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Weak lower semicontinuity in problems of variational calculus

Komise pro obhajoby doktorských disertací v oboru: Matematická analýza a příbuzné obory

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1 Summary

Minimization is a reoccurring theme in many mathematical disciplines ranging from pure to applied ones. Of particular importance is the minimization of integral functionals that is studied within the calculus of variations. Proofs of the existence of minimizers usually rely on a fine property of the involved functional called *(sequential)* weak lower semicontinuity. While early studies of weak lower semicontinuity go back to the beginning of the 20th century, the milestones of the modern theory were set by C.B. Morrey Jr. [80] in 1952 and N.G. Meyers [79] in 1965. We first discuss weak lower semicontinuity of integral functionals in problems arising in continuum mechanics of solids and in magnetism. Special attention is paid to applications where physical models do not allow for weak lower semicontinuity of energy functionals. In this case, we search for a lower semicontinuous envelope of the original problem. Here, generalized convexity notions (quasiconvexity, rank-one onvexity, and polyconvexity) play a key role. In the he second part of the thesis, we review quasiconvexity and its refinement important for a characterization of parametrized measures generated by gradients and give some aplications to weak lower semicontinuity of integral functionals for signed integrands. Besides, we mention results in lower semicontinuity of functionals along sequences satisfying differential constraints and some interesting properies of quasiconvex functions.

2 Preface

Many tasks in the world surrounding us can be mathematically formulated as minimization or maximization problems. For example, in physics we minimize the energy, in economy one tries to minimize the cost and maximize the profit, entrepreneurs may try to minimize the investment risk. In addition, minimization problems appear in many more specific tasks: in a fitting procedure, or more generally inverse problems, one tries to minimize the deviation of the model prediction from the experimental observation or training of a neuronal network is based on minimizing a suitable cost function.

In a very general manner, we may express these problems as

minimize
$$I$$
 over \mathcal{Y} , (2.1)

where \mathcal{Y} is a set over which the minimum is sought and $I : \mathcal{Y} \to \mathbb{R}$ is a functional whose meaning may be the energy, cost, risk, or gain, for instance. From the mathematical point of view, two questions are immediate when inspecting problem (2.1): firstly whether (2.1) is solvable, that is if I possesses minimizers on \mathcal{Y} , and secondly how to find a solution (i.e. a minimizer) to (2.1).

Calculus of variations is devoted to solving (2.1) when \mathcal{Y} is (a subset) of an infinitedimensional vector space. Its starting point may have been a question of Johann Bernoulli on which curve a mass point will descent the fastest in a gravitational field; the so-called *brachistochrone problem*. In the most typical situation (that covers the brachistochrone problem in particular), I in (2.1) is an integral functional depending on functions $u: \Omega \to \mathbb{R}^m$ with $\Omega \subset \mathbb{R}^n$ and their derivatives. In the easiest case, in which n = m = 1, $\Omega = [a, b]$, and $f: \Omega \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a suitable integrand, the functional reads

$$I(u) := \int_{a}^{b} f(x, u(x), u'(x)) \, \mathrm{d}x \quad \text{with } u(a) = u_a \text{ and } u(b) = u_b, \tag{2.2}$$

where u_a and u_b are given boundary data. The task is to either solve (2.1) or at least to prove existence of minimizers.

Foundations of the calculus of variations were laid down in the 18th century by L.P. Euler and J.L. Lagrange who also realized its important connections to physics and to mechanics. black These early works quite naturally concentrated on the question on how to find (candidates for) solutions of (2.1). The classical method to do so, is to consider so-called *variations*. Indeed, if u_0 is a minimizer of I then

$$I(u_0) \le I(u_0 + \varepsilon \varphi) \quad \text{for all } \varphi \in C_0^{\infty}([a, b]),$$

$$(2.3)$$

where $\varepsilon \varphi$ is called a variation of the minimizer. Now, assume that f is twice continuously differentiable and $u_0 \in C^2([a, b])$, then by the classical calculus (2.3) implies that $\frac{\mathrm{d}}{\mathrm{d}\varepsilon}I(u_0(x) + \varepsilon \varphi(x))\Big|_{\varepsilon=0}$ vanishes for all $\varphi \in C_0^{\infty}([a, b])$. This is equivalent to solving

$$\frac{\partial f}{\partial r}(x, u_0, u_0') - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial f}{\partial s}(x, u_0, u_0') = 0 \quad \text{on } [a, b],$$
(2.4)

where $\frac{\partial f}{\partial r}$ and $\frac{\partial f}{\partial s}$ denote the partial derivative of f with respect to the second and third variable, respectively. Equation (2.4) is referred to as the *Euler-Lagrange equation* and solving it is the classical path to finding solutions of (2.1). Of course, any critical point of I (and not only the minimizer) is a solution to (2.4) but solving (2.4) is still an efficient approach to (2.1) at least in a situation in which all critical points are minimizers, for example if f is convex. For more details, see for example the book by Bolza [18].

Nevertheless, solving the Euler-Lagrange equation naturally relies on smoothness properties of f which might not be available. Therefore, it is often advantageous to address existence of solutions to (2.1) in a non-constructive way by using suitable compactness properties of \mathcal{Y} and continuity properties of I. For example, if \mathcal{Y} is a bounded closed interval of reals and $I: \mathcal{Y} \to \mathbb{R}$ is a function then (2.1) has a solution whenever I is continuous. This observation goes back to Bernard Bolzano who proved it in his work "Function Theory" in 1830 and is called the *Extreme Value Theorem*. Later on, it was independently shown by Karl Weierstrass. The main ingredient of the proof, namely the fact that one can extract a convergent subsequence from a closed bounded interval of reals, is nowadays known as the Bolzano-Weierstrass theorem.

The results of Bolzano and Weierstrass easily extend to the situation when \mathcal{Y} is a bounded and closed set of a *finite-dimensional* vector space. However, they cannot be generalized to the situation in which, for example, \mathcal{Y} is a ball in an infinite dimensional vector space since the Bolzano-Weierstrass theorem is false in this case.

Thus, the only hope to transfer a variant of the Bolzano-Weierstrass theorem to infinite dimensional spaces is to seek compactness in a "weaker" topology than the one induced by the norm. This possibility has been opened by Riesz and Hilbert who used the *weak topology* on Hilbert spaces from the beginning of the 20th century and by Stefan Banach who defined it on other normed spaces around 1930.

Having the weak topology at hand, a generalization of the Bolzano extreme value theorem becomes possible and is today known as the *direct method of the calculus of variations*. This algorithm was proposed by David Hilbert around 1900, to show (in a non-constructive way) the existence of a solution to the minimization problem (2.1). It consists of three steps:

- 1. We find a minimizing sequence along which I converges to its infimum on \mathcal{Y} .
- 2. We show that a subsequence of the minimizing sequence converges to an element of \mathcal{Y} in some topology τ .

3. We prove that this limit element is a minimizer.

The third step of the direct needs to rely on suitable semicontinuity properties of I; a sufficient and widely used condition is the *(sequential)* lower semicontinuity of I with respect to the weak/weak* topology:

Definition 2.1 Let \mathcal{Y} be a subset of a Banach space. We say that the functional $I: \mathcal{Y} \to \mathbb{R}$ is (sequentially) weakly/weakly* lower-semicontinuous on \mathcal{Y} if for every sequence $\{u_k\}_{k\in\mathbb{N}}\subset\mathcal{Y}$ converging weakly/weakly* to $u \in \mathcal{Y}$, we have that

$$I(u) \le \liminf_{k \to \infty} I(u_k).$$

If I is not weak/weak* lower semicontinuous solutions to (2.1) need not to exist. However, weak lower semicontinuity of I is not a necessary condition for the existence of minimizers. These facts are demonstrated by the following example.

Example 2.2 Consider the following special case of (2.2):

$$I(u) = \int_0^1 \left(1 - (u'(x))^2\right)^2 + (u(x))^2 \,\mathrm{d}x \tag{2.5}$$

with

$$\mathcal{Y} := \{ u \in W^{1,\infty}(0,1); -1 \le u' \le 1, u(0) = u(1) = 0 \}$$

We can see, for example by the Lebesgue dominated convergence theorem, that I is continuous on $W^{1,\infty}(0,1)$ but it is not weakly lower semicontinuous. To show this, define

$$u(x) = \begin{cases} x & \text{if } 0 \le x \le 1/2 \\ -x+1 & \text{if } 1/2 \le x \le 1 \end{cases}$$

and extend it periodically to the whole \mathbb{R} . Let $u_k(x) := k^{-1}u(kx)$ for all $k \in \mathbb{N}$ and all $x \in \mathbb{R}$. Notice that $\{u_k\}_{k\in\mathbb{N}}\subset\mathcal{Y}$.

The sequence of "zig-zag" functions $\{u_k\}_{k\in\mathbb{N}}$ converges weakly* to zero in $W^{1,\infty}(0,1)$. It is not hard to see that $I(u_k) \to 0$ for $k \to \infty$ but

$$1 = I(0) > \lim_{k \to \infty} I(u_k) = 0;$$

so that I is not weakly^{*} lower semicontinuous on $W^{1,\infty}(0,1)$ and, in fact, no minimizer exists in this case.

Indeed, $0 = \inf_{\mathcal{V}} I \neq \min_{\mathcal{V}} I$ because $I \geq 0$ and $I(u_k) \to 0$, so that $0 = \inf_{\mathcal{V}} I$. However, I(u) > 0 for every $u \in \mathcal{Y}$, for otherwise it would mean that we could find a Lipschitz function whose derivative is ± 1 almost everywhere on (0,1) but the function value is identically zero.

If we, however, consider a slight modification of \mathcal{Y} by changing the boundary condition at x = 1, and consider

$$\mathcal{Y}_1 := \{ u \in W^{1,\infty}(0,1); -1 \le u' \le 1, u(0) = 0, u(1) = 1 \}$$

then $\min_{\mathcal{Y}_1} I = 1/3$ and the unique minimizer is u(x) = x for $x \in (0, 1)$. Firstly, this shows that weak/weak* lower semicontinuity of I is not necessary for the existence of a minimizer, and, secondly, it stresses the influence of boundary conditions on the solvability of (2.1). This phenomenon is even more pronounced in higher dimensions.

Although the study of weak lower semicontinuity is motivated by understanding minimization problems, it has become an independent subject in mathematical literature that has been studied for its own right. In the case of integral functionals as in (2.2), further properties of the integrand besides continuity are needed to assure weak/weak* lower-semicontinuity: the right additional property is always some type of *convexity* of f. Indeed, notice that I in Example 2.2 is not convex.

The importance of convexity for weak/weak* lower semicontinuity for integral functionals has been discovered by Tonelli in 1920 [102], who pioneered the study of lower semicontinuity of an integral functional rather than studying the associated Euler-Lagrange equation. *Connections of convexity notions and weak lower semicontinuity are a central theme of this thesis.* The first chapter is devoted to *relaxation* of variational problems which consists in finding the largest lower semicontinuous envelope of a given functional. These problems naturally appear in continuum physics of solids. The first paper is [67]. It deals with a model of shape memory single crystals describing their rate-independent evolution. The weak lower semicontinuity is a key ingredient of the theory. The second part of Chapter 1 is devoted to mathematical modeling of ferromagnetic materials. It includes a review paper [69] which partly maps my research in mathematical aspects of ferromagnetism and the paper [68] which proposes and analyses an algorithm for solving a static relaxed problem. Here again convexity plays a crucial role. Specifically, the first chapter includes the following papers (here we refer to items in the structured bibliography where one also finds list of papers citing each particular article):

- [C1]20 KRUŽÍK, M., MIELKE A., ROUBÍČEK, T.: Modeling of microstructure and its evolution in shape memory-alloy single-crystals, in particular in CuAlNi. *Meccanica* 40 (2005), 389-418.
- [C1]10 KRUŽÍK, M., PROHL, A.: Young measure approximation in micromagnetics. Num. Math. 90 (2001), 291–307.
- [C1]22 KRUŽÍK, M., PROHL, A.: Recent developments in modeling, analysis, and numerics of ferromagnetism. SIAM Rev. 48 (2006), 439–483.

The second chapter of the thesis studies various convexity conditions and their relation to weak lower semicontinuity of integral functionals with integrands whose negative part has the same growth as the positive one. Then, besides oscillations, also concentrations of sequences along which we study weak lower semicontinuity play an important role. The chapter consists of the following articles:

- [C1]6 KRUŽÍK, M.: On the composition of quasiconvex functions and the transposition, J. Convex Anal. 6 (1999), 207–213.
- [C1]27 KALAMAJSKA, A., KRUŽÍK, M.: Oscillations and concentrations in sequences of gradients. *ESAIM Control Optim. Calc. Var.* 14 (2008), 71-104.
- [C1]33 FONSECA, I., KRUŽÍK, M.: Oscillations and concentrations generated by A-free mappings and weak lower semicontinuity of integral functionals. ESAIM Control Optim. Calc. Var. 16 (2010), 472–502.
- [C1]44 KRUŽÍK, M.: Quasiconvexity at the boundary and concentration effects generated by gradient. *ESAIM Control Optim. Calc. Var.* **19** (2013), 679–700.

These papers reviews my work on generalized Young measures, called here DiPerna-Majda measures, which are able to detect and record not only oscillations but also concentrations. Analysis of oscillations and concentrations generated by sequences of gradients Sobolev mappings allows us to discover interesting connections between weak lower semicontinuity of certain integral functionals and concentrations of the sequence on the closure of the domain. In what follows we discuss the content of both chapters in more detail. Main mathematical features discussed in both chapters can be also found in [13] which is a new review article accepted for publication in SIAM Review.

3 Overview of Chapter 1

The aim of [67] is to propose a computational method for solving non(quasi)convex vectorial and multidimensional variational problems and to prove convergence of discrete solutions to a solution of the original problem.

