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Magnetization reversal

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Poznań 2019

Maciej Urbaniak

Magnetization reversal

- Beyond Stoner-Wohlfarth model
- Landau-Lifshitz-Gilbert equation
- Micromagnetism
- Langevin-Landau-Lifshitz-Gilbert equation
- Thiele equation

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Statement of the micromagnetic problem

- In the original Stoner-Wolfarth (SW) model the particle was single domain, i.e., its has a single magnetic moment (macrospin)
- We searched for an equilibrium orientation of the moment as a function of magnitude and direction an external magnetic field
- The dynamic effects played no role in the model
- In the fifth lecture we studied the rate dependent hysteresis in 1 dimension (angle of rotation of the moment) assuming some fictional energy landscape (similar to the one in SW model) but still within macrospin approximation
- We want now to introduce the formalism allowing the reasonable predictions of the behavior of the magnetic sample composed of many magnetic moments and evolving under the influence of:
- external magnetic field

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- exchange, RKKY-like, and Dzyaloshinskii–Moriya coupling between neighboring spins
- local anisotropies (magnetocrystalline, stress etc.)
- influence of the flow (current, heat etc.)
- long range magnetostatic interactions between the magnetic moments (shape anisotropy)



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Statement of the micromagnetic problem

- First we will describe the behavior of a rectangular prism sample with a single magnetic moment
- The raise time of the magnetic field is always larger than zero but in micromagnetics the field changes are approximated by step-wise varying magnetic field – the field changes are instantaneous

The analytical formulas for demagnetizing factors for rectangular prisms are given by A. Aharoni in J. Appl. Phys. **83**, 3432 (1998)

> Raise-time of the field is determined primarily by a self-inductance of the the coils/electromagnet

Statement of the micromagnetic problem

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- In the simulation we want to predict the changes of the orientation of the magnetic moments as the external field changes
- The position of the moment is assumed to be fixed no changes due to magnetostriction, phonons, magnons etc.



Landau-Lifshitz-Gilbert (LLG) equation of spin motion

- The change of angular momentum of a rigid body under the influence of the torque is given by:
- given by: $\vec{\tau} = \frac{d\vec{J}}{dt}$ The torque acting on magnetic moment in magnetic field is: $\vec{\tau} = \vec{m} \times \vec{B}$ With gyromagnetic ratio defined as $\gamma = \frac{|\vec{m}|}{|\vec{\tau}|}$ we get: For an electron we have: $<math>\vec{m}_e = -g_e \frac{e}{2m} \vec{S}$ $|S| = \frac{h}{2\pi} \frac{\sqrt{3}}{2} S_z = \frac{h}{2\pi} \frac{1}{2} g^{\approx 2}$ $\gamma = \frac{\vec{m}_e}{\vec{S}} = -\frac{e}{m}$

 $\frac{d\,\vec{m}}{dt} = \gamma\,\vec{m}\times\vec{B}$

This equation can be used to describe motion of the electron's magnetic moment. The electron itself is fixed in space.

Larmor precession [3] • Vector rotating with angular velocity Ω changes according to the formula:

$$\frac{d\vec{A}}{dt} = \vec{\Omega} \times \vec{A}$$

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• From equation for time change of **m** we get:

$$\frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B} = -\gamma \vec{B} \times \vec{m} = -\omega_L \times \vec{m}$$

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•The velocity is called *Larmor angular velocity* and is given by:

$$\vec{\Omega}_L = \gamma \vec{B}$$

•The corresponding *Larmor frequency* is:

$$f_L = \frac{1}{2\pi} \gamma B$$

•For electron *Larmor frequency* is approximately 1.761×10¹¹ rad s⁻¹T⁻¹ *

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R E S •Landau and Lifshitz have introduced **a damping term** to the precession equation:

$$\frac{d\vec{m}}{dt} = \gamma \,\vec{m} \times \vec{B} - \frac{\alpha_L}{|\vec{m}|} (\vec{m} \times (\vec{m} \times \vec{B})), \qquad (1)$$

where α_L is a dimensionless parameter [5].

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- •As can be seen the damping vector $-\vec{m} \times (\vec{m} \times \vec{B})$ is directed toward **B** and vanishes when **m** and **B** become parallel.
- •As can be seen from Eq. (1) the relaxation of m towards B is greater the higher the damping constant α_L . Gilbert [6] pointed out that this is nonphysical and that Eq. (1) can be used for small damping only [5].



