4\pi\rho_m(\vec{r})$$

$$\rho_m(\vec{r}) \equiv -\nabla \bullet \vec{M}(\vec{r})$$

The pole density, or (magnetic) charge density, ρ_m(**r**) is the source of magnetic field due to magnetization density **M**

Poles and demagnetizing fields

So the equations for the field **H** are then

$$\boxed{\begin{aligned}
&\nabla\times\vec{H}(\vec{r})=\nabla\times\vec{B}(\vec{r})-4\pi\nabla\times\vec{M}(\vec{r})\\
&=\frac{4\pi}{c}\vec{j}(\vec{r})-\frac{4\pi}{c}\vec{j}_{bound}(\vec{r})=\frac{4\pi}{c}\vec{j}_{free}(\vec{r})\\
&\nabla\bullet\vec{H}(\vec{r})=4\pi\rho_m(\vec{r})
\end{aligned}}$$

Write this in terms of integrals over sources:

$$\vec{H}(\vec{r})=-\nabla\Phi(\vec{r})+\frac{1}{c}\nabla\times\int\frac{\vec{j}_{free}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}d\vec{r}\,',$$

$$\Phi(\vec{r})\equiv\int\frac{\rho_m(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}d\vec{r}\,'$$

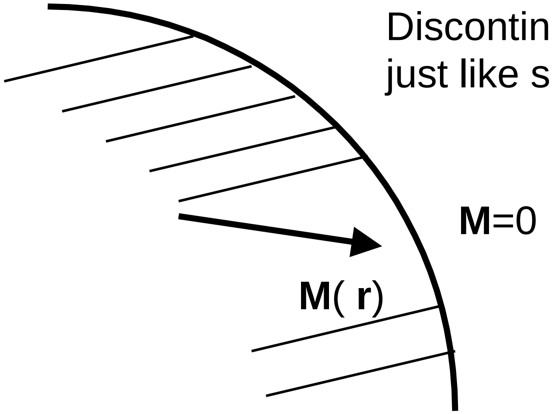
For magnetized medium, we can then write for the induced field $\mathbf{H}_d$, the *demagnetizing field,*

$$\vec{H}_d(\vec{r})=-\nabla_r\int\frac{\rho_m(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}d\vec{r}\,'=\nabla_r\int\frac{\nabla\bullet\vec{M}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}d\vec{r}\,'$$

integrated over the volume of the magnetized medium

Poles and demagnetizing fields

Separate out volume and surface contributions:



Discontinuities in ρ_m at surfaces give rise to magnetic fields just like surface electric charges give rise to electric fields.

Field from magnetized body, including bulk and surface charges:

$$\vec{H}_d(\vec{r}) = -\int_V dV \frac{\nabla \bullet \vec{M}(\vec{r})(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3} + \int_S dS \frac{\hat{n}(\vec{r}\,') \bullet \vec{M}(\vec{r}\,')(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3},$$

$\hat{n}(\vec{r}\,')$ is outward pointing normal at $\vec{r}\,'$, S is bounding surface of volume V

Magnetostatic interactions (energies due to demagnetizing fields) are *long-range* - the effect of surface and volume charges will affect the magnetic state over a large distance.

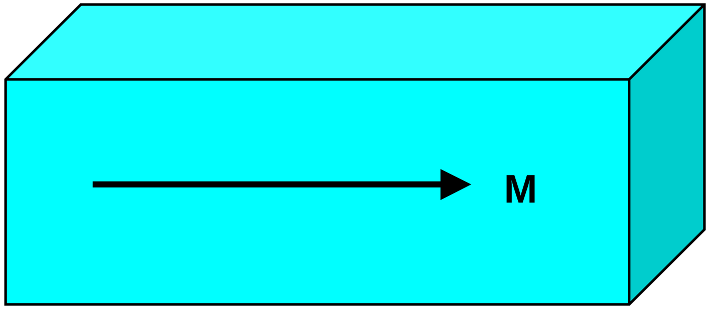
Poles and demagnetizing fields

Sources of magnetic field from magnetized body:

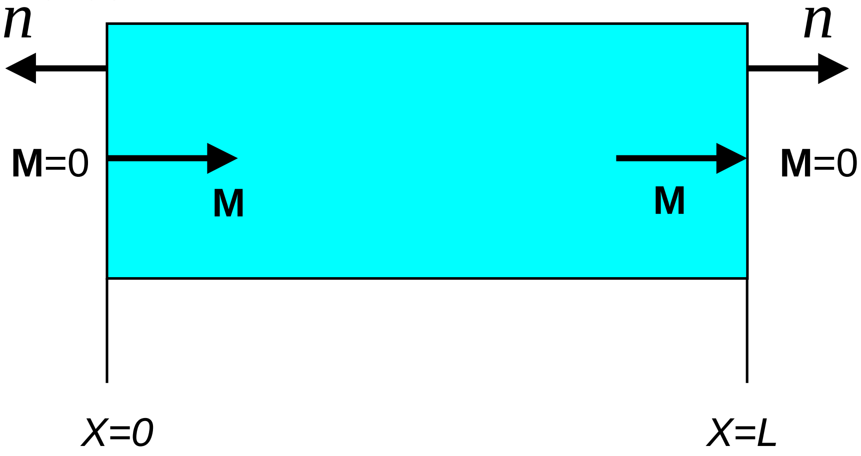
$-\nabla \bullet \vec{M}(\vec{r})$ - volume charge density

$\hat{n}(\vec{r}) \bullet \vec{M}(\vec{r})$ on bounding surface - surface charge density

Uniformly magnetized bar



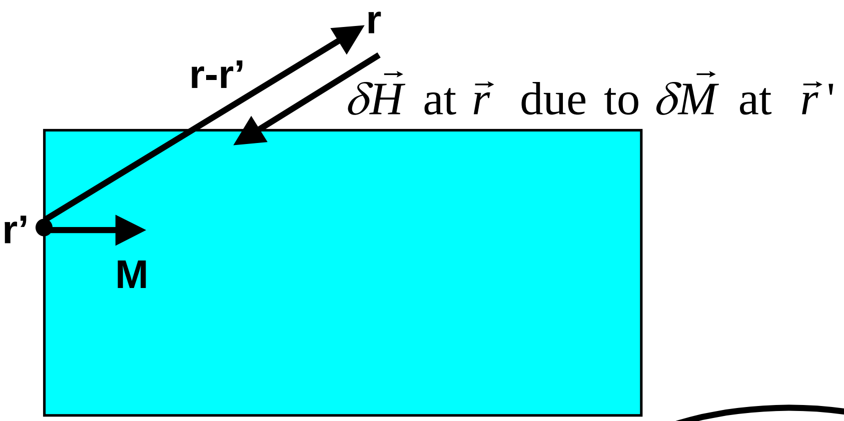
Sources of demagnetizing field are poles at the ends

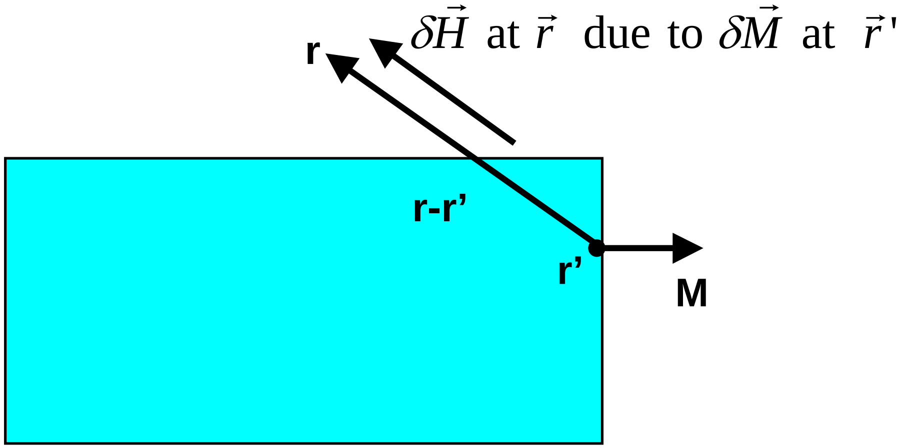


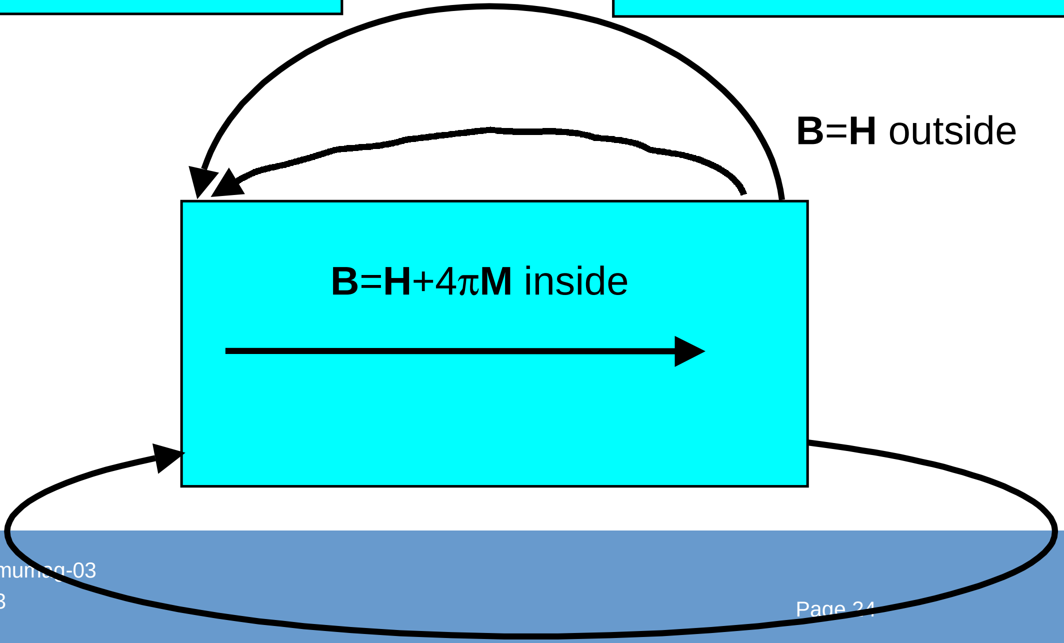
Poles and demagnetizing fields

$$\text{At } x = 0,\ \hat{n} \bullet \vec{M} = -M$$

$$x = L,\ \hat{n} \bullet \vec{M} = M$$



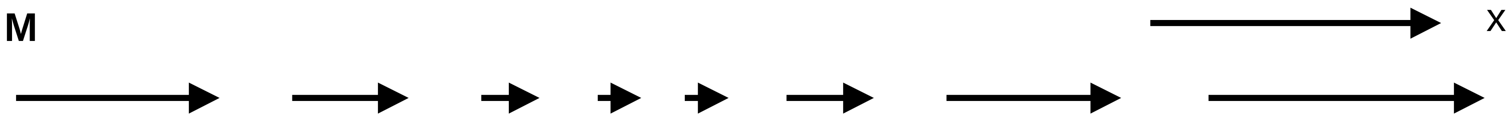




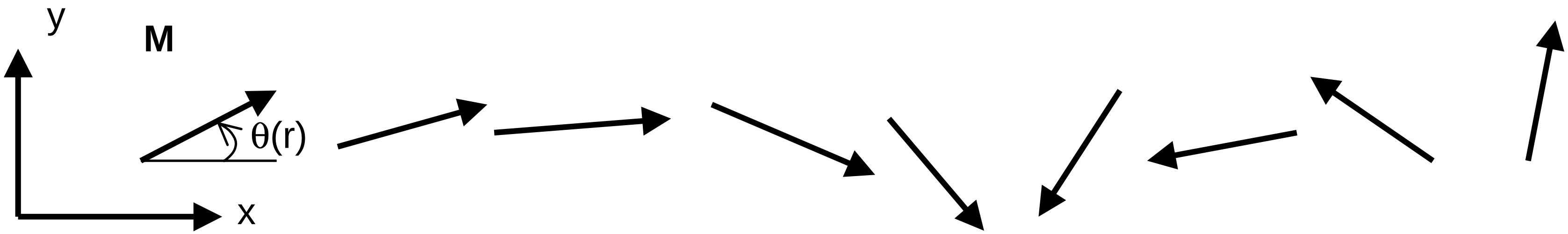
Poles and demagnetizing fields

Volume charge density: $\nabla \bullet \vec{M}(\vec{r}) = \frac{\partial M_x}{\partial x} + \frac{\partial M_y}{\partial y} + \frac{\partial M_z}{\partial z}$

In general, when **M** is changing direction and/or direction, there will be volume charges



$$\vec{M} = \hat{x} M(x), \quad \frac{\partial M_x}{\partial x} \neq 0$$



$$|\vec{M}| = \text{const.}, \quad \vec{M}(\vec{r}) = M(\cos\theta(x), \sin\theta(x)) = M(\cos kx, \sin kx)$$

$$\nabla \bullet \vec{M}(\vec{r}) = -kM(\sin kx, \cos kx) \neq 0 \Rightarrow \text{induced fields}$$

Demagnetizing fields

Demagnetizing field $\mathbf{H}_d$ is field due to surface charges $\hat{n} \bullet \vec{M}$ and volume charges $\nabla \bullet \vec{M}$ of a magnetized body. Demagnetizing fields strive to *reduce* the total magnetic field $\mathbf{B}=\mathbf{H}_{applied}+\mathbf{H}_d$ (hence the name).

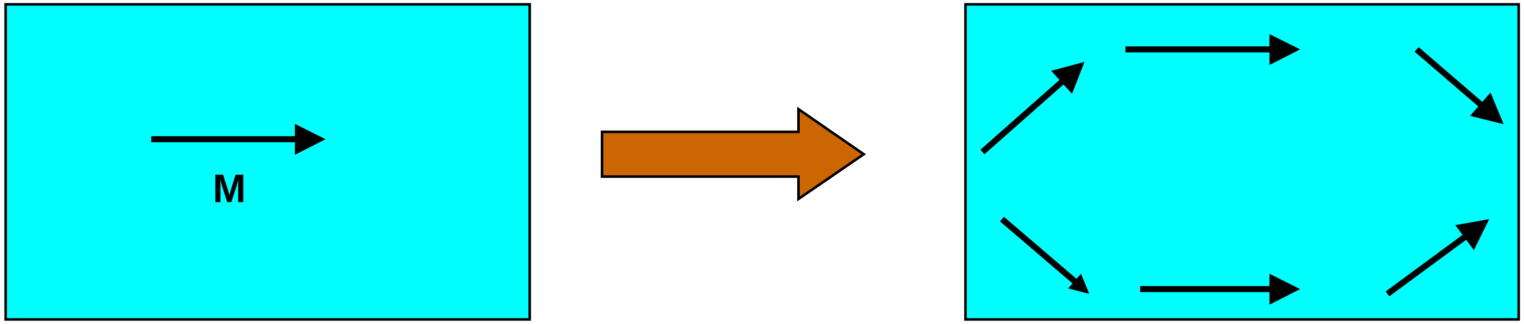
This is expressed by the *pole avoidance principle:* The energy E_d due to demagnetizing fields is positive semi-definite:

$$E_d = \frac{1}{8\pi} \int (H_d)^2 dV \geq 0$$

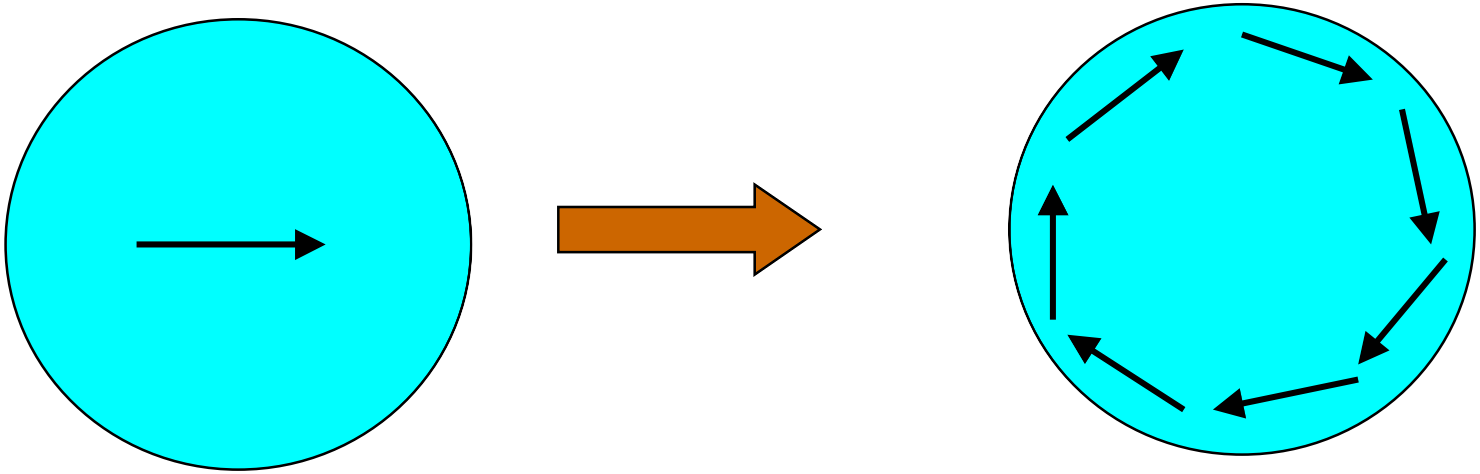
Therefore, the system strives to reduce the total energy by reducing the `poles' (surface and volume charges) in order to reduce E_d.