Modeling of multi-scale physical phenomena in mechanics and electromagnetics is an active area with ambitious applications in high technology industry like the development of "smart materials" or new recording media. Physical phenomena appearing on larger scales are usually different from those on microscales which makes their mathematical description a challenging task. Many effects are accompanied by creation of microstructures which crucially influence physical properties of the material and are often created to follow some extremum principle as the minimal energy principle, for instance. The mathematical analysis of microstructures usually neglects the atomic scale and considers already a continuum model. One of possible approaches to their modeling are variational models which deal with systems spontaneously creating microstructures supposing that the microstructure satisfies some optimality criteria. The reason for formation of fine structures is usually the nonexistence of an exact optimum. Mathematical modeling must typically cope with nonconvexity and nonexistence of solutions in Sobolev (Lebesgue) spaces, which has its drawback in numerical schemes. Mathematically, the formation of microstructures is demonstrated by finer and finer spatial oscillations of minimizing sequences. Those oscillations can only be limited by effects on the atomic scale like, for example, surface energies but these issues are mostly neglected. An important problem is to extract relevant information from minimizing sequences. This is, roughly speaking, the idea of *relaxation*; see e.g. Dacorogna [23] or Müller [83]. The basic approach is to find some effective macroscopic energy density of the system as, e.g., an effective stored energy density of an elastic material or an effective anisotropy energy density of a ferromagnet which governs behavior of the system. In problems, which we have in mind, the effective energy enjoys suitable convexity properties which damp out oscillations. In applications to elasticity theory, oscillations appear in the gradient and the appropriate convexity property is *quasiconvexity* introduced by Morrey [81] in 1952. We recall that $W : \mathbb{R}^{m \times n} \to \mathbb{R}$ is quasiconvex if for all $\psi \in W_0^{1,\infty}(\Omega; \mathbb{R}^m)$ and all $F \in \mathbb{R}^{m \times n}$ it holds that

$$W(F)|\Omega| \le \int_{\Omega} W(F + \nabla \psi(x)) \,\mathrm{d}x \;. \tag{3.1}$$

Here $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain with the *n*-dimensional Lebesgue measure $|\Omega|$. The effective energy density is (under some technical assumptions) the quasiconvex envelope (i.e. the largest quasiconvex function below the density) of the elastic energy density. This is a common situation in a description of elastic crystals undergoing martensitic phase transitions with negligible hysteresis effects. A similar situation occurs in micromagnetics, however, in this case the quasiconvex envelope reduces to the usual convex one. One possible way how to evaluate these envelopes is to use parametrized measures, the so-caled Young measures [108]. If we include hysteretic behavior in models then typically the evolution of Young measures contributes to dissipation of materials.

3.1 Young measures

It is well known [6] that if $\{z_k\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{m\times n})$, $1 \leq p < +\infty$, is bounded then there exists a subsequence (not relabeled) and a family $\nu = \{\nu_x\}_{x\in\Omega}$ of probability measures on Ω such that for all $g \in L^{\infty}(\Omega)$ and all $f \in C(\mathbb{R}^{m\times n})$ such that $\{f(z_k)\}_{k\in\mathbb{N}}$ is uniformly integrable in $L^1(\Omega)$ it holds that

$$\lim_{k \to \infty} \int_{\Omega} f(z_k(x))g(x)) \, \mathrm{d}x = \int_{\Omega} \int_{\mathbb{R}^{m \times n}} f(s)\nu_x(\mathrm{d}s)g(x) \, \mathrm{d}x \,. \tag{3.2}$$

Conversely, if $\nu = \{\nu_x\}_{x\in\Omega}$ is such that ν_x is for almost all $x \in \Omega$ a probability measure on $\mathbb{R}^{m\times n}$, $x \mapsto \int_{\mathbb{R}^{m\times n}} f(s)\nu_x(\mathrm{d}s)$ is measurable for all $f \in C_0(\mathbb{R}^{m\times n})$, and $\int_{\Omega} \int_{\mathbb{R}^{m\times n}} |s|^p \nu_x(\mathrm{d}s) \mathrm{d}x < +\infty$ then there exists a sequence $\{z_k\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{m\times n})$ such that (3.2) holds. The family $\nu = \{\nu_x\}$ is called Young measure and $\{z_k\}$ its generating sequence. It is well-known that every Young measure ν as above can be generated by a sequence $\{z_k\}$ such that $\{f(z_k)\}$ is uniformly integrable for every continuous $f \in C_p(\mathbb{R}^{m\times n}) := \{f \in C(\mathbb{R}^{m\times n}); |f| \leq C(1+|\cdot|^p), C > 0\}.$

ated by a sequence $\{z_k\}$ such that $\{J(z_k)\}$ is uniformly integrable for every continuous $f \in C_p(\mathbb{R}^{m \times n}) := \{f \in C(\mathbb{R}^{m \times n}); |f| \leq C(1 + |\cdot|^p), C > 0\}.$ We will be interested in Young measures generated by gradients, i.e. $z_k := \nabla u_k$ for some sequence $\{u_k\} \subset W^{1,p}(\Omega; \mathbb{R}^m)$. Such a Young measure will be refered to as gradient Young measure. Fixing $1 \leq p < +\infty$, we denote the set of gradient Young measures generated by $\{\nabla u_k\}$ for $\{u_k\} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ by $\mathcal{G}^p(\Omega; \mathbb{R}^{m \times n})$. Thus, if $\{u_k\} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ is bounded and $\{W(\nabla u_k)\}$ equiintegrable, we have (up to a subsequence) that

$$\lim_{k \to \infty} V(u_k) = \int_{\Omega} \int_{\mathbb{R}^{m \times n}} W(s) \nu_x(\mathrm{d}s) \,\mathrm{d}x \;,$$

where $V(u) = \int_{\Omega} W(\nabla u(x)) dx$. Let us mention that if W is coercive with superlinear growth at infinity and $\{u_k\}$ is minimizing for V then the equiintegrability condition holds. The following well-known result of Kinderlehrer and Pedregal [85] characterizes the set of gradient Young measures.

Lemma 3.1 Let $1 . A Young measure <math>\nu = {\{\nu_x\}_{x \in \Omega}}$ belongs to $\mathcal{G}^p(\Omega; \mathbb{R}^{m \times n})$ if and only if the following three conditions are satisfied simultaneously: (i) there is $y \in W^{1,p}(\Omega; \mathbb{R}^n)$ such that for a.a. $x \in \Omega$

$$\nabla y(x) = \int_{\mathbb{R}^{m \times n}} F \nu_x(\mathrm{d}F) , \qquad (3.3)$$

(ii) for this y and all quasiconvex functions $v : \mathbb{R}^{m \times n} \to \mathbb{R}$, $|v| \leq C(1 + |\cdot|^p)$, it holds that for a.a. $x \in \Omega$

$$v(\nabla y(x)) \le \int_{\mathbb{R}^{m \times n}} v(F)\nu_x(\mathrm{d}F) , \qquad (3.4)$$

(iii) it holds that

$$\int_{\Omega} \int_{\mathbb{R}^{m \times n}} |F|^p \nu_x(\mathrm{d}F) \,\mathrm{d}x < +\infty \ . \tag{3.5}$$

Extending the validity of (ii) to all rank-one convex functions with *p*-growth at infinity defines a subset of $\mathcal{G}^p(\Omega; \mathbb{R}^{m \times n})$ called laminates [85].

An example of a Young measure $\nu \in \mathcal{G}^p(\Omega; \mathbb{R}^{3\times 3})$ describing a so-called 1st-order *laminate* with an underlying macroscopic deformation $y \in W^{1,p}(\Omega; \mathbb{R}^3)$ is

$$\nu = \{\nu_x\}_{x \in \Omega}, \qquad \nu_x = \xi_0(x)\delta_{F_1(x)} + (1 - \xi_0(x))\delta_{F_2(x)}, \qquad (3.6a)$$

$$\left[\xi_0 F_1 + (1 - \xi_0) F_2\right](x) = \nabla y(x), \quad F_1(x) - F_2(x) = a_0(x) \otimes n_0(x), \quad (3.6b)$$

$$0 \le \xi_0(x) \le 1,$$
 $a_0(x), n_0(x) \in \mathbb{R}^3.$ (3.6c)

This process can be re-iterated: a 2nd-order laminate with the macroscopic deformation y as above is $\nu = {\nu_x}_{x\in\Omega}$, where

$$\nu_{x} = \xi_{0}(x)\xi_{1}(x)\delta_{F_{1}(x)} + \xi_{0}(x)(1-\xi_{1}(x))\delta_{F_{2}(x)} + (1-\xi_{0}(x))\xi_{2}(x)\delta_{F_{3}(x)} + (1-\xi_{0}(x))(1-\xi_{2}(x))\delta_{F_{3}(x)} , \qquad (3.7)$$

with (dropping for simplicity a dependence on x)

$$F_1 - F_2 = a_1 \otimes n_1, \qquad F_3 - F_4 = a_2 \otimes n_2 , \qquad (3.8a)$$

$$\xi_1 F_1 + (1 - \xi_1) F_2 - \xi_2 F_3 - (1 - \xi_2) F_4 = a_0 \otimes n_0 , \qquad (3.8b)$$

$$\nabla y = \xi_0 \xi_1 F_1 + \xi_0 (1 - \xi_1) F_2 + (1 - \xi_0) \xi_2 F_3 + (1 - \xi_0) (1 - \xi_2) F_4$$
(3.8c)

and $0 \leq \xi_i \leq 1$, $a_i, n_i \in \mathbb{R}^3$, $i \in \{0, 1, 2\}$. Analogously, we can get laminates of an arbitrary order which are often called sequential laminates.

Young measures are an important tool in the mathematical treatment of various nonconvex variational problems. A prominent example is the relaxation of energy functionals in the modeling of shape memory materials.

3.2 Shape memory alloys

Shape-memory alloys (SMAs) are active materials, and have been the subject of intensive theoretical and experimental research during the past decades. Existing or potential applications can be found, for example, in medicine and mechanical or aerospace engineering. Shape-memory alloys are crystalline materials that exhibit specific hysteretic stress / strain / temperature response; they have the ability to recover a trained shape after deformation and subsequent reheating. This is called the shape-memory effect. It is based on the ability of the alloy to rearrange atoms in different crystallographic configurations (in particular, with different symmetry groups). The stability depends on the temperature. Normally, at higher temperatures a high-symmetry (for example, cubic) lattice is stable, which is referred to as the austenite phase. At lower temperatures, a lattice of lower symmetry (for example, tetragonal, orthorhombic, monoclinic, or triclinic) becomes stable, called the martensite phase. Due to the loss of symmetry, this phase may occur in different variants. The number of variants M, is the quotient of the order of the high-symmetry phase and the order of the low-symmetry group. So for a cubic high-symmetry phase, M = 3, 6, 12, or 4 for the tetragonal, orthorhombic, monoclinic, respectively triclinic martensites mentioned above. The variants can be combined coherently with each other, forming so-called twins of two variants.

The mathematical and computational modeling of SMAs represents a tool for the theoretical understanding of phase transition processes in solids. Such an analysis may complement experimental results, predict the response of new materials, or facilitate the usage of SMAs in applications. SMAs are genuine multi-scale materials and create a variety of challenges for mathematical modeling. We refer the reader to [92] for a survey of a wide menagerie of SMA models ranging from nano- to macro-scales. In this article, we focus on a mesoscopic model in the framework of continuum mechanics. Beside the macroscopic deformation and its gradient, the model also involves the volume fractions of phases and variants and gradients of volume fraction. This seems a reasonable compromise, since it allows for the modeling scales of large single crystals or polycrystals.

Although the natural physical dimension is three we will assume that our specimen occupies a bounded domain $\Omega \subset \mathbb{R}^n$ and the deformation y maps Ω to \mathbb{R}^m . This allows us to consider various variational problems. Nevertheless for shape memory applications we obviously assume that m = n = 3. The stress-free parent austenite is a natural state of the material which makes it, in the context of continuum mechanics, a canonical choice for the reference configuration. As usual, $y: \Omega \to \mathbb{R}^m$ denotes the deformation and $u: \Omega \to \mathbb{R}^m$ the displacement, which are related to each other via the identity y(x) = x + u(x), where $x \in \Omega$. Hence the deformation gradient is $F := \nabla y = I + \nabla u$. Unfortunately, not every $\nu \in \mathcal{G}^p(\Omega; \mathbb{R}^{3\times 3})$ is of the form of a sequential laminate, or even

Unfortunately, not every $\nu \in \mathcal{G}^p(\Omega; \mathbb{R}^{3\times 3})$ is of the form of a sequential laminate, or even cannot be attained by sequential laminates, which can be interpreted that microstructures might be much more chaotic; This might be connected with the Šverák's famous counterexample [99] that rank-one convexity does not imply quasiconvexity. Moreover, an efficient description of $\mathcal{G}^p(\Omega; \mathbb{R}^{3\times 3})$ is not available, which is related to the lack of a local characterization of quasiconvex functions; cf. [58].

Starting from 1D-numerical experiments by Nicolaides and Walkington [84], there are numerical studies involving gradient Young measures as e.g. [66] but, due to the mentioned impossibility of an efficient description of the whole set $\mathcal{G}^p(\Omega; \mathbb{R}^{3\times 3})$, they eventually have to deal with laminates of an order $\kappa \geq 1$, let us denote this set as

$$\mathcal{G}_{\text{lam}}^{p,\kappa}(\Omega;\mathbb{R}^{3\times3}) := \big\{\nu \in \mathcal{G}^p(\Omega;\mathbb{R}^{3\times3}); \quad \nu_x \text{ is a } \kappa \text{-order laminate for a.a. } x \in \Omega \big\}.$$
(3.9)

Nevertheless, laminates enable us to describe volume fractions of particular phases/variants at a given material point. The idea of looking at volume fractions (sometimes in simplified situations leading to a transformation strain as an independent variable) occurred in various other models, too, see Frémond [35, 36], often meant for polycrystals so that the fine (and in context of single-crystals very important) issues related with rank-one connections are often not accounted for.

3.3 Stored energy and its minimization

The specific energy stored in the inter-atomic links in the continuum $\hat{W} = \hat{W}(F)$ is phenomenologically described as a function of the deformation gradient F; recall that we consider temperature constant. The *frame-indifference*, i.e. $\hat{W}(F) = \hat{W}(RF)$ for any $R \in SO(3)$, the group of orientation-preserving rotations, requires that \hat{W} in fact depends only on the (right) *Cauchy-Green stretch* tensor $C := F^{\top}F$. As $F = \mathbb{I} + \nabla u$, we can express the specific stored energy in terms of the displacement gradient as

$$W = W(\nabla u) = \hat{W}(\mathbb{I} + \nabla u).$$
(3.10)

The absence of an explicit dependence on x is related to homogenous single crystals considered. The *Piola-Kirchhoff stress* $\sigma : \mathbb{R}^{3\times 3} \to \mathbb{R}^{3\times 3}$ is given by $\sigma = W'(\nabla u)$ with W' denoting the tensor-valued gradient.