•He introduced other phenomenological form of equation which can be used for arbitrary damping. Damping is introduced as dissipative term [7] of the effective field acting on the moment:

$$\vec{B} \rightarrow \vec{B} - \eta \frac{d \vec{m}}{dt}$$

(2)

•Inserting Eq. (2) into precession equation (3 slides back) we obtain:

$$\frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B} \Rightarrow \gamma \vec{m} \times \left(\vec{B} - \eta \frac{d\vec{m}}{dt}\right) = \gamma \vec{m} \times \vec{B} - \gamma \eta \vec{m} \times \frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B} - \frac{\alpha}{|\vec{m}|} \vec{m} \times \frac{d\vec{m}}{dt}, \text{ with } \alpha = \gamma \eta |\vec{m}|$$

•The equation can be transformed by substituting itself into righ-hand side:

$$\frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B} - \frac{\alpha}{|\vec{m}|} \vec{m} \times \frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B} - \frac{\alpha}{|\vec{m}|} \vec{m} \times \left(\gamma \vec{m} \times \vec{B} - \frac{\alpha}{|\vec{m}|} \vec{m} \times \frac{d\vec{m}}{dt}\right)$$

•Multiplying out we get:

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$$\frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B} - \frac{\alpha \gamma}{|\vec{m}|} \vec{m} \times \vec{m} \times \vec{B} + \frac{\alpha^2}{|\vec{m}|^2} \vec{m} \times \vec{m} \times \frac{d\vec{m}}{dt}$$
(3)

•Using vector identity $\vec{a} \times (\vec{b} \times \vec{c}) = \vec{b} (\vec{a} \cdot \vec{c}) - \vec{c} (\vec{a} \cdot \vec{b})$ we have: $\vec{m} \times \vec{m} \times \frac{d\vec{m}}{dt} = \vec{m} (\vec{m} \cdot \frac{d\vec{m}}{dt}) - \frac{d\vec{m}}{dt} |\vec{m}|^2$

•Since the magnitude of *m* is assumed to be constant* there can be no component of ² which is parallel to *m*; we get then:

$$\vec{m} \times \vec{m} \times \frac{d\vec{m}}{dt} = -\frac{d\vec{m}}{dt} |\vec{m}|^2 \qquad (4$$

*if the system consists of a number of individual moments, each of which is damped slightly differently, the magnitude of the total magnetic moment may not be conserved; one should use Bloch equation then.

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Landau-Lifshitz-Gilbert (LLG) equation of spin motion

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• Inserting Eq. (4) into Eq. (3) we obtain: $\frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B} - \frac{\alpha \gamma}{ \vec{m} } \vec{m} \times \vec{m} \times \vec{B} - \alpha^2 \frac{d\vec{m}}{dt}$	$\frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B} - \frac{\alpha \gamma}{ \vec{m} } \vec{m} \times \vec{m} \times \vec{B} + \frac{\alpha^2}{ \vec{m} ^2} \vec{m} \times \vec{m} \times \frac{d\vec{m}}{dt} $ (3) $-\frac{d\vec{m}}{dt} \vec{m} ^2 = \vec{m} \times \vec{m} \times \frac{d\vec{m}}{dt} $ (4)	G N E T I C
$\frac{d\vec{m}}{dt}(1+\alpha^2) = \gamma \vec{m} \times \vec{B} - \frac{\alpha \gamma}{ \vec{m} } \vec{m} \times \vec{m} \times \vec{B}$	$\alpha = \gamma \eta \left \vec{m} \right $	M A T
And finally:		Ē
Landau-Lifshitz-Gilbert equation		R
		I.
$\left(\frac{d\vec{m}}{dt} = \frac{\gamma}{(1+\alpha^2)}\vec{m} \times \vec{B} - \frac{\alpha}{(1+\alpha^2)}\frac{\gamma}{ \vec{m} }\vec{m} \times \vec{m} \times \vec{B}\right)$		A L S
 In general the magnetic induction should 	be replaced by the effective field B _{eff} [9, p. 178]:	A N
$\vec{B}_{n} = \mu \left(\nabla^{2} \vec{M} + \vec{H} + \frac{\partial}{\partial m} F \right)$		D
$\partial \vec{m}^{\text{anisotropy}}$		H Y
	Other energy terms, like Dzyaloshinskii–Moriya interaction or magneto-elastic effects, may	S T