In small systems, E_d can be a very large contribution to the total energy (or, the demagnetizing fields are large compared to applied fields). Then the demagnetizing effects (magnetostatic self-interactions) largely determine the magnetic state of the system.

Pole avoidance principle (simple examples)



Uniform magnetization gives rise to large surface charges (poles), which cost a large energy. The system reduces the energy by trying to align the magnetization density with boundaries, which reduces the surface charges (at a small cost in volume charge density).



Demagnetizing fields

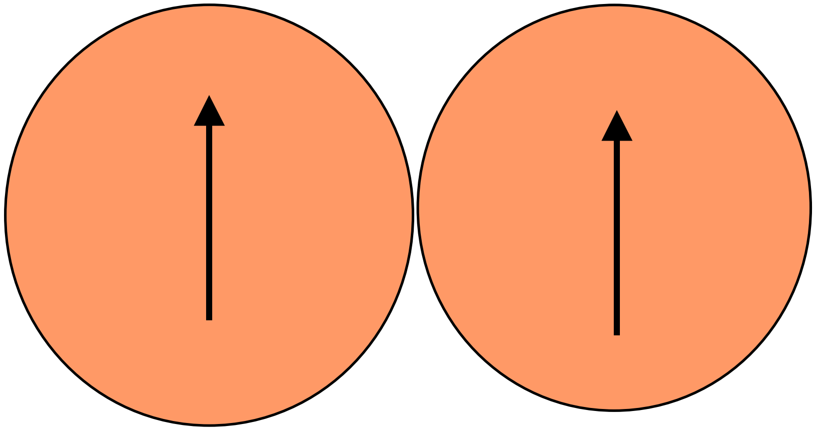
The effect of demagnetizing fields become increasingly more severe with decreasing system size. For example, for a sheet film, the only relevant effect of the demagnetizing field is to make the magnetization point in the plane of the film, but in the interior of the film, demagnetizing effects due to the boundaries of the film can be ignored. This is basically because even though the demag interactions are long-ranged, they do decay with distance and eventually become negligible.

However, if the system is small enough, demag fields due to boundaries cannot be ignored and may in fact be the dominant effect determining the magnetic state of the system. For example, in sheet film stacks, demag effects can be ignored but <u>not in small patterned magnetic elements.</u>

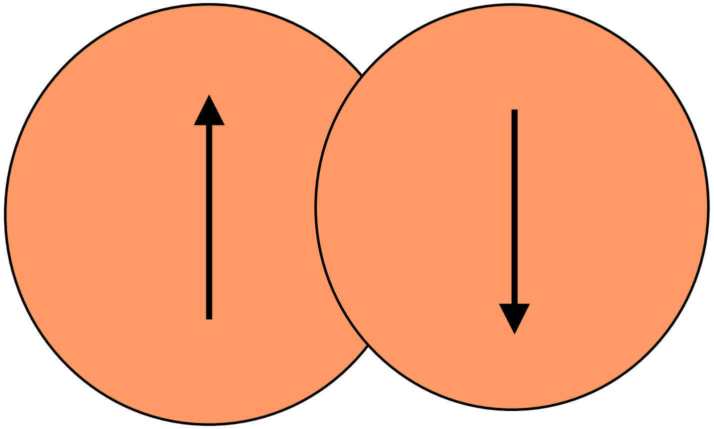
Ferromagnets

Electron spin magnetic moments interact with one another through *exchange coupling*.

What is exchange coupling? Its origin is quantum mechanical and comes from the Pauli exclusion principle: two electrons cannot occupy the same quantum state (here spin-up and spin-down states) at the same place and time. If a spin-up electron is located at position **r**, we cannot put another spin-up electron in the same quantum state at that position. As a consequence, two electrons with the same spin orientation is kept apart by the Pauli exclusion principle, which lowers their electrostatic (Coulomb) interaction energy. Hence, the Pauli exclusion principle makes the total energy of the two parallel spins *lower* than that of two electrons with *anti*-parallel spins. The amount by which the Coulomb energy is reduced is called *exchange energy,* and denoted by *J*.



Electrons with parallel spin are kept apart by the Pauli exclusion principle - this lowers the Coulomb energy



Electrons with anti-parallel spin can overlap, which costs electrostatic energy

Ferromagnets and exchange (cont'd)

The spin-statistics theorem dictates that the total wavefunction of identical spin-1/2 particles be antisymmetric under exchange of positions of any two particles. Consider two identical neighboring atoms and orbital electrons states $|\alpha>$ and $|\beta>$. We want to construct a two-electron wavefunction in which both electrons are in the same spin-state (triplet). Then the total orbital wavefunction must be antisymmetric, and can be constructed in the following way:

$$\Psi(\vec{r}_1,\vec{r}_2)=\frac{1}{\sqrt{2}}\left[\phi_\alpha(\vec{r}_1)\phi_\beta(\vec{r}_2)-\phi_\alpha(\vec{r}_2)\phi_\beta(\vec{r}_1)\right]$$

This wavefunction is manifestly antisymmetric under interchange of the two electrons ($\mathbf{r}_1$ -> $\mathbf{r}_2$, $\mathbf{r}_2$ -> $\mathbf{r}_1$). This procedure can be generalized to *N* electrons (Slater determinants).

Magnetic state of a body

When an external field **H** is applied to a body, it will induce a magnetization density **M**. The magnetization density gives rise to magnetic charge density $\rho_m(\mathbf{r})$, which in turns gives rise to and induced demagnetizing field $\mathbf{H}_d$. This changes to total field **B,** which changes the induced magnetization density, and so on…..

The magnetic state of a body has to be found by self-consistently finding the magnetization in the presence of the external field **H** such that the total energy is minimized.

Self-consistency:
- Apply external field **H**
- Find induced magnetization density **M**
- Find total field **B**
- Find new magnetization density due to total field
- Find new total field **B**……..
- Continue until the magnetization density does not change between steps.

The equations that describe these must be derived from an energy minimization principle.

Micromagnetic energy

OK, let's think about the energy of a ferromagnet in an external field and see if we can put together an energy minimization principle.

Note: We write the external field H_{ext}, keeping in mind that this field can be considered to be generated by some external currents

Ferromagnets - Heisenberg model and exchange energy

Pauli exclusion principle lowers the interaction energy by -2*J* for parallel spins on neighboring sites.

This suggests a simple model of exchange interaction of electron spins on two neighboring sites 1 and 2:

$$H = -J\vec{S}_1 \bullet \vec{S}_2,$$

$$\vec{S}_1 = \text{total spin vector (classical) of electron at site 1}$$

$$\vec{S}_2 = \text{total spin vector (classical) of electron at site 2}$$

For a system of N electron spins on N sites, we can then write the classical Heisenberg Hamiltonian

$$H = -\frac{J}{2}\sum_{<i,j>} \vec{S}_i \bullet \vec{S}_j,$$

$$\text{where} < i, j > \text{means } i \text{ and } j \text{ are neighboring sites}$$

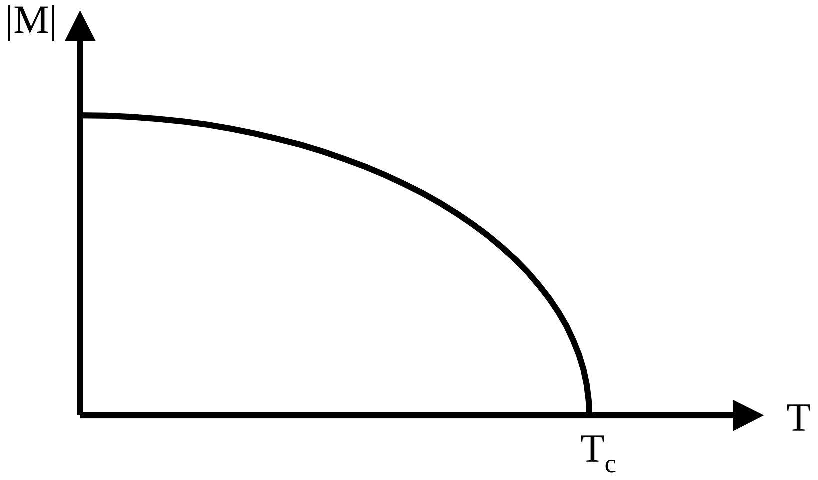
This is a good model to represent the collective behavior (magnetism) due to interacting spins. It does *not* represent individual atomic moments in transition metals, but rather the average magnetization in some small volume.

Ferromagnets - Heisenberg model

At T=0, lowest-energy state is that with all spins parallel in an arbitrary direction,

$$E_0 = -NJS^2, \; |M| = S\mu_B \frac{N}{V}$$

At finite, non-zero temperatures, entropy S increases and free energy $F = U - TS$ is minimized. As entropy is increased, |M| decreases and vanishes at the Curie temperature T_c.



For $T>T_c$, |M|=0. For $T<T_c$, there will be spontaneous magnetization.

Ferromagnets - Heisenberg model

If we measure the magnetization in a macroscopic ferromagnet (e.g., a piece of Fe or Co), we will observe $|\mathbf{M}|=0$ when the system is cooled through the Curie temperature in zero external field.

Why?

Domains. The magnetic state is *not* homogeneous with a uniform magnetization density.

To understand the magnetic state of ferromagnets, we turn to a micromagnetic description.

This is a classical model which includes all relevant energy contributions on scales larger than some 10 nm. This means that as a rule of thumb, in actual calculations, the grid size used should be less than 10 nm or so.

Micromagnetic exchange energy

Continuum limit of Heisenberg exchange: assume direction of magnetization density changes slowly on scale of atomic lattice constant *a*, but that the magnitude of the magnetization density is constant at the saturation magnetization density M_s (T=0 limit!). Then

$$E = -\frac{J}{2}\sum_{<i,j>}\vec{S}_i \bullet \vec{S}_j = -\frac{JS^2}{2}\sum_{<i,j>}\sin\theta_i\cos\theta_j\cos(\varphi_i-\varphi_j)$$

Assume θ, φ vary slowly on scale a of atomic spacing. Then

$$\theta_j \approx \theta_i + \Delta\vec{r}_{ij} \bullet \nabla\theta_i,$$

$$\varphi_j \approx \varphi_i + \Delta\vec{r}_{ij} \bullet \nabla\varphi_i,$$

$$\cos(\theta_i - \theta_j) \approx \cos(\theta_i - \theta_{ij} - \Delta\vec{r}_{ij} \bullet \nabla\theta_i) = 1 - \frac{1}{2}\left(\Delta\vec{r}_{ij} \bullet \nabla\theta\right)^2$$

$$E \approx \text{const.} + \frac{1}{2}C\int\left[\left(\nabla m_x\right)^2 + \left(\nabla m_y\right)^2 + \left(\nabla m_z\right)^2\right]dV,$$

$$C = \frac{2JS^2}{a}c, \quad \text{with } c = 1,2,4 \text{ for sc, bcc, fcc lattices, } \left[C\right] = \left[\text{energy/length}\right]$$

$m_\alpha, \alpha = x, y, z$ are the Cartesian components of a unit vector along the local magnetization direction

Micromagnetic exchange energy

Redefine zero of energy to absorb the unimportant constant. Then

$$E_{\text{ex}} = \frac{1}{2} C \int \left[(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2 \right] dV$$

$$C \approx 10^{-6} \text{ erg/cm for NiFe}$$

One can also derive this form of the exchange energy without appealing to an underlying Heisenberg Hamiltonian. Instead, one starts with a (macroscopic) continuum theory and expands the exchange energy about a uniformly magnetized state. The lowest-order surviving term dictated by symmetry is then

$$E_{\text{ex}} = \frac{1}{2} C \int \left[(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2 \right] dV$$

To do calculations, space has to be divided into cells of some size *l.* It must be noted that this form of the exchange energy is valid *only for small angles* between adjacent cells. If in a calculation the angles between magnetization directions in adjacent cells change by a large amount, the calculation is invalid, the results nonsense, and the calculation has to be done over again on a finer cell size.

Micromagnetic Zeeman energy

Add energy term due to interaction of the magnetization density with the external field.

For a magnetic moment μ**=M**V**,** the Zeeman energy is

$$\vec{\mu}\cdot\vec{B}=\vec{\mu}\cdot(\vec{H}_{ext}+4\pi\vec{M})=\vec{\mu}\cdot(\vec{H}_{ext}+4\pi\vec{\mu}/V)$$

The self-interaction term does not make much sense here, so we will drop it. Thus for the whole ferromagnetic body the Zeeman energy

$$E_Z=-\mu_B\sum_i\vec{S}_i\bullet\vec{H}_{\mathrm{ext},i}\approx -M_s\int\vec{m}(\vec{r})\bullet\vec{H}_{ext}(\vec{r})dV,$$

where $\vec{H}_{\mathrm{ext}}(\vec{r})$ is the applied external field at $\vec{r}$

Micromagnetic magnetostatic self-interactions

Add another energy term: a finite system must have a demagnetizing field (even if the magnetization density is uniform and homogeneous in the magnetized body). Add energy due to magnetostatic self-interactions (demagnetizing energy):

$$E_d = -\frac{1}{2}\mu_B \sum_i \vec{S}_i \bullet \vec{H}_{d,i} \approx -\frac{1}{2} M_s \int \vec{m}(\vec{r}) \bullet \vec{H}_d(\vec{r}) dV$$

where the factor of 1/2 is inserted to avoid double-counting, and

$$\vec{H}_d(\vec{r}) = -\int_V dV \frac{\nabla \bullet \vec{M}(\vec{r})(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3} + \int_S dS \frac{\hat{n}(\vec{r}\,') \bullet \vec{M}(\vec{r}\,')(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3}$$

If we expand this expression in moments of the magnetization in each cell, the first term is just the dipole-dipole interaction between to magnets at **r** and **r**':

$$E_{\text{dipole}} = M_s^2 V^2 \frac{\vec{m}(\vec{r}) \bullet \vec{m}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3} - M_s^2 V^2 \frac{3\left(\vec{m}(\vec{r}) \bullet (\vec{r}-\vec{r}\,')\right)\left(\vec{m}(\vec{r}\,') \bullet (\vec{r}-\vec{r}\,')\right)}{|\vec{r}-\vec{r}\,'|^5}$$

This term makes the magnets want to line up parallel to the vector **r-r**'.

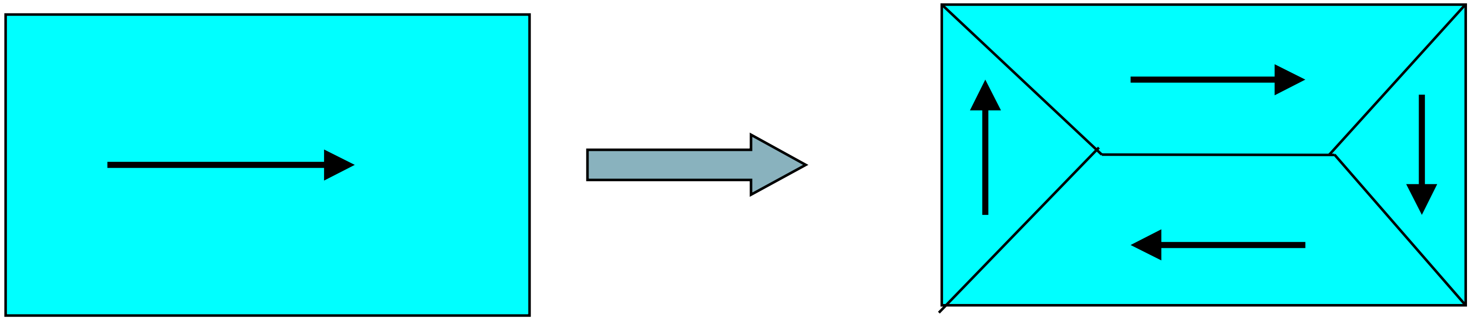
Micromagnetic model, so far

- Space divided into cells of size *l* and volume *dV*, with *l* much greater than lattice spacing *a*
- Each cell has a fixed magnitude of magnetization density equal to saturation magnetization density M_s and a total magnetic moment equal to M_s *dV*
- Temperature is effectively 0
- Direction **m**(**r**) of magnetization density changes slowly on length scale *l*
- Exchange energy: tries to keep direction of magnetization density constant
- Magnetostatic self-interactions: try to minimize demagnetizing field by (typically) aligning magnetization density parallel to bounding surfaces
- Zeeman energy: tries to align magnetization direction with external field.

