Progress in Nonlinear Differential Equations
and Their Applications

Variational Problems in Materials Science

Gianni dal Maso
Antonio DeSimone
Franco Tomarelli
Editors

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Volume 68

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Preface

This volume contains the proceedings of the international workshop *Variational Problems in Materials Science*, which was jointly organized by the International School for Advanced Studies (SISSA) of Trieste and by the Dipartimento di Matematica "Francesco Brioschi" of the Politecnico di Milano. The conference took place at SISSA from September 6 to 10, 2004.

The study of variational problems in materials science has a long history, and it has contributed a lot in shaping our understanding on how materials work and perform. There is, however, a recent renewed interest in this subject as a consequence of the fruitful interaction between mathematical analysis and the modelling of new, technologically advanced materials. On one hand, a sizable group of analysts has found in materials science a valuable source of inspiration for new variational theories and interesting problems. On the other hand, workers in the fields of theoretical, applied, and computational mechanics are increasingly using innovative variational techniques. The workshop intended to review some of the recent advances stemming from the successful interaction between the two communities, and to identify promising areas for further cooperation.

Talks were devoted to a wide spectrum of analytical techniques and of physical systems and phenomena. They included the study of BV vector fields, path functionals over Wasserstein spaces, variational approaches to quasi-static evolution, free-discontinuity problems with applications to fracture and plasticity, systems with hysteresis or with interfacial energies, evolution of interfaces, multiscale analysis in ferromagnetism and ferroelectricity, variational techniques for the study of crystal plasticity, of dislocations, and of concentrations in Ginzburg–Landau functionals, concentrated contact interactions, and phase transitions in biaxial liquid crystals.

This volume collects contributions authored or co-authored by 11 out of the 20 speakers invited to deliver lectures at the workshop. They all contain original results in fields which are at the forefront of current research, and in rapid evolution.

More than sixty researchers with quite different disciplinary expertise (calculus of variations, computational mechanics, continuum mechanics, geometric measure theory, materials science) attended the workshop. The list of participants appears at the end of the volume. We thank them all for their lively and friendly contributions to the scientific discussions, and to the pleasant atmosphere of the event.

The meeting enjoyed the financial support of SISSA, Politecnico di Milano, MIUR (through the National Research Group "Calculus of Variations"), and of the Istituto Nazionale di Alta Matematica "Francesco Severi" through the groups GNAMPA and GNFM. We are grateful to all these Institutions for their contributions.

Most of the burden of organizing the logistics fell on Andrea Brunetta. We wish to warmly thank him for his excellent job.

Finally, it is our pleasure to thank once again all the lecturers, and we are especially grateful to those who contributed to this volume.

Milano and Trieste, November 15, 2005

Gianni Dal Maso
Antonio DeSimone
Franco Tomarelli

Invited Lectures

Luigi Ambrosio (Scuola Normale Superiore, Pisa)
On the Cauchy problem for BV vector fields

Kaushik Bhattacharya (Caltech)
Ferroelectric ceramics

Andrea Braides (Università di Roma Tor Vergata)
Surface energies in discrete systems

Giuseppe Buttazzo (Università di Pisa)
Path functionals over Wasserstein spaces

Antonin Chambolle (École Polytechnique)
On the initiation of cracks in Griffith's model

Gianpietro Del Piero (Università di Ferrara)
Bi-modal cohesive energies

Irene Fonseca (Carnegie Mellon University)
Variational methods in materials science: the study of foams and quantum dots

Ilaria Fragalà (Politecnico di Milano)
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David Kinderlehrer (Carnegie Mellon University)
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Stefan Müller (Max Planck Institute for Mathematics in the Sciences, Leipzig)

A hierarchy of plate and shell theories derived from three-dimensional nonlinear elasticity by Gamma-convergence

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Discrete crystal plasticity

Felix Otto (University of Bonn)

Multiscale analysis in micromagnetics

Danilo Percivale (Università di Genova)

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Phenomenology of concentrated contact interactions in simple continuous bodies

Lev Truskinovsky (École Polytechnique)

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Remarks on a Multiscale Approach to Grain Growth in Polycrystals

Katayun Barmak, David Kinderlehrer, Irine Livshits
and Shlomo Ta'asan*

Abstract. Nearly all technologically useful materials are polycrystalline. Their ability to meet system level specifications of performance and reliability is influenced by the types of grain boundaries present and their connectivity. To engineer the grain boundary network to achieve these objectives, we seek predictive models of growth at various mesoscale levels. Here we discuss a master equation description of normal grain growth derived from large scale simulations and compare the results with recent experiments.

Introduction

A central problem in materials science is the understanding and control of microstructure, the ensemble of grains that comprise polycrystalline materials. Macroscopic properties of these materials are affected by grain size, texture and other mesoscale properties. The orientations and arrangements of the grains and their network of boundaries are implicated in many properties across wide scales, for example, functional properties, like conductivity in microprocessors, and lifetime properties, like fracture toughness in structures. Modeling and simulation of the grain evolution at the mesoscale plays an increasingly important role in resolving this central problem. With the implementation of automated data acquisition, based on orientation imaging microscopy, in the Mesoscale Interface Mapping Project, a strategy has emerged for determining interfacial energy and mobility in polycrystals, [1]. Our present task is to investigate microstructural evolution.

Here we examine the issues related to simulations of grain boundary network evolution subject to the conventions of normal grain growth and compare these with new experimental work on aluminum thin films. Normal grain growth consists

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of the Mullins Equations of curvature driven growth [16, 10] in a two-dimensional setting with appropriate boundary conditions at triple junctions, where boundaries meet. This paradigm system is the most studied in theory and corresponds in experiment to a columnar grain structure, which is what we shall actually see in the experiment. Are there general laws of evolution for ensembles of grains? Such questions have been studied for many generations and now become accessible by means of a very large scale reliable and accurate approach to simulation.

To engage this issue we are led to another. The simulated coarsening process is a large metastable system with a precise formulation, for example, consisting of some 50,000 nonlinear partial differential equations. This must be replaced at a larger scale by some distribution functions, or stochasticized, in order to be interpreted. Which distribution functions to choose may be a matter of history, art, or intuition, but there remains the necessity of deriving their stability and robustness. The problem, after all, is all mathematics. The issue is yet more compelling since we are ultimately asked to compare the simulation with experimental results. We are not able to directly pass from the mesoscopic scale of the simulation to the more macroscopic scale, but we shall seek to derive some theory for the distribution functions which is simulation based. This vast multiscale arena has many challenges.

1. Recapitulation of grain growth

We review very briefly the Mullins Equation for the evolution of a two dimensional grain boundary system. Our concern here is limited to systems with constant energy and mobility. Consider a curve family, or an evolving curve,

$$\Gamma : x = \xi(s,t), \quad 0 \leqq s \leqq L, \ t > 0, \tag{1.1}$$

with

$$b = \frac{d\xi}{ds} \text{ (tangent)} \quad \text{and} \quad n = Rb \text{ (normal)}.$$

Let γ denote the energy density and μ the mobility of Γ. The equation of motion is then

$$v_n = \mu\gamma\kappa \ \text{ on } \Gamma, \quad \kappa = \text{curvature}. \tag{1.2}$$

We assume that only triple junctions are stable and impose the Herring condition, [10], where three curves meet. This condition reduces to: if $\Gamma^{(1)}, \Gamma^{(2)}, \Gamma^{(3)}$ meet at p, then they meet at angles of $2\pi/3$. It is the natural boundary condition in equilibrium for the functional

$$F = \sum_{i=1\ldots3} \int_{\Gamma_i} \gamma ds$$

under the assumption that the three curves meet at the triple junction p. Consider a network of grains bounded by $\{\Gamma_i\}$ subject to some conditions at the border of

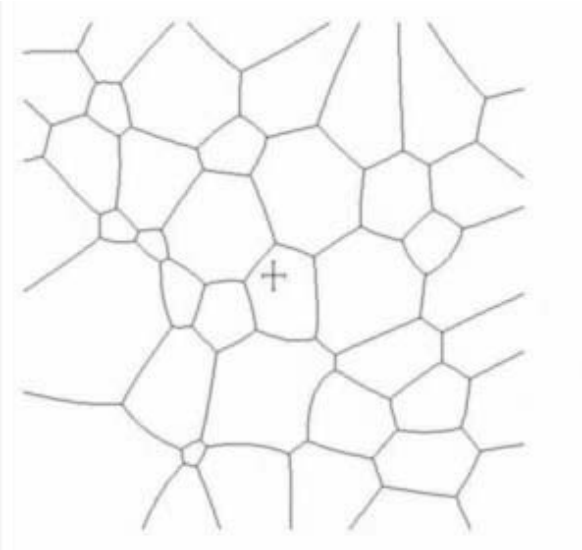

FIGURE 1. A snapshot of a network of grain boundaries from the simulation

the region they occupy, like fixed end points or periodicity, cf. Figure 1. The total energy of this system

$$E(t) = \sum_{\{\Gamma_i\}} \int_{\Gamma_i} \gamma ds$$

during evolution in the absence of topological events satisfies

$$\frac{d}{dt} E(t) \leqq 0,$$

and thus the system is dissipative. Our simulation is designed to preserve this feature at the discrete level and to enforce it during topological events, [14].

The well-posedness of (1.2) with the Herring condition was discovered by Bronsard and Reitich, [5], and long time existence established in [11]. Details of the simulation method may be found in [13], [14].

2. Master equation approach to evolution

The idea of the master equation approach is to replace the original mesoscale system of many equations with a simpler set of equations that still provides desired information. In this implementation, the connectivity of the grain boundary network is abandoned in favor of side class distributions motivated by the Mullins-von Neumann $n - 6$ rule. The strategy is to discover such a system of equations by interrogating the simulation, a strategy made possible because we have at hand a

reliable large scale simulation. As suggested, here we are primarily interested in the stationary relative area histogram.

Suppose a grain with n sides or facets evolves subject to (1.2) and the Herring Condition. Then, according to the Mullins-von Neumann Rule, [16] and also von Neumann in [17], its area $A(t)$ satisfies

$$\frac{d}{dt}A(t) = \alpha(n-6), \quad t > 0, \quad \alpha = \frac{\pi}{3}\mu\gamma. \tag{2.1}$$

A grain is subject to events which may increase or decrease its number of sides, usually called topological events or critical events, so through its history, we may think of a given grain with area x as satisfying an equation like

$$\frac{d}{dt}x(t) = \alpha(n(t)-6), \quad t > 0, \tag{2.2}$$

where $n(t)$ may increase or decrease by 1 at a time at various times and if $x(t) = 0$, the grain is deleted from the system. Thus $x(t)$ is like the sample path of a stochastic process. Deducing a master equation for the ensemble of grains based on this notion does not seem possible, but the perception that there should be such a master equation is what motivates our thinking.

Let

$f_n(x,t)$ be the density of n-sided grains with area x at time t,
$g_n(t) = \int_0^\infty f_n(x,t)dx$ density of grains with n-sides surviving at time t,
$g(t) = \sum g_n(t)$ density of (surviving) grains at time t.

In a time interval during which n-sided grains experience no topological changes, $(T, T+\tau)$, the density f_n changes only through transport so

$$\frac{\partial f_n}{\partial t} + \alpha(n-6)\frac{\partial f_n}{\partial x} = 0, \quad x > 0, \ T < t < T+\tau$$

which leads us to seek a system of equations of the form

$$\begin{aligned} \frac{\partial f_n}{\partial t} + \alpha(n-6)\frac{\partial f_n}{\partial x} &= A_{nn-1}f_{n-1} + A_{nn}f_n + A_{nn+1}f_{n+1}, \\ &\qquad x > 0, \ t > 0, \ n = n_{\min}, \dots, n_{\max} \\ f_n(0,t) = 0, &\qquad t > 0, \ n = 6, \dots, n_{\max} \end{aligned} \tag{2.3}$$

satisfying the conservation conditions

$$\sum_{n_{min} \leqq i \ \leqq n_{max}} A_{ij} = 0, \quad \text{and} \quad A_{ii-1} \geqq 0, \ A_{ii} \leqq 0, \ A_{ii+1} \geqq 0. \tag{2.4}$$

We take $n_{\min} = 3$ and typically in simulation $M \equiv n_{\max} = 11$ or 12. The equations (2.3) have the appearance of a birth/death process with transport; for sufficiently small $\tau > 0$,

$$\mathbf{1} + \tau A, \quad A = (A_{ij})$$

is a probability matrix.

On this basis, we may make several quick observations. Assume that

$$\begin{aligned} A_{nn-1} &> 0, \quad 3 < n \leqq M \\ A_{nn} &< 0, \quad 3 \leqq n \leqq M \\ A_{nn+1} &> 0, \quad 3 \leqq n < M \end{aligned}$$

and that $f_n(x,0) \geqq 0$. Then $f_n(x,t) \geqq 0$, since at the first time t where $f_n(x,t) = 0$ for some x, f_n has a minimum, so $\partial f_n/\partial t \geqq 0$ and f_n is increasing. Now suppose that n-sided grains are extinguished at some time t_0, namely,

$$f_n(x,t_0) = 0, \quad x > 0, \quad \text{some fixed } t_0.$$

Then

$$\frac{\partial f_n}{\partial t} = \frac{\partial f_n}{\partial x} = 0$$

and

$$A_{nn-1} f_{n-1} + A_{nn+1} f_{n+1} = 0$$

so $f_{n-1} = f_{n+1} = 0$, and so forth, whence the solution is extinguished for time $t \geqq t_0$. These arguments may be refined and, essentially, have to do with the ergodicity of the Markov Chain with matrix $\mathbf{1} + \tau A$. We shall not actually be entitled to impose the conditions above on A, but we believe the conclusions to hold nonetheless.

There are two special constraints on (2.3) and (2.4). From the Euler formula (♯ polygons − ♯ edges + ♯ vertices = 1), the average number of sides per grain in the network is 6 since curves can meet only at triple junctions, except for a small number on the outside border, cf. Smith [17]. Assuming this for the initial conditions, we then need that

$$\frac{d}{dt} \sum_n (n-6) \int_0^\infty f_n dx = 0.$$

Now,

$$\begin{aligned} \frac{d}{dt} \sum_n (n-6) \int_0^\infty f_n dx &= \sum_n (n-6)^2 \int_0^\infty \frac{\partial f_n}{\partial t} dx \\ &= -\alpha \sum_n (n-6)^2 \int_0^\infty \frac{\partial f_n}{\partial x} dx + \sum_{nj} (n-6) \int_0^\infty A_{nj} f_j dx \\ &= \alpha \sum_3^5 (n-6)^2 f_n(0,t) + \sum_{n,j} (n-6) \int_0^\infty A_{nj} f_j dx. \end{aligned}$$

Hence, since only grains with 3, 4, or 5 sides can vanish,

$$\alpha \sum_3^5 (n-6)^2 f_n(0,t) = -\sum_{n,j} (n-6) \int_0^\infty A_{nj} f_j dx. \tag{2.5}$$

Secondly, the total area of the configuration remains constant, so

$$\sum_n \int_0^\infty f_n x dx = \text{const.} \tag{2.6}$$

(2.6) is implied by (2.5). It is also easy to check that

$$\frac{d}{dt} g(t) = \alpha \sum_{\mu=3..5} (\mu - 6) f_\mu(0,t) \leqq 0, \tag{2.7}$$

representing that grains are being deleted from the system. To date, it is the only dissipation we have found in the system. The reciprocal of the proportion of the surviving grains is a measure of the average grain area at time t. We shall use the expression

$$\langle \text{area}(t) \rangle = \frac{g(0)}{g(t)}. \tag{2.8}$$

Let us discuss briefly how the matrix A arises from the simulation. There are two possible contributions to non-zero A_{nj}, from grain deletion and from facet switching. Grain disappearance is not a random event, since grains with less than 6 sides tend to vanish, however the grains affected by the vanishing of a given grain may be regarded as having been randomly selected from the ensemble. We limit discussion to grain deletion events in the limited space provided us here.

From (2.1), in a short time τ, a 3-, 4-, or 5-sided grain may disappear. When a 3 sided grain disappears, each of its three neighboring grains loses a side, and, in general, if a μ sided grain disappears, $6 - \mu$ sides are lost. Hence the rate of boundaries lost is

$$\psi(t) = \lim_{\tau \to 0} \sum_3^5 \frac{\mu - 6}{\tau} \int_0^{\alpha(6-\mu)\tau} f_\mu(x,t) dx \tag{2.9}$$

$$= \alpha \sum_3^5 (\mu - 6)^2 f_\mu(0,t) \tag{2.10}$$

consistent with (2.5). This factor is apportioned among the various n in a way determined by interrogation of the simulation. We find that

$$\begin{aligned} A_{nn+1} &= \frac{\psi(t)}{g_{n+1}(t)} a_{n+1} + A^{\text{facet}}_{nn+1}, \\ A_{nn} &= -\frac{\psi(t)}{g_n(t)} a_n + A^{\text{facet}}_{nn}, \\ A_{nn-1} &= A^{\text{facet}}_{nn-1}, \end{aligned} \tag{2.11}$$

where $a_j \geqq 0$ are *constants* with $a_3 + \cdots + a_M = 1$. A^{facet}_{nj} refers to the contribution to A_{nj} from facet interchange and it also depends on t alone and this dependence is through g_j and g. In the product

$$A_{nj} f_j(x,t) = \pm \psi_j(t) a_j \ \frac{f_j(x,t)}{g_j(t)} + \cdots$$

the fraction is the probability density that a grain of j sides has area x and a_j is the conditional probability that a grain loses a side given that it has j sides. As observed, ψ is a measure of the rate, or number of edges, lost through grain disappearance at time t. Facet interchange can change the side class of a grain but not cause its disappearance. The grains affected by switching are selected randomly from the ensemble. If we compromise and replace the terms g_j and g which occur in denominators by $\epsilon + g_j$ and $\epsilon + g$, then the conclusions based on the ergodicity of the Markov Chain are available to us.

We know little about this system of equations. A first objective is to show that the average grain area (2.8) grows linearly in time. Actually, to our knowledge, none of the grain growth models based on the $n-6$ rule have been shown to have this property. There should, in addition be some form of self-similar solution. This means that the relative area density

$$\rho(x,t) = \frac{1}{g(t)} \sum_{n=3\ldots M} f_n(x,t) \tag{2.12}$$

should have a self-similar form for large t. For a range of parameter values, including those derived from the large scale simulation, this seems reasonable. However this self-similar form may depend on the initial data. Perhaps there is a manifold of self-similar solutions.

We present a few results of simulations. Figure 2 shows $\rho(x,0)$ determined from the initial configuration of the large scale simulation and Figure 3 is a typical comparison of $\rho(x,t)$ computed from the master equations with the histogram gathered from the simulation. The master equation description gives quite good agreement with the large scale simulation. The values near $x = 0$ are close and they are subsequently nearly coincident. Decay as $x \to 1$ is of the form $\exp(-\lambda x)$.

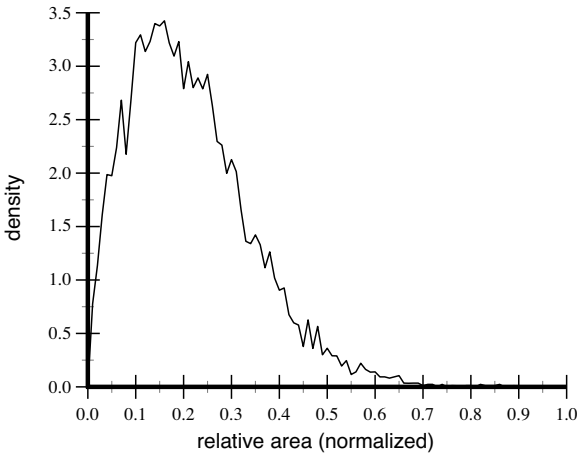

FIGURE 2. Initial relative area histogram gathered from the large scale simulation

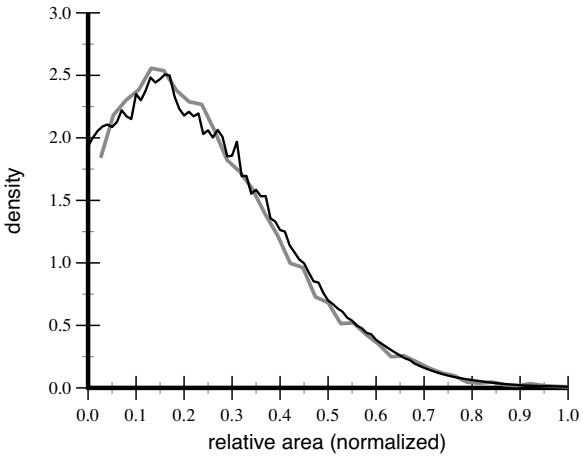

FIGURE 3. Relative area histograms from large scale simulation (thick gray) and from master equation (black)

The evolution of the relative area histogram may be discussed from a long time standpoint by analyzing data collected at 20 to 25 time steps during the simulation, [12]. This results in a Fokker-Planck equation and thus suggests some diffusion behavior in the system, confirmed by computing that the decay of the sequence of histograms to their stationary state is linearly exponential. Although this may be a consequence of the long time interval separating the histograms, which may allow some details of the statistics to equilibrate, transport systems – if not single transport equations – can exhibit diffusive behavior, [15].

The large scale simulations are insensitive to grain boundary energy, even when it depends on both normal angle and lattice misorientation, and agree well with Monte Carlo type simulations. As we discuss in the next section, they do not compare very well with our recent experiments on *Al* thin films, which is a columnar structure.

Other derivations of master equation type systems starting from the $n - 6$ rule have been given in the past, e.g., by Fradkov, [7], and Flyvbjerg, [6]. They are reviewed in [18].

3. Comparison with experiments

Grain growth was examined in 25 and 100 nm thick films of aluminum deposited onto oxidized silicon wafers. Film texture for the 100 nm thick films was characterized through pole figures and found to be strongly $\langle 111 \rangle$ fiber-textured, with little strengthening of this texture upon annealing. The grain structure of the films was characterized by transmission electron microscopy. Additional experimental details are given in [2], [3], cf. also [4].

Aluminum thin films			
Annealing time (h)	Average radius (nm)	Standard deviation	Number of measured grains
0	68	29	1497
0.5	87	42	1304
1	134	73	1100
2	139	68	1353
4	146	75	1455
10	137	45	2022

TABLE 1. Data for 100 nm thick Al grains annealed at 400°C.

Table 1 gives the mean grain size and its standard deviation as a function of annealing time for the 100 nm thick *Al* film. It is clear that grain growth stagnates after one hour, when the grains have nearly doubled in diameter from 68 nm to 134 nm. The subsequent evolution is not exactly self-similar, although the various distributions are not greatly different. The main feature is that the relative area histogram is more shifted toward the left and there is an increased fraction of small grains. This indicates that small grains persist in the structure longer than expected. At the same time, the tails of the distributions show a small but significant number of grains 5 to 18 times larger than the mean. By contrast, very few grains are generally found with areas more than 5 times the mean in simulation.

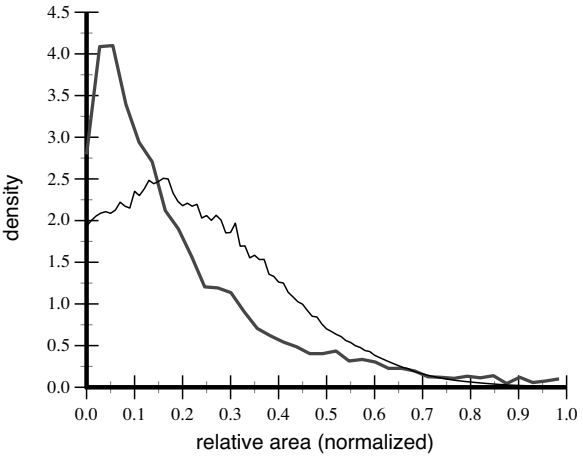

FIGURE 4. Comparison of normalized relative area probabilities for Al thin films (thick gray) at stagnation and the master equation simulation (black)

It is useful to address the issue of stagnation in the thin film. Pinning of grain boundaries by either grooves formed at the film surface or by solute drag has been proposed as a mechanism for stagnation. Solute drag due to Fe impurities cannot explain this behavior, but cf. [8]. Grooves are not expected to form in this film owing to the very stable oxide of Al which forms on exposure to air. In addition, grooving should pin boundaries with low curvature, but small grains, which by necessity have high curvature, are the most affected. Contributions other than grain boundary energy reduction can promote grain growth in thin films. Examples include surface, elastic strain, or plastic strain energies. Minimization of these energies typically promotes development of certain subpopulations of grains and leads to development of strong film texture. Here, however, the films initially had a strong $\langle 111 \rangle$ texture and annealing resulted in minimally enhancing this texture. Finally, the films are in zero stress or low compressive steady state stress state at the annealing temperature. Thus film stress and relaxation are also not expected to play a significant role in observed grain growth and subsequent stagnation. To conclude, the origins of film stagnation in the present context are not understood. Further, it is obvious that the film has not experienced what we generally interpret as normal grain growth.

The simulation and the model of the simulation given by the master equation system we have discussed envisions a long time evolutionary process, so it is not surprising that their grain size statistics differ considerably from the experiment. Nonetheless, there are other statistical features which are quite similar, in particular the relative populations of grains with a given number of sides. We shall have more to report on this in a future work.

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Another Brick in the Wall

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Abstract. We study the homogenization of a linearly elastic energy defined on a periodic collection of disconnected sets with a unilateral condition on the contact region between two such sets, with the model of a brick wall in mind. Using the language of Γ-convergence we show that the limit homogenized behavior of such an energy can be described on the space of functions with bounded deformation using the masonry-type functionals studied by Anzellotti, Giaquinta and Giusti. In this case, the limit energy density is given by the homogenization formula related to the brick-wall type energy.

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1. Introduction

The modeling of 'masonry-like materials' can be undertaken both from a 'macroscopic' and a 'microscopic' standpoint. In the first case the masonry structure is viewed as an elastic continuum sustaining compression but (little or) no tension. The translation of this approach in mathematical terms and within a linearized elasticity theory can be performed by introducing energies of the form

$$\mathcal{F}(u) = \int_\Omega f\big(P_{K^\perp}\mathcal{E}u\big)\,dx, \tag{1.1}$$

where Ω is a reference configuration, $\mathcal{E}u$ is the linearized strain of the deformation u, K is the 'cone of tensile strains' (correspondingly, $K^\perp$ is the cone of 'compressive strains' defined by duality from K), and f is a linear elastic energy density. The operator $P_{K^\perp}$ is the *projection* on the cone of compressive strains. Note that for a uniform compressive strain, when $\mathcal{E}u \equiv A \in K^\perp$ then $f\big(P_{K^\perp}\mathcal{E}u\big) = f(\mathcal{E}u)$ and the material response is linearly elastic, while for a uniform tensile strain, when $\mathcal{E}u \equiv A \in K$, we have $P_{K^\perp}A = 0$, so that $f\big(P_{K^\perp}\mathcal{E}u\big) \equiv 0$. This degeneracy corresponds to the inability of the material to sustain tension. Note that this

degenerate behavior renders the problem mathematically ill-posed, so that in order to solve some problems involving the energy $\mathcal{F}$ within the framework of the direct methods of the Calculus of Variations, it is necessary to extend the definition of $\mathcal{F}$ to the space $BD(\Omega)$ of *functions of bounded deformations* on Ω consisting of functions whose distributional strain Eu is a measure.

Conversely, a masonry structure can be described 'microscopically' as a domain with a structure of a brick wall, with (linear) elastic elements that can be detached from one another at the expense of no energy, but satisfy some unilateral condition at their common boundaries. In the simplest situation, by taking as a model the geometry in Fig. 1, we can consider a periodic 2-dimensional closed set B (in that figure, the union of the boundary of the rectangles in the reference configuration) that subdivides the reference configuration $\Omega \setminus B$ into connected sets. On each of these subsets the material is linearly elastic; i.e., upon possibly changing the norm on the space of symmetric matrices, the energy density of a deformation u is simply $\|\mathcal{E}u\|^2$. If we denote by $\nu(x)$ the normal to B at a point x (that we assume exists almost everywhere with respect to the surface measure) and by $u^{\pm}(x)$ the traces on both sides of B at x (that exist almost everywhere since automatically $u \in H^1(\Omega \setminus B)$) then a unilateral condition can be again expressed by considering a cone of matrices K_0 and requiring that

$$(u^+(x) - u^-(x)) \otimes \nu(x) \in K_0 \tag{1.2}$$

for a.e. $x \in B$. This expression includes for example the constraints $\langle u^+(x) - u^-(x), \nu(x)\rangle \geq 0$ or $u^+(x) - u^-(x) = \lambda\nu(x)$ with $\lambda \geq 0$ a.e. on B, that express a linearized condition of impenetrability.

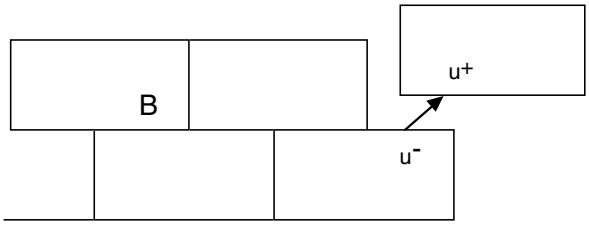

FIGURE 1. Admissible deformation for a brick wall

In this paper we make a connection between the two standpoints described above by showing that the first 'macroscopic' model can be obtained by *homogenization* of the second 'microscopic' one. Namely, we introduce a small parameter ε and consider the energies

$$\mathcal{F}_\varepsilon(u) = \int_{\Omega\setminus\varepsilon B} \|\mathcal{E}u\|^2\,dx \qquad (u^+ - u^-) \otimes \nu^\varepsilon \in K_0 \text{ a.e. on } \varepsilon B \tag{1.3}$$

($\nu^\varepsilon(x)$ is a fixed normal to εB in x), and we show that these energies Γ-converge as $\varepsilon \to 0^+$ to an energy $\mathcal{F}_{\rm hom}$ of the form (1.1) (more precisely, its extension to

$BD(\Omega)$) that may be written as

$$\mathcal{F}_{\rm hom}(u) = \int_\Omega f_{\rm hom}\big(P_{K_{\rm hom}^\perp}\mathcal{E}u\big)\,dx, \tag{1.4}$$

where the cone of *homogenized tensile stresses* $K_{\rm hom}$ and the *effective homogenized energy density* $f_{\rm hom}$ depend both on the 'microgeometry' described by B and on the constraint imposed by K_0, and are expressed by suitable homogenization formulas.

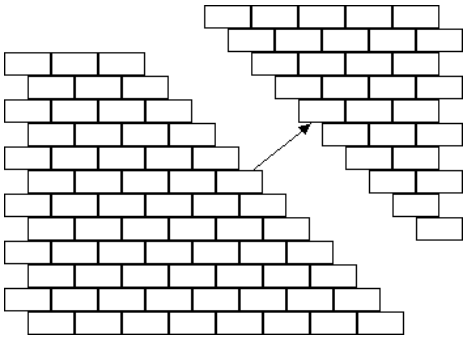

FIGURE 2. A limit macroscopic discontinuity

The proof relies on the localization techniques of Γ-convergence and on results of the BD-theory of masonry-like energies as in (1.1) by Anzellotti [4], Giaquinta and Giusti [16], etc. It has some strong connections with a recent result by Braides, Defranceschi and Vitali [11], where the relaxation of energies of the form

$$\mathcal{H}(u) = \int_{\Omega\setminus J_u} \|\mathcal{E}u\|^2\,dx \qquad (u^+ - u^-)\otimes\nu \in K_0 \text{ a.e. on } J_u \tag{1.5}$$

is performed, where u is constrained to be a piecewise-smooth function outside a closed set J_u (that is itself a variable of the problem). In this case the relaxed energy is again of the form (1.4) but the effective homogenized energy density depends solely on K_0. A detailed analysis when K_0 is related to a no-slip condition in contained in [10]. A mechanical insight in the subject cam be found in [15].

2. Statement of the problem and main result

We denote by $Y = [0,1)^n$ the unit cube of $\mathbb{R}^n$; a set $B \subset \mathbb{R}^n$ is Y-periodic if $B + k = B$ for all $k \in \mathbb{Z}^n$ $\mathbb{M}^{n\times n}$ denotes the space of $n \times n$ real matrices, ${}^tA$ is the transposed of the matrix A, and $A^s := \frac{1}{2}(A + {}^tA)$ its symmetric part. If $a, b \in \mathbb{R}^n$ are vectors then $a \odot b = \frac{1}{2}(a \otimes b + b \otimes a)$ is their symmetric tensor product (i.e., $a\odot b$ is the symmetric part of the tensor product $a\otimes b$) $\mathbb{M}^{n\times n}_{\rm sym}$ denotes the subspace of symmetric matrices of $\mathbb{M}^{n\times n}$ (i.e., such that $A{=}{}^tA$). We fix a scalar product on $\mathbb{M}^{n\times n}_{\rm sym}$ that will be denoted by $\langle A, B\rangle$ and the corresponding norm $\|A\|^2 = \langle A, A\rangle$.

$\mathcal{M}(\Omega;\mathbb{M}^{n\times n})$ is the set of $\mathbb{M}^{n\times n}$-valued measures on Ω with finite total variation. We will use standard notation for Lebesgue and Sobolev spaces.

The space $BD(\Omega)$ is defined by

$$BD(\Omega)=\{u\in L^1(\Omega;\mathbb{R}^n) : Eu\in\mathcal{M}(\Omega;\mathbb{M}^{n\times n})\},$$

where Eu is the *linearized strain tensor*, whose entries are defined by $E_{ij}u=\frac{1}{2}(D_iu_j+D_ju_i)$, where Du denotes the distributional gradient of u. For the measure Eu the Radon-Nikodym decomposition $Eu=\mathcal{E}u\,dx+E_su$ holds. For a function $u\in BD(\Omega)$ the symbol J_u denotes the set of essential discontinuity points for u; we will denote by $SBD(\Omega)$ (*special functions of bounded deformation*) the set of all functions $u\in BD(\Omega)$ such that $|E_su|(\Omega\setminus J_u)=0$. For such functions we have the representation

$$E_su=(u^+-u^-)\odot\nu_u\mathcal{H}^{n-1}\llcorner J_u,$$

where $\mathcal{H}^k$ is the k-dimensional Hausdorff measure, ν_u is the normal to J_u and $u^\pm$ are the traces of u on both sides of J_u (see [1], [2]).

We fix a closed rectifiable Y-periodic $(n-1)$-dimensional subset B of $\mathbb{R}^n$ and a closed cone K_0 of $\mathbb{M}^{n\times n}_{\rm sym}$ contained in $\{a\odot b : a,b\in\mathbb{R}^n\}$. We suppose that K_0 satisfies the following condition:

$$a\odot(b+c)\in K_0 \text{ whenever } a\odot b \text{ and } a\odot c\in K_0. \tag{2.1}$$

A possible choice for K_0 is the set $\{a\odot b:\ a,b\in\mathbb{R}^n,\langle a,b\rangle\geq 0\}$.

Let Ω be a bounded open subset of $\mathbb{R}^n$. For all $\varepsilon>0$ we define

$$\mathcal{U}_\varepsilon(\Omega)=\{u\in SBD(\Omega) : J_u\subseteq\varepsilon B,(u^+-u^-)\odot\nu_u\in K_0\mathcal{H}^{n-1}\text{−a.e.}\},$$

the set of all special functions with bounded deformation whose discontinuity set is contained in εB and such that the density of their singular part belongs to the cone K_0.

In this paper we deal with the homogenization of integral functionals $F_\varepsilon(u):BD(\Omega)\to[0,+\infty]$ of the form

$$F_\varepsilon(u)=\begin{cases}\displaystyle\int_\Omega\|\mathcal{E}u\|^2\,dx & \text{if } u\in\mathcal{U}_\varepsilon(\Omega)\\ +\infty & \text{otherwise,}\end{cases} \tag{2.2}$$

More precisely, we will study the asymptotic behavior of F_ε as $\varepsilon\to 0$ in the sense of Γ-convergence, with respect to the L^2 convergence on $BD(\Omega)\cap L^2(\Omega;\mathbb{R}^n)$.

We define the *homogenized energy density* as

$$\begin{aligned}f_{\rm hom}(A) \;=\; &\inf\Big\{\int_Y\|\mathcal{E}u\|^2dx : u\in BD_{\rm loc}(\mathbb{R}^n),\\ &J_u\subseteq B,(u^+-u^-)\odot\nu_u\in K_0,\ u-Ax\ Y\text{−periodic}\Big\},\end{aligned} \tag{2.3}$$

and the corresponding kernel

$$K_{\rm hom}=\{A\in\mathbb{M}^{n\times n} : f_{\rm hom}(A)=0\}. \tag{2.4}$$

The orthogonal cone $K_{\rm hom}^{\perp}$ is defined by

$$K_{\rm hom}^{\perp} = \{B \in \mathbb{M}^{n\times n}_{\rm sym} : \langle A, B\rangle \le 0 \text{ for all } A \in K_{\rm hom}\}$$

We will prove the following result.

Theorem 2.1. *Suppose that the function $f_{\rm hom}$ satisfies*

$$f_{\rm hom}(A) = f_{\rm hom}\big(P_{K_{\rm hom}^{\perp}} A\big), \tag{2.5}$$

and that it is a convex function on $K_{\rm hom}^{\perp}$; then the family F_ε Γ-converges to F where

$$F(u) = \begin{cases} \displaystyle\int_\Omega f_{\rm hom}(Du)dx & \text{if } u \in \mathcal{U}_{hom}(\Omega) \\ +\infty & \text{otherwise,} \end{cases} \tag{2.6}$$

where

$$\mathcal{U}_{\rm hom} = \{u \in BD(\Omega) : P_{K_{\rm hom}^{\perp}}(E_s u) = 0\}. \tag{2.7}$$

Note that by Korn's inequality indeed all functions in $\mathcal{U}_\varepsilon(\Omega)$ belong to $H^1(\Omega'\setminus \varepsilon B)$ for all $\Omega' \subset\subset \Omega$.

Example. Our theorem applies to a number of model geometries described as follows. For the sake of simplicity we treat the two-dimensional case only.

The simplest geometry is given by taking as B the square lattice

$$B_1 = \{(x, y) \in \mathbb{R}^2 : x \in \mathbb{Z} \text{ or } y \in \mathbb{Z}\}.$$

The usual brick-wall structure can be parameterized by

$$B_2 = \{(x, y) : 2y \in \mathbb{Z}\} \cup \{(x, y) : [2y] \text{ even}, x \in \mathbb{Z}\} \cup \{(x, y) : [2y] \text{ odd}, x + 1/2 \in \mathbb{Z}\}$$

(see Fig. 3 (a) and (b)).