We will use a *St. Venant-Kirchhoff*-like form of the stored energy of each particular phase variants which allows for an explicit reference to measured data and can easily be applied to various materials. We consider M variants of martensite determined, in the stress-free state, by *distortion matrices* U_{ℓ} , $\ell = 1, ..., M$, while the cubic austenite corresponds to $U_0 = \mathbb{I}$. The frame-indifferent stored energy of particular phases or phase variants is considered

The frame-indifferent stored energy of particular phases or phase variants is considered as a function of the *Green strain* tensor ε^{ℓ} related to the distortion of this phase (variant). In the simplest case (cf. [86, Sect.6.6], e.g.), one can consider a function quadratic in terms of ε^{ℓ} of the form

$$\hat{W}_{\ell}(F) = \frac{1}{2} \sum_{i,j,k,l=1}^{d} \varepsilon_{ij}^{\ell} \mathcal{C}_{ijkl}^{\ell} \varepsilon_{kl}^{\ell} + d_{\ell}, \qquad \varepsilon^{\ell} = \frac{R_{\ell}^{\top} (U_{\ell}^{\top})^{-1} F^{\top} F U_{\ell}^{-1} R_{\ell} - \mathbb{I}}{2}, \quad (3.11)$$

where $C^{\ell} = \{C_{ijkl}^{\ell}\}$ is the 4th-order tensor of elastic moduli satisfying the usual symmetry relations depending also on symmetry of the specific phase (variant) ℓ , d_{ℓ} is some offset; d_{ℓ} depends on temperature which is, however, considered as fixed – this dependence differs in various phases due to various heat capacities, which is just what makes the shape-memory effect.

The simplest way to assembly the overall *multi-well* stored energy \hat{W} relying on that materials naturally tend to minimize stored energy is to put

$$\hat{W} := \min_{\ell=0,\dots,M} \hat{W}_{\ell} .$$
(3.12)

The total stored energy in the bulk occupying, in its reference configuration, the domain Ω is then

$$V(u) := \int_{\Omega} W(\nabla u) \, \mathrm{d}x. \tag{3.13}$$

Basic variational principle is minimization of the stored energy. Due to the multi-well character W and here also due to the chosen St.Venant-Kirchhoff form of W, minimizing sequences of V tend to develop, in general, faster and faster spatial oscillations of their gradients, which is related to development of the finer and finer microstructures when the stored energy is to be minimized. The minimum of V, under specific boundary conditions for u, say

$$u|_{\Gamma_{\mathrm{D}}} = u_{\mathrm{D}} \tag{3.14}$$

where $\Gamma_{\rm D}$ is a part of the (Lipschitz) boundary $\partial\Omega$ of Ω , need not ever be attained on the space $W^{1,p}(\Omega; \mathbb{R}^3)$, however. This effect is due to neglecting the (usually small) energy stored in the interfaces like the twinning plane which is certainly relevant approach on meso- and macroscopic level. However, the minimum is attained, under suitable coercivity conditions, on Young measures. For this, we need to extend V by continuity for such measures. Considering now the configuration as the couple $(u, \nu) \in W^{1,p}(\Omega; \mathbb{R}^3) \times \mathcal{G}^p(\Omega; \mathbb{R}^{3\times 3})$, the extended functional is

$$\bar{V}(u,\nu) := \int_{\Omega} \int_{\mathbb{R}^{3\times3}} W(A)\,\nu_x(\,\mathrm{d}A)\,\mathrm{d}x = \int_{\Omega} \int_{\mathbb{R}^{3\times3}} \hat{W}(\mathbb{I}+A)\,\nu_x(\,\mathrm{d}A)\,\mathrm{d}x.$$
(3.15)

The set of admissible configurations is now

$$\left\{ (u,\nu) \in W^{1,p}(\Omega;\mathbb{R}^3) \times \mathcal{G}^p(\Omega;\mathbb{R}^{3\times3}); (3.14) \text{ holds and} \right. \\ \left. \int_{\mathbb{R}^{3\times3}} A \nu_x(\,\mathrm{d}A) = \nabla u \text{ for a.a. } x \in \Omega \right\},$$
(3.16)

and the minimum of \overline{V} on this set is the infimum of V on $W^{1,p}(\Omega; \mathbb{R}^3)$ under (3.14). The process of extension V to \overline{V} is called *relaxation*, cf. [85].

3.4 Dissipation energy and its maximization

Phase transformation (PT) in SMAs is, to a large extent, a *rate-independent, activated process* and leads to a specific dissipation which results in a hysteretic response in stress/strain diagrams. Its modelling is equally important as the stored energy but the related phenomenology is still less understood than the stored-energy one; indeed, as pointed out by Bhattacharya et al. [17], 'much remains unknown concerning the nucleation and evolution of microstructure, and the resultant hysteresis'. Let us recall that the orbits $SO(3)U_{\ell}$ and $SO(3)U_{\ell}$ are *rank-1 connected* if

$$\exists R \in \mathrm{SO}(3): \quad \mathrm{Rank}(U_{\ell} - RU_{l}) = 1.$$
(3.17)

There seems to be two main approaches to the dissipation problem:

- (A) the hysteresis (and the related rate-independent dissipation) is determined by the stored-energy landscape, advocated essentially by Abeyaratne, Knowles [2], Ball et al. [7, 8], Goldstein [38], James and Zhang [47], Šilhavý [96], etc. The common philosophy is that, if the orbits $SO(3)U_{\ell}$ and $SO(3)U_{l}$ are rank-1 connected, then the dissipation within PT between these (phase) variants is small, or rather zero, otherwise it is related with metastability and a stress which the material must inevitably withstand to move out of the bottoms of the wells during the PT.
- (B) The hysteresis is quite independent of the stored energy and needs a separate phenomenology (recording, e.g, various impurities and dislocations in the atomic grid that lead to bigger dissipation), advocated essentially (besides authors' own previous works) by Frémond [35] or Hackl et al. [41] and many others.

It is likely that both these approaches combine mutually. Besides, for completeness let us mention that there are attempts to apply a phenomenology like (B) but through a modification of the stored energy which then causes a hysteresis like in the case (A), see Abeyaratne, Chu, James [1].

We adopt a (to some extent quite simplified) standpoint that the amount of dissipated energy within the particular PT between austenite and a martensitic variant or between two martensitic variants can be described by a specific energy (of the dimension $J/m^3=Pa$). For this, we need to identify the particular phases or phase variants and thus we define a continuous mapping $\mathcal{L} : \mathbb{R}^{3\times 3} \to \Delta$ where

$$\Delta := \left\{ \zeta \in \mathbb{R}^{1+M} \; ; \; \zeta_{\ell} \ge 0, \; \ell = 0, ..., M, \; \sum_{\ell=0}^{M} \zeta_{\ell} = 1 \right\}$$
(3.18)

is a simplex with M+1 vertexes, M = the number of martensitic variants as in Section 3.3. As in (3.10), we assume

$$\mathcal{L}(\nabla u) = \hat{\mathcal{L}}(\mathbb{I} + \nabla u) \quad \text{with} \quad \hat{\mathcal{L}} : \mathbb{R}^{3 \times 3} \to \Delta.$$
(3.19)

Here $\hat{\mathcal{L}}$ is related with the material itself and thus is to be frame indifferent. We assume, beside $\hat{\mathcal{L}}_{\ell} \geq 0$ and $\sum_{\ell=0}^{M} \hat{\mathcal{L}}_{\ell} = 1$, that $\hat{\mathcal{L}}_{\ell}(F) = 1$ if F is in the ℓ -th (phase) variant, i.e. Fis in a vicinity of ℓ -th well SO(3) U_{ℓ} of W, which can be identified according to the stretch tensor $F^{\top}F$ close to $U_{\ell}^{\top}U_{\ell}$, cf. [77, 78]. If $\hat{\mathcal{L}}(F)$ is not in any vertex of Δ , then it means that F in the spinodal region where no definite (phase) variant is specified; we assume, however, that the wells are sufficiently deep and the (phase) variants geometrically sufficiently far from each other that the tendency for minimization of the stored energy will essentially prevent Fto range the spinodal region and thus the concrete form of $\hat{\mathcal{L}}$ does not seem to be important as long as $\hat{\mathcal{L}}$ enjoys the above properties. Hence \mathcal{L} plays the role of what is often called a vector of order parameters or a vector-valued internal variable.

The dissipation-energy phenomenology itself is considered through the choice of a "norm" on \mathbb{R}^{1+M} (not necessarily Euclidean and even not symmetric), let us denote it by $|\cdot|_M$; its physical dimension will be J/m^3 =Pa. The desired meaning is to set up the specific energy $\mathcal{E}_{\ell l}$ needed for PT of a phase (variant) ℓ to l as $|e_{\ell} - e_l|_M$, where $e_{\ell} = (0, ..., 0, 1, 0, ...0) \in$ \mathbb{R}^{1+M} is the unit vector with 1 at the position ℓ . The set $\{\mathcal{E}_{\ell l}\}_{\ell,l=0,...,M}$ can reflect both the presence/lack of rank-one connections (A) and the influence of various impurities (B).

Referring to a mesoscopic description through a Young measure $\nu \in \mathcal{G}^p(\Omega; \mathbb{R}^{3\times 3})$, the *meso-scopic volume fractions* $\lambda = \lambda(x)$ at a current "macroscopic" point x is then

$$\lambda(x) := \int_{\mathbb{R}^{3\times 3}} \mathcal{L}(A)\nu_x(\,\mathrm{d}A) = \int_{\mathbb{R}^{3\times 3}} \hat{\mathcal{L}}(\mathbb{I}+A)\nu_x(\,\mathrm{d}A). \tag{3.20}$$

As a mesoscopic configuration, we will consider a triple $q = (u, \nu, \lambda)$, i.e. the macroscopic displacement, the Young measure describing the microstructure, and the volume fraction field; of course, they are linked with each other by (3.20) and also by the constraint in (3.16). In terms of $\frac{d}{dt}q$, the (pseudo) potential of dissipative forces R that corresponds to this phenomenology is

$$R\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right) = R\left(\frac{\mathrm{d}u}{\mathrm{d}t}, \frac{\mathrm{d}\nu}{\mathrm{d}t}, \frac{\mathrm{d}\lambda}{\mathrm{d}t}\right) := \int_{\Omega} \left|\frac{\partial\lambda(t, x)}{\partial t}\right|_{M} \mathrm{d}x.$$
(3.21)

This means, considering a process over the time interval $[t_1, t_2]$, the overall dissipated energy by all undergone PTs in the whole specimen Ω will be

$$\int_{t_1}^{t_2} \int_{\Omega} \left| \frac{\partial \lambda}{\partial t} \right|_M \, \mathrm{d}x \, \mathrm{d}t = \int_{\Omega} \quad \underset{t \in [t_1, t_2]}{\operatorname{Var}} \lambda(t, x) \, \mathrm{d}x \tag{3.22}$$

where the total variation "Var" with respect to the (possibly nonsymmetric) norm $|\cdot|_M$ counts which PTs (and how many times) have been undergone at the point x. The important property of R is that it satisfies the triangle inequality, i.e.

$$\forall q_1, q_2, q_3 \in Q: \qquad R(q_1 - q_3) \le R(q_1 - q_2) + R(q_2 - q_3), \tag{3.23}$$

which follows immediately from convexity and the degree-1 homogeneity.

The dissipation mechanism through the convex, degree-1 homogeneous potential R is intimately related with Hill's maximum-dissipation principle [42]. The desired energy balance, i.e. the rate of Helmholtz' stored energy \bar{V} plus the dissipation rate equal to the power of the external force, is

$$\frac{\mathrm{d}V}{\mathrm{d}t} + R\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right) = \left\langle f, \frac{\mathrm{d}u}{\mathrm{d}t} \right\rangle \tag{3.24}$$

where the degree-1 homogeneous dissipation rate R can be written in the form

$$R\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right) = \int_{\Omega} \omega(t,x) \cdot \frac{\partial \lambda(t,x)}{\partial t} \,\mathrm{d}x \quad \text{with} \quad \omega(t,x) \in \left[\partial |\cdot|_{M}\right] \left(\frac{\partial \lambda(t,x)}{\partial t}\right) \tag{3.25}$$

with $\partial |\cdot|_M$ denoting the subdifferential of $|\cdot|_M$. The last inclusion can be written as

$$\left\langle \frac{\partial \lambda(t,x)}{\partial t}, \omega(t,x) \right\rangle = \max_{z \in \mathbb{Z}} \left\langle \frac{\partial \lambda(t,x)}{\partial t}, z \right\rangle \quad \text{with} \quad \mathbb{Z} := \left[\partial |\cdot|_M \right](0).$$
(3.26)

This says that, for the considered volume-fraction rate $\frac{\partial}{\partial t}\lambda$, the driving stress (or specific activation energies) ω in Pa (=J/m³) makes the dissipation caused by the PTs maximal among all other admissible driving stresses, i.e. those from the convex set $Z \subset \mathbb{R}^{1+M}$. In plasticity theory, this maximum-dissipation principle can alternatively be expressed as a normality in the sense that the rate of plastic deformation belongs to the cone of outward normals to the elasticity domain. Here, this would result in the observation that the rate $\frac{\partial}{\partial t}\lambda(t,x)$ of PTs at (t,x) belongs to the normal cone of the "elasticity domain" Z at the point $\omega(t,x)$. In particular, (3.26) says that $\frac{\partial}{\partial t}\lambda = 0$ (i.e. the volume fractions do not evolve) if $\omega(t,x)$ is inside Z (i.e. there in not enough stress to activate PTs at (t,x)). Also recall that ∂R is maximal responsive. For a discussion in a 1D-case see also [74, Remark 4.5]. However, we saw that (3.26) contains, in fact, only a rather small portion of information about the evolution and other principles can be considered at this context, too.

3.5 Energetic solution and its discretization

We want to present briefly the model of evolution of microstructure described "mesoscopically" and governed by the principles from Sections 3.3–3.4, as well as its mathematical analysis. It exploits the definition of the so-called energetic solution invented in [77] (see also the book [75]). We consider here a "soft-device" loading through time-varying Neumann's boundary conditions.

