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Mini-Workshop: Mathematics of Magnetoelastic Materials

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ABSTRACT. The unifying theme of the workshop was the mathematical modeling, analysis, and numerical simulation of materials which involve magnetic and elastic interactions. During the workshop we identified several open problems from the calculus of variations, partial differential equations and modeling which appear to be essential in the understanding of the behavior of magnetoelastic materials.

Mathematics Subject Classification (2010): 35Q74, 35Q35, 49Sxx, 70-XX, 74F15.

Introduction by the Organisers

The mini-workshop *Mathematics of Magnetoelastic Materials*, organized by Carlos J. García-Cervera (Santa Barbara), Martin Kružík (Prague), Chun Liu (University Park), and Anja Schlömerkemper (Würzburg), was attended by 15 participants from the US and Europe. The workshop brought together specialists in mathematical analysis, applied mathematics, numerical computations and engineering. We had 15 extended talks on various aspects of new modeling and mathematical approaches to magnetoelastic materials. Finally, we had a lively closing discussion on open problems. The atmosphere of the mini-workshop was stimulating and very collaborative. During every talk, several questions were posed and interesting problems were pointed out.

Magnetoelasticity describes the mechanical behavior of solids under magnetic effects. The magnetoelastic coupling is based on the presence of small magnetic domains in the material. In the absence of an external magnetic field, these magnetic domains are randomly oriented but when exposed to a field they become

aligned along the field and their rotations induce a deformation of the specimen. As the intensity of the magnetic field increases, more and more magnetic domains orientate themselves so that their principal axes of anisotropy are collinear with the magnetic field in each region and finally saturation is reached. The mathematical modeling of magnetoelasticity is a vibrant area of research, triggered by the interest on ferromagnetic shape-memory alloys, magnetorheological elastomers and magnetic fluids. Mathematical tools include weak convergence methods, lower semicontinuity, compactness, multiscale methods, homogenization, and various approximations.

The main open problems that we worked out during the workshop are:

- What is the role and importance of the saturation constraint for the magnetization with respect to modeling and analysis?
- Resolve the discrepancy between the modeling of different physical effects that occur on different length scales, as e.g., exchange energies and rate-independent dissipation mechanisms.
- What are reasonable models for dissipation? Can one derive them from microscopic considerations?
- Show (non-)existence of minimizers of energy functionals arising in magnetoelasticity.
- Can one read off hysteresis from material parameters? What is the role of nucleation?
- What is the effective static and dynamical behavior of composite materials with microscopic structure and magnetic interactions?

These are important problems which will help to construct more accurate mathematical models for magnetoelasticity. We are convinced that they will also lead to new mathematical developments.

Generally speaking, the participants felt that the mini-workshop format with fifteen researchers was particularly successful in promoting discussions and new interactions. The organizers thank the Institute's staff for having provided an inspiring and comfortable environment for the participants.

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Abstracts

Understanding the Role of Magnetoelasticity in Magnetoelectric Heterostructures

LONG-QING CHEN

(joint work with Jia-Mian Hu)

Magnetolectric heterostructures integrate magnetic and dielectric materials to produce new functionalities, e.g., magnetolectric responses that are absent in each of the constituent materials.[1, 2] The magnetolectric coupling in these materials is achieved through the interfaces between the two different types of materials, and the coupling effect is measured by the degree of mutual conversion between magnetic and electric signals in the absence of an electric current. Magnetolectric heterostructures are attractive for applications in many energy-efficient devices and systems since they avoid electric current and offer a wide range of materials selection and possible geometrical and microstructural designs. Here, we theoretically and computationally discuss how magnetoelasticity affects the magnetolectric coupling in magnetolectric heterostructures.

Depending on the type of the constituent dielectric materials, the mechanism of magnetolectric coupling can vary. For example, if the dielectric material is also piezoelectric (meaning that it permits a mutual conversion between an electric field and a mechanical force), and if the magnetic material has a relatively large magnetoelastic coupling, a stress-transfer-based magnetolectric coupling can be achieved (see Figure 1).

This can be quantitatively understood using the equation below,

$$(1) \quad \alpha_{i,j} = \frac{dM_i}{dE_j} = \left(\frac{\partial M_1}{\partial \sigma_{ij}} \right)_{E,H} \eta \left(\frac{\partial \sigma_{jk}}{\partial \epsilon_{pq}} \right)_{E,H} \left(\frac{\partial \epsilon_{pq}}{\partial E_j} \right)_{\sigma,E},$$

where α_{ij} indicates the magnetolectric coupling coefficient; the first term in brackets on the right describes the magnetoelastic coupling coefficient; the second and the third terms represent, respectively, the elastic and electromechanical coupling coefficients of the piezoelectric; the η ($0 < \eta < 1$) denotes the efficiency of stress transfer across the interface of the two constituent phases.

The role of magnetoelasticity in magnetolectric coupling can also be understood from the energetics of magnets. The total magnetic free energy of the magnetolectric heterostructure can be written as [2]

$$(2) \quad F_{\text{tot}} = \int \left(\underbrace{A|\nabla m|^2}_{\text{exchange}} + \underbrace{f_{\text{ani}}(m)}_{\text{magneto-crystalline}} + \underbrace{0.5(\epsilon - \epsilon^0(m)) \cdot c \cdot (\epsilon - \epsilon^0(m))}_{\text{elastic}} \right. \\ \left. + \underbrace{K_s(1 - (m \cdot n)^2)/d}_{\text{surface and interface}} - \underbrace{0.5\mu_0 M_s(H_d \cdot m)}_{\text{stray field}} - \underbrace{\mu_0 M_s(H_{\text{ex}} \cdot m)}_{\text{external field}} \right) dV$$

where m is the normalized magnetization vector ($=M/M_s$, where M_s is the saturation magnetization) with $|m| = 1$; A is the phenomenological exchange coupling coefficient describing the local interaction between neighboring magnetic spins; K_s is the surface anisotropy coefficient; μ_0 is the vacuum permeability; H_d is the magnetic stray field obeying the magnetostatic equilibrium equation $\nabla \cdot (\mu_0 H_d + M) = 0$; H_{ex} denotes the externally applied magnetic field. The spontaneous deformation in a magnetoelastic body is described using a stress-free strain ϵ^0 ,

$$(3) \quad \epsilon_{ij}^0(r) = \frac{3}{2} \lambda_{ijkl} \left(m_k(r) m_l(r) - \frac{1}{3} \delta_{kl} \right),$$

where λ is the magnetostrictive coefficient, and δ is the Kronecker delta. The total strain ϵ can be separated into a homogeneous part ϵ^{hom} and a heterogeneous part ϵ^{het} to describe the global and local deformation, respectively [3]. The heterogeneous strain, the volume integral of which is zero, can be obtained by solving the mechanical equilibrium equation,

$$(4) \quad \nabla \cdot \left(c_{ijkl}(r) (\epsilon_{kl}^{\text{het}}(r) - \epsilon_{ij}^0(r)) \right) = 0.$$

When applying an electric field to a magnetic-piezoelectric heterostructure, both ϵ^{hom} and ϵ^{het} of the piezoelectric phase are modified due to piezoelectric coupling. This further changes the ϵ^{hom} and ϵ^{het} of the magnetic phase. Since the elastic energy density is an even function of m (see equation (2) and (3)), the electrically induced change in strain can merely shift the global minima of the total magnetic free energy from for example $m_i = 1$ or -1 ($i = 1, 2, 3$) to $m_i = 0$. This suggests an at most 90 rotation of the magnetization vector under an applied electric field, leading to a magnetoelectric coupling coefficient with a maximum magnitude of $\mu_0 M_s / |E|$. Such strain-mediated electric-field-induced 90 magnetization switching has been utilized to design a novel magnetoelectric random access memory the performance of which eclipses competing technologies [4].

The role of magnetoelasticity in magnetoelectric coupling can also be understood from a dynamic perspective. Strain-mediated electric-field-induced dynamic evolution of m can be described by solving the Landau-Lifshitz-Gilbert equation,

$$(5) \quad \frac{\partial m(r)}{\partial t} = -\gamma_0 (m(r) \times H_{\text{eff}}(r)) + \alpha_G \left(m(r) \times \frac{\partial m(r)}{\partial t} \right),$$

where γ_0 is the gyromagnetic ratio describing the ratio of an atom's magnetic momentum to its angular momentum; α_G is the Gilbert damping coefficient describing the energy dissipation during magnetization evolution.

$H_{\text{eff}}(r) = -(1/\mu_0)(\delta F_{\text{tot}}/\delta M(r))$ denotes the effective magnetic field. A combination of equation (2)-(5) represents the key of a computational model for modeling the strain-mediated electric-field-induced magnetization dynamic in magnetoelectric heterostructures. The numerical solution of equation (4) depends on the specific mechanical boundary condition of a magnetoelectric heterostructure, e.g., a continuous magnetic thin film or an isolated magnetic island fabricated on a piezoelectric substrate. Notably, by exploiting the magnetization dynamics, we recently

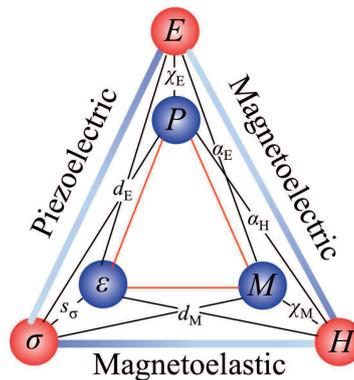


FIGURE 1. Coupling of physical properties in magnetoelectric systems, showing order parameters (blue) and conjugate fields (red), notably electric field E , stress field σ , and magnetization M . Other symbols represent coupling coefficients.

used this computational model to predict a full 180 magnetization switching driven purely by a dynamic electromechanical strain [5] This could double the magnitude of magnetoelectric coupling coefficient, with a new maximum of $2\mu_0 M_s/|E|$.