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to be read as $\frac{\partial}{\partial \vec{m}} f = \hat{x} \frac{\partial}{\partial m_x} f + \hat{y} \frac{\partial}{\partial m_y} f + \hat{z} \frac{\partial}{\partial m_z} f$ [9, p.178]

contribute to the effective field

Landau-Lifshitz-Gilbert equation

$$\frac{d\vec{m}}{dt} = \frac{\gamma_G}{(1+\alpha_G^2)} \vec{m} \times \vec{B} - \frac{\alpha_G}{(1+\alpha_G^2)} \frac{\gamma_G}{|\vec{m}|} \vec{m} \times \vec{m} \times \vec{B}$$

•With the replacement $\gamma_L = \frac{\gamma_G}{1 + \alpha_G^2}$, $\alpha_L = \frac{\alpha_G \gamma_G}{1 + \alpha_G^2}$ both equations have similar form but...

 $\frac{d\vec{m}}{dt} = \gamma_L \vec{m} \times \vec{B} - \frac{\alpha_L}{|\vec{m}|} (\vec{m} \times (\vec{m} \times \vec{B}))$

Landau-Lifshitz equation

the dependencies of precessional and relaxation terms on damping constant are quite different [8]:

 According to LL equation the relaxation becomes faster with increasing damping α_L (red dashed curve) which is counter intuitive.

 In case of LLG equation the behavior of both terms agree with the expectations for the dynamics of damped precession [8].

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Landau-Lifshitz-Gilbert (LLG) equation of spin motion – inclusion of moment of inertia

Landau-Lifshitz-Gilbert equation

$$\frac{d\vec{m}}{dt} = \frac{\gamma_G}{(1+\alpha_G^2)} \vec{m} \times \vec{B} - \frac{\alpha_G}{(1+\alpha_G^2)} \frac{\gamma_G}{|\vec{m}|} \vec{m} \times \vec{m} \times \vec{B}$$

- Investigation of spin dynamics at very high frequencies requires taking into account • moments of inertia of a system (not limited to spins)
- Calculations set "the time scale of the inertial contribution to the femtosecond (10-15 s) regime. It, therefore, defines magnetization dynamics on a time scale that is one or more orders of magnitude shorter compared to, e.g., the precessional dynamics of the magnetic moment."

which is composed of precessional and damping terms driving the dynamics to an equilibrium. By including the moment of inertia, we arrive at a generalized LLG equation

$$\dot{\mathbf{M}} = \mathbf{M} \times (-\gamma \mathbf{B} + \hat{\mathbf{G}} \, \dot{\mathbf{M}} + \hat{\mathbf{I}} \, \ddot{\mathbf{M}}), \tag{1}$$

where $\hat{\mathbf{G}}$ and $\hat{\mathbf{I}}$ are the Gilbert damping and the moment of inertia tensors, respectively. In this equation the effective field **B** includes both the external and internal fields, of which the latter includes the exchange coupling and anisotropy effects. Here, we will for convenience include the anisotropy arising from the classical dipole-dipole

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FIG. 1. arising from the effective magnetic field, and the superimposed effects from the Gilbert damping and the moment of inertia, respectively.





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 Let us* consider the LLG equation describing the orientation of a single moment (monodomain state) of magnetized sphere fixed in space (no translational motion)**:

 $\tau = \frac{t M \gamma \mu_0}{(1+q^2)}$

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$$\frac{d\vec{M}}{dt} = \frac{\gamma \mu_0}{(1+\alpha^2)} (\vec{M} \times \vec{H} - \frac{\alpha}{M} [\vec{M} \times (\vec{M} \times \vec{H})])$$

- For simplicity the time scale is changed: $M^{2} \frac{d\vec{M}}{d\tau} = M \vec{M} \times \vec{H} - \alpha \left[\vec{M} \times (\vec{M} \times \vec{H}) \right]$
- We assume that the external field is applied along z-direction [$B_a/\mu_0=(0,0,H_z)$]. The demagnetizing field inside the sphere is (H_d=-1/3 H_z). With $H=H_a$ - H_d we obtain:

$$M^{2} \frac{dM_{x}}{d\tau} = -\alpha H_{z} M_{x} M_{z} + H_{z} M_{y} M$$
$$M^{2} \frac{dM_{y}}{d\tau} = -\alpha H_{z} M_{y} M_{z} - H_{z} M_{x} M$$
$$M^{2} \frac{dM_{z}}{d\tau} = \alpha \left(H_{z} M_{x}^{2} + H_{z} M_{y}^{2}\right)$$

• Verifying that $d\mathbf{M}$ is perpendicular to $\mathbf{M} ([dM_x, dM_y, dM_z) \cdot \vec{M} = 0]$ we see that the length of the magnetization vector is preserved as expected.