We denote the set Q^0 of the admissible configurations q's, i.e.

$$Q^{0} = \left\{ \begin{array}{ll} (u, \nu, \lambda) \in Q ; & \lambda = \mathcal{L} \bullet \nu \text{ a.e.} \right\}, \quad \text{where} \quad (3.27)$$
$$Q := \left\{ q = (u, \nu, \lambda) \in W^{1, p}(\Omega; \mathbb{R}^{3}) \times \mathcal{G}^{p}(\Omega; \mathbb{R}^{3 \times 3}) \times L^{1}(\Omega; \mathbb{R}^{1+M}) ; \\ \nabla u(x) = \int_{\mathbb{R}^{3 \times 3}} \mathcal{A} \nu_{x}(\mathrm{d}A), \quad \lambda(x) \in \Delta \text{ a.e. on } \Omega, \quad u|_{\Gamma_{\mathrm{D}}} = u_{\mathrm{D}} \right\},$$

where we abbreviated

$$\lambda = \mathcal{L} \bullet \nu \quad \text{where} \quad \left[\mathcal{L} \bullet \nu\right](x) := \int_{\mathbb{R}^{3\times 3}} \mathcal{L}(A) \,\nu_x(\,\mathrm{d}A). \tag{3.28}$$

We distinguished, just for numerical purposes later, Q, which "forgets" the constraint $\lambda = \mathcal{L} \bullet \nu$, from Q_0 .

The Gibbs' stored energy which also counts for the time-dependent boundary conditions and which is regularized by $\rho > 0$ is

$$G(t,q) := G(t,u,\nu,\lambda) = \bar{V}(u,\nu) + \int_{\Gamma_{\rm N}} f(t,x) \cdot u(x) \,\mathrm{d}x + \rho |\lambda|_{\alpha,r}^r \text{ on } Q, \qquad (3.29)$$

$$G^{0}(t,q) := \begin{cases} G(t,q) & \text{on } Q^{0}, \\ +\infty & \text{on } Q \backslash Q^{0}, \end{cases}$$
(3.30)

with \overline{V} from (3.15), $f:[0,T] \times \Gamma_{\mathrm{N}} \to \mathbb{R}^3$ a prescribed "soft-device" loading, $\Gamma_{\mathrm{N}} \subset \partial\Omega$, T > 0 a fixed time horizon, and with the semi-norm in the Sobolev-Slobodetskiĭ space $W^{\alpha,r}(\Omega;\mathbb{R}^{1+M})$ considered as

$$\left|\lambda\right|_{\alpha,r} := \left(\frac{1}{4} \int_{\Omega} \int_{\Omega} \frac{\left|\lambda(x) - \lambda(\tilde{x})\right|^{r}}{|x - \tilde{x}|^{3 + r\alpha}} \, \mathrm{d}\tilde{x} \, \mathrm{d}x\right)^{1/r},\tag{3.31}$$

for a fixed parameter $0 < \alpha < 1$. Such a regularizing term in (3.29) gives some (possibly very small) energy to spatial variation of mesoscopic volume fractions and is exploited for a rigorous proof of existence of energetic solutions as well as convergence of numerical approximations. Gradients of mesoscopic volume fractions have already been used in Frémond's model [35, p.364]. Our form (3.31) corresponds to the only " α -fractional gradient" which is compactifying, namely the embedding $W^{\alpha,r}(\Omega; \mathbb{R}^{1+M}) \subset L^1(\Omega; \mathbb{R}^{1+M})$ is compact. Also it allows for an element-wise affine approximation of λ , because $W^{\alpha,r}(\Omega; \mathbb{R}^{1+M}) \supset W^{1,\infty}(\Omega; \mathbb{R}^{1+M})$ or, if $\alpha < 1 - 3(r-1)/r$ with some 1 < r < 3/2, for an element-wise constant approximation which has necessarily discontinuities on 2-dimensional manifolds requiring then $W^{\alpha,r}(\Omega; \mathbb{R}^{1+M}) \supset W^{1,1}(\Omega; \mathbb{R}^{1+M})$; later in (3.36) we choose the latter option. In [74] such a regularization was interpreted as a limit from the Ericksen-Timoshenko model scrutinized by Ren, Rogers, and Truskinovsky [89] who also proposed a nonlocal term like (3.31) in the 1D case with either positive or also, for different purposes, non-positive kernels. One can interprete the energy (3.31) as associated to a sort of non-local microstress measuring nonlocal interactions related to spatial microstructural variations.

Definition 3.2 The process $q : [0,T] \mapsto Q^0$ will be called an *energetic solution* to the problem given by the triple (G^0, R, q_0) , i.e. by the data $(W, \mathcal{L}, |\cdot|_M, f, u_D, q_0, \rho)$, if it satisfies the initial condition $q(0) = q_0$, the static *stability condition*:

$$\forall t \in [0,T] \quad \forall \tilde{q} \in Q^0: \qquad G^0(t,q(t)) \le G^0(t,\tilde{q}) + R(\tilde{q}-q(t)), \tag{3.32}$$

and the *energy equality*

$$\forall s, t \in [0, T]: \quad G^0(t, q(t)) + \operatorname{Var}_R(q; s, t) = G^0(s, q(s)) + \int_s^t \frac{\partial G^0}{\partial \vartheta}(\vartheta, q(\vartheta)) \, \mathrm{d}\vartheta. \quad (3.33)$$

Here $\operatorname{Var}_R(q; s, t)$ is the total variation of the process $q = (u, \nu, \lambda) : [0, T] \to Q$ over the time interval [s, t] with respect to the norm $|\cdot|_M$, namely

$$\operatorname{Var}_{R}(q;s,t) := \sup \sum_{i=1}^{k} R(q(t_{i}) - q(t_{i-1})) = \sup \sum_{i=1}^{k} \int_{\Omega} |\lambda(t_{i},x) - \lambda(t_{i-1},x)|_{M} \, \mathrm{d}x \quad (3.34)$$

where the supremum is taken over all partition $s = t_0 < t_1 < ... < t_k = t, k \in \mathbb{N}$. The definition of stability (3.32) and energy balance (3.33) could also be defined on all of Q, since G^0 equals $+\infty$ on $Q \setminus Q^0$. It will be useful to define the *stability set* $\mathcal{S}^0(t)$ by

$$\mathcal{S}^{0}(t) := \left\{ q \in Q \; ; \; G^{0}(t,q) < +\infty, \; \forall \tilde{q} \in Q : \; G^{0}(t,q) \le G^{0}(t,\tilde{q}) + R(\tilde{q}-q) \right\}.$$
(3.35)

Let us note that the stability (3.32) just means that $q(t) \in S^0(t)$ for all $t \in [0, T]$. Under some qualification of the data $(W, \mathcal{L}, |\cdot|_M, f, u_D, q_0, \rho)$, the existence of some energetic solution can be proved by a constructive way by approximation of the implicit Euler formula and the spacial finite-element-like discretization combined with laminated Young measures (3.9) and a penalization of the equality (3.20), which also suggest a numerical strategy. As already emphasized, the set $\mathcal{G}^p(\Omega; \mathbb{R}^{3\times3})$ cannot be explicitly implemented so we employ the smaller set $\mathcal{G}_{\text{lam}}^{p,k}(\Omega; \mathbb{R}^{3\times3})$ from (3.9), which, however, brings a necessity to treat the relation $\lambda = \mathcal{L} \bullet \nu$ with a "tolerance", because, due to the compactness in λ 's caused by the regularizing nonlocal ρ -term in (3.29), it behaves like a constraint which, if treated without any tolerance, might destroy the convergence.

To construct approximate solutions, we consider time steps $\tau > 0$, assuming that T/τ is integer and that $\tau \to 0$. Beside of this time discretization we will employ the finite-element method as space discretization. We assume that Ω is a polyhedral domain triangulated by simplicial triangulations, denoted by \mathcal{T}_h , where h > 0 is a mesh parameter satisfying $h \ge \max_{S \in \mathcal{T}_h} \operatorname{diam}(S)$. We consider a countable set of h's with $h \to 0$ which are nested, i.e. \mathcal{T}_{h_1} is a refinement of \mathcal{T}_{h_2} if $h_2 \ge h_1 > 0$. We fix an order of lamination $\kappa \ge 0$ in (3.9); the concrete value of κ does not affect

We fix an order of lamination $\kappa \geq 0$ in (3.9); the concrete value of κ does not affect the theoretical convergence results but may, of course, substantially influence the rate of convergence and thus numerical results of concrete computational experiments if taken too small. We introduce the spatially discretized state space as

$$Q_{h} = \left\{ q = (u, \nu, \lambda) \in Q; \ \nu \in \mathcal{G}_{\text{lam}}^{p, \kappa}(\Omega; \mathbb{R}^{3 \times 3}) \text{ and constant on each simplex of } \mathcal{T}_{h}, \\ \lambda \text{ constant on each simplex of } \mathcal{T}_{h} \right\}$$
(3.36)

Note that each u with $(u, \nu, \lambda) \in Q_h$ is inevitably piecewise affine on \mathcal{T}_h , since ∇u is piecewise constant.

In addition to the two small parameters $\tau > 0$ and h > 0 we introduce a third small parameter $\varepsilon > 0$ which is used to relax the constraint $\lambda = \mathcal{L} \bullet \nu$. For this we introduce the relaxed, spatially discretized energy

$$G_{h}^{\varepsilon}(t,q) = \begin{cases} G(t,q) + \frac{1}{\varepsilon} \| \lambda - \mathcal{L} \bullet \nu \| ^{2} & \text{for } q \in Q_{h}, \\ +\infty & \text{for } q \in Q \backslash Q_{h}, \end{cases}$$
(3.37)

where $\mathcal{L} \bullet \nu$ is from (3.28) and where $\| \cdot \|$ is the norm in a space to which $L^{\infty}(\Omega; \mathbb{R}^{1+M}) + W^{\alpha,r}(\Omega; \mathbb{R}^{1+M})$ is embedded compactly, e.g. the space $H^{-1}(\Omega; \mathbb{R}^{1+M}) := W_0^{1,2}(\Omega; \mathbb{R}^{1+M})^*$; recall that L^{∞} stands, as standard, for the space of measurable essentially bounded functions.

With these definitions, we consider a fully implicit algorithm based on the following incremental problem: Let $q_{\tau}^0 = q_0$ be a given initial condition, and, for $k = 1, ..., T/\tau$ we define $(q_{\tau,h}^{\varepsilon,k})_{k=1,...,T/\tau}$ to be a solution of the minimization problems

$$\begin{array}{ll}
\text{Minimize} & G_h^{\varepsilon}(k\tau, q) + R(q - q^{k-1}) \\
\text{subject to} & q = (u, \nu, \lambda) \in Q_h.
\end{array} \right\}$$
(3.38)

Let us denote by $q_{\tau,h}^{\varepsilon}$ the piecewise constant approximate solution, i.e. $q_{\tau,h}^{\varepsilon}(t) := q_{\tau,h}^{\varepsilon,k}$ for $(k-1)\tau < t \leq k\tau, k = 0, ..., T/\tau$. Beside the standard notation for $W^{\alpha,p}$ and L^{p} -spaces already explained, we now use also "BV" for the space of functions with bounded variations.

The main result is the following theorem showing approximation properties of the the sequence of discreized problems.

Theorem 3.3 Let $\{q_{\tau,h}^{\varepsilon}\}_{(\tau,h,\varepsilon)}$ be a family of approximations constructed as above such that $(\tau, h, \varepsilon) \to 0$, such that

$$q_{\tau,h}^{\varepsilon}(0) \in \mathcal{S}_{h}^{\varepsilon}(0), \quad q_{\tau,h}^{\varepsilon}(0) \stackrel{*}{\rightharpoonup} q_{0}, \text{ and } \quad G_{h}^{\varepsilon}(0, q_{\tau,h}^{\varepsilon}(0)) \to G^{0}(0, q_{0}).$$
(3.39)

Then, there exists a subsequence $\{(\tau_k, h_k, \varepsilon_k)\}_{k \in \mathbb{N}}$ with $(\tau_k, h_k, \varepsilon_k) \to (0, 0, 0)$ for $k \to \infty$ satisfying the stability criterion $h_k \leq H(\varepsilon_k)$ and a limit process $q : [0, T] \to Q$ with $q(0) = q_0$, such that the following holds. (We shortly write $q_k = (u_k, \nu_k, \lambda_k)$ for $q_{\tau_k, h_k}^{\varepsilon_k} = (u_{\tau_k, h_k}^{\varepsilon_k}, \nu_{\tau_k, h_k}^{\varepsilon_k}, \lambda_{\tau_k, h_k}^{\varepsilon_k})$.) (i) $q : [0, T] \to Q^0 \subset Q$ is an energetic solution, i.e., q satisfies (3.32) and (3.33), and also it holds $\lambda \in L^{\infty}([0, T]; W^{\alpha, r}(\Omega; \mathbb{R}^{1+M})) \cap BV([0, T], L^1(\Omega; \mathbb{R}^{1+M}))$ and $u : [0, T] \to Q^{\alpha, r}(\Omega; \mathbb{R}^{1+M})$

- $W^{1,p}(\Omega; \mathbb{R}^3)$ is bounded.
- For all $t \in [0,T]$ we have $\lambda_k(t) \rightharpoonup \lambda(t)$ in $W^{\alpha,r}(\Omega; \mathbb{R}^{1+M})$. (ii)
- (iii) For all $t \in [0, T]$ we have $\operatorname{Var}_R(q_k; 0, t) \to \operatorname{Var}_R(q; 0, t)$.
- (iv) For all $t \in [0,T]$ we have $G_{h_k}^{\varepsilon_k}(t,q_k(t)) \to G^0(t,q(t))$.

(v)
$$\frac{\partial}{\partial t}G_{h_k}^{\varepsilon_k}(\cdot, q_k(\cdot)) \xrightarrow{*} \frac{\partial}{\partial t}G^0(\cdot, q(\cdot))$$
 in $L^{\infty}(0, T)$.

(vi) For all $t \in [0,T]$ there is a subsequence $\{k_l\}_{l \in \mathbb{N}}$ such that $q_{k_l}(t) \stackrel{*}{\rightharpoonup} q(t)$ in Q.