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Variational modeling of magnetic-shape-memory crystals

ULISSE STEFANELLI

Magnetic shape-memory alloys (MSMAs) are *active* materials: strains as large as 10% can be *activated* by thermal, mechanical, or magnetic stimuli [7]. This results from a solid-solid phase transition between different crystallographic variants of the materials, namely austenite (high symmetry phase) and ferromagnetic martensites (low symmetry) [5]. The strong magnetoelastic behavior of MSMAs is hence mainly triggered by magnetic-driven martensitic reorientation.

The phenomenology of nonmagnetic SMAs is well described by the so-called *Souza-Auricchio* model [6, 11]. By focusing on the single-crystal, cubic-to-tetrahedral transformation regime, this is specified by identifying the local solid phase

$\mathbf{p} \in \{(p_1, p_2, p_3) \in \mathbb{R}^3 : 0 \leq p_i \leq 1, p_1 + p_2 + p_3 = 1\}$ and the Gibbs free energy

$$G_{\text{mech}}(\boldsymbol{\sigma}, \mathbf{p}) = -\boldsymbol{\sigma} : \mathbb{C}^{-1}\boldsymbol{\sigma}/2 - \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_0(\mathbf{p}) + F_{\text{mech}}(\mathbf{p}).$$

Here, $\boldsymbol{\sigma} \in \mathbb{R}_{\text{sym}}^{3 \times 3}$ is the stress, \mathbb{C} is the elasticity tensor, $\boldsymbol{\varepsilon}_0(\mathbf{p}) = \sum_i \boldsymbol{\varepsilon}_0^i p_i \in \mathbb{R}_{\text{dev}}^{3 \times 3}$ (deviatoric) is the stress-free strain at phase \mathbf{p} with $\boldsymbol{\varepsilon}_0^i = \varepsilon_L \text{dev}(\mathbf{e}_i \otimes \mathbf{e}_i)/\sqrt{6}$, $\varepsilon_L > 0$ maximal reorientation strain, and \mathbf{e}_i is the i unit versor, and the convex function F_{mech} encodes nonquadratic, temperature-dependent hardening.

The evolution of the material is governed by the interplay between energy-storage and dissipation mechanisms. This last is modulated by the dissipation potential $D(\dot{\mathbf{p}}) = r|\dot{\mathbf{p}}|$ where $r > 0$ is a given yield stress. The material constitutive relation has the rate-independent form $\partial D(\dot{\mathbf{p}}) + \partial_{\mathbf{p}} G_{\text{mech}}(\boldsymbol{\sigma}, \mathbf{p}) \ni \mathbf{0}$ (∂ is the subdifferential) and admits a complete mathematical and numerical discussion [2].

Building upon the original formulation of the Souza-Auricchio model, one can include the description of magnetic effects by explicitly relating \mathbf{p} with the *easy* magnetization axis of martensites. Under the assumption of *strong magnetic anisotropy* (i.e., no magnetization rotation w.r.t. the easy axis) one can define

$$G(\boldsymbol{\sigma}, \mathbf{h}, \mathbf{p}, \alpha) = G_{\text{mech}}(\boldsymbol{\sigma}, \mathbf{p}) - \alpha^2/(2\delta) + I_{[-1,1]}(\alpha) + \mu_0 \mathbf{h} \cdot m_{\text{sat}} \alpha \mathbf{p}.$$

Here, \mathbf{p} is the easy axis for phase \mathbf{p} (in the present cubic-to-tetragonal setting), $\alpha \in [-1, 1]$ is the signed proportion of magnetic domains oriented in direction \mathbf{p} , $\delta > 0$ is a user-defined parameter controlling the tendency of α to equilibrate at 0, $I_{[-1,1]}$ is the indicator function of the interval $[-1, 1]$, $\mu_0 > 0$ is vacuum permittivity, $m_{\text{sat}} > 0$ is the saturation magnetization, and \mathbf{h} is the applied magnetic field. By assuming α to be nondissipative the material relation reduces to

$$(1) \quad \partial D(\dot{\mathbf{p}}) + \partial_{\mathbf{p}} F_{\text{mech}}(\mathbf{p}) - \partial_{\mathbf{p}} F_{\text{mag}}(\mathbf{h} \cdot \mathbf{p}) \ni \boldsymbol{\sigma} : \mathbf{E}$$

where and $\mathbf{E}_{ijk} = (\partial_{\mathbf{p}} \boldsymbol{\varepsilon}_0(\mathbf{p}))_{ijk} = (\boldsymbol{\varepsilon}_0^k)_{ij}$ and the convex function $F_{\text{mag}} \in C^{1,1}$ is $F_{\text{mag}}(r) = (\delta \mu_0 m_{\text{sat}} r)^2 / (2\delta)$ if $|\delta \mu_0 m_{\text{sat}} r| \leq 1$ and $F_{\text{mag}}(r) = (2(\delta \mu_0 m_{\text{sat}} r) - 1) / (2\delta)$ otherwise. In particular, the effective energy driving the evolution of \mathbf{p} turns out to be the sum of a mechanical convex and a magnetic concave part [1].

Existence of *energetic* solutions [8] to (1) is proved in [3]. By augmenting the constitutive equation by the nonlocal term $\int_{\Omega} |\nabla \mathbf{p}|$, giving indeed rise to a scale effect which penalizes martensitic boundaries, the quasistatic evolution problem consisting in coupling (1) with the equilibrium system $\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$ (with boundary conditions) is energetically solvable as well. The nonmagnetic Souza-Auricchio model can be rigorously recovered by letting $\delta \rightarrow 0$ [9] and both temperature evolution [10] and magnetic-control problems can be addressed [12].

By dropping the strong-anisotropy assumption one is forced to include the magnetization \mathbf{m} in the list of state variables and define the total energy as [4]

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{u}) - \boldsymbol{\varepsilon}_0(\mathbf{p})) : \mathbb{C}(\boldsymbol{\varepsilon}(\mathbf{u}) - \boldsymbol{\varepsilon}_0(\mathbf{p})) + \int_{\Omega} F_{\text{mech}}(\mathbf{p}) + \int_{\Omega} |\nabla \mathbf{p}| \\ & + \frac{\mu_0}{2} \int_{\mathbb{R}^3} |\nabla v_m|^2 + \kappa_m \int_{\Omega} |\nabla \mathbf{m}|^2 - \mu_0 \kappa_{\text{ani}} \int_{\Omega} (\mathbf{m} \cdot \mathbf{p})^2 - \mu_0 \int_{\Omega} \mathbf{h} \cdot \mathbf{m} \end{aligned}$$

under the constraint $|\mathbf{m}| = m_{\text{sat}}$ and the Maxwell equation $\nabla \cdot (-\mu_0 \nabla v_{\mathbf{m}} + \mathbf{m} \chi_{\Omega}) = \mathbf{0}$ in \mathbb{R}^3 (χ_{Ω} is the characteristic function of Ω). The energy features the *Zeeman term* $-\mu_0 \mathbf{h} \cdot \mathbf{m}$ and the *exchange energy* term with $\kappa_{\mathbf{m}} > 0$. The anisotropic term $-\mu_0 \kappa_{\text{ani}} \int_{\Omega} (\mathbf{m} \cdot \mathbf{p})^2$ is minimized when \mathbf{m} is parallel to the easy axis \mathbf{p} .

By prescribing the dissipation in the form $D(\dot{\mathbf{p}}, \dot{\mathbf{m}}) = \int_{\Omega} R_{\mathbf{p}} |\dot{\mathbf{p}}| + \int_{\Omega} R_{\mathbf{m}} |\dot{\mathbf{m}}|$ one can prove the existence energetic solutions [4]. Moreover, again by [9] one can prove that by letting $R_{\mathbf{m}} \rightarrow \infty$ the model rigorously reduces to the purely mechanical one and by taking $R_{\mathbf{p}} \rightarrow \infty$ a micromagnetic model is obtained [4].

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The magnetization ripple revisited

FELIX OTTO

(joint work with Lukas Döring, Radu Ignat)

The magnetization ripple in a ferromagnetic thin-film sample is its response to polycrystallinity. The fact that the sample is made up of randomly oriented grains leads to an easy axis for the magnetization m that is a random field, and thus acts like quenched noise. In experiments, the response to that noise manifests itself as an in-plane oscillation of m , predominantly in direction of the main magnetization direction. This *anisotropic* response of m to the isotropic noise comes from its non-local interaction mediated by the stray-field.

Starting from the three-dimensional micromagnetic (variational) model, we heuristically derive a reduced model that zooms in on the (different) longitudinal and transversal characteristic scales of the ripple. The reduced model is a two-dimensional, non-local variational model formulated in terms of the transversal magnetization component m_2 . Because the grains are typically smaller than the characteristic ripple scales, the random easy axis acts like a transversal field of white-noise character. This derivation, which essentially follows [1, Section V], is self-consistent.

We point out two challenges of the reduced model. The first challenge can already be seen on the level of the simplification that gets rid of the anharmonic term in the energy. The ensuing linear Euler-Lagrange equation can be explicitly solved in Fourier space — however the highest-order term in the energy, the exchange contribution, diverges. Hence the ripple should rather be analyzed on the level of the Euler-Lagrange equation than by the direct method of the calculus of variations.