(-α Hz Mx Mz +Hz My M,-α Hz My Mz -Hz Mx M, α (Hz Mx Mx +Hz My My)).(Mx,My,Mz)=0

*Ryoichi Kikuchi, J. Appl. Phys. 27, 1352 (1956)

**Kikuchi uses this form of the equation; for $\alpha \ll 1$ it reduces to Landau-Lifshitz equation

•We can then rewrite the equation for M_z obtaining the equation of motion that does not depend on M_x and M_y :

•Integrating between the final and the initial values of M_z we have:

$$\alpha H_{z} \tau = \int_{M_{z}^{i}}^{M_{z}^{f}} \frac{M^{2}}{(M^{2} - M_{z}^{2})} dM_{z} = M \operatorname{ArcTanh} \left[\frac{M_{z}}{M} \right]_{M_{z}^{i}}^{M_{z}^{f}} = M \ln \left| \sqrt{\frac{-1 - M_{z}/M}{\sqrt{-1 + M_{z}/M}}} \right|_{M_{z}^{i}}^{M_{z}^{f}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i}} = M \ln \left| \sqrt{\frac{-1 - M_{z}^{f}/M}{-1 + M_{z}^{f}/M}} \right|_{M_{z}^{i}}^{M_{z}^{i$$

•Going back to the actual time we get for the time for M_z to change from the initial to final value:

$$\tau = \frac{l M y \mu_0}{(1+a^2)}$$

$$t_{F} = \frac{1}{2 \gamma H_{z}} \frac{1 + \alpha^{2}}{\alpha} \ln \left| \frac{(M + M_{z}^{f})(M - M_{z}^{i})}{(M - M_{z}^{f})(M + M_{z}^{i})} \right|$$

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$$\underbrace{t_{F} = \frac{1}{2 \gamma H_{z}} \frac{1 + \alpha^{2}}{\alpha} \ln \left| \frac{(M + M_{z}^{f})(M - M_{z}^{i})}{(M - M_{z}^{f})(M + M_{z}^{i})} \right| }_{\mathbf{A}}$$

If at t=0 the magnetization/moment points exactly along z-axis (M_z=-M) then t_F would be undefined, for M_z approaching -M it would approach infinity – **no switching**.
If there is no damping (α approaches 0) then t_F would tend to infinity – the moment of the sample would precess around the external field direction.



•The shortest switching time is obtained for finite value of damping coefficient (α =1).

•The value of the critical damping constant depends on the shape of the sample.

•For single domain thin film the critical α is about 0.013.

•For permalloy films the minimum switching time, as obtained from the similar calculations is about **1 ns**.

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- Time evolution of magnetic moment orientation for low and high damping:
- initial orientation of magnetic moment: (0,0.001,1) -
- magnetic field instantaneously switched on to value: (0,0,-1)



H||z axis

- Time evolution of magnetic moment orientation for low and high damping:
- initial orientation of magnetic moment: (0,0.001,1) +
- magnetic field instantaneously switched on to value: (0,0,-1)



- blue dots mark the same time intervals
- the end of moment moves from top to R bottom

HIIz axis

Ryoichi Kikuchi, J. Appl. Phys. 27, 1352 (1956)

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- Time evolution of magnetic moment orientation for low and high damping:
- initial orientation of magnetic moment: (0,0.001,1)
- magnetic field instantaneously switched on to value: (0,0,-1)



- blue dots mark the same time intervals
- the end of moment moves from top to bottom

HIIz axis

- the total time of movement is the same as on the previous page
- note that due to weaker damping the moment did not change its orientation to -z – the switching is delayed

ng Ryoichi Kikuchi, J. Appl. Phys. 27, 1352 (1956)

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- Time evolution of magnetic moment orientation for low and high damping:
- initial orientation of magnetic moment: (0,0.001,1) +
- magnetic field instantaneously switched on to value: (0,0,-1)