3.6 Evolutionary problems in magnetism

The second part of Chapter 1 mainly deals with evolutionary problems of magnetism and includes papers [68] and [69]. A large part of my research in this subject consists of mesoscopic models of magnetic hysteresis. This phenomenon is very complex, and it is not yet fully understood, nothwithstanding many attempts which have been made to develop mathematical models of it for ferromagnetic and ferrimagnetic materials. See for example [15, 19, 104, 105, 106] for various models of hysteresis. To obtain a hysteresis loop for a general shape of a ferromagnet and general magnetization regimes, one must rely only on experimental measurements or numerical simulations. The latter option, we are focusing in the thesis, seems difficult to be obtained by conventionally used models which either treat the microstructure in too much detail (so that the multi-level character of macroscopical/microscopical effects cannot be properly modeled because of capacity of usual computers) or replaces the important information about the microstructure by mere phenomenology and smears thus out the complex interrelations counting macroscopical geometry of a specimen. The former sort of (domain-like) models includes Gilbert-Landau-Lifshitz' one [37, 72] and is discussed in detail in the paper [69], while the later one involves, e.g., models based on Rayleigh's modification [88] of Prandtl's and Ishlinskii's model or Preisach's model [87] (see also Jiles [48], Mayergoyz [73], or Visintin [104]). Another one is, e.g., due to Jiles and Atherton [50] and its modifications as, e.g., [49, 57].

3.7Mesoscopic models

It can roughly be said that, in our model, we combine the so-called *dry-friction* idea with the mesoscopical-level description of microstructure by using basically volume fractions expressed by Young measures. In fact, the notion of "dry-friction" is related to the maximumdissipation principle used in (quasi)plasticity. Dry-friction is very natural in the context of ferromagnetism, and has been already used in a Jiles-Atherton-like model by Bergqvist [14], in a micromagnetical-type model and in a model based on macroscopical magnetization by Visintin in [105] and [106], respectively. The mesoscopical description of the magnetization has been used by DeSimone [24], James and Kinderlehrer [46], and Rogers [89] (see also [53]) but only for minimization of the Gibbs energy.

The theory of rigid ferromagnetic bodies [21, 72] assumes that a magnetization $m: \Omega \to \mathbb{R}^n$, describing the state of a body $\Omega \subset \mathbb{R}^n$, n = 2, 3, is subjected to the Heisenberg-Weiss constraint, i.e., has a given (in general, temperature dependent) magnitude

$$|m(x)| = M_s$$
 for almost all $x \in \Omega$.

where $M_{\rm s} > 0$ is the saturation magnetization, considered here Here we relax this constraint and only assume that the magnetization is penalized if its magnitude is not constant for given temperature.

In the no-exchange formulation, which is valid for large bodies [24], the Helmholtz free energy of a rigid ferromagnetic body $\Omega \subset \mathbb{R}^n$ consists of two parts. The first part is the anisotropy energy $\int_{\Omega} \varphi(m(x)) dx$ related crystallographic properties of the ferromagnet. A typical $\varphi : S^{n-1} := \{s \in \mathbb{R}^n; |s| = M_s\} \to \mathbb{R}$ is a nonnegative function vanishing only at a few isolated points on S^{n-1} determining directions of easy magnetization, e.g. at two points for uniaxial materials or at six (or eight) for cubic ones. Throughout the paper we will assume that φ is a restriction of some smooth function $\tilde{\varphi}$, i.e.,

$$\varphi = \tilde{\varphi}|_{S^{n-1}}; \ \tilde{\varphi} \in C^{\infty}(\mathbb{R}^n) \ , \ \tilde{\varphi} \ge 0 \ \text{and even} \ .$$

$$(3.40)$$

The second part of the Helmholtz energy, $\frac{1}{2} \int_{\mathbb{R}^n} |\nabla u_m(x)|^2 dx$, is the energy of the demagnetizing field ∇u_m self-induced by the magnetization m; its potential u_m is governed by

$$\operatorname{div}(-\nabla u_m + m\chi_{\Omega}) = 0 \quad \text{in } \mathbb{R}^n, \qquad (3.41)$$

where $\chi_{\Omega} : \mathbb{R}^n \to \{0, 1\}$ is the characteristic function of Ω . The demagnetizing-field energy thus penalizes non-divergence-free magnetization vectors. Standardly, we will understand (3.41) in the weak sense, i.e. $u_m \in W^{1,2}(\mathbb{R}^n)$ will be called a weak solution to (3.41) if the integral identity $\int_{\mathbb{R}^n} (m\chi_{\Omega} - \nabla u_m(x)) \cdot \nabla v(x) \, dx = 0$ holds for all $v \in W^{1,2}(\mathbb{R}^n)$, where $W^{1,2}(\mathbb{R}^n) \equiv W^{1,2}(\mathbb{R}^n)$ denotes the Sobolev space of functions from $L^2(\mathbb{R}^n)$ with all first derivatives (in the distributional sense) also in $L^2(\mathbb{R}^n)$. Altogether, the Helmholtz energy E(m), has the form

$$E(m) = \int_{\Omega} \varphi(m(x)) \,\mathrm{d}x + \frac{1}{2} \int_{\mathbb{R}^n} |\nabla u_m(x)|^2 \,\mathrm{d}x \ . \tag{3.42}$$

If the ferromagnetic specimen is exposed to some external magnetic field h = h(x), the socalled Zeeman's energy of interactions between this field and magnetization vectors equals to $H(m) := -\int_{\Omega} h(x) \cdot m(x) \, dx$. Finally, the following variational principle governs equilibrium configurations:

minimize
$$G(m) := E(m) - H(m)$$
$$= \int_{\Omega} (\varphi(m(x)) - h(x) \cdot m(x)) \, \mathrm{d}x + \frac{1}{2} \int_{\mathbb{R}^n} |\nabla u_m(x)|^2 \, \mathrm{d}x , \qquad (3.43)$$
subject to (3.41), $(m, u_m) \in \mathcal{A} \times W^{1,2}(\mathbb{R}^n)$,

where the introduced notation G stands for *Gibbs' energy* and \mathcal{A} is the set of admissible magnetizations

$$\mathcal{A} := \{ m \in L^{\infty}(\Omega; \mathbb{R}^n); \ |m(x)| = M_{\rm s} \text{ for almost all } x \in \Omega \} .$$

As \mathcal{A} is not convex we cannot rely on direct methods in proving the existence of a solution. In fact, the solution to (3.43) need not exist in $\mathcal{A} \times W^{1,2}(\mathbb{R}^n)$; cf. [46] for the uniaxial case. Due to nonconvexity of \mathcal{A} weak limits of minimizing sequences of (3.43) do not necessarily live in $\mathcal{A} \times W^{1,2}(\mathbb{R}^n)$.

It is, therefore, natural to look for an extension (=relaxation) of our problem in which we would properly describe behavior of (3.43) along minimizing sequences. It is well-known [24, 85] that such relaxation can be achieved by extending the Helmholtz energy by continuity on the convex set of Young measures

$$\bar{E}(\nu) = \int_{\Omega} \varphi \bullet \nu \, \mathrm{d}x + \frac{1}{2} \int_{\mathbb{R}^n} |\nabla u_{(\mathrm{id} \bullet \nu)}(x)|^2 \, \mathrm{d}x \,, \qquad (3.44)$$

where $[v \bullet \nu](x) := \int_{\mathbb{R}^n} v(s)\nu_x(\mathrm{d}s)$ and $\mathrm{id} : \mathbb{R}^n \to \mathbb{R}^n$ is the identity.

This model represents a so-called *mesoscopic level* model because, a minimizing Young measure ν records some, but not full information about spatial oscillations of a minimizing sequence of (3.43) around each "macroscopic" point x through volume fractions described as the probability distribution ν_x . This information makes possible to describe the effective magnetic properties by means of the first moment, the "macroscopic" magnetization $m = id \cdot \nu$, and moreover seems sufficient for designing a dissipative mechanism in a good agreement with experiments, which will be just exploited further.

3.8 Rate-independent dissipation

For usual loading regimes and magnetically hard materials, one must consider a certain dissipation. Moreover, the dissipation mechanism in ferromagnets can be influenced by impurities in the material without affecting substantially the stored energy. Hence, both mechanisms (energy storage and dissipation) are, to some extent, independent of each other and, as the dissipation mechanisms are determined on the atomistic level, it seems that the only efficient way how to incorporate them in a higher-level model is phenomenology.

Our, to some extent simplified, standpoint is that the amount of dissipated energy within the phase transformation from one pole to the other can be described by a single, phenomenologically given number (of the dimension $J/m^3=Pa$) depending on the coercive force H_c [22]. Hence, we need to identify the particular poles according to the magnetization vector. Inspired by [77, 78] and considering L poles (L = 2 for uniaxial magnets or 6 or 8 for cubic magnets), we define a continuous mapping $\mathcal{L} : S^{n-1} \to \Delta_L$ where $\Delta_L := \{\xi \in \mathbb{R}^L; \xi_i \geq 0, i = 1, ..., L, \sum_{i=1}^L \xi_i = 1\}$. In other words, $\{\mathcal{L}_1, ..., \mathcal{L}_L\}$ forms a partition of unity on S^{n-1} such that $\mathcal{L}_i(s)$ is equal 1 if s is in *i*-th pole, i.e. $s \in S^{n-1}$ is in a neighborhood of *i*-th easy-magnetization direction. Of course, $\mathcal{L}(m)$ in the (relative) interior of Δ_L indicates m in the region where no definite pole is specified. Hence \mathcal{L} plays the role of what is often called an order parameter.

In terms of the mesoscopic microstructure described by the Young measure ν , the "mesoscopic" order parameter is naturally defined as

$$\lambda = \Lambda \nu := \mathcal{L} \bullet \nu \tag{3.45}$$

where $[\mathcal{L} \bullet \nu](x) := \int_{S^{n-1}} \mathcal{L}(s)\nu_x(\mathrm{d} s)$. Thus Λ is just a continuous extension of the mapping $m \mapsto \mathcal{L}(m)$, i.e. if $\{m_k\}$ converges to ν weakly* in $L^{\infty}(\Omega; \mathbb{R}^n)$, then $\mathcal{L}(m_k) \rightharpoonup \Lambda \nu$ weakly* in $L^{\infty}(\Omega; \mathbb{R}^L)$.

To described phenomenologically the dissipative energetics, one must prescribe a (pseudo)*potential of dissipative forces* as a function of the rate of λ . For rate-independent processes, this potential must be convex and homogeneous of degree one. Considering a norm $|\cdot|_L$ on \mathbb{R}^L , one can postulate $\varrho(\dot{\lambda}) = H_c |\dot{\lambda}|_L$. The energy needed to transform *i*-th pole to *j*-pole is then $H_c |e_i - e_j|_L$ with e_i the unit vector with 1 at the *i*-th position.

(at a given time t) will be described by the couple $q = q(t) \equiv (\nu, \lambda) = (\{\nu_{x,t}\}_{x \in \Omega}, \lambda(\cdot, t))$. Let us denote by \mathcal{Q} the convex set of admissible configurations:

$$\mathcal{Q} := \left\{ q = (\nu, \lambda) \in \mathcal{Y}(\Omega; S^{n-1}) \times L^{\infty}(\Omega; \mathbb{R}^{L}) \\ \lambda(x) \in \Delta_{L}, \quad \Lambda \nu = \lambda \text{ for a.a. } x \in \Omega \right\}$$
(3.46)

For the analysis, we will need to consider rather a certain *regularization* of the stored energy \mathcal{E} which would control spatial smoothness of λ . For this, we will augment \mathcal{E} by a higher-order term

$$\mathcal{E}_{\rho}(\nu,\lambda) := \bar{E}(\nu) + \begin{cases} \rho ||\lambda||_{W^{\alpha,2}(\Omega;\mathbb{R}^{L})}^{2} & \text{if } \lambda \in W^{\alpha,2}(\Omega;\mathbb{R}^{L}), \\ +\infty & \text{otherwise,} \end{cases}$$
(3.47)

where $W^{\alpha,2}(\Omega)$ denotes the usual Sobolev-Slobodetskiĭ space and where we assume

$$\alpha, \rho > 0, \text{ fixed.} \tag{3.48}$$

From now on, we will work with this regularized relaxed stored energy \mathcal{E}_{ρ} rather than \mathcal{E} . Following [77] we define the "dissipation distance" by ("co" denotes the convex hull):

$$d(\lambda_1, \lambda_2) := \inf \left\{ \int_0^1 \varrho(\frac{\mathrm{d}\lambda}{\mathrm{d}t}) \, \mathrm{d}t; \quad \lambda \in C^1([0, 1]; \mathbb{R}^L), \qquad (3.49) \right.$$
$$\lambda(t) \in \mathrm{co}\mathfrak{L}(S^{n-1}), \ \lambda|_{t=0} = \lambda_1, \ \lambda|_{t=1} = \lambda_2 \left. \right\}.$$

Let us still introduce the total "dissipation distance"

$$\mathcal{D}(q_1, q_2) := \int_{\Omega} d(\lambda_1, \lambda_2) \, \mathrm{d}x, \quad q_i = (\nu_i, \lambda_i). \tag{3.50}$$

Let us abbreviate the Gibbs energy by

$$\mathcal{G}(t,q) := \mathcal{E}_{\rho}(q) - \langle \mathcal{H}(t), q \rangle , \qquad (3.51)$$

where

$$\langle \mathcal{H}(t), q \rangle = [H(t)](\mathrm{id} \bullet \nu) = \langle \nu, h(\cdot, t) \otimes \mathrm{id} \rangle.$$
 (3.52)

Let us agree to identify quite naturally the mapping $t \mapsto \nu(t) = \{ [\nu(t)]_x \}_{x \in \Omega}$ with a Young measure $(x, t) \mapsto \nu_{x,t}$.

Definition 3.4 We say that a process q = q(t) is stable if

$$\forall \tilde{q} \in \mathcal{Q}: \qquad \mathcal{G}(t,q) \le \mathcal{G}(t,\tilde{q}) + \mathcal{D}(q(t),\tilde{q}) \tag{3.53}$$

for all $t \in [0, T]$.