The second challenge is more subtle and more serious: The nonlinearity in the Euler-Lagrange equation is too singular for its rhs given by white noise ξ . More dramatically, one of the quadratic terms in the Euler-Lagrange equation cannot be given a path-wise unambiguous sense even when one plugs in the solution of the linear Euler-Lagrange equation. This situation is similar to certain classes of stochastic partial differential equation (SPDE); ie time-dependent nonlinear parabolic equations driven by space-time white noise. While noise in SPDEs typically models *thermal* noise and our noise is of *quenched* nature, and while these SPDEs are typically parabolic and our Euler-Lagrange equation is of (non-local) elliptic character, the mathematical challenges are identical.

In fact, the issue is to make sense of the product of a function and a distribution. This can be done in an unambiguous sense provided the function is more regular than the distribution is irregular. In the context of a PDE, regularity has to be measured in a way that is consistent with the (leading-order) linear part of the equation. While in the parabolic case, this requires function spaces that respect the fact that the time derivative is worth two space derivatives, in our case we have the relationship that two x_2 -derivates are worth three x_1 -derivatives. When the distribution of the driving noise remains stationary under shifts, like is the case of white noise, there is no loss in using the scale of Hölder spaces — and thus wrt to a (Carnot-Carathéodory) metric that respects the above scaling. On the scale of these Hölder spaces, the crucial product turns out to be border-line singular: The function in this product is slightly worse than $C^{\frac{3}{4}}$ while the distribution is slightly worse than $C^{-\frac{3}{4}}$.

This situation is reminiscent of a fundamental problem in stochastic (ordinary) differential equations (SDE): The theory requires, at a minimum, to give a (distributional) sense of the product of (multi-dimensional) Brownian motion and of its derivative, ie (temporal) white noise. Brownian motion is known to be slightly

worse than $C^{\frac{1}{2}}$ and thus white noise slightly worse than $C^{-\frac{1}{2}}$. Stochastic analysis has found two ways out of this (specific) border-line singular situation: Ito calculus, and more recently Lyons' rough path theory. While Ito calculus uses the Martingale structure of Brownian motion and thus is not easily amenable to a treatment of irregular *spatial* noise, rough path theory is oblivious to this structure. Hairer and coworkers have extended rough path theory from SDEs to SPDEs. We follow their approach in our – simpler – situation.

This approach consists of two parts: The first part gives an “off-line” definition to the singular product with the solution of the linear (constant-coefficient) equation v plugged in. This product F is the product of two *Gaussian* fields and can be characterized by Gaussian calculus: Thanks to stochastic cancellations, an *almost-sure* (distributional) sense may be given to this product that is unambiguous in the sense that it is stable under regularization of white noise by convolution.

The second part consists in setting up a completely *deterministic* (ie path-wise) fixed-point problem in $w := u - v$, where u denotes the solution of the nonlinear problem, with a rhs given by the distribution $F \in C^{-\frac{3}{4}-}$. All the further nonlinearities in the PDE are regular. For this second part, we have to show 1) that for our (anisotropic and nonlocal) linear operator \mathcal{L} we have $\mathcal{L}^{-1}C^{\alpha-2} \subset C^{\alpha}$ and 2) that $C^{\alpha} \times C^{\beta} \subset C^{\beta}$ for $\beta < 0 < \alpha$ with $\alpha + \beta > 0$ (ie the regular case). We do both with help of a set of tools recently introduced for SPDEs [2, Section 2].

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A Variationally Consistent Approach to Micro-Magnetic Domain Evolution at Large Deformations

MARC-ANDRÉ KEIP

(joint work with A. Sridhar)

This contribution presents a variational formulation of micro-magnetic domain evolution at finite deformations, cf. [1, 2]. Such approach is of particular importance for the understanding of micro-magnetic domain evolution in large-strain scenarios. A prototype example is given by magnetorheological elastomers, in which ferromagnetic particles are embedded in a soft elastomeric matrix [3, 4].

The macroscopic boundary-value-problem of a ferromagnetic body \mathcal{B} embedded in a general free space box Ω is a coupled multifield problem. Primary variables are the *deformation map* φ , the *magnetic self-potential* $\tilde{\phi}$ and the *reference magnetization director* \mathbf{M} given by,

$$\varphi : \begin{cases} \Omega \times \mathcal{T} \rightarrow \mathcal{R}^d \\ (\mathbf{x}, t) \mapsto \varphi(\mathbf{X}, t) \end{cases}, \quad \tilde{\phi} : \begin{cases} \Omega \times \mathcal{T} \rightarrow \mathcal{R} \\ (\mathbf{X}, t) \mapsto \tilde{\phi}(\mathbf{X}, t) \end{cases}, \quad \mathbf{M} : \begin{cases} \mathcal{B} \times \mathcal{T} \rightarrow \mathcal{S}^{d-1} \\ (\mathbf{X}, t) \mapsto \mathbf{M}(\mathbf{X}, t) \end{cases}.$$

The magnetization director has the geometric property such that $|\mathbf{M}| = 1$ with the rate $\dot{\mathbf{M}} = \boldsymbol{\omega} \times \mathbf{M}$, where $\boldsymbol{\omega}$ is the *spin of the magnetization*. The three-field rate-type saddle-point variational principle is given as,

$$(1) \quad \{\dot{\boldsymbol{\varphi}}, \tilde{\boldsymbol{\phi}}, \dot{\mathbf{M}}\} = \arg \left\{ \inf_{\dot{\boldsymbol{\varphi}} \in \mathcal{R}^d} \sup_{\tilde{\boldsymbol{\phi}} \in \mathcal{R}} \inf_{\dot{\mathbf{M}} \in T_{\mathbf{M}} \mathcal{S}^{d-1}} \Pi'(\dot{\boldsymbol{\varphi}}, \tilde{\boldsymbol{\phi}}, \dot{\mathbf{M}}) \right\},$$

where the *rate-type magneto-mechanical potential* Π' appears as,

$$\Pi'(\dot{\boldsymbol{\varphi}}, \tilde{\boldsymbol{\phi}}, \dot{\mathbf{M}}) := \frac{d}{dt} E'(\boldsymbol{\varphi}, \tilde{\boldsymbol{\phi}}, \mathbf{M}) + D(\dot{\mathbf{M}}; \mathbf{C}) - L^{mech}(\dot{\boldsymbol{\varphi}}; t) - L^{mag}(\dot{\mathbf{M}}; t).$$

Here, E' is the *mixed energy-enthalpy functional* that contains the energy stored in the magnetized body as well as the *free-space contribution*. D is the *dissipation potential* that describes the dynamic evolution of the order parameter. L^{mech} and L^{mag} are the *mechanical and magnetic loading contributions*. It has to be noted here that the dissipation potential and the magnetic loading contributions have to be formulated in terms of the *objective rates* of the magnetization such that,

$$L^{mag}(\dot{\mathbf{M}}; t) = \int_{\varphi_t(\mathcal{B})} \rho \mu_0 m_s \bar{\mathbf{h}} \cdot \boldsymbol{\mathcal{L}}_v \mathbf{m} \, dv = \int_{\mathcal{B}} \rho_0 \mu_0 m_s \bar{\mathbf{h}} \cdot \mathbf{F} \dot{\mathbf{M}} \, dV,$$

$$D(\dot{\mathbf{M}}; \mathbf{C}) = \int_{\varphi_t(\mathcal{B})} \rho \frac{\eta}{2} \text{tr}[\boldsymbol{\mathcal{L}}_v \mathbf{m} \otimes \boldsymbol{\mathcal{L}}_v \mathbf{m}] = \int_{\mathcal{B}} \frac{\eta}{2} \rho_0 \text{tr}[\mathbf{C}(\dot{\mathbf{M}} \otimes \dot{\mathbf{M}})] \, dV.$$

Taking the consistent first variation of the potential Π' with $\dot{\mathbf{M}} = \boldsymbol{\omega} \times \mathbf{M}$, gives the Euler-Lagrange equations as,

$$\text{Div}[\partial_{\mathbf{F}} \Psi] = \mathbf{0}, \quad \mathbf{M} \times (\eta \mathbf{C} \dot{\mathbf{M}} - \text{Div}(\partial_{\nabla \mathbf{M}} \Psi) - \mu_0 m_s \mathbf{F}^T \bar{\mathbf{h}}) = \mathbf{0}, \quad \text{Div}[-\partial_{\bar{\mathbf{H}}} \Psi] = 0.$$

We identify the *balance of momentum*, *Gauss's law* and the *large-deformation LLG equation*.

In order to arrive at a numerically more feasible formulation, we propose a penalty-type approach to the geometric property of the magnetization director, such that we rewrite (1) as,

$$(2) \quad \{\dot{\boldsymbol{\varphi}}, \tilde{\boldsymbol{\phi}}, \dot{\mathbf{M}}\} = \arg \left\{ \inf_{\dot{\boldsymbol{\varphi}} \in \mathcal{R}^d} \sup_{\tilde{\boldsymbol{\phi}} \in \mathcal{R}} \inf_{\dot{\mathbf{M}} \in \mathcal{R}^d} \Pi^{aug}(\dot{\boldsymbol{\varphi}}, \tilde{\boldsymbol{\phi}}, \dot{\mathbf{M}}) \right\}$$

where the *augmented rate-type magneto-mechanical potential* Π^{aug} is given as,

$$\Pi^{aug}(\dot{\boldsymbol{\varphi}}, \tilde{\boldsymbol{\phi}}, \dot{\mathbf{M}}) := \frac{d}{dt} (E'(\boldsymbol{\varphi}, \tilde{\boldsymbol{\phi}}, \mathbf{M}) + E^{pen}) + D(\dot{\mathbf{M}}; \mathbf{C}) - L^{mech}(\dot{\boldsymbol{\varphi}}; t) - L^{mag}(\dot{\mathbf{M}}; t).$$

Here, the *penalty functional* $E^{pen} = \frac{\epsilon}{2} (\|\mathbf{M}\| - 1)^2$ penalizes the violation of the unity constraint. Taking the first variation of the augmented potential gives us the evolution of the magnetization which contains the penalty contribution,

$$\eta \mathbf{C} \dot{\mathbf{M}} + \partial_{\mathbf{M}} \Psi + \epsilon \{ \|\mathbf{M}\| - 1 \} \frac{\mathbf{M}}{\|\mathbf{M}\|} - \text{Div}(\partial_{\nabla \mathbf{M}} \Psi) - \mu_0 m_s \mathbf{F}^T \bar{\mathbf{h}} = \mathbf{0}.$$

In combination with a staggered solution algorithm [2], the above model was implemented into the Finite Element Method, see Fig. 1 for an example application.