Note that in both cases we have that $\nu \in \{\pm e_1, \pm e_2\}$ $\mathcal{H}^1$-a.e. on B.

We can consider the two cones of matrices

$$K_1 = \{a \odot b : a = \lambda b,\ \lambda \ge 0\}$$

and

$$K_2 = \{a \odot b : \langle a, b\rangle \ge 0\}.$$

Correspondingly, we have four cases in which $f_{\rm hom}$ can be easily described.

(1) When considering the geometry given by $B = B_1$ and $K_0 = K_1$ the function $f_{\rm hom}$ is given on symmetric matrices by

$$f_{\rm hom}\begin{pmatrix} a & b \\ b & c \end{pmatrix} = (a_-)^2 + b^2 + (c_-)^2,$$

the minimum in problem (2.3) being given by the function $u(x, y) = (-a_- x + by, -c_- y + bx)$. The corresponding kernel is

$$K_{\rm hom} = \left\{\begin{pmatrix} a & 0 \\ 0 & c \end{pmatrix} :\ a \ge 0,\ c \ge 0\right\}.$$

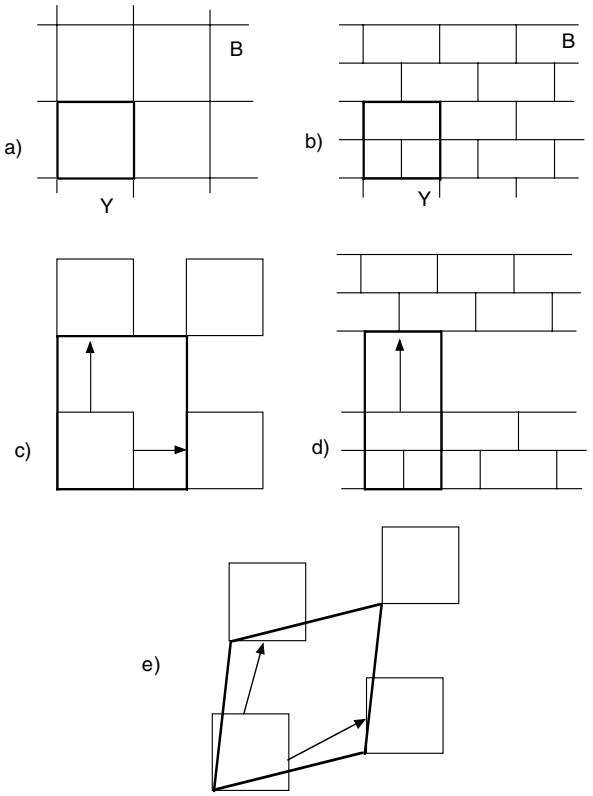

FIGURE 3. The geometries of the example and related zero-energy displacements

(2) If $B = B_2$ and $K_0 = K_1$ the function $f_{\rm hom}$ is given on symmetric matrices by

$$f_{\rm hom}\begin{pmatrix} a & b \\ b & c \end{pmatrix} = a^2 + b^2 + (c_-)^2,$$

a minimum in problem (2.3) being given by the function $u(x, y) = (ax+by, -c_-y+bx)$. The corresponding kernel is

$$K_{\rm hom} = \left\{ \begin{pmatrix} 0 & 0 \\ 0 & c \end{pmatrix} : c \geq 0 \right\}.$$

(3) In the two remaining cases with $K_0 = K_2$ the function $f_{\rm hom}$ is given on symmetric matrices by

$$f_{\rm hom}\begin{pmatrix} a & b \\ b & c \end{pmatrix} = (a_-)^2 + (c_-)^2.$$

The corresponding kernel is

$$K_{\hom} = \left\{ \begin{pmatrix} a & b \\ b & c \end{pmatrix} : \ a \geq 0, \ c \geq 0 \right\}.$$

In the case $B = B_1$ the minimum in problem (2.3) is given by the function $u(x, y) = (-a_- x, -c_- y)$, and similarly in the case $B = B_2$.

In Fig. 3 (c)–(e) we have pictured three displacement fields with zero energy, related to case (1)–(3), respectively. The area with a thick contour represents the image of Y through $I + A$.

3. Proof of the result

The result can be proven in part following the usual localization methods of Γ-convergence, and in part using recent (and less recent) results on energies defined on BD with constraints on the strain. The proof can be divided into three steps: 1) existence and representation of the Γ-limit on $H^1(\Omega; \mathbb{R}^n)$; 2) Γ-liminf inequality by a convolution argument and translation invariance; 3) Γ-limsup inequality by density.

Step 1. As customary, we localize the energies on open subsets U of Ω by setting

$$F_\varepsilon(u, U) = \begin{cases} \displaystyle\int_{U \setminus \varepsilon B} \|\mathcal{E}u\|^2 \, dx & \text{if } u \in \mathcal{U}_\varepsilon(\Omega) \\ +\infty & \text{otherwise.} \end{cases} \tag{3.1}$$

By a density argument we may assume that the Γ-limit $F(u, U)$ exists for all u and for U in a dense class $\mathcal{D}$ of open sets (e.g., all polyrectangles with rational vertices). The extension of such a set function $F(u, \cdot)$ can be proved to be a measure (the crucial point is to prove the subadditivity with respect to the set variable; this can be done as in [11] Step 5 in the proof of Theorem 5.1). By comparing (the extension of) F with the pointwise limit on $H^1(\Omega; \mathbb{R}^n)$ we have that

$$F(u, U) \leq \int_U \|\mathcal{E}u\|^2 \, dx \leq c \int_U |Du|^2 \, dx;$$

hence we may apply the usual integral representation theorems on $H^1(\Omega; \mathbb{R}^n)$ (see [9] Section 9,[12]) to conclude that there exists a function f such that

$$F(u, U) = \int_U f(x, Du) \, dx.$$

It is easily seen that indeed $f(x, Du)$ does not depend on x (see e.g. [9] Proposition 14.3). Moreover, f depends only on the symmetric part of the gradient; i.e., $f(A) = f(B)$ whenever $A^s = B^s$. In fact, If $u_\varepsilon \to Ax$ is a sequence in $\mathcal{U}_\varepsilon(\Omega)$ such that

$$|\Omega| f(A) = \lim_{\varepsilon \to 0^+} F_\varepsilon(u_\varepsilon),$$

then we may set $v_\varepsilon = u_\varepsilon + (B-A)x$ and note that $v_\varepsilon \in \mathcal{U}_\varepsilon(\Omega)$, $v_\varepsilon \to Bx$ and $Ev_\varepsilon = Eu_\varepsilon$, so that

$$|\Omega| f(B) \le \liminf_{\varepsilon\to 0^+} F_\varepsilon(v_\varepsilon) = \lim_{\varepsilon\to 0^+} F_\varepsilon(u_\varepsilon) = |\Omega| f(A).$$

Hence, we have $f(B) \le f(A)$ and by symmetry $f(B) = f(A)$.

It remains then to check that f is given by the homogenization formula (2.3). To this end, choose $U = (0,1)^n$, and a sequence $u_\varepsilon \to Ax$ in $\mathcal{U}_\varepsilon((0,1)^n)$ such that

$$f(A) = \lim_{\varepsilon\to 0^+} F_\varepsilon(u_\varepsilon). \tag{3.2}$$

Fix $\delta > 0$ and define $\varphi(y) = \Big(\frac{1}{\delta}\mathrm{dist}(y,\partial Y)\Big) \wedge 1$ and $S_\delta = \{y \in Y : \mathrm{dist}(y,\partial Y)\Big) < \delta\}$. Set

$$v_\varepsilon = \varphi u_\varepsilon + (1-\varphi)Ax,$$

and note that

$$(v_\varepsilon^+ - v_\varepsilon^-) \odot \nu_{v_\varepsilon} = \varphi(u_\varepsilon^+ - u_\varepsilon^-) \odot \nu_{u_\varepsilon}$$

on εB, so that $v_\varepsilon \in \mathcal{U}_\varepsilon((0,1)^n)$. We extend v_ε to a function defined on $\varepsilon[\frac{1}{\varepsilon}+1]Y$ ($[t]$ is the integer part of t) by setting

$$w_\varepsilon(y) = \begin{cases} v_\varepsilon(y) & \text{if } y \in Y \\ Ay & \text{if } y \in \varepsilon[\frac{1}{\varepsilon}+1]Y \setminus Y. \end{cases}$$

The function w_ε is then extended to all $\mathbb{R}^n$ by requiring that $w_\varepsilon(y) - Ay$ be $\varepsilon[\frac{1}{\varepsilon}+1]Y$periodic. If we set

$$z_\varepsilon(y) = \frac{1}{\varepsilon} \sum_{k\in\{0,\dots,[\frac{1}{\varepsilon}]\}^n} w_\varepsilon(\varepsilon y + \varepsilon k),$$

then z_ε is Y-periodic and ad admissible test function for the computation of $f_{\mathrm{hom}}(A)$. By the periodicity of w_ε and Jensen's inequality we have

$$\begin{aligned} f_{\mathrm{hom}}(A) &\le \int_Y \|\mathcal{E} z_\varepsilon\|^2\,dy \\ &= \frac{1}{\varepsilon^n[\frac{1}{\varepsilon}+1]^n} \int_{\varepsilon[\frac{1}{\varepsilon}+1]Y} \|\mathcal{E} z_\varepsilon\|^2\,dy \le \frac{1}{\varepsilon^n[\frac{1}{\varepsilon}+1]^n} \int_{\varepsilon[\frac{1}{\varepsilon}+1]Y} \|\mathcal{E} w_\varepsilon\|^2\,dy \\ &\le \int_Y \|\mathcal{E} v_\varepsilon\|^2 + \|A^s\|\Big(\varepsilon^n[\frac{1}{\varepsilon}+1]^n - 1\Big). \end{aligned} \tag{3.3}$$

We then have to estimate this last term. Let $\eta > 0$; we have (for a suitable constant c_η)

$$\begin{aligned}\int_{(0,1)^n} \|\mathcal{E}v_\varepsilon\|^2\,dy &= \int_{(0,1)^n\setminus S_\delta} \|\mathcal{E}u_\varepsilon\|^2\,dy \\ &\quad + \int_{S_\delta} \|\varphi\mathcal{E}u_\varepsilon + (1-\varphi)A^s + D\varphi\odot(u_\varepsilon - Ay)\|^2\,dy \\ &\le (1+\eta)\int_{(0,1)^n} \|\mathcal{E}u_\varepsilon\|^2\,dy \\ &\quad + c_\eta|S_\delta|\|A^s\|^2 + c_\eta\frac{1}{\delta^2}\int_{(0,1)^n}|u_\varepsilon - Ay|^2\,dy.\end{aligned}$$

By letting first $\varepsilon\to 0^+$, $\delta\to 0^+$ and $\eta\to 0^+$ we get

$$\limsup_{\varepsilon\to 0^+}\int_{(0,1)^n}\|\mathcal{E}v_\varepsilon\|^2\,dy \le \limsup_{\varepsilon\to 0^+}\int_{(0,1)^n}\|\mathcal{E}u_\varepsilon\|^2\,dy, \tag{3.4}$$

so that, by (3.3), (3.4) and (3.2),

$$f_{\rm hom}(A) \le \liminf_{\varepsilon\to 0^+}\int_Y \|\mathcal{E}z_\varepsilon\|^2\,dy \le \lim_{\varepsilon\to 0^+}\int_Y\|\mathcal{E}u_\varepsilon\|^2\,dy \le f(A).$$

The converse inequality is obtained by estimating $f(A)$ using the liminf inequality of Γ-convergence upon choosing $u_\varepsilon\to Ay$ of the form $u_\varepsilon(x) = \varepsilon u(x/\varepsilon)$, where u is an admissible test function for (2.3).

Step 2. To prove the lower-bound inequality we use a convexity method through convolutions (see [14], [9] Section 14.3.2). We first remark that, setting $u^y(x) = u(x-y)$, we have that if the Γ-limit $F(u,U)$ exists then we have

$$F(u^y, y+U) = F(u,U).$$

Next, we choose a sequence U_k converging increasingly to Ω with $U_k\subset\subset\Omega$, and we suppose (upon subsequences) that

$$F(u,U) = \Gamma\text{-}\lim_j F_{\varepsilon_j}(u,U)$$

for all $U = U_k$ and for $U=\Omega$ (this is not restrictive upon enlarging the class $\mathcal{D}$ above). By Step 1 we have that

$$F(u,U) = \int_U f_{\rm hom}(\mathcal{E}u)\,dx$$

on such U. By hypothesis (2.5) we may also write

$$F(u,U) = \int_U f_{\rm hom}\Big(P_{K^\perp_{\rm hom}}\mathcal{E}u\Big)\,dx.$$

Let ρ_j be a sequence of mollifiers with supports in $B_{1/j}(0)$. We then have

$$\begin{aligned} F_\#(\rho_j * u, U_k) &= F(\rho_j * u, U_k) \\ &\le \int_{B_{1/j}(0)} \rho_j(y) F(u^y, U_k)\, dy \\ &\le \int_{B_{1/j}(0)} \rho_j(y) F(u, \Omega)\, dy = F(u, \Omega). \end{aligned}$$

By [4, 11] the functional

$$F_\#(u, U) = \begin{cases} \displaystyle\int_U f_{\rm hom}\Big(P_{K^\perp_{\rm hom}} \mathcal{E}u\Big)\, dx & \text{if } P_{K^\perp_{\rm hom}} \mathcal{E}_s u = 0 \\ +\infty & \text{otherwise} \end{cases}$$

is weakly lower semicontinuous on BD. We can then pass to the limit as $j \to +\infty$ to obtain

$$F_\#(u, U_k) \le \liminf_j F_\#(\rho_j * u, U_k) \le F(u, \Omega).$$

We may then take the supremum in k to get

$$F_\#(u, \Omega) \le F(u, \Omega).$$

By the arbitrariness of the sequence (ε_j) we obtain

$$F_\#(u, \Omega) \le \Gamma\text{-}\liminf_{\varepsilon \to 0^+} F_\varepsilon(u, \Omega).$$

Note in particular that $F(u, \Omega) = +\infty$ if $u \notin \mathcal{U}(\Omega)$.

Step 3. To prove the upper bound we use an approximation result by Anzellotti (see [4] Theorem 10.2) that states that for all $u \in \mathcal{U}(\Omega)$ there exists a sequence $u_k \in H^1(\Omega; \mathbb{R}^n)$ converging weakly* to u such that

$$P_{K^\perp_{\rm hom}} \mathcal{E}u_k \to P_{K^\perp_{\rm hom}} \mathcal{E}u$$

strongly in L^2, and hence in particular

$$F_\#(u, \Omega) = \liminf_k F_\#(u_k, \Omega).$$

By the lower semicontinuity of the Γ-lim sup we then obtain

$$\begin{aligned} \Gamma\text{-}\limsup_{\varepsilon \to 0^+} F_\varepsilon(u, \Omega) &\le \liminf_k \Big(\Gamma\text{-}\limsup_{\varepsilon \to 0^+} F_\varepsilon(u_k, \Omega)\Big) \\ &= \lim_k F_\#(u_k, \Omega) = F_\#(u, \Omega) \end{aligned}$$

as desired. □

4. Perspectives

The results presented here lead to various additional questions. One is whether assumption (2.5) on the effective energy density $f_{\rm hom}$ can be altogether dropped, or some general assumptions on the set B and the cone K_0 can be found that ensure its validity. Another direction of investigation may be adding some energy on the discontinuity set B, and consider energies of the form

$$F_\varepsilon(u) = \int_\Omega \|\mathcal{E}u\|^2\,dx + \int_{\Omega\cap\varepsilon B} \varphi_\varepsilon(u^+ - u^-)\,d\mathcal{H}^{n-1}.$$

Referring to the sets K_1 and K_2 in the example the functions φ_ε may satisfy different growth conditions when $u^+ - u^-$ points in the direction of ν, mimicking a plastic or an elastic behavior, and when it is orthogonal to ν (to mimic, e.g., friction). In this case the results of the present paper should be integrated with those in [3] (see also [9] Section 18). Furthermore, most of these problems can be rephrased in a nonlinearly elastic framework, where some of the analog of the results in [10, 11] are still to be proved. Part of these questions will be addressed in [8].

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Variational Problems for Functionals Involving the Value Distribution

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Abstract. We study variational problems involving the measure of level sets, or more precisely the push-forward of the Lebesgue measure. This problem generalizes variational problems with finitely many (discrete) volume constraints. We obtain existence results for this general framework. Moreover, we show the surprising existence of asymmetric solutions to symmetric variational problems with this type of volume constraints.

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1. Introduction

Variational problems consist of a functional $\mathcal{F}$ and a class $\mathcal{A}$ of admissible functions on a set $\Omega \subset \mathbb{R}^N$ among which the functional has to be minimized (or maximized).

There are many possible constraints that can be posed on the functions in $\mathcal{A}$, e.g., regarding regularity or the average of the function on Ω.

In the last years, classes $\mathcal{A}$ which are connected with the measure of level sets of the functions have been studied in different frameworks. In particular, there is a series of works where the measure of certain level sets is prescribed. As a prototypical example we may prescribe the measure of the sets $u^{-1}(0) = \{x \in \Omega;\ u(x) = 0\}$ and $u^{-1}(1) = \{x \in \Omega;\ u(x) = 1\}$ for all functions $u \in \mathcal{A}$. Such constraints are called "volume–" or "level set constraints". Here the geometrical and topological shape of the level sets $u^{-1}(0)$ and $u^{-1}(1)$ is *a priori* completely arbitrary.

A typical variational problem with volume constraints reads as

$$\text{Minimize } \mathcal{F}(u) := \int_\Omega |\nabla u(x)|^2 \, dx \tag{1.1}$$

among all functions in

$$\mathcal{A} := \Big\{ u \in H^1(\Omega, \mathbb{R});\ |\{x \in \Omega,\ u(x) = 0\}| = \alpha,\ |\{x \in \Omega,\ u(x) = 1\}| = \beta \Big\},$$

where $|\cdot|$ denotes the Lebesgue measure of a set, and α and β are positive constants with $\alpha + \beta < |\Omega|$.

Similar minimization problems but with only one volume constraint have been studied by various authors, see, e.g., [2]. Recently problems with two or more constraints have caught attention [4, 17, 18, 19, 21, 22, 23], partially motivated by physical problems related to immiscible fluids [14] and mixtures of micromagnetic materials [1].

These problems have a very different nature than problems with only one volume constraint: In the case of one volume constraint, only additional boundary conditions or the form of the energy can induce transitions of the solution between different values. Two or more volume constraints, on the other hand, force transitions of the solution by their very nature. Ambrosio, Marcellini, Fonseca and Tartar [4] studied this class of problems for the first time and proved an existence result for the problem of two (or more) level set constraints with an energy density of the form

$$\mathcal{F}(u) = \int_\Omega f(|\nabla u|).$$

It turned out that unlike usual variational problems, lower order terms in the function f pose hard problems for the analysis and can lead, even in very easy examples, to nonexistence of optimal solutions [17, 19]. However, under certain regularity assumptions on the energy density the existence results were extended to quite general energy functionals depending on ∇u and u [19]. For the special case of one space dimension a somewhat complete analysis of existence and uniqueness has been given in [17]. These results have been partially extended to the higher dimensional setting in [18].

The original motivation for this paper was to generalize these ideas from finitely many prescribed levels to more arbitrary (possibly infinitely many). In fact, it is possible to define a notion of volume constraints on arbitrary levels, even on the whole range of a function. As an illustration imagine a transparency which casts a shadow, see Fig. 1. The density of the shadow will then be determined by the shape of the transparency. A typical problem could be to find the optimal shape of the transparency under the constraint of a prescribed shadow density. The mathematical equivalent of the shadow density is the push-forward $u^\#$ of the Lebesgue measure through u, as will be explained in Section 2. The study of $u^\#$ leads to a class of minimization problems which entail not only classical volume constrained problems, but also variational problems that have been investigated in connection with vortex dynamics [9, 10, 11] and plasma physics (compare [16] and the references therein).

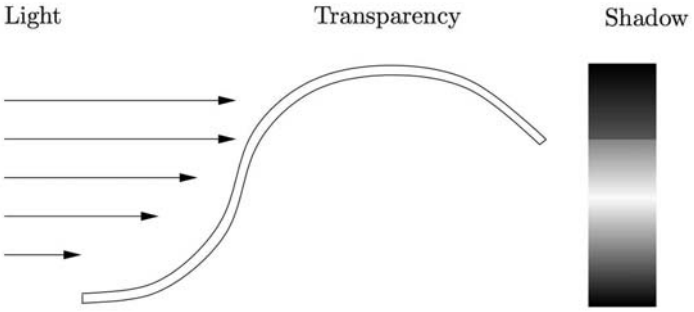

FIGURE 1. Interpretation of the push-forward $u^{\#}$ as the shadow of a curved transparency.

The connection of our general setting to the classical volume constrained problems is explained in more details in Section 3. Additionally, we present existence results for a certain class of generalized volume constrained problems. A number of examples conclude the section.

In the final Section 4, we apply methods from symmetric rearrangements to discuss the symmetry behavior of these problems and to construct some examples with interesting symmetry breaking solutions.

2. Value distributions and optimization problems

In all the paper Ω will be a bounded open subset of $\mathbb{R}^N$ with a Lipschitz boundary. We recall that, for every $u \in L^1(\Omega)$, the distribution measure $u^{\#}$ associated to u is the push-forward of the measure $\mathscr{L}^N \llcorner \Omega$ through u, that is

$$u^{\#}(E) = \mathscr{L}^N\big(\Omega \cap u^{-1}(E)\big) \tag{2.1}$$

for every Borel subset E of $\mathbb{R}$, where $\mathscr{L}^N$ denotes the N-dimensional Lebesgue measure. It turns out that $u^{\#}$ is a nonnegative measure on the real line, such that

$$u^{\#}(\mathbb{R}) = \mathscr{L}^N(\Omega). \tag{2.2}$$

We sometimes call $u^{\#}$ the *value distribution* of u.

Example 2.1. If $u(x) = c$ is a constant function, by (2.1) we have $u^{\#} = \mathscr{L}^N(\Omega) \cdot \delta_c$ where δ_c is the Dirac mass at the point $c \in \mathbb{R}$.

Analogously, if we denote the characteristic function of a set A by χ_A and consider the piecewise constant function $u = \sum_{i \in I} c_i \chi_{\Omega_i}$, we have that $u^{\#} = \sum_{i \in I} \mathscr{L}^N(\Omega_i) \cdot \delta_{c_i}$.

Example 2.2. In the case $N = 1$, if $u\colon (a, b) \to \mathbb{R}$ is a monotone nondecreasing function, then it is easy to see that $u^{\#} = (u^{-1})' \llcorner (\alpha, \beta)$ where $(u^{-1})'$ is the distributional derivative of the monotone nondecreasing function u^{-1} and $\alpha, \beta \in [-\infty, +\infty]$ are defined by $\alpha = \lim_{\varepsilon \to 0} u(a + \varepsilon)$, $\beta = \lim_{\varepsilon \to 0} u(b - \varepsilon)$.

The following result relates the convergence of a sequence of functions to the one of the corresponding value distributions.

Proposition 2.3. *Assume that $u_n \to u$ strongly in $L^1(\Omega)$. Then $u_n^\# \to u^\#$ in the weak$\star$-convergence of measures.*

Proof. By (2.2) the measures $u_n^\#$ have bounded total mass; therefore, it is enough to show that for every smooth function $\varphi : \mathbb{R} \to \mathbb{R}$ with compact support we have

$$\int_{\mathbb{R}} \varphi \, du_n^\# \to \int_{\mathbb{R}} \varphi \, du^\# \ .$$

By a change of variables we obtain

$$\lim_{n\to\infty} \int_{\mathbb{R}} \varphi \, du_n^\# = \lim_{n\to\infty} \int_\Omega \varphi\big(u_n(x)\big)\, dx = \int_\Omega \varphi\big(u(x)\big)\, dx = \int_{\mathbb{R}} \varphi \, du^\# \ , \qquad (2.3)$$

where in the second equality we used the fact that $u_n \to u$ in $L^1(\Omega)$ and that φ is smooth. □

The variational problems we consider are of the form

$$\min\big\{F(u) + G(u^\#) \ : \ u \in X\big\} \qquad (2.4)$$

where:

- the function space X is either a Sobolev space $W^{1,p}(\Omega)$, $W_0^{1,p}(\Omega)$ $(1 \le p \le \infty)$ or the space $BV(\Omega)$ of functions with bounded variation;
- the functional F is sequentially lower semicontinuous with respect to the weak $W^{1,p}(\Omega)$ convergence (if $p < \infty$) or the weak$\star$-convergence $\big($in the cases $X = W^{1,\infty}(\Omega)$ or $X = BV(\Omega)\big)$;
- the functional G is sequentially lower semicontinuous with respect to the weak$\star$-convergence on measures.

The following existence theorem is straightforward.

Theorem 2.4. *In addition to the conditions above we assume:*

(i) *F is coercive on X, that is for every $c \in \mathbb{R}$ the set $\{F(u) \le c\}$ is sequentially compact for the weak convergence $\big($weak$\star$ if $X = W^{1,\infty}(\Omega)$ or $X = BV(\Omega)\big)$;*

(ii) *there exists at least one function $u_0 \in X$ such that $F(u_0) + G(u_0^\#) < +\infty$.*

Then the minimum problem (2.4) *admits at least one solution.*

Proof. It follows by a straightforward application of the direct methods of the calculus of variations, taking into account Proposition 2.3. □

A typical choice for F is to consider integral functionals like

$$F(u) = \int_\Omega f(x, u, Du)\, dx \qquad (2.5)$$

where $f : \Omega \times \mathbb{R} \times \mathbb{R}^N \to [0, +\infty]$ is a Borel integrand such that $f(x, \cdot, \cdot)$ is lower semicontinuous and $f(x, s, \cdot)$ is convex. Then (see for instance [12, 13]) the functional in (2.5) turns out to be sequentially lower semicontinuous with respect

to the weak convergence in $W^{1,p}(\Omega)$ (weak$\star$ if $p = \infty$). Some extra assumptions on the regularity of the integrand f are required in the case $X = BV(\Omega)$, as well as a refinement of the definition of the functional F, since the gradient Du is in this case a vector measure. We refer the interested reader to [5, 12] for further details.

In the case of functionals of the form (2.5) the coercivity condition (i) of Theorem 2.4 is fulfilled whenever

- $f(x, s, z) \geq \alpha|z|^p$ (with $\alpha > 0$) if $X = W^{1,p}(\Omega)$ with $1 < p < \infty$;
- $f(x, s, z) \geq \alpha|z|$ (with $\alpha > 0$) if $X = BV(\Omega)$;
- $f(x, s, z) \geq H(|z|)$ with H superlinear, that is $\lim_{t\to+\infty} H(t)/t = +\infty$, if $X = W^{1,1}(\Omega)$;
- $f(x, s, z) = +\infty$ for $|z| > \alpha$ (with $\alpha > 0$) if $X = W^{1,\infty}(\Omega)$.

In order to define the functional G, it is convenient to decompose any measure μ into an absolutely continuous part (with respect to the Lebesgue measure) with a density $\rho \in L^1$, and a singular part, which we denote by σ. The singular measure σ can be further decomposed into a Cantor part σ^c and an atomic part σ^0, so that we obtain

$$\mu = \rho \cdot dx + \sigma^c + \sigma^0 \ .$$

An index u to the measures $\mu, \rho, \sigma, \sigma^c, \sigma^0$ stands to denote that they are related to u via the equality $\mu_u = u^\#$.

The class of weakly$\star$ lower semicontinuous functionals on measures have been systematically studied by Bouchitté and Buttazzo in [6, 7, 8]; for simplicity here we limit ourselves to the ones which are invariant under translations in the x-variable. Then, in our case we have the characterization formula

$$G(\mu) = \int_{\mathbb{R}} g(\rho)\, dt + \int_{\mathbb{R}} g^\infty(\sigma^c) + \int_{\mathbb{R}} \vartheta(\sigma^0)\, d\mathscr{H}^0 \tag{2.6}$$

where:

- g is convex and lower semicontinuous;
- g^∞ is the recession function of g given by $g^\infty(z) = \lim_{s\to+\infty} g(sz)/s$;
- $\mathscr{H}^0$ is the counting measure;
- ϑ is a subadditive function satisfying the compatibility condition

$$g^\infty(z) = \lim_{s\to 0^+} \frac{\vartheta(sz)}{s} \ .$$

Example 2.5. Consider the functional (of *desired distribution penalization*)

$$G(\mu) = \begin{cases} \int_{\mathbb{R}} |\rho(t) - \rho_0(t)|^2\, dt & \text{if } \sigma \equiv 0 \\ +\infty & \text{otherwise.} \end{cases} \tag{2.7}$$

where ρ_0 is a given L^2 function. Then by Theorem 2.4 the minimization problem

$$\min\Big\{ \int_\Omega |Du|^2\, dx + \int_{\mathbb{R}} |\rho_u(t) - \rho_0(t)|^2\, dt \ : \ u \in H^1_0(\Omega),\ u^\# \ll \mathscr{L}^N \Big\}$$

admits at least one solution.

Example 2.6. Consider the Mumford-Shah like functional

$$G(\mu) = \begin{cases} \alpha \int_{\mathbb{R}} \rho^2(t)\,dt + \beta \mathscr{H}^0(\text{supp } \sigma^0) & \text{if } \sigma^c \equiv 0 \\ +\infty & \text{otherwise.} \end{cases}$$

(with $\alpha, \beta > 0$) which is weakly$\star$ lower semicontinuous by the arguments above. Then by Theorem 2.4 the minimization problem

$$\min \Big\{ \int_\Omega |Du|^2\,dx + \alpha \int_{\mathbb{R}} \rho_u^2(t)\,dt + \beta \mathscr{H}^0(\text{atoms of } u^\#) \ : \ u \in H_0^1(\Omega),\ (u^\#)^c \equiv 0 \Big\}$$

admits at least one solution. In the one-dimensional case, with $\Omega = (-1,1)$, it is easy to see that the minimum value of the problem is $\beta \wedge 6\alpha^{2/3}$, reached at $u \equiv 0$ if $\beta \le 6\alpha^{2/3}$ and at $u(x) = \alpha^{1/3}(1 - |x|)$ if $\beta \ge 6\alpha^{2/3}$.

The framework above can be repeated in the case of vector valued functions $u : \Omega \to \mathbb{R}^m$. Setting again

$$u^\#(E) = \mathscr{L}^N\big(\Omega \cap u^{-1}(E)\big)$$

for every Borel subset E of $\mathbb{R}^m$, we have that $u^\#$ is a nonnegative measure on $\mathbb{R}^m$, with $u^\#(\mathbb{R}^m) = \mathscr{L}^N(\Omega)$. For instance, in the case $N = m$, if $u : \Omega \to \mathbb{R}^N$ is a regular invertible function we have that

$$u^\# = |\det Du^{-1}| \cdot \mathscr{L}^N \llcorner u(\Omega)\ .$$

By the way, this formula allows to define the Jacobian for nonregular functions v by

$$|\det Dv| := (v^{-1})^\#,$$

compare, e.g., [20].

The previous tools, as Proposition 2.3 and Theorem 2.4, still hold and we may obtain existence results for minimum problems of the form (2.4) where now:

- F is a variational integral like

$$F(u) = \int_\Omega f(x, u, Du)\,dx$$

  with $f(x, s, \cdot)$ quasiconvex and coercive (we refer to [13] for the lower semicontinuity results of integral functionals in the vector valued setting);
- G is a weakly$\star$ lower semicontinuous functional on measures.

For instance, as in Examples 2.5 and 2.6, the minimum problems

$$\min \Big\{ \int_\Omega f(Du)\,dx \quad + \int_{\mathbb{R}^m} |\rho_u(y) - \rho_0(y)|^2\,dy \\ : \ u \in W_0^{1,p}(\Omega;\mathbb{R}^m),\ u^\# \ll \mathscr{L}^N \Big\}$$

and

$$\min \Big\{ \int_\Omega f(Du)\,dx \quad + \alpha \int_{\mathbb{R}^m} \rho_u^2(y)\,dy + \beta \mathscr{H}^0(\text{atoms of } u^\#) \\ : \ u \in W_0^{1,p}(\Omega;\mathbb{R}^m),\ (u^\#)^c \equiv 0 \Big\}$$

both admit a solution, provided f is quasiconvex and $f(z) \ge c|z|^p$ with $c > 0$ and $p > 1$.

3. Generalized volume constraints

3.1. Smooth rearrangements and existence

In this section we consider a special case of the problem (2.4) by setting for a given measure μ_0 and a set $S \subset \mathbb{R}$:

$$G(\mu) := \begin{cases} 0 & \text{if } \mu|_S = \mu_0|_S \\ +\infty & \text{otherwise.} \end{cases} \tag{3.1}$$

This class of problems includes standard problems with volume constraints (also called "level set constraints") as considered, e.g., in [4, 17, 19, 23]. In fact, by setting $S := \{m_1, m_2, \dots, m_n\}$ and $\mu_0 = \sum_{i=1}^n \alpha_i \delta_{m_i}$ we obtain the classical volume constraints

$$|\{x \in \Omega :\ u(x) = m_i\}| = \alpha_i, \quad \text{for } i = 1, \dots, n. \tag{3.2}$$

Obviously, problem (3.1) is in general not solvable. Take, e.g., the measure $\mu_0 = 0$, the set $\Omega = (0, 1)$, $S = \mathbb{R}$ and the Sobolev space $X = H^1(\Omega)$, then there is simply no function $u \in X$ such that $u^\# \equiv 0$. A first necessary condition is therefore $\int_S \mu_0 \le |\Omega|$ (with equality if $S = \mathbb{R}$), compare (2.2). However, this condition is not sufficient, as it can be seen from the examples in [19] and [17]. One of the difficulties is that a minimizing sequence satisfying the constraint (3.1) may have a limit which does not satisfy the constraint. Indeed, it is easy to see that this can happen whenever S is not open. In other words, we have the following proposition:

Proposition 3.1. *The functional G defined by* (3.1) *is weakly$\star$ lower semicontinuous if and only if S is open.*

In the classical setting of finitely many volume constraints as in (3.2), S is a finite union of points and hence not open, which leads to a lack of semicontinuity of G, and allows for non-existence of solutions to the minimization problem, compare [17, 19].

In the following, we want to consider the case where S is open. For simplicity, we assume $S = \mathbb{R}$. Similar problems have been considered, e.g., in [9, 16].

According to Theorem 2.4, it is sufficient for the existence of a minimizer to prove that there is at least one function $u_0 \in X$ such that $F(u_0) + G(u_0^\#) < +\infty$. In the case of G given by (3.1), this can be restated as

$$K_{\mu_0}(X) := \{u \in X;\ u^\# = \mu_0\} \neq \emptyset.$$

Hence we arrive at the problem of finding a "smooth rearrangement" of a given value distribution μ_0. The following theorem gives sufficient conditions for this problem which are sharp for certain spaces X:

Theorem 3.2. *Let $\Omega \subset \mathbb{R}^N$ be a bounded open set with Lipschitz boundary and let $1 < p < +\infty$. Let μ_0 be a nonnegative measure with $|\mu_0| = |\Omega|$ and absolutely continuous part ρ, and let $S := \operatorname{conv}(\operatorname{supp} \mu_0)$, where $\operatorname{conv}(A)$ denotes the convex envelope of A.*

Then we have:

(i) *If* $\rho \geq C > 0$ *on* S, *then* $K_{\mu_0}(W^{1,\infty}_{(0)}(\Omega)) \neq \emptyset$,

(ii) *If* $1/\rho \in L^{p-1}(S)$ (*for* $p > 1$), *then* $K_{\mu_0}(W^{1,p}_{(0)}(\Omega)) \neq \emptyset$,

(iii) *If* S *is bounded, then* $K_{\mu_0}(\mathrm{BV}(\Omega)) \neq \emptyset$.

Here $W^{1,p}_{(0)}$ *means that a zero boundary condition can be* (*optionally*) *imposed as long as* $0 \in S$. *The condition* (iii) *is sharp,* (i) *and* (ii) *are not* (*see examples below*).

An immediate consequence of Theorem 3.2 and Theorem 2.4 is the following corollary:

Corollary 3.3. *The minimization problem* (2.4) *with* G *defined by* (3.1) *and* F *weakly lower semicontinuous with respect to the function space* $X \in \{\mathrm{BV}, W^{1,p}\}$, *where* $1 < p \leq +\infty$, *admits a solution whenever the nonnegative measure* μ_0 *satisfies* $|\mu_0| = |\Omega|$ *and the corresponding condition* (i), (ii) *or* (iii) *from Theorem* 3.2 *holds.*

We define $\Omega_t := \{x \in \Omega;\ \mathrm{dist}(x, \partial\Omega) > t\}$ and $\mathrm{Per}(\Omega_t) := \mathscr{H}^{N-1}(\partial\Omega_t)$. The following lemma collects some results on these functions:

Lemma 3.4. *Let* $\Omega \subset \mathbb{R}^N$ *be a bounded set with* $\partial\Omega$ *Lipschitz. Let* $\omega(t) := |\Omega_t|$. *Then* $\omega'(t)$ *and* $\mathrm{Per}(\Omega_t)$ *are uniformly bounded for a.e.* $t \geq 0$.

Proof. The uniform bound on $\mathrm{Per}(\Omega_t)$ follows from the following result by Ambrosio, compare Theorem 3.8 in [3]:

Theorem 3.5. *Let* $A \subset \mathbb{R}^N$ *and* $\theta, \tau > 0$ *such that*

$$\mathscr{H}^{N-1}(A \cap B_\rho(x)) \geq \theta\rho^{N-1} \quad \text{for all } x \in A,\ \rho \in (0, \tau). \tag{3.3}$$

Then there exists a constant $\Gamma < \infty$ *only depending on* N *and* θ *such that*

$$\text{ess sup}\left\{\mathscr{H}^{N-1}(\{x \in \mathbb{R}^N;\ d(x, A) = t\});\ 0 < t < R\right\} \leq \Gamma\left(\frac{R}{\tau}\right)^{N-1}\mathscr{H}^{N-1}(A).$$

We can apply this theorem, since a Lipschitz continuous boundary $\partial\Omega$ satisfies (3.3).