An important notion is the so-called set of stable states, S(t), at a time instant t

$$S(t) = \{ q \in \mathcal{Q}; \ \forall \tilde{q} \in \mathcal{Q} : \mathcal{G}(t,q) \le \mathcal{G}(t,\tilde{q}) + \mathcal{D}(q,\tilde{q}) \}$$
(3.54)

Definition 3.5 We say that the process q = q(t) satisfies the energy inequality if for a.a. $s \in [0,T]$ and a.a. $t \in [0,T]$, $s \leq t$,

$$\underbrace{\mathcal{G}(t,q(t))}_{\text{effective Gibbs'}} + \underbrace{\operatorname{Var}(\mathcal{D},q;s,t)}_{\text{dissipated energy}} \leq \underbrace{\mathcal{G}(s,q(s)))}_{\text{Gibbs' energy at time 0}} - \underbrace{\int_{s}^{t} \left\langle \frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t},q(\theta) \right\rangle \mathrm{d}\theta}_{\text{reduced work of external field}} (3.55)$$

where the total variation over the time interval [s,t] is defined standardly, without using explicitly any time derivative, as

$$\operatorname{Var}(\mathcal{D}, q; s, t) := \sup \sum_{i=1}^{J} \mathcal{D}(q(t_{i-1}), q(t_i))$$

$$\equiv \sup \sum_{i=1}^{J} \int_{\Omega} d(\lambda(t_{i-1}), \lambda(t_i)) \, \mathrm{d}x,$$
(3.56)

where the supremum is taken over all $J \in \mathbb{N}$ and over all partitions of [s,t] in the form $s = t_0 < t_1 < ... < t_{J-1} < t_J = t$.

Definition 3.6 The process q = q(t), $q \equiv (\nu, \lambda)$, will be considered as a solution if $\nu \in \mathcal{Y}(\Omega \times [0,T]; S^{n-1})$, $\lambda \in BV([0,T]; L^1(\Omega; \mathbb{R}^L))$ and $q(t) \in \mathcal{Q}$ for all $t \in [0,T]$, and it is stable in the sense (3.53) for all $t \in [0,T]$ and satisfies the energy inequality (3.55) for a.a. $s, t \in [0,T]$, $s \leq t$.

The paper [68] proposes an efficient algorithm based on first-order optimality conditions which is then applied to numerical solution of the static problem. The survey article [69] reviews variety of effects in magnetism, in particular, its multiscale nature due to different inherent spatio-temporal physical and geometric scales, together with nonlocal phenomena and a nonconvex side-constraint, which are also the reason for severe problems in analysis, model validation, reductions, and numerics.

4 Overview of Chapter 2

Chapter 2 consists of papers [62, 52, 31, 64]. The main topic is a detailed analysis of oscillations and concentrations phenomena generated by sequences of gradients of Sobolev maps and, more generally, sequences of maps from the kernel of a first-order partial differential operator [31]. The emphasize in the gradient case is put on results describing behavior of sequences in the vicinity of the domain boundary. This issue seems to be omitted in existing literature. Interestingly, a condition which we isolate in [64] to deal with *p*-homogeneous integrands and which characterizes the subset of probability measures generated by gradients on the boundary is the so-called *quasiconvexity at the boundary* discovered by Ball and Marsden in 1984 [9] to characterize local minimizers of variational integrals in nonlinear elasticity. In what follows, we discuss the main results achieved in mentioned papers. The first one concerns an interesting property of quasiconvex functions.

4.1 Quasiconvexity and transposition

The first paper in the Chapter 2 is concerned with quasiconvexity and its properties. We again recall that $W : \mathbb{R}^{m \times n} \to \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$ is called quasiconvex at $A \in \mathbb{R}^{m \times n}$ if for any $\varphi \in W(\mathbb{R}^n; \mathbb{R}^m) := \{\theta \in W^{1,\infty}(\mathbb{R}^n; \mathbb{R}^m); \theta \text{ is } (0,1)^n\text{-periodic}\}$ (or equivalently any $\varphi \in W_0^{1,\infty}((0,1)^n; \mathbb{R}^m))$ (see e.g. [23])

$$W(A) \le \int_{(0,1)^n} W(A + \nabla \varphi(x)) \,\mathrm{d}x \tag{4.1}$$

whenever the integral on the right hand side exists. We say that W is quasiconvex if the previous inequality is valid for any $A \in \mathbb{R}^{m \times n}$. Quasiconvexity is the key property in the calculus of variations. Namely, if W is only finite valued then quasiconvexity of W is equivalent to sequential weak lower semicontinuity (omitting some growth conditions) of the functional

$$I(u) = \int_{\Omega} W(\nabla u(x)) \,\mathrm{d}x$$

where $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain and $u : \Omega \to \mathbb{R}^m$ smooth enough; cf. e.g. [3, 23]. If W attains also the value $+\infty$ then it is known that quasiconvexity is the necessary condition for sequential weak lower semicontinuity of I; cf. [23]. Unfortunately, quasiconvexity is very difficult to verify even in particular cases. On the other hand, there are known sufficient conditions and necessary conditions for quasiconvexity.

One sufficient condition is *polyconvexity*; cf. [5]. W given above is polyconvex if there is a convex function ϕ such that, for any $A \in \mathbb{R}^{m \times n}$, $W(A) = \phi(T(A))$, where T(A) is a vector of all subdeterminants of A, thus, $T : \mathbb{R}^{m \times n} \to \mathbb{R}^N$ where $N := \sum_{l=1}^{\min(m,n)} {m \choose l} {n \choose l}$. Dacorogna [23] showed that W is polyconvex at $A \in \mathbb{R}^{m \times n}$ if and only if

$$W(A) = \inf\left\{\sum_{i=1}^{N+1} \lambda_i W(A_i); \ \sum_{i=1}^{N+1} \lambda_i T(A_i) = T(A), \ \sum_{i=1}^{N+1} \lambda_i = 1, \ \lambda_i \ge 0, \ A_i \in \mathbb{R}^{m \times n}\right\} \ . (4.2)$$

The necessary (if W is real-valued) condition is rank-one convexity. The function W (as above) is called rank-one convex if $W(\lambda A + (1 - \lambda)B) \leq \lambda W(A) + (1 - \lambda)W(B)$ for any $0 \leq \lambda \leq 1$ and any $A, B \in \mathbb{R}^{m \times n}$, rank(A - B) = 1; cf. e.g. [23].

If $\min(m, n) = 1$ then quasiconvexity, polyconvexity and rank-one convexity are equivalent to usual convexity. The question whether or not rank-one convexity implies quasiconvexity if $\min(m, n) > 1$ has been open for many years. In 1992 Šverák [99] found a counterexample showing that this is not the case when $m \ge 3$ and $n \ge 2$. In particular, he showed that for any $\varepsilon > 0$ there is $k = k(\varepsilon) > 0$ such that the function $f_k^{\varepsilon} : \mathbb{R}^{3\times 2} \to \mathbb{R}$

$$f_k^{\varepsilon}(A) = f(PA) + \varepsilon(|A|^2 + |A|^4) + k|A - PA|^2$$
(4.3)

is rank-one convex but there is $\varepsilon > 0$ such that f_k^{ε} is not quasiconvex for any k > 0 at the point A = 0. Above, $P : \mathbb{R}^{3 \times 2} \to \mathbb{R}^{3 \times 2}$ is an orthogonal projector given by

$$P\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \\ A_{31} & A_{32} \end{pmatrix} = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \\ \frac{A_{31} + A_{32}}{2} & \frac{A_{31} + A_{32}}{2} \end{pmatrix}$$

and

$$f(PA) = -\frac{A_{11}A_{22}(A_{31} + A_{32})}{2} \, ,$$

where A_{ij} , i = 1, 2, 3, j = 1, 2 mean the entries of A and $|\cdot|$ is the Euclidean norm.

The aim of [62] is to discuss properties of the function $F_k^{\varepsilon}: \mathbb{R}^{2 \times 3} \to \mathbb{R}$ defined as

$$F_k^{\varepsilon}(A) = f_k^{\varepsilon}(A^t) \tag{4.4}$$

and its limit for $k \to \infty$. The superscript "t" denotes the transposition (i.e. $A_{ij}^t = A_{ji}$). Namely, we show that $\lim_{k\to\infty} F_k^{\varepsilon}$ is quasiconvex although $\lim_{k\to\infty} f_k^{\varepsilon}$ is not.

4.2 Gradient DiPerna-Majda measures

Let us take a complete (i.e. containing constants, separating points from closed subsets and closed with respect to the Chebyshev norm) separable ring \mathcal{R} of continuous bounded functions $\mathbb{R}^{m \times n} \to \mathbb{R}$. It is known [28, Sect. 3.12.21] that there is a one-to-one correspondence $\mathcal{R} \mapsto \beta_{\mathcal{R}} \mathbb{R}^{m \times n}$ between such rings and metrizable compactifications of $\mathbb{R}^{m \times n}$; by a compactification we mean here a compact set, denoted by $\beta_{\mathcal{R}} \mathbb{R}^{m \times n}$, into which $\mathbb{R}^{m \times n}$ is embedded homeomorphically and densely. For simplicity, we will not distinguish between $\mathbb{R}^{m \times n}$ and its image in $\beta_{\mathcal{R}} \mathbb{R}^{m \times n}$. Similarly, we will not distinguish between elements of \mathcal{R} and their unique continuous extensions on $\beta_{\mathcal{R}} \mathbb{R}^{m \times n}$.

Let $\sigma \in \mathcal{M}(\bar{\Omega})$ be a positive Radon measure on a bounded domain $\bar{\Omega} \subset \mathbb{R}^n$. A mapping $\hat{\nu} : x \mapsto \hat{\nu}_x$ belongs to the space $L^{\infty}_w(\bar{\Omega}, \sigma; \mathcal{M}(\beta_{\mathcal{R}}\mathbb{R}^{m\times n}))$ if it is weakly^{*} σ -measurable (i.e., for any $v_0 \in C_0(\mathbb{R}^{m\times n})$, the mapping $\bar{\Omega} \to \mathbb{R} : x \mapsto \int_{\beta_{\mathcal{R}}\mathbb{R}^{m\times n}} v_0(s)\hat{\nu}_x(ds)$ is σ -measurable in the usual sense). If additionally $\hat{\nu}_x \in \operatorname{rca}_1^+(\beta_{\mathcal{R}}\mathbb{R}^{m\times n})$ for σ -a.a. $x \in \bar{\Omega}$ the collection $\{\hat{\nu}_x\}_{x\in\bar{\Omega}}$ is the so-called Young measure on $(\bar{\Omega}, \sigma)$ [108], see also [6, 91, 100, 103, 107].

DiPerna and Majda [25] shown that having a bounded sequence in $L^{\hat{p}}(\Omega; \mathbb{R}^{m \times n})$ with $1 \leq p < +\infty$ and Ω an open domain in \mathbb{R}^n , there exists its subsequence (denoted by the same indices), a positive Radon measure $\sigma \in \mathcal{M}(\bar{\Omega})$, and a Young measure $\hat{\nu} : x \mapsto \hat{\nu}_x$ on $(\bar{\Omega}, \sigma)$ such that $(\sigma, \hat{\nu})$ is attainable by a sequence $\{y_k\}_{k \in \mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{m \times n})$ in the sense that $\forall g \in C(\bar{\Omega}) \ \forall v_0 \in \mathcal{R}$:

$$\lim_{k \to \infty} \int_{\Omega} g(x) v(y_k(x)) \, \mathrm{d}x = \int_{\bar{\Omega}} \int_{\beta_{\mathcal{R}} \mathbb{R}^{m \times n}} g(x) v_0(s) \hat{\nu}_x(\,\mathrm{d}s) \sigma(\,\mathrm{d}x) \,, \tag{4.5}$$

where

$$v \in \Upsilon^p_{\mathcal{R}}(\mathbb{R}^{m \times n}) := \{ v_0(1+|\cdot|^p); v_0 \in \mathcal{R} \}.$$

In particular, putting $v_0 = 1 \in \mathcal{R}$ in (4.5) we can see that

$$\lim_{k \to \infty} (1 + |y_k|^p) = \sigma \quad \text{weakly* in } \mathcal{M}(\bar{\Omega}) .$$
(4.6)

If (4.5) holds, we say that $\{y_k\}_{\in\mathbb{N}}$ generates $(\sigma, \hat{\nu})$. Let us denote by $\mathcal{DM}_{\mathcal{R}}^p(\Omega; \mathbb{R}^{m \times n})$ the set of all pairs $(\sigma, \hat{\nu}) \in \mathcal{M}(\bar{\Omega}) \times L^{\infty}_{w}(\bar{\Omega}, \sigma; \mathcal{M}(\beta_{\mathcal{R}}\mathbb{R}^{m \times n}))$ attainable by sequences from $L^p(\Omega; \mathbb{R}^{m \times n})$; note that, taking $v_0 = 1$ in (4.5), one can see that these sequences must be inevitably bounded in $L^p(\Omega; \mathbb{R}^{m \times n})$. We also denote by $\mathcal{GDM}_{\mathcal{R}}^p(\Omega; \mathbb{R}^{m \times n})$ measures from $\mathcal{DM}_{\mathcal{R}}^p(\Omega; \mathbb{R}^{m \times n})$ generated by a sequence of gradients of some bounded sequence in $W^{1,p}(\Omega; \mathbb{R}^m)$. The explicit description of the elements from $\mathcal{DM}_{\mathcal{R}}^p(\Omega; \mathbb{R}^{m \times n})$, called DiPerna-Majda measures, for unconstrained sequences was given in [70, Theorem 2]. In fact, it is easy to see that (4.5) can be also written in the form

$$\lim_{k \to \infty} \int_{\Omega} h(x, y_k(x)) \, \mathrm{d}x = \int_{\bar{\Omega}} \int_{\beta_{\mathcal{R}} \mathbb{R}^{m \times n}} h_0(x, s) \hat{\nu}_x(\,\mathrm{d}s) \sigma(\,\mathrm{d}x) \,, \tag{4.7}$$

where $h(x,s) := h_0(x,s)(1+|s|^p)$ and $h_0 \in C(\overline{\Omega} \otimes \beta_{\mathcal{R}} \mathbb{R}^{m \times n})$.