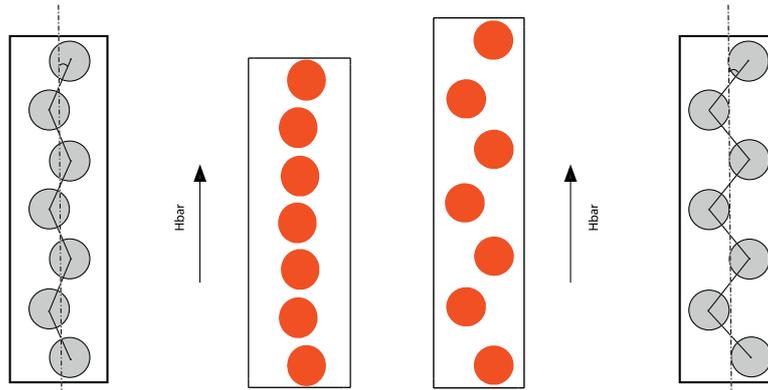


FIGURE 1. Formation of *particle chains* and associated deformations for different micro-structures under external field \bar{h} [3, 5].

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Second Order Γ -Convergence for the (Nonlocal) Modica-Mortola Functional

IRENE FONSECA

Variational models in micromagnetics exhibit competition between the anisotropic energy, that favors the formation of domains according to the easy axes of the magnetization director, and the exchange energy that penalizes the creation of interfaces. More broadly, in this talk we discussed the asymptotic behavior of anisotropic Cahn-Hilliard-type functionals that are the prototype of singularly perturbed bulk energies with multi-wells energy densities and with higher order perturbations accounting for interface energy when domains are formed, as the small parameter ε that determines the width of the transition layer tends to zero.

We recall the anisotropic Cahn-Hilliard functional (see, e.g., [11], [14], [13])

$$(1) \quad \mathcal{W}_\varepsilon(u) := \int_{\Omega} (W(u(x)) + \varepsilon^2 \Phi^2(\nabla u(x))) \, dx,$$

where Ω is a bounded open set in \mathbb{R}^N , $N \geq 2$, with Lipschitz boundary. Here $W : \mathbb{R} \rightarrow [0, +\infty)$ is an even function of class C^1 such that $W(s) = 0$ if and

only if $s = \pm 1$, with $W(s) = |s - 1|^\beta$ near $s = 1$ for some $1 < \beta < 2$, and $\Phi : \mathbb{R}^N \rightarrow [0, +\infty)$ is convex, even, and positively homogeneous of degree one.

We impose a mass constraint and a boundary condition

$$(2) \quad u \in H^1(\Omega), \quad \int_{\Omega} u(x) \, dx = m, \quad \text{and} \quad u = 1 \text{ on } \partial\Omega,$$

where $-|\Omega| < m < |\Omega|$. To study the asymptotic behavior of $\mathcal{W}_\varepsilon(u)$, we rescale the energies as

$$\mathcal{F}_\varepsilon(u) := \int_{\Omega} \left(\frac{1}{\varepsilon} W(u(x)) + \varepsilon \Phi^2(\nabla u(x)) \right) dx$$

if (2) is satisfied, and we extend \mathcal{F}_ε to $L^1(\Omega)$ by setting $\mathcal{F}_\varepsilon(u) := +\infty$ if (2) is not satisfied.

The first order term in the asymptotic development by Γ -convergence is well-known (see [3], [4], [9], [17]), and is related to a suitable anisotropic perimeter of the interface

$$(3) \quad \mathcal{F}_0(u) := c_W P_\Phi(E)$$

if

$$(4) \quad u = u_E := 1 - 2\chi_E, \quad E \subset \Omega, \quad P(E) < +\infty, \quad \text{and} \quad |E| = \frac{|\Omega| - m}{2},$$

while $\mathcal{F}_0(u) := +\infty$ if (4) is not satisfied. Here

$$c_W := 2 \int_{-1}^1 \sqrt{W(s)} \, ds$$

and P_Φ is the Φ -perimeter, defined for every $E \subset \mathbb{R}^n$ with finite perimeter by

$$P_\Phi(E) := \int_{\partial^* E} \Phi(\nu_E(x)) \, d\mathcal{H}^{N-1}(x),$$

where $\partial^* E$ is the reduced boundary of E , ν_E is the measure theoretic outer unit normal of E , and \mathcal{H}^{N-1} is the $(N - 1)$ -dimensional Hausdorff measure. Observe that in contrast with the results in the literature just quoted, due to the boundary condition in (2) in (3), we obtain the full Φ -perimeter of E as opposed to the relative Φ -perimeter of E in Ω .

Jointly with Gianni Dal Maso and Giovanni Leoni, in [7] we studied the second order term $\mathcal{W}^{(2)}$ for (1). We recall the notion of *asymptotic development by Γ -convergence of order k* :

$$F_\varepsilon \stackrel{\Gamma}{=} F^{(0)} + \varepsilon F^{(1)} + \dots + \varepsilon^k F^{(k)} + o(\varepsilon^k)$$

if $F_\varepsilon \xrightarrow{\Gamma} F^{(0)}$ and

$$F_\varepsilon^{(i)} := \frac{F_\varepsilon^{(i-1)} - \inf_X F^{(i-1)}}{\varepsilon} \xrightarrow{\Gamma} F^{(i)}$$

for $i = 1, \dots, k$, where $F_\varepsilon^{(0)} := F_\varepsilon$ (see [1], [2], [5, Section 1.10]).

Under some additional assumptions on Ω and W , we proved that $\mathcal{W}^{(2)}(u) = 0$ if u is a minimizer of \mathcal{F}_0 and $\mathcal{W}^{(2)}(u) = +\infty$ otherwise. This was somewhat

disappointing as we were hoping to use this higher order Γ -limit to narrow further the selection criteria invoking, e.g., the curvature of the interfaces. In fact, a similar problem was studied in [2] for the single-well potential $W(s) = s^2$ without imposing the mass constraint and assuming a strictly positive boundary condition g . This forces a transition near $\partial\Omega$ and leads to a second order term $\mathcal{W}^{(2)}$ in the asymptotic expansion of the form $\frac{1}{2} \int_{\partial\Omega} g^2 K d\mathcal{H}^{n-1}$, where K is the mean curvature of $\partial\Omega$.

This problem is very sensitive to the hypotheses we place on W . The assumption that W is even is used in a crucial way to cancel many terms in the estimates due to symmetry arguments. The hypothesis that $W(s) = |s - 1|^\beta$ near $s = 1$ for some $1 < \beta < 2$ is also fundamental, since it implies that the solution z of the Cauchy problem

$$z'(t) = \sqrt{W(z(t))}, \quad z(0) = 0.$$

reaches 1 and -1 in “finite time”, and this property was central to our proofs. Without assuming the boundary condition in (2), it can be shown that $\mathcal{W}^{(2)}$ may be different from zero if either $1 < \beta < 2$ but W is not even or $\beta = 2$ and W is even (see [12]).

As observed by Bronsard and Kohn in [6], Grant in [10], Otto and Westdickenberg in [16], among others, identifying the (static) Γ -limit yields an estimate on the rate of convergence for the dynamics of the related gradient flow. In [7] we use what we know on the Γ -limit to “prepare well the initial data” of the Allen-Cahn equation (the L^2 gradient flow for the Cahn-Hilliard energy) and deduce slow motion of the interface, here on a ε^{-1} time scale (see also [15]).

Further, we note that on our recent work [8] we studied nonlocal Cahn-Hilliard-type singularly perturbed functionals. The kernels considered included those leading to Gagliardo’s fractional seminors for gradients. The integral representation of the Γ -limit energy is again characterized as an anisotropic energy of the interfaces separating the different phases.

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Thermodynamics of magnetoelastic materials at large strains

TOMÁŠ ROUBÍČEK

The theory of elastic magnets at large strains is formulated merely in the reference (material) configuration $\Omega \subset \mathbb{R}^d$, i.e. using the Lagrangian approach which is convenient for solids. The basic variables are thus the deformation $y : \Omega \rightarrow \mathbb{R}^d$ and the magnetisation $m : \Omega \rightarrow \mathbb{R}^d$, and the material response is determined by the free energy $\psi = \psi(F, m)$ with F a placeholder for ∇y . On the other hand, some data (as the external magnetic field h_{ext}) are naturally given in the space, i.e. in the actual deformed configuration, and the same concerns demagnetising field generated by the magnetisation $m_s : y(\Omega) \rightarrow \mathbb{R}^d$ in the deformed configuration, i.e. the push-forward of m given by $m_s = [Fm / \det F] \circ y^{-1}$. In turn, the external field can be pulled-back into the reference configuration as $h_{\text{ext},r} = F^\top(h_{\text{ext}} \circ y)$, cf. Fig. 1. Let us note that the pulled-back field $h_{\text{ext},r}$ is defined only on Ω , in contrast to h_{ext} which is defined on the whole “universe” \mathbb{R}^d . Then, for example, for the energy of magnetisation in the external field (Zeeman’s energy), it holds

$$\int_{\Omega} h_{\text{ext},r}(x) \cdot m(x) \, dx = \int_{\Omega} \left([\nabla y]^\top(x) h_{\text{ext}}(y(x)) \right) \cdot m(x) \, dx = \int_{y(\Omega)} h_{\text{ext}}(z) \cdot m_s(z) \, dz.$$

Actually, the middle form is most natural because it combines the given field h_{ext} with the magnetisation in the reference configuration where all equations are formulated within the Lagrangean approach. Similar transformation applies for the demagnetising field.