Theorem 3.5 together with the fact that $\mathrm{Per}(\Omega_t) = 0$ for all $t > \mathrm{diam}(\Omega)/2$ proves the uniform bound on $\mathrm{Per}(\Omega_t)$.

Now using the Coarea Formula for the characteristic function of Ω_t we deduce

$$\omega(t) = \int_t^\infty \mathrm{Per}(\Omega_\tau)\, d\tau.$$

With this we can compute

$$\omega'(t) = \lim_{h\to 0}\frac{\omega(t+h) - \omega(t)}{h} = \lim_{h\to 0}\frac{1}{h}\int_t^{t+h}\mathrm{Per}(\Omega_\tau)\, d\tau.$$

Using the boundedness of $\mathrm{Per}(\Omega_t)$ a.e., the right hand side is bounded a.e. Hence a limit exists and is bounded a.e. □

We remark that the use of Theorem 3.5 for the proof of Lemma 3.4 can be replaced at least in the two-dimensional case by a much easier result using some simple geometrical observations:

Lemma 3.6. *Let $\Omega \subset \mathbb{R}^2$ be a bounded set with $\partial\Omega$ Lipschitz. Then*

$$\mathrm{Per}(\Omega_t) \leq \mathrm{Per}(\Omega) - 2\pi t(1 - h(\Omega)),$$

where $h(\Omega)$ denotes the number of holes in Ω, i.e., the number of bounded connected components of $\mathbb{R}^2 \setminus \Omega$. (This number is finite since Ω is bounded and $\partial\Omega$ is Lipschitz.)

Proof. By polygonal approximation of $\partial\Omega$ from inside and by the weak semi-lower-continuity of the perimeter we can reduce the problem to the case where Ω is a polygon with k sides.

Let us assume for simplicity that Ω is simply connected. Let E_i denote the edges of Ω and α_i the angle between E_i and E_{i+1} for $i = 1, \ldots, k$ (where $E_{k+1} := E_1$). Then an easy geometric construction shows that

$$\begin{aligned} \mathrm{Per}(\Omega_t) &\leq \sum_{i=1}^{N} \big(\mathscr{H}^1(E_i) + (\alpha_i - \pi)t\big) \\ &= \mathrm{Per}(\Omega) - 2\pi t, \end{aligned}$$

since the sum of all angles in a k-sided polygon is $(k-2)\pi$.

The proof can be easily modified to the general case where Ω is not simply connected by an additional approximation of the holes by polygons. □

Proof of Theorem 3.2. We only need to construct a function u in the class X, satisfying the constraint $u^{\#} = \mu_0$.

In case (iii), since in one-dimension BV functions are bounded, the boundedness of S is a necessary condition. In cases (i) and (ii), we have $\rho \in L^1$ and $1/\rho \in L^\varepsilon$ for some $\varepsilon > 0$ and a short computation using Jensen's Inequality shows that therefore the support of ρ must be bounded. Hence S is bounded as well.

For all three cases, we apply the following construction:

Define $\sigma := \mu_0 - \rho\, dt$ and $R' := \rho$ (R exists, since ρ is integrable). Using standard mollifiers ψ_ε one can set $\rho_\varepsilon := \rho + \sigma * \psi_\varepsilon$ where ρ_ε is absolutely continuous and $\lim_{\varepsilon\to 0} \rho_\varepsilon = \rho$. We remark that if ρ nonnegative, then also the (partially) mollified measures ρ_ε are nonnegative. Similar as above we define $R'_\varepsilon := \rho_\varepsilon$.

Then we can make the following ansatz, using $t(x) := \mathrm{dist}(x, \partial\Omega)$:

$$u_\varepsilon(x) := g_\varepsilon(t(x)),$$

where we set

$$g_\varepsilon(t) := R_\varepsilon^{-1}(\omega(t)).$$

The function R_ε is invertible, since by assumption $1/\rho \in L^{p-1}(S)$ and hence $|\{\rho = 0\}| = 0$ and $|\{\rho_\varepsilon = 0\}| = 0$.

Computing the gradient of u_ε we get

$$\begin{aligned} |\nabla u_\varepsilon(x)| \;=\; |g_\varepsilon'(t(x))| \;&=\; \left|\frac{1}{\rho_\varepsilon(R_\varepsilon^{-1}(\omega(t(x))))}\right|\omega'(t) \\ &\le\; \left|\frac{1}{\rho(R_\varepsilon^{-1}(\omega(t(x))))}\right|\omega'(t). \end{aligned} \tag{3.4}$$

In the last step we used that σ is nonnegative and hence $\rho_\varepsilon = \rho + \sigma * \psi_\varepsilon \ge \rho$.

Case (i): If $\rho \ge C > 0$, we see from (3.4) that $|\nabla u_\varepsilon(x)|$ is bounded uniformly, independently of ε. Thus we can take the limit in $W^{1,\infty}$ (for a subsequence) and obtain a limit function u which is Lipschitz continuous. Together with $u_\varepsilon^\# = \mu_\varepsilon$ and Proposition 2.3 we derive $u^\# = \mu_0$. Hence case (i) is proved.

Cases (ii)–(iii): We compute the $W^{1,p}$-seminorm (for $p \in [1,\infty)$), introducing geometric constants $c_i > 0$, depending only on the space dimension and on the shape of Ω:

$$\begin{aligned} \int_\Omega |\nabla u_\varepsilon(x)|^p\,dx \;&=\; \int_\Omega \frac{1}{|\rho_\varepsilon(R_\varepsilon^{-1}(\omega(t(x))))|^p}|\omega'(t)|^p\,dx \\ &\le\; \int_\Omega \frac{1}{|\rho_\varepsilon(R_\varepsilon^{-1}(\omega(t(x))))|^p}c_1\,dx \\ &\le\; \int_0^T \frac{c_2}{|\rho(R_\varepsilon^{-1}(\omega(t))|^p}\,dt, \end{aligned}$$

where T is the largest distance of a point in Ω from $\partial\Omega$.

Using the transformation $s := \omega(t)$ (remember that ω is a decreasing function and ω' is bounded) and $\xi := R_\varepsilon^{-1}(s)$, and defining $a := R_\varepsilon^{-1}(0)$ and $b := R_\varepsilon^{-1}(T)$ we obtain:

$$\int_\Omega |\nabla u_\varepsilon(x)|^p\,dx \;\le\; c_3\int_a^b \frac{1}{|\rho(\xi)|^{p-1}}\,d\xi. \tag{3.5}$$

Since the function R is bounded by $\mu_0(\mathbb{R}) = |\Omega| < \infty$, the $W^{1,p}$-seminorm is uniformly bounded. The L^p-norm is obviously finite, since u_ε is bounded. Thus there exists a subsequence of u_ε converging to a function u in $W^{1,p}$. Together with $u_\varepsilon^\# = \mu_\varepsilon$ and Proposition 2.3 we obtain $u^\# = \mu_0$.

In case (iii) we define

$$\tilde\mu_\varepsilon := (1-\varepsilon)\mu_0 + \varepsilon\frac{\mathscr{L}^1 \llcorner S}{|S|},$$

where $\mathscr{L}^1 \llcorner S$ denotes the Lebesgue measure restricted to the set S.

Since S is by assumption bounded, each $\tilde\mu_\varepsilon$ satisfies the condition of case (i), i.e., $\tilde\mu_\varepsilon \ge C > 0$. Hence we can construct a Lipschitz continuous function $\tilde u_\varepsilon$ with $\tilde u_\varepsilon^\# = \tilde\mu_\varepsilon$ and obtain an estimate for $|D\tilde u_\varepsilon|$ corresponding to (3.5) for the special case $p = 1$, i.e.,

$$\int_\Omega |\nabla \tilde u_\varepsilon(x)|\,dx \;\le\; c_3(b-a). \tag{3.6}$$

Since this estimate is independent of ε, and on the other hand the sequence $\tilde{u}_\varepsilon$ converges in $L^1(\Omega)$ to a function u, a standard result on BV-functions gives that $u \in BV(\Omega)$. Moreover, by Proposition 2.3 we obtain $u^\# = \mu_0$. Thus we have proved case (iii). □

3.2. Examples

We consider first some elementary situations:

Example 3.7. *Let* $\mu_0 = \alpha\delta_a + \beta\delta_b$ *and* $|\Omega| = \alpha + \beta$.

According to Theorem 3.2, we can find a function $u \in \mathrm{BV}(\Omega)$ with $u^\# = \mu_0$. Indeed, any BV-function which takes the value a on a set of measure α and b on a set of measure β satisfies this constraint. It is easy to see that if $a \neq b$ no $W^{1,p}$-function u satisfies the equality $u^\# = \mu_0$.

This example occurs for instance in shape optimization problems when we search for the optimal distribution of two materials a and b of given amounts α and β in a set Ω. Here the function u satisfying the above constraint corresponds to such a distribution.

Example 3.8. *Let* $\mu_0 = \chi_{[0,1]}\, dy$ *and* $\Omega = (0, 1)$.

Again by Theorem 3.2, we can find a function $u \in W^{1,\infty}(\Omega)$ with $u^\# = \mu_0$. In fact, we can simply choose $u(x) := x$. However, we may also choose $u(x) := 2x \wedge 4 - 2x$ and other highly oscillating functions (see Fig. 2). We could even choose a function u which has a jump, take, e.g.,

$$u(x) := \begin{cases} 2x & \text{for } x \leq 1/2, \\ 2x - 2 & \text{for } x > 1/2. \end{cases}$$

The control on $u^\#$ gives therefore no more regularity than the obvious L^∞.

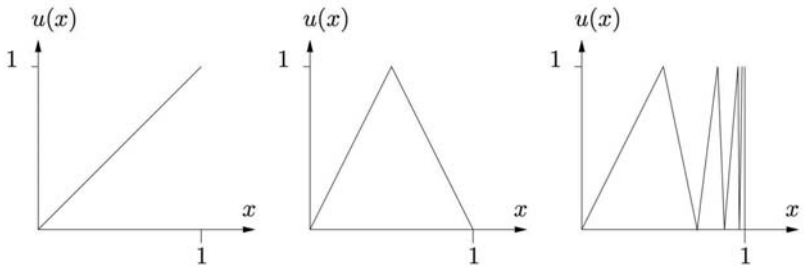

FIGURE 2. Functions satisfying the constraint of Example 3.8.

This example shows that a naive attempt to a characterization of Sobolev functions via their value distribution fails. However, we could try to impose a local condition in the following way: For all open subsets $\omega \subset \Omega$ assume that $\mu := (u|_\omega)^\#$ satisfies the condition (i), i.e., ρ, the absolutely continuous part of μ, fulfills the estimate $\rho \geq C > 0$ on $S := \mathrm{conv}(\mathrm{supp}\, \mu)$. This excludes examples with jumps,

since in a small neighborhood of a jump the set S has a "gap", i.e. $\rho = 0$ on a non-zero subset of S. However, the following example shows, that such a "local" classification fails as well:

Example 3.9. *Let* $u : (-1, 1) \to \mathbb{R}$ *be given by*

$$u(x) := \begin{cases} 2^n(x + 2^{1-n}) & \text{for } -2^{1-n} < x \le -2^{-n},\ n \text{ odd}, \\ 1 - 2^n(x + 2^{1-n}) & \text{for } -2^{1-n} < x \le -2^{-n},\ n \text{ even}, \\ 0 & \text{for } x = 0 \end{cases}$$

and $u(x) := u(-x)$ *for* $0 < x < 1$, *see Fig.* 3.

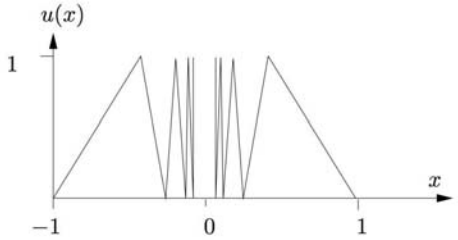

FIGURE 3. The non-continuous function of Example 3.9.

Then in any neighborhood ω of the "irregular" point $x_0 = 0$ the corresponding value distribution $\mu = \rho\,dx + \sigma$ satisfies $\rho \ge C > 0$ on $S := \mathrm{conv}(\mathrm{supp}\,\mu)$ for some constant $C = C(\omega)$.

We conclude with a two-dimensional example on a disk:

Example 3.10. *Let* $\Omega := B(0, 1) \subset \mathbb{R}^2$, $\mu = c(1 - y)^\alpha \chi_{[0,1]}$ *where the constant* c *is chosen such that* $|\mu| = |\Omega|$.

Using the computation of the proof of Theorem 3.2, we get $u(x) = R^{-1}(\omega(1 - |x|)$. With $\omega(1 - |x|) = c_1(1 - |x|)^n$ and $R(t) = c\alpha^{-1}(1 - t)^{\alpha+1} + c_4$, we finally compute that $u(|x|)$ is proportional to $|x|^2\alpha + 1$ (modulo a constant, needed to adjust the boundary value). Hence we get (compare Fig. 4),

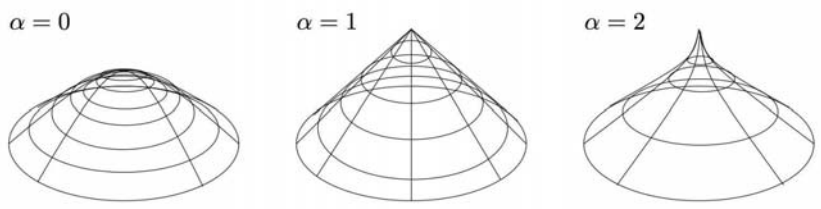

FIGURE 4. Functions u with $u^\# = c(1 - y)^\alpha \chi_{[0,1]}$ for different values of α.

- for $\alpha = 0$, the solution u is of order $O(|x|^2)$ near $x = 0$;
- for $\alpha = 1$, the solution u is of order $O(|x|)$ near $x = 0$;
- for $\alpha = 2$, the solution u is of order $O(|x|^{2/3})$ near $x = 0$.

This means in particular that for $\alpha = 1$ we have Lipschitz continuity, although the condition (i) of Theorem 3.2 is violated. The potential regularity problem disappears, since the critically small value of the measure $u^{\#}$ at $y = 1$ is mapped to a point. If it were mapped to a line (for instance, if we imposed the boundary condition $u = 1$), the gradient of u had to grow too fast to allow for Lipschitz regularity.

In the next section we will use this observation for the construction of a symmetry breaking solution.

4. Symmetry breaking solutions

It is interesting to study the symmetry of solutions in symmetric domains. As an immediate consequence of standard results on symmetric rearrangements we first obtain the following theorem.

Theorem 4.1. *Let Ω be a unit ball and assume that there exists a minimizer $u \in W_0^{1,2}(\Omega)$ to a functional $E(u) := \int_\Omega f(|\nabla u|, u)\,dx + G(u^{\#})$ where f is strictly increasing and convex in the first variable and G is defined as in* (3.1)*. Then there exists a minimizer which is* radially symmetric*.*

Proof. This follows immediately by applying the Schwarz rearrangement (see [15]), since the push-forward of a function does not change when the function is rearranged. □

It is clear that this result strongly depends on the symmetry of the domain Ω. However, it is interesting to see that its generalization to arbitrary radially symmetric domains may fail. In fact, we can construct an example where a radially symmetric problem admits only asymmetric solutions. (As we will show later, even on the ball such examples exists when we omit the zero boundary condition.)

A "symmetry breaking" variational problem can be constructed by taking in the plane $\mathbb{R}^2$ the annulus $\Omega = \{1 < |x| < 2\}$ and the function (compare Fig. 5)

$$\rho(t) := \begin{cases} c & \text{if } -1 \le t \le 0, \\ k(1-t) & \text{if } 0 < t \le 1, \end{cases}$$

with $c = 11\pi/12$ and $k = \pi/2$. If B is the ball centered at $(3/2, 3/2)$ and with radius $1/2$ (compare Fig. 6), we can easily check that

$$\int_{-1}^{0} \rho(t)\,dt = |\Omega \setminus B|, \qquad \int_0^1 \rho(t)\,dt = |B|.$$

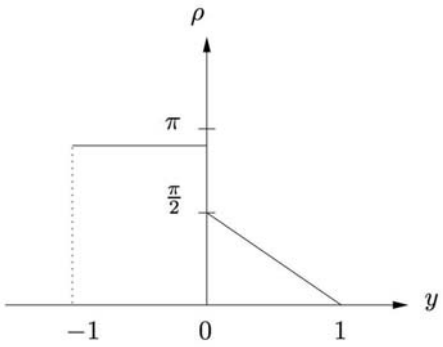

FIGURE 5. The auxiliary function ρ.

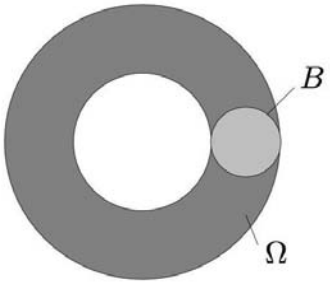

FIGURE 6. Construction of a symmetry breaking solution.

Theorem 4.2. *The minimization problem*

$$\min\Big\{\int_\Omega |\nabla u|^2\,dx \;:\; u\in H^1_0(\Omega),\ u^{\#}=\rho\cdot dt\Big\} \tag{4.1}$$

admits a solution, and every solution is asymmetric.

Proof. We first prove that K_μ is nonempty. To this aim we define

$$u_1(r)=1-\sqrt{2-4r^2}\qquad r\in[0,1/2]$$

inside the ball B, where r stands for the corresponding radial coordinate. In particular, $u_1\in H^1_0(B)$. By using Theorem 3.2 we then find a function u_2 such that:

$$u_2\in H^1_0(\Omega\setminus B),\qquad u_2^{\#}=\rho\cdot dt\llcorner\mathbb{R}^-.$$

We finally glue u_1 to u_2 and we obtain the function

$$u(x):=\begin{cases} u_1(x) & \text{if } x\in B,\\ u_2(x) & \text{if } x\in\Omega\setminus B,\end{cases}$$

which satisfies:

$$u \in H_0^1(\Omega), \qquad u^{\#} = \rho \cdot dt.$$

The existence of a solution to problem (4.1) is therefore guaranteed by Theorem 2.4.

It remains to prove the nonexistence of a radially symmetric solution. Let us assume that such a solution u exists. Since the decreasing rearrangement does not increase the Dirichlet integral $\int_\Omega |\nabla u|^2\,dx$ and does not change the push-forward measure $u^{\#}$, we may also assume that u coincides with its decreasing rearrangement. By the coarea formula we then obtain

$$\begin{aligned}\int_\Omega |\nabla u|^2\,dx &= \int_{-1}^{1} \Big(\int_{\{u=t\}} |\nabla u|\,d\mathscr{H}^1 \Big)\,dt \\ &= \int_{-1}^{1} \frac{|2\pi u^{-1}(t)|^2}{\rho(t)}\,dt \geq 4\pi^2 \int_{-1}^{1} \frac{1}{\rho(t)}\,dt.\end{aligned}$$

This is clearly a contradiction, since $1/\rho(t)$ is not summable on $(-1,1)$ as it is easily checked. □

Heuristically, this symmetry breaking can be explained in the following way: A function satisfying the constraint has to have very small level sets close to $y = 1$. This is either possible if the set $u^{-1}(1)$ is a point (and hence the surrounding level sets can shrink making $u^{\#}$ small), or if the function becomes very steep (which is also making $u^{\#}$ small). In the latter case, the function has a singularity and hence is not admissible for the variational problem. However, the first case is excluded by the geometry of Ω when we allow only radially symmetric functions.

We can use this idea to construct a similar example on the ball which shows that the possibility for a "symmetry breaking solution" is not restricted to topological complicated domains, but is a natural property of our variational problem:

Theorem 4.3. *Let Ω be the open unit ball in $\mathbb{R}^2$ and $\rho(t) := \pi - \pi|t|$ for $t \in [-1,+1]$. Then the minimization problem*

$$\min \Big\{ \int_\Omega |\nabla u|^2\,dx \;:\; u \in H^1(\Omega),\ u^{\#} = \rho \cdot dt \Big\} \tag{4.2}$$

admits a solution, and every solution is asymmetric.

Proof. Again, we first construct an admissible function. This time we cut out two small disjoint balls in Ω on which we define u explicitly as above with values in $(-1,-1+\varepsilon)$ and $(1-\varepsilon,1)$ for suitable $\varepsilon > 0$. Then the problem on the remaining set can be solved by Corollary 3.3 (with only minor modifications due to the slightly different boundary condition).

To prove that there cannot be a radially symmetric solutions, we observe that $u(0)$ can only take the value of one of the "critical" points -1 and $+1$. The other one has to be stretched out along a circle which leads to an infinite Sobolev norm as in the example above. □

The above examples also work for non-constrained situations as the following simple observation shows:

Remark 4.4. *Minimize* $\int_\Omega |\nabla u|^2 + \lambda |u^\# - \rho|^2 \, dx$ *without constraints on* $u^\#$*. Then for* λ *sufficiently large, the symmetry breaking examples above still hold, since* $u^\#$ *will be forced to be sufficiently close to* ρ*.*

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Bi-Modal Cohesive Energies

Gianpietro Del Piero

Abstract. A unified treatment of several aspects of material behavior is provided by a one-dimensional model based on the decomposition of the energy of a body into the sum of two parts, bulk and cohesive. This note deals with a specific form of the cohesive energy, called *bi-modal*. Using the example of a bar subject to axial elongation, it is shown that a cohesive energy of this form captures two aspects of material response which, at a first glance, look very different: stress oscillation, and damage.

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Keywords. Theories of material behavior, One-dimensional elasticity, One-dimensional damage.

1. Introduction

In the model which forms the object of this note the presence of jump discontinuities in the displacement field is allowed, and a *cohesive energy* is associated with the formation of such discontinuities. The analytical form of this energy has a strong influence on the macroscopic behavior of the body. In particular, some of the fundamental types of material response met in the experiments, such as fracture, yielding, or damage, can be obtained from some specific forms of the cohesive energy. This opens the way to a unified treatment of phenomena which are traditionally studied by different ad hoc theories.

The model of an elastic bar with cohesive energy has been discussed in several papers. Earlier stages of development can be found in [4] and [5], and a systematic presentation is in preparation, in collaboration with L. Truskinovsky [10]. Other papers deal with specific forms of the cohesive energy and with the corresponding material responses. For example, it has been shown that a concave energy leads to Barenblatt's theory of fracture [2], and that a convexity in a neighborhood of the origin determines a plastic-like response [3]. In [6], the plastic-like model has been

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refined to account for elastic unloading, and in [7] its relation with the theory of structured deformations has been analyzed.

The bi-modal energy, which is a concave energy with a convex segment away from the origin, has been studied in [8] and [9]. A peculiar property of this energy is that, as shown in Fig. 1, the intermediate convex segment separates two distinct energy levels, one responsible for the formation of a micro-cracked zone (the process zone), and one responsible for final collapse.

In this note, after briefly introducing the conditions for equilibrium and stability, the response curves for a bar subject to a prescribed axial elongation are constructed. In them, the interplay of the concave and convex parts of the energy diagram determine an oscillatory behavior of the stress. In the last section I show how these oscillations can be related to those observed in standard uniaxial tension tests, and how an equilibrium branch of the response curve characterized by a specific number of jumps can be associated with a *damaged state* of the material.

2. The model

Consider a rectilinear bar of length l, whose axial displacement u may have jump discontinuities. Mathematically, u can be thought as a function of bounded variation on $(0, l)$. The jump set of u will be denoted by $S(u)$, while $[u](x)$ and u' will denote the jump of u at x and the absolutely continuous part of the derivative, respectively.

Two types of energy are assumed to coexist in the bar: an *elastic strain energy* diffused over the bulk, whose density w depends on u', and a *cohesive energy* θ concentrated at the jump set and depending on the amplitude of the jumps. For simplicity, both w and θ are assumed to be the same at all points of the bar. Thus, the strain energy of the bar is

$$E(u) \,=\, \int_0^l w(u'(x))\,dx + \sum_{x\in S(u)} \theta([u](x))\,. \tag{2.1}$$

The bar is assumed to be held fixed at the end $x = 0$ and to be subject to an axial displacement βl at the end $x = l$. This type of boundary condition is called a *hard device*. To within an inessential rigid translation, it is expressed by the equation

$$\int_0^l u'(x)\,dx + \sum_{x\in S(u)} [u](x) \,=\, \beta l\,. \tag{2.2}$$

In the absence of body forces, $E(u)$ coincides with the total energy of the bar. The list of the basic equations of the model is completed by the inequality

$$[u](x) \,\geq\, 0 \qquad \forall x \in S(u)\,, \tag{2.3}$$

which prevents interpenetration at the jump points.

The bulk energy w is assumed to be smooth, convex, non-negative, and with $w(0) \,=\, w'(0) \,=\, 0$. The various forms of θ mentioned in the Introduction are

shown in Fig. 1. Of them, the Griffith cohesive energy leads to brittle fracture, the energy of Barenblatt yields both ductile and brittle fracture, and the convex-concave energy leads to plastic-like behavior. As shown in the picture, a bi-modal energy is characterized by the presence of two inflection points H, K, separating a central convex part from the two concave lateral parts.

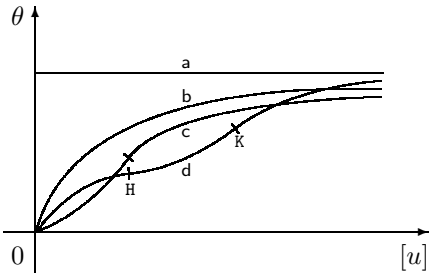

FIGURE 1. Some types of cohesive energy:
(a) Griffith, (b) Barenblatt, (c) convex-concave, (d) bi-modal.

3. Equilibrium

An *equilibrium configuration* is a displacement field u for which

$$\lim_{\varepsilon \to 0} \frac{E(u+\varepsilon\eta) - E(u)}{\varepsilon} \geq 0 \tag{3.1}$$

for all perturbations η of bounded variation which preserve the length of the bar:

$$\int_0^l \eta'(x)\, dx + \sum_{x \in S(\eta)} [\eta](x) = 0\,. \tag{3.2}$$

Notice that the standard requirement of the vanishing of the first variation is replaced here by an inequality. This is due to the presence of the unilateral constraint (2.3).

It has been proved in [10] that u is an equilibrium configuration if and only if

$$\begin{gathered} u'(x) =: \varepsilon \quad \forall x \in (0,l) \backslash S(u)\,, \\ \theta'([u](x)) = w'(\varepsilon) =: \sigma \quad \forall x \in S(u)\,, \\ \sigma \leq \theta'(0+)\,. \end{gathered} \tag{3.3}$$

Thus, at an equilibrium configuration the deformation u' is the same at all points not in the jump set; its value ε is the *strain*. Moreover, the derivative of θ is the same at all jump points, and coincides with the derivative of w at ε. The common value of the derivatives is the *stress* σ. Finally, the stress is bounded from above by the right derivative of θ at the origin, which is the *ultimate stress* for the bar.

Since we are interested in the energy minimizers and (3.1) is a necessary condition for a minimum, it is convenient to restrict our attention to equilibrium

configurations. For them, the expressions (2.1), (2.2) of the total energy and of the hard device take the simpler form

$$E(u) \,=\, lw(\varepsilon) + \sum_{x\in S(u)} \theta([u](x))\,, \tag{3.4}$$

$$\varepsilon l + \sum_{x\in S(u)} [u](x) \,=\, \beta l\,, \tag{3.5}$$

and after elimination of ε the total energy can be rewritten as

$$F_\beta(q) \,=\, lw\big(\beta - l^{-1}\sum_{h=1}^{N(q)} q_h\big) + \sum_{h=1}^{N(q)} \theta(q_h)\,. \tag{3.6}$$

The energy being assumed to depend on the amplitudes of the jumps but not on their position, to eliminate the reference to x the jumps $[u](x)$ have been re-named q_h. The symbol q on the left side denotes the *jump vector* with components q_h, and $N(q)$ is the number of these components. The energy E has been re-named F_β, both to emphasize the change of the independent variable from u to q and to remark its explicit dependence on β.

The fact that the independent variable has changed from a function to a vector does not mean that the problem has become finite-dimensional. Indeed, the number of the jumps is not fixed a priori, and it could well be infinite. Nevertheless, as discussed in the next section, for the purpose of energy minimization the problem can be reduced to a sequence of finite-dimensional problems.

4. Energy minimizers

A *stable equilibrium configuration* is an equilibrium configuration which is a local minimizer for the energy E. In the preceding section, with any displacement field u in the domain of E it has been associated a jump vector q whose components q_h are the jumps of u, and over such vectors an energy F_β has been defined, such that $F_\beta(q) = E(u)$. In [10], two theorems on the local minimum properties of F_β have been proved. The first guarantees that, for an appropriate choice of the topologies of the domains of definition of the two energies, all local minima are preserved in the transition from E to F_β.

Theorem 4.1. *A displacement field u is a local minimizer for E with respect to the norm of the total variation*

$$\|u\| \,=\, \int_0^l |u'(x)|\,dx + \sum_{x\in S(u)} |u(x)| \tag{4.1}$$

if and only if the corresponding jump vector q is a local minimizer for F_β with respect to the norm

$$[\![\, q \,]\!] \,=\, \sum_{h=1}^{N(q)} |q_h|\,. \tag{4.2}$$

The second theorem states that every local minimizer q for F_β is also a minimizer for the same functional in a finite-dimensional space of dimension $N(q)$.

Theorem 4.2. *Let ℓ^+ be the set of all vectors q with $q_h \geq 0$, and let ℓ^+_n be the set of all q in ℓ^+ with $N(q) = n$. Then q_0 is a local minimizer for F_β in ℓ^+ if and only if it is a local minimizer for F_β in $\ell^+_{N(q_0)}$.*

Thus, all local minimizers for F_β can be detected by finite-dimensional minimization over the sets ℓ^+_n. A possible strategy for finding all local minimizers for F_β is then to look for the local minimizers for a fixed n, and to repeat the procedure for all n.

For each n, the minimum problem for a given β coincides with the minimum problem for the chain of atoms connected in series by non-linear elastic springs shown in Fig. 2. More precisely, for a given n there are $n+1$ springs, n with the energy θ and one with the energy lw. Note that, while the energy of the first n springs only depend on the amplitude of the jumps, the energy of the last spring also depends on l and β.

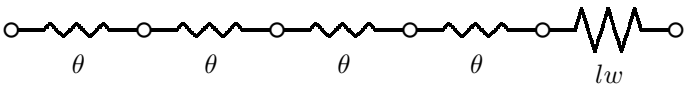

FIGURE 2. An atom chain representing the finite-dimensional version of the problem.

This model has been studied in [14]. From the stability analysis it comes out that for each fixed n there are only three types of stable equilibrium configurations:

(i) the equilibrium configurations without jumps,
(ii) the equilibrium configurations with $\theta''(q_h)$ non-negative for all h,
(iii) the equilibrium configurations with one of the $\theta''(q_h)$ negative and all remaining $\theta''(q_h)$ positive, such that

$$lw''(\beta - l^{-1}\sum_{h=1}^{n} q_h)^{-1} + \sum_{h=1}^{n} (\theta''(q_h))^{-1} \leq 0\,. \tag{4.3}$$

These are necessary conditions for stability. Sufficient conditions are obtained by replacing *non-negative* by *positive* in (ii), and by taking the strong inequality in (iii).

5. Equilibrium branches and response curves

Let us fix n, and let us rewrite the equilibrium condition $(3.3)_2$ in the form

$$\theta'(q_k) \;=\; w'(\beta - l^{-1}\sum_{h=1}^{n} q_h)\,, \qquad k \in \{1, 2, \ldots, n\}. \tag{5.1}$$

This is a system of n equations in the n unknowns q_k, depending on the parameter β. After solving the system for each β, we get a one-parameter family

$$q \,=\, \hat{q}(\beta) \tag{5.2}$$

of equilibrium configurations. This family can be represented by a piecewise continuous curve in the n-dimensional space; a continuous segment of this curve will called an *equilibrium branch*. *Stable* equilibrium branches are those which are made of stable equilibrium configurations.

Within each branch, one may define the energy

$$\hat{E}(\beta) \,=\, F_\beta(\hat{q}(\beta))\,, \tag{5.3}$$

and the stress

$$\hat{\sigma}(\beta) \,=\, \frac{1}{l}\,\frac{d}{d\beta}\,\hat{E}(\beta)\,. \tag{5.4}$$

The resulting energy-elongation and stress-elongation curves are the *response curves* of the bar. The following characterization of stable equilibrium branches in terms of the slope of the stress-elongation curve is given in [10].

Theorem 5.1. *An equilibrium branch made of configurations either without jumps or with all $\theta''(q_h)$ positive is stable if the slope of the stress-elongation curve is positive. An equilibrium branch made of configurations with one $\theta''(q_h)$ negative is stable if the slope of the stress-elongation curve is negative.*

6. Response curves for a bi-modal cohesive energy

Consider again the equilibrium conditions (3.3) and the hard device (3.5):

$$\sigma \,=\, w'(\varepsilon) \,=\, \theta'(q_h)\,, \qquad \sigma \,\le\, \theta'(0+)\,, \tag{6.1}$$

$$\varepsilon + l^{-1}\sum_{h=1}^{N(q)} q_h \,=\, \beta\,. \tag{6.2}$$

If w is convex, w' is an increasing function of ε as represented in Fig. 3a. For a bi-modal cohesive energy, the qualitative properties of the derivative θ' are shown in Fig. 3b: the diagram has a local maximum at 0 and $p_{\mathtt{K}}$ and a local minimum at $p_{\mathtt{H}}$. It is assumed here that $\theta'(0+)$ is greater than $\theta'(p_{\mathtt{K}})$.

Let us determine the local minimizers for each fixed n. For $n = 0$, since there are no jumps, we get $\varepsilon = \beta$ from (6.2) and $\sigma = w'(\beta)$ from $(6.1)_1$. By $(6.1)_3$, this holds for all β smaller than the "critical" value

$$\beta_c \,=\, (w')^{-1}(\theta'(0+))\,. \tag{6.3}$$

Then for $n = 0$ we have the equilibrium branch

$$\{\sigma \,=\, w'(\beta)\,, \quad \beta < \beta_c\} \tag{6.4}$$

shown in Fig. 3c.

For $n = 1$ there is only one jump q_1, and the corresponding equilibrium curve can be traced by points in the following way. Fix a $\sigma < \theta'(0+)$. Then equation

$(6.1)_1$ determines the strain $\varepsilon = w^{-1}(\sigma)$, and $(6.1)_2$ determines q_1. More precisely, it determines three possible values $p_i(\sigma)$ of q_1 if σ is included in $(\theta'(p_{\mathrm{H}}), \theta'(p_{\mathrm{K}}))$, and only one value $p_1(\sigma)$ otherwise. By (6.2), the corresponding values of β are

$$\beta_i(\sigma) \;=\; (w')^{-1}(\sigma) + l^{-1} p_i(\sigma)\,. \tag{6.5}$$

For a specific value of σ, the $p_i(\sigma)$ are shown in Fig. 3b and the $\beta_i(\sigma)$ are shown in Fig. 3c. Since the points $(\beta_i(\sigma),\, \sigma)$ belong to the response curve for $n = 1$, the curve can be constructed by determining the abscissas $\beta_i(\sigma)$ for a suitable number of values of σ.

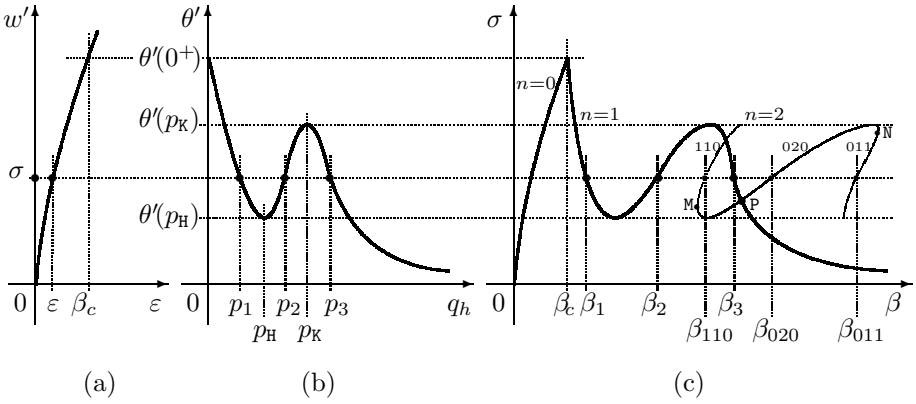

FIGURE 3. Stress-strain (a), stress-jump amplitude (b), and stress-elongation (c) curves for small l.

The stable branches of the curve can be detected with the aid of Theorem 5.1. It tells us that a branch of the response curve in Fig. 3c corresponding to an ascending branch of the constitutive curve in Fig. 3b is stable if its slope is positive, and one corresponding to a descending branch is stable if its slope is negative. In the specific case shown in the picture these conditions are satisfied everywhere, and so the whole curve $n = 1$ is stable.

For $n > 1$, the values of β corresponding to equilibrium configurations with a given σ in $(\theta'(p_{\mathrm{H}}), \theta'(p_{\mathrm{K}}))$ are

$$\beta_{n_1 n_2 n_3}(\sigma) \;=\; (w')^{-1}(\sigma) + l^{-1}\big(n_1 p_1(\sigma) + n_2 p_2(\sigma) + n_3 p_3(\sigma)\big)\,, \tag{6.6}$$

with $p_i(\sigma)$ as above and with n_1, n_2, n_3 non-negative integers such that $n_1 + n_2 + n_3 = n$. For example, for $n = 2$ we have six possible values of β, one for each of the triples

$$(200),\;\; (110),\;\; (101),\;\; (020),\;\; (011),\;\; (002).$$

For σ not in $(\theta'(p_{\mathrm{H}}), \theta'(p_{\mathrm{K}}))$ there is only one value of β, given by (6.6) with $n_2 = n_3 = 0$ if $\sigma < \theta'(q_{\mathrm{H}})$ and with $n_1 = n_2 = 0$ if $\sigma > \theta'(q_{\mathrm{K}})$.

By Theorem 5.1, the configurations of the type (020) are stable, those of the type (200), (101) and (002) are unstable, and those of the type (110) and (011) are

stable only if they lie on an equilibrium curve with negative slope. In Fig. 3c, the branches (020), (110), (011) are represented by a thin line, and the values β_{020}, β_{110}, β_{011} of β are shown for a specific σ. If we denote by M and N the points at which the tangents to the two branches are vertical, we have that the stable part of the curve $n = 2$ is the part comprised between M and N.