We say that $\{y_k\}$ generates $(\sigma, \hat{\nu})$ if (4.5) holds. Moreover, we denote $d_{\sigma} \in L^1(\Omega)$ the absolutely continuous (with respect to the Lebesgue measure) part of σ in the Lebesgue decomposition of σ .

Let us recall that for any $(\sigma, \hat{\nu}) \in \mathcal{DM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$ there is precisely one $(\sigma^{\circ}, \hat{\nu}^{\circ}) \in \mathcal{DM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$ such that

$$\int_{\Omega} \int_{\mathbb{R}^{m \times n}} v_0(s) \hat{\nu}_x(\,\mathrm{d}s) g(x) \sigma(\,\mathrm{d}x) = \int_{\bar{\Omega}} \int_{\mathbb{R}^{m \times n}} v_0(s) \hat{\nu}_x^{\circ}(\,\mathrm{d}s) g(x) \sigma^{\circ}(\,\mathrm{d}x) \tag{4.8}$$

for any $v_0 \in C_0(\mathbb{R}^{m \times n})$ and any $g \in C(\Omega)$ and $(\sigma^\circ, \hat{\nu}^\circ)$ is attainable by a sequence $\{y_k\}_{k \in \mathbb{N}}$ such that the set $\{|y_k|^p; k \in \mathbb{N}\}$ is relatively weakly compact in $L^1(\Omega)$; see [70, 91] for details. We call $(\sigma^\circ, \hat{\nu}^\circ)$ the nonconcentrating modification of $(\sigma, \hat{\nu})$. We call $(\sigma, \hat{\nu}) \in \mathcal{DM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$ nonconcentrating if

$$\int_{\bar{\Omega}} \int_{\beta_{\mathcal{R}} \mathbb{R}^{m \times n} \setminus \mathbb{R}^{m \times n}} \hat{\nu}_x(\mathrm{d}s) \sigma(\mathrm{d}x) = 0 \; .$$

There is a one-to-one correspondence between nonconcentrating DiPerna-Majda measures and Young measures; cf. [91].

We wish to emphasize the following fact: if $\{y_k\} \in L^p(\Omega; \mathbb{R}^{m \times n})$ generates $(\sigma, \hat{\nu}) \in \mathcal{DM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$ and σ is absolutely continuous with respect to the Lebesgue measure it generally **does not** mean that $\{|y_k|^p\}$ is weakly relatively compact in $L^1(\Omega)$. A simple examples can be found e.g. in [71, 91].

Having a sequence bounded in $L^p(\Omega; \mathbb{R}^{m \times n})$ generating a DiPerna-Majda measure $(\sigma, \hat{\nu}) \in \mathcal{DM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$ it also generates an L^p -Young measure $\nu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{m \times n})$. It easily follows from [91, Th. 3.2.13] that

$$\nu_x(\mathrm{d}s) = d_{\sigma^\circ}(x) \frac{\hat{\nu}_x^\circ(\mathrm{d}s)}{1+|s|^p} \quad \text{for a.a. } x \in \Omega .$$
(4.9)

Note that (4.9) is well-defined as $\hat{\nu}_x^{\circ}$ is supported on $\mathbb{R}^{m \times n}$. As pointed out in [70, Remark 2] for almost all $x \in \Omega$

$$d_{\sigma}(x) = \left(\int_{\mathbb{R}^{m \times n}} \frac{\hat{\nu}_x(\mathrm{d}s)}{1+|s|^p}\right)^{-1} . \tag{4.10}$$

In fact, that (4.8) can be even improved to

$$\int_{\Omega} \int_{\mathbb{R}^{m \times n}} v_0(s) \hat{\nu}_x(\,\mathrm{d}s) g(x) \sigma(\,\mathrm{d}x) = \int_{\bar{\Omega}} \int_{\mathbb{R}^{m \times n}} v_0(s) \hat{\nu}_x^\circ(\,\mathrm{d}s) g(x) \sigma^\circ(\,\mathrm{d}x) \tag{4.11}$$

for any $v_0 \in \mathcal{R}$ and any $g \in C(\overline{\Omega})$. The one-to-one correspondence between Young and DiPerna-Majda measures, in particular (see (4.9) and (4.11))

$$\int_{\mathbb{R}^{m \times n}} v(s)\nu_x(ds) = d_{\sigma}(x) \int_{\mathbb{R}^{m \times n}} v_0(s)\hat{\nu}_x(ds)$$

whenever $v \in \Upsilon^p_{\mathcal{R}}(\mathbb{R}^{m \times n})$, finally yields that $\forall g \in C(\overline{\Omega}) \ \forall v \in \Upsilon^p_{\mathcal{R}}(\mathbb{R}^{m \times n})$:

$$\lim_{k \to \infty} \int_{\Omega} g(x) v(y_k(x)) \, \mathrm{d}x = \int_{\Omega} \int_{\mathbb{R}^{m \times n}} v(s) g(x) \nu_x(\mathrm{d}s) \, \mathrm{d}x + \int_{\bar{\Omega}} \int_{\beta_{\mathcal{R}} \mathbb{R}^{m \times n} \setminus \mathbb{R}^{m \times n}} \frac{v(s)}{1 + |s|^p} \hat{\nu}_x(\mathrm{d}s) g(x) \sigma(\mathrm{d}x) , \quad (4.12)$$

where $\nu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{m \times n})$ and $(\sigma, \hat{\nu}) \in \mathcal{DM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$ are Young and DiPerna-Majda measures generated by $\{y_k\}_{k \in \mathbb{N}}$, respectively. We will denote elements from $\mathcal{DM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$ which are generated by $\{\nabla u_k\}_{k \in \mathbb{N}}$ for some bounded $\{u_k\} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ by $\mathcal{GDM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$.

The following two theorems were proved in [52].

Theorem 4.1 Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with Lipschitz boundary, 1 $and <math>(\sigma, \hat{\nu}) \in \mathcal{DM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$. Then then there is $u \in W^{1,p}(\Omega; \mathbb{R}^m)$ and a bounded sequence $\{u_k - u\}_{k \in \mathbb{N}} \subset W^{1,p}_0(\Omega; \mathbb{R}^m)$ such that $\{\nabla u_k\}_{k \in \mathbb{N}}$ generates $(\sigma, \hat{\nu})$ if and only if the following three conditions hold

for a.a.
$$x \in \Omega$$
: $\nabla u(x) = d_{\sigma}(x) \int_{\beta_{\mathcal{R}} \mathbb{R}^{m \times n}} \frac{s}{1 + |s|^p} \hat{\nu}_x(\mathrm{d}s) ,$ (4.13)

for almost all $x \in \Omega$ and for all $v \in \Upsilon^p_{\mathcal{R}}(\mathbb{R}^{m \times n})$ the following inequality is fulfilled

$$Qv(\nabla u(x)) \le d_{\sigma}(x) \int_{\beta_{\mathcal{R}}\mathbb{R}^{m\times n}} \frac{v(s)}{1+|s|^p} \hat{\nu}_x(\,\mathrm{d}s) \,, \qquad (4.14)$$

for σ -almost all $x \in \overline{\Omega}$ and all $v \in \Upsilon^p_{\mathcal{R}}(\mathbb{R}^{m \times n})$ with $Qv > -\infty$ it holds that

$$0 \le \int_{\beta_{\mathcal{R}} \mathbb{R}^{m \times n} \setminus \mathbb{R}^{m \times n}} \frac{v(s)}{1 + |s|^p} \hat{\nu}_x(\mathrm{d}s) \ . \tag{4.15}$$

The next theorem addresses DiPerna-Majda measures generated by gradients of maps with possibly different traces.

Theorem 4.2 Let Ω be an arbitrary bounded domain, $1 and <math>(\sigma, \hat{\nu}) \in \mathcal{GDM}^p_{\mathcal{R}}(\Omega; \mathbb{R}^{m \times n})$ be generated by $\{\nabla u_k\}_{k \in \mathbb{N}}$ such that $w - \lim_{k \to \infty} u_k = u$ in $W^{1,p}(\Omega; \mathbb{R}^m)$. Then the conditions (4.13), (4.14) hold, and (4.15) is satisfied for σ -a.a. $x \in \Omega$.

Remark 4.3 (i) It can happen that under the assumptions of Theorem 4.2 formula (4.15) does not hold on $\partial\Omega$. See an example in [10] showing the violation of weak sequential continuity of $W^{1,2}(\Omega; \mathbb{R}^2) \to L^1(\Omega) : u \mapsto \det \nabla u$ if $\Omega = (-1, 1)^2$. (ii) In terms of Young measures, conditions (4.13) and (4.14) read, respectively: there is $u \in W^{1,p}(\Omega; \mathbb{R}^m)$:

$$\nabla u(x) = \int_{\mathbb{R}^{m \times n}} s \nu_x(\mathrm{d}s) , \qquad (4.16)$$

for all $v : \mathbb{R}^{m \times n} \to \mathbb{R}, |v| \le C(1 + |\cdot|^p)$:

$$Qv(\nabla u(x)) \le \int_{\mathbb{R}^{m \times n}} v(s)\nu_x(\mathrm{d}s) \ . \tag{4.17}$$

Finally, we have the following result from [52].

Theorem 4.4 Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain. Let $0 \leq g \in C(\overline{\Omega})$, $v \in C(\mathbb{R}^{m \times n})$, $|v| \leq C(1 + |\cdot|^p)$, C > 0, quasiconvex, and $1 . Then the functional <math>I : W^{1,p}(\Omega; \mathbb{R}^m) \to \mathbb{R}$ defined as

$$I(u) := \int_{\Omega} g(x)v(\nabla u(x)) \,\mathrm{d}x \tag{4.18}$$

is sequentially weakly lower semicontinuous in $W^{1,p}(\Omega; \mathbb{R}^m)$ if and only if for any bounded sequence $\{w_k\} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ such that $\nabla w_k \to 0$ in measure we have $\liminf_{k\to\infty} I(w_k) \ge I(0)$.

Moreover, oscillations and concentrations effects generated by sequences from a kernel of a first-order linear differential operator are studied in [31].

In particular, following [33], we consider linear operators $A^{(i)} : \mathbb{R}^m \to \mathbb{R}^d$, $i = 1, \ldots, n$, and define $\mathcal{A} : L^p(\Omega; \mathbb{R}^m) \to W^{-1,p}(\Omega; \mathbb{R}^d)$ by

$$\mathcal{A}u := \sum_{i=1}^{n} A^{(i)} \frac{\partial u}{\partial x_i} , \text{where } u : \Omega \to \mathbb{R}^m , \qquad (4.19)$$

i.e., for all $w \in W_0^{1,p'}(\Omega; \mathbb{R}^d)$

$$\langle \mathcal{A}u, w \rangle = -\sum_{i=1}^{n} \int_{\Omega} A^{(i)} u(x) \cdot \frac{\partial w(x)}{\partial x_{i}} \, \mathrm{d}x$$

For $w \in \mathbb{R}^n$ we define the linear map

$$\mathbb{A}(w) := \sum_{i=1}^{n} w_i A^{(i)} : \mathbb{R}^m \to \mathbb{R}^d , \qquad (4.20)$$

and assume that there is $r \in \mathbb{N} \cup \{0\}$ such that

rank
$$\mathbb{A}(w) = r$$
 for all $w \in \mathbb{R}^n$, $|w| = 1$,

i.e., \mathcal{A} has the so-called *constant-rank property*. Corresponding weak lower semicontinuity results and characterization of DiPerna-Majda measures can be found in [31].

4.3 Quasiconvexity at the boundary

Oscillations and/or concentrations appear in many problems in the calculus of variations, partial differential equations, or optimal control theory, which admit only L^p but not L^{∞} apriori estimates. While Young measures [108] successfully capture oscillatory behavior (see e.g. [66, 83, 93, 94]) of sequences they completely miss concentrations. There are several tools how to deal with concentrations. They can be considered as generalization of Young measures, see for example Alibert's and Bouchitté's approach [4], DiPerna's and Majda's treatment of concentrations [25], or Fonseca's method described in [30]. An overview can be found in [91, 101]. Moreover, in many cases, we are interested in oscillation/concentration effects generated by sequences of gradients. A characterization of Young measures generated by gradients was completely given by Kinderlehrer and Pedregal [54, 56], cf. also [83, 85]. The first attempt to characterize both oscillations and concentrations in sequences of gradients is due to Fonseca, Müller, and Pedregal [32]. They dealt with a special situation of $\{gv(\nabla u_k)\}_{k\in\mathbb{N}}$ where v coincides with a positively p-homogeneous function at infinity (see (4.26) for a precise statement), $u_k \in W^{1,p}(\Omega; \mathbb{R}^m)$, p > 1, with g continuous and van-ishing on $\partial\Omega$. Later on, a characterization of oscillation/concentration effects in terms of DiPerna's and Majda's generalization of Young measures was given in [52] for arbitrary integrands and in [31] for sequences living in the kernel of a first-order differential operator. Recently, Kristensen and Rindler [59] characterized oscillation/concentration effects in the case p = 1. Nevertheless, a complete analysis of boundary effects generated by gradients is still missing. We refer to [52] for the case where $u_k = u$ on the boundary of the domain. As already observed by Meyers [79], concentration effects at the boundary are closely related to the sequential weak lower semicontinuity of integral functionals $I : W^{1,p}(\Omega; \mathbb{R}^m) \to \mathbb{R}$: $I(u) = \int_{\Omega} v(\nabla u(x)) \, dx$ where $v : \mathbb{R}^{m \times n} \to \mathbb{R}$ is continuous and such that $|v| \leq C(1+|\cdot|^p)$ for some constant C > 0, cf. also [60] for recent results. Indeed, consider $u \in W_0^{1,p}(B(0,1);\mathbb{R}^m)$, where B(0,1) is the unit ball in \mathbb{R}^n centered at 0, and extend it by zero to the whole \mathbb{R}^n . Define for $x \in \mathbb{R}^n$ and $k \in \mathbb{N}$ $u_k(x) := k^{n/p-1}u(kx)$, i.e., $u_k \to 0$ in $W^{1,p}(B(0,1);\mathbb{R}^m)$ and consider a smooth convex domain $\Omega \in \mathbb{R}^n$ such that $0 \in \partial\Omega$, ρ is the outer unit normal to $\partial\Omega$ at 0 and let there be $x \in \Omega$ such that $\rho \cdot x < 0$. Moreover, take a function v to be positively p-homogeneous, i.e., $v(\alpha s) = \alpha^p v(s)$ for all $\alpha \ge 0$. Then if I is weakly lower semicontinuous then

$$0 = I(0) \leq \liminf_{k \to \infty} \int_{\Omega} v(\nabla u_k(x)) \, \mathrm{d}x = \liminf_{k \to \infty} \int_{B(0,1) \cap \Omega} v(\nabla u_k(x)) \, \mathrm{d}x$$
$$= \liminf_{k \to \infty} \int_{B(0,1) \cap \{x \in \mathbb{R}^n; \ \varrho \cdot x < 0\}} v(\nabla u(kx)) \, \mathrm{d}x$$
$$= \int_{B(0,1) \cap \{x \in \mathbb{R}^n; \ \varrho \cdot x < 0\}} v(\nabla u(y)) \, \mathrm{d}y \;. \tag{4.21}$$