The magnitude of magnetization is not constrained by the Heisenberg constraint (otherwise discutable, except very low temperatures) but the temperature-dependent saturation magnetisation is reflected through the free energy ψ , cf. [2]. This allows for ferro-to-paramagnetic phase transformation as well as for the interpretation as ferroelectric instead of ferromagnetic materials.

The model can be augmented by possible diffusion and heat flow governed by Fick’s and Fourier’s laws in the deformed (Eulerian) configuration, respectively. Then $\psi = \psi(F, m, \zeta, \theta)$ with ζ the concentration of a diffusant and θ temperature.

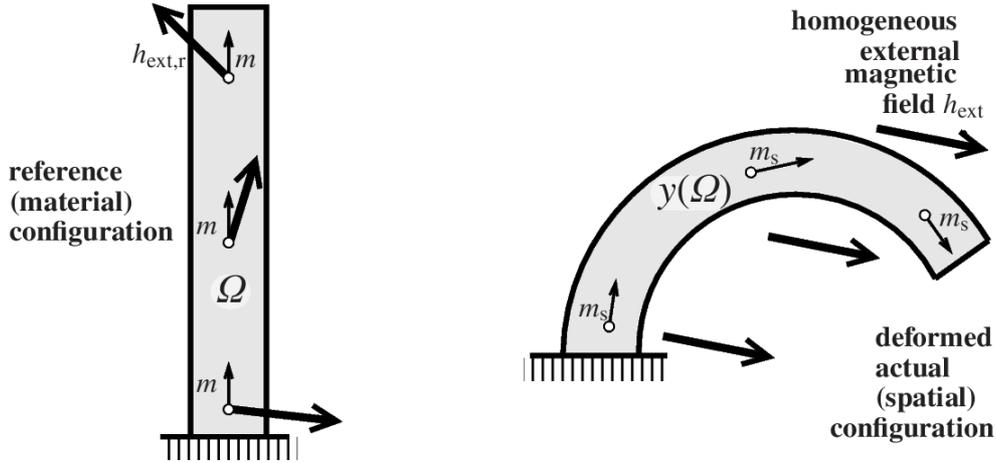


FIGURE 1. An illustration how the magnetization and the magnetic field transform. An elastically soft but magnetically hard specimen with a homogeneous magnetization m fixed at the bottom by Dirichlet condition is deformed in a homogeneous external magnetic field h_{ext} . Alternatively, an interpretation of polarization and electric field in case of elastic ferroelectric materials can be considered, too.

These transport processes are formulated naturally in the actual configuration and then pulled back into the reference configuration. The concepts of nonlocal non-simple materials and viscous Cahn-Hilliard equations are used.

Except the static (or quasistatic) problems, the demagnetising field is ignored (which is legitimate rather for long magnets like in Figure 1, otherwise its influence may be quite essential [1]) and only local non-selfpenetration is considered. In the dynamic case, the governing system of equations is

$$\begin{aligned} \varrho \ddot{y} &= \text{div}(\partial_F \psi(\nabla y, m, \zeta) - (h_{\text{ext}} \circ y) \otimes m - \text{div} \mathfrak{H}(\nabla^2 y)) + ((\nabla h_{\text{ext}}) \circ y)^\top \nabla y m, \\ \tau_1 \dot{m} &= \kappa_1 \Delta m - \partial_m \psi(\nabla y, m, \zeta, \theta) + (\nabla y)^\top h_{\text{ext}} \circ y, \\ \dot{\zeta} - \text{div}(M(\nabla y, m, \zeta, \theta) \nabla \mu) &= 0 \quad \text{with} \quad \mu = \partial_\zeta \psi(\nabla y, m, \zeta, \theta) + \tau_2 \dot{\zeta} - \kappa_2 \Delta \zeta, \\ c_v(m, \zeta, \theta) \dot{\theta} - \text{div}(K(\nabla y, m, \zeta, \theta) \nabla \theta) &= \tau_1 |\dot{m}|^2 + \tau_2 \dot{\zeta}^2 \\ &\quad + M(\nabla y, m, \zeta, \theta) \nabla \mu \cdot \nabla \mu + \theta \partial_{m\theta}^2 \psi(m, \zeta, \theta) \cdot \dot{m} + \theta \partial_{\zeta\theta}^2 \psi(m, \zeta, \theta) \dot{\zeta} \end{aligned}$$

where the dot-notation stands for the time derivative, ϱ is the mass density, $c_v(m, \zeta, \theta) = -\theta \partial_{\theta\theta}^2 \psi$ the heat capacity, τ 's and κ 's are given constants, M is the pulled-back mobility tensor and K the heat-conductivity tensor, and \mathfrak{H} is a (nonlocal) hyperstress realizing the nonsimple-material concept. The existence of weak solutions of an initial-boundary value problem for this system is proved by a careful regularization and approximation by a Galerkin method.

Either ignoring or combining particular aspects, the model has numerous applications as ferro-to-paramagnetic transformation in elastic ferromagnets, diffusion of solvents in polymers possibly accompanied by magnetic effects (magnetic gels), or metal-hydride phase transformation in some intermetallics under diffusion of hydrogen (as studied in [3] at small strains) accompanied by magnetic effects.

The talk was in large parts based on a joint work with Giuseppe Tomassetti [4].

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Relaxation, deformation and thermal fluctuation of a quasi-spherical body

LIPING LIU

(joint work with Miao Yu, Hao Lin, Ramsey Foty)

Motivated by recent experiments on vesicles, cells and cell aggregates, we consider a general viscoelastic model that consists of a 2D membrane encapsulating a 3D bulk. Quantifying the mechanical properties of vesicles, cells and cell aggregates requires analytical and numerical solutions to suitable boundary value problems. In the first part of the talk [1], I present a framework for quick explicit and numerical solutions for a variety of different 2D elastic models including (i) constant surface tension model, (ii) Helfrich-Canham bending model and (iii) Gurtin-Murdoch surface elasticity. These solutions can be used to extract properties of postulated material models for cells or cell aggregates. In the second part of the talk [2], I present a statistical-physics based model that explains the origin of nonlinear volume-dependent surface (or cortex) tension of vesicles (or cells). Though we start from a model assuming incompressible bulk and area-preserving membrane, thermal fluctuations give rise to an effective model that the bulk is compressible with a nonlinear bulk modulus and the surface is stretchable with a nonlinear surface tension.

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Magnetic domains in thin ferromagnetic films with strong perpendicular anisotropy

HANS KNÜPFER

(joint work with Cyrill B. Muratov, Florian Nolte)

This talk summarizes the results of our upcoming paper [3], in which we investigate the scaling of the ground state energy and optimal domain patterns in thin ferromagnetic films with strong uniaxial anisotropy and easy axis perpendicular to the film plane. Starting from the full three-dimensional micromagnetic model, we identify the critical scaling where the transition from single domain states to multi-domain states such as bubble or maze patterns occurs. Furthermore, we analyze the asymptotic behavior of the energy in two regimes separated by the transition. In the single domain regime, the energy Γ -converges towards a much simpler two-dimensional and local model. In the second regime, we derive the scaling of the minimal energy and deduce a scaling law for the typical domain size.

More precisely, we show that, in the regimes we consider, the main part of the micromagnetic energy, upon rescaling and subtracting a constant, is given by the following two-dimensional functional

$$(1) \quad F_{\varepsilon, \lambda}[m] = \begin{cases} \int_{\mathbb{T}^2} \frac{\varepsilon |\nabla m|^2}{2} + \frac{(1 - m_3^2)}{2\varepsilon} \, d^2x - \frac{\lambda}{|\log \varepsilon|} \int_{\mathbb{T}^2} |\nabla^{1/2} m_3|^2 \, d^2x, & \text{if } m \in H^1(\mathbb{T}^2; \mathbb{S}^2), \\ +\infty, & \text{otherwise} \end{cases}$$

In (1), $\mathbb{T}^2 = \mathbb{R}^2/\mathbb{Z}^2$ denotes the flat square torus and we have assumed for simplicity that $m : \mathbb{T}^2 \rightarrow \mathbb{S}^2$ is periodic to avoid boundary effects. The main part of our analysis is concerned with the asymptotic behavior of (1) as $\varepsilon \rightarrow 0$ for different values of $\lambda > 0$. Note that the last term in (1) occurs with a negative sign and hence prefers oscillations of m_3 .