The equilibrium curves for higher values of n can be constructed in a similar way. If we analyze the response of the bar to an increasing elongation β, we see that for $\beta < \beta_c$ the equilibrium configurations have no jumps, while for $\beta > \beta_c$ all equilibrium configurations have jumps. The transition occurs for $\beta = \beta_c$ and $\sigma = \theta'(0+)$. When β crosses this threshold a jump point is created in the bar, and the growth of β beyond β_c is accompanied by a smooth decrease of the stress.

Very different is the situation at the intersections between curves corresponding to non-null values of n. Consider, for example the intersection between the curve $n = 1$ and the stable branch of the curve $n = 2$. This is the point P in Fig. 2.3c. This point represents two different configurations, one with one jump and one with two jumps, and the distance (4.2) of the two configurations is not zero. A continuous path joining the two configurations is a non-equilibrium path, and crossing this path requires the overcoming of energy barriers. Therefore, a bar in a configuration with $n = 1$ cannot switch to $n = 2$, even if $n = 2$ were a branch with lower energy, unless some dramatic perturbation occurs. The same conclusion holds for the intersections of the curve $n = 1$ with all curves for $n > 1$. The conclusion is that for increasing β the bar follows the curve $n = 1$, and reaches the lowest part of that curve after a single oscillation.

But this is not the end of the story, neither is the most interesting part of it. An important point, not emphasized hitherto, is that, as shown by equation (6.5), the $\beta_i(\sigma)$ depend on the length l of the bar. This implies that the responses of two bars made of the same material but of different length are different. In fact, there is experimental evidence that large bodies are more brittle than small bodies. In fracture mechanics, this phenomenon is known as *size effect*. Let us see how this effect is embodied in the present model.

By (6.5), the $\beta_i(\sigma)$ decrease with increasing l. Then for sufficiently large l some parts of the curve $n = 1$ change their slope from negative to positive and become unstable. Then it may happen that, as shown in Fig. 4, at $\beta = \beta_c$ the smooth transition between the regimes $n = 0$ and $n = 1$ be replaced by a non-smooth transition, accompanied by a sudden drop in the stress. This new type of transition is essentially dynamic, and is not described by the model.

What is provided by the model is a complete landscape of the stable equilibrium configurations. They are organized in a number of disconnected branches, one for each n, plus the descending branch of the curve $n = 1$. The disconnected branches are essentially ascending branches, in which the stress ranges from $\theta'(p_{\mathtt{H}})$ to $\theta'(p_{\mathtt{K}})$; along the descending branch of the curve $n = 1$, the stress reaches the lowest values which can be taken as representative of collapse. Thus, under a growing elongation β, the stress in the bar oscillates, and each oscillation is accompanied by the creation of a new jump. The precise points at which the transitions occur

are not specified by the model, neither is clear whether and when the oscillatory regime eventually comes to an end, and the bar switches to the descending branch of the curve $n = 1$.

In the following section I show how, in spite of these limits, the model succeeds in predicting and qualitatively describing two specific aspects of material behavior, stress oscillation and progressive damage.

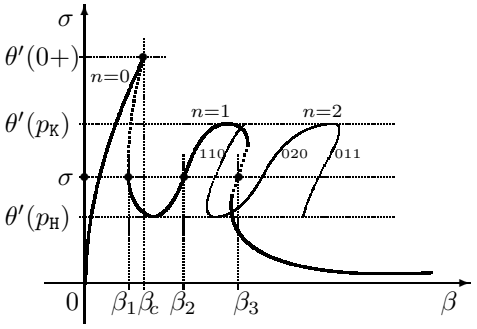

FIGURE 4. Stress-elongation curves for large l.

7. Stress oscillation and damage

Assume that, as shown in Fig. 5a, the stresses $\theta'(p_{\mathtt{H}})$ and $\theta'(p_{\mathtt{K}})$ be close to each other and not much smaller than the ultimate stress $\theta'(0+)$. Then, as shown in Fig. 5b, the response curve has a peak at β_c followed by small-amplitude stress oscillations. As shown by comparison with Fig. 5c, this is a rather good approximation of the initial part of the stress-strain curve for a metallic material, such as mild steel or certain aluminum alloys, tested in a *hard* machine.[1] There has been a period, across the thirties and the forties of the past century, in which there was a lot of speculation about the stress peak and the subsequent oscillations. A precursory attribution of these phenomena to loss of stability is due to F. Nakanishi [13], and their dependence on the hardness of the testing machine and on the speed of stretching was made evident by J. Miklowitz [12].

In the view of Nakanishi and of other contemporary experimenters, these phenomena were regarded as manifestations of plastic behavior. According to the present model, both stress oscillation and stress peak are manifestations of a discrete phenomenon, the transition between equilibrium branches corresponding to different n.[2] Yielding is rather associated with a convex-concave energy [3], [6], in which this element of discreteness disappears, and stress oscillation is rather associated with damage, as I am going to show in a moment.

[1]The model fails in reproducing the subsequent hardening, shown in the picture by a dotted line.
[2]Clearly, the stress peak disappears if $\theta'(p_{\mathtt{K}}) > \theta'(0+)$ [8]. This is the case, for example, of the response curve shown in [1], Sect. 4.24, obtained by Elam in a hard test on an aluminum alloy.

The discrete nature of the stress-strain evolution in a tensile test was noticed early in the history of experimental mechanics.[3] The experiments of Mc Reynolds with a soft machine and of Elam with a hard machine[4] are in a good agreement with the qualitative predictions of the present model. The progressive formation and growth of weakened zones in the bulk of the bar observed by Mc Reynolds has been recently confirmed by experiments made by Froli and Royer Carfagni [11].

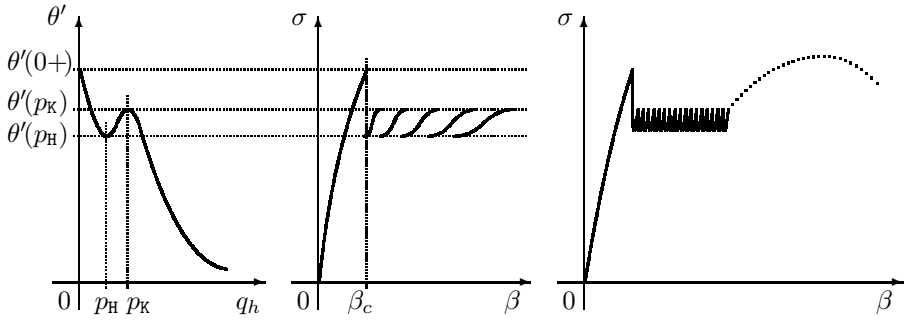

FIGURE 5. A particular shape of θ' (a) determining a response curve with stress peak and stress oscillation (b), compared with the response of a mild steel bar tested in a hard machine (c). In (c), the dotted line shows the phenomenon of *work-hardening*, not described by the present model.

Now let us see how damage is described within the present model. For simplicity, assume that w is quadratic

$$w(\varepsilon) \;=\; \tfrac{1}{2}\, k\, \varepsilon^2\,, \tag{7.1}$$

and take the cohesive energy

$$\theta(p) \;=\; \begin{cases} 0 & \text{for } p = 0\,, \\ \theta_{\mathrm{H}} + \tfrac{1}{2}\, c\, p^2 & \text{for } 0 < p < p_{\mathrm{K}}\,, \\ \theta_{\mathrm{H}} + \tfrac{1}{2}\, c\, p_{\mathrm{K}}^2 & \text{for } p > p_{\mathrm{K}}\,, \end{cases} \tag{7.2}$$

with k, c, θ_{H} and p_{K} given positive constants. The graph of θ is shown in Fig. 6a, and that of θ' in Fig. 6b. In the latter, the first descending branch of the curve in Fig. 3b degenerates into the vertical half-line $\{p = 0,\, \theta' \geq 0\}$, so that the ultimate stress rises to infinity, the ascending branch is the segment $\{0 < p < p_{\mathrm{K}},\, \theta' = cp\}$, and the second descending branch is the horizontal half-line $\{p \geq p_{\mathrm{K}},\, \theta' = 0\}$.

[3] In [1], Sect. 4.31, the first observation of the phenomenon is attributed to Duleau (1813), and the first systematic study to Savart and Masson in the 1840's. However, the phenomenon bears the names of Portevin and Le Chatelier, who re-discovered it in the 1920's.
[4] See [1], Sect. 4.31.

The stress-elongation response curves are shown in Fig. 6c. The half-line $\{\beta \geq 0,\ \sigma = k\beta\}$ is the response curve for $n = 0$, and k can be identified with the *Young modulus* of the material. For $n > 0$, equations (6.1), (6.2) take the form

$$\sigma \,=\, k\varepsilon \,=\, c\,p\,, \qquad \varepsilon + nl^{-1}p \,=\, \beta\,, \tag{7.3}$$

and after elimination of ε and p we get the response curves[5]

$$\sigma \,=\, \Big(1+\frac{nk}{lc}\Big)^{-1} k\,\beta\,, \qquad 0<\beta<\Big(1+\frac{nk}{lc}\Big)\frac{cp_{\mathrm{K}}}{k}\,. \tag{7.4}$$

When subject to increasing β, the bar first follows the line $n = 0$. The model does not tell us when the bar leaves this regime to reach an equilibrium branch with $n > 0$.[6] But once this is done, since for each n the values of β are bounded by $(7.4)_2$, for growing β we have transitions to higher and higher n. At each transition, there is a reduction in the slope of the equilibrium curve, measured by the factor

$$\alpha(n) \,=\, \Big(1+\frac{nk}{lc}\Big)^{-1}\,. \tag{7.5}$$

This means that the bar becomes weaker and weaker with the increase of β. In damage theory, this weakening is represented as a reduction of Young's modulus, and the factor α is known as the *damage factor*. In the present model, rather than the weakening of the material, $\alpha(n)$ measures the weakening of the whole structure, since a *size effect* is given by the presence of l in the right side of (7.5).

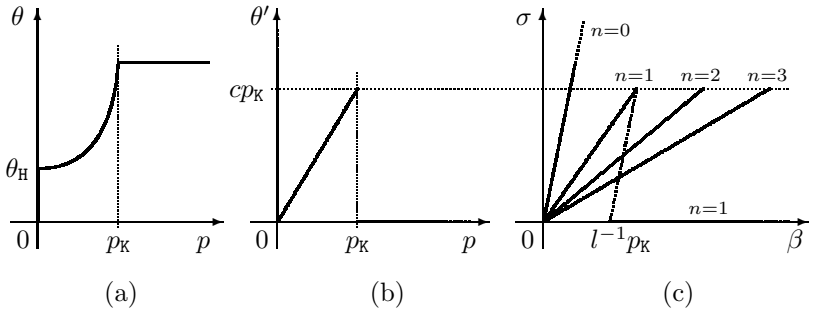

FIGURE 6. An elementary model for damage: the cohesive energy (a), its derivative (b), and the stress-elongation response curves (c).

[5]For $n = 1$ we also have the unstable branch represented by a dotted line in Fig. 6c, plus the half-line $\{\beta \geq l^{-1}p_{\mathrm{K}},\ \sigma = 0\}$, which corresponds to collapse.

[6]This inconvenience can be eliminated by giving a finite slope to the vertical portion of the θ diagram.

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Criterion for Tricritical Points in Liquid Crystal Phases

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Abstract. We propose a criterion to find the symmetric tricritical points of an ordering phase transition in liquid crystals described by more than one scalar order parameter. Our criterion extends the one already put forward in the literature, which is based on the classical Griffiths's criterion valid when all phases are described by a single order parameter. When applied to a recently proposed model for biaxial liquid crystals, the criterion presented here predicts the existence of a new tricritical point.

Mathematics Subject Classification (2000). Primary 76A15; Secondary 82B27, 82B26.

Keywords. Liquid crystals, Critical phenomena, Phase transitions.

1. Introduction

In general, tricritical points occur whenever *three* coexisting fluid phases become simultaneously identical [1]. A tricritical point is thus different from both a critical point, where only two coexisting phases become identical, and a critical end point, where two phases become identical, in the presence of a third dissimilar phase. Ordered soft matter systems other than fluid mixtures can also exhibit tricritical points: there, three ordered phases become identical. Often two such phases are conjugated by a symmetry transformation: when this is the case, the tricritical points are referred to as being symmetric [1]. Symmetric tricritical points are the object of this paper, especially in liquid crystals, where the underling molecular symmetry is more likely to induce them [2, 3, 4, 5]. In Griffiths's terminology [6], a tricritical point is also a point on a phase diagram where a first-order transition becomes second-order (the equivalence between the above two definitions of a tricritical point is well explained, for example, on pp. 29–30 of [7]; [8] is another relevant general reference).

Within a simplified model describing the ordered phase of a system in terms of a single order parameter ψ, the free energy $\mathcal{F}$ can be given the following Landau expansion:

$$\mathcal{F} = a_2\psi^2 + a_4\psi^4 + \psi^6 + o(\psi^6), \tag{1.1}$$

where only even powers of ψ are retained since ψ and $-\psi$ are thought of as corresponding to one and the same state. The coefficients a_2 and a_4 in (1.1) depend on a set of physical field variables, generally including the temperature. The coefficient of ψ^6, which must be positive for thermodynamic stability, is set equal to unity, as its specific value is inessential [9]. In this simplified setting, the criterion for the existence of a tricritical point is given by the equations [1, 9]:

$$a_2 = a_4 = 0. \tag{1.2}$$

These equations have been extended to multi-component fluid mixtures [11, 10], though the reasoning leading to them was essentially left unchanged. In liquid crystals, however, the occurrence of tricritical points is more likely related to ordered phases that need to be described by more than a single order parameter [2, 3, 12]. The existing criterion for tricritical points in the liquid crystal literature [13, 14, 15] appears as an extension of the classical criterion (1.2) based on the assumption that all order parameters can be seen as functions of a leading one, still conventionally denoted by ψ, which is different from zero only in the ordered phase and which in turn makes all other order parameters differ from zero as well. Under this assumption, $\mathcal{F}$ can again be given an effective form as in (1.1), but with both a_2 and a_4 expressed in terms of the coefficients of the Landau expansion of $\mathcal{F}$ thought of as a function of all independent order parameters. Accordingly, the criterion for tricriticality is still derived from equations (1.2) [13, 14].

Here we take a different avenue. We consider a general ordered system with two independent order parameters, symmetric in one of them. Our motivation came from the study of a molecular model for biaxial phases in nematic liquid crystals [12], which represents a special case of the model envisaged by Straley [16]. Straley's model introduces four independent order parameters to describe a fully developed biaxial phase, while essentially two of them suffice in the simpler model studied in [12]. The occurrence of a tricritical point in the phase diagram predicted by this model called for a more general criterion fit to identify both such points and the portion of the critical manifold that indeed corresponds to second-order phase transitions.

This paper is organized as follows. In Section 2, we derive the criterion and in Section 3 we show how it is able to identify correctly the tricritical points already known in the phase diagrams for smectic and biaxial liquid crystals. Moreover, we heed that it predicts the existence of a new tricritical point for biaxial liquid crystals (see also [17]). In Section 4, we contrast the criterion worked out here with the one already known in the literature. Finally, in Section 5, we draw the main conclusion of this paper and comment on the perspectives that it opens.

2. Criterion

In this paper we study a model system with ordered phases described by two order parameters, X and Y, for which we confine attention to states homogeneous in space. We assume that the free energy $\mathcal{F}$ is a smooth function of X, Y, and several physical parameters $\{\beta, \lambda_1, \ldots, \lambda_n\}$, among which is $\beta := \frac{U_0}{\kappa_B t}$, where κ_B is the Boltzmann constant, t is the absolute temperature and U_0 a typical energy of the system. In the following, we denote by $\lambda := (\lambda_1, \ldots, \lambda_n)$ the vector of $\mathbb{R}^n$ comprising all parameters independent of the temperature. In general, the admissible parameters λ range in a subset of $\mathbb{R}^n$, which we denote by $\mathbb{A}$. For simplicity, we further assume that $\mathcal{F}$ enjoys the symmetry property

$$\mathcal{F}(X, Y, \beta, \lambda) = \mathcal{F}(X, -Y, \beta, \lambda), \tag{2.1}$$

which makes equilibria with $Y = 0$ the natural candidates for states whence a second-order phase transition could develop. Though these assumptions might appear to be quite restrictive at first glance, they are valid for disparate mean-field models of liquid crystals, as shown in Section 3 below.

In equilibrium, for given β and λ, the order parameters of the system solve the equations

$$\frac{\partial \mathcal{F}}{\partial X}(X, Y, \beta, \lambda) = 0, \tag{2.2}$$

$$\frac{\partial \mathcal{F}}{\partial Y}(X, Y, \beta, \lambda) = 0. \tag{2.3}$$

These equations may possess more than a single root (X, Y), each of which represents an equilibrium phase. We call *locally stable* a phase where $\mathcal{F}$ attains a relative minimum and *globally stable* a phase where $\mathcal{F}$ attains its absolute minimum.

We assume that the system always admits a globally stable phase in $\mathbb{A}$. Let first λ_0 be given in $\mathbb{A}$. Suppose that for all β in an appropriate range I there is an equilibrium phase described by $X = X_0(\beta, \lambda_0)$ and $Y = 0$. Conventionally, we say that $(X_0, 0)$ represents a *reference state* for the system. It may represent a stable phase of the system and it may not: it could be any equilibrium state of the system whose vicinity is worth exploring.

We denote by $[H_0]$ the Hessian matrix of $\mathcal{F}$ at the point $(X_0, 0)$. By the symmetry requirement (2.1), $[H_0]$ is diagonal, and its two eigenvalues are given by

$$\Sigma_X(\beta, \lambda_0) := \frac{\partial^2 \mathcal{F}}{\partial X^2}(X_0(\beta, \lambda_0), 0, \beta, \lambda_0), \tag{2.4}$$

$$\Sigma_Y(\beta, \lambda_0) := \frac{\partial^2 \mathcal{F}}{\partial Y^2}(X_0(\beta, \lambda_0), 0, \beta, \lambda_0). \tag{2.5}$$

Our strategy will be to look for other equilibrium phases near a given reference state and, if there are some, to see which is likely to be locally stable. The success of this strategy will clearly depend on the choice of the reference state. We expand

the free energy $\mathcal{F}$ in power series about $(X_0, 0)$:

$$\begin{aligned}\mathcal{F}(X_0+\delta X, Y) &= \mathcal{F}(X_0,0) + F_1 Y^2 + F_2 Y^4 + F_3 Y^2 \delta X + F_4 (\delta X)^2 \\ &+ F_5 (\delta X)^4 + F_6 Y^2 (\delta X)^2 + F_7 (\delta X)^3 + O(5), \end{aligned} \tag{2.6}$$

where use has been made again of the symmetry requirement (2.1). The coefficients $\{F_j\}_{j=1\ldots7}$ are related to the partial derivatives of $\mathcal{F}$ with respect to X and Y at the reference state: they are all functions of (β, λ_0). In particular, also by (2.4) and (2.5),

$$F_1 := \frac{1}{2}\Sigma_Y(\beta, \lambda_0), \tag{2.7}$$

$$F_2 := \frac{1}{24}\left(\frac{\partial^4 \mathcal{F}}{\partial Y^4}\right)_{(X_0,0)}, \tag{2.8}$$

$$F_3 := \frac{1}{2}\left(\frac{\partial^3 \mathcal{F}}{\partial Y^2 \partial X}\right)_{(X_0,0)}, \tag{2.9}$$

$$F_4 := \frac{1}{2}\Sigma_X(\beta, \lambda_0). \tag{2.10}$$

If there exist equilibrium phases near the reference state, they can be found by requiring the function in (2.6) to be stationary, that is, by solving the equations

$$F_3 Y^2 + 2F_4 \delta X + 4F_5 (\delta X)^3 + 2F_6 Y^2 \delta X + 3F_7 (\delta X)^2 = 0, \tag{2.11}$$

$$F_1 Y + 2F_2 Y^3 + F_3 Y \delta X + F_6 Y (\delta X)^2 = 0. \tag{2.12}$$

Under the assumption that $Y \neq 0$, to the lowest approximation, these equations reduce to the following linear system

$$\begin{pmatrix} 2F_4 & F_3 \\ F_3 & 2F_2 \end{pmatrix} \begin{pmatrix} \delta X \\ Y^2 \end{pmatrix} = \begin{pmatrix} 0 \\ -F_1 \end{pmatrix}. \tag{2.13}$$

It is apparent from (2.13) that a new single equilibrium phase fails to exist whenever

$$\Delta F := 4F_2 F_4 - F_3^2 = 0. \tag{2.14}$$

This condition actually identifies a set in the space $I \times \mathbb{A}$, which we call the *singular manifold*. More properly, we should momentarily think of λ as being freed from the assigned value λ_0 and of $(X_0(\beta, \lambda), 0)$ as the continuation in λ of the equilibrium solution $(X_0(\beta, \lambda_0), 0)$. Thus, (2.14) explicitly becomes

$$\begin{aligned}\Delta F(\beta, \lambda) := &\frac{\partial^4 \mathcal{F}}{\partial Y^4}(X_0(\beta,\lambda), 0, \beta, \lambda) \frac{\partial^2 \mathcal{F}}{\partial X^2}(X_0(\beta,\lambda), 0, \beta, \lambda) \\ &- 3\left(\frac{\partial^3 \mathcal{F}}{\partial Y^2 \partial X}(X_0(\beta,\lambda), 0, \beta, \lambda)\right)^2 = 0. \end{aligned} \tag{2.15}$$

When (β, λ_0) does not belong to the singular manifold, the solution to equation (2.13) is *admissible*, that is, it gives $Y^2 > 0$, only if

$$F_1 F_4 \Delta F < 0. \tag{2.16}$$

Moreover, the new equilibrium phase is close to the reference state $(X_0, 0)$, if F_1 is infinitesimal. For this reason we choose the reference state $(X_0, 0)$ such that (β, λ_0) is near the *critical manifold* in the space $I \times \mathbb{A}$, which is defined by the conditions

$$\Sigma_Y(\beta, \lambda) := \frac{\partial^2 \mathcal{F}}{\partial Y^2}(X_0(\beta, \lambda), 0, \beta, \lambda) = 0, \tag{2.17}$$

$$\Sigma_X(\beta, \lambda) := \frac{\partial^2 \mathcal{F}}{\partial X^2}(X_0(\beta, \lambda), 0, \beta, \lambda) > 0, \tag{2.18}$$

where the latter ensures that the equilibrium phase $(X_0(\beta, \lambda), 0)$ is locally stable against all perturbations in the X order parameter. When (β, λ_0) lies precisely on the critical manifold, F_1 vanishes in (2.13) and the new equilibrium phases reduce to the reference state: all equilibrium solutions corresponding to the critical manifold can be thought of as states whence new equilibria are to bifurcate. Choosing (β, λ_0) near the critical manifold captures the bifurcation onset, and so makes it successful the strategy of finding new equilibrium phases near the reference state.

As a consequence of inequality (2.18), F_4 is positive in (2.11) and this reduces the admissibility condition (2.16) to

$$F_1 \Delta F < 0. \tag{2.19}$$

This inequality is central to the following stability analysis. At the lowest approximation, the Hessian matrix of $\mathcal{F}$ computed at $(X_0 + \delta X, Y)$, where $(\delta X, Y)$ solves equation (2.13), is

$$[H] = \begin{pmatrix} 2F_4 & 2F_3 Y \\ 2F_3 Y & 2F_1 + 12F_2 Y^2 + 2F_3 \delta X \end{pmatrix}. \tag{2.20}$$

Since $F_4 > 0$, the sign of $\det[H]$ suffices to characterize the local stability of $(X_0 + \delta X, Y)$:

$$\det[H] = 4F_1 F_4 + 6Y^2 \left(4F_2 F_4 - F_3^2\right) = -8F_1 F_4. \tag{2.21}$$

Moreover, within the same approximation, the energy difference reads as

$$\Delta\mathcal{F} := \mathcal{F}(X_0 + \delta X, Y) - \mathcal{F}(X_0, 0) = -\frac{F_1^2 F_4}{\Delta F}. \tag{2.22}$$

Our general assert is that the intersection between the critical and the singular manifolds, if not empty, is constituted by tricritical points, which represent states where the character of a phase transition changes from first- to second-order. Here we prove our assert in a special case. In Figure 1, only for illustration purposes, we describe the case where λ is a single parameter model. The following analysis can be easily extended to the general case where $\lambda \in \mathbb{R}^n$, though it becomes more cumbersome. Both the critical and the singular manifolds now become curves, which in Figure 1 are represented in the $(\lambda, 1/\beta)$-plane. We assume that these curves cross at the point C. In Figure 1, ΔF vanishes along the singular curve $\mathcal{S}$, and Σ_Y vanishes along the critical curve $\mathcal{C}$. Near C, a tubular neighborhood of the critical curve is divided into four parts by $\mathcal{S}$ and $\mathcal{C}$, which we denote

by $\mathcal{A}_1$, $\mathcal{A}_2$, $\mathcal{A}_3$, and $\mathcal{A}_4$. For definiteness, we assume that $\Sigma_Y > 0$ in $\mathcal{A}_2 \cup \mathcal{A}_3$ and $\Sigma_Y < 0$ in $\mathcal{A}_1 \cup \mathcal{A}_4$, while $\Delta F > 0$ in $\mathcal{A}_1 \cup \mathcal{A}_3$ and $\Delta F < 0$ in $\mathcal{A}_2 \cup \mathcal{A}_4$.

By inequality (2.19), $\mathcal{A}_1 \cup \mathcal{A}_2$ is the *admissible set*, that is, the set where there are equilibrium phases near the reference state. By (2.21) and (2.22), in $\mathcal{A}_1$ the new equilibrium phase is locally stable since $\det[H] > 0$ and it possesses less energy than the reference state since $\Delta\mathcal{F} < 0$. Moreover, since there $\Sigma_Y < 0$, the reference state is unstable. Clearly, in $\mathcal{A}_1$ a new stable phase bifurcates from the reference state. Similarly, in $\mathcal{A}_2$ $\det[H] < 0$ and $\Delta\mathcal{F} > 0$, while $\Sigma_Y > 0$. This means that the new equilibrium phase is unstable and it possesses higher energy than the reference state, while the reference state is still stable. Here no bifurcation occurs. Away from the admissible set, the reference state is not accompanied by any other equilibrium phase in its vicinity. The reference state itself is locally stable in $\mathcal{A}_3$ and unstable in $\mathcal{A}_4$. Since here we assume that a globally stable phase always exists for the system, when the parameters are chosen in $\mathcal{A}_4$, this phase must lie away from the reference state. On the other hand, in $\mathcal{A}_2$ the reference state could be either locally or globally stable.

Taking now the reference state in $\mathcal{A}_3$ as globally stable, we conclude from the foregoing discussion that it migrates slightly upon crossing the critical curve $\mathcal{C}$ from $\mathcal{A}_3$ into $\mathcal{A}_1$, whereas it jumps abruptly upon crossing the point C from $\mathcal{A}_3$ into $\mathcal{A}_4$. Such a behavior is indicative of the presence of a first-order transition line emanating from C within $\mathcal{A}_2$; the portion of the curve $\mathcal{C}$ that separates $\mathcal{A}_1$ and $\mathcal{A}_3$ is to be interpreted as a second-order transition line.

C is a *tricritical* point, because there two different transition lines meet: one is first-order, the other is second-order. In Figure 1, according to Griffiths's notation [6], first-order transitions are represented by a solid line, while second-order transitions are represented by a broken line.

The situation envisaged in Figure 1 can easily be extended. As shown in Figure 2, the critical curve $\mathcal{C}$ and the singular curve $\mathcal{S}$ can have multiple intersections. Here the admissible set $\mathcal{A}_1 \cup \mathcal{A}_2$ has more than two adjacent components, but it is still connected; a first-order transition line joins two tricritical points, whence two distinct second-order transition lines emerge.

In conclusion, in the general formulation employed above, we may hold that the *tricritical manifold* is defined by equations (2.15) and (2.17) and that the conditions

$$\frac{\partial^2\mathcal{F}}{\partial Y^2}\left(X_0\left(\beta,\lambda\right),0,\beta,\lambda\right) = 0 \tag{2.23a}$$

$$\frac{\partial^4\mathcal{F}}{\partial Y^4}\left(X_0\left(\beta,\lambda\right),0,\beta,\lambda\right)\frac{\partial^2\mathcal{F}}{\partial X^2}\left(X_0\left(\beta,\lambda\right),0,\beta,\lambda\right) - 3\left(\frac{\partial^3\mathcal{F}}{\partial Y^2\partial X}\left(X_0\left(\beta,\lambda\right),0,\beta,\lambda\right)\right)^2 > 0, \tag{2.23b}$$

determine the submanifold of the critical manifold consisting of second-order transition points.

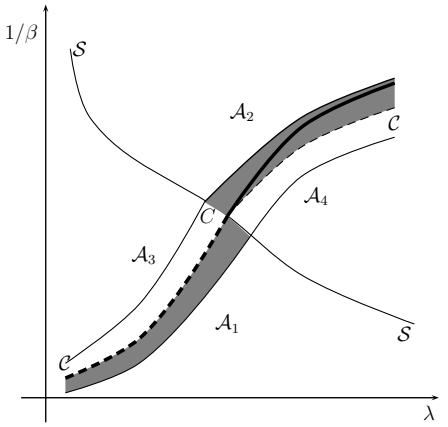

FIGURE 1. The tricritical point C is identified as the intersection between the critical curve $\mathcal{C}$ and the singular curve $\mathcal{S}$ in the plane $(\lambda, 1/\beta)$. $\mathcal{A}_1 \cup \mathcal{A}_2$ is the admissible set, where there is an equilibrium phase near the reference state. The heavy dashed line is a second-order transition line, while the heavy solid line is a first-order transition line.

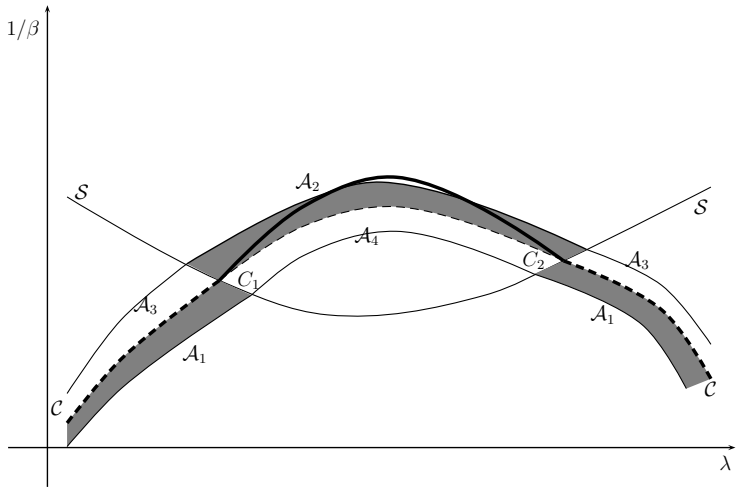

FIGURE 2. The critical curve $\mathcal{C}$ and the singular curve $\mathcal{S}$ cross in two tricritical points, C_1 and C_2, connected by a first-order transition line (heavy solid line). The second-order transition line has two distinct components (heavy dashed lines).

Finally, we note that a better approximation for the equilibrium phase near the reference state can be obtained in the admissible set from (2.11) and (2.12):

$$\delta X = \frac{F_1 F_3}{4F_2F_4 - F_3^2 - 2F_1F_6}, \tag{2.24}$$

$$Y^2 = \frac{(F_1F_6 - 2F_2F_4)}{4F_2F_4 - F_3^2 - 2F_1F_6}\frac{F_1}{F_2}. \tag{2.25}$$

These formulae are useful in sketching the bifurcating solution branches and to continue them numerically. A similar improvement of the lowest approximation employed above can be obtained for both the determinant of the Hessian matrix and the energy difference along the bifurcating branches.

3. Applications

In this section we apply the criterion presented above to two different molecular models. These are mean-field models for smectic and biaxial phases in liquid crystals. In both cases, the reference state is one of the equilibrium phases predicted by Maier-Saupe's molecular model for nematic liquid crystals [18].

3.1. McMillan's model for smectics

McMillan's mean-field theory for smectics is a two-order-parameter theory [2]. This theory extends Maier-Saupe's by accounting for the possibility that the slender liquid crystal molecules be also subject to a positional ordering superimposed to the orientational ordering. At variance with Maier-Saupe's pair potential, McMillan's pair potential V_{12} also includes a part depending on the intermolecular distance r_{12}:

$$V_{12}\left(r_{12}, \cos\vartheta_{12}\right) = -\left(\frac{V_0}{N r_0^3 \pi^{\frac{3}{2}}}\right) \exp\left[-\left(\frac{r_{12}}{r_0}\right)^2\right]\left(\frac{3}{2}\cos^2\vartheta_{12} - \frac{1}{2}\right), \tag{3.1}$$

where ϑ_{12} is the angle between the orientations of two interacting molecules, V_0 is a typical interaction energy, N is the number density of particles, r_0 is a typical molecular length. In this equation, V_{12} decays exponentially with r_{12}, thus reflecting the short range character of the interaction.

Within the mean-field theory, one assumes that each molecule feels a mean potential V_1, which can be viewed as an average of the pair potential V_{12}. Under the further assumption that all molecules are preferentially aligned along the z-axis and that their centers of mass tend to lie on planes parallel to the (x, y)-plane, at the distance d from one another, McMillan arrived at the following expression for V_1

$$V_1\left(z, \cos\vartheta\right) = -V_0\left[S + \sigma\alpha\cos\left(\frac{2\pi z}{d}\right)\right]\left(\frac{3}{2}\cos^2\vartheta - \frac{1}{2}\right), \tag{3.2}$$

where ϑ is the angle that the individual molecule makes with the z-axis, S and σ are order parameters, and $\alpha := 2\exp\left[-\left(\pi r_0/d\right)^2\right]$ is a model parameter ranging in the interval $[0, 2]$. S is the classical Maier-Saupe order parameter [18], which

expresses the orientational order of molecules, while σ is a smectic order parameter, which expresses the degree of positional order within the layer structure of the molecular centers of mass. S ranges in the interval $\left[-\frac{1}{2}, 1\right]$, while σ ranges in the interval $[-1, 1]$.

Within the mean-field approximation, the partition function and the free energy per molecule of this system are, respectively,

$$Z(S, \sigma, \beta, \alpha) = \int_0^{2\pi} d\varphi \int_0^1 du \exp\left[\beta (S + \alpha\sigma \cos\varphi)\left(u^2 - \frac{1}{3}\right)\right] \tag{3.3}$$

and

$$\mathcal{F}(S, \sigma, \beta, \alpha) = \frac{1}{2} V_0 \left\{ \left(S^2 + \alpha\sigma^2\right) - \frac{3}{\beta} \ln \frac{Z(S, \sigma, \beta, \alpha)}{2\pi} \right\}, \tag{3.4}$$

where $\beta := \frac{3}{2} \frac{V_0}{\kappa_B t}$ and κ_B is the Boltzmann constant [2]. It should be noted that $\mathcal{F}$ is even in σ:

$$\mathcal{F}(S, \sigma, \beta, \alpha) = \mathcal{F}(S, -\sigma, \beta, \alpha),$$

and so it falls within the class of free energies to which the criterion presented in the preceding section can be directly applied, with the identifications $X = S$ and $Y = \sigma$.

When α is sufficiently small, McMillan's model appears to be a perturbation to Maier-Saupe's. As is well-known, this latter predicts that the isotropic phase corresponding to $S = 0$ is accompanied by another locally stable equilibrium phase as soon as $\beta > \beta^* \approx 6.73$. This is the oriented nematic phase, which is characterized by the largest positive root $S_+(\beta)$ of the equilibrium equation

$$\frac{\partial \mathcal{F}}{\partial S} = 0,$$

which for $\alpha = 0$ becomes

$$\frac{2}{3} S + \frac{1}{3} + \frac{1}{2S\beta} - \frac{\exp(S\beta)}{\sqrt{\pi S\beta}\, Erfi\left(\sqrt{S\beta}\right)} = 0, \tag{3.5}$$

where

$$Erfi(x) := \frac{2}{\sqrt{\pi}} \int_0^x e^{t^2} dt \quad \text{for all } x \in \mathbb{R}. \tag{3.6}$$

For $\beta > \beta_c \approx 6.81$, the nematic phase has indeed lower free energy than the isotropic phase, which is still locally stable, and so the system undergoes a first-order phase transition. For $\beta > \beta_* = \frac{15}{2}$, the isotropic phase becomes locally unstable and another equilibrium ordered phase with a negative order parameter $S_-(\beta)$ arises; in the absence of any external field, this phase never attains the least energy, and so it fails to be globally stable.

When $\alpha = 0$, the only phase transition undergone by the system occurs at $\beta = \beta_c$, where S condenses in S_+, but when $\alpha > 0$, this is followed by a smectic transition which establishes an equilibrium value of $\sigma \neq 0$ for $\beta > \beta_c' > \beta_c$. This secondary transition can be either first- or second-order [2]: we show now how our criterion is able to locate correctly the tricritical point where the change of type in the secondary phase transition occurs. Specifically, for $\alpha > 0$ and $\beta > \beta^*$, we

take the state with $S = S_+(\beta)$ and $\sigma = 0$ as reference state. The eigenvalues Σ_σ and Σ_S defined in (2.17) and (2.18) here become

$$\Sigma_S(\beta,\alpha) := \frac{\partial^2 \mathcal{F}}{\partial S^2}(S_+(\beta),0) = \frac{5}{2} + \frac{\beta}{3}\left(2S_+^2(\beta) - S_+(\beta) - 1\right), \tag{3.7}$$

$$\Sigma_\sigma(\beta,\alpha) := \frac{\partial^2 \mathcal{F}}{\partial \sigma^2}(S_+(\beta),0) = \alpha\left[1 - \alpha\left(\frac{\beta}{6}(S_+(\beta)+1) - \frac{3}{4}\right)\right], \tag{3.8}$$

whence it follows that Σ_S is actually independent of α and it is positive for $\beta > \beta^*$.

The critical line defined in Section 2 by equation (2.17) is here represented by the equation

$$\Sigma_\sigma(\beta,\alpha) = 0, \tag{3.9}$$

while the singular line defined by (2.15) is here (see also the Appendix)

$$\begin{aligned}\frac{3\alpha^4}{128S_+^2}\Bigg[&75 + 20\beta\left(S_+^2 + S_+ - 1\right) + \frac{16}{27}\beta^3 S_+\left(3 + 19S_+ + 15S_+^2 - 17S_+^3\right)\\ &+ \frac{4}{3}\beta^2\left(1 - 12S_+ - 36S_+^2 + 6S_+^3\right)\\ &+ \frac{16}{81}\beta^4 S_+^2\left(10S_+^3 + S_+^2 - 8S_+ - 3\right)\Bigg] = 0.\end{aligned} \tag{3.10}$$

Thus, the tricritical points are identified as the common roots of (3.9) and (3.10), where $S_+ = S_+(\beta)$ is the largest root of (3.5).