Micromagnetic energy competition

Exchange energy tries to keep magnetization uniform and parallel. But constant magnetization up to boundaries creates poles which cost a lot of `demag' energy - `demag' energy tries to line up magnetization parallel to bounding surfaces which makes the magnetization direction change.

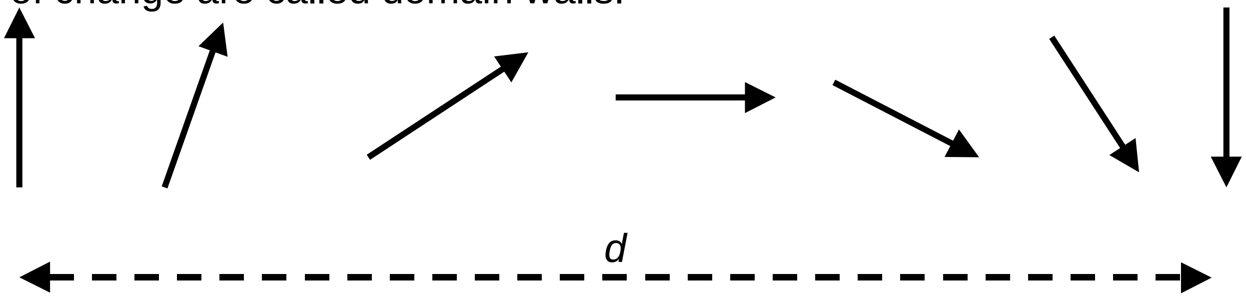
Compromise: Divide up the system into chunks, *domains*, each of which has uniform magnetization, but the direction of the magnetization in different domains is different. This minimizes exchange energy within each domain, and minimizes exchange energy between domains and boundaries by closing flux loops.



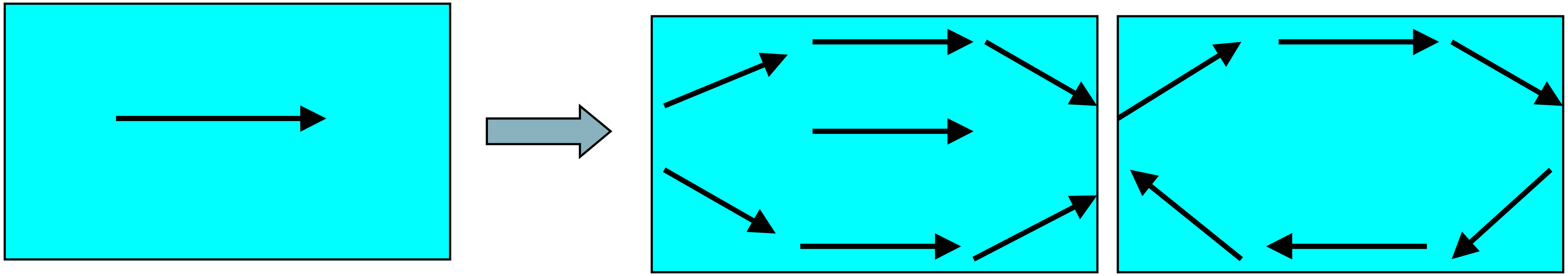
Whether or not the system breaks up into domains depends on if the increase in exchange energy of the domain walls more than offset by the decrease in demag energy.

Micromagnetic energy competition

There is a finite length *d* over which the magnetization changes from one domain to another. The regions of change are called domain walls.



For a small system, the exchange and magnetostatic energy cost of domain walls can be too high and the system can form, *e.g.,* a single domain or a vortex state



Domain walls

What is the cost in exchange energy of a domain wall?

Suppose magnetization direction changes only along *x*, and is constant along *y* and *z*.

Magnetization angle θ:

$$\theta(x) = \frac{\pi x}{d}, \text{ from some initial } x = 0, \theta = 0, \text{ to } x = d, \theta = \pi$$

$$m_x = \cos\theta = \cos\frac{\pi x}{d},$$

$$m_y = \sin\theta = \sin\frac{\pi x}{d}$$

$$\nabla m_x = \hat{x}\frac{dm_x}{dx} = -\frac{\pi}{d}\sin\frac{\pi x}{d}$$

$$\nabla m_y = \hat{x}\frac{dm_y}{dx} = \frac{\pi}{d}\cos\frac{\pi x}{d}$$

$$\left|\nabla m_x\right|^2 = \left(\frac{\pi}{d}\right)^2 \sin^2\frac{\pi x}{d}$$

$$\left|\nabla m_y\right|^2 = \left(\frac{\pi}{d}\right)^2 \cos^2\frac{\pi x}{d}$$

$$E_{\mathrm{ex}} \approx A\frac{C}{2}\left(\frac{\pi}{d}\right)^2 \int_0^d dx = \frac{AC\pi^2}{2d}, \text{ with } A \text{ area in } yz\text{-plane}$$

Domain walls - scaling of exchange energy and demag energy

Suppose we have a magnet of width L and make the magnetization twist from -1 to +1 across the width L. The domain wall (exchange) energy of this twist scales as 1/L, that is, as

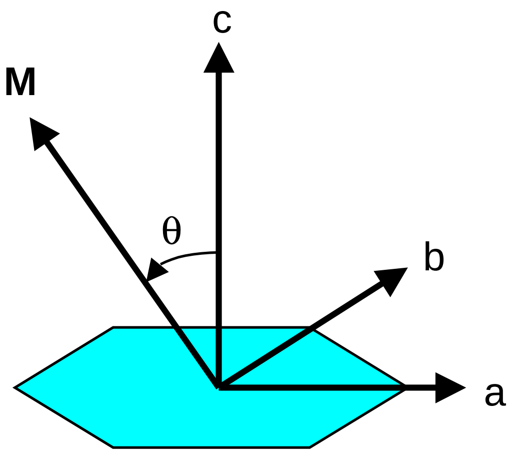
1/(linear dimension) of the system. In contrast, demag energy scales as (Volume ~L^3). This means that when the size L approaches the scale of a domain wall, the system will become very stiff: the cost in exchange energy to change the direction of magnetization across the system will start to become prohibitive.

Domain walls and anisotropy

What is the size *d* of a domain wall, and what determines *d*? In order to answer this in more detail, we need to introduce another energy term: anisotropy energy.

Crystal axes in a material are in general not equivalent due to spin-orbit coupling between the spin magnetic moment and the orbital magnetic moment of electrons. This makes some axes preferred for the magnetization direction.

Hexagonal crystals (*e.g,* Co): Uniaxial anisotropy.



The anisotropy energy density depends only on angle θ to *c*-axis, and is symmetric with respect to *ab*-plane

$$\varepsilon_{\mathrm{ani}}(\cos\theta) = \varepsilon_{\mathrm{ani}}\left[\cos(\pi-\theta)\right]$$

$$\cos(\pi-\theta) = \cos\pi\cos\theta = -\cos\theta \Rightarrow$$

$$\text{Expand in } \cos\theta\text{, no odd powers}$$

$$\varepsilon_{\mathrm{ani}} \approx -K_1\cos^2\theta + K_2\cos^4\theta = -K_1 m_z^2 + K_2 m_z^4$$

In most hexagonal crystals, *c*-axis is easy axis with $K_1>0$ and

$|K_1| >> |K_2|$

Domain walls and anisotropy

Cubic anisotropy:

The anisotropy energy density must be invariant with respect to interchange of the crystal axes. Expandin cubic harmonics:

$$\varepsilon_{\text{ani}} \approx K_1\left(m_x^2 m_y^2 + m_x^2 m_z^2 + m_y^2 m_z^2\right) + K_2 m_x^2 m_y^2 m_z^2$$

$K_1>0$ for Fe (easy axis along (100) direction)

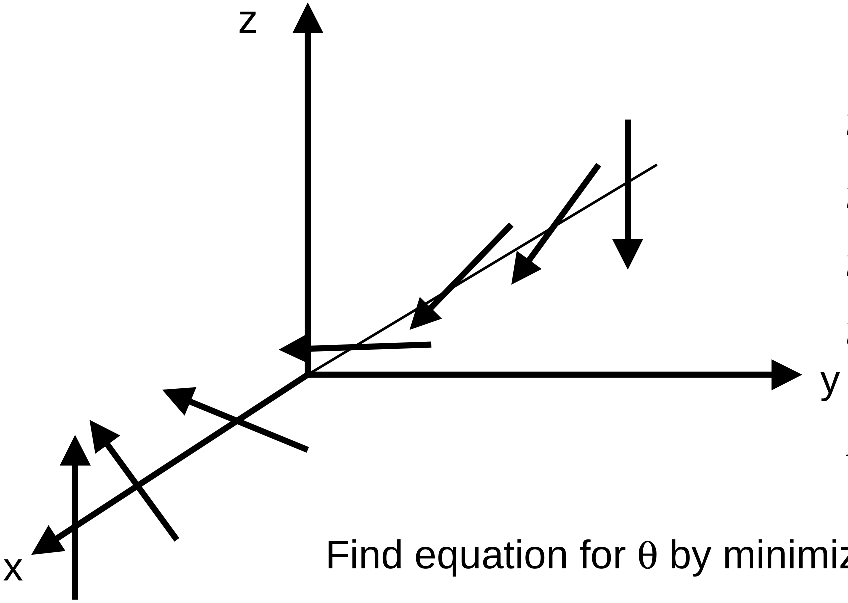
$K_1<0$ for Ni (easy axis along (111) direction)

Domain walls have to fight:

- increased exchange energy due to non-collinear spins in domain wall
- magnetostatic energy due to pole density $\nabla \bullet \vec{M}$
- anisotropy energy as the magnetization direction deviates from easy axis direction(s)

Domain walls and anisotropy

Estimate typical size *d* of domain wall (so-called Landau-Lifshitz wall). Use a simple model of an infinite crystal, no demag energy, uniaxial anisotropy, easy axis=*z* axis



$$\vec{m}(\vec{r}) = m_y(x)\hat{y} + m_z(x)\hat{z} = \sin\theta(x)\hat{y} + \cos\theta(x)\hat{z}$$

$$m_z \to -1 \text{ for } z \to -\infty,$$

$$m_z \to +1 \text{ for } z \to +\infty$$

$$m_x = 0 \Rightarrow \nabla \bullet \vec{m} = 0 \text{ so no demag energy}$$

$$E = \int dV\varepsilon \approx \int dV\left[K_1 \sin^2\theta(x) + K_2 \sin^4\theta(x) + \frac{C}{2}\left(\frac{d\theta}{dx}\right)^2\right]$$

Find equation for θ by minimizing this energy. Euler-Lagrange equations:

$$0 = \frac{\partial\varepsilon}{\partial\theta} - \frac{\partial}{\partial x}\frac{\partial\varepsilon}{\partial(d\theta/dx)}$$

$$C\frac{d^2\theta}{dx^2} - 2K_1\sin\theta\cos\theta - 4K_2\sin^3\theta\cos\theta = 0,$$

$$\left(\frac{d\theta}{dx}\right)_{x\to\pm\infty} = 0$$

Domain walls and anisotropy

First integral

$$\frac{C}{2}\left(\frac{d\theta}{dx}\right)^2 - K_1 \sin^2\theta - K_2 \sin^4\theta = \text{const}$$

$$x \to \pm\infty \Rightarrow \frac{d\theta}{dx} = 0 \Rightarrow \text{const} = 0$$

$$\text{Then } \frac{d\theta}{dx} = \pm\sqrt{\frac{2K_1}{C}}\left[1+\frac{K_2}{K_1}\sin^2\theta\right]^{1/2} \sin\theta$$

Integrate:

$$\int \frac{dx}{\sin x\sqrt{1+k^2\sin^2 x}} = \frac{1}{2}\ln\frac{\sqrt{1+k^2\sin^2 x}-\cos x}{\sqrt{1+k^2\sin^2 x}+\cos x} \Rightarrow$$

$$\cos\theta = \frac{\sqrt{1+\frac{K_1}{K_2}}\tanh\sqrt{\frac{2K_1}{C}}x}{\sqrt{1+\frac{K_1}{K_2}\tanh^2\sqrt{\frac{2K_1}{C}}x}}$$

Domain walls and anisotropy

Characteristic scale of domain wall is $\delta = \sqrt{\frac{C}{2K_1}}$, with δ the *exchange length.* This is of the order of 10^3 A.

Note:

- Exchange coupling *C* tries to spread out the size of the domain wall in order to minimize exchange energy
- Anisotropy energy tries to reduce the size of the domain wall since it costs energy not to have the magnetization along an easy axis
- In finite-size devices such as spin valves, demagnetizing fields add an effective uniaxial anisotropy which will also contribute to the effective exchange length.

Micromagnetic energy

The total magnetic energy for some system with saturation magnetization density M_s is then

$$E = E_{\mathrm{ex}} + E_{\mathrm{d}} + E_{\mathrm{Z}} + E_{\mathrm{ani}},$$

$$E_{\mathrm{ex}} = \frac{1}{2} C \int \left[(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2 \right] dV$$

$$E_d = -\frac{1}{2} \mu_B \sum_i \vec{S}_i \bullet \vec{H}_{d,i} \approx -\frac{1}{2} M_s \int \vec{m}(\vec{r}) \bullet \vec{H}_d(\vec{r}) dV$$

$$\vec{H}_d(\vec{r}) = -\int_V dV \frac{\nabla \bullet \vec{M}(\vec{r})(\vec{r} - \vec{r}\,')}{|\vec{r} - \vec{r}\,'|^3} + \int_S dS \frac{\hat{n}(\vec{r}\,') \bullet \vec{M}(\vec{r}\,')(\vec{r} - \vec{r}\,')}{|\vec{r} - \vec{r}\,'|^3}$$

$$E_Z = -\mu_B \sum_i \vec{S}_i \bullet \vec{H}_{\mathrm{ext},i} \approx -M_s \int \vec{m}(\vec{r}) \bullet \vec{H}_{\mathrm{ext}}(\vec{r}) dV$$

E_{ani} depends on the specific form of anisotropy.

Surface anisotropy has not been included here.

Note:

- Exchange energy depends on *C* but not (directly) on M_s
- Zeeman energy depends on M_s
- Demag energy depends on $M_s^2 V$ times a *dimensionless* shape function

Micromagnetic energy minimization

Find equation for magnetization density by minimizing the energy expression with respect to **m**(**r**).

The ensuing algebra is a bit cumbersome, but the final result is

$$\vec{m}(\vec{r}) \times \left(C\nabla^2 \vec{m}(\vec{r}) + M_s \vec{H}_{\text{applied}}(\vec{r}) + M_s \vec{H}_{\text{d}}(\vec{r}) - \frac{\partial \varepsilon_{\text{ani}}}{\partial \vec{m}(\vec{r})} \right) = 0$$

This may look formidable, but simply expresses that the minimum-energy state is such that the torque exerted locally by the local effective field on the magnetization (or magnetic moment per cell) is zero. **The equilibrium magnetization is parallel to the local effective field $\mathbf{H}_{\mathbf{eff}}$ given by**

$$\vec{H}_{\text{eff}}(\vec{r}) = \frac{C}{M_s} \nabla^2 \vec{m}(\vec{r}) + \vec{H}_{\text{applied}}(\vec{r}) + \vec{H}_{\text{d}}(\vec{r}) - \frac{1}{M_s} \frac{\partial \varepsilon_{\text{ani}}}{\partial \vec{m}(\vec{r})}$$

Micromagnetic energy minimization

- Since **A**x**A**=0 for any vector **A**, we can add an arbitrary vector proportional to **M**(**r**) without changing anything. This is a convenient degree of freedom in actual calculations.
- The physics of the equilibrium state suggests a simple algorithm for calculations:

  1. Assign an initial magnetization density (good guess, random, whatever)
  2. Calculate the effective field at each cell
  3. Align the magnetization of each cell with its local effective field
  4. If the change in angle in the magnetization is small enough, exit, otherwise go to 2.