Ryoichi Kikuchi, J. Appl. Phys. 27, 1352 (1956) 2019

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- Note that further increase of damping constant α slows down the switching of magnetic moment (more blue dots)





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Magnetic moment reversal - thin film

- •Time evolution of magnetic moment orientation for low and high damping:
- nitial orientation of magnetic moment: (-1,0.001,0) in plane of the sample
- magnetic field instantaneously switched on to value: (+1,0,0) HIIz axis



- α→0
- the end of moment moves from behind to the front
- blue dots mark the same time intervals
- in thin films, contrary to the case of the single domain sphere, the demagnetizing field is, in general*, not parallel to magnetic moment and Α exerts a torque on it \Rightarrow the switching Ν time depends on the magnetization

• for large α:

 $t_F \propto \frac{\alpha}{M}$

 \vec{H}_{demag} $=-\hat{z}M_{z}$

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Magnetic moment reversal – thin film

- •Time evolution of magnetic moment orientation for low and high damping:
- initial orientation of magnetic moment: (-1,0.001,0) in plane of the sample
- magnetic field instantaneously switched on to value: (+1,0,0)



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Element-resolved precessional dynamics

- Sputtered, 0.35 mm wide Cu(75nm)/Py(25nm)/Cu(3nm) trilayer
- Current pulses through thick Cu layer (10ns duration) create field pulses (Oersted field) perpendicular to the film stripline (in plane of the film)
- A bias field *H*_b can be applied parallel to the stripline in order to align the initial magnetization prior to excitation.
- Element-selective x-ray resonant magnetic scattering (XRMS)



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Figure 1. Schematic of the setup and fields applied at the sample region. The 350 μ m stripline is centred on a Si substrate and oriented perpendicular to the scattering plane. A pair of coils provides the bias field $H_{\rm b}$ along the *y*-axis, the pulse field from the stripline is parallel to the *x*-axis. With our setup the change in the M_x -component is measured while the magnetization precesses around the effective field direction $H_{\rm eff}$.

authors' "data show that Fe and Ni moments are aligned parallel to each other at all times, while they oscillate around the effective field direction given by the step field pulse and applied bias field"

Figure **5**. Comparison of the magnetization dynamics measured at the **Fe** (full) and **Ni** (open symbols) resonant edges for a set of different bias fields. The detected intensity is converted into opening angle ϕ according to the hysteresis curves.

2019 S. Buschhorn, F. Brüssing, R. Abrudan and H. Zabel, J. Phys. D: Appl. Phys. 44, 165001 (2011)

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Micromagnetism

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- Micromagnetism*, as a refinement of *domain theory*, begins in 1930ies (Landau, Lifshitz) [9].
- In most cases of interest the use of atomistic description is too computationally demanding.
- In micromagnetism microscopic details of the atomic structure are ignored and the material is considered from the macroscopic point of view as **continuous** [9].
- Spins are replaced by classical vectors motion of which is described by LLG equation



micromagnetic description



• The exchange interaction energy among spins*, assuming that coupling is non-zero between nearest neighbors only, can be written as [9]:

$$E_{ex} = -JS^2 \sum_{neighbours} \cos\phi_{i,j}$$

 $E_{ex} \approx \frac{1}{2} J S^2 \sum_{neighbours} \phi_{i,j}^2$

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 The angles between the magnetic moments of neighboring spins are always small due to high strength of exchange coupling [8]. The angle between spins can be expanded in series coefficients**. In one dimensional case we have:

$$E_{ex} = -JS^2 \sum_{neighbours} \cos\phi_{i,j} = -JS^2 \sum_{neighbours} \left(1 - \frac{1}{2}\phi_{i,j}^2 + \dots \right) \approx -JS^2 \sum_{neighbours} 1 + JS^2 \sum_{neighbours} \frac{1}{2}\phi_{i,j}^2$$

• If we use the state with all spins aligned ($\varphi_{ij}=0$) as a reference state we get:



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•If the angle between neighboring magnetic moments is small it can be expressed as:

$$|\phi_{i,j}| \approx |\vec{m}_i - \vec{m}_j|$$

•If M (magnetization vector) is a continuous variable we can use first-order expansion in Taylor series [9] to get Δm dependence on r:

$$|\vec{m}_i - \vec{m}_j| = \left| \left(dr_x \frac{\partial}{\partial x} + dr_y \frac{\partial}{\partial y} + dr_z \frac{\partial}{\partial z} \right) \vec{m} \right| = \left| (\vec{dr} \cdot \nabla) \vec{m} \right|$$