Figure 3 shows both critical and singular lines described by (3.9) and (3.10) on the plane $(\alpha, 1/\beta)$. In particular, since the critical line is meaningful only when $\Sigma_S > 0$, the curve corresponding to (3.9) is restricted to the region where $\beta > \beta^*$, and so it ends at the point E_1, where $\beta = \beta^*$. Moreover, since for all $\alpha > 0$ the roots of (3.10) are independent of α, the singular line has indeed equation $\beta = \beta_t$, where β_t is a root of the function of β between brackets in (3.10). It can be shown numerically that there is only one such root. The tricritical point C in Figure 3 has the following co-ordinates:

$$(\beta_t, \alpha_t) \approx (7.831, 0.707) \tag{3.11}$$

with $S_t := S_+(\beta_t) \approx 0.657$. This tricritical point coincides with the one found by McMillan [2] by solving directly the equilibrium equations of the model: it is also the same found by Kloczkowski and Stecki [13] by another method (see the discussion in the following section). By applying (2.23b), we finally conclude that the portion of critical line that marks a second-order transition between nematic and smectic phases is the one heavily dashed in Figure 3.

Figure 3 also depicts the line $\beta = \beta_c$, where the first-order transition between isotropic and nematic phases takes place, and a sketch of the first-order line originated in C; when this line meets the line $\beta = \beta_c$, a first-order direct transition between isotropic and smectic phases takes place. In principle, along this line there could be another tricritical point, where the isotropic-to-smectic transition becomes second-order, in complete analogy with the ideal situation illustrated in Figure 2. To see whether this putative tricritical point does actually exist, we now

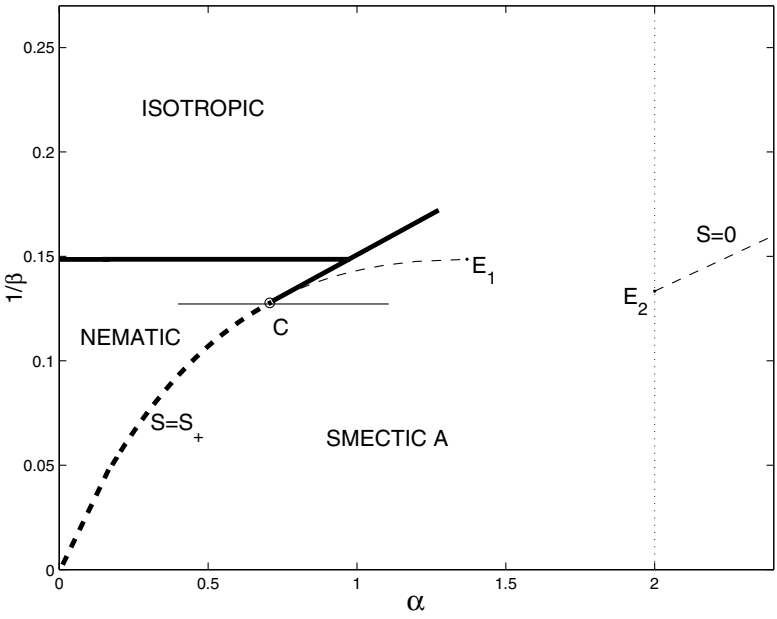

FIGURE 3. Phase diagram in the plane $(\alpha, 1/\beta)$ associated with McMillan's model for smectics A. The critical line relative to the nematic state $S = S_+$ and $\sigma = 0$ starts from the origin and ends in E_1: it is confined to the stable manifold $\beta > \beta^*$. The dashed portion of this line, bounded by line $\beta = \beta_t$, marks the second-order transition between nematic and smectic phases. C is the tricritical point. The critical line relative to the isotropic phase $S = \sigma = 0$ is confined to the stable manifold $\beta < \frac{15}{2}$: it starts from the point E_2 where $\alpha = 2$ and falls entirely outside the range of validity of the model. The heavy solid line represents first-order transitions: both between isotropic and nematic phases, and between isotropic and smectic phases.

apply our criterion, taking the isotropic phase as reference state. Thus we compute both Σ_S and Σ_σ for $S = \sigma = 0$:

$$\Sigma_S(\beta, \alpha) := \frac{\partial^2 \mathcal{F}}{\partial S^2}(0,0) = 1 - \frac{2\beta}{15}, \tag{3.12}$$

$$\Sigma_\sigma(\beta, \alpha) := \frac{\partial^2 \mathcal{F}}{\partial \sigma^2}(0,0) = \alpha - \frac{\alpha^2 \beta}{15}. \tag{3.13}$$

It follows from (3.12) that $\Sigma_S > 0$ for $\beta < \frac{15}{2}$ and that the critical line is represented by the equation

$$\frac{1}{\beta} = \frac{\alpha}{15}. \tag{3.14}$$

The singular line is now represented by (see also the Appendix)

$$\alpha^4\beta^3\,(35+22\beta)=0. \tag{3.15}$$

It is clear that equations (3.14) and (3.15) have no common root for $\alpha > 0$. Moreover, by (3.14), Σ_S would be positive on the critical line only for $\alpha > 2$, that is, away from the range of validity of the model. Thus, the only tricritical point compatible with McMillan's model is the one in (3.11): the direct phase transition isotropic-to-smectic predicted by this model remains first-order for all admissible values of α.

3.2. Model for biaxial nematics

Recently, much attention has again be devoted to thermotropic biaxial nematic phases, both theoretically [12, 19, 20] and experimentally [21, 22, 23] (we refer the reader to [24] for a short, but effective update on the most recent developments in this rapidly evolving field).

In particular, in [12] Straley's molecular pair potential [16] has also been studied beyond the range of validity of London's dispersion forces approximation and Freiser's model [25]. In [12], the general form of Straley's pair potential V is expressed by representing each interacting molecule by a pair of traceless, symmetric, second-rank tensors $(\mathbf{q},\mathbf{b})$, where

$$\mathbf{q} := \boldsymbol{m}\otimes\boldsymbol{m}-\frac{1}{3}\mathbf{I} \tag{3.16}$$

is purely uniaxial around the long molecular axis $\boldsymbol{m}$, and

$$\mathbf{b} := \boldsymbol{e}\otimes\boldsymbol{e}-\boldsymbol{e}_\perp\otimes\boldsymbol{e}_\perp \tag{3.17}$$

is fully biaxial and orthogonal to $\mathbf{q}$. The orthonormal basis $\{\boldsymbol{e},\boldsymbol{e}_\perp,\boldsymbol{m}\}$ is the eigenframe of any molecular polarizability tensor. Letting $(\mathbf{q},\mathbf{b})$ and $(\mathbf{q}',\mathbf{b}')$ represent two interacting molecules, we write V as

$$V=-U_0\left\{\mathbf{q}\cdot\mathbf{q}'+\gamma\left(\mathbf{q}\cdot\mathbf{b}'+\mathbf{b}\cdot\mathbf{q}'\right)+\lambda\mathbf{b}\cdot\mathbf{b}'\right\}, \tag{3.18}$$

where $U_0 > 0$ is a typical interaction energy, and λ and γ are model parameters.

Macroscopically the liquid crystal is described by two order tensors, both defined as ensemble averages:

$$\mathbf{Q} := \langle\mathbf{q}\rangle\,, \qquad \mathbf{B} := \langle\mathbf{b}\rangle\,.$$

Under the assumption that $\mathbf{Q}$ and $\mathbf{B}$ have a common eigenframe $\{\boldsymbol{e}_x,\boldsymbol{e}_y,\boldsymbol{e}_z\}$, which is plausible in the absence of any external distorting cause, they can be represented as follows

$$\mathbf{Q}=S\left(\boldsymbol{e}_z\otimes\boldsymbol{e}_z-\frac{1}{3}\mathbf{I}\right)+T\left(\boldsymbol{e}_x\otimes\boldsymbol{e}_x-\boldsymbol{e}_y\otimes\boldsymbol{e}_y\right), \tag{3.19}$$

$$\mathbf{B}=S'\left(\boldsymbol{e}_z\otimes\boldsymbol{e}_z-\frac{1}{3}\mathbf{I}\right)+T'\left(\boldsymbol{e}_x\otimes\boldsymbol{e}_x-\boldsymbol{e}_y\otimes\boldsymbol{e}_y\right), \tag{3.20}$$

where S, T, S', T' are the order parameters of the system. $\mathbf{Q}$ represents the average quadrupolar distribution of the long molecular axis: its degree of biaxiality

measured by T reflects the lack of axial symmetry in the orientational distribution function. $\mathbf{B}$ reflects on a macroscopic scale the intrinsic biaxiality of molecules and the role this plays in the molecular interaction: like $\mathbf{Q}$, in general, $\mathbf{B}$ has both a uniaxial and a biaxial component. S is precisely Maier-Saupe's order parameter: when T, S', and T' all vanish, the resulting phase is purely uniaxial. We would call a phase uniaxial even when only S and S' do not vanish, though the origin of S' is to be retraced in the intrinsic molecular biaxiality. Similarly, T and T' express degrees of biaxiality of two different origins.

In the mean-field approximation adopted in [12], a single molecule feels the pseudo-potential

$$U(\mathbf{q}, \mathbf{b}) = -U_0 \{\mathbf{Q} \cdot \mathbf{q} + \gamma (\mathbf{Q} \cdot \mathbf{b} + \mathbf{B} \cdot \mathbf{q}) + \lambda \mathbf{B} \cdot \mathbf{b}\}. \tag{3.21}$$

Accordingly, the partition function Z and the free energy F are

$$Z(\mathbf{Q}, \mathbf{B}, \beta, \lambda, \gamma) = \int_{\mathbb{T}} \exp(\beta (\mathbf{Q} \cdot \mathbf{q} + \gamma (\mathbf{Q} \cdot \mathbf{b} + \mathbf{B} \cdot \mathbf{q}) + \lambda \mathbf{B} \cdot \mathbf{b})), \tag{3.22}$$

$$\mathcal{F}(\mathbf{Q}, \mathbf{B}, \beta, \lambda, \gamma) = U_0 \left\{ \frac{1}{2} \mathbf{Q} \cdot \mathbf{Q} + \gamma \mathbf{Q} \cdot \mathbf{B} + \frac{1}{2} \lambda \mathbf{B} \cdot \mathbf{B} - \frac{1}{\beta} \ln \left(\frac{Z(\mathbf{Q}, \mathbf{B}, \beta, \lambda, \gamma)}{8\pi^2} \right) \right\}, \tag{3.23}$$

where $\mathbb{T}$ is the manifold described by all possible molecular orientations $\{\boldsymbol{e}, \boldsymbol{e}_\perp, \boldsymbol{m}\}$, and $\beta := \frac{U_0}{\kappa_B t}$. In [12], the case where $\gamma = 0$ and λ ranges in the interval $\left[0, \frac{1}{3}\right]$ was extensively considered and a tricritical point was discovered in the phase diagram. More precisely, it was shown that for small enough values of λ the classical Maier-Saupe first-order transition from the isotropic phase is followed, at a large enough value of β, by a second-order transition to a biaxial phase characterized by $T' \neq 0$ and with both T and S' almost vanishing. This *scenario* changes qualitatively when λ grows: the transition to the biaxial phase becomes first-order, as shown by solving numerically the equilibrium equations, thus disclosing a tricritical point.

Here we apply the criterion presented in Section 2 to this model predicting biaxial phases. Though all admissible states are described by four scalar order parameters, instead of two, our criterion is still directly applicable since T and S' can be set equal to zero at all equilibrium phases [12] and the free energy $\mathcal{F}$ in (3.23) turns out to be even in T'. Thus, we identify X with S and Y with T' in our formal development above. Taking again as reference state Maier-Saupe's uniaxial phase described by the pair $(S_+(\beta), 0)$, with S_+ as above, we compute the following eigenvalues of the Hessian matrix $[H_0]$:

$$\Sigma_S(\beta) = \frac{2}{3} \left[\frac{5}{2} + \frac{\beta}{3} (2S_+^2 - 2S_+ - 1) \right], \tag{3.24}$$

$$\Sigma_{T'}(\beta, \lambda) = \frac{1}{12} \lambda [24 + (3 - 10\beta - 14S_+\beta)\lambda], \tag{3.25}$$

where the expression for Σ_S is proportional to the one in (3.7), and so again $\Sigma_S > 0$ for $\beta > \beta^* \approx 6.73$. The critical and the singular lines are represented by the equations

$$\Sigma_{T'} = 0 \tag{3.26}$$

and

$$\begin{aligned}\frac{\lambda^4}{27648 S_+^2}\big[&2025 + 180(-3 + 17S_+ + 3S_+^2)\beta \\ &+ 12(3 - 184S_+ - 652S_+^2 + 74S_+^3)\beta^2 \\ &+ 80S_+(3 + 97S_+ + 181S_+^2 + 7S_+^3)\beta^3 \\ &+ 16S_+^2(-65 - 192S_+ + 3S_+^2 + 254S_+^3)\beta^4\big] = 0,\end{aligned} \tag{3.27}$$

respectively (see also the Appendix). Thus, the tricritical points are identified as the common roots of equations (3.26) and (3.27), where $S_+ = S_+(\beta)$ is defined precisely as above.

In complete analogy with our development in the above subsection, Figure 4 shows both critical and singular lines described by (3.26) and (3.27) in the plane $(\lambda, 1/\beta)$. In particular, since the critical line is meaningful only when $\Sigma_S > 0$, the curve corresponding to (3.26) is restricted to the region where $\beta > \beta^*$, and so it ends at the point E_1, where $\beta = \beta^*$. Moreover, since for $\lambda > 0$ the roots of (3.27) are independent of λ, the singular line has equation $\beta = \beta_t$, where β_t is a root of the function of β within brackets in (3.27). By use of the asymptotic behavior of S_+ for $\beta \to \infty$,

$$S_+(\beta) \simeq \frac{1}{2}\left(1 + \sqrt{1 - \frac{6}{\beta}}\right), \tag{3.28}$$

it is easily shown that there exists a single root $\beta_t^{(1)}$. The tricritical point C_1 in Figure 4 has the following co-ordinates:

$$\left(\beta_t^{(1)}, \lambda_t^{(1)}\right) \approx (7.07, 0.20), \tag{3.29}$$

with $S_t = S_+(\beta_t^{(1)}) \approx 0.53$. It coincides with the point found in [12] by inspecting the numerical solutions to the equilibrium equations. By applying (2.23b), we conclude that the portion of critical line that marks a second-order transition between uniaxial and biaxial phases is the one heavily dashed in Figure 4. This figure also depicts the lines of first-order transitions computed for $0 < \lambda < \frac{1}{3}$ in [12].

It could also be asked for this model the same question asked for McMillan's model: as to whether the transition between isotropic and biaxial phases can possibly become second-order. To answer this question, we also study this model for $\lambda > \frac{1}{3}$ and we take the isotropic phase as reference state in our criterion.

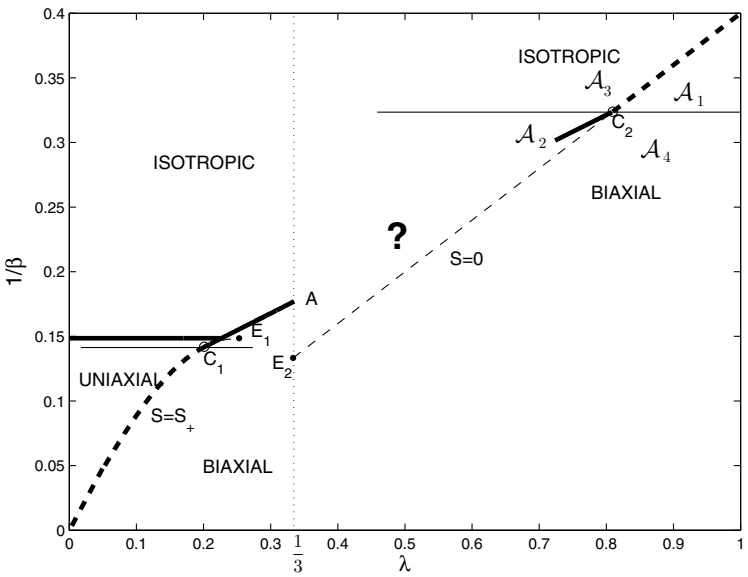

FIGURE 4. Phase diagram in the plane $(\lambda, 1/\beta)$ associated with a model for biaxial nematics [12]. The critical line relative to the uniaxial state $S = S_+$ and $T' = 0$ starts from the origin and ends in E_1: it is confined to the stable manifold $\beta > \beta^*$. The dashed portion of this line, bounded by line $\beta = \beta_t^{(1)}$, marks the second-order transition between uniaxial and biaxial phases. C_1 is the first tricritical point. The critical line relative to the isotropic phase $S = T' = 0$ is confined to the stable manifold $\beta < \frac{15}{2}$: it starts from the point E_2 and goes to infinity. It hosts the second tricritical point C_2 at $\beta = \beta_t^{(2)}$; the regions $\mathcal{A}_1$, $\mathcal{A}_2$, $\mathcal{A}_3$, and $\mathcal{A}_4$ have the same meaning as in Section 2. The heavy dashed line starting from C_2 represents a second-order transition between isotropic and biaxial phases. The heavy line represents first-order phase transitions computed for $0 < \lambda < \frac{1}{3}$ [12]: a bifurcation analysis is needed to know how the points A and C_2 are to be joined [27].

We compute both Σ_S and $\Sigma_{T'}$, for $S = T' = 0$:

$$\Sigma_S(\beta, \lambda) := \frac{\partial^2 \mathcal{F}}{\partial S^2}(0,0) = \frac{1}{3} - \frac{2\beta}{45}, \tag{3.30}$$

$$\Sigma_{T'}(\beta, \lambda) := \frac{\partial^2 \mathcal{F}}{\partial T'^2}(0,0) = \lambda - \frac{2\lambda^2 \beta}{5}. \tag{3.31}$$

It follows from (3.30) that $\Sigma_S > 0$ for $\beta < \frac{15}{2}$ and that the critical line is represented by the equation

$$\frac{1}{\beta} = \frac{2\lambda}{5}. \tag{3.32}$$

The singular line is now (see also the Appendix)

$$\beta^3\lambda^4\,(34\beta - 105) = 0. \tag{3.33}$$

It is clear that equations (3.32) and (3.33) have only the following root

$$\left(\beta_t^{(2)}, \lambda_t^{(2)}\right) = \left(\frac{105}{34}, \frac{17}{21}\right), \tag{3.34}$$

which identifies a second tricritical point C_2. By (2.23b), the heavy dashed line emanating in Figure 4 from C_2 represents the locus of second-order transitions between isotropic and biaxial phases.

The criterion presented here can only predict the existence of this second tricritical point, where the phase transition between isotropic and biaxial phases becomes second-order. It says nothing on how to complete the phase diagram in the plane $(\lambda, 1/\beta)$ for $\frac{1}{3} < \lambda < \lambda_t^{(2)}$: this requires a bifurcation analysis of the equilibrium phases, which will be undertaken elsewhere [27].

4. Comparison

We derived a criterion to identify the symmetric tricritical points for a general ordered system described by two order parameters, X and Y, knowing only the free energy $\mathcal{F} = \mathcal{F}(X, Y)$. Our criterion is embodied by equations (2.15) and (2.17). Moreover, since our reasoning rests essentially on a local stability analysis, we were also able to characterize the subset of the critical manifold bordered by the tricritical manifold where the transition is genuinely second-order (see inequality (2.23b) above). In general, the criterion proposed here is valid if the free energy is however given in terms of the order parameters; this is always the case for a molecular field theory, as was for the applications shown in Section 3.

We already mentioned in the Introduction another criterion to find tricritical points between liquid crystal phases [13, 14]. It stems from extending Griffiths's criterion to a system with more than one order parameter, under the assumption that there is always a single leading order parameter, from which all others depend in the ordered phase. Taking in our setting Y as the leading order parameter and denoting by f the function linking $\delta X := X - X_0$ to Y, so that $\delta X = f(Y)$, we easily see that the path of equilibrium states in the vicinity of the reference state $(X_0, 0)$, where $\delta X = Y = 0$, is described by the equations

$$\frac{\partial(\Delta\mathcal{F})}{\partial Y}(f(Y), Y) = 0, \qquad \frac{\partial(\Delta\mathcal{F})}{\partial(\delta X)}(f(Y), Y) = 0, \tag{4.1}$$

where $\Delta\mathcal{F}$ is defined as in (2.22). It follows from the second of equations (4.1) that

$$\frac{\partial^2(\Delta\mathcal{F})}{\partial(\delta X)\partial Y} + \frac{\partial^2(\Delta\mathcal{F})}{\partial(\delta X)^2} f' = 0, \tag{4.2}$$

where a prime denotes differentiation with respect to Y. Since $\Delta\mathcal{F}$ is symmetric in Y, also by (2.18), (4.2) implies that f' vanishes at the reference state $(X_0, 0)$,

whenever this lies on the critical manifold. Thus, evaluating both $(\Delta\mathcal{F})''$ and $(\Delta\mathcal{F})''''$ at the reference state, we find that there

$$(\Delta\mathcal{F})'' = \left(\frac{\partial^2\mathcal{F}}{\partial Y^2}\right)_{(X_0,0)},$$
$$(\Delta\mathcal{F})'''' = \left(\frac{\partial^4\mathcal{F}}{\partial Y^4}\right)_{(X_0,0)} - \frac{3}{\left(\frac{\partial^2\mathcal{F}}{\partial X^2}\right)_{(X_0,0)}}\left(\frac{\partial^3\mathcal{F}}{\partial Y^2\partial X}\right)^2_{(X_0,0)}.$$

Requiring both $(\Delta\mathcal{F})''$ and $(\Delta\mathcal{F})''''$ to vanish, as prescribed by Griffiths's criterion, reproduces our equations (2.15) and (2.17). This shows that the existing criterion [13, 14], which assumes the existence of a leading order parameter, reduces to ours, which, strictly speaking, does not require that assumption.

5. Conclusion

It was remarked in [12] that the model proposed there for biaxial nematics has a striking resemblance to McMillan's model for smectics A, in that it predicts a similar phase diagram with a tricritical point. The original motivation of our study was to find a criterion to identify tricritical points for liquid crystal phases, sufficiently general both to encompass the tricritical points known in the cases just recalled and to predict other such points, possibly unknown.

We arrived at a criterion of this kind building on existing criteria. The main outcome of our study was to predict the existence of another tricritical point for biaxial nematics according to the model employed in [12]. As explained in Section 3, this makes this model and McMillan's qualitatively very different, as our criterion confirmed for the latter the existence of a single tricritical point.

A bifurcation analysis of the whole class of equilibrium phases predicted by the model for biaxial nematics in [12] is still needed to complete the phase diagram. This study will be presented in [27].

Appendix A. Smectics

In this and in the following appendix we list the coefficients of the expansion in (2.6) for the free energy $\mathcal{F}$ that enter the definitions of both the critical and singular lines for the specific models studied above. For each model we distinguish explicitly two cases: the one where $S = S_0 \neq 0$ and the one where $S = 0$. In the former case, repeated use of (3.5) is made.

A.1. $S = S_0$

$$
\begin{aligned}
F_1\left(S_0,\beta,\alpha\right) =& \frac{1}{2}\Sigma_\sigma\left(\beta,\alpha\right) = -\frac{1}{8}\alpha\left[-4+\frac{2}{3}\alpha\left(\beta S_0+\beta-\frac{9}{2}\right)\right],\\
F_2\left(S_0,\beta,\alpha\right) =& \frac{\alpha^4}{512S_0^2}\left[105+\frac{8}{27}\beta^3S_0^2\left(1+3S_0+4S_0^2\right)\right.\\
&\left.-\frac{4}{3}\beta^2S_0\left(-2+S_0+8S_0^2\right)+2\beta\left(-7-15S_0+12S_0^2\right)\right],\\
F_3\left(S_0,\beta,\alpha\right) =& \frac{\alpha^2}{16S_0}\left[-15+2\beta\left(1+2S_0-2S_0^2\right)+\frac{4}{9}\beta^2S_0\left(-1-S_0+2S_0^2\right)\right],\\
F_4\left(S_0,\beta\right) =& \frac{1}{2}\Sigma_S\left(\beta\right) = \frac{1}{4}\left[5+\frac{2}{3}\beta\left(-1-S_0+2S_0^2\right)\right].
\end{aligned}
$$

A.2. $S = 0$

$$
\begin{aligned}
F_1\left(\beta,\alpha\right) =& \frac{1}{2}\Sigma_\sigma\left(\beta,\alpha\right) = \frac{\alpha}{2}\left(1-\frac{\alpha\beta}{15}\right),\\
F_2\left(\beta,\alpha\right) =& -\frac{\alpha^4\beta^3}{37800},\\
F_3\left(\beta,\alpha\right) =& -\frac{2\alpha^2\beta^2}{315},\\
F_4\left(\beta\right) =& \frac{1}{2}\Sigma_S\left(\beta\right) = \frac{1}{2}\left(1-\frac{2\beta}{15}\right).
\end{aligned}
$$

Appendix B. Biaxials

B.1. $S = S_0$

$$
\begin{aligned}
F_1(S_0,\beta,\lambda) =& \frac{1}{2}\Sigma_{T'}\left(\beta,\lambda\right) = \frac{1}{24}\lambda\left[24+(3-10\beta-14S_0\beta)\lambda\right],\\
F_2(S_0,\beta,\lambda) =& \frac{\lambda^4}{18432S_0^2}\left[945+18\beta(8S_0^2-135S_0-7)\right.\\
&\left.+12S_0\beta^2(26+287S_0-112S_0^2)+8S_0^2\beta^3(392S_0^2+185S_0-1)\right]\\
F_3(S_0,\beta,\lambda) =& \frac{\lambda^2}{144S_0}\left[-45+\beta(6+132S_0-12S_0^2)+28S_0\beta^2(2S_0^2-S_0-1)\right],\\
F_4(S_0,\beta) =& \frac{1}{2}\Sigma_S\left(\beta\right) = \frac{1}{18}\left[15+(-2-2S_0+4S_0^2)\beta\right].
\end{aligned}
$$

B.2. $S = 0$

$$F_1(\beta,\lambda) = \frac{1}{2}\Sigma_{T'}(\beta,\lambda) = \lambda\left(1 - \frac{2\beta\lambda}{5}\right),$$
$$F_2(\beta,\lambda) = \frac{4\beta^3\lambda^4}{175},$$
$$F_3(\beta,\lambda) = -\frac{8\beta^2\lambda^2}{105},$$
$$F_4(\beta) = \frac{1}{2}\Sigma_S(\beta) = \frac{1}{3} - \frac{2\beta}{45}.$$

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Asymptotics of Boundary Value Problems for Supercritical Ginzburg-Landau Energies

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Abstract. We present a result of variational convergence for Ginzburg-Landau type energies having "supercritical" growth, under a prescribed Dirichlet boundary condition. This is obtained modifying our previous result proved in [4] about the Γ-convergence of the unconstrained functionals, and allows us to obtain the asymptotic behavior of minimizers.

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1. Introduction

Let Ω be an open and regular bounded domain in $\mathbb{R}^{n+k}$, where the integers k and n satisfy $k \geq 2$ and $n \geq 0$. For $u \in W^{1,p}(\Omega;\mathbb{R}^k)$, let us consider the integral functionals

$$F_\varepsilon(u) := \int_\Omega \big[|\nabla u|^p + \frac{1}{\varepsilon^p} W(u)\big] d\mathcal{L}^{n+k} \ , \tag{1.1}$$

where $p > 1$ is a real exponent, $\mathcal{L}^{n+k}$ is the Lebesgue measure on $\mathbb{R}^{n+k}$, and W is a nonnegative continuous potential on $\mathbb{R}^k$, vanishing only on the unit sphere S^{k-1}. Minimizers of F_ε are trivially constant functions with values into the unit sphere, as long as no additional constraint is imposed in the minimization process. On the other hand, if v is an assigned boundary datum in the natural trace space $W^{1-1/p,p}(\partial\Omega, S^{k-1})$, the asymptotics of the minimum problems

$$\min\Big\{F_\varepsilon(u) \ : \ u \in W^{1,p}(\Omega;\mathbb{R}^k) \ , \ u = v \text{ on } \partial\Omega\Big\} \tag{1.2}$$

may be nontrivial provided $p \geq k$. Indeed, when this last condition holds, the Dirichlet datum v can be chosen so that the space of functions in $W^{1,p}(\Omega; S^{k-1})$ with trace v on $\partial\Omega$ is empty [8]. Thus, a competition arises between the two terms in the integral functionals F_ε, as the first one penalizes spatial inhomogeneity, while the second one penalizes values far from the unit sphere. In particular, as $\varepsilon \to 0$,

energy concentration is expected near an n-dimensional singular set M (recalling that n is the difference of dimension between the domain and the codomain of the admissible functions, M may be intuitively thought as the zero level set of u, see Section 2.4). Moreover, M can be endowed with an integer multiplicity, which takes into account the degree of the singularity. Thus, one is led in a natural way to study the problem in the setting of currents. In particular, the concentration phenomenon can be tackled by looking at the Jacobians of admissible functions, seen as n-dimensional currents. This approach was developed in [2], where the limit behavior of the minimum problems (1.2) is completely determined under the assumption that the growth exponent p is equal to the dimension k of the target space (see also [11] for the special case $p = k = 2$). Quite roughly, the main result of [2] tells that, as $\varepsilon \to 0$, the Jacobians of maps solving problem (1.2) for $p = k$ converge in a suitable sense to n-currents which are mass minimizing in a certain class of rectifiable currents with prescribed boundary. This result may be regarded as an extension of the celebrated Modica-Mortola theorem [12] to the case of vector-valued functions. Let us add that such extension is quite far from being straightforward: it requires a deep investigation on the behavior of the Jacobians, as well as many fine tools from currents theory.

In our previous work [4], we studied the variational convergence of the energies F_ε in the supercritical case $p > k$ (the word "supercritical" being due to the above mentioned fact that $p = k$ is the smallest exponent for which energy concentration may occur). By following the same approach as in [2], we proved that for $p > k$ the Γ-limit of the functionals F_ε can be characterized as a suitable integral functional on a class of rectifiable n-boundaries M supported in Ω. Moreover, the most interesting feature of the limit energy is that it depends on the multiplicity of M through a family of optimal profile constants τ_d, for d varying in $\mathbb{Z}$: heuristically, τ_d represents the minimal energetic cost needed for a singularity of degree d (see Section 2.6). Thus the case $p > k$ is not a trivial adaptation of the case $p = k$, and in particular for the sake of simplicity we confined ourselves to studying the variational convergence of the unconstrained functionals F_ε. In other words, we considered F_ε as defined on the entire space of $W^{1,p}(\Omega;\mathbb{R}^k)$ functions, without imposing any boundary datum. This kind of result, though individuates a meaningful Γ-limit, does not allow to consider Dirichlet minimum problems of the type (1.2). To that aim, one has to extend the Γ-convergence result proved in [4], by including a prescribed boundary condition. This is precisely the aim of the present paper. Since the fixed trace requires many nontrivial modifications, and a lot of technicalities are involved, here we limit ourselves to present the result, referring to [3] for the proof. On the other hand, the paper is conceived so as to be self-contained, and to enlighten as possible the statement of the result.

The contents are organized as follows. All the required preliminaries are summarized in Section 2. In Section 3, after recalling the Γ-convergence theorem for the unconstrained case, we state the corresponding result for the constrained functionals, together with the corollary on the asymptotics of their minimizers. In Section 4, some clarifying comments and remarks are gathered.

2. Notation and preliminaries

2.1. Currents

We set $\mathcal{D}^h(\Omega)$ the class of all smooth h-forms (maps from Ω into the space of h-covectors in $\mathbb{R}^{n+k}$) with compact support in Ω. The dual of $\mathcal{D}^h(\Omega)$ may be identified with the space $\mathcal{D}_h(\Omega)$ of *h-currents* over Ω, namely distributions with values into the space of h-vectors in $\mathbb{R}^{n+k}$.
For $h \geq 1$, the *boundary* of an h-current T is the $(h-1)$-current ∂T defined by the identity $\partial T(\omega) := T(d\omega)$, being $d\omega$ the differential of the $(h-1)$-form ω.
Let us adopt the standard notation $\mathcal{H}^h$ for the h-dimensional Hausdorff measure. Let $M \subseteq \Omega$ be an h-rectifiable set (namely the union, up to an $\mathcal{H}^h$-negligible set, of countably many h-surfaces of class C^1), endowed with an orientation ξ (namely a mapping which associates with $\mathcal{H}^h$-a.e. $x \in M$ a simple unitary h-vector spanning the approximate tangent space to M at x), and a multiplicity σ (namely a real function locally integrable with respect to the measure $\mathcal{H}^h$ on M). We set (M, ξ, σ) the current defined by

$$(M, \xi, \sigma)(\omega) := \int_M \sigma(\omega \cdot \xi)\, d\mathcal{H}^h \qquad \forall \omega \in \mathcal{D}^h(\Omega) \quad ,$$

where $\omega \cdot \xi$ stands for the standard scalar product between h-covectors and h-vectors in $\mathbb{R}^{n+k}$. When σ is integer-valued, currents of the form (M, ξ, σ) are said to be *rectifiable*. A rectifiable current whose boundary is in turn rectifiable is said to be *integral*. By *h-integral boundary*, we mean an h-current T which is rectifiable and is also a boundary (so that $\partial T = 0$, thanks to the definition of boundary and the identity $d^2\omega = 0$).
For a broad description of currents theory, we refer the reader to [5, 6, 13].

2.2. Flat norm

When a current $T \in \mathcal{D}_h(\Omega)$ is a finite measure with values into the space of h-vectors, we say that T has finite mass. In this case, we denote by $|T|$ the variation of the measure T, by $\|T\| := |T|(\Omega)$ the total variation of T, and by $\|T\|_A = |T|(A)$ the mass of T in the open set $A \subset \Omega$.
For $T \in \mathcal{D}_h(\Omega)$, we shall denote by $\mathbb{F}_\Omega(T)$ the following *flat norm* (see [2]):

$$\mathbb{F}_\Omega(T) := \begin{cases} \inf\{\|S\| : S \in \mathcal{D}_{h+1}(\Omega) \text{ of finite mass, } T = \partial S\} & \text{if } T \text{ is a boundary} \\ +\infty & \text{otherwise.} \end{cases}$$

We point out that $\mathbb{F}_\Omega$ is strictly related with the usual flat norm $\mathcal{F}_\Omega$ for integral currents, as defined in [5, §4.1.24]. In particular, if $S_i \to S$ in the flat norm $\mathcal{F}_\Omega$, we have $\mathbb{F}_\Omega(\partial S_i - \partial S) \to 0$, which in turn implies $\partial S_i \to \partial S$ in the dual of forms of class C^1_0, see [2] for more details.

2.3. Jacobians

Given a smooth map $u : \Omega \to \mathbb{R}^k$, its Jacobian is the k-form defined on Ω by

$$Ju := u^\sharp(dy) = du^1 \wedge \cdots \wedge du^k \ , \tag{2.1}$$

where $dy = dy_1 \wedge \cdots \wedge dy_k$ is the standard volume form on $\mathbb{R}^k$, and the 1-form du^i is the differential of the i^{th} component of u. As long as u is of class $W^{1,k}(\Omega;\mathbb{R}^k)$, (2.1) makes sense as a k-form with L^1 coefficients. Now observe that

$$Ju = \frac{1}{k} d(u^\sharp \omega_0) \ , \tag{2.2}$$

where, denoting by $\widehat{dy_i}$ the wedge product of all dy_j with $j \neq i$, ω_0 is the k-form $\omega_0(y) := \sum_i (-1)^{i-1} y_i \widehat{dy_i}$. Let us stress that, differently from (2.1), the weak definition (2.2) makes sense as a distribution even for maps $u : \Omega \to \mathbb{R}^k$ of class $L^\infty_{\text{loc}} \cap W^{1,k-1}_{\text{loc}}$ (cf. [10] and references therein).

For a more geometric interpretation of the Jacobian, it is convenient to consider, following [2], the n-current $\star Ju$, obtained via the standard identification $\star$ of k-vectors and n-covectors. (We recall that, given a multiindex α of order k, $\star dx_\alpha$ is the n-vector $\text{sgn}(\hat\alpha, \alpha) e_{\hat\alpha}$, where $\hat\alpha = (j_1, \ldots, j_n)$ is the set of indices not contained in α, $e_{\hat\alpha}$ is the n-vector $e_{j_1} \wedge \cdots \wedge e_{j_n}$, and $\text{sgn}(\hat\alpha, \alpha)$ is the sign of the permutation $(\hat\alpha, \alpha)$.) The identification $\star$ extends in a natural way to an operator bringing k-forms into n-currents. Such operator transforms differentials into boundaries, as one can check that, for every $\omega \in \mathcal{D}^k(\Omega)$, there holds $\star(d\omega) = (-1)^n \partial(\star\omega)$. Since, in view of (2.2), Ju is always a differential, the Jacobian current $\star Ju$ is always a boundary. In particular, for S^{k-1}-valued maps u which are smooth outside an n-surface M without boundary, the restriction of $\star Ju$ to $\Omega \setminus M$ vanishes. More generally, for $u \in W^{1,k-1}(\Omega, S^{k-1})$, there holds [1, Theorem 3.8]

$$\star Ju = \alpha_k \partial N \ , \tag{2.3}$$

being N an $(n+1)$-rectifiable current in Ω and α_k the Lebesgue measure of the unit ball in $\mathbb{R}^k$. It follows from (2.3) and the Federer-Fleming rectifiability theorem [13, Theorem 30.3] that, for maps $u \in W^{1,k-1}(\Omega; S^{k-1})$, $\alpha_k^{-1} \star Ju$ is an n-integral boundary whenever it has a finite mass.