- Whatever technique is used to solve the equations for minimum energy magnetization, we are only guaranteed to find a local minimum. With a different initial state, we may reach a different equilibrium magnetization. A converged solutions has to be tested for stability: if we find an equilibrium state (local energy minimum), poke at it to see if the system recovers the same state or if another, different, minimum-energy state is reached.

Landau-Lifshitz-Gilbert (LLG) equations

We can also find a dynamic equation for the magnetization density. Start with the torque equation for a magnetic moment in an external field:

$$\frac{d\vec{M}(\vec{r},t)}{dt} = -\gamma_0 \vec{M}(\vec{r},t) \times \vec{H}_{\text{eff}}(\vec{r},t),$$

$$\text{with } \gamma_0 = \frac{g\,|e|}{2m_e c},$$

$$\vec{H}_{\text{eff}}(\vec{r}) = \frac{C}{M_s}\nabla^2 \vec{m}(\vec{r},t) + \vec{H}_{\text{applied}}(\vec{r},t) + \vec{H}_{\text{d}}(\vec{r},t) - \frac{1}{M_s}\frac{\partial \varepsilon_{\text{ani}}}{\partial \vec{m}(\vec{r},t)}$$

This equation describes the undamped (no energy dissipation) precessional motion of a moment in an effective magnetic field. We add a phenomenological damping by assuming that the driving field is reduced by an amount proportional to the time-rate of change of the magnetization:

$$\vec{H}_{\text{eff}}(\vec{r},t) \to \vec{H}_{\text{eff}}(\vec{r},t) - \eta \frac{d\vec{M}(\vec{r},t)}{dt}$$

with η a phenomenological damping constant. Thus

$$\frac{d\vec{M}(\vec{r},t)}{dt} = -\gamma_0 \vec{M}(\vec{r},t) \times \vec{H}_{\text{eff}}(\vec{r},t) + \gamma_0 \eta \vec{M}(\vec{r},t) \times \frac{d\vec{M}(\vec{r},t)}{dt}$$

Landau-Lifshitz-Gilbert (LLG) equations

This can also be written

$$\frac{d\vec{M}(\vec{r},t)}{dt} = -\gamma_0^{'}\vec{M}(\vec{r},t)\times\vec{H}_{\text{eff}}(\vec{r},t) - \lambda\vec{M}(\vec{r},t)\times\left[\vec{M}(\vec{r},t)\times\vec{H}_{\text{eff}}(\vec{r},t)\right],$$

$$\gamma_0^{'} = \frac{\gamma_0}{1+\gamma_0^2\eta^2M_s^2},$$

$$\lambda = \frac{\gamma_0\eta}{1+\gamma_0^2\eta^2M_s^2}$$

This form is a little more convenient for calculations. The dynamic LLG equation can be used both to find the time-dependent response and to find an equilibrium state. In the latter case, one just cranks up the damping constant and lets the system evolve until excess energy has dissipated and a stable time-independent state has been reached. The structure of the equation guarantees that M^2 is a constant of the motion. This latter approach is convenient numerically because it is faster than the previous torque-method. Note that here to we may reach different equilibrium states depending on what we set the damping constant to be (the system may evolve farther with less damping and reach a different state than with higher damping)!

Landau-Lifshitz-Gilbert (LLG) equations

Questions:

1. What are the microscopic damping processes?

2. Is there any justification for the form of the damping term in the LLG equations from more fundamental considerations?

One damping mechanism is due to coupling between spin waves (normal modes of the magnetization motion) and the lattice, the so-called magnetoelastic coupling (H. Suhl, IEEE Trans. Mag., **34,** 1834 (1998))

Basic physics: Magnetization motion gives rise to strain (fundamentally due to spin-orbit coupling) which gives rise to phonons, which dissipate energy.

$$F = \mu \sum_{i,j} e_{ij}(\vec{r}) \cdot e_{ij}(\vec{r}) + \sum_{i,j} B e_{ij}(\vec{r}) m_i(\vec{r}) m_j(\vec{r}),$$

$$F = \text{elastic energy}$$

$$e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i}\right) \text{ is strain tensor}$$

$$\vec{u}(\vec{r}) \text{ is displacement vector at } \vec{r},\ \vec{r} = (r_1, r_2, r_3) \text{ is position vector}$$

$$\mu \text{ is shear modulus, } B \text{ is magnetoelastic coupling constant}$$

Landau-Lifshitz-Gilbert (LLG) equations

Combine equation of motion for the strains:

$$\eta \frac{\partial e_{ij}}{\partial t} + \mu e_{ij} + \frac{1}{2} B m_i m_j = 0$$

(viscous stress tensor+elastic stress tensor equals zero),

with that for the magnetization:

$$\frac{\partial \vec{m}}{\partial t} = \gamma_0 \vec{m} \times \left(\frac{\partial F}{\partial \vec{m}} \right)$$

(time-rate of change equals torque exerted by force). For small viscosity η one can obtain an asymptotic expression (long times) which has the form of the LLG damping term.

Nitty-gritties

OK, how do we actually do computations? Why would I write my own code when there are free (eg OOMMF from NIST) or commercial (eg Scheinfein’s LLG code) packages? Well,

- canned codes do well what they were written to do, which is almost never exactly what you are interested in
- you are anal-retentive and want to write your own code anyhow because you don’t trust anybody else’s coding
- You’re a graduate student and have infinite time at your hands and you don’t have anything better to do.

Nitty-gritties

The main pain in the rear is calculating the demag term. This can be done by

- direct evalution (pair-wise summation). Extremely time consuming. Not smart.
- multi-pole expansion. Has theoretical appeal in that one can in theory go to larger length scales, but in the practical calculations of the kind that I do multi-pole expansions do not pay off.
- FFT. Very fast, but requires a regular lattice. The main drawback is that the cell size of the lattice must be small enough that the magnetization direction does not change much from cell to cell (otherwise the exchange energy is garbage). Typical cell size is 10 nm or less. So the amount of memory (RAM) available and the time and patience (for execution) available put serious constraints on the size of systems that can be modeled without resorting to some kind of parallelization (which is not easy because of the overhead in communications between nodes).

Nitty-gritties (cont'd)

So let's decide on a Cartesian grid of cells of volume *abc* and use the FFT method. The coordinate to the center of cell *i* is $\mathbf{r}_i$, and the magnetization is taken to be constant in each cell *i*. The 'demag' field at cell *i* is then expressed in terms of a demag-tensor N:

$$\vec{H}_d(\vec{r}) = \int d^3\vec{r}\,'\,\overleftrightarrow{N}'(\vec{r}-\vec{r}\,')\bullet\vec{M}(\vec{r}\,') \Rightarrow$$

$$\vec{H}_d(\vec{r}_i) = \sum_j \overleftrightarrow{N}(\vec{r}_i-\vec{r}_j)\bullet\vec{M}(\vec{r}_j)$$

The problem is then reduced to evaluating the demag tensor. Since the magnetization is constant in each cell, we only need the contributions from

$\vec{M}_j \cdot \hat{n}_j$ at all the surfaces of volume j. These integrals are found in the literature. There are two different versions:

- field-at-center. The demag field from cell *j* is evaluated at the center of cell *i*. This is good for cubic systems but not for general parallelepipeds.

- volume-averaged field. The field from cell *j* is averaged over the volume of cell *i*. This is considered more accurate and is my recommended form.

Nitty-gritties (cont'd)

Let *X*,*Y*,*Z* be the relative coordinates between cells *i* and *j*, and define $\xi = X - x'$, $\eta = Y - y'$, $\zeta = Z - z'$, and $r = \sqrt{\xi^2 + \eta^2 + \zeta^2}$. Then

$$\overleftrightarrow{N} = \frac{1}{abc}\,\overleftrightarrow{n}\,\Big|_{x'=-a/2}^{x'=a/2}\Big|_{y'=-b/2}^{y'=b/2}\Big|_{z'=-c/2}^{z'=c/2}\Big|_{\xi=X-x'-a/2}^{\xi=X-x'+a/2}\Big|_{\eta=Y-y'-b/2}^{\eta=Y-y'+b/2}\Big|_{\zeta=Z-z'-c/2}^{\zeta=Z-z'+c/2}$$

The matrix elements of $\overleftrightarrow{n}$ are

$$n_{xx}(\xi,\eta,\zeta) = \xi\eta\zeta\tan^{-1}\left(\frac{\eta\zeta}{\xi}\right) - \frac{\zeta\left(\xi^2-\eta^2\right)}{2}\ln\left(r-\zeta\right) - \frac{\eta\left(\xi^2-\zeta^2\right)}{2}\ln\left(r-\eta\right) + \frac{r^3}{3} - \frac{r\xi^2}{2}$$

$$n_{xy}(\xi,\eta,\zeta) = \xi\eta\zeta\ln\left(r-\zeta\right) + \left(\frac{\eta^3}{6} - \frac{\eta\zeta^2}{2}\right)\ln\left(r+\xi\right) + \left(\frac{\xi\zeta^2}{2} - \frac{\xi^3}{6}\right)\ln\left(r-\eta\right) + \frac{\xi^2\zeta}{2}\tan^{-1}\left(\frac{\eta\zeta}{\xi r}\right)$$

$$+\frac{\eta^2\zeta}{2}\tan^{-1}\left(\frac{\zeta\xi}{\eta r}\right) + \frac{\zeta^3}{6}\tan^{-1}\left(\frac{\xi\eta}{\zeta r}\right) + \frac{\xi\eta r}{3}$$

Nitty-gritties (cont'd)

Luckily, the other matrix elements are given by symmetry and cyclic permutations of the arguments:

$$n_{yy}(\xi,\eta,\zeta)=n_{xx}(\eta,\zeta,\xi)$$

$$n_{zz}(\xi,\eta,\zeta)=n_{xx}(\zeta,\xi,\eta)$$

$$n_{xy}(\xi,\eta,\zeta)=n_{yx}(\xi,\eta,\zeta)$$

$$n_{xz}(\xi,\eta,\zeta)=n_{zx}(\xi,\eta,\zeta)=n_{xy}(\zeta,\xi,\eta)$$

$$n_{yz}(\xi,\eta,\zeta)=n_{zy}(\xi,\eta,\zeta)=n_{xy}(\eta,\zeta,\xi)$$

It's still a bit of a pain to code up – be careful about the signs for the different limits of integration, and be careful with the forms of matrix elements in the limit of one (or more) argument going to zero! When debugging, carefully check that your calculated matrix elements satisfy all the symmetries above.

Note: for a cube, the self-demag field of a cell is parallel to the magnetization of that cell and exerts no torque. Therefore, the self-demag field can be omitted. *This is not true for general parallelepipeds.*

Nitty-gritties (cont'd)

The strategy is then to calculate the demag tensor in the beginning of the calculation, FFT and store. To calculate the demag field, FFT the magnetization density in each cell, FFT, multiply with the FFT of the demag tensor, and back-transform. See Numerical Recipes for implementations – I use the fftpack routines with F90 drivers for 2D and 3D FFT. This is up to seven times faster than the cxml library routines for 3D FFT!

To zero-pad or not to zero-pad?

Note that FFT introduces a spurious periodicity since the approach assumes a periodic system. There are standard ways in which one can avoid these periodicities in the resulting magnetization density by enlarging the demag tensor and filling up the new elements with zeros (zero-padding) – again, see Numerical Recipes for a detailed discussion. However, this is not necessary for magnetic systems – the demag tensor is a function of the difference coordinate, and the magnetization array has to be enlarged to the same dimension before FFT and convolution with the demag tensor, and the enlarged elements have zeros. These are the elements which *would* cause spurious periodicities were they not zero. Since they are, no spurious periodicities are introduced and we save some space in RAM (I invite you to try with and without zero-padding and see what the difference is!)

Nitty-gritties (cont'd)

Exchange energy: Evaluate the exchange field according to a numerical implementation of

$$\vec{H}_{\mathrm{ex}}(\vec{r}) = \frac{C}{M_s}\nabla^2 \vec{m}(\vec{r},t)$$

The vector Laplacian can be evaluated using some standard numerical scheme – usually a three-point scheme (along each coordinate direction) works just fine. Note

- there is no need to include the magnetization at point *i* in the evaluation of the exchange field at point *i.* This is because this would give a contribution which exerts no torque on the magnetization at point *i.* So the mid-point in the three-point scheme can be excluded. There may perhaps sometimes be some advantage from a stability point-of view to included it, but as a rule I have seen no advantage to doing so.

- the exchange field is not scale invariant – if the cell size is decreased by a factor of 2, the exchange field increases in strength by a factor of 4.

Nitty-gritties (cont'd)

The whole code is just a loop:

- First define geometry – magnetization density, exchange coupling etc
- calculate demag tensor, FFT and store
- Initialize magnetization direction vectors
- Define external field
- Converge using torque minimization or LLG
- Dump data
- New external field

Initialization: Try not to build in any symmetries in the initial state. For example, if you are calculating a magnetization loop (M vs. H) and start with a large applied field and seed the magnetization to be parallel to the initial external field, you will get *incorrect* results (too large coercivity). The reason is you built in a symmetry which is preserved and which the system does not exhibit in reality. It is much safer to start with a random initial magnetization direction in each cell.

Nitty-gritties (cont'd)

LLG method and convergence.

Let's assume we'll only use the LLG method. To reach an equilibrium state, we crank up the damping α, use some standard numerical integrator and let it rip.

Note

- *You must renormalize each magnetization vector after each update!* Numerical integrators do not usually preserve norm, and if you don't renormalize, the norms of the magnetization vectors will change and you get crap.

- Pick a suitable time step and α. If the time step is too large, you get garbage (numerical instabilities), too slow is time-consuming. Similarly, α too large can lead to instabilities and α too small leads to longer times before the precessional motions are damped out. As rules of thumbs, α in the range of 0.5 – 2 and time steps in the range of 0.1 ps to 0.5 ns usually work. You may want to be careful and check the maximum rotation of each magnetization vector in each update and limit the time step so this maximum rotation does not exceed some value like 5 degrees.

- Convergence. You have to have pretty tight convergence criterion in order to avoid numerical 'noise'. For example, you can check the maximum rotation of each magnetization vector or the difference between the magnetization direction and effective field in each cell and require that either one is less than, say, 0.00001 radians.

Nitty-gritties (cont'd)

Code sanity checks

So you have put together a code, it compiles, links, runs without crashing, and gives some output that doesn't look too stupid. How do you know the output is correct?

Some suitable code sanity checks can be obtained by checking the 'standard' problems at the NIST micromagnetic group's Web site:
http://www.ctcms.nist.gov/~rdm/mumag.org.html

Also, try some simple checks: set the magnetization to be uniform for a large parallelepiped (bar magnet). Check the demag field with available analytical expressions.

Examples – dynamics (J. van Ek and M. Plumer)

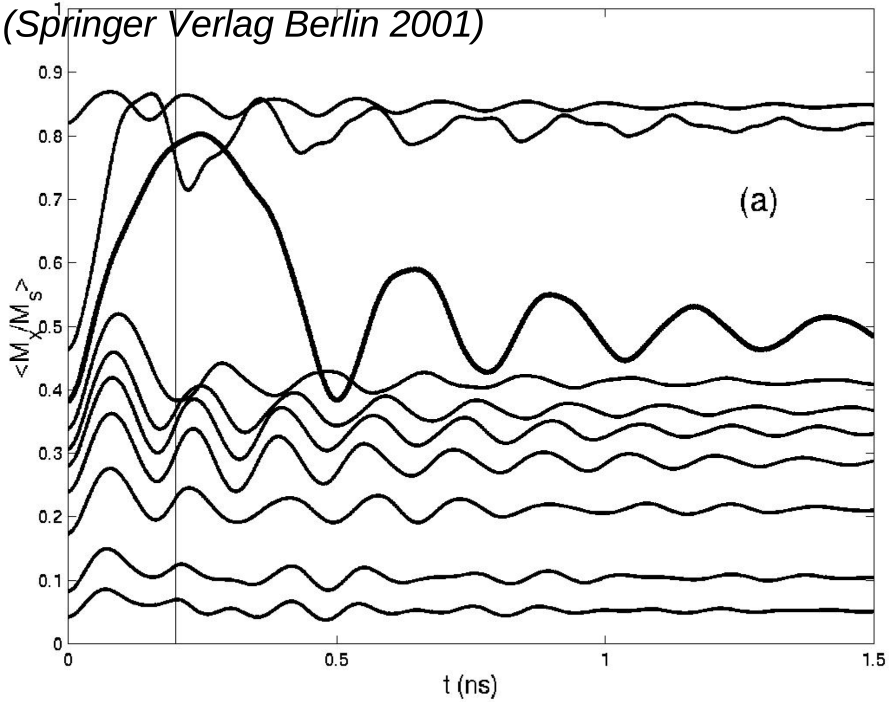
Impact of shape anisotropy on the characteristic precession frequencies of small ferromagnetic platelets

2.5 nm thick platelets with M_s=1440 emu/cc ($Co_{80}Fe_{20}$).