Thus, we see that

$$0 \le \int_{B(0,1) \cap \{x \in \mathbb{R}^n; \ \varrho \cdot x < 0\}} v(\nabla u(y)) \, \mathrm{d}y$$

for all $u \in W_0^{1,p}(B(0,1);\mathbb{R}^m)$ forms a necessary condition for weak lower semicontinuity of I. Here we show that the weak lower semicontinuity of the above defined functional I is intimately related to the so-called quasiconvexity at the boundary defined by Ball and Marsden in [9] and that this notion of quasiconvexity plays a crucial role in the characterization of parametrized measures generated by sequences of gradients. Moreover, we show that if $\{u_k\} \subset W^{1,2}(\Omega;\mathbb{R}^3), u_k \rightarrow u, \text{ and } h(x,s) := [\operatorname{Cof} s] \cdot (a(x) \otimes \varrho(x))$ ("Cof" denotes the cofactor matrix) for some $a, \varrho \in C(\bar{\Omega};\mathbb{R}^3)$ such that ϱ coincides with the outer unit normal to $\partial\Omega$ on the boundary $\partial\Omega$ of a smooth bounded domain $\Omega \subset \mathbb{R}^3$ then $h(\cdot, \nabla u_k) \rightarrow h(\cdot, \nabla u)$ weakly* in Radon measures supported in $\bar{\Omega}$. If, additionally, $h(x, \nabla u_k(x)) \geq 0$ for all $k \in \mathbb{N}$ and almost all $x \in \Omega$ then the above convergence is even in the weak topology of $L^1(\Omega)$. Hence, there is a continuous function $\psi : [0, +\infty) \rightarrow [0, +\infty)$ such that $\lim_{t\to\infty} \psi(t)/t = +\infty$ and $\sup_{k\in\mathbb{N}} \int_{\Omega} \psi(h(x, \nabla u_k(x))) \, dx < +\infty$. This result, which can be generalized to higher dimensions, too, is an analogy to the celebrated S. Müler's result on higher integrability of determinants [82]. See also [43, 55]. Nevertheless, there are indications [51] that the problem might be more complicated for quasiconvexity at the boundary.

Following [9, 96, 98] we define the notion of quasiconvexity at the boundary. In order to proceed, we first define the so-called *standard boundary domain*.

Definition 4.5 Let $\varrho \in \mathbb{R}^n$ be a unit vector and let Ω_{ϱ} be a bounded open Lipschitz domain. We say that Ω_{ϱ} is a standard boundary domain with the normal ϱ if there is $a \in \mathbb{R}^n$ such that $\Omega_{\varrho} \subset H_{a,\varrho} := \{x \in \mathbb{R}^n; \ \varrho \cdot x < a\}$ and the (n-1)- dimensional interior Γ_{ϱ} of $\partial \Omega_{\varrho} \cap \partial H_{a,\varrho}$ is nonempty.

We are now ready to define the quasiconvexity at the boundary. We put for $1 \le p \le +\infty$

$$W^{1,p}_{\Gamma_{\varrho}}(\Omega_{\varrho};\mathbb{R}^m) := \{ u \in W^{1,p}(\Omega_{\varrho};\mathbb{R}^m); \ u = 0 \text{ on } \partial\Omega_{\varrho} \setminus \Gamma_{\varrho} \} .$$

$$(4.22)$$

Definition 4.6 ([9]) Let $\varrho \in \mathbb{R}^n$ be a unit vector. A function $v : \mathbb{R}^{m \times n} \to \mathbb{R}$ is called quasiconvex at the boundary at $s_0 \in \mathbb{R}^{m \times n}$ with respect to ϱ (shortly v is qcb at (s_0, ϱ)) if there is $q \in \mathbb{R}^m$ such that for all $u \in W^{1,\infty}_{\Gamma_{\varrho}}(\Omega_{\varrho}; \mathbb{R}^m)$ it holds

$$\int_{\Gamma_{\varrho}} q \cdot u(x) \, \mathrm{d}S + v(s_0) |\Omega_{\varrho}| \le \int_{\Omega_{\varrho}} v(s_0 + \nabla u(x)) \, \mathrm{d}x \, . \tag{4.23}$$

It will be convenient to define the following notion recalling the quasiconvex envelope of v at zero. Here, however, we integrate only over a standard boundary domain with a given normal. If $\rho \in \mathbb{R}^n$ has a unit length then put

$$Q_{b,\varrho}v(0) := \inf_{u \in W_{\Gamma_{\varrho}}^{1,\rho}(\Omega_{\varrho};\mathbb{R}^m)} \frac{1}{|\Omega_{\varrho}|} \int_{\Omega_{\varrho}} v(\nabla u(x)) \,\mathrm{d}x \,.$$

$$(4.24)$$

Remark 4.7 If v is positively p homogeneous with p > 1 then either $Q_{b,\varrho}v(0) = 0$ or $Q_{b,\varrho}v(0) = -\infty$. We also have that $Q_{b,\varrho}v(0) \leq Qv(0)$.

4.3.1 Compactification of $\mathbb{R}^{m \times n}$ by the sphere

In what follows we will work mostly with a particular compactification of $\mathbb{R}^{m \times n}$, namely, with the compactification by the sphere. We will consider the following ring of continuous bounded functions

$$\mathcal{S} := \left\{ v_0 \in C(\mathbb{R}^{m \times n}) : \text{ there exist } c \in \mathbb{R}^{m \times n} , v_{0,0} \in C_0(\mathbb{R}^{m \times n}), \text{ and } v_{0,1} \in C(S^{(m \times n)-1}); \\ v_0(s) = c + v_{0,0}(s) + v_{0,1} \left(\frac{s}{|s|}\right) \frac{|s|^p}{1 + |s|^p} \text{ if } s \neq 0 \text{ and } v_0(0) = c + v_{0,0}(0) \right\}, \quad (4.25)$$

where $S^{m \times n-1}$ denotes the (mn - 1)-dimensional unit sphere in $\mathbb{R}^{m \times n}$. Then $\beta_{\mathcal{S}} \mathbb{R}^{m \times n}$ is homeomorphic to the unit ball $\overline{B(0,1)} \subset \mathbb{R}^{m \times n}$ via the mapping $d : \mathbb{R}^{m \times n} \to B(0,1)$, d(s) := s/(1+|s|) for all $s \in \mathbb{R}^{m \times n}$. Note that $d(\mathbb{R}^{m \times n})$ is dense in $\overline{B(0,1)}$.

For any $v \in \Upsilon^p_{\mathcal{S}}(\mathbb{R}^{m \times n})$ there exists a continuous and positively *p*-homogeneous function $v_{\infty} : \mathbb{R}^{m \times n} \to \mathbb{R}$ (i.e. $v_{\infty}(\alpha s) = \alpha^p v_{\infty}(s)$ for all $\alpha \ge 0$ and $s \in \mathbb{R}^m$) such that

$$\lim_{|s| \to \infty} \frac{v(s) - v_{\infty}(s)}{|s|^p} = 0 .$$
(4.26)

Indeed, if v_0 is as in (4.25) and $v = v_0(1 + |\cdot|^p)$ then set

$$v_{\infty}(s) := \left(c + v_{0,1}\left(\frac{s}{|s|}\right)\right) |s|^p \text{ for } s \in \mathbb{R}^{m \times n} \setminus \{0\}.$$

By continuity we define $v_{\infty}(0) := 0$. It is easy to see that v_{∞} satisfies (4.26). Such v_{∞} is called the *recession function* of v.

Our main result is the following explicit characterization of DiPerna-Majda measures from $\mathcal{DM}^p_{\mathcal{S}}(\Omega; \mathbb{R}^{m \times n})$ which are generated by gradients.

Theorem 4.8 Let $\Omega \subset \mathbb{R}^n$ be a smooth (at least C^1) bounded domain, $1 , and <math>(\sigma, \hat{\nu}) \in \mathcal{DM}^p_{\mathcal{S}}(\Omega; \mathbb{R}^{m \times n})$. Then then there is a bounded sequence $\{u_k\}_{k \in \mathbb{N}} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ such that $\{\nabla u_k\}_{k \in \mathbb{N}}$ generates $(\sigma, \hat{\nu})$ if and only if the following three conditions hold

for a.a.
$$x \in \Omega$$
: $\nabla u(x) = d_{\sigma}(x) \int_{\beta_{\mathcal{S}} \mathbb{R}^{m \times n}} \frac{s}{1 + |s|^p} \hat{\nu}_x(\mathrm{d}s) ,$ (4.27)

for almost all $x \in \Omega$ and for all $v \in \Upsilon^p_{\mathcal{S}}(\mathbb{R}^{m \times n})$ the following inequality is fulfilled

$$Qv(\nabla u(x)) \le d_{\sigma}(x) \int_{\beta_{\mathcal{S}}\mathbb{R}^{m\times n}} \frac{v(s)}{1+|s|^p} \hat{\nu}_x(\,\mathrm{d}s) \,, \qquad (4.28)$$

for σ -almost all $x \in \Omega$ and all $v \in \Upsilon^p_{\mathcal{S}}(\mathbb{R}^{m \times n})$ with $Qv_{\infty} > -\infty$ it holds that

$$0 \le \int_{\beta_{\mathcal{S}} \mathbb{R}^{m \times n} \setminus \mathbb{R}^{m \times n}} \frac{v(s)}{1 + |s|^p} \hat{\nu}_x(\mathrm{d}s) , \qquad (4.29)$$

and for σ -almost all $x \in \partial \Omega$ with the outer unit normal to the boundary $\varrho(x)$ and all $v \in \Upsilon^p_{\mathcal{S}}(\mathbb{R}^{m \times n})$ with $Q_{b,\varrho(x)}v_{\infty}(0) = 0$ it holds that

$$0 \le \int_{\beta_{\mathcal{S}} \mathbb{R}^{m \times n} \setminus \mathbb{R}^{m \times n}} \frac{v(s)}{1 + |s|^p} \hat{\nu}_x(\mathrm{d}s) \ . \tag{4.30}$$

The following results show that sequential weak lower semicontinuity of I from (4.18) puts serious restrictions on v.

Theorem 4.9 Let $\Omega \subset \mathbb{R}^n$ be a smooth bounded domain and $1 . Let <math>0 \leq g \in C(\overline{\Omega}), 0 < g$ on $\partial\Omega, v \in C(\mathbb{R}^{m \times n})$, and $|v| \leq C(1+|\cdot|^p), C > 0$, quasiconvex such that there is a positively p-homogeneous function $v_{\infty} : \mathbb{R}^{m \times n} \to \mathbb{R}$ satisfying $\lim_{|s|\to\infty} (v(s) - v_{\infty}(s))/|s|^p = 0$. Then the functional I defined by (4.18) is sequentially weakly lower semicontinuous in $W^{1,p}(\Omega; \mathbb{R}^m)$ if and only if $Q_{b,\varrho}v_{\infty}(0) = 0$ for every ϱ a unit outer normal to $\partial\Omega$.

Theorem 4.10 Let $\Omega \subset \mathbb{R}^n$ be a smooth bounded domain and $1 . Let <math>0 \leq g \in C(\bar{\Omega})$, 0 < g on $\partial\Omega$, $v \in C(\mathbb{R}^{m \times n})$, and $|v| \leq C(1 + |\cdot|^p)$, C > 0, quasiconvex such that there is a positively p-homogeneous function $v_{\infty} : \mathbb{R}^{m \times n} \to \mathbb{R}$ satisfying $\lim_{|s|\to\infty} (v(s) - v_{\infty}(s))/|s|^p = 0$. Let $\{u_k\} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ weakly converge to $u \in W^{1,p}(\Omega; \mathbb{R}^m)$. Let $|\nabla u_k|^p \to \sigma$ weakly* in $\mathcal{M}(\bar{\Omega})$. Then the functional I defined by (4.18) satisfies $I(u) \leq \liminf_{k\to\infty} I(u_k)$ if $Q_{b,\varrho(x)}v_{\infty}(0) = 0$ for every $\varrho(x)$, a unit outer normal to $\partial\Omega$ at $x \in \partial\Omega$, for σ -a.a. $x \in \partial\Omega$.

Theorem 4.11 Let $\Omega \subset \mathbb{R}^3$ be a smooth bounded domain. Let $\{u_k\} \subset W^{1,2}(\Omega; \mathbb{R}^3)$ be such that $u_k \to u$ weakly in $W^{1,2}(\Omega; \mathbb{R}^3)$. Let $h(x, s) = \operatorname{Cof} s \cdot (a(x) \otimes \varrho(x))$, where $a, \varrho \in C(\overline{\Omega}; \mathbb{R}^3)$, ϱ coincides at $\partial\Omega$ with the outer unit normal to $\partial\Omega$. Then for all $g \in C(\overline{\Omega})$

$$\lim_{k \to \infty} \int_{\Omega} g(x)h(x, \nabla u_k(x)) \,\mathrm{d}x = \int_{\Omega} g(x)h(x, \nabla u(x)) \,\mathrm{d}x \ . \tag{4.31}$$

If, moreover, for all $k \in \mathbb{N}$ $h(\cdot, \nabla u_k) \geq 0$ almost everywhere in Ω then $h(\cdot, \nabla u_k) \rightarrow h(\cdot, \nabla u)$ weakly in $L^1(\Omega)$.

A more general compactifications that the one by the sphere are considered in [61]. In particular, a general relaxation result for possibly noncoercive integrands is proved there; see [61, Theorem 3.2].

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