Let us finally mention how one can define the Jacobian of a map v in the trace space $W^{1-1/p,p}(\partial\Omega;\mathbb{R}^{n+k})$ (where $p \geq k$). So far, for any $u \in W^{1,p}(\Omega;\mathbb{R}^k)$, we have defined its Jacobian as a current on Ω. Let us now extend it to zero out of Ω, thus obtaining an n-current on the entire space $\mathbb{R}^{n+k}$, still denoted by $\star Ju$. Clearly, since in view of (2.3) $\star Ju$ has no boundary in Ω, the current $\partial(\star Ju)$ is supported on $\partial\Omega$. Moreover, for any $u \in W^{1,p}(\Omega;\mathbb{R}^k)$, $\partial(\star Ju)$ turns out to depend only on the trace v of u on $\partial\Omega$, and to coincide with the classical Jacobian of v in case u is smooth. This leads to define the Jacobian of any map v in the trace space $W^{1-1/p,p}(\partial\Omega;\mathbb{R}^{n+k})$ as [7]

$$\star Jv := \partial(\star Ju) \ , \tag{2.4}$$

being u *any* map in $W^{1,p}(\Omega;\mathbb{R}^k)$ with trace v on $\partial\Omega$. Similarly as above, $\alpha_k^{-1} \star Jv$ is an n-integral boundary whenever it has a finite mass (cf. Lemma 3.2 below).

For more details on the properties of the Jacobians, we refer the reader to [2, 7, 9].

2.4. Regular level currents

The level sets of a map $u \in W^{1,p}(\Omega;\mathbb{R}^k)$ can be endowed in a natural way with a structure of rectifiable n-currents. More precisely, let E be the set of points of approximate differentiability of u, and define

$$M_y = M_y(u) := u^{-1}(y) \cap E \qquad \forall y \in \mathbb{R}^k \ .$$

Then the sets M_y are n-rectifiable with $\mathcal{H}^n(M_y) < +\infty$ for $\mathcal{L}^k$-a.e. y. For any such y, equipping M_y with constant multiplicity equal to 1 and with the orientation $\star Ju/|\star Ju|$ gives a rectifiable n-current, that we still denote by M_y.
It turns out that $\mathcal{L}^k$-a.e. $y \in \mathbb{R}^k$ is a *regular value* of u, meaning that the map $y \mapsto M_y$ from $\mathbb{R}^k$ into the Banach space of n-currents with finite mass is approximately continuous at y in the weak * sense. Whenever y is a regular value of u, we shall call $M_y = M_y(u)$ a *regular level current*. We refer to [1, §7.5] for further details.

2.5. Cobordism

Let M_1 and M_2 be rectifiable n-currents in $\mathbb{R}^{n+k}$, with $n \geq 1$, and let K be a compact subset of $\mathbb{R}^{n+k}$. We say that M_1 and M_2 are *cobordant in* K if $M_1 - M_2 = \partial N$, being N an integral $(n+1)$-current supported in K. This immediately implies that $\partial M_1 = \partial M_2$. Conversely, if the difference current $M_1 - M_2$ is supported into K and has no boundary, not necessarily it is itself a boundary, unless the nth integral homology group $H_n(K,\mathbb{Z})$ is trivial. When this last condition holds, M_1 and M_2 are cobordant in K if and only if $\mathrm{supp}(M_1 - M_2) \subset K$ and $\partial M_1 = \partial M_2$.

2.6. Optimal profile constants

For every $d \in \mathbb{Z}$, let ϕ_d be a fixed Lipschitz map from the sphere S^{k-1} into itself of degree d. We say that a map $u \in W^{1,p}_{\mathrm{loc}}(\mathbb{R}^k;\mathbb{R}^k)$ has *trace* ϕ_d *at infinity*, and we write $\mathrm{tr}(u,\infty) = \phi_d$ if there exists $\overline{r} > 0$ such that $u(x) = \phi_d(x/|x|)$ for all x with $|x| \geq \overline{r}$. Then we set

$$\tau_d := \inf \left\{ F_1(u,\mathbb{R}^k) \ : \ u \in W^{1,p}_{\mathrm{loc}}(\mathbb{R}^k;\mathbb{R}^k) \text{ such that } \mathrm{tr}(u,\infty) = \phi_d \right\} . \qquad (2.5)$$

In [4, Section 4], it is proved that the above definition of τ_d depends only on d, *i.e.*, it turns out to be *independent* of the choice of the function ϕ_d. Further, it is shown that the constants τ_d are strictly positive for every integer d (more precisely, they are superlinear, namely $\tau_d \geq c|d|$ for a positive constant $c = c(W)$), and that they are subadditive with respect to d (hence in particular $\tau_d \leq \tau_1|d|$). Thus, for suitable positive constants c, C independent of d, we have the inequalities

$$c|d| \leq \tau_d \leq C|d| \qquad \forall d \in \mathbb{Z} \ . \qquad (2.6)$$

3. Results

Let k and n be integers with $k \geq 2$ and $n \geq 0$, and let p be a real exponent with $p > k$. Let $\Omega \subset \mathbb{R}^{n+k}$ be a bounded domain with a Lipschitz boundary. Assume

that $W : \Omega \to [0, +\infty)$ is a continuous potential, with $\{W = 0\} = S^{k-1}$, satisfying the growth conditions

$$\liminf_{|y|\to 1} \frac{W(y)}{(1-|y|)^{p/(p-k+1)}} > 0 \qquad \text{and} \qquad \liminf_{|y|\to+\infty} \frac{W(y)}{|y|^p} > 0 \ .$$

For any measurable subset $A \subset \mathbb{R}^{n+k}$ and any map $u \in W^{1,p}(A; \mathbb{R}^k)$, we set

$$E_\varepsilon(u, A) = \int_A \left[\varepsilon^{p-k} |\nabla u|^p + \frac{1}{\varepsilon^k} W(u)\right] \ .$$

For any A as above and any rectifiable n-current M with multiplicity σ, we denote by $\mathcal{E}(M, A)$ the energy given by

$$\mathcal{E}(M, A) := \int_{M\cap A} \tau_{\sigma(x)} \, d\mathcal{H}^n(x) \ ,$$

where $\tau_{\sigma(x)}$ is defined according to (2.5).
Finally, we denote by α_k the Lebesgue measure of the unit ball in $\mathbb{R}^k$.
The variational behavior of the functionals $\{E_\varepsilon\}$ in the limit as $\varepsilon \to 0$ is described as follows.

Theorem 3.1 (unconstrained case). *Under the above assumptions, the following statements hold.*

(i) Compactness and Γ-lim inf inequality: *whenever* $\sup_\varepsilon E_\varepsilon(u_\varepsilon, \Omega) < +\infty$*, up to subsequences we have* $\mathbb{F}_\Omega(\star J u_\varepsilon - \alpha_k M) \to 0$*, where* M *is an* n*-integral boundary in* Ω*; moreover*

$$\liminf_\varepsilon E_\varepsilon(u_\varepsilon, \Omega) \geq \mathcal{E}(M, \Omega) \ ; \tag{3.1}$$

(ii) Γ-lim sup inequality: *for every* n*-integral boundary* M *in* Ω *there exists a sequence* $\{u_\varepsilon\} \subset W^{1,p}(\Omega; \mathbb{R}^k)$ *such that* $\mathbb{F}_\Omega(\star J u_\varepsilon - \alpha_k M) \to 0$ *and*

$$\lim_\varepsilon E_\varepsilon(u_\varepsilon, \Omega) = \mathcal{E}(M, \Omega) \ . \tag{3.2}$$

Proof. See [4, Theorem 1.1]. □

As mentioned in the Introduction, Theorem 3.1 does not allow to deal with non-trivial minimum problems. To that aim, we are going to consider the Γ-convergence of the energies $\{E_\varepsilon\}$ on the space of maps having a prescribed trace v on $\partial\Omega$. Then, in view of (2.4), the Jacobian currents of all admissible maps will have the same boundary (when extended to zero out of Ω). Consequently, we are led to compute the Γ-limit with respect to the flat convergence on the whole of $\mathbb{R}^{n+k}$, and to expect – as domain of the limit energy – currents on $\mathbb{R}^{n+k}$ belonging to a fixed cobordism class over $\overline{\Omega}$. Next lemma allows to individuate such cobordism class. From now on, all the involved currents are tacitely intended on $\mathbb{R}^{n+k}$, and all the definitions introduced in Section 2 are in use.

Lemma 3.2. *Let $v \in W^{1-1/p,p}(\partial\Omega; S^{k-1})$ be fixed. Let u be any map in $W^{1,p}(\Omega;\mathbb{R}^k)$ with trace v on $\partial\Omega$, and let y be any regular value of u. Then the cobordism class in $\overline{\Omega}$ of any regular level current $M_y = M_y(u)$ depends neither on the choice of u nor on the choice of y. More precisely, if $|y| > 1$, $M_y(u)$ is cobordant to 0 in $\overline{\Omega}$ while, if $|y| < 1$, then*

$$\partial M_y(u) = \alpha_k^{-1} \star Jv \ . \tag{3.3}$$

In particular, by (3.3) *and the boundary rectifiability theorem, $\alpha_k^{-1}\star Jv$ is rectifiable whenever it has a finite mass.*

Proof. See [2, §5.2]. □

We are now in a position to state the variational convergence result in the constrained case.

Theorem 3.3 (constrained case). *Under the same assumptions of Theorem* 3.1*, fix a boundary datum $v \in W^{1-1/p,p}(\partial\Omega, S^{k-1})$. Choose $u \in W^{1,p}(\Omega,\mathbb{R}^k)$ with trace v on $\partial\Omega$, and a regular level current $M_y = M_y(u)$ with $|y| < 1$. Then the following statements hold.*

(i) Compactness and Γ-lim inf inequality: *for every sequence $\{u_\varepsilon\} \subset W^{1,p}(\Omega;\mathbb{R}^k)$ such that $u_\varepsilon = v$ on $\partial\Omega$ and $\sup_\varepsilon E_\varepsilon(u_\varepsilon,\Omega) < +\infty$, up to subsequences we have $\mathbb{F}_{\mathbb{R}^{n+k}}(\star Ju_\varepsilon - \alpha_k M) \to 0$, where M is a rectifiable n-current in $\mathbb{R}^{n+k}$ supported in $\overline{\Omega}$ and therein cobordant to M_y; moreover, for every open set $A \subset \mathbb{R}^{n+k}$*

$$\liminf_\varepsilon E_\varepsilon(u_\varepsilon, A\cap\Omega) \geq \mathcal{E}(M,A) \ ; \tag{3.4}$$

(ii) Γ-lim sup inequality: *for every rectifiable n-current M in $\mathbb{R}^{n+k}$, supported in $\overline{\Omega}$ and therein cobordant to M_y, there exists a sequence $\{u_\varepsilon\} \subset W^{1,p}(\Omega;\mathbb{R}^k)$ such that $u_\varepsilon = v$ on $\partial\Omega$, $\mathbb{F}_{\mathbb{R}^{n+k}}(\star Ju_\varepsilon - \alpha_k M) \to 0$, and*

$$\lim_\varepsilon E_\varepsilon(u_\varepsilon,\Omega) = \mathcal{E}(M,\mathbb{R}^{n+k}) \ . \tag{3.5}$$

Proof. For statement (i), see [3, Chapter 11]; for statement (ii), see [3, Chapter 12]. □

As a consequence of Theorem 3.3, we obtain the following concentration result for minimizing sequences.

Corollary 3.4. *Under the same assumptions of Theorem* 3.3*, set*

$$(\mathcal{P}_\varepsilon) \qquad m_\varepsilon := \min\Big\{ E_\varepsilon(u,\Omega) \ : \ u \in W^{1,p}(\Omega,\mathbb{R}^k) \ , \ u = v \text{ on } \partial\Omega \Big\} \ .$$

Then m_ε are of order 1.
Moreover, for any sequence $\{u_\varepsilon\}$ of admissible maps in the minimum problems $(\mathcal{P}_\varepsilon)$ such that $E_\varepsilon(u_\varepsilon,\Omega) - m_\varepsilon = o(1)$, up to subsequences $\mathbb{F}_{\mathbb{R}^{n+k}}(\star Ju_\varepsilon - \alpha_k M) \to 0$, where M solves the limit problem

$$(\mathcal{P}_0) \quad m_0 := \min\left\{ \mathcal{E}(M,\mathbb{R}^{n+k}) \ : \ \begin{array}{l} M \text{ is a rectifiable } n\text{-current supported} \\ \text{in } \overline{\Omega} \text{ and therein cobordant to } M_y \end{array} \right\} \ .$$

Proof. To show that m_ε are of order 1, choose any rectifiable n-current M with finite mass, supported in $\overline{\Omega}$, and therein cobordant to any regular level current $M_y = M_y(u)$ of a map $u \in W^{1,p}(\Omega;\mathbb{R}^k)$, with $u = v$ on $\partial\Omega$ and $|y| < 1$. For such M, let $\{u_\varepsilon\}$ be a sequence as in the statement of Theorem 3.3 (ii). Then, by definition,

$$m_\varepsilon \le E_\varepsilon(u_\varepsilon, \Omega) \to \mathcal{E}(M, \mathbb{R}^{n+k}) < +\infty \ ,$$

where the last inequality holds since, by the right inequality in (2.6), the limit energy $\mathcal{E}$ is controlled from above by the mass.
Assume now that $\{u_\varepsilon\}$ is a sequence of admissible maps in the minimum problems $(\mathcal{P}_\varepsilon)$ such that $E_\varepsilon(u_\varepsilon, \Omega) - m_\varepsilon = o(1)$. Then $E_\varepsilon(u_\varepsilon, \Omega) = O(1)$ and, by Theorem 3.3 (i), up to subsequences $\mathbb{F}_{\mathbb{R}^{n+k}}(\star J u_\varepsilon - \alpha_k M) \to 0$ and $\liminf E_\varepsilon(u_\varepsilon, \Omega) \ge \mathcal{E}(M, \mathbb{R}^{n+k})$, where M is an admissible current in the limit problem $(\mathcal{P}_0)$. On the other hand, for any other admissible current M' in the minimum problem $(\mathcal{P}_0)$, we may find a sequence $\{u'_\varepsilon\}$ as in the statement of Theorem 3.3 (ii). Then we have

$$\mathcal{E}(M, \mathbb{R}^{n+k}) \le \liminf_\varepsilon E_\varepsilon(u_\varepsilon, \Omega) = \liminf_\varepsilon m_\varepsilon \le \lim_\varepsilon E_\varepsilon(u'_\varepsilon, \Omega) = \mathcal{E}(M', \mathbb{R}^{n+k}) \ .$$

By the arbitrariness of M', we deduce that M solves the minimum problem $(\mathcal{P}_0)$. □

4. Comments and remarks

4.1. Comparison with the case $p = k$

When the exponent p in the definition of the functionals F_ε in (1.1) is taken equal to k, the very same statements of Theorems 3.1 and 3.3 hold, provided the sequence $\{E_\varepsilon\}$ is defined via a different scaling, precisely as $E_\varepsilon := |\log\varepsilon|^{-1} F_\varepsilon$, and the limit energy $\mathcal{E}(M, A)$ is replaced by a multiple of the mass, namely $\beta_k \|M\|_A$ for a dimensional constant β_k. The corresponding results were proved by Alberti, Baldo and Orlandi in [2].
We stress that we do not know whether in our case $p > k$ the limit energy $\mathcal{E}$ is still a multiple of the mass, because it is currently an open problem to establish whether the optimal profile constants τ_d are additive with respect to d (this would imply that $\tau_d = \tau_1 |d|$, and, in turn, that $\mathcal{E}(\cdot, A) = \tau_1 \|\cdot\|_A$). However, for $p > k$ the limit energy does depend on the choice of the potential W, differently from the case $p = k$.

4.2. About the statement of Theorem 3.3

Thanks to Lemma 3.2, the cobordism class in $\overline{\Omega}$ of the currents M in the statement of Theorem 3.3 does not depend on the choice of the extension u and of the regular value y. Moreover, since (3.3) holds, the cobordancy equivalence between M and M_y forces M to obey the prescribed boundary condition

$$\partial M = \alpha_k^{-1} \star J v \ . \tag{4.1}$$

In the special case when the nth homology group $H_n(\Omega, \mathbb{Z})$ is trivial, fixing the cobordism class of M as done in Theorem 3.3 is in fact equivalent to asking condition (4.1) above (cf. Section 2.5).

4.3. Comparison between Theorems 3.3 **and** 3.1

We remark that the basic features distinguishing Theorem 3.3 from Theorem 3.1, due to the presence of the boundary datum, are:

(i) the convergence of the Jacobian currents of sequences $\{u_\varepsilon\}$ is taken in the flat norm $\mathbb{F}_{\mathbb{R}^{n+k}}$ on the entire $\mathbb{R}^{n+k}$, instead of in the flat norm $\mathbb{F}_\Omega$;

(ii) the limit currents M of the Jacobians are supported on $\overline{\Omega}$ instead of Ω: while the part of M supported on Ω is just the current given by the statement of Theorem 3.1, it may happen that part of the mass of M can be located also on $\partial\Omega$ (*cf.* (3.4) and (3.5)).

4.4. About Corollary 3.4

When $H_n(\Omega, \mathbb{Z})$ is trivial, the minimum problem $(\mathcal{P}_0)$ can be reformulated as

$$(\mathcal{P}_0) \qquad m_0 := \min\left\{\mathcal{E}(M, \mathbb{R}^{n+k}) : \begin{array}{l} M \text{ is a rectifiable } n\text{-current} \\ \text{supported in } \overline{\Omega} \text{ satisfying (4.1)} \end{array}\right\} .$$

If in addition $\star Jv = 0$ (which happens, *e.g.*, when v belongs to $W^{1,k}$), then (4.1) turns into $\partial M = 0$, so that the solution to $(\mathcal{P}_0)$ is trivially the zero current (notice that, by the left inequality in (2.6), the limit energy $\mathcal{E}$ is controlled from below by the mass).

Let us also point out that we do not know whether the current M in Corollary 3.4 is mass-minimizing as in case $p = k$ (cf. Section 4.1). However, since the limit energy $\mathcal{E}$ depends on the choice of the potential W, for $p > k$ it is no longer true that the potential part of the energy of a sequence $\{u_\varepsilon\}$ satisfying (3.5) is asymptotically negligible as it happens for $p = k$ (see Corollary 5.6 in [2]).

4.5. About the proof of Theorem 3.3

The proof of statement (i) in Theorem 3.3 is based on statement (i) in Theorem 3.1. More precisely, given a sequence $\{u_\varepsilon\}$, the basic idea is to apply Theorem 3.1 (i) to a sequence of maps $\{u'_\varepsilon\}$ which extend u_ε on a domain $\Omega' \supset \Omega$ so that the energy amount paid by u'_ε on $\Omega' \setminus \Omega$ is small, and the Jacobians $\star Ju'_\varepsilon$ converge to a current M' whose restriction to $\overline{\Omega}$ belongs to the appropriate cobordism class. This construction follows essentially the same outline of the corresponding result obtained for $p = k$ in [2].

The proof of statement (ii) in Theorem 3.3 is a little bit more delicate. Indeed, the basic idea is now to apply Theorem 3.1 (ii) on a subdomain $\Omega'' \subset \Omega$. Then the recovery sequence $\{u''_\varepsilon\}$ on Ω'' has to be pasted, with a small energy cost, with a suitable sequence $\{v_\varepsilon\}$, defined on $\Omega \setminus \Omega''$ and having trace v on $\partial\Omega$. In this process, though the strategy is again similar as in case $p = k$, an additional difficulty arises: indeed, in order to control the energy needed for pasting together the maps u''_ε and v_ε, the potential term comes into play. Since the choice of W

affects the form of our Γ-limit $\mathcal{E}$, one cannot reduce to deal with the simplified case when the potential W is constant inside the unit ball, as done in [2]. Therefore, the energy estimate on $\Omega \setminus \Omega''$ requires some nontrivial adaptations (compare Lemma 7.1 in [2] with Lemma 12.4 in [3]).

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An Introduction to H-measures and Their Applications

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Abstract. These notes attempt a simple introduction to H-measures (microlocal defect measures), a tool designed independently by P. GÉRARD and by L. TARTAR to compute weak limits of quadratic products of oscillating fields. The canvas around which the concepts are presented is that of the linear wave equation with smooth coefficients and rapidly oscillating initial data. The weak limit of the energy density is computed and a compactness result of the L^6-norm of the field (in $\mathbb{R}^3$) at each time is established.

Keywords. Symbolic calculus, microlocal analysis, oscillations, compactness, wave equation.

1. Introduction

In these notes, I attempt a self-contained treatment of H-measures, which are also called microlocal defect measures. The concept was introduced under the former name by L. TARTAR, and under the latter by P. GÉRARD at the beginning of the 1990's. The key references are [13], [4].

In a nutshell, the basic mathematical issue is that of the computation of the weak limit of quadratic products of weakly converging fields. Older tools are available.

In an elliptic setting, compensated compactness often proves successful (see, e.g., [14, 9, 10]). The "div-curl" lemma provides a prototypical example. That lemma states that, if $u^\varepsilon \in L^p(\Omega;\mathbb{R}^N)$, $v^\varepsilon \in L^{p'}(\Omega;\mathbb{R}^N)$ $(1 < p < \infty,\ 1/p + 1/p' = 1)$ are such that

$$u^\varepsilon \rightharpoonup u, \quad \text{weakly in } L^p(\Omega;\mathbb{R}^N)$$
$$v^\varepsilon \rightharpoonup v, \quad \text{weakly in } L^{p'}(\Omega;\mathbb{R}^N)$$

while curl u^ε and div v^ε lie in a compact set of $W^{-1,p}_{\rm loc}(\Omega;\mathbb{R}^N)$ and $W^{-1,p'}_{\rm loc}(\Omega;\mathbb{R}^N)$ respectively, then,

$$u^\varepsilon.v^\varepsilon \rightharpoonup u.v, \text{ weak-* in } \mathcal{D}'(\mathbb{R}^N).$$

Although very handy in the study of elliptic equations in divergence form, compensated compactness does not allow a general computation for any quadratic product, precisely because it requires specific compensations between the various derivatives of the weakly converging quantities.

YOUNG measures, on the other hand, compute the weak limit of any non-linear function of the weakly converging fields (see, e.g., [14, 1]): if

$$u^\varepsilon \rightharpoonup u, \text{ weakly in } L^p(\Omega),\ 1 < p < \infty,$$

there exists a subsequence, still indexed by ε and, for a.e. $x \in \Omega$, a probability measure ν_x on $\mathbb{R}$, such that, for any $f \in \mathcal{C}^0(\Omega)$ with $|f(t)| \leq cst.(1 + |t|^q),\ q < p$,

$$f(u^\varepsilon(x)) \rightharpoonup \int_{\mathbb{R}} f(\lambda)\, d\nu_x(\lambda), \text{ weakly in } L^r(\Omega),\ rq < p.$$

The measure ν_x has adequate weak measurability properties in x, so as to lend a meaning to the above limit. Unfortunately, the determination of the YOUNG measure is in general impossible, unless the investigated problem possesses a variational structure (see, e.g., [11]). In essence, YOUNG measures fail to inherit any kind of differential structure from the equations satisfied by the field u^ε, with the notable exception of certain classes of conservation laws (see, e.g., [14], [2]).

H-measures may be seen as a middle ground between compensated compactness and YOUNG measures. In contrast to the former, no compensation is necessary in order to pass to the limit in quadratic products, while, in contrast to the latter, the differential structure of the investigated problem results in localization and transport properties for the H-measures.

The notes will articulate around the non-homogeneous wave equation in $\mathbb{R}^N$ (with mostly $N = 3$) with oscillating initial conditions. From a mathematical standpoint, such a setting demonstrates the power of the method and eventually leads to a beautiful result of P. GÉRARD on the generic compactness in $L^{\frac{2N}{N-2}}(\mathbb{R}^N)$, at each time t, of the solution $u^\varepsilon(x,t)$ to the classical wave equation with oscillating initial data. From a mechanical standpoint, the computation of the limit of the energy density associated to the solution $u^\varepsilon(x,t)$ is a key to the investigation of energy transfer from high frequencies into heat, a prerequisite to the determination of a sound thermomechanical model.

Consider, for any $\rho, k \in \mathcal{C}^\infty(\mathbb{R}^N)$ with

$$0 < \alpha \leq \rho(x), k(x) \leq \beta < \infty \tag{1.1}$$

the following wave equation:

$$\begin{array}{c} \rho \dfrac{\partial^2 u^\varepsilon}{\partial t^2} - \operatorname{div}(k \operatorname{grad} u^\varepsilon) = 0 \\ u^\varepsilon(0) = u_0^\varepsilon \\ \dfrac{\partial u^\varepsilon}{\partial t}(0) = v_0^\varepsilon \end{array},$$

with

$$\left\{ \begin{array}{ll} u_0^\varepsilon \rightharpoonup u_0 & \text{weakly in } H^1(\mathbb{R}^N) \\ v_0^\varepsilon \rightharpoonup v_0 & \text{weakly in } L^2(\mathbb{R}^N) \end{array} \right. ,$$

and let us assume, for simplicity sake, that

$$\text{supp } u_0^\varepsilon, \text{supp } v_0^\varepsilon \subset \text{ a fixed compact K.}$$

Take $\Omega \supset K'(\text{compact}) \supset K$ and solve the wave equation on $\Omega \times [0,T]$ with T chosen such that supp $u^\varepsilon(t) \subset K'$; this is always possible if T is small enough because the wave equation has finite speed of propagation, no greater than $\sqrt{\frac{\beta}{\alpha}}$. Thus, on the time interval $[0,T]$, u^ε is equivalently defined as the solution of the same wave equation, formulated on Ω with DIRICHLET boundary conditions.

Elementary energy estimates imply that u^ε is uniformly bounded in

$$\mathcal{E}_T := L^\infty(0,T;H_0^1(\Omega)) \cap W^{1,\infty}(0,T;L^2(\Omega)),$$

so that, for a subsequence still indexed by ε,

$$u^\varepsilon \rightharpoonup u, \text{ weakly in } \mathcal{E}_T,$$

with u solution of the same wave equation. Furthermore, AUBIN's classical compactness lemma (see, e.g., [12]) implies that

$$\left\{ \begin{array}{rcll} u^\varepsilon(0) & \longrightarrow & u(0) & \text{in } L^2(\Omega) \\ \rho(x)\dfrac{\partial u^\varepsilon}{\partial t}(0) & \longrightarrow & \rho(x)\dfrac{\partial u}{\partial t}(0) & \text{in } H^{-1}(\Omega) \end{array} \right. ,$$

so that $u(0) = u_0$ and $\dfrac{\partial u}{\partial t}(0) = v_0$. Summing up, u solves the same wave equation with u_0 and v_0 as initial data.

Further, by virtue of energy conservation,

$$\begin{aligned} E^{(\varepsilon)}(t) &:= 1/2 \int_\Omega \left\{ \rho(x)(\frac{\partial u^{(\varepsilon)}}{\partial t})^2 + k(x)|\operatorname{grad} u^{(\varepsilon)}|^2 \right\} dx \\ &= E_0^{(\varepsilon)} := 1/2 \int_\Omega \left\{ \rho(x)(v_0^{(\varepsilon)})^2 + k(x)|\operatorname{grad} u_0^{(\varepsilon)}|^2 \right\} dx. \end{aligned}$$

Thus,

$$\liminf E^\varepsilon(t) \geq E(t),$$

with equality if and only if

$$\left\{ \begin{array}{l} u_0^\varepsilon \longrightarrow u_0, \text{ in } H^1(\mathbb{R}^N) \\ v_0^\varepsilon \longrightarrow v_0, \text{ in } L^2(\mathbb{R}^N) \end{array} \right. .$$

Generically, some energy has been lost during the limit process. Quantifying that loss *pointwise* is the goal of our study.

Setting

$$v^\varepsilon := u^\varepsilon - u \tag{1.2}$$

reduces the analysis to

$$\rho \frac{\partial^2 v^\varepsilon}{\partial t^2} - \operatorname{div}(k \operatorname{grad} v^\varepsilon) = 0 \tag{1.3}$$

with initial conditions

$$\begin{array}{rl} v^\varepsilon(0) = u_0^\varepsilon - u_0 := V_0^\varepsilon & \rightharpoonup 0, \text{ in } H^1(\mathbb{R}^N) \\ \dfrac{\partial v^\varepsilon}{\partial t}(0) = v_0^\varepsilon - v_0 := Z_0^\varepsilon & \rightharpoonup 0, \text{ in } L^2(\mathbb{R}^N), \end{array} \tag{1.4}$$

so that

$$v^\varepsilon \rightharpoonup 0, \text{ weakly in } \mathcal{E}_T.$$

The energy density

$$e^\varepsilon(t,x) := 1/2\Big\{\rho(x)(\frac{\partial v^{(\varepsilon)}}{\partial t})^2 + k(x)|\operatorname{grad} v^{(\varepsilon)}|^2\Big\}(t,x) \tag{1.5}$$

is bounded in $L^\infty(0,T;L^1(\mathbb{R}^N))$, so that a subsequence, still indexed by ε converges weak-* in $L^\infty(0,T;\mathcal{M}(\mathbb{R}^N))$ to $e(t,x) \in L^\infty(0,T;\mathcal{M}(\mathbb{R}^N))$, where $\mathcal{M}(\mathbb{R}^N)$ denotes the bounded RADON measures on $\mathbb{R}^N$.

The second section is devoted to the determination of the H-measure associated to $(\dfrac{\partial v^\varepsilon}{\partial t}, \operatorname{grad} v^\varepsilon)$ (see Theorem 2.14 below) and to the ensuing determination of $e(t,x)$. To this effect, H-measures are defined and their localization and transport properties are analyzed, then specialized to the adequate setting for the wave equation.

The third section briefly introduces semi-classical measures, as a convenient tool in the proof, in dimension $N = 3$, of a microlocal theorem (see Theorem 3.7 below), due to P. GÉRARD [5], which improves a classical result of compactness of P.L. LIONS [8]. The original result, specialized to a three-dimensional setting, is the following

Theorem 1.1. *If*

$$w^n \rightharpoonup 0, \text{ weakly in } H^1(\mathbb{R}^3),$$

while

$$\left\{ \begin{array}{cl} |\operatorname{grad} w^n|^2 & \rightharpoonup M, \text{ weak-* in } \mathcal{M}(\mathbb{R}^3) \\ (w^n)^6 & \rightharpoonup R, \text{ weak-* in } \mathcal{M}(\mathbb{R}^3) \end{array} \right. ,$$

then R has its support on the atoms of M.

The improved version is then applied to the solution v^ε of the wave equation with the help of the results of Section 2, and it yields the already mentioned generic (in time) compactness of $v^\varepsilon(x,t)$, hence of $u^\varepsilon(x,t)$, in $L^6(\mathbb{R}^3)$ (see Theorem 3.9 below).

In matters of notation, we will sometimes use Einstein's summation convention. The letter C will always denote a generic constant, so that for example $2C$ will be replaced by C. In dealing with the wave equation, we will denote the time variable, either by t or by x_0, as convenient, while the associated FOURIER variable will always be denoted by ξ_0; x will always mean the N-tuple $x_1, \ldots, x_N \in \mathbb{R}^N_x$, with associated FOURIER variable $\eta \in \mathbb{R}^N_\eta$(or S^{N-1}_η), while

y will always mean the $(N+1)$-tuple $x_0, x_1, \ldots, x_N \in \mathbb{R}^{N+1}_y$, with associated FOURIER variable $\xi \in \mathbb{R}^{N+1}_\eta$(or S^N_η).Also,

$$\{\!\{p,q\}\!\} := \frac{\partial p}{\partial \xi_j}\frac{\partial q}{\partial y_j} - \frac{\partial p}{\partial y_j}\frac{\partial q}{\partial \xi_j}$$

will denote the Poisson bracket of two functions p, q of y and ξ. For any set A, χ_A will denote the characteristic function of that set. Finally, we will be somewhat loose in our writing of measures: for example by $\nu(x,\eta)$ we will denote a measure that leaves on the phase space $\mathbb{R}^N_x \times \mathbb{R}^N_\eta$(or S^{N-1}_η), while $\nu(x+t\eta)$ will denote the translate ν under $(x,\eta) \to (x-t,\eta)$; $\mathcal{L}^N(\xi)$ will denote the N-dimensional LEBESGUE measure on $\mathbb{R}^N$.

2. H-measures or microlocal defect measures

In a first subsection, we introduce elementary notions of the pseudo-differential calculus; the second subsection is devoted to the definition and basic properties of localization and transport of H-measures with a focus on the wave equation, while the third subsection particularizes the obtained results to the homogeneous wave equation.

2.1. Pseudo-differential operators

We first define a convenient class of pseudo-differential operators, namely

Definition 2.1.

$$S^m_M(\mathbb{R}^Q) := \Big\{ p(y,\xi) \in \mathcal{C}^\infty(\mathbb{R}^Q_y \times \mathbb{R}^Q_\xi; \mathbb{C}^{M^2}) : \text{ for any } K \subset \mathbb{R}^Q,$$

$$\text{and for any } n\text{-tuples } \gamma, \delta, \ |D^\gamma_y D^\delta_\xi p(y,\xi)| \le C(K,\gamma,\delta)(1+|\xi|^{m-|\delta|}\Big\}.$$

Then the standard pseudo-differential operator P of order m, with symbol $\sigma(P) = p$, is defined as the mapping

$$\left\{ \begin{array}{ccc} [\mathcal{C}^\infty_0(\mathbb{R}^Q)]^M & \to & [\mathcal{C}^\infty(\mathbb{R}^Q)]^M \\ u & \to & Pu(y) = 1/(2\pi)^Q \displaystyle\int_{\mathbb{R}^Q_\xi} e^{iy.\xi} p(y,\xi)\hat{u}(\xi)d\xi \end{array} \right.$$

The mapping P extends as a mapping from $[H^t(\mathbb{R}^Q)]^M$ into $[H^{t-m}_{\rm loc}(\mathbb{R}^Q)]^M$, and if $C(K,\gamma,\delta)$ is independent of K, then P maps $[H^t(\mathbb{R}^Q)]^M$ into $[H^{t-m}(\mathbb{R}^Q)]^M$. We denote the set of such mappings by $\Sigma^m_M(\mathbb{R}^Q)$.

For those readers that are somewhat unfamiliar with pseudo-differential operators, note that the above properties are easily established through various manipulations of the FOURIER transform, together with application of the following PETREE's inequality that holds true for any pair $(\xi,\xi') \in (\mathbb{R}^N)^2$ and any $s \in \mathbb{R}$:

$$(1+|\xi|^2)^s \le 2^{|s|}(1+|\xi-\xi'|^2)^{|s|}(1+|\xi'|^2)^s. \tag{2.1}$$

We further define

Definition 2.2.

$$\Psi^m_M(\mathbb{R}^Q) := \Big\{ P \in \Sigma^m_M(\mathbb{R}^Q) : \sigma(P)(y,\xi) = p^m(y,\xi)\chi(\xi) + p^{m-1}(y,\xi) :$$
$$p^m \in \mathcal{C}^\infty(\mathbb{R}^Q_y \times (\mathbb{R}^Q_\xi \setminus \{\xi = 0\}); \mathbb{C}^{M^2}) \text{ homogeneous of degree } m \text{ in } \xi,$$
$$\chi \in \mathcal{C}^\infty(\mathbb{R}^Q_\xi) \text{ with } \chi \equiv 0 \text{ in a neighborhood of } \xi = 0, p^{m-1} \in S^{m-1}_M(\mathbb{R}^Q)\Big\},$$

and $\Psi^m_{M,c}(\mathbb{R}^Q)$ is the subset of $\Psi^m_M(\mathbb{R}^Q)$ of y-compactly supported operators.

Further, $\sigma^m(P) := p^m$ is then called the principal symbol of P and p^{m-1} the lower order symbol of P.

Remark 2.3. Note that $\sigma^m(P)$ is uniquely determined whenever $P \in \Psi^m_M(\mathbb{R}^Q)$ while changing χ only modifies P by a smoothing operator$(\in \cap_m \Sigma^m_M(\mathbb{R}^Q))$.

We now give, without proof, the two properties of pseudo-differential operators that we will use later (see [7] for a proof); note that the first lemma deals with principal symbols whereas the second one deals with the full symbols.

Lemma 2.4. *If P^* denotes the adjoint operator to $P \in \Psi^m_{M,c}(\mathbb{R}^Q)$, and $Q \in \Psi^n_{M,c}(\mathbb{R}^Q)$,*

(1) *$P^* \in \Psi^m_{M,c}$ and $\sigma^m(P^*) = \overline{\sigma^m(P)}^t =: \sigma^m(P)^*$;*
(2) *$PQ \in \Psi^{m+n}_{M,c}(\mathbb{R}^Q)$ and $\sigma^{m+n}(PQ) = \sigma^m(P)\sigma^n(Q)$.*

Lemma 2.5. *If $P \in \Psi^m_{M,c}, Q \in \Psi^n_{M,c}(\mathbb{R}^Q)$,*

$$(1)\ \ \sigma(P^*) - \sigma(P)^* - 1/i \sum_1^Q \frac{\partial^2 \sigma(P)^*}{\partial y_j \partial \xi_j} \in S^{m-2}_M(\mathbb{R}^Q);$$

$$(1)\ \ \sigma(PQ) - \sigma(P)\sigma(Q) - 1/i \sum_1^Q \frac{\partial \sigma(P)}{\partial \xi_j} \frac{\partial \sigma(Q)}{\partial y_j} \in S^{m+n-2}_M(\mathbb{R}^Q).$$

Thus, if $\sigma(P)$ commutes with $\sigma(Q)$, then $[P,Q] := PQ - QP \in S^{m+n-1}_M(\mathbb{R}^Q)$ with symbol $1/i\{\!\{\sigma(P), \sigma(Q)\}\!\}$.

2.2. H-measures

We begin with a definition/lemma for H-measures.