As it turns out, the value of the parameter λ is crucial - in fact, we will show that the asymptotic behavior changes at $\lambda_c = \frac{\pi}{2}$, which is a singular point in the terminology of [2]. For $\lambda < \lambda_c$ the Γ -limit $F_{*, \lambda} := \Gamma(L^1)\text{-}\lim_{\varepsilon \rightarrow 0} F_{\varepsilon, \lambda}$ measures the length of the interface separating regions with $m \approx e_3$ and $m \approx -e_3$

$$(2) \quad F_{*, \lambda}[m] = \begin{cases} \left(1 - \frac{\lambda}{\lambda_c}\right) \int_{\mathbb{T}^2} |\nabla m_3| \, d^2x, & \text{for } m \in BV(\mathbb{T}^2; \{\pm e_3\}), \\ +\infty, & \text{otherwise.} \end{cases}$$

(Note that the last term in (1) leads to a reduction of the interfacial cost by $\frac{\lambda}{\lambda_c}$ compared to the classical result [1] for $\lambda = 0$.) On the other hand, for $\lambda > \lambda_c$, the scaling of the minimal energy changes

$$(3) \quad \min F_{\varepsilon, \lambda} \sim -\frac{\lambda \varepsilon^{\frac{\lambda_c - \lambda}{\lambda}}}{|\log \varepsilon|} \xrightarrow{\varepsilon \rightarrow 0} -\infty,$$

and sequences $\{m_\varepsilon\}_{\varepsilon>0}$ which achieve the optimal scaling $F_{\varepsilon,\lambda}[m_\varepsilon] \sim \min F_{\varepsilon,\lambda}$ are highly oscillatory in the sense that

$$(4) \quad \int_{\mathbb{T}^2} |\nabla(m_\varepsilon)_3| dx \sim \varepsilon \frac{\lambda_c - \lambda}{\lambda} \xrightarrow{\varepsilon \rightarrow 0} +\infty.$$

Furthermore, for $\lambda \geq \lambda_c$, the leading order contributions of all three terms in (1) cancel. The main difficulty in the proof is to find asymptotically optimal estimates for the non-local term.

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Injectivity in magnetoelasticity

BARBORA BENEŠOVÁ

(joint work with Malte Kampschulte, Martin Kružík)

In continuum mechanics the primary state variable is the *deformation* of the specimen $y : \Omega \rightarrow y(\Omega)$. Here and in the sequel $\Omega \subset \mathbb{R}^n$ ($n = 2, 3$) is a bounded Lipschitz domain, the reference configuration.

It is generally postulated [2] that an element of the set of admissible deformations should be an *orientation-preserving* and *injective* map with a suitably integrable weak gradient; one usually assumes that $y \in W^{1,p}(\Omega; \mathbb{R}^n)$ with $1 < p \leq +\infty$.

The injectivity constraint is of particular importance in magnetoelasticity where the observables are not only the deformation but also the magnetization M , defined in the current configuration. Then, the stable states are obtained by minimizing the magnetoelastic energy of the form

$$(1) \quad \psi(y, M) = \underbrace{A \int_{y(\Omega)} |\nabla M|^2 dx}_{\text{exchange energy}} + \underbrace{\int_{\Omega} \phi(\nabla y, M \circ y) dx}_{\text{anisotropy energy}} + \underbrace{\frac{\mu_0}{2} \int_{\mathbb{R}^3} |H|^2 dx}_{\text{stray field energy}} \\ + \underbrace{\int_{\Omega} W(\nabla y) dx}_{\text{elastic energy}} - \underbrace{\mu_0 \int_{y(\Omega)} M \cdot H_{\text{ext}} dx}_{\text{Zeeman energy}},$$

where A is a constant, μ_0 is the permeability of vacuum, H_{ext} is the applied magnetic field and the stray field $H : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ (defined in the whole space, even if $\Omega \subset \mathbb{R}^2$) is obtained from (possibly a reduced set) of the Maxwell equations.

As we see from (1), the purely magnetic parts of the energy (such as the exchange or Zeeman one) are defined in the deformed configuration while the ones

referring to elasticity in the reference one. Thus, in order to allow for a transformation between the two configurations, we need the deformation to be invertible or even to be a homeomorphism. On a more technical level, one might look, for example, at the composition $M \circ y$ that appears in the anisotropy energy. This may not be Lebesgue measurable even if M and y are measurable themselves.¹

In this talk, we concentrated on two types of set admissible deformations *in the plane*: the *quasiconformal maps*

$$\mathcal{QC}(\Omega; \mathbb{R}^2) = \left\{ y \in W^{1,2}(\Omega; \mathbb{R}^2) : y \text{ is a homeomorphism and } \exists K \geq 1 \text{ such that} \right. \\ \left. |\nabla y|^2 \leq K \det(\nabla y) \text{ a.e. in } \Omega \right\},$$

as well as the bi-Lipschitz maps

$$W^{1,\infty,-\infty}(\Omega; \mathbb{R}^2) = \left\{ y \in W^{1,\infty}(\Omega; \mathbb{R}^2) : y \text{ is injective, } \det(\nabla y) > 0 \right. \\ \left. \text{and } y^{-1} \in W^{1,\infty}(y(\Omega); \Omega) \right\};$$

and studied conditions on the stored energy W that assure weak lower semicontinuity of the elastic energy in (1)

$$(2) \quad I(y) := \int_{\Omega} W(\nabla y) \, dx$$

along sequences in $\mathcal{QC}(\Omega; \mathbb{R}^2)$ or $W^{1,\infty,-\infty}(\Omega; \mathbb{R}^2)$.

The relevant condition that we identified with this respect is the so-called *bi-quasiconvexity* or *quasiconformal quasiconvexity*:

Definition. We say that a Borel measurable and bounded from below function $W : \mathbb{R}^{2 \times 2} \rightarrow \Omega$ is *bi-quasiconvex* if

$$(3) \quad \mathcal{L}^2(\Omega)W(A) \leq \int_{\Omega} W(\nabla \varphi(x)) \, dx$$

for all $\varphi \in W_+^{1,\infty,-\infty}(\Omega; \mathbb{R}^2)$, $\varphi = Ax$ on $\partial\Omega$ and all A with $\det A > 0$.

We say that W is *quasiconformally quasiconvex* if (3) holds for all A with $\det(A) > 0$ and all $\varphi \in \mathcal{QC}(\Omega; \mathbb{R}^2)$ such that $\varphi(x) = Ax$ on $\partial\Omega$.

With this definition at hand, we have the following result:

Proposition (see [4, 3]). Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain. Let W be continuous on the set of matrices 2×2 with a positive determinant. Then W is *bi-quasiconvex* if and only if I in (2) is *sequentially weakly** lower semicontinuous on $W_+^{1,\infty,-\infty}(\Omega; \mathbb{R}^2)$.

Moreover, let W satisfy $0 \leq f(A) \leq c(1+|A|^2)$ with $c > 0$ on the set of matrices with a positive determinant. Then W is *quasiconformally quasiconvex* if and only if I is *weakly lower semicontinuous* on $\mathcal{QC}(\Omega; \mathbb{R}^2)$.

¹However, measurability of the composition can be assured if either M is continuous (which however is not physically required) or y is an homeomorphism, which is the physical requirement that we aim to study.

Let us highlight that weak lower semicontinuity of I is proved from quasi-convexity without assuming that W locally bounded on $\mathbb{R}^{2 \times 2}$. This is generally considered to be a difficult task in the calculus of variations (cf. [1]) but it is physically important because the stored energy should be infinite on matrices with a non-positive determinant to yield (with further restrictions) injectivity of the deformation.

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Coupling and numerical integration of the Landau–Lifshitz–Gilbert equation

MICHELE RUGGERI

(joint work with Dirk Praetorius and Bernhard Stiftner)

The understanding of the magnetization dynamics plays an essential role in the design of many technological applications, e.g., storage devices, sensors, actuators, electric motors, and generators. The availability of reliable numerical tools to perform large-scale micromagnetic simulations of magnetic systems is therefore of fundamental importance. Time-dependent micromagnetic phenomena are usually described by the Landau–Lifshitz–Gilbert (LLG) equation

$$(1) \quad \partial_t \mathbf{m} = -\mathbf{m} \times [\mathbf{h}_{\text{eff}} + \mathbf{\Pi}(\mathbf{m})] + \alpha \mathbf{m} \times \partial_t \mathbf{m} \quad \text{in } \Omega \times (0, T).$$

Here, $\Omega \subset \mathbb{R}^3$ is a bounded Lipschitz domain, while T and α are positive constants. The unknown is the normalized magnetization $\mathbf{m} \in L^2(0, T; \mathbf{H}^1(\Omega)) \cap H^1(0, T; \mathbf{L}^2(\Omega))$, which satisfies $|\mathbf{m}| = 1$ a.e. in Ω . The effective field takes the form $\mathbf{h}_{\text{eff}} = -\frac{\delta \mathcal{E}(\mathbf{m}, \mathbf{f})}{\delta \mathbf{m}} = \mathbf{\Delta} \mathbf{m} + \mathbf{\pi}(\mathbf{m}) + \mathbf{f}$, where the energy is given by

$$\mathcal{E}(\mathbf{m}, \mathbf{f}) = \frac{1}{2} \|\nabla \mathbf{m}\|_{\mathbf{L}^2(\Omega)}^2 - \frac{1}{2} \langle \mathbf{\pi}(\mathbf{m}), \mathbf{m} \rangle - \langle \mathbf{f}, \mathbf{m} \rangle.$$

The bounded, linear, and self-adjoint operator $\mathbf{\pi} : \mathbf{L}^2(\Omega) \rightarrow \mathbf{L}^2(\Omega)$, the function $\mathbf{f} \in H^1(0, T; \mathbf{L}^2(\Omega))$, and the bounded operator $\mathbf{\Pi} : \{\mathbf{m} \in \mathbf{H}^1(\Omega) : |\mathbf{m}| = 1 \text{ a.e. in } \Omega\} \rightarrow \mathbf{L}^2(\Omega)$ are general \mathbf{m} -dependent, \mathbf{m} -independent, and nonenergetic field contributions, respectively. The LLG equation is usually supplemented with homogeneous Neumann boundary conditions $\partial_n \mathbf{m} = \mathbf{0}$ on $\partial\Omega \times (0, T)$ and initial condition $\mathbf{m}(0) = \mathbf{m}^0$ in Ω , where $\mathbf{m}^0 \in \mathbf{H}^1(\Omega)$ satisfies $|\mathbf{m}^0| = 1$ a.e. in Ω .