•The exchange energy then becomes:

$$E_{ex} \approx \frac{1}{2} J S^2 \sum_{neighbours} \phi_{i,j}^2 \approx \frac{1}{2} J S^2 \sum_i \sum_{\vec{dr}_i} \left((\vec{dr} \cdot \nabla) \vec{m} \right)^2$$

summation from lattice point to all its neighbors



If ϕ_{ij} is small the vector $\mathbf{m}_i \cdot \mathbf{m}_j$ is approximately of the same length as arc. Μ

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- As an example consider a simple cubic lattice with following six vectors to the nearest neighbors:
- $-\vec{dr}$: (1,0,0), (0,1,0), (-1,0,0), (0,-1,0), (0,0,1), (0,0,-1)
- We substitute the above vectors into the sum from previous page. We have:

$$+ \sum_{dr_{i}} \left[\left(\vec{dr} \cdot \nabla \right) \vec{m} \right]^{2} = 2 \left(\frac{\partial}{\partial x} m_{x} \right)^{2} + 2 \left(\frac{\partial}{\partial y} m_{x} \right)^{2} + 2 \left(\frac{\partial}{\partial z} m_{x} \right)^{2} + 2 \left(\frac{\partial}{\partial z} m_{y} \right)^{2} + 2 \left(\frac{\partial}{\partial z} m_{y} \right)^{2} + 2 \left(\frac{\partial}{\partial z} m_{y} \right)^{2} + 2 \left(\frac{\partial}{\partial z} m_{z} \right)^{2} + 2 \left(\frac{\partial}{\partial z} m_{y} \right)^{2} + 2 \left(\frac{\partial}{\partial z} m_$$

 Changing the summation to integration over the ferromagnetic body we obtain for cubic systems [9,14 p. 134]:

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

C - constant

• For lower symmetries of crystal lattice the expression for exchange energy density has slightly different forms . *"But for most cases of any practical interest this equation can be taken as a good approximation for the exchange energy, in as much as the assumption of the continuous material is a good approximation to the physical reality."*-A. Aharoni [9]

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• Constant C depends on lattice type [9]:

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

 For hexagonal crystal, such as cobalt, one obtains the same form of expression but the value of constant C is different:

 $C = \frac{4\sqrt{2}JS^2}{1}$, where **a** is nearest neighbors' distance

- It is common ([8] for example) to write the expression for exchange energy density without the factor $\frac{1}{2}$; a different constant $A = \frac{1}{2}C$ is defined then.
- Both A and C are referred to as "exchange constant of the material" [9] or exchange stiffness constant (A) [8].
- Constant A is of the order of 10×10⁻¹² Jm⁻¹ in ferromagnetic materials.
- The exchange constant is roughly proportional to Curie temperature [15]:

 $A \approx \frac{k_B T_C}{2a_c}$, a_0 -lattice parameter in a simple structure

 $C = \frac{2JS^2}{c}$

J- exchange integral, S – spin, a-lattice constant. c- constant

lattice	С
SC	1
bcc	2
fcc	4

	A[pJ m⁻¹]*
α-Fe	21
Со	31
Ni	7
Ni ₈₀ Fe ₂₀ [7]	11

*from H. Kronmüller. M. Fähnle. Micromagnetism... [8]

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Equilibrium condition

• We have the expression for the effective field [7, 9]:

$$\vec{B}_{eff} = \mu_0 \left(\nabla^2 \vec{M} + \vec{H} + \frac{\partial}{\partial \vec{m}} E_{anisotropy} \right)$$

• If one is interested in magnetization distribution static equilibrium the only condition that must be satisfied is [7,14]:

 $\vec{m} \times \vec{H}_{eff} = 0$

 $\frac{\partial \vec{m}}{\partial \vec{n}} = 0$

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A K **M** must point at each point along the direction of the effective field

• Symmetry breaking of exchange interactions at outer surfaces brings additional so called *free boundary conditions* [7,14 p.135]:

Effective field is an extension of magnetostatic energy terms of different origin:

$$E_{magn} = -\vec{M} \cdot \vec{B}$$
$$\vec{H}_{eff} = -\frac{1}{\mu_0 M_s} \frac{\partial}{\partial \vec{m}} E_{total}$$

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to be read as
$$\frac{\partial}{\partial \vec{m}} f = \hat{x} \frac{\partial}{\partial m_x} f + \hat{y} \frac{\partial}{\partial m_y} f + \hat{z} \frac{\partial}{\partial m_z} f$$
 ([9, p.178], [14, p. 126])

Lets us assume that a sample possesses uniaxial anisotropy with easy axis along *z*-axis

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The anisotropy energy can be described as (where θ is a polar angle of magnetic moment of the sample):



The effective field of anisotropy – an example

... or, using direction cosines, to:

$$E = -K m_z^2$$

Using the definition of vector derivative we arrive at:

$$\rightarrow \frac{\partial}{\partial \vec{m}} E = \hat{z} \frac{\partial}{\partial m_z} E = -2 K m_z$$

and finally have:

$$B_{eff} = \frac{2 K m_z}{M_s} \hat{z}$$

Note that B_{eff} depends on the orientation of magnetic moment, but in some cases, when we are interested only in **small deviations from easy axis** we can use the approximation [15,25]:

$$B_{eff} \approx \frac{2K}{M_s} \hat{z}$$

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In the case of constant B_{eff} "A magnetic field defines an easy direction, not an easy axis." [Coey, 25, p. 171]:

to be read as
$$\frac{\partial}{\partial \vec{m}} f = \hat{x} \frac{\partial}{\partial m_x} f + \hat{y} \frac{\partial}{\partial m_y} f + \hat{z} \frac{\partial}{\partial m_z} f$$
 ([9, p.178], [14, p. 126])

Effective field is an extension of magnetostatic energy terms of different origin:

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$$= \frac{E_{magn}}{\vec{H}_{eff}} = -\frac{\vec{M} \cdot \vec{B}}{\mu_0 M_s} \frac{\partial}{\partial \vec{m}} E_{total}$$

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The effective field of anisotropy – an example

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and finally have:

$$B_{eff} = \frac{2 K m_z}{M_s} \hat{z}$$

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Note too, that "the exact" effective field gives the proper dependence of the anisotropy energy^{*} on the angle γ :

$$\Delta E_{m_{z1} \rightarrow m_{z2}} = \int_{m_{z1}}^{m_{z2}} -B_{eff} \cdot dm M_s = \int_{m_{z1}}^{m_{z2}} -B_{eff}^z \cdot dm_z M_s = \int_{m_{z1}}^{m_{z2}} -\frac{2Km_z}{M_s} dm_z M_s = \left[-Km_z^2\right]_{m_{z2}}^{m_{z1}}$$
$$= -K(\cos^2(\gamma_2) - \cos^2(\gamma_1)) \rightarrow \gamma_1 = 0: \begin{bmatrix} E(\gamma) = -K\cos^2(\gamma) \\ E(\theta) = -K\cos^2(\theta), \end{bmatrix} K > 0$$

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Finite difference micromagnetism

• In the so called *field based approach* [7] one is seeking a numerical solution to LLG equation by first calculating the effective field and then inserting it into LLG equation.

$$\vec{H}_{eff} = -\frac{1}{\mu_0 M_S} \frac{\partial}{\partial \vec{m}} E_{total}$$

- The most difficult task is the calculation of long range magnetostatic interactions
- Exchange interactions and magnetocrystalline anisotropy are calculated locally:
- exchange energy depends on the magnetic moment orientation of nearest neighbors (nn) (6-neighbor exchange in simple cubic crystals) or nnn
- magnetocrystalline energy depends only on the orientation of the moment itself



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Finite difference micromagnetism – demagnetizing field evaluation

- Demagnetizing field evaluation can be calculated in formalism of volume and surface charges (lecture 2).
- The volume of magnetic body is divided into a number of discretization cells.
- It can be assumed that each cell has *constant* magnetization divergence within its volume and surface tiles with magnetic charge density [14].
- The demagnetizing field in a given cell is averaged across its volume for integrating LLG equation.
- It can be assumed too that the magnetization within each cell is homogeneous [8].
- The discretization cell must not necessarily be a cube [16].