Lemma 2.6. *Let $V^\varepsilon \in [L^2(\mathbb{R}^Q)]^M$ be such that $V^\varepsilon \rightharpoonup O$. There exists a subsequence $\{\varepsilon'\} \subset \{\varepsilon\}$ and a $M \times M$ matrix μ_{ij} of* RADON *measures on $\mathbb{R}^Q_y \times S^{Q-1}_\xi$ such that, for any $P \in \Psi^0_{M,c}(\mathbb{R}^Q)$,*

$$\lim_{\varepsilon'} \int_{\mathbb{R}^Q_y} PV^{\varepsilon'} . \overline{V}^{\varepsilon'} dx =: \lim_{\varepsilon'} \langle PV^{\varepsilon'}, V^{\varepsilon'} \rangle = \int_{\mathbb{R}^Q_y \times S^{Q-1}_\xi} \sigma^0(P)_{ij} d\mu_{ij} =: \langle \mu, \sigma^0(P) \rangle.$$

Furthermore, μ is non-negative and Hermitian, i.e.,

$$\begin{cases} \mu_{ij} = \overline{\mu}_{ji} \\ \sum_{i,j=1}^{Q} \mu_{ij} c_i \overline{c}_j \geq 0,\ c \in \mathbb{C}^Q. \end{cases}$$

Sketch of proof. Take $P \in \Psi^0_{M,c}(\mathbb{R}^Q)$. Since $V^\varepsilon \overset{[L^2(\mathbb{R}^Q]^M}{\rightharpoonup} 0$, for a subsequence $\{\varepsilon'\} \subset \{\varepsilon\}$,

$$\langle \mu, P \rangle := \lim_{\varepsilon'} \langle PV^{\varepsilon'}, V^{\varepsilon'} \rangle.$$

A simple diagonalization process, together with Stone–Weierstrass' theorem, imply that μ can be defined for any element $P \in \Psi^0_{M,c}(\mathbb{R}^Q)$. But, if $\sigma^0(P) = \sigma^0(Q),\ P, Q \in \Psi^0_{M,c}(\mathbb{R}^Q)$, then $P - Q$ maps $L^2(\mathbb{R}^Q)$ into $H^1_c(\mathbb{R}^Q)$, so that Rellich's theorem implies that $\langle \mu, P - Q \rangle = 0$. Thus $\langle \mu, P \rangle$ only depends upon $\sigma^0(P)$, and we can redefine $\langle \mu, P \rangle$ as $\langle \mu, \sigma^0(P) \rangle$, a linear functional on $\mathcal{C}^\infty_0(\mathbb{R}^Q_y \times S^{Q-1}_\xi; \mathbb{C}^{M^2})$.

Let us show the additional properties of μ. The Hermitian character of μ is evident from its definition. To demonstrate that μ is a non-negative matrix of Radon measures, we consider, for any scalar valued $\sigma^0(P) \geq 0 \in \mathcal{C}^\infty_0(\mathbb{R}^Q_y \times S^{Q-1}_\xi)$, the quantity $\langle \mu, \sigma^0(P) c \otimes \overline{c} \rangle,\ c \in \mathbb{C}^M$. Introduce $\Phi \in \mathcal{C}^\infty_0(\mathbb{R}^Q_y \times S^{Q-1}_\xi)$, with $\Phi \geq 0$ and $\equiv 1$ on $\mathrm{supp}(\sigma^0(P))$ and consider, for $\delta > 0$, the element $b_\delta := \sqrt{\sigma^0(P) + \delta\Phi}$ which belongs to $\mathcal{C}^\infty_0(\mathbb{R}^Q_y \times S^{Q-1}_\xi)$. Then, if $B_\delta \in \Psi^0_{M,c}(\mathbb{R}^Q)$ is defined as any element such that $\sigma^0(B_\delta) = b_\delta d \otimes \overline{d}$ with

$$d := \frac{c}{\sqrt{\sum_{k=1,\dots,M} |c_k|^2}},$$

Lemma 2.4 and the very definition of μ imply that

$$0 \leq \langle \mu, \sigma^0(B^*_\delta B_\delta) \rangle = \langle \mu, (\sigma^0(P) + \delta\Phi) c \otimes \overline{c} \rangle$$

or still,

$$\langle \mu, \sigma^0(P) c \otimes \overline{c} \rangle \geq -\delta \langle \mu, \Phi c \otimes \overline{c} \rangle.$$

The result is obtained upon letting $\delta \searrow 0$, because a non-negative linear functional on $\mathcal{C}^\infty_0(\mathbb{R}^Q_y \times S^{Q-1}_\xi)$ is a non-negative Radon measure. □

Remark 2.7. If $P \in \Psi^0_{M,c}(\mathbb{R}^Q)$ has a principal symbol of the form $\sigma^0(P) = a(x)b(\xi)$, define, for any $V \in [L^2(\mathbb{R}^Q)]^M$ (and any χ smooth cut-off around $\xi = 0$),

$$\tilde{P}V(y) := \int_{\mathbb{R}^Q_\xi} \chi(\xi) b(\xi) \widehat{aV}(\xi) e^{iy.\xi} d\xi;$$

it is then a simple exercise that uses, e.g., (2.1) to show that

$$PV^\varepsilon - \tilde{P}V^\varepsilon \overset{[L^2(\mathbb{R}^Q)]^M}{\to} 0.$$

Consequently, an equivalent definition of μ for such symbols is (see [13])

$$\langle \mu, \sigma^0(P) \rangle = \lim_{\varepsilon'} \langle \tilde{P} V^{\varepsilon'}, V^{\varepsilon'} \rangle.$$

As a corollary, for any $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^Q_y)$, $\varphi^2 \mu$ is the H-measure associated to $\varphi V^{\varepsilon'}$.

Example 2.8. We now give two examples where the H-measure is explicitly computable.

Periodic oscillations: Assume that $v \in L^2(\mathcal{T})$, $\int_{\mathcal{T}} v dy = 0$ where $\mathcal{T}$ is the unit Q-dimensional torus and define the oscillating sequence $v^\varepsilon(y) := v(\frac{y}{\varepsilon}) \overset{L^2_{\rm loc}(\mathbb{R}^Q)}{\rightharpoonup} 0$. For $\varphi \in \mathsf{S}(\mathbb{R}^Q)$ – the set of rapidly decreasing functions – look at the H-measure μ_φ associated to (a subsequence of) $\{v^\varepsilon \varphi\}$. Then, the whole sequence actually admits a H-measure μ_φ defined as

$$\mu_\varphi = \sum_{k \neq 0} |\hat{v}_k|^2 \varphi(y) dy \otimes \delta_{\frac{k}{|k|}}(\xi),$$

where $\hat{v}_k$ is the kth-FOURIER coefficient of v.

Indeed, assume that $\hat{\varphi}$ has compact support. Then, $\widehat{\varphi v^\varepsilon} = \sum_{k \neq 0} \hat{v}_k \hat{\varphi}(\xi - \frac{k}{\varepsilon})$ is such that, for $k \neq k'$ and ε small enough, the supports of $\hat{\varphi}(\xi - \frac{k}{\varepsilon})$ and of $\hat{\varphi}(\xi - \frac{k'}{\varepsilon})$ are disjoint.

Defining $\sigma^0(P) := \varphi^2(y) b(\frac{\xi}{|\xi|})$ with $b \in \mathcal{C}^\infty(S^{Q-1})$, PLANCHEREL's identity yields

$$\langle \tilde{P} v^\varepsilon, v^\varepsilon \rangle = \int_{\mathbb{R}^Q_\xi} \chi(\xi) b(\frac{\xi}{|\xi|}) (\sum_{k \neq 0} |\hat{v}_k|^2 |\hat{\varphi}(\xi - \frac{k}{\varepsilon})|^2 d\xi,$$

so that, upon performing the change of variables $\eta := \xi - \frac{k}{\varepsilon}$, we obtain

$$\lim_\varepsilon \langle \tilde{P} v^\varepsilon, v^\varepsilon \rangle = (\sum_{k \neq 0} |\hat{v}_k|^2 b(\frac{k}{|k|})) \int_{\mathbb{R}^Q_\eta} |\hat{\varphi}(\eta|^2 d\eta.$$

The result follows through a density argument.

Concentrations: Assume that $f \in L^2(\mathbb{R}^Q)$ and define the concentrating sequence $v^\varepsilon(y) := \varepsilon^{-\frac{Q}{2}} f(\frac{y - z}{\varepsilon}) \overset{L^2(\mathbb{R}^Q)}{\rightharpoonup} 0$. Then it is easily shown that the whole sequence admits an H-measure μ with

$$\mu = \delta_z(y) \otimes [1/(2\pi)^Q \int_0^\infty |\hat{f}(t\xi)|^2 t^{Q-1} dt] d\xi.$$

Remark 2.9. When, as in the examples above, the *whole* sequence admits an H-measure, we say that *the sequence is pure.*

We now derive a localization lemma for the support of an H-measure.

Lemma 2.10. *Consider* $V^\varepsilon \overset{[L^2(\mathbb{R}^Q)]^M}{\rightharpoonup} 0$ *with associated H-measure* μ. *If, for some* $R \in \Psi^m_M(\mathbb{R}^Q)$, $RV^\varepsilon \in$ compact of $[H^{-m}_{\rm loc}(\mathbb{R}^Q)]^M$, *then*

$$\sigma^m(R) \mu = 0,$$

or, in indices,

$$\sum_{j=1}^{M} \sigma^m(R)_{ij}\mu_{jq} = 0,\ 1 \le i \le M, 1 \le q \le M.$$

Proof. Assume $M = 1$ for simplicity. Consider, for $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^Q_y), b(\xi) \in S^{Q-1}_\xi$, the pseudo-differential operator $T \in \Psi^{-m}_{1,c}(\mathbb{R}^Q)$ with associated principal symbol $\varphi(y)b(\frac{\xi}{|\xi|})|\xi|^{-m}$.

Then, $TRV^\varepsilon \in$ compact of $[L^2_{\rm loc}(\mathbb{R}^Q)]$, thus $\langle TRV^\varepsilon, V^\varepsilon\rangle \to 0$, or in other words $\langle \mu, \sigma^m(R)|\xi|^{-m}b(\xi)\varphi(y)\rangle = 0$. The arbitrariness of the choice of φ and b yields the lemma. □

First application to the wave equation. In the framework of Section 1 (see (1.2)) introduce

$$V^\varepsilon := (\frac{\partial v^\varepsilon}{\partial t}, \operatorname{grad} v^\varepsilon) \overset{L^\infty(\mathbb{R}_t;[L^2(\mathbb{R}^Q)]^M)}{\rightharpoonup} 0$$

and remark that such a sequence will fit within the H-measure framework, provided we multiply it by a smooth compactly supported function of t which is identically 0 if $|t|$ is large enough. In the remainder of the paper we will do as if there were no such multiplier in dealing with the solution to the wave equation, favoring simplicity over rigor.

The H-measure associated to (a subsequence of) V^ε is a $N \times N$ matrix μ. Let us apply the localization lemma. First, we express the commutativity of mixed derivatives, namely

$$\frac{\partial V^\varepsilon_j}{\partial y_i} = \frac{\partial V^\varepsilon_i}{\partial y_j},\ i, j = 0, \dots, N.$$

Thanks to the localization lemma, we obtain

$$\xi_i\mu_{jk} = \xi_j\mu_{ik},\ i, j, k = 0, \dots, N.$$

Thus $\mu_{ik} = \xi_i\nu_k,\ i, k = 0, \dots, N$, and since μ is Hermitian, i.e., $\mu_{ik} = \overline{\mu}_{ki}$, $\nu_i = \xi_i\nu,\ i = 0, \dots, N$ with ν a non-negative scalar RADON measure. Thus

$$\mu = (\xi \otimes \xi)\,\nu. \tag{2.2}$$

Then, we write the actual wave equation, namely

$$\rho(x)\frac{\partial V^\varepsilon_0}{\partial x_0} - \sum_{j=1,N} \frac{\partial}{\partial x_j}(k(x)V^\varepsilon_j) = 0,$$

or still

$$\rho(x)\frac{\partial V^\varepsilon_0}{\partial x_0} - k(x)\sum_{j=1,N} \frac{\partial V^\varepsilon_j}{\partial x_j} = \sum_{j=1,N} \frac{\partial k(x)}{\partial x_j}V^\varepsilon_j.$$

The right-hand side of the previous equality belongs to a bounded set of $L^2(\mathbb{R}^{N+1})$, hence to a compact set in $H^{-1}_{\rm loc}(\mathbb{R}^{N+1})$ and the localization theorem applies yielding

$$\rho(x)\xi_0\mu_{0k} - k(x)\sum_{j=1,\dots,N} \xi_j\mu_{jk} = 0,\ k = 0, \dots, N,$$

or still in view of (2.2) and because not all ξ_k may cancel at the same time ($|\xi| = 1$),

$$q(x,\xi)\nu = 0. \tag{2.3}$$

where

$$q(x,\xi) := \rho(x)\xi_0^2 - k(x)\sum_{j=1,\dots,N}\xi_j^2. \tag{2.4}$$

Thanks to (2.2), the limit of (a subsequence of) the energy density e^ε defined in (1.5) is given by

$$\lim_\varepsilon e^\varepsilon = 1/2\int_{S_\xi^N}(\rho(x)\xi_0^2 + k(x)\sum_{i=1,\dots,N}\xi_i^2)d\nu(y,\xi). \tag{2.5}$$

It thus remains to determine ν subject to the support restriction (2.3). This will be performed with the help of the following transport lemma specialized to the context of the wave equation. Note that, as emphasized in the introduction, this lemma is the outstanding feature which permits a complete characterization of H-measures as solutions of a transport equation, in contrast to YOUNG measures which are not constrained by any type of partial differential equation.

Lemma 2.11. *Consider* $V^\varepsilon \overset{[L^2(\mathbb{R}^Q)]^M}{\rightharpoonup} 0$ *with associated H-measure* μ. *Consider also* $R \in \Psi_M^m(\mathbb{R}^Q)$ *such that*

- $\sigma^m(R)$ *is self-adjoint;*
- *the lower order symbol of* P *defines an element in* $\Psi_M^{m-1}(\mathbb{R}^Q)$ *with principal symbol* $\sigma^{m-1}(R)$,

and assume that $RV^\varepsilon \in$ compact of $[H^{-m+1}_{\rm loc}(\mathbb{R}^Q)]^M$.

Then, for any $a \in \mathcal{C}_0^\infty(\mathbb{R}_y^Q \times S_\xi^{Q-1})$,

$$\langle \mu, \{\!\{\sigma^m(R), a\}\!\} + \Big[i\Big((\sigma^{m-1}(R))^* - \sigma^{m-1}(R)\Big) + \frac{\partial^2\sigma^m(R)}{\partial y_j\partial\xi_j} + (m-1)\xi_j\frac{\partial\sigma^m}{\partial y_j}\Big]a\rangle = 0.$$

Remark 2.12. Note that the hypotheses on R are automatically satisfied if R is a differential operator with self-adjoint higher-order terms.

Proof. Take an arbitrary $A \in \Psi_{1,c}^0(\mathbb{R}^Q)$, with $a := \sigma^0(A)$, and define $Q := (-\Delta)^{-\frac{m-1}{2}}R$, so that, according to Lemma 2.4(2), $Q \in \Psi_{M,c}^1(\mathbb{R}^Q)$ and $\sigma^1(Q) = |\xi|^{-(m-1)}\sigma^m(R)$. Actually, according to Lemma 2.5(2),

$$\sigma(Q) = |\xi|^{-(m-1)}\sigma(R) + 1/i\frac{\partial}{\partial\xi_j}(|\xi|^{-(m-1)})\frac{\partial\sigma(R)}{\partial y_j} + q'(\in S_M^{-1}(\mathbb{R}^Q)),$$

hence, according to Lemma 2.5(1),

$$\begin{aligned}\sigma(Q^*) = |\xi|^{-(m-1)}\sigma(R)^* &- \frac{1}{i}\frac{\partial}{\partial\xi_j}(|\xi|^{-(m-1)})\frac{\partial\sigma(R)^*}{\partial y_j}\\ &+ \frac{1}{i}\frac{\partial^2}{\partial y_j\partial\xi_j}(|\xi|^{-(m-1)}\sigma(R)^*) + q''\end{aligned}$$

with $q'' \in S_M^{-1}(\mathbb{R}^Q)$). But, by hypothesis, $\sigma^m(R)$ is self-adjoint and the lower order symbol of P defines an element in $\Psi_M^{m-1}(\mathbb{R}^Q)$ with principal symbol $\sigma^{m-1}(R)$, thus $Q^* - Q \in \Psi_M^0(\mathbb{R}^Q)$ with principal symbol

$$\begin{aligned}\sigma^0(Q^*-Q) &= |\xi|^{-(m-1)}\Big((\sigma^{m-1}(R))^* - \sigma^{m-1}(R)\Big)\\ &\quad -\frac{2}{i}\frac{\partial}{\partial\xi_j}(|\xi|^{-(m-1)})\frac{\partial\sigma^m(R)}{\partial y_j} + \frac{1}{i}\frac{\partial^2}{\partial y_j\partial\xi_j}(|\xi|^{-(m-1)}\sigma^m(R))\\ &= |\xi|^{-(m-1)}\Big((\sigma^{m-1}(R))^* - \sigma^{m-1}(R)\Big)\\ &\quad +\frac{2}{i}(m-1)|\xi|^{-(m+1)}\xi_j\frac{\partial\sigma^m(R)}{\partial y_j} + \frac{1}{i}\frac{\partial^2}{\partial y_j\partial\xi_j}(|\xi|^{-(m-1)}\sigma^m(R))\end{aligned}$$

or still,

$$\begin{aligned}\sigma^0(Q^*-Q) &= |\xi|^{-(m-1)}\Big((\sigma^{m-1}(R))^* - \sigma^{m-1}(R)\Big)\\ &\quad +\frac{1}{i}(m-1)|\xi|^{-(m+1)}\xi_j\frac{\partial\sigma^m(R)}{\partial y_j} + \frac{1}{i}|\xi|^{-(m-1)}\frac{\partial^2\sigma^m(R)}{\partial y_j\partial\xi_j}.\end{aligned} \tag{2.6}$$

Now, application of Lemma 2.5(2) to A and Q implies, since a commutes with $\sigma(Q)$, that $[A,Q] \in \Sigma_M^0(\mathbb{R}^Q)$, with $\sigma([A,Q]) = 1/i\{\!\{a,\sigma(Q)\}\!\}$, and consequently since $A \in \Psi_{1,c}^0(\mathbb{R}^Q)$ and $Q \in \Psi_{M,c}^1(\mathbb{R}^Q)$, that $[A,Q]$ actually belongs to $\Psi_M^{0,c}(\mathbb{R}^Q)$ with principal symbol

$$\begin{aligned}\sigma^0([A,Q]) &= 1/i\{\!\{a,\sigma^1(Q)\}\!\} = 1/i\{\!\{a,|\xi|^{-(m-1)}\sigma^m(R)\}\!\}\\ &= 1/i\Big(|\xi|^{-(m-1)}\{\!\{a,\sigma^m(R)\}\!\} + (m-1)|\xi|^{-(m+1)}\xi_j\frac{\partial a}{\partial y_j}\sigma^m(R)\Big)\ .\end{aligned} \tag{2.7}$$

We now apply the definition of μ to the sequence $\langle [A,Q]V^\varepsilon, V^\varepsilon\rangle$. Noting that $QV^\varepsilon \in$ compact of $[L^2_{\rm loc}(\mathbb{R}^Q)]^M$, we immediately conclude that, as $\varepsilon \searrow 0$,

$$\begin{cases}\langle AQV^\varepsilon, V^\varepsilon\rangle \to 0\\ \langle AV^\varepsilon, QV^\varepsilon\rangle \to 0\end{cases}$$

so that,

$$\lim_\varepsilon \langle [A,Q]V^\varepsilon, V^\varepsilon\rangle = \lim_\varepsilon \langle (Q^*-Q)AV^\varepsilon, V^\varepsilon\rangle,$$

or still, appealing to (2.6,2.7),

$$\begin{aligned}&\langle \mu, 1/i\Big(|\xi|^{-(m-1)}\{\!\{a,\sigma^m(R)\}\!\} + (m-1)|\xi|^{-(m+1)}\xi_j\frac{\partial a}{\partial y_j}\sigma^m(R)\Big)\rangle\\ &= \langle \mu, \Big[|\xi|^{-(m-1)}\Big((\sigma^{m-1}(R))^* - \sigma^{m-1}(R)\Big) + \frac{1}{i}(m-1)|\xi|^{-(m+1)}\xi_j\frac{\partial\sigma^m(R)}{\partial y_j}\\ &+\frac{1}{i}|\xi|^{-(m-1)}\frac{\partial^2\sigma^m(R)}{\partial y_j\partial\xi_j}\Big]a\rangle.\end{aligned}$$

The localization lemma 2.10 implies that $\sigma^m(R)\mu = 0$, so that the last term in the left-hand side of the previous equality disappears; furthermore, $|\xi| \equiv 1$ on the support of μ. Rearranging terms, we are left with the transport equation stated in the lemma. □

Second application to the wave equation. To analyze the transport properties of the measure ν introduced in (2.2), it is more convenient to introduce the $(N+1)$-vector

$$W^\varepsilon := (\sqrt{\rho}V^\varepsilon, \sqrt{k}V_i^\varepsilon)$$

with associated H-measure

$$\pi = (L(x)\xi \otimes L(x)\xi)\nu \tag{2.8}$$

where

$$L(x) := \begin{pmatrix} \sqrt{\rho} & 0 & \dots & 0 \\ 0 & \sqrt{k} & \dots & \dots \\ \dots & \dots & \dots & 0 \\ 0 & \dots & 0 & \sqrt{k} \end{pmatrix}.$$

Then it is easily checked that the commutativity properties of the mixed derivatives, together with the wave equation, now expressed in those new variables, become

$$iRW^\varepsilon = 0$$

with

$$iR := \begin{pmatrix} \dfrac{\partial}{\partial t} & -\dfrac{1}{\sqrt{\rho}}\dfrac{\partial(\sqrt{k}\,.)}{\partial x_1} & \dots & -\dfrac{1}{\sqrt{\rho}}\dfrac{\partial(\sqrt{k}\,.)}{\partial x_3} \\ -\sqrt{k}\dfrac{\partial(\frac{1}{\sqrt{\rho}}\,.)}{\partial x_1} & \dfrac{\partial}{\partial t} & 0 & \dots \\ \dots & \dots & \dots & \dots \\ -\sqrt{k}\dfrac{\partial(\frac{1}{\sqrt{\rho}}\,.)}{\partial x_3} & \dots & 0 & \dfrac{\partial}{\partial t} \end{pmatrix}.$$

Note that $R \in \Psi_M^{1,c}(\mathbb{R}^Q)$ with

$$\sigma^1(R) = \begin{pmatrix} \xi_0 & -\xi_1\sqrt{\dfrac{k}{\rho}} & \dots & -\xi_3\sqrt{\dfrac{k}{\rho}} \\ -\xi_1\sqrt{\dfrac{k}{\rho}} & \xi_0 & 0 & 0 \\ \dots & \dots & \dots & \dots \\ -\xi_3\sqrt{\dfrac{k}{\rho}} & 0 & 0 & \xi_0 \end{pmatrix}. \tag{2.9}$$

Further, the lower order symbol defines an element in $\Psi_M^{0,c}(\mathbb{R}^Q)$ with (full) symbol

$$\sigma^0(R) = \begin{pmatrix} 0 & \frac{i}{\sqrt{\rho}}\frac{\partial\sqrt{k}}{\partial x_1} & \cdots & \frac{i}{\sqrt{\rho}}\frac{\partial\sqrt{k}}{\partial x_3} \\ i\sqrt{k}\frac{\partial\frac{1}{\sqrt{\rho}}}{\partial x_1} & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots \\ i\sqrt{k}\frac{\partial\frac{1}{\sqrt{\rho}}}{\partial x_3} & 0 & 0 & \xi_0 \end{pmatrix}. \tag{2.10}$$

In view of (2.9, 2.10), the transport Lemma 2.11 straightforwardly yields

$$\langle \pi, \{\!\{\sigma^1(R), a\}\!\} \rangle = 0,$$

a relation we now explicit with the help of (2.8). The computation is straightforward, but a bit tedious. It only uses the localization equation (2.3), and is safely left to the reader.

We finally obtain the following transport equation:

$$\langle \nu, \xi_0 \{\!\{q, a\}\!\} \rangle = 0, \quad \text{for any } a \in \mathcal{C}_0^\infty(\mathbb{R}_y^{N+1} \times S_\xi^N). \tag{2.11}$$

Consequences 2.13. The following four remarks complete the study of the H-measure for the wave equation:

i. Since the support of ν lies in the zero set of $q(x,\xi)$ on S_ξ^N, and in view of (1.1),

$$\{\xi \in S_\xi^N : \xi_0 = 0\} \subset (\text{supp } \nu)^c$$

so that we are at liberty to choose a in (2.11) of the form $\dfrac{1}{\xi_0}\zeta(\xi)a$ where $\zeta \in \mathcal{C}^\infty(S_\xi^N)$ is such that $\zeta(0,\xi_1,\ldots,\xi_N) = 0$ and $\zeta \equiv 1$ on supp ν. Then, since q does not depend upon $x_0 = t$ or ξ_0,

$$0 = \langle \nu, \xi_0 \{\!\{q, \frac{1}{\xi_0}\zeta a\}\!\} \rangle = \langle \nu, \{\!\{q, \zeta a\}\!\} \rangle = \langle \nu, \{\!\{q, a\}\!\} \rangle$$

and the transport equation reads more simply as

$$\langle \nu, \{\!\{q, a\}\!\} \rangle = 0, \quad \text{for any } a \in \mathcal{C}_0^\infty(\mathbb{R}_y^{N+1} \times S_\xi^N); \tag{2.12}$$

ii. We have referred several times to (2.11, 2.12) as "transport equations". In the case of the wave equation, it is actually shown in [3], Section 3.2.1, that ν remains constant along the projections onto $\mathbb{R}_y^{N+1} \times S_\xi^N$ of the integral curves of

$$\begin{cases} \dfrac{d\overline{y}_i}{ds} = \dfrac{\partial(q/|\xi|)}{\partial\xi_i}(\overline{y},\overline{\xi}) \\ \dfrac{d\overline{\xi}_i}{ds} = -\dfrac{\partial(q/|\xi|)}{\partial y_i}(\overline{y},\overline{\xi}) \end{cases} \quad \left(|\xi| := (\sum_0^N \xi_j^2)^{1/2}\right)$$

with initial conditions

$$\begin{cases} \overline{y}(0) = y \\ \overline{\xi}(0) = \xi \end{cases} \quad \text{with } q(y,\xi) = 0,\ \xi \in S^N_\xi.$$

The principle leading to the above statement is simple. Assume for a moment that the weak form (2.12) was for test functions $a \in \mathcal{C}^\infty_0(\mathbb{R}^{N+1}_y \times \mathbb{R}^{N+1}_\xi)$. Then, a simple integration by parts would immediately yield

$$\{\!\{q, \nu\}\!\} = 0$$

and ν would then be constant along the integral curves of

$$\begin{cases} \dfrac{d\overline{y}_i}{ds} = \dfrac{\partial q}{\partial \xi_i}(\overline{y}, \overline{\xi}) \\ \dfrac{d\overline{\xi}_i}{ds} = -\dfrac{\partial q}{\partial y_i}(\overline{y}, \overline{\xi}) \end{cases}$$

with

$$\begin{cases} \overline{y}(0) = y \\ \overline{\xi}(0) = \xi. \end{cases}$$

The difficulty in our context is that the ξ variable only lives on the sphere S^N_ξ;

iii. The transport equation (2.12) only makes sense once the initial value of ν is determined. This is not completely immediate because the H-measure associated to the initial conditions (1.4) *a priori* leaves in $\mathbb{R}^N_x \times S^{N-1}_\eta$; there is thus a reduction of *2* dimensions. The following theorem is established in [3] (see Corollary 3.1):

Theorem: *If $\tilde{\nu}^\pm$ are the H-measures associated to (a subsequence of) $\{v^\varepsilon_{\pm 0}\}$ with $v^\varepsilon_{\pm 0} := \sqrt{\rho} Z^\varepsilon_0 \pm i\sqrt{k}|D_x| V^\varepsilon_0$ ($V^\varepsilon_0, Z^\varepsilon_0$ defined in* (1.4)*), then*

$$\nu(t=0) = \frac{1}{4\rho\xi_0^2}(\tilde{\pi}^+ + \tilde{\pi}^-)$$

where, for any $\phi \in \mathcal{C}^\infty_0(\mathbb{R}^N_y \times S^N_\xi)$,

$$\langle \tilde{\pi}^\pm, \phi \rangle := \int_{\mathbb{R}^N_x \times S^{N-1}_\eta} \phi\Big(x, \pm(\frac{k(x)}{\rho(x)+k(x)})^{1/2}, (\frac{\rho(x)}{\rho(x)+k(x)})^{1/2}\eta_1, \dots\Big) d\tilde{\nu}^\pm.$$

We will not establish this here, but merely note that the above definition of $\tilde{\pi}^\pm$ permits to transform the H-measures $\tilde{\nu}^\pm$ that live on $\mathbb{R}^N_x \times S^{N-1}_\eta$ into measures on $\mathbb{R}^N_\xi \times S^N_\xi$, which is precisely what we need to obtain a meaningful initial condition for ν. Also note that $|D_x|$ is the element of $\Psi^1_1(\mathbb{R}^N)$ with principal symbol $|\xi|$.

iv. According to Remark 3.10 in [3], any point in the support of ν can be reached by a unique projection of an integral curve, and that integral curve intersects $t = 0$.

Coalescing items i and iii of Consequences 2.13, we finally obtain the following

Theorem 2.14. *The H-measure associated to* (*a subsequence of*)

$$V^\varepsilon := (\frac{\partial v^\varepsilon}{\partial t}, \operatorname{grad} v^\varepsilon)$$

associated to v^ε *defined in* (1.2) *is of the form* $(\xi\otimes\xi)\nu$, *where* ν *lives on the zero set of* $q(x,\xi)$ *defined in* (2.4). *Furthermore* ν *remains constant along the projections onto* $\mathbb{R}^{N+1}_y \times S^N_\xi$ *of the integral curves of*

$$\left\{\begin{array}{rcl} \dfrac{d\overline{y}_i}{ds} & = & \dfrac{\partial(q/|\xi|)}{\partial\xi_i}(\overline{y},\overline{\xi}) \\ \dfrac{d\overline{\xi}_i}{ds} & = & -\dfrac{\partial(q/|\xi|)}{\partial y_i}(\overline{y},\overline{\xi}) \end{array}\right. \quad \left(|\xi| := (\sum_0^N \xi_j^2)^{1/2}\right)$$

with initial conditions

$$\left\{\begin{array}{l} \overline{y}(0) = y \\ \overline{\xi}(0) = \xi \end{array}\right. \quad \text{with } q(y,\xi) = 0,\ \xi \in S^N_\xi.$$

These are also called bicharacteristic strips. Finally,

$$\nu(t=0) = \frac{1}{4\rho\xi_0^2}(\tilde{\pi}^+ + \tilde{\pi}^-)$$

where $\tilde{\pi}^\pm$ *has been defined in item iii of Consequences* 2.13.

The limit of the energy density is then given by (2.5).

Particular Case 2.15. We conclude this section with an investigation of the particular case of the homogeneous wave equation, that is of the case where $k(x) = \rho(x) \equiv 1$. In such a case the bicharacteristic strips are easily determined. We obtain

$$\left\{\begin{array}{rcl} \overline{\xi} & = & \xi \\ \xi_0\overline{x}_i + \xi\overline{t} & = & \xi_0 x_i,\ 1 \le i \le N \end{array}\right. \quad \left(\xi_0^2 = \sum_1^N \xi_i^2,\ |\xi| = 1\right).$$

Then the H-measure ν is explicitly computable by virtue of Theorem 2.14; we get:

$$\nu(t,x,\xi_0,\eta) = \frac{1}{4\xi_0^2}(\tilde{\pi}^+ + \tilde{\pi}^-)(x + \frac{\eta}{\xi_0}t, \xi_0, \eta),$$

or still, in terms of $\tilde{\nu}^\pm$,

$$\nu(t,x,\xi_0,\eta) = 2^{\frac{N-2}{2}}\Big\{\tilde{\nu}^+(x+\sqrt{2}\eta t, \sqrt{2}\eta)\delta_{\xi_0=\frac{1}{\sqrt{2}}} + \tilde{\nu}^-(x-\sqrt{2}\eta t, \sqrt{2}\eta)\delta_{\xi_0=-\frac{1}{\sqrt{2}}}\Big\}. \tag{2.13}$$

Since there is nothing special about time $t = 0$, the H-measure ν is also

$$\begin{array}{rl} \nu(t,x,\xi_0,\eta) & = 2^{\frac{N-2}{2}}\Big\{ \quad \tilde{\nu}^+_{t_0}(x+\sqrt{2}\eta(t-t_0), \sqrt{2}\eta)\delta_{\xi_0=\frac{1}{\sqrt{2}}} \\ & \qquad +\tilde{\nu}^-_{t_0}(x-\sqrt{2}\eta(t-t_0), \sqrt{2}\eta)\delta_{\xi_0=-\frac{1}{\sqrt{2}}}\Big\}, \end{array} \tag{2.14}$$

where $\tilde{\nu}^{\pm}_{t_0}$ are the H-measures associated to $\dfrac{\partial v^\varepsilon(t_0)}{\partial t} \pm i|D_x|v^\varepsilon(t_0)$. Comparison of (2.13) and (2.14) immediately implies that

$$\tilde{\nu}^{\pm}_t(x,\eta) = \tilde{\nu}^{\pm}(x \mp \eta t, \eta). \tag{2.15}$$

We denote by ν_t the measure on $\mathbb{R}^N_x \times S^{N-1}_\eta$ such that, for a subsequence of v^ε, and any $A \in \Psi^0_{1,c}(\mathbb{R}^N)$,

$$\langle \nu_t, \sigma^0(A)\rangle = 1/2 \lim_\varepsilon \Big\{ \langle A \frac{\partial v^\varepsilon(t)}{\partial t}, \frac{\partial v^\varepsilon(t)}{\partial t}\rangle + \langle A \frac{\partial v^\varepsilon(t)}{\partial x_i}, \frac{\partial v^\varepsilon(t)}{\partial x_i}\rangle \Big\}. \tag{2.16}$$

For almost any given time t, the existence of such a subsequence is a direct consequence of the $L^\infty(0,T;H^1_0(\mathbb{R}^N)) \cap W^{1,\infty}(0,T;L^2(\mathbb{R}^N))$-bound on v^ε, together with Lemma 2.6. It can actually be shown that the subsequence can be picked *independently of* $t \in [0,T]$ and that the convergence in (2.16) is locally uniform in time (see [5], Proposition 4.4).

A simple computation would show that

$$\langle \nu_t, \sigma^0(A)\rangle = 1/4 \lim_\varepsilon \Big(\sum_\pm \langle A(\frac{\partial v^\varepsilon(t)}{\partial t} \pm i|D_x|v^\varepsilon(t)), \frac{\partial v^\varepsilon(t)}{\partial t} \pm i|D_x|v^\varepsilon(t)\rangle \Big)$$

In view of (2.15), this also reads as

$$\nu_t(x,\eta) = 1/4 \Big\{ \tilde{\nu}^+(x - \eta t, \eta) + \tilde{\nu}^-(x + \eta t, \eta) \Big\}, \tag{2.17}$$

a relation that will be used in Subsection 3.3 below.

3. A compactness theorem for the wave equation

In a first subsection, we briefly introduce semi-classical measures as a tool for the further investigation of the solution to the wave equation investigated in the particular case 2.15. The following subsection is devoted to the proof of a microlocal compactness theorem of P. GÉRARD (Theorem 3.7 below). As a corollary, we obtain in the short third subsection the compactness result (Theorem 3.9) announced in the introduction.

3.1. Semi-classical measures

Whenever the problem under consideration exhibits a characteristic scale, say ε, it is of special interest to investigate the oscillations that take place at that scale. In the sake of simplicity, we only consider scalar problems.

To this effect, we consider the regularizing standard pseudo-differential operators $A(\varepsilon D) \in \cap_m \Sigma^m_1(\mathbb{R}^Q)$ with symbols $\sigma(A)(y,\varepsilon\xi)$, where $\sigma(A)(y,\xi) \in \mathsf{S}(\mathbb{R}^Q_y \times \mathbb{R}^Q_\xi)$. Note that

$$u^\varepsilon \text{ bounded in } L^2(\mathbb{R}^Q) \Longrightarrow A(\varepsilon D)u^\varepsilon \text{ bounded in } L^2(\mathbb{R}^Q).$$

An existence lemma analogous to Lemma 2.6 holds true.

Lemma 3.1. *Let $v^\varepsilon \overset{L^2(\mathbb{R}^Q)}{\rightharpoonup} v$. There exists a subsequence $\{\varepsilon'\} \subset \{\varepsilon\}$ and a nonnegative* RADON *measure m on $\mathbb{R}^Q_y \times \mathbb{R}^Q_\xi$ such that, for any $\sigma(A) \in \mathsf{S}(\mathbb{R}^Q_y \times \mathbb{R}^Q_\xi)$,*

$$\lim_{\varepsilon'} \int_{\mathbb{R}^Q_y} A(\varepsilon' D) v^{\varepsilon'} \overline{v}^{\varepsilon'} dx =: \lim_{\varepsilon'} \langle A(\varepsilon' D) v^{\varepsilon'}, v^{\varepsilon'} \rangle = \int_{\mathbb{R}^Q_y \times R^Q_\xi} \sigma(A) dm =: \langle m, \sigma(A) \rangle.$$

Remark 3.2. In contrast to the definition of H-measures, the weak limit of v^ε is not taken to be 0. In problems involving semi-classical measures, the weak limit of the oscillating field is not always easily identifiable.