The numerical integration of (1) poses several challenges: strong nonlinearities, a nonconvex pointwise constraint, an intrinsic energy law, which combines conservative and dissipative effects, as well as the presence of nonlocal field contributions which require the coupling with other partial differential equations (PDEs).

In this contribution, we discuss some of our recent results [1, 7, 2, 3, 9, 10]. To discretize (1), we extend the numerical scheme of [4]. We consider a quasi-uniform family $\{\mathcal{T}_h\}$ of tetrahedral triangulations of Ω with mesh size h and a uniform partition $\{t_i = ik : 0 \leq i \leq M\}$ of the time interval $(0, T)$ with time-step size $k = T/M$. We denote by $\mathcal{S}^1(\mathcal{T}_h)$ the space of piecewise linear and globally continuous polynomials. The orthogonality $\mathbf{m} \cdot \partial_t \mathbf{m} = 0$ from (1) is introduced at the discrete level only at the nodes of \mathcal{T}_h by considering the discrete tangent space

$$\mathcal{K}_{\mathbf{m}_h} := \{\phi_h \in \mathcal{S}^1(\mathcal{T}_h)^3 : \mathbf{m}_h(z) \cdot \phi_h(z) = 0 \text{ for any node } z\} \text{ for } \mathbf{m}_h \in \mathcal{S}^1(\mathcal{T}_h)^3.$$

Given $0 \leq \theta \leq 1$, the time-marching scheme is based on an equivalent reformulation of (1) and consists, for every $0 \leq i \leq M - 1$, of the following steps:

- (i) Compute $\mathbf{v}_h^i \in \mathcal{K}_{\mathbf{m}_h^i}$ such that, for all $\phi_h \in \mathcal{K}_{\mathbf{m}_h^i}$,

$$\begin{aligned} & \alpha \langle \mathbf{v}_h^i, \phi_h \rangle + \langle \mathbf{m}_h^i \times \mathbf{v}_h^i, \phi_h \rangle + \theta k \langle \nabla \mathbf{v}_h^i, \nabla \phi_h \rangle \\ & = -\langle \nabla \mathbf{m}_h^i, \nabla \phi_h \rangle + \langle \boldsymbol{\pi}_h(\mathbf{m}_h^i), \phi_h \rangle + \langle \mathbf{f}_h^i, \phi_h \rangle + \langle \boldsymbol{\Pi}_h(\mathbf{m}_h^i), \phi_h \rangle; \end{aligned}$$

- (ii) Define $\mathbf{m}_h^{i+1} \in \mathcal{S}^1(\mathcal{T}_h)^3$ by $\mathbf{m}_h^{i+1}(z) = \frac{\mathbf{m}_h^i(z) + k\mathbf{v}_h^i(z)}{|\mathbf{m}_h^i(z) + k\mathbf{v}_h^i(z)|}$ for every node z .

Here, $\mathbf{m}_h^i \approx \mathbf{m}(t_i)$ and $\mathbf{v}_h^i \approx \partial_t \mathbf{m}(t_i)$. The pointwise constraint is enforced by nodal projection of the computed solution at each time-step. Despite all the nonlinearities, the algorithm requires only the solution of one linear system per time-step. Under suitable stability and convergence assumptions on \mathbf{m}_h^0 , $\{\mathbf{f}_h^i\}$, $\boldsymbol{\pi}_h$, and $\boldsymbol{\Pi}_h$, the sequence of discrete approximations converges towards a weak solution of the problem [7]. If $1/2 < \theta \leq 1$ and the triangulation additionally satisfies a weak acuteness condition, the convergence is unconditional, i.e., the analysis does not impose any CFL-type condition between the time-step size and the mesh size. Moreover, a fully linear projection-free variant of the method, which omits the nodal projection in (ii), preserves the (unconditional) convergence result [1].

One particular focus of our work is on the efficient treatment of coupled systems, for which we show that an approach based on the decoupling of the time integration of the LLG equation and the coupled PDE reduces the computational cost, but still leads to time-marching algorithms that are unconditionally convergent. This approach was successfully applied to the coupling of the LLG equation with the Maxwell equations [8, 6] and with a balance law for the linear momentum to model the magnetoelastic interaction [5]. As an application of the theory, we analyze several extensions of the micromagnetic model for the simulation of spintronic devices. As an example, we consider the system

$$\begin{aligned} \partial_t \mathbf{m} &= -\mathbf{m} \times \mathbf{h}_{\text{eff}} + \alpha \mathbf{m} \times \partial_t \mathbf{m} - \mathbf{m} \times \mathbf{s}, \\ \partial_t \mathbf{s} &= \nabla \cdot [(\mathbf{I}_{3 \times 3} - \beta \beta' \mathbf{m} \otimes \mathbf{m}) \nabla \mathbf{s}] - \mathbf{s} - \mathbf{s} \times \mathbf{m} - \beta \nabla \cdot (\mathbf{m} \otimes \mathbf{j}_e), \end{aligned}$$

where the LLG equation is nonlinearly coupled with a parabolic equation, which models the evolution of the spin accumulation \mathbf{s} in the presence of a spin-polarized electric current \mathbf{j}_e in magnetic multilayer structures. Numerical experiments support our theoretical findings and demonstrate the applicability of the method for the simulation of practically relevant problem sizes [2, 9, 3, 10].

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Phase transformations and magnetism

RICHARD D. JAMES

Many interesting problems are emerging from problems in which magnetism is combined with phase transformations. Typical interesting phenomena include cases in which the two phases have diverse magnetic properties — one phase is ferromagnetic and the other non-ferromagnetic (or anti-ferromagnetic), one phase soft-magnetic, the other hard etc. These lead to challenging problems in the calculus of variations for which there, as yet, does not appear even an existence theorem.

Other older problems that remain unsolved include the “coercivity paradox” and the “permalloy problem”. The former is, from the mathematical point of view, the failure of linear stability analysis. But there is no clear resolution though methods that are adapted to analyze “large localized disturbances” could be relevant. In the permalloy problem the challenge is to understand, from a predictive viewpoint, the particular compositions 45% Ni and 78.5 % Ni (in the $\text{Fe}_x\text{Ni}_{1-x}$ system) at which the alloys become exceptionally soft.

Two open mathematical problems concerning ferroelectric solids

KAUSHIK BHATTACHARYA

Ferroelectric materials are the electrical analogs of magnets as they are spontaneously electrically polarized.

The first problem concerns understanding the physical origins of electrical polarization from microscopic physics. We seek to understand if commonly used macroscopic models based on polarization arise as the large body limit of microscopic models based on electron density. We conjecture this to be true and support the conjecture with an upper bound. The lower bound remains open. This is based on joint work with Saurabh Puri.

The second problem concerns the phase diagram of a commonly used material which is a solid solution of lead titanate and lead zirconate. We propose a model similar to a random field Ising model with long-range interactions, and show through numerical simulation that particular features of the phase diagram arise from a competition between the short-range disorder (from the chemistry) and long-range order (from the electrostatic and mechanical interaction). A systematic analysis of this model remains open. This is based on joint work with Jiangyu Li and Jeong Ho You.

Polyconvexity in magnetoelasticity and phase transitions

MARTIN KRUŽÍK

In this talk, we first review results obtained in [6]. Here we investigate a variational theory for magnetoelastic solids under the incompressibility constraint. The state of the system is described by deformation and magnetization. While the domain of the deformation is the reference configuration, magnetization is defined in the deformed configuration instead. We discuss the existence of energy minimizers without relying on second-order deformation gradient terms cf. [7] where, on the other hand, no incompressibility constraint was imposed. Then, by introducing a suitable positively 1-homogeneous dissipation, a quasistatic evolution model is proposed and analyzed within the frame of energetic solvability.

The state of a magnetostrictive material is described by its deformation $y : \Omega \rightarrow \mathbb{R}^3$ from the reference configuration $\Omega \subset \mathbb{R}^3$ and by its magnetization $m : \Omega^y \rightarrow \mathbb{R}^3$ which is defined on the deformed configuration $\Omega^y := y(\Omega)$ instead. This difficulty is exclusively related to large deformation regimes that magnetostrictive materials can undergo. Relying standardly on a variational approach, we define the magnetoelastic energy as

$$(1) \quad E(y, m) := \int_{\Omega} W(\nabla y, m \circ y) \, dx + \frac{\alpha}{2} \int_{\Omega^y} |\nabla m|^2 \, dx + \frac{\mu_0}{2} \int_{\mathbb{R}^3} |\nabla u_m|^2 \, dx \\ - \left(\int_{\Omega^y} h \cdot m + \int_{\Omega} f \cdot u + \int_{\partial\Omega} g \cdot u \right).$$

Here, W stands for the elastic energy density, the second term is the so-called *exchange* energy and $\alpha > 0$ is related to the typical size of ferromagnetic texture.

The next term represents magnetostatic energy, $\mu_0 = 4\pi \times 10^{-7} \text{N/A}^2$ is the permeability of the vacuum, and u_m is the magnetostatic potential generated by m . In particular, u_m is a solution to the Maxwell equation

$$(2) \quad \nabla \cdot (-\mu_0 \nabla u_m + \chi_{\Omega^y} m) = 0 \quad \text{in } \mathbb{R}^3,$$

where χ_{Ω^y} is the characteristic function of the deformed configuration Ω^y . Finally, h , f , and g are external magnetic field, and densities of volume and surface forces applied to the specimen, respectively. We consider E under the constraints

$$(3) \quad \det \nabla y = 1 \quad \text{and} \quad |m| = 1 \quad \text{almost everywhere in } \Omega,$$

which correspond to incompressibility and magnetic saturation.