Excited with short pulses (200 ps) of a weak external field (10 Oe), or subject to a harmonic (frequencies from 0.5 to 2 GHz) strong driving force (200 Oe amplitude).

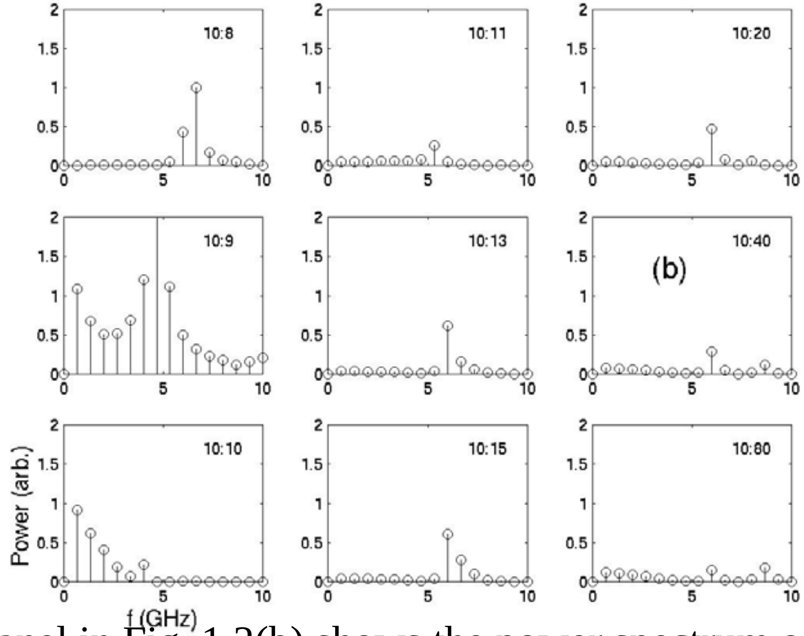
Examples – dynamics (J. van Ek and M. Plumer)

From *The Physics of Ultra-High-Density Magnetic Recording, M. Plumer, J. van Ek, and D. Weller (eds) (Springer Verlag Berlin 2001)*



Systems with varying aspect ratio *W/L*, but constant *W*=100 nm, were excited with weak, short field pulses along the *x*-direction (along *W*). A constant 10 Oe bias field was applied along the *y*-direction. The temporal evolution of M_x is monitored for samples ranging in size from *W* x *L*=100 x80 nm^2 to 100x800 nm^2. The cell size in the LLG calculation was 10x10x2.5 nm^3 and the damping parameter was α=0.01. At the 10:8 aspect ratio (*W*x*L*=100x80 nm^2) the remnant state (*t*=0) is largely magnetised along the *x*-direction, constrained by shape anisotropy (upper curve). After a short field pulse the system is dissipating energy through viscous damping, but the magnetisation never deviates substantially from the remnant state.

Examples – dynamics (J. van Ek and M. Plumer)



The upper right panel in Fig. 1.2(b) shows the power spectrum of the temporal evolution of M_x. A relatively narrow mode at 6.3 GHz dominates the spectrum.

The oscillatory mode softens and broadens when the aspect ratio approaches unity. At this aspect ratio the combined bias and the pulse fields make the state with diagonal magnetisation (M_x=0.71 M_s) energetically favourable, and the system strives toward this state. Once the field pulse vanishes, the system relaxes with roughly half the precessional frequency observed at the 10:8 aspect ratio.

When the aspect ratio decreases, shape anisotropy poses well-defined constraints on the magnetisation of the sample. The excitation narrows (Fig. 1.2(b)) and has shifted to slightly lower frequency (5.7 GHz). At very small aspect ratio of 10:40 and 10:80, spectral power develops at even higher frequency (8.6 GHz). The origin of this beating phenomenon is not clear.

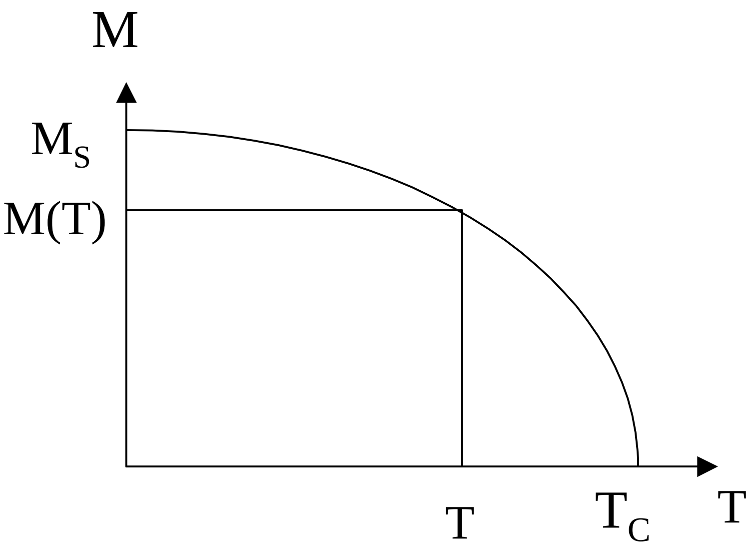
Finite temperatures: background and motivation

Micromagnetic simulations assume *fixed* saturation magnetization

Fluctuations are ignored

Thermal excitations over energy barriers ignored

At finite T, magnetization density is reduced



Finite temperatures - background and motivation

- How can we include finite temperature effects (reduced equilibrium magnetization, fluctuations) in micromagnetic simulations?
- How does equilibrium magnetic configuration change with element dimensions and temperature?
- For magnetic sensors: What is the noise due to thermal magnetic fluctuations?

Magnetic systems at finite temperatures

- Standard micromagnetics simulations are inherently 0-temperature techniques which do not in any way include the effects of finite temperatures.

- At finite temperatures the local magnetization will fluctuate due to thermal excitations. The probability that a new magnetization configuration at a change in energy ΔE will be reached is given by the Boltzmann factor

$$\exp\left[-\Delta E/\left(k_B T\right)\right]$$

- The frequency f_0 with which the system tries to reach new configurations (the *attempt frequency*) is of the order of 10^{-10} Hz and is due to magnon-phonon interactions and magnon-quasiparticle interactions.

- The effect of thermal fluctuations can be studied using statistical mechanics. Effects include reduced magnetization density *M(T)* compared to the T=0 value, finite-range correlations functions such as susceptibility

$$\chi_{\alpha\beta}(\vec{q}) = \sum_{\vec{r}\,'} \left\langle M_\alpha(\vec{r}+\vec{r}\,')M_\beta(\vec{r})\right\rangle e^{i\vec{q}\cdot\vec{r}\,'}$$

Magnetic systems at finite temperatures

- Standard finite-temperature Monte Carlo (MC) simulations can be used to calculate thermal averages of any quantity.Unfortunately, MC simulations do not contain any time scale and are not based on an equation of motion, so it is difficult (at best) to obtain any dynamics information (e.g. frequency behavior) using MC simulations.

- Another approach which *does* contain time scales is the Langevin equation. This approach is based on a clear separation of time scales. That is, the thermal fluctuations of a particle(s) of interest is due to interactions with some other bath of particles. The timescale of the particle of interest is much slower than the time scale of the particles in the bath. The effect of the interactions with the particles in the bath can then be expressed as a random force. As an example, the equation of motion for a particle of mass *m* in contact with a thermal bath is then (in 1D)

$$m\frac{dv}{dt} = R(r) - \beta v$$

where $R(r)$ is the random force due to the interactions with the bath.

- The solution is

$$v(t) = v(0)\exp\left[-\frac{\beta}{m}t\right] + \frac{1}{m}\int_0^t \exp[-(t-\tau)\beta/m]R(\tau)d\tau$$

To proceed, use the fact that integration and averaging commute

$$v(t) = \langle v(0)\rangle \exp\left[-\frac{\beta}{m}t\right] + \frac{1}{m}\int_0^t \exp[-(t-\tau)\beta/m]\langle R(\tau)\rangle d\tau$$

On the average, the stochastic force has to vanish: $\langle R(t)\rangle = 0$

At any two different times the random force is uncorrelated (this is based on the separation of time scales!):

$$\langle R(t)R(t')\rangle = q\delta(t-t')$$

Must now determine the strength of the noise q.

- **Define the spectral density of a stochastic variable *z*(*t*) as**

$$S(f) = \lim_{T\to\infty} \frac{2}{T} |A(f)|^2, \text{ where}$$

$$A(f) = \int_0^T z(t)\exp\left(-2\pi i f t\right)dt. \text{ If } \langle z(t) \rangle = 0, \langle z(t)z(t+\tau)\rangle = q\delta(\tau), \text{ then}$$

$$G(f) = 2\int_{-\infty}^{\infty} \exp(-2\pi i f\tau) q\delta(\tau) = 2q.$$

Fourier-transforming the formal solution to $v(t)$ and taking the modules, one then gets

$$G_v(f) = \frac{2q/m^2}{(\beta/m)^2 + (2\pi f)^2}. \text{ Then } \langle v^2 \rangle = \int_0^{\infty} G_v(f)df = \frac{2}{2\beta m}.$$

The equipartition theorem states that $\langle v^2 \rangle = k_B T/m,$ so therefore $q = 2\beta k_B T.$

- Next, need a distribution for the random force – will take it as Gaussian, so

$$\langle R(t)\rangle = 0,\ \langle R(t)R(0)\rangle = 2\beta k_B T\delta(t),\ \text{and}$$

$$P(R) = \frac{1}{\sqrt{2\pi\langle R^2\rangle}}\exp\left(-\frac{R^2}{\langle R^2\rangle}\right).$$

How do we then integrate the stochastic equation of motion numerically (cannot make a Dirac delta function numerically, so what should the *numerical* variance of the stochastic force be?). The velocity and random force correlation times are

$$t_v = \frac{1}{\langle v^2\rangle}\int_0^\infty \langle v(t)v(0)\rangle dt,\ \text{and}$$

$$t_R = \frac{1}{\langle R^2\rangle}\int_0^\infty \langle R(t)R(0)\rangle dt,\ \text{which obey}$$

$$t_v t_R = \frac{\langle v^2\rangle m^2}{\langle R^2\rangle}.\ \text{Here}\ t_v = m/\beta\ \text{and}\ t_R = \frac{\beta k_B T}{\langle R^2\rangle}.$$

- **By assumption, the correlation time for the random force is much smaller than the correlation time for the velocity. For a finite time step *h* in the numerical algorithm, we**
then assume that the random force is constant and that the correlation time of the random force is *h*.Thus

$$\langle R^2 \rangle = \beta k_B T / h,$$

and the system of equations is closed.

Stochastic LLG equation

Use the ideas from the Langevin equation to write a stochastic LLG equation. The magnetization is interacting with phonons and quasiparticles with much faster timescales, and the interactions give rise to a **fluctuating magnetic field.**

LLG equation: $\frac{d\vec{m}(\vec{r},\tau)}{d\tau} = -\vec{m}\times\vec{h} - \alpha\vec{m}\times\left(\vec{m}\times\vec{h}\right),$

where the field and time have been scaled appropriately. Add a random field to the effective fields give the stochastic LLG equation

$$\frac{d\vec{m}(\vec{r},\tau)}{d\tau} = -\vec{m}\times(\vec{h}+\vec{h}_{fl}) - \alpha\vec{m}\times\left(\vec{m}\times(\vec{h}+\vec{h}_{fl})\right),$$

Note: the stochastic field here enters multiplicatively, in contrast to the standard Langevin equation, where the stochastic field is additive. There must be a rule how to interpret the equation – Stratanovich stochastic calculus. One then has to be careful that the numerical algorithm converges in the Stratanovich sense.

Stochastic LLG

- Assume that the stochastic field is uncorrelated in time,

$$\left\langle h_{fl,i}(t), h_{fl,j}(t')\right\rangle \propto \delta(t-t')$$

Still need to find the amplitude of the correlations (at *t*=*t'*). This was done by Brown for an ensemble of non-interacting Stoner-Wohlfahrt particles as the form of the equilibrium distribution function is known for them.

It is *not* easy to do for an interacting system (like a soft ferromagnetic film). Can get certain approximate solutions from studying asymptotic behavior of the Fokker-Planck equation. The stochastic field correlation function is taken as (Brown)

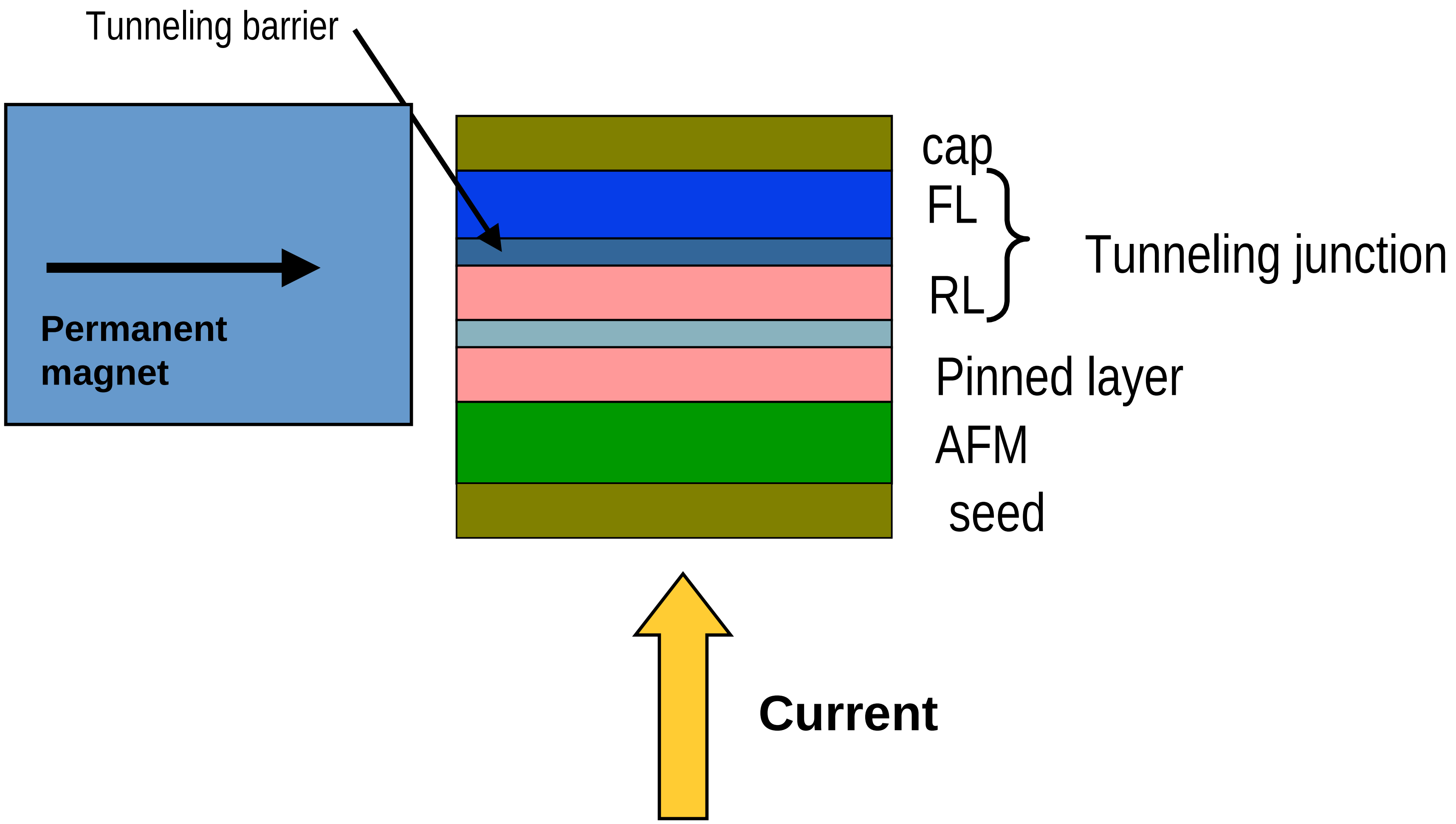
$$\left\langle h_{fl,i}(t), h_{fl,j}(t')\right\rangle \propto \frac{2k_B T\alpha}{M_s V\gamma}\delta_{i,j}\delta(t-t')$$

Use a second-order semi-implicit Heun scheme with added magnetization renormalization for numerical integration. For an excellent guide for implementation, see Ref. 13.