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- The required resolution of discretization (the maximum sizes of cells) is determined by the smallest features which may appear in the solution of micromagnetic problem [17].
- In micromagnetism there are three typical length scales [7,8]:

-magnetocrystalline exchange length – related to the width of the Bloch wall (π I_k)

$$l_k = \sqrt{A/K_1}$$

-magnetostatic exchange length* [10] – related to the width of the Néel wall (π l_s)

$$l_k = \sqrt{\frac{2A}{\mu_0 M_s^2}}$$

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-thermal exchange length [13]

$$l_{k} = \sqrt{\frac{A}{\mu_{0}M_{s}H_{th}}}, \qquad H_{th} = \sqrt{\frac{2\alpha k_{b}T}{\Delta \gamma \mu_{0}M_{s}l^{3}}}$$

- The discretization cell should be smaller than the smallest of three lengths defined above [17].
- The magnetostatic exchange length rarely exceeds a few nanometers in 3d ferromagnetic metals or alloys; it imposes a severe constraint on the mesh size in numerical simulations [7].

*that length is sometimes defined without ,,2" under square root [7].

Finite difference micromagnetism – exchange lengths

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• The magnetostatic exchange length rarely exceeds a few nanometers in 3d ferromagnetic metals or alloys; it imposes a severe constraint on the mesh size in numerical simulations [7].

	<i>l</i> _k [nm]	/ _s [nm]	
α-Fe	21	3.3	
Со	8.3	4.9	table data from: H Kronmüller M Fähnle
Ni	7	8.7	Micromagnetism and the Microstructure of
SmCo₅	0.84	5.3	Ferromagnetic Solids, Cambridge University Press 2003
		1	2000



• At a distance roughly equal to the appropriate exchange length the spin configuration is that of unperturbed state:

- the local perturbation can be a grain with high magnetocrystalline anisotropy with easy direction perpendicular to the applied field (here, on the drawing, directed to the right)
- it can be laser-heated region of the sample in which magnetocrystalline anisotropy vanishes and the spin is directed along the external field (this time directed upward), etc.

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- In micromagnetic simulation every discretization cell interacts with every other cell by magnetostatic interactions.
- The shortest exchange length determines which energy term contributes the largest amount to the total energy [8].
- In soft magnetic materials the spin arrangements are more or less divergence free pole avoidance principle [9].





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- each cell is a source of magnetic field either due to volume or to surface magnetic charges
- to compute the average field through the cell the demagnetizing factors for rectangular ferromagnetic prisms are used.

- In micromagnetic simulation every discretization cell interacts with every other cell by • magnetostatic interactions.
- The shortest exchange length determines which energy term contributes the largest amount to the total energy [8].
- In soft magnetic materials the spin arrangements are more or less divergence free ٠ pole avoidance principle [9].



There exist analytical formulas for interaction energy between rectangular blocks which are used to calculate effective field, due to all blocks in the simulation, acting on a magnetic moment of a given block:

A.J. Newell, W. Williams, D.J. Dunlop Journal of Geophysical Research 98, 9551 (1993)

- In dynamic micromagnetic simulation the effective field is calculated as the input of LLG equation (for example OOMMF) [18].
- The magnetic moments of the cells are then updated according to angular velocities obtained from LLG equation.
- The time step is adjusted so that the "the total energy of the system decreases, and the maximum error between the predicted and final M is smaller than a nominal value" [18]



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Finite difference micromagnetism – exemplary simulation

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- The oommf simulation of a "sample" consisting of four discretization cells
- In simulation of the hysteresis, in contrast to study of dynamics, we usually assume relatively high damping constant to make the simulation time shorter



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Finite difference micromagnetism – exemplary simulation

- The oommf simulation of a "sample" consisting of four discretization cells
- In simulation of the hysteresis, in contrast to study of dynamics, we usually assume relatively high damping constant to make the simulation time shorter



... and the corresponding time variations of the Cartesian components of the resultant moment

Trajectory of the resultant moment corresponding to the simulation from the previous slide ...

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- Remanent state of thin 900×900nm NiFe film; discretization cell 3×3×1nm³
- Simulation time 6ns (simulated with OOMMF [18])



 Magnetization tends to be align along outer edges of the specimen – minimization of surface charges М

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 Exchange anisotropy forces moments to be parallel to each other – central part of the specimen

each arrow corresponds to 11×11 discretization cells

Langevin-Landau-Lifshitz-Gilbert equation ...

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