As to the stored energy density, we assume that for some $p > 3$ and the rotation group $\text{SO}(3)$ it holds that

$$(4a) \quad \exists c > 0 \forall F, m : -1/c + c|F|^p \leq W(F, m),$$

$$(4b) \quad \forall R \in \text{SO}(3) : W(RF, Rm) = W(F, m),$$

$$(4c) \quad \forall F, m : W(F, m) = W(F, -m),$$

$$(4d) \quad \forall F, m : W(F, m) = \hat{W}(F, \text{cof } F, m),$$

where $\hat{W}(\cdot, \cdot, m)$ is convex. The last condition (4d) is just polyconvexity of $W(\cdot, m)$. Polyconvexity was introduced in [1] to show existence of minimizers for energy functionals arising in nonlinear elasticity. Here, $\text{cof } F$ denotes the cofactor matrix of F . Incompressibility is expressed by the requirement that $\det F = 1$ which implies that $\text{cof } F = F^{-\top}$. Polyconvexity allows us to incorporate injectivity of y and it is also relatively easy to construct polyconvex functions.

In many situations, however, one cannot rely on polyconvexity; see [2] for a recent survey. This is, for example, the case of magnetic shape memory materials where $W(\cdot, m \circ y)$ has a multiwell structure. Each well describes a stress free state of a particular variant of the material. Energy minimizing deformations exhibit fine microstructures composed of various material variants. In many mathematical models, this feature is manifested by non-existence of minimizers because minimizing sequences exhibit finer and finer oscillations. A possible way out was proposed by Šilhavý in [8] who introduced the so-called interfacial polyconvexity. We call a function $g : \mathbb{R}^{3 \times 3} \times S^2 \rightarrow \mathbb{R}$ interfacial polyconvex if there is a convex and positively 1-homogeneous function Ψ such that $g(F, n) = \Psi(n, F \times n, \text{Cof } F n)$. Here n is the unit vector and $F \in \mathbb{R}^{3 \times 3}$ is such that $F n = 0$. Moreover, $F \times n$ is defined by the formula $(F \times n)a := F(n \times a)$ for every $a \in \mathbb{R}^3$. If F is the surface gradient and n is the unit normal to the surface between two different variants then $F \times n$ measures the curvature of the interface in the deformed configuration while $\text{Cof } F n$ accounts for the area of the deformed interface. A model for quasistatic evolution of shape memory materials using interface polyconvexity can be found in [5], its phase-field approximation in [4], and an analogous model for ferromagnetic shape memory alloys in [3].

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On some model for magnetoelasticity with Eulerian description

ANJA SCHLÖMERKEMPER

(joint work with B. Benešová, J. Forster, C. García-Cervera and C. Liu)

A fundamental issue in the modeling of magnetoelastic materials is that elasticity is phrased in Lagrangian coordinates whereas magnetism is phrased in Eulerian coordinates. We discuss a model that is completely phrased in Eulerian coordinates and show existence of weak solutions, cf. [1, 2, 4]. The model presented is a system of partial differential equations that contains (i) a Navier-Stokes equation with magnetic and elastic terms in the stress tensor obtained by a variational approach, (ii) a regularized transport equation for the deformation gradient and (iii) the Landau-Lifshitz-Gilbert equation for the dynamics of the magnetization.

Let $\Omega_0 \subset \mathbb{R}^d$, $d = 2, 3$ be the reference configuration of the body considered. Its elements X are referred to as Lagrangian coordinates. The current/deformed configuration at time $t \in [0, T]$ is denoted by $\Omega \subset \mathbb{R}^d$ and is identified with Ω_0 at $t = 0$. The deformation or flow map of the body

$$x : \Omega_0 \times [0, T] \rightarrow \Omega, \quad (X, t) \mapsto x(X, t), \quad \text{where } x(X, 0) = X,$$

maps the reference configuration onto the deformed/current configuration at time t . The velocity is a mapping $v : \Omega \times [0, T] \rightarrow \mathbb{R}^d$ such that $v(x(X, t), t) = \frac{\partial}{\partial t} x(X, t)$ for all $t > 0$. The deformation gradient is defined as $\tilde{F} : \Omega_0 \times [0, T] \rightarrow \mathbb{R}^{d \times d}$ with $\tilde{F}(X, t) := \frac{\partial x}{\partial X}(X, t)$ and becomes $F(x(X, t), t) = \tilde{F}(X, t)$ in Eulerian coordinates. As in [6], the following transport equation allows us to determine the deformation gradient in Eulerian coordinates from the velocity:

$$(1) \quad F_t + (v \cdot \nabla)F - \nabla v F = 0 \quad \text{in } \Omega \times [0, T].$$

For the beginning, we work in the framework of incompressible materials

$$(2) \quad \operatorname{div} v = 0 \quad \text{in } \Omega \times [0, T].$$

The energetic variational approach starts from an action functional, which is an integral of the difference of the kinetic energy and the free energy of the system, as well as a dissipation term due to viscosity. The first variation of this action functional with respect to the flow map yields the balance of momentum

$$(3) \quad v_t + (v \cdot \nabla)v - \operatorname{div} \mathcal{T} = 0 \quad \text{in } \Omega \times [0, T],$$

where $\mathcal{T} = -p \operatorname{Id} + \nu \nabla v + \mathcal{T}_{\text{mag-ela}}$ is the stress tensor with p denoting the pressure, Id denotes the identity matrix, and $\nu \nabla v$, $\nu > 0$ represents the viscous stress, which in fact makes the model magnetoviscoelastic. The formula for $\mathcal{T}_{\text{mag-ela}}$ follows from a variation with respect to the flow map x of the corresponding free energy ψ phrased in Eulerian coordinates.

The magnetization $M : \Omega \times [0, T] \rightarrow \mathbb{R}^3$ is phrased in Eulerian coordinates and satisfies $|M(x, t)| = 1$ almost everywhere in $\Omega \times [0, T]$. Based on the standard micromagnetic energy, the free energy reads

$$\begin{aligned} \psi(F, M) = & \underbrace{\frac{1}{2} \int_{\Omega} |\nabla M|^2 dx}_{\text{exchange energy}} + \underbrace{\int_{\Omega} \Phi(F, M) dx}_{\text{anisotropy energy}} + \underbrace{\frac{1}{2} \int_{\mathbb{R}^3} |H|^2 dx}_{\text{stray field energy}} \\ & + \underbrace{\int_{\Omega} W(F) dx}_{\text{elastic energy}} - \underbrace{\int_{\Omega} M \cdot H_{\text{ext}} dx}_{\text{Zeeman energy}}, \end{aligned}$$

where $\Phi : \mathbb{R}^{d \times d} \times \mathbb{R}^3 \rightarrow \mathbb{R}$ describes the impact of the crystalline structure on the magnetization and is allowed to depend on F and M here. Further, H_{ext} is the applied magnetic field, and the magnetic field $H : \mathbb{R}^d \rightarrow \mathbb{R}^3$ is the solution of Maxwell's equations for magnetostatics.

The dynamics of the magnetization vector is governed by the Landau-Lifshitz-Gilbert equation (LLG), where the usual time-derivative $\frac{dM}{dt}$ needs to be replaced by the convective or material derivative,

$$(4) \quad M_t + (v \cdot \nabla)M = M \times \frac{\delta \psi}{\delta M} + M \times \left(M \times \frac{\delta \psi}{\delta M} \right) \quad \text{in } \Omega \times [0, T],$$

with $\frac{\delta \psi}{\delta M}$ denoting the variational derivative of ψ with respect to M . The LLG equation inherits a coupling of F and M from ψ .

The system of PDEs describing the evolution of magnetoelastic materials is then given by the equations (1)–(4) and certain boundary and initial conditions for F , M and v , see [4] for details.

In [1] we prove existence of weak solutions to a special version of this system in $d = 2$ for small initial data. In the special system, the stray field energy and anisotropy energy are neglected, the elastic energy W is assumed convex and the transport equation for F is regularized. On $\Omega \times [0, T]$ the system then reads

$$\begin{aligned} v_t + (v \cdot \nabla)v + \nabla p + \operatorname{div}(\nabla^T M \nabla M - W'(F)F^T) &= \nu \Delta v + \nabla^T H_{\text{ext}} M, \\ \operatorname{div} v &= 0, \\ F_t + (v \cdot \nabla)F - \nabla v F &= \kappa \Delta F, \\ (5) \quad M_t + (v \cdot \nabla)M &= -M \times (\Delta M + H_{\text{ext}}) - M \times (M \times (\Delta M + H_{\text{ext}})) \end{aligned}$$

for some $\kappa > 0$ and certain boundary and initial conditions.

We prove global in time small data existence of weak solutions in two dimensions, and locally in time also in three dimensions [1]. The proof is based on a Galerkin method and a fixed-point argument; it combines ideas from the analysis of models for the flow of liquid crystals [5] and of the Landau-Lifshitz equation [3]. For a corresponding result in $d = 2, 3$ for a gradient flow for M instead of (5) we refer to [2, 4].

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Topics in energetic variational approaches

CHUN LIU

In this talk, I present a general framework of variational approaches. The approaches are motivated by earlier work of Rayleigh and Onsager. It had been proven to be extremely useful to derive thermodynamically consistent coupled systems; such as those of liquid crystals, magnetohydrodynamics, electrorheological fluids and polymeric fluids. It emphasizes the coupling between the kinematic transport of the phase variables and the induced elastic stresses. For example, we

look at the Eulerian description of an incompressible Hookean elasticity and the well-posedness results of viscoelastic fluids. Finally, by looking at the examples of fine interface motion in mixtures and MHD dynamics, we demonstrate the underlying structure of these systems as well as the specifics of the individual ones.

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