Note:

- The damping used is the phenomenological Gilbert damping. Need better physics…
- For practical implementations, the time step has to be very small (sub-ps). This is of the order of the time-scale of the thermal bath (e.g. phonons) and so violates the very foundation of separation of time-scales which underpins the Langevin equation

Tunneling reader cartoon



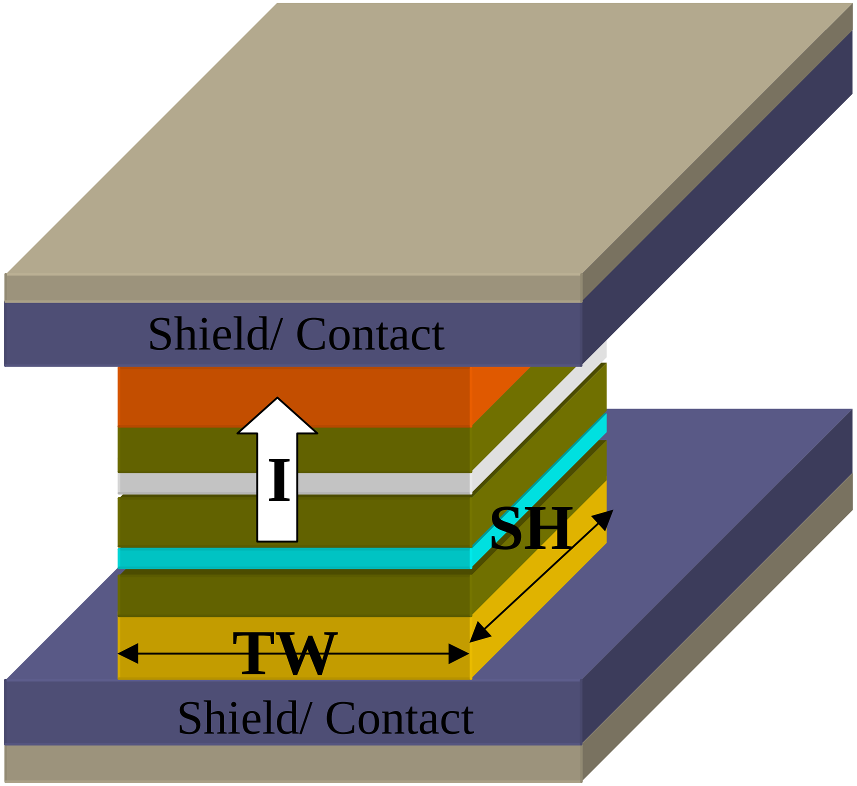
Tunneling barrier

Permanent magnet

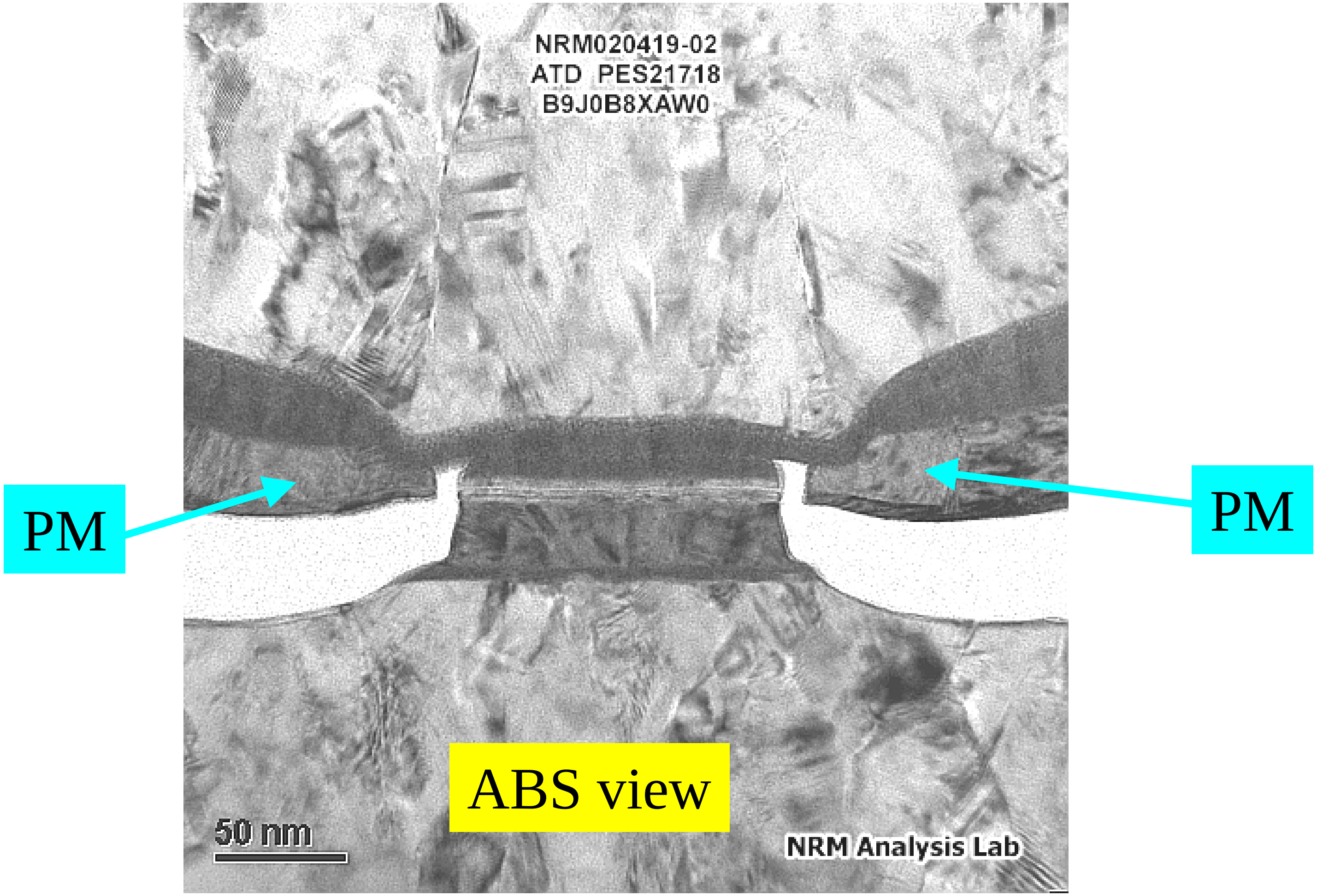
cap
FL
RL
Tunneling junction
Pinned layer
AFM
seed

Current

Example: noise in tunneling magnetoresistive reader. Cartoon of tunneling reader.

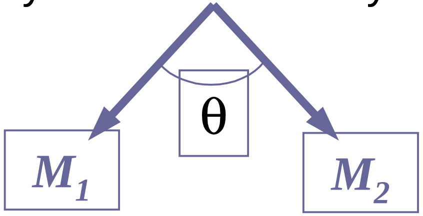


Tunneling Magnetoresistive Read Head - TEM



Example: noise in tunneling magnetoresistive reader

The signal voltage in a tunneling reader is generated by the difference in magnetization direction between the reference layer and the free layer.



$$\boxed{R = R_0\left[1 + \frac{1}{2}\frac{\Delta R}{R_0}(1-\cos\theta)\right]}$$

For a fixed applied bias current I_b thee signal voltage is

$$V_s = I_b\Delta R = \frac{1}{2}I_b R_0\left(\frac{\Delta R}{R_0}\right)(1-\cos\theta)$$

Thermal fluctuations in the magnetization in the free layer and reference layer will create voltage fluctuations – noise, $\langle v_s{}^2\rangle \sim \langle\cos\theta^2\rangle$. Using the stochastic LLG we can directly calculate the magnetization fluctuations and the noise voltage, which is a rather complicated correlation function between magnetization in free and reference layers.

Background - noise

Consider a electronic device to which a constant potential difference V is applied. The noise power is related to the fluctuations in current from its average value $\langle I \rangle$:

$$P_n = V\langle \Delta I \rangle^2 = V\langle I - \langle I \rangle \rangle^2 = V\left[\langle I^2 \rangle - \langle I \rangle^2\right]$$

The noise is characterized by its spectral density, which is the Fourier transform of the current-current correlation function:

$$S(\omega) = 2\int_{-\infty}^{\infty} dt e^{i\omega t} \langle \Delta I(t + t_0) \Delta I(t_0) \rangle$$

with the brackets indicating an ensemble average, or, equivalently, and average over initial times t_0.

Background, cont'd

Thermal noise (V=0, T>0) is related to the conductance G_{SD} (Source to Drain) through the fluctuation-dissipation theorem:

$$S_{SD} = 2k_B T(G_{SD} + G_{DS})$$

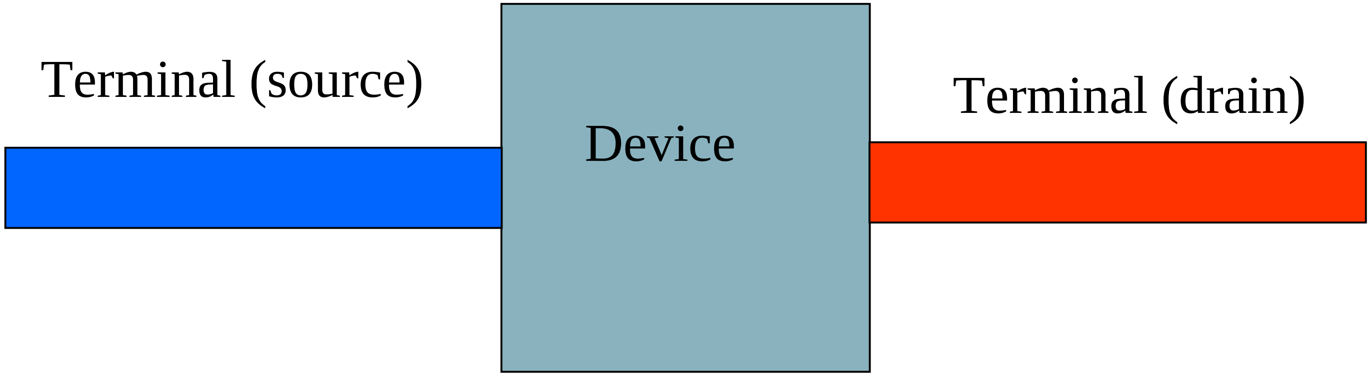
For systems which obey time-reversal invariance, $S_{SD} = 4k_B T G_{SD}$

Shot noise (V>0, T=0) is due to temporal correlations between electrons. In tunneling junctions and vacuum tubes, electrons are transmitted randomly and independently of each other - described by Poisson statistics (events uncorrelated in time) . For these devices, shot noise is maximum at

$$S_P = 2eI$$

In both cases, the noise is white (no dependence on frequency).

Background, cont'd



Source emits electrons in *n* channels (different bands) at the Fermi energy. Each channel *n* has a probability T_n of being transmitted to the drain, and a probability $R_n = 1 - T_n$ of being reflected back to the source. In the presence of a voltage V between the source and drain, the (linear response) conductance is (Landauer)

$$G = \frac{e^2}{h} \sum_n T_n$$

Background, cont'd

Using the Landauer formula at finite temperature, 'one can show that' the noise spectral density is

$$S(\omega) = 2\frac{e^2}{h}\sum_n \left[2k_B T T_n^2 + T_n(1-T_n)eV\coth(eV/2k_B T)\right]$$

This equation describes thermal noise at eV<<k_BT and the classical shot noise formula for $T_n << 1$ at T=0. In the limit of zero temperature (2k_BT<<eV), we get

$$S(\omega) = \frac{2e^3|V|}{h}\sum_n T_n(1-T_n)$$

For arbitrary temperature and $T_n << 1$ we get

$$S = \coth(eV/2k_B T)S_{Poisson}$$

Background, cont'd

Define the *Fano factor*

$$F(\omega) = \frac{S(\omega)}{S_P(\omega)} = \frac{\sum_n T_n(1 - T_n)}{\sum_n T_n}$$

- Zero-temperature shot noise is always suppressed compared to the Poisson limit (F<1) – neither closed (T=0) nor open (T=1) channels contribute to the shot noise.

- In metallic diffuse wires F=1/3

Example: noise in tunneling magnetoresistive reader

Calculate noise current spectral density (constant voltage)

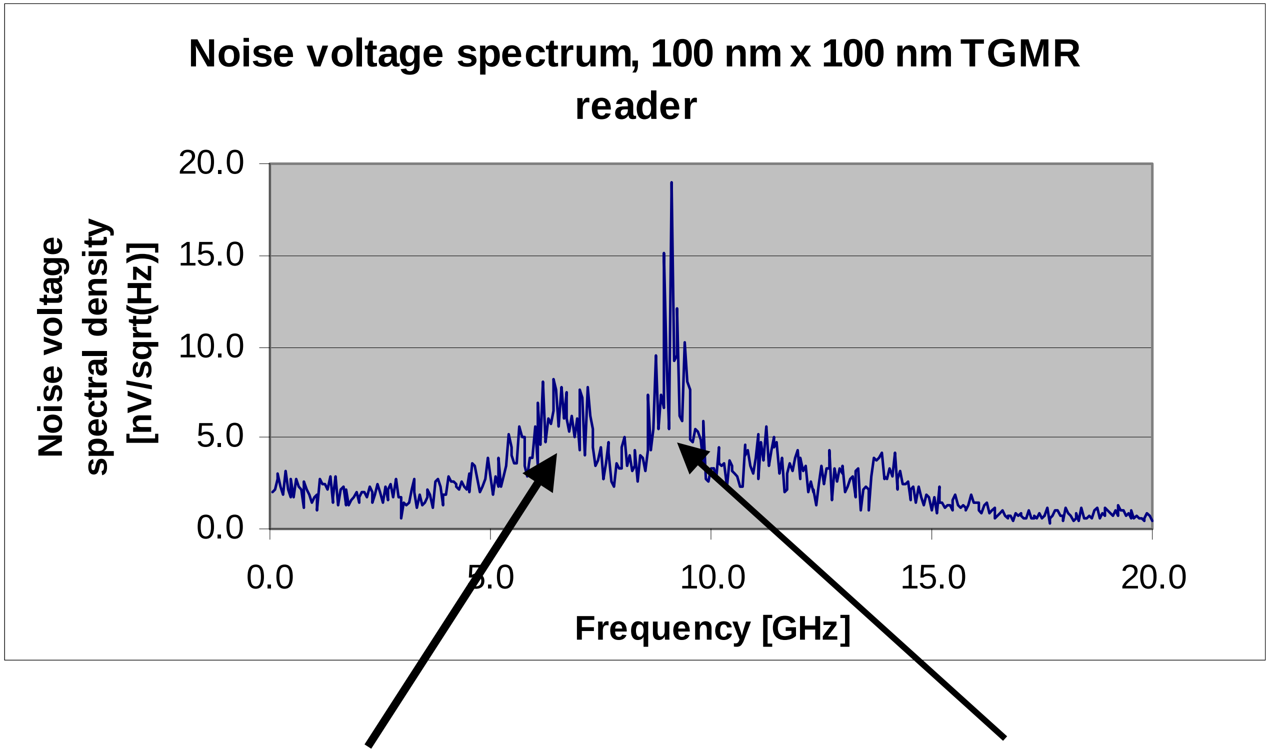
$$S_I(\omega) = 2\int_{-\infty}^{\infty} dt e^{i\omega t} \left\langle \Delta I(t+t_0)\Delta I(t_0)\right\rangle$$

or noise voltage spectral density (constant current)

$$S_V(\omega) = 2\int_{-\infty}^{\infty} dt e^{i\omega t} \left\langle \Delta V(t+t_0)\Delta V(t_0)\right\rangle$$

directly using stochastic LLG - sample voltage at timesteps over a long time (100 ns), calculate voltage-voltage correlation function

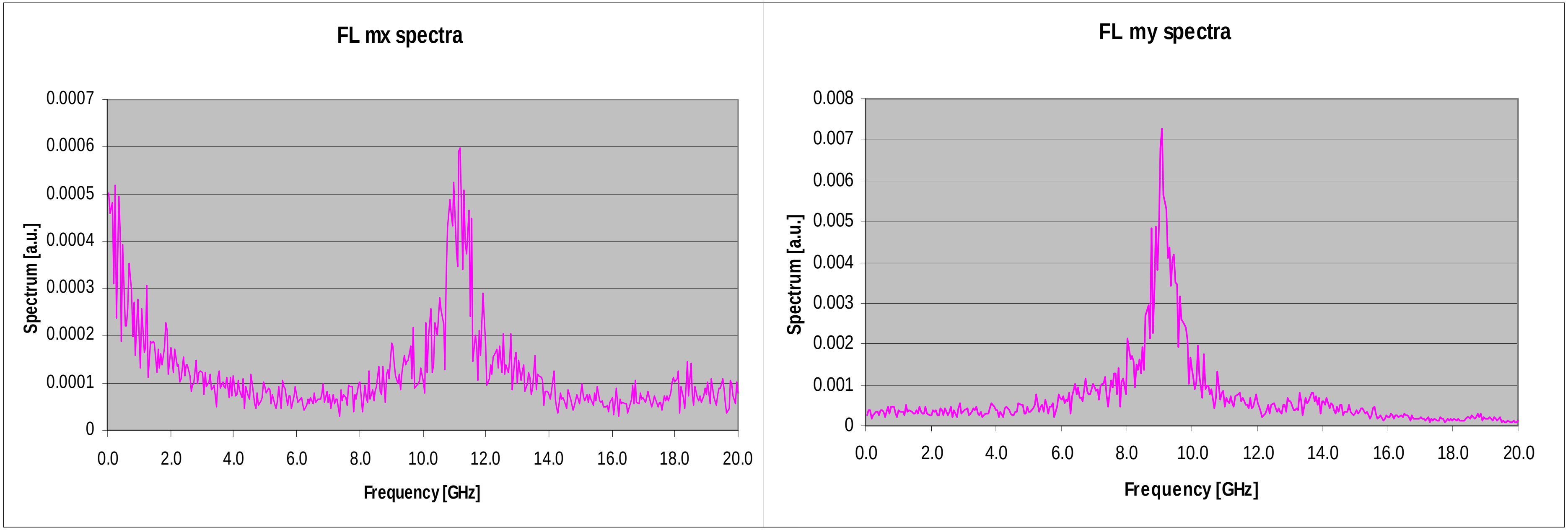
Example: noise in tunneling magnetoresistive reader



What is this?

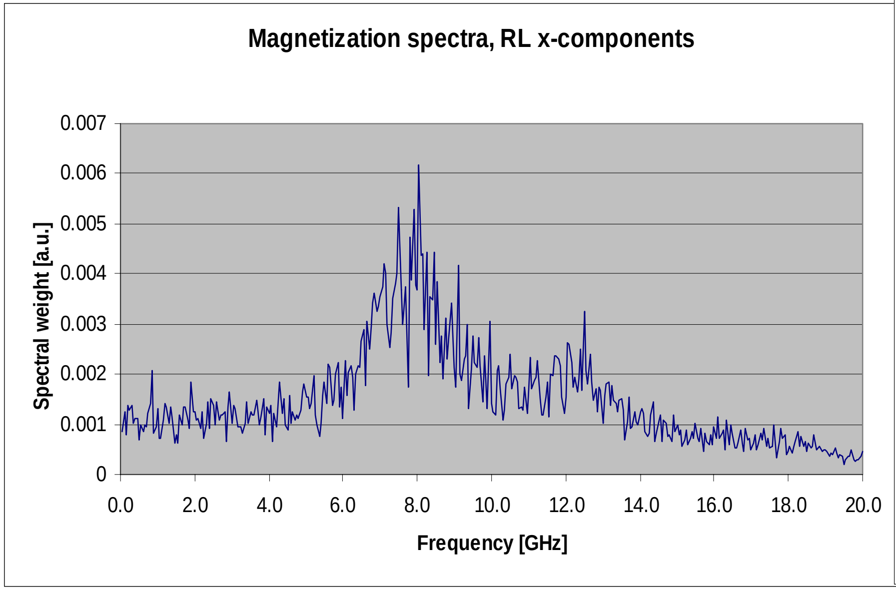
FMR peak (?)

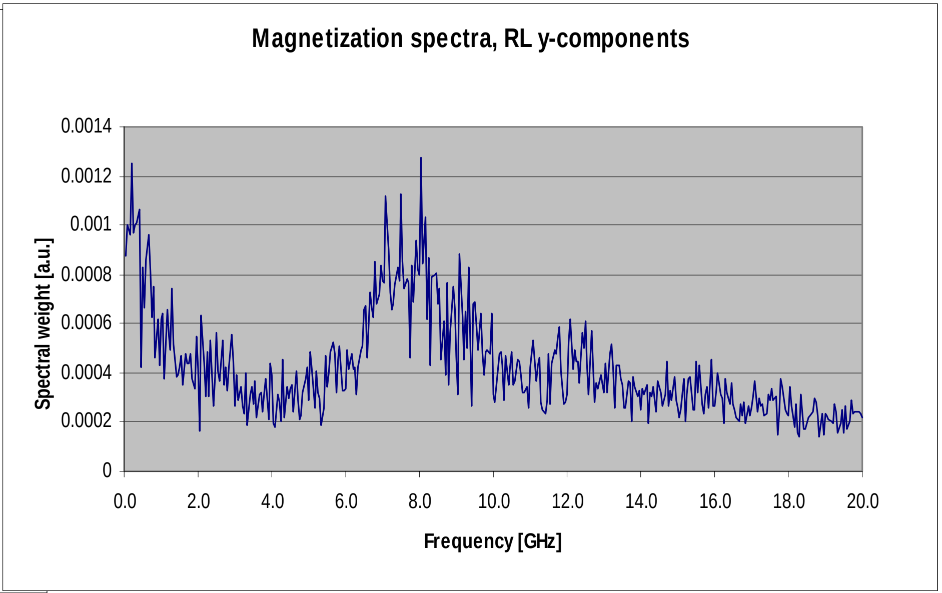
Magnetization motion spectra 100 nm x 100 nm TGMR readers – free layer motion



- Clear FMR peak seen at about 9 GHz
- x-component shows evidence of 1/f-ish stuff
- The peak in the noise voltage spectral density at about 8 GHz comes from the reference layer motion – uncorrelated with the free layer motion

Magnetization motion spectra 100 nm x 100 nm TGMR readers


Magnetization spectra, RL x-components


Magnetization spectra, RL y-components

- Reference layer has a lower peak structure around 8 GHz and some 1/f-ish stuff at lower frequencies

References:

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2. Introduction to Magnetic Recording, R M. White (editor) (IEEE Press 1985). A bit outdated but an excellent reference for the basics of magnetism and magnetic recording (media, readers, writers, shields, the whole ball of wax).

3. *The Theory of Magnetism I,* D.C. Mattis (Springer Verlag, 1988). Much more oriented towards quantum theories of magnetization and the origin of magnetism.

4. *Classical Electrodynamics,* J.D. Jackson (Wiley, 1975). All-purpose reference and textbook on Electrodynamics, even if a bit dull and outdated.

5. *Quantum Mechanics,* Gacziorovics. Good reference for Hunds' rules, for those who want to know more about that.

6. *Solid State Theory,* W. Harrison (Dover, 1979) Good introduction to band theory and transition metals.

7. *Theory of Solids,* J. Ziman (Cambridge, 1972). Also good all-purpose introduction to what electrons do in solids and metals.

8. *Introduction to Solid State Physics*, C. Kittel (Wiley, 19xx). This standard introduction is on its um-teenth edition. Good introduction to spin waves (which is one of the areas where Kittel has made some important contributions himself).

9. *Condensed Matter Physics. Dynamic Correlations,* by Stephen W. Lovesey (Benjamin/Cummins, Reading, MA 1980). Nice little monograph on correlation functions, Langevin equation.

10. *Quantum Dissipative Systems*, by U. Weiss. My favorite reference for this topic.

References:

11. W.F. Brown, Jr., *Phys. Rev.* **130**, 1677 (1963). Classic reference for stochastic LLG equation.

12. R. Kubo and N. Hashitsume, *Prog. Theor. Phys. Suppl.* **46**, 210 (1970). Kubo and Hashitsume's work on stochastic LLG.

13. J. L. Garcia-Palacios and F. J. Lazaro, *Phys. Rev. B* **58**, 14 937 (1998). In my opinion the clearest reference for stochastic LLG and its implementation

14. *Numerical Recipes,* and *Numerical Recipes in Fortran 90*, by Press, Teukolsky, Vetterling, and Flannery. The Bible of numerical work.

15. *Spin Electronics,* M. Ziese and M.J. Thornton (eds) (Springer-Verlag, Berlin 2001). Nice reference on spintronics, micromagnetics, GMR, CMR, MRAMs etc.

Extra slides

Paramagnets, diamagnets, and ferromagnets

Paramagnets:

- Induced magnetization is parallel in direction and proportional to in magnitude to the applied external field $\mathbf{H}_{ext}$. $\mathbf{M}$=0 if $\mathbf{H}$=0.
- Well-defined permeability and susceptibility
- No significant temperature dependence of response
- Most materials

Microscopic picture: spins of electrons act as independent magnetic moments, not interacting with one another but only with external fields (Pauli paramagnetism). Orbital motion (and ensuing orbital magnetic moment) is insignificant.

Antiferromagnets

The exchange interaction between local moments in a sea of conduction electrons actually oscillates in sign (the so-called RKKY interaction). This means that for some lattices, the interaction between local moments actually favors anti-parallel moments, which gives rise to anti-ferromagnets. These are also usually described by a Heisenberg model, but now

$$H = \frac{J}{2} \sum_{<j,j>} \vec{S}_i \bullet \vec{S}_j, \quad J > 0.$$

Paramagnets

Apply and external field **B** to a metal with Fermi energy ε_F.

Electrons with spins anti-parallel to magnetic field lowers energy, Fermi energy shifts to $\varepsilon_F + g\mu_B B$.

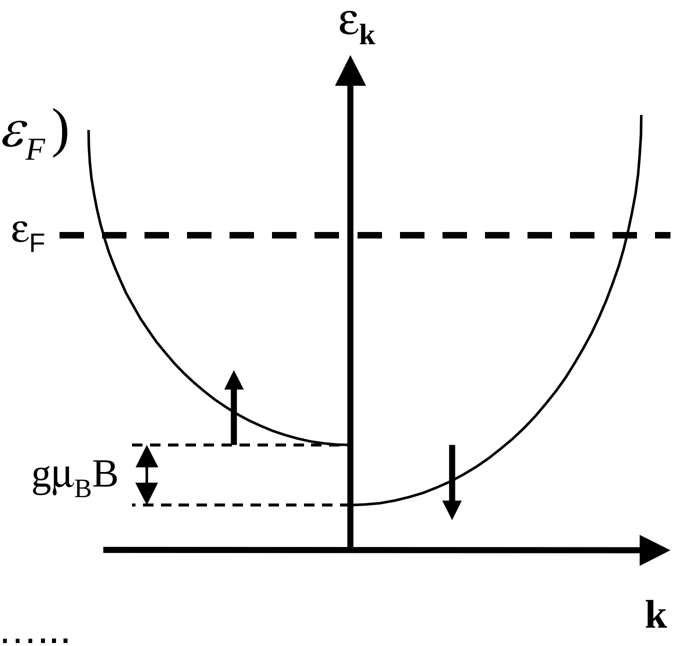
Electrons with spin parallel to magnetic field increase energy, Fermi energy shifts to $\varepsilon_F - g\mu_B B$.

Find number of down- and up-spin electrons:

$$N_{\downarrow} = \frac{1}{2}\int_{-g\mu_B B}^{\varepsilon_F} d\varepsilon D(\varepsilon)(\varepsilon + g\mu_B B) \approx \frac{1}{2}\int_{0}^{\varepsilon_F} d\varepsilon D(\varepsilon) + \frac{1}{2} g\mu_B B D(\varepsilon_F)$$

$$N_{\uparrow} \approx \frac{1}{2}\int_{0}^{\varepsilon_F} d\varepsilon D(\varepsilon) - \frac{1}{2} g\mu_B B D(\varepsilon_F)$$

$$M = g\mu_B (N_{\downarrow} - N_{\uparrow}) = g^2 \mu_B^2 D(\varepsilon_F) B = \frac{3g^2 N \mu_B^2}{2k_B T_F} B$$



Temperature dependence only in T/T_F, and T_F is about 10000 K…...

Diamagnets

Orbital motion gives rise to magnetic moment which couples to external fields. Magnetization is *anti*-parallel to external field. No significant temperature dependence. Orbital motion responds according to Lenz' law with induced magnetic moment antiparallel to the external field

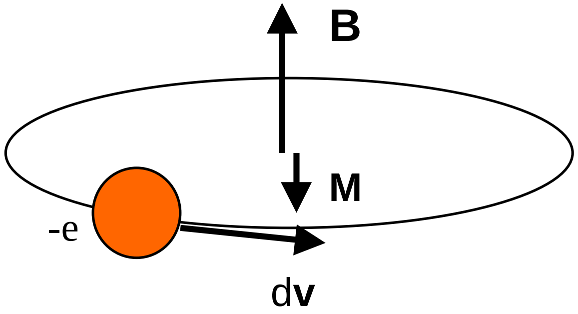
$$\vec B = B\hat z$$

$$\hat H = \frac{1}{2m}\left(\hat{\vec p} + \frac{e}{c}\vec A(\vec r)\right)^2$$

$$A_x = -\frac{1}{2}yB$$

$$A_y = \frac{1}{2}xB$$

$$\hat H = \frac{1}{2m}\hat p^2 + \frac{ie\hbar B}{2mc}\underbrace{\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)}_{\propto L_z \text{ (gives rise only to paramagnetism)}} + \frac{e^2B^2}{8mc^2}\left(x^2+y^2\right)$$



Last term gives an energy shift (1st order perturbation theory)

$$\Delta E \approx \langle 0|\frac{e^2B^2}{8mc^2}\left(x^2+y^2\right)|0\rangle = \frac{e^2B^2}{12mc^2}\langle 0|r^2|0\rangle \text{ for spherically symmetric system, where } |0\rangle \text{ is the ground state}$$

$$\mu = -\frac{\partial(\Delta E)}{\partial B} = -\frac{e^2\langle r^2\rangle}{6mc^2}B$$

$$M = \frac{N\mu}{V} < 0$$

Transition metals

Transition metals: Rows 4, 5, 6 in the periodic table.

Row 4: (K,Ca), Sc, Ti, V, Cr, Mn, Fe, Co, Ni (Cu, Zn, Ga, Ge, As, Se, Br, Kr)

Row 5: (Rb, Sr), Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd (Ag, Cd, In, Sn, Sb, Te, I, Xe)

Row 6: (Cs, Ba), La (Lanthanides), Hf, Ta, W, Re, Os, Ir, Pt (Au, Hg, Tl, Pb, Bi, Po, At, Rn)

- Filled inner shells up to ns^2, (n-1)d shells empty in alkali metals and alkaline earths, but filling up in the transition metals.

Example: K($4s^1$), Ca($4s^2$), Sc($3d^1\,4s^2$), Ti ($3d^2\,4s^2$), V ($3d^3\,4s^2$), Cr ($3d^5\,4s^1$), Mn ($3d^5\,4s^2$), Fe ($3d^6\,4s^2$),

Co ($3d^7\,4s^2$), Ni ($3d^8\,4s^2$), Cu ($3d^{10}\,4s^1$)

The order of filling the d shell is described by Hund’s rules, which give

n	$l_z=2$	$l_z=1$	$l_z=0$	$l_z=-1$	$l_z=-1$	S	$L=\lvert\Sigma\, l_z\rvert$	J
1	-1/2					½	2	3/2 (=|L-S|)
2	-1/2	-1/2				1	3	2 (=|L-S|)
3	-1/2	-1/2	-1/2			3/1	3	3/2 (=|L-S|)
4	-1/2	-1/2	-1/2	-1/2		2	2	0 (=|L-S|)
5	-1/2	-1/2	-1/2	-1/2	-1/2	5/2	0	5/2
6	-1/2,+1/2	+1/2	+1/2	+1/2	+1/2	2	2	4 (=L+S)
7	-1/2,+1/2	-1/2,+1/2	+1/2	+1/2	+1/2	3/2	3	9/2 (=L+S)
8	-1/2,+1/2	-1/2,+1/2	-1/2,+1/2	+1/2	+1/2	1	3	4 (=L+S)
9	-1/2,+1/2	-1/2,+1/2	-1/2,+1/2	-1/2,+1/2	+1/2	½	2	5/2 (=L+S)
10	-1/2,+1/2	-1/2,+1/2	-1/2,+1/2	-1/2,+1/2	-1/2,+1/2	0	0	0

Transition metals

Note: Magnetism in transition metals is not well described by starting with a picture of atoms with local moments equal to those of isolated atoms, and these moments are coupled by exchange coupling. The moment per atom in, for example, crystalline Fe, Co, Ni is not equal to the moment of isolated atoms. Furthermore, just calculating the exchange coupling blindly can give rise to anti-ferromagnetic coupling.

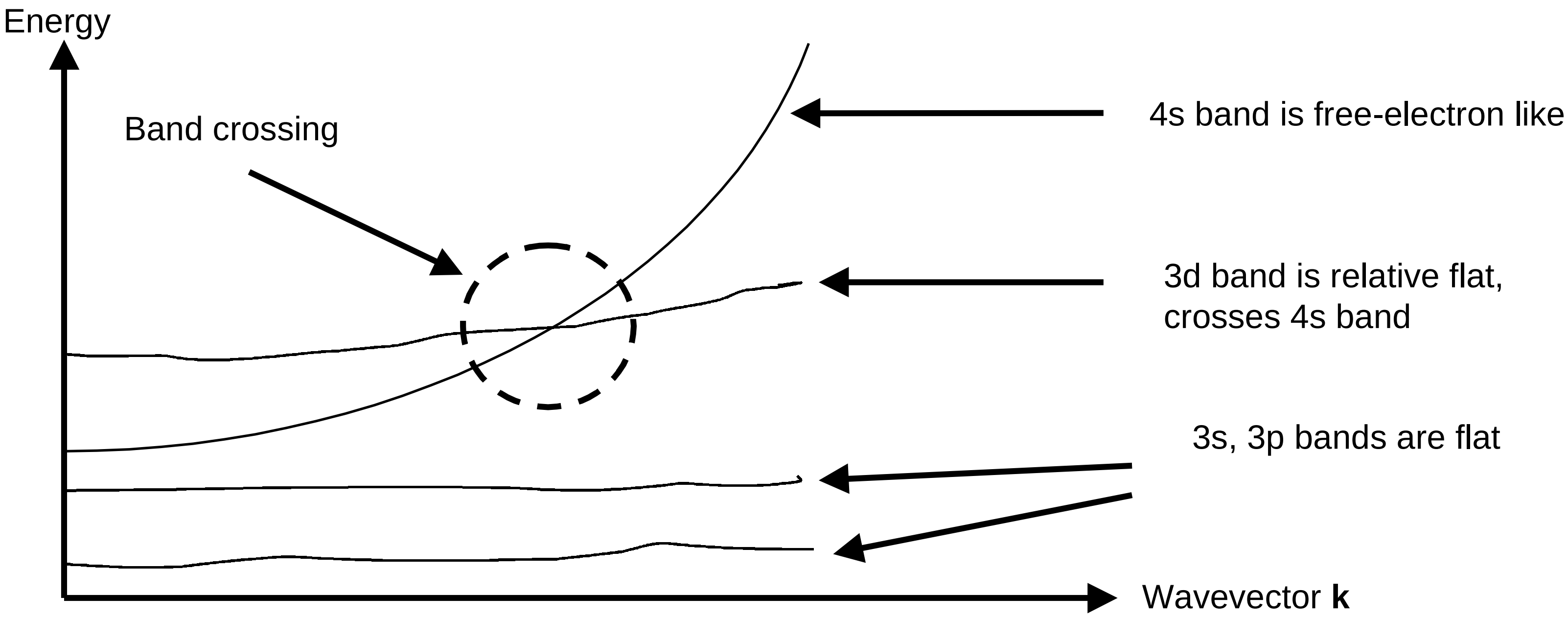
The magnetic transition metals are not individual isolated moments (local moments) which interact with near-neighbors. Instead, the magnetism is distributed throughout spin-split d-bands (itinerant magnetism) and one must look to the band structure to understand the cause of the magnetism.

Transition metals

3s and 3p (or 4s, 4p, 5s, 5p) states are strongly localized near the core of the atoms due to strong Coulomb attraction to nucleus and do not overlap with states on neighboring sites. 3d states are also strongly localized, but do overlap a little with neighboring sites, and overlap with 4s conduction electrons.

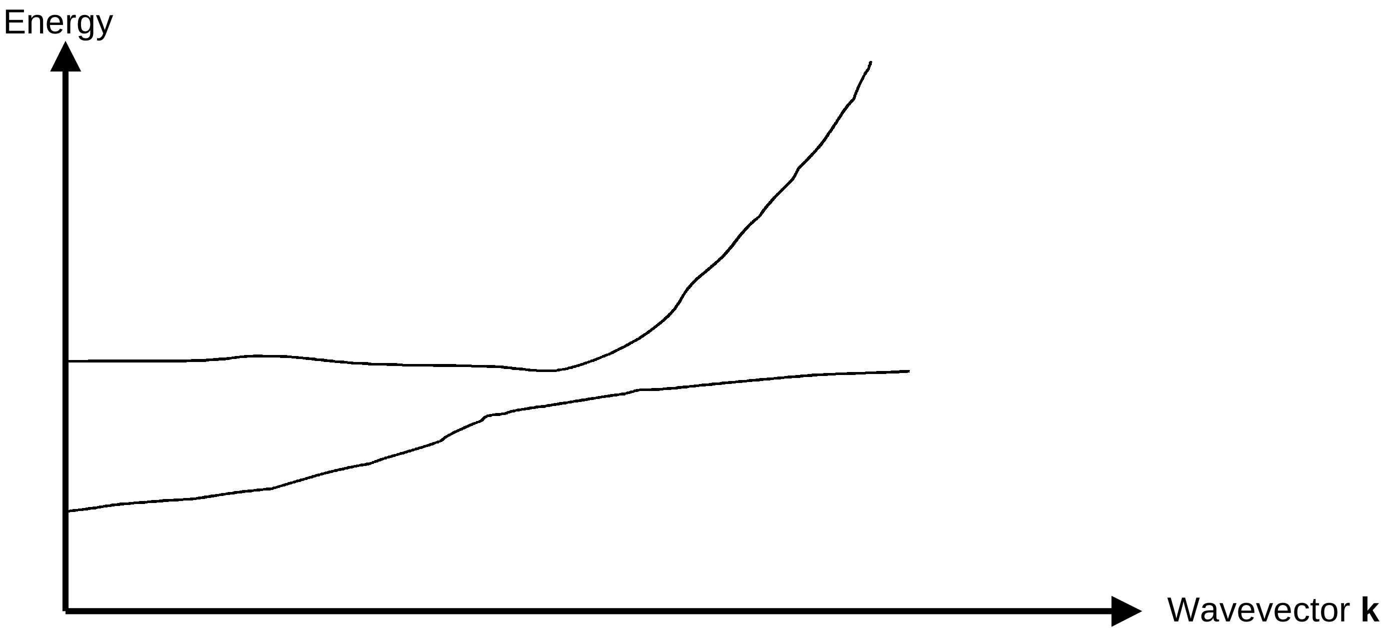
Non-overlapping states ⇨ energy levels are approximately those of states in single atoms and do not broaden into bands as the levels mix.

3d bands are relatively flat due to small mixing, 4s bands are free-electron like (near parabolic).



Transition metals

At the band crossing, 3d and 4s states hybridize (mix), and a gap opens up at the crossing



Opening the gap may cause the paramagnetic state to be unstable with respect to formation of a ferromagnetic ground state (more spin-up than spin down)

Transition metals - ferromagnetic instability

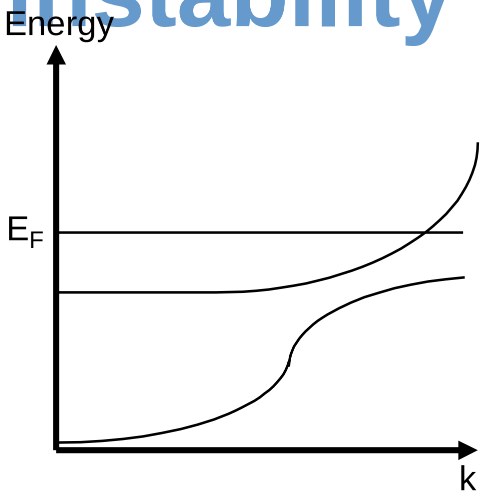


Fig. 1

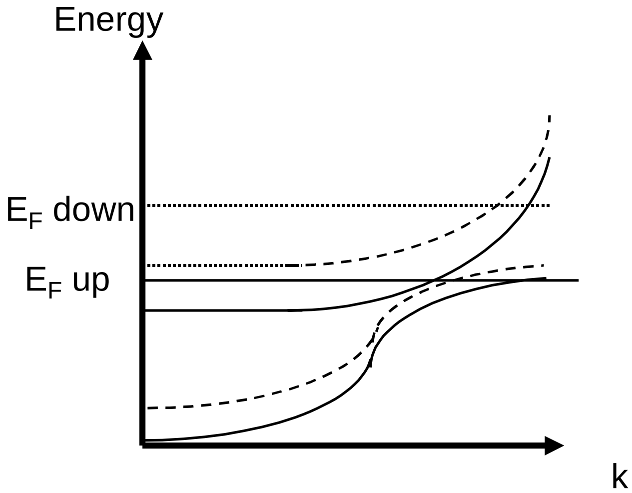


Fig. 2

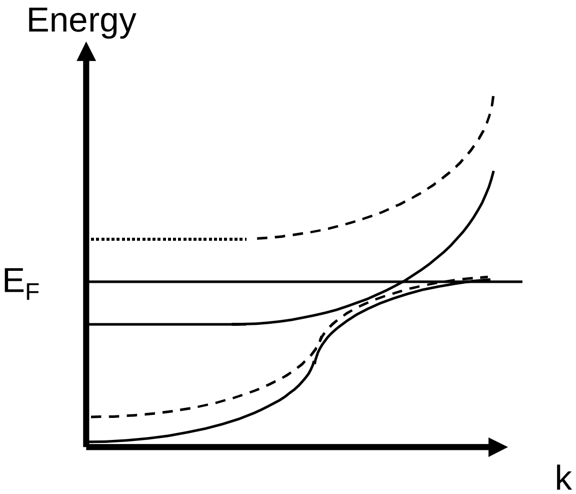


Fig. 3

Why are some transition metals ferromagnets? The reason is that they can achieve lower total energy in a ferromagnetic state than in a paramagnetic state. Consider first a transition metal in a paramagnetic state. The up-and down-spin bands are identical and have equal populations of electrons up to the common Fermi energy E_F (Fig. 1). In the presence of a band gap, the system may try to move some down-spin electrons to up-spin electrons so that the spin populations are unequal. This changes the exchange energy of the bands, and tends to move up-spin bands to lower energy, and down-spin bands to higher energy. As a consequence, the Fermi energies of the spin orientations will be changed and be unequal if the occupations of up-and down-spin bands are assumed to be held constant (Fig. 2). If the Fermi energy of the up-spin electrons is *lowered*, more electrons can be transferred from down-spin states to up-spin states until the Fermi energies are equalized - the paramagnetic state was unstable with respect to formation of a ferromagnetic state (Fig. 3).

Stoner-Wohlfart model

Simple model to describe magnetic material, hysteresis and coercivity. Assume material consists of a collection of uniformly magentized ellipsoids with their axes pointing in arbitrary directions. For an ellipsoid, the demagnetizing field can easily be obtained :

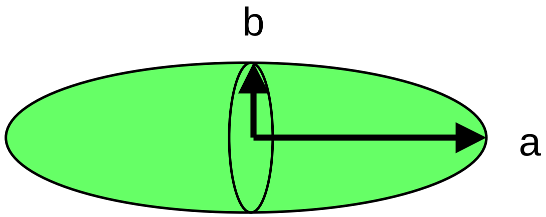
$$\vec{H}_\mathrm{d} = \overleftrightarrow{N} \bullet \vec{M}_s,$$

$$\overleftrightarrow{N} = \begin{pmatrix} N_a & 0 & 0 \\ 0 & N_b & 0 \\ 0 & 0 & N_b \end{pmatrix},$$

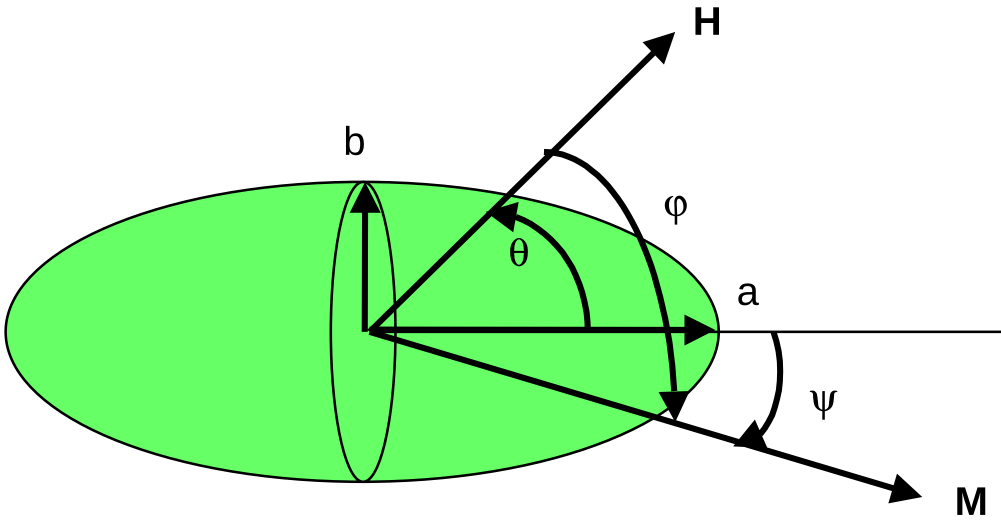
$$N_a = \frac{4\pi}{a^2/b^2 - 1}\left[\frac{(a/b)\ln\left[a/b + (a^2/b^2-1)^{1/2}\right]}{(a^2/b^2-1)^{1/2}} - 1\right],$$

$$N_b = \frac{2\pi}{1 - b^2/a^2} - \frac{4\pi}{a^2/b^2 - 1}\left[\frac{(a/b)\ln\left[a/b + (a^2/b^2-1)^{1/2}\right]}{(a^2/b^2-1)^{1/2}}\right]$$

$$\mathrm{Tr}\left[\overleftrightarrow{\mathrm{N}}\right] = N_a + 2N_b = 4\pi$$



Stoner-Wohlfart model



$$E_{\mathrm{d}} = -\frac{1}{2}\vec{M} \bullet \vec{H}_{\mathrm{d}} = -\frac{1}{2}\vec{M}_s \bullet \left(\overleftrightarrow{N} \bullet \vec{M}_s\right)$$

$$= \frac{M_s^2}{4}\left[\left(N_a + N_b\right) + \left(N_a - N_b\right)\cos 2\psi\right]$$

$$E_Z = -M_s H \cos\varphi$$

$$E = E_{\mathrm{d}} + E_Z$$

Stoner-Wohlfart model

Minimize total energy by setting

$$\frac{dE}{d\varphi} = 0, \quad \text{and} \quad \frac{d^2E}{d\varphi^2} > 0 \Rightarrow$$

$$\frac{1}{2}\sin 2(\varphi - \theta) + h\cos\varphi = 0$$

$$\cos 2(\varphi - \theta) + h\cos\varphi > 0,$$

$$h \equiv \frac{H}{(N_a - N_b)M_s}$$

Set second derivative to zero to find instability of solution for given θ gives critical field at which magnetization jumps to new orientation:

$$h_c = -\frac{(1 - t^2 + t^4)^{1/2}}{(1 + t^2)}, \quad t = \tan^{1/3}\theta$$

Stoner-Wohlfart model

Find hysteresis loop by evaluating average orientation over an ensemble of particles with different orientations as a function of external field:

$$\langle \cos\varphi \rangle = \frac{\int_0^{\pi/2} 2\pi \cos\varphi \sin\theta d\theta}{\int_0^{\pi/2} 2\pi \sin\theta d\theta}$$

Numerical evaluation gives a coercivity of $H_c=0.479(N_a-N_b)M_s$, and a remnant magnetization of $M_s/2$

Note:

- Particle-particle interactions changes the coercivity
- Rotation of individual particles can be incoherent (not coherent as assumed here)
- If the ellipsoid is made large enough, the magnetization will not be uniform but domains will be formed to lower the total energy.