Usually, we a priori know that v^ε oscillates at the scale of ε; that is for example the case when both v^ε and $\varepsilon D v^\varepsilon$ are bounded in $L^2(\mathbb{R}^Q)$ (think of $v^\varepsilon(x) := v(\frac{x}{\varepsilon}), v \in L^2(\mathcal{T})$). In such a case, we label the sequence ε-oscillatory; this gives rise to the following

Definition 3.3. *The sequence $v^\varepsilon \overset{L^2(\mathbb{R}^Q)}{\rightharpoonup} v$ is called ε-oscillatory if*

$$\lim_{R \nearrow \infty} \limsup_{\varepsilon} \int_{|\xi| \geq R/\varepsilon} |\widehat{\varphi v^\varepsilon}(\xi)|^2 d\xi = 0, \ \varphi \in \mathcal{C}_0^\infty(\mathbb{R}^Q).$$

Then, the following result holds true:

Lemma 3.4. *Assume that $v^\varepsilon \overset{L^2(\mathbb{R}^Q)}{\rightharpoonup} v$ admits m as semi-classical measure.*

i. *If v^ε is ε-oscillatory, then the measure limit of $(v^\varepsilon)^2$ is given by $\int_{\mathbb{R}^Q_\xi} dm(y, \xi)$;*

ii. *If $m(\mathbb{R}^Q \times \{0\}) = 0$, then $v = 0$ and if, further v^ε is ε-oscillatory, v^ε admits a H-measure defined, for any $A \in \Psi^0_{1,c}(\mathbb{R}^Q)$, as*

$$\langle \mu, \sigma^0(A) \rangle = \int_{\mathbb{R}^Q_y \times (\mathbb{R}^Q_\xi \setminus \{0\})} \sigma^0(A)(y, \frac{\xi}{|\xi|}) dm(y, \xi); \ \textit{and}$$

iii. *If $v^\varepsilon \overset{L^2(\mathbb{R}^Q)}{\rightharpoonup} 0$ and admits both a H-measure and a semi-classical measure (it is both pure and ε-pure), then*

$$\langle \mu, \sigma^0(A) \rangle \geq \int_{\mathbb{R}^Q_y \times (\mathbb{R}^Q_\xi \setminus \{0\})} \sigma^0(A)(y, \frac{\xi}{|\xi|}) dm(y, \xi).$$

Proof. The proof of item i. is as follows. Take $\varphi, \psi \in [\mathcal{C}_0^\infty(\mathbb{R}^Q)]^2$ with $0 \leq \psi \leq 1$ and $\psi \equiv 1$ in a neighborhood of $\xi = 0$ and consider $\sigma(A) := \varphi^2(y) \psi(\frac{\xi}{R}), \ \sigma(\Psi) := \psi(\xi)$. It is easily checked (in the spirit of Remark 2.7) that φv^ε admits $\varphi^2(y) m$ as semi-classical measure. Denote the measure limit of (a subsequence of) $(v^\varepsilon)^2$ by M; then, with obvious notation,

$$\langle m(y, \xi), \varphi^2(y) \psi(\frac{\xi}{R}) \rangle = \langle M(y), \varphi^2(y) \rangle - \lim_{\varepsilon} \langle 1 - \Psi(\varepsilon D/R) \varphi v^\varepsilon, \varphi v^\varepsilon \rangle.$$

But, in view of the definition of ψ and since v^ε is ε-oscillatory, the last term in the above equality tends to 0 as $R \nearrow \infty$. LEBESGUE dominated convergence implies that the left-hand side of the same equality goes to $\langle m(y, \xi), \varphi^2(y) \rangle$ as $R \nearrow \infty$, which proves item i.

To prove ii., we consider $\sigma(A_n)(\xi) \geq 0 \in \mathcal{C}_0^\infty(\mathbb{R}^Q)$. Then, invoking PLANCHEREL's identity,

$$\langle (A_n(\varepsilon D)v^\varepsilon, v\rangle = \int_{\mathbb{R}^Q_\xi} \sigma((A_n)(\varepsilon\xi)\hat{v}^\varepsilon \overline{\hat{v}}\, d\xi \overset{\varepsilon \rightharpoonup 0}{\rightharpoonup} \sigma((A_n)(0)\|v\|^2_{L^2(\mathbb{R}^Q)}.$$

But, appealing to CAUCHY–SCHWARTZ inequality,

$$\begin{aligned} \limsup_\varepsilon \langle (A_n(\varepsilon D)v^\varepsilon, v\rangle &\leq \lim_\varepsilon \langle (A_n(\varepsilon D)v^\varepsilon, v^\varepsilon\rangle^{1/2} \lim_\varepsilon \langle (A_n(\varepsilon D)v, v\rangle^{1/2} \\ &= \langle m, \sigma((A_n)\rangle^{1/2} \sigma((A_n)^{1/2}(0)\|v\|_{L^2(\mathbb{R}^Q)}, \end{aligned}$$

so that

$$\sigma((A_n)^{1/2}(0)\|v\|_{L^2(\mathbb{R}^Q)} \leq \langle m, \sigma((A_n)\rangle^{1/2}.$$

Choosing $\sigma(A_n)(\xi) \overset{n}{\rightharpoonup} \begin{cases} 0, \ \xi \neq 0 \\ 1, \ \xi = 0 \end{cases}$, we obtain ii. since m does not charge $\{\xi = 0\}$.

Assume now that v^ε is ε-oscillatory. Take $a(\xi) \in \mathcal{C}^\infty(\mathbb{R}^Q_\xi)$ and $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^Q_y)$. Consider $\chi(\xi) \in \mathcal{C}^\infty(\mathbb{R}^Q_\xi)$ with $\chi \equiv 0$ in a neighborhood of $\xi = 0$ and $\chi \equiv 1$ for $|\xi| \geq 1$. Define $\sigma^0(A)(y,\xi) := \varphi^2(y)a(\frac{\xi}{|\xi|})$ as the (principal) symbol of an element $A \in \Psi^0_{1,c}(\mathbb{R}^Q)$; then, according to Remark 2.7,

$$\begin{aligned} \langle A\varphi v^\varepsilon, \varphi v^\varepsilon\rangle &= \int_{\mathbb{R}^Q_\xi \setminus \{0\}} a(\frac{\xi}{|\xi|})\chi(\frac{\xi}{r})\widehat{\varphi v^\varepsilon}(\xi)\overline{\widehat{\varphi v^\varepsilon}}(\xi)d\xi \\ &= \int_{\mathbb{R}^Q_\xi \setminus \{0\}} a(\frac{\varepsilon\xi}{\varepsilon|\xi|})\widehat{\varphi v^\varepsilon}(\xi)\overline{\widehat{\varphi v^\varepsilon}}(\xi)d\xi + \\ &\quad \int_{\mathbb{R}^Q_\xi \setminus \{0\}} a(\frac{\varepsilon\xi}{\varepsilon|\xi|})(\chi(\frac{\xi}{r}) - 1)\widehat{\varphi v^\varepsilon}(\xi)\overline{\widehat{\varphi v^\varepsilon}}(\xi)d\xi \\ &= \int_{\mathbb{R}^Q_\xi \setminus \{0\}} a(\frac{\varepsilon\xi}{\varepsilon|\xi|})\chi(\varepsilon r\xi)\widehat{\varphi v^\varepsilon}(\xi)\overline{\widehat{\varphi v^\varepsilon}}(\xi)d\xi + \\ &\quad \int_{\mathbb{R}^Q_\xi \setminus \{0\}} \chi(\frac{\xi}{\eta})a(\frac{\varepsilon\xi}{\varepsilon|\xi|})(1 - \chi(\varepsilon r\xi))\widehat{\varphi v^\varepsilon}(\xi)\overline{\widehat{\varphi v^\varepsilon}}(\xi)d\xi + \\ &\quad \int_{\mathbb{R}^Q_\xi \setminus \{0\}} (1 - \chi(\frac{\xi}{\eta}))a(\frac{\varepsilon\xi}{\varepsilon|\xi|})(1 - \chi(\varepsilon r\xi))\widehat{\varphi v^\varepsilon}(\xi)\overline{\widehat{\varphi v^\varepsilon}}(\xi)d\xi + \\ &\quad \int_{\mathbb{R}^Q_\xi \setminus \{0\}} a(\frac{\varepsilon\xi}{\varepsilon|\xi|})(\chi(\frac{\xi}{r}) - 1)\widehat{\varphi v^\varepsilon}(\xi)\overline{\widehat{\varphi v^\varepsilon}}(\xi)d\xi. \end{aligned} \tag{3.1}$$

Since v^ε is ε-oscillatory,

$$\limsup_{r \searrow 0} \limsup_\varepsilon \int_{\mathbb{R}^Q_\xi} \chi(\varepsilon r\xi)|\widehat{\varphi v^\varepsilon}|^2(\xi)d\xi = 0,$$

so that the first term in the right-hand side of the last equality in (3.1) tends to 0 as ε then r tend to 0.

As $\varepsilon \searrow 0$, the second term in the right-hand side of the last equality in (3.1) tends to $\langle \varphi^2(y)m(y,\xi), (1-\chi(r\xi))a(\frac{\xi}{|\xi|})\chi(\frac{\xi}{\eta})\rangle$. Thus, because by assumption $m(\mathbb{R}^Q \times \{0\}) = 0$, the dominated convergence theorem yields

$$\begin{aligned}
&\lim_{\eta\searrow 0}\lim_{r\searrow 0}\lim_{\varepsilon}\int_{\mathbb{R}^Q_\xi}\chi(\frac{\xi}{\eta})a(\frac{\varepsilon\xi}{\varepsilon|\xi|})(1-\chi(\varepsilon r\xi))\widehat{\varphi v^\varepsilon}(\xi)\overline{\widehat{\varphi v^\varepsilon}}(\xi)d\xi = \\
&= \lim_{\eta\searrow 0}\langle \varphi^2(y)m(y,\xi), a(\frac{\xi}{|\xi|})\chi(\frac{\xi}{\eta})\rangle = \langle \varphi^2(y)m(y,\xi), a(\frac{\xi}{|\xi|})\chi_{\{\xi\neq 0\}}\rangle \qquad (3.2)\\
&= \langle \varphi^2(y)m(y,\xi), a(\frac{\xi}{|\xi|})\rangle.
\end{aligned}$$

The third and fourth terms in that equality can be bounded from above by

$$C\int_{\mathbb{R}^Q_\xi\setminus\{0\}}|\chi(\frac{\xi}{\eta})-1| \text{ (resp. } |\chi(\frac{\xi}{r})-1|)|\widehat{\varphi v^\varepsilon}|^2(\xi)d\xi.$$

If we denote by $\hat{R}_\varphi$ the measure limit of (a subsequence of) $|\widehat{\varphi v^\varepsilon}|^2(\xi)$, we obtain

$$\limsup_{r\searrow 0}\lim_{\varepsilon} C\int_{\mathbb{R}^Q_\xi\setminus\{0\}}|\chi(\frac{\xi}{r})-1||\widehat{\varphi v^\varepsilon}|^2(\xi)d\xi \leq \int_{\mathbb{R}^Q_\xi\setminus\{0\}}\chi_{\{\xi=0\}}d\hat{R}_\varphi(\xi) = 0.$$

Collecting the various limits above, we conclude that the limit of the left-hand side of (3.1) is that computed in (3.2), that is

$$\lim_{\varepsilon}\langle A\varphi v^\varepsilon, \varphi v^\varepsilon\rangle = \langle \varphi^2(y)m(y,\xi), a(\frac{\xi}{|\xi|})\rangle. \qquad (3.3)$$

If the principal symbol of A is of the general form $a(y,\xi) \in \mathcal{C}_0^\infty(\mathbb{R}^Q_y \times S^{Q-1}_\xi)$, an approximation of $\sup\{a,0\}$ and $\sup\{-a,0\}$ in $\mathcal{C}_0^0(\mathbb{R}^Q_y \times S^{Q-1}_\xi)$ by symbols of the form $\varphi^2(y)a(\xi)$ implies that (3.3) still holds for such symbols, that is that v^ε admits a H-measure μ given by

$$\langle \mu, \sigma^0(A)\rangle = \langle m(y,\xi), a(y,\frac{\xi}{|\xi|})\rangle,$$

hence the second part of item ii.

The proof of iii. is implicit in the proof of the second part of item ii. above. □

Remark 3.5. Note that in the course of deriving the first part of the previous lemma we have actually shown that the measure-limit M of $(v^\varepsilon)^2$ satisfies

$$M \geq \int_{\mathbb{R}^Q_\xi} dm(y,\xi).$$

Remark 3.6. Localization and transport results of the type obtained in the previous section can be analogously derived within the framework of semi-classical measures (see [6], (3.12) and Proposition 3.5*)*.

3.2. An improvement of P.L. Lions ' compactness result

As mentioned in the introduction, the microlocal tools of H and semi-classical measures are fundamental in P. Gérard's following improvement (see [5], Corollary 5) of P.L. Lions' compactness Theorem 1.1 which we now state and prove in a three-dimensional setting for simplicity sake.

Theorem 3.7. *Let* $w^n \rightharpoonup 0$, *weakly in* $H^1(\mathbb{R}^3)$.

Assume that $\operatorname{grad} w^n$ *admits a H-measure* $(\xi \otimes \xi)\mu$ *such that*

$$\mu(y,\xi) \perp \delta(y-z) \otimes d\sigma(\xi),\ \forall z \in \mathbb{R}^3,$$

where σ *is the superficial* Lebesgue *measure on* S^2_ξ.

Then,

$$w^n \to 0,\ \textit{strongly in}\ L^6_{\rm loc}(\mathbb{R}^3).$$

We offer a complete proof of the theorem; the proof provides an elegant application of the interplay between semi-classical and H-measures displayed in Lemma 3.4, together with a rather striking use of a Sobolev–Besov type imbedding.

Proof. The following imbedding estimate is pivotal in the subsequent proof:

Lemma 3.8. *Define, for any* $1 < p < \infty$ *the space* B_p *of all* $f \in L^2(\mathbb{R}^3)$ *such that*

$$\|f\|_{B_p} := \sup_{k\in\mathbb{Z}} \|\widehat{\Delta_k f}\|_{L^p} < \infty$$

with $\widehat{\Delta_k f} := \chi_{\{2^k \le |\xi| < 2^{k+1}\}}(\xi)\hat{f}(\xi)$.

Then, for any $1 < p \le \frac{6}{5}$, *there exists* $0 < s \le 1$ *and a constant* C *such that, for any* $u \in H^s(\mathbb{R}^3) \cap B_p$,

$$\|u\|_{L^6} \le C\|D^s u\|^{1/3}_{L^2}\|u\|^{2/3}_{B_p}.$$

The actual value of s *is* $\frac{6(p-1)}{p}$.

Proof of Lemma. Define, for any $A > 0$, $\widehat{u_{>A}}(resp.\ \widehat{u_{\le A}}) := \chi_{\{|\xi|>(resp.\ \le)A\}}\hat{u}(\xi)$ and write $u = u_{\le A} + u_{>A}$. Then,

$$\|u_{\le A}\|_{L^\infty} \le C\|\widehat{u_{\le A}}\|_{L^1} \le C \sum_{k(\in\mathbb{Z})\le k(A)} \|\chi_{\{2^k\le|\xi|<2^{k+1}\}}\hat{u}\|_{L^1},$$

where $2^{k(A)} \le A < 2^{k(A)+1}$. Now, by Hölder's inequality, for $p > 1$,

$$\|\chi_{\{2^k\le|\xi|<2^{k+1}\}}\hat{u}\|_{L^1} \le C2^{3k(\frac{p-1}{p})}\Big(\int_{2^k\le|\xi|\le 2^{k+1}} |\hat{u}|^p d\xi\Big)^{1/p}.$$

thus,

$$\|u_{\le A}\|_{L^\infty} \le CA^{3(\frac{p-1}{p})}\|u\|_{B_p}.$$

Now,

$$\|u\|^6_{L^6} = 6\int_0^\infty \lambda^5 \mathcal{L}^3(\{|u| > \lambda\})d\lambda.$$

Set, for any $\lambda > 0$, $A(\lambda) := \Big(\dfrac{\lambda}{2C\|u\|_{B_p}}\Big)^{\frac{p}{3(p-1)}}$, so that $\|u_{\leq A(\lambda)}\|_{L^\infty} \leq \frac{\lambda}{2}$. Then,

$$\mathcal{L}^3(\{|u| > \lambda\}) \leq \mathcal{L}^3(\{|u_{>A(\lambda)}| > \lambda/2\}) \leq \frac{4}{\lambda^2}\|u_{>A(\lambda)}\|_{L^2}^2 = \frac{4}{\lambda^2}\|\widehat{u_{>A(\lambda)}}\|_{L^2}^2.$$

Consequently,

$$\|u\|_{L^6}^6 \leq 24\int_0^\infty \lambda^3 \|\widehat{u_{>A(\lambda)}}\|_{L^2}^2 d\lambda,$$

or still, invoking Fubini's theorem,

$$\|u\|_{L^6}^6 \leq 24\int_0^\infty \Big(\int_0^{4C|\xi|^{\frac{3(p-1)}{p}}\|u\|_{B_p}} \lambda^3 d\lambda\Big)|\hat{u}|^2(\xi)d\xi,$$

which finally implies that

$$\|u\|_{L^6}^6 \leq C\|u\|_{B_p}^4 \|D^{\frac{6(p-1)}{p}}u\|_{L^2}^2;$$

hence the lemma. □

We now address the proof of Theorem 3.7. To this effect, we define

$$\rho(y,\xi) := (y, \frac{\xi}{|\xi|})$$

and apply item iii. of Lemma 3.4 to the current setting for any subsequence $\{n'\}$ of $\{n\}$ such that $\operatorname{grad} w^{n'}$ admits a semi-classical measure $(\xi\otimes\xi)m$ and also such that $|\operatorname{grad} w^{n'}|^2$ admits a measure limit M. Thus, because by assumption

$$\mu(y,\xi) \perp \delta(y-z)\otimes d\sigma(\xi),\ z\in\mathbb{R}^3,$$

a fortiori

$$\rho(\chi_{\{\xi\neq 0\}}m(y,\xi)) \perp \rho(\chi_{\{\xi\neq 0\}}\delta(y-z)\otimes\mathcal{L}^3(\xi)),\ z\in\mathbb{R}^3,$$

or still, since $\mathcal{L}^3(\xi) \perp \delta_{\xi=0}$,

$$m(y,\xi) \perp \delta(y-z)\otimes\mathcal{L}^3(\xi). \tag{3.4}$$

Consider now, for $\theta\in\mathcal{C}_0^\infty(B(0,1))$ with $0\leq\theta(y)\leq 1$, $\theta(0)=1$,

$$z_\delta^n(y) := \theta(\frac{y-z}{\delta})w^n(y).$$

Now,

$$\limsup_n \|z_\delta^n\|_{B_p} = \limsup_n \sup_k \|\widehat{\Delta_k z_\delta^n}\|_{L^p}$$

and, at fixed δ, $\widehat{z_\delta^n} \overset{L^2_{\mathrm{loc}}(\mathbb{R}^3)}{\to} 0$ because $w^n \overset{L^2(\mathbb{R}^3)}{\rightharpoonup} 0$ and $\theta(\frac{y-z}{\delta})$ has compact support. Thus, each term $\|\widehat{\Delta_k z_\delta^n}\|_{L^p}$, $p\leq 2$ goes to 0 with n and

$$\limsup_n \|z_\delta^n\|_{B_p} = \limsup_{n\nearrow\infty} \|\widehat{\Delta_{k_n} z_\delta^n}\|_{L^p}, \tag{3.5}$$

$\{k_n\}$ being a sequence that tends to ∞ with n.

We choose $p = \frac{6}{5}$.

Set $\varepsilon_n := 2^{-k_n}$ and consider a subsequence $\{n'\} \subset \{n\}$ (in all rigor, a subsequence that depends upon $\{\varepsilon_n\}$) such that $\operatorname{grad} w^{n'}$ admits a semi-classical measure $(\xi \otimes \xi)m$ (with associated k'_n). Then, applying Hölder's inequality,

$$\begin{aligned} \|\widehat{\Delta_{k'_n} z_\delta^{n'}}\|_{L^{\frac{6}{5}}} &\leq C(\varepsilon_{n'})^{-1} \|\widehat{\Delta_{k'_n} z_\delta^{n'}}\|_{L^2} \\ &\leq C(\varepsilon'_n)^{-1} \Big(\int_{\mathbb{R}^3_\xi} \chi_{\{1 \leq \varepsilon_{n'}|\xi| < 2\}}(\xi) (\varepsilon_{n'})^2 |\xi|^2 |\widehat{z_\delta^{n'}}|^2 d\xi \Big)^{1/2}, \end{aligned} \tag{3.6}$$

or still,

$$\|\widehat{\Delta_{k'_n} z_\delta^{n'}}\|_{L^{\frac{6}{5}}} \leq C \Big(\int_{\mathbb{R}^3_\xi} \chi_{\{1 \leq \varepsilon_{n'}|\xi| < 2\}}(\xi) |\xi|^2 |\widehat{z_\delta^{n'}}|^2 d\xi \Big)^{1/2}. \tag{3.7}$$

Note that $\widehat{\operatorname{grad} z_\delta^{n'}} = (\theta(\frac{\cdot - z}{\delta}) \widehat{\operatorname{grad} w^{n'}(.)}) +$(a term that converges strongly to 0 in $L^2(\mathbb{R}^3)$), so that (3.7) also reads as

$$\|\widehat{\Delta_{k'_n} z_\delta^{n'}}\|_{L^{\frac{6}{5}}} \leq C \Big(\int_{\mathbb{R}^3_\xi} \chi_{\{1 \leq \varepsilon_{n'}|\xi| < 2\}}(\xi) |(\theta(\frac{\cdot - z}{\delta}) \widehat{\operatorname{grad} w^{n'}(.)})|^2 d\xi \Big)^{1/2} + \omega(n), \tag{3.8}$$

with $\omega(n) \overset{n \nearrow \infty}{\to} 0$. Now, in the spirit of Remark 2.7, the previous inequality can be rewritten as

$$\|\widehat{\Delta_{k'_n} z_\delta^{n'}}\|_{L^{\frac{6}{5}}} \leq C < \Theta_z(\varepsilon_{n'} D) \operatorname{grad} w^{n'}, \operatorname{grad} w^{n'} >^{1/2}, \tag{3.9}$$

where Θ_z is the pseudo-differential operator with symbol

$$\sigma(\Theta_z) := \theta(\frac{y - z}{\delta}) \chi_{\{1 \leq |\xi| < 2\}}(\xi).$$

At the expense of a smoothing of the symbol $\sigma(\Theta_z)$, we are in a position to compute the limit of the right-hand side of (3.9) in terms of the semi-classical limit m associated to $\operatorname{grad} w^{n'}$. Consequently, in view of (3.8), (3.5) becomes

$$\limsup_n \|\widehat{\Delta_{k_n} z_\delta^n}\|_{L^{\frac{6}{5}}} \leq C \langle |\xi|^2 m(y, \xi), \theta(\frac{y - z}{\delta}) \chi_{\{1 \leq |\xi| < 2\}}(\xi) \rangle^{1/2}, \tag{3.10}$$

which we rewrite as

$$\limsup_n \|\widehat{\Delta_{k_n} z_\delta^n}\|_{L^{\frac{6}{5}}} \leq C \Big\{ \int_{\mathbb{R}^3_\xi} d\nu^\delta(m)(\xi) \Big\}^{1/2} \tag{3.11}$$

with

$$\nu^\delta(m)(\xi) := |\xi|^2 \chi_{\{1 \leq |\xi| < 2\}}(\xi) \int_{\mathbb{R}^3_y} \theta(\frac{y - z}{\delta}) dm(y, \xi).$$

Using the Radon–Nikodym theorem, we decompose $\nu^\delta(m)$ as

$$\nu^\delta(m) = \nu^\delta_{\mathcal{L}}(m) \mathcal{L}^3 + \nu^\delta_s(m),$$

where $\nu^\delta_{\mathcal{L}}(m)$ is the density of the Lebesgue-absolutely continuous part of $\nu^\delta(m)$ and $\nu^\delta_s(m)$ is the Lebesgue-singular part of that measure. We then consider, for any $\beta > 0$, $0 \leq \zeta_{\mathcal{L}}, \zeta_s \leq 1 \in \mathcal{C}^0(\mathbb{R}^3_\xi)$ such that:

- supp $\nu^\delta_{\mathcal{L}}(m) \subset \{\zeta_{\mathcal{L}} \equiv 1\}$;
- $\nu^\delta_s(m)\Big(\text{supp } \zeta_{\mathcal{L}}\Big) < \beta$;
- supp $\nu^\delta_s(m) \subset \{\zeta_s \equiv 1\}$;
- $\int_{\mathbb{R}^3_\xi} \zeta_s d\xi < \beta$;
- $\zeta_{\mathcal{L}} + \zeta_s \equiv 1$.

Then, rewriting $\|\widehat{\Delta_{k_{n'}} z^{n'}_\delta}\|_{L^{\frac{6}{5}}}$ as $\|\widehat{\Delta_{k_{n'}} z^{n'}_\delta}(\xi)(\zeta_{\mathcal{L}}+\zeta_s)(\varepsilon^{n'}\xi)\|_{L^{\frac{6}{5}}}$, an argument identical to that of (3.6)–(3.11) would lead to

$$\begin{aligned}\limsup_n \|\widehat{\Delta_{k_n} z^n_\delta}\|_{L^{\frac{6}{5}}} \quad &\leq \quad C\Big\{\Big(\int_{\mathbb{R}^3_\xi} \zeta_{\mathcal{L}} d\nu^\delta(m)(\xi)\Big)^{\frac{3}{5}}\Big(\int_{\{1\leq|\xi|<2\}} \zeta_{\mathcal{L}} d\xi\Big)^{\frac{2}{5}} \\ &\quad + \Big(\int_{\mathbb{R}^3_\xi} \zeta_s d\nu^\delta(m)(\xi)\Big)^{\frac{3}{5}}\Big(\int_{\{1\leq|\xi|<2\}} \zeta_s d\xi\Big)^{\frac{2}{5}}\Big\}^{\frac{5}{6}},\end{aligned}$$

or still, in view of the properties of $\zeta_{\mathcal{L}}, \zeta_s$,

$$\begin{aligned}\limsup_n \|\widehat{\Delta_{k_n} z^n_\delta}\|_{L^{\frac{6}{5}}} \quad &\leq \quad C\Big\{\Big(\int_{\mathbb{R}^3_\xi} d\nu^\delta_{\mathcal{L}}(m)(\xi) + C\beta\Big)^{\frac{3}{5}} \\ &\quad + \Big(\int_{\mathbb{R}^3_\xi} d\nu^\delta_s(m)(\xi) + C\beta\Big)^{\frac{3}{5}}\beta^{\frac{2}{5}}\Big\}^{\frac{5}{6}}.\end{aligned}$$

Letting $\beta \searrow 0$, we obtain the following refinement of (3.11):

$$\limsup_n \|\widehat{\Delta_{k_n} z^n_\delta}\|_{L^{\frac{6}{5}}} \leq C\Big\{\int_{\mathbb{R}^3_\xi} d\nu^\delta_{\mathcal{L}}(m)(\xi)\Big\}^{\frac{1}{2}}. \tag{3.12}$$

At this point, we recall (3.4) and apply it to m, which immediately implies that

$$\nu^\delta_{\mathcal{L}}(m) = \nu^\delta_{\mathcal{L}}(m\chi_{\{y\neq z\}}(y)). \tag{3.13}$$

Note that the above would not be true for $\nu^\delta(m)$ itself; just take, for ξ_0 such that $|\xi_0| = 3/2$, $m = \delta_{y\neq z} \otimes \delta_{\xi=\xi_0} \perp \delta(y-z) \otimes \mathcal{L}^3(\xi)$ (the reader can easily construct a sequence which admits such a measure as semi-classical measure), yet the associated $\nu^\delta(m)$ is $|\xi_0|^2\delta_{\xi=\xi_0}$, while $\nu^\delta(m\chi_{\{y\neq z\}}(y)) = 0$.

In any case, thanks to (3.13), we rewrite (3.12) as

$$\limsup_n \|\widehat{\Delta_{k_n} z^n_\delta}\|_{L^{\frac{6}{5}}} \leq C\Big\{\int_{\mathbb{R}^3_\xi} d\nu^\delta_{\mathcal{L}}(m\chi_{\{y\neq z\}})(\xi)\Big\}^{1/2},$$

and, *a fortiori*,

$$\limsup_n \|\widehat{\Delta_{k_n} z^n_\delta}\|_{L^{\frac{6}{5}}} \leq C\langle|\xi|^2\chi_{\{y\neq z\}}m(y,\xi), \theta(\frac{y-z}{\delta})\chi_{\{1\leq|\xi|<2\}}(\xi)\rangle^{1/2}.$$

Appealing to Remark 3.5 immediately implies that the right-hand side of the previous inequality can be bounded from above by

$$C\int_{\mathbb{R}^3_y} \chi_{\{y\neq z\}}|\theta(\frac{y-z}{\delta})|^2 dM(y),$$

where we recall that M is the measure limit of $|\operatorname{grad} w^{n'}|^2$. Since $0 \leq \theta \leq 1$, we thus get that

$$\limsup_n \|\widehat{\Delta_{k_n} z_\delta^n}\|_{L^{\frac{6}{5}}} \leq CM(B(z,\delta) \setminus \{\delta\}).$$

Letting $\delta \searrow 0$ finally yields

$$\limsup_\delta \limsup_n \|\widehat{\Delta_{k_n} z_\delta^n}\|_{L^{\frac{6}{5}}} = 0,$$

hence, in view of (3.5),

$$\limsup_\delta \limsup_n \|z_\delta^n\|_{B_{\frac{6}{5}}} = 0. \tag{3.14}$$

We now apply Lemma 3.8 and obtain,

$$\limsup_\delta \limsup_n \|z_\delta^n\|_{L^6} \leq C\ 0 \times \limsup_\delta \limsup_n \|\operatorname{grad} z_\delta^n\|_{L^2}^{1/3}. \tag{3.15}$$

But,

$$\limsup_n \|\operatorname{grad} z_\delta^n\|_{L^2}^{1/3} \leq \limsup_n (\|\operatorname{grad} w^n\|_{L^2} + C/\delta \|w^n\|_{L^2(B(z,\delta))})_{L^2}^{1/3}$$

or still, by virtue of Rellich's theorem applied to w^n on $L^2(B(z,\delta))$,

$$\limsup_n \|\operatorname{grad} z_\delta^n\|_{L^2}^{1/3} \leq \limsup_n \|\operatorname{grad} w^n\|_{L^2}^{1/3}.$$

Thus, (3.15) actually reads as

$$\limsup_\delta \limsup_n \|z_\delta^n\|_{L^6} = 0,$$

that is, if R denotes the measure limit of (a subsequence of) $(w^n)^6$,

$$\limsup_\delta \int_{\mathbb{R}^3_y} |\theta(\frac{y-z)}{\delta})|^6 dR(y) = R(\{z\}) = 0.$$

Since z is arbitrary, we conclude that R does not charge atoms; application of Theorem 1.1 then yields the desired result. □

3.3. A compactness result for the homogeneous wave equation

In this subsection, the results of the Particular case 2.15 and of Theorem 3.7 coalesce to produce a pointwise in time compactness result for the solution v^ε to the homogeneous wave equation.

The following theorem is due to P. Gérard (see [5], Theorem 9).

Theorem 3.9. *Let* $V_0^\varepsilon \rightharpoonup 0$, *in* $H^1(\mathbb{R}^N)$, $Z_0^\varepsilon \rightharpoonup 0$, *in* $L^2(\mathbb{R}^N)$ *with* supp V_0^ε *and* supp $Z_0^\varepsilon \subset K$ (*compact of* $\mathbb{R}^3$). *Consider the homogeneous wave equation*

$$\frac{\partial^2 v^\varepsilon}{\partial t^2} - \operatorname{div}(\operatorname{grad} v^\varepsilon) = 0$$

with initial conditions

$$v^\varepsilon(0) = u_0^\varepsilon - u_0 := V_0^\varepsilon$$
$$\frac{\partial v^\varepsilon}{\partial t}(0) = v_0^\varepsilon - v_0 := Z_0^\varepsilon.$$

Then the complement in $\mathbb{R}^+$ *of the set* $\{t \geq 0 : \|v^\varepsilon(t)\|_{L^6(\mathbb{R}^3)} \to 0\}$ *is at most countable.*

Proof. Because of the finite speed of propagation, supp $v^\varepsilon(t)$ lies in a compact subset of $\mathbb{R}^3$ for any $t \geq 0$. Assume that for some $t \geq 0$,

$$\limsup_\varepsilon \|v^\varepsilon(t)\|_{L^6(\mathbb{R}^3)} > 0. \tag{3.16}$$

Then, according to Theorem 3.7, a subsequence of $\{\operatorname{grad} w^\varepsilon(t)\}$ – possibly depending on t – admits a H-measure $\xi \otimes \xi\kappa_t$ and a point $x_t \in \mathbb{R}^3$ such that κ_t and $\delta(x - x_t) \otimes d\sigma(\eta)$ are not mutually singular.

Recall the Particular case 2.15. Since, obviously, $\kappa_t \leq \nu_t$, we *a fortiori* have that ν_t and $\delta(x-x_t)\otimes d\sigma(\eta)$ are not mutually singular, or, in other words, appealing to (2.17) that $1/4\Big\{\tilde\nu^+(x - \eta t, \eta) + \tilde\nu^-(x + \eta t, \eta)\Big\}$ and $\delta(x - x_t) \otimes d\sigma(\eta)$ are not mutually singular. Now, this means that either $\tilde\nu^+(x, \eta)$ and $\delta(x + \eta t - x_t) \otimes d\sigma(\eta)$ are not mutually singular, or that $\tilde\nu^-(x, \eta)$ and $\delta(x - \eta t - x_t) \otimes d\sigma(\eta)$ are not mutually singular.

Consequently, either $\tilde\nu^+(x, \eta)$ or $\tilde\nu^-(x, \eta)$ are not singular with respect to the superficial Lebesgue measure on a sphere of center x_t and radius t. But, such superficial measures are pairwise mutually singular for distinct t's, whether the x_t's are distinct or not. Since a Radon measure cannot have a non-zero Radon–Nykodim derivative with respect to more than a countable set of mutually singular measures, there cannot be more than a countable set of times t's for which (3.16) holds. □

Remark 3.10. The same result holds for the solution to the heterogeneous wave equation (1.3, 1.4) as could be derived at the expense of a revisiting of the particular case 2.15 in the more general context of arbitrary ρ's and k's.

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A Singular Perturbation Result with a Fractional Norm

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Abstract. Let I be an open bounded interval of $\mathbb{R}$ and W a non-negative continuous function vanishing only at $\alpha, \beta \in \mathbb{R}$. We investigate the asymptotic behavior in terms of Γ-convergence of the following functional

$$G_\varepsilon(u) := \varepsilon^{p-2} \iint_{I\times I} \left| \frac{u(x)-u(y)}{x-y} \right|^p dxdy + \frac{1}{\varepsilon}\int_I W(u)\,dx \quad (p>2),$$

as $\varepsilon \to 0$.

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1. Introduction

The classical variational model for phase transition is related to the so called Cahn-Hilliard functional

$$F_\varepsilon(u) = \varepsilon \int_\Omega |\nabla u|^2 dx + \frac{1}{\varepsilon}\int_\Omega W(u)\,dx, \tag{1.1}$$

where W is a two well potential vanishing in two point, α and β.

The study of the Γ-limit of this functional, due to Modica and Mortola [15] (see also [14]), provided a connection between the singular perturbation of the two well potential and the (classical) surface tension model. They indeed proved that F_ε Γ-converges to the functional defined in $BV(\Omega, \{\alpha, \beta\})$ given by

$$c_W \mathrm{Per}(\{u = \alpha\});$$

i.e., its value is proportional to the measure of the surface which separates the two phases.

After this result it has been proved that many other kinds of singular perturbation give the same type of limit. For the case of local singular perturbation see for instance [6].

In the case of nonlocal singular perturbation the first result is due to Alberti, Bouchitté and Seppecher. In [4] they consider the following 1-dimensional functional

$$\varepsilon \iint_{I\times I} \left| \frac{u(x)-u(y)}{x-y} \right|^2 dxdy + \lambda_\varepsilon \int_I W(u)\,dx, \tag{1.2}$$

where $\varepsilon \log \lambda_\varepsilon \to k \in (0,+\infty)$. Again the limit is defined in $BV(I,\{\alpha,\beta\})$ and is given by

$$F(u) = 2k(\beta-\alpha)^2 \mathcal{H}^0(Su), \quad u \in BV(I,\{\alpha,\beta\}),$$

where the jump set Su is the complement of the set of Lebesgue points of u and $\mathcal{H}^0$ denotes the measure that counts points.

Other kinds of similar nonlocal phase transition problems in the case of both singular and regular kernels can be found in [2], [3], [5], [12] and [13].

The main difference between the nonlocal energy with singular kernel (1.2) and the classical Modica-Mortola functional (1.1) is the optimal profile problem that approximately describes the shape of the optimal transitions. In fact, the asymptotical behavior of (1.1) is characterized by the equipartition of the energy between the two terms in the functional and by a scaling property which provides an optimal profile problem that determines the constant c_W in the limit. Instead, the logarithmic natural scaling for functional (1.2) produces no equipartition of the energy, the limit comes only from the nonlocal part of the energy, it does not depend on W, and any profile is optimal as far as the transition occurs on a layer of order ε.

In this paper, we study the following nonlocal singularly perturbed energy

$$G_\varepsilon(u) := \varepsilon^{p-2} \iint_{I\times I} \left| \frac{u(x)-u(y)}{x-y} \right|^p dxdy + \frac{1}{\varepsilon} \int_I W(u)\,dx,$$

where W is the usual two well potential, with wells at α and β, and $p > 2$; ε^{p-2} being the natural scaling.

In contrast with what happens in the case of energy (1.2) (with $p = 2$) here the functional satisfies a useful scaling property and hence the limit is characterized by an optimal profile problem; i.e., G_ε Γ-converges to $\gamma_p \mathcal{H}^0(S_u)$, where γ_p is given by

$$\gamma_p := \inf \left\{ \iint_{\mathbb{R}\times\mathbb{R}} \left| \frac{v(x)-v(y)}{x-y} \right|^p dxdy + \int_{\mathbb{R}} W(v)\,dx : v \in W^{1-\frac{1}{p},p}_{\mathrm{loc}}(\mathbb{R}), \right.$$
$$\left. \lim_{x\to-\infty} v(x) = \alpha, \ \lim_{x\to+\infty} v(x) = \beta \right\}. \tag{1.3}$$

In this respect the case $p = 2$ represents the critical case in the context of this type of nonlocal singular perturbations.

A similar dichotomy occurs in the case of Ginzburg-Landau problems (see for instance Alberti, Baldo and Orlandi [1] for the case $p = 2$ and Desenzani and Fragalà [10] for the case $p > 2$).

2. The Γ-convergence result

Let $p > 2$ be a real number and W a non-negative continuous function vanishing only at $\alpha, \beta \in \mathbb{R}$ $(0 < \alpha < \beta)$, with growth at least linear at infinity. By I we denote an open bounded interval of $\mathbb{R}$.

For every $\varepsilon > 0$ we consider the functional G_ε defined in the fractional Sobolev space $W^{1-\frac{1}{p},p}(I)$,

$$G_\varepsilon(u) := \varepsilon^{p-2} \iint_{I\times I} \left| \frac{u(x) - u(y)}{x - y} \right|^p dxdy + \frac{1}{\varepsilon} \int_I W(u)\, dx. \tag{2.1}$$

Notice that the first terms of G_ε is the p-power of the semi-norm in $W^{1-\frac{1}{p},p}(I)$.

The asymptotic behavior in term of Γ-convergence of G_ε is described by the functional

$$G(u) := \gamma_p \mathcal{H}^0(Su)\,, \qquad u \in BV(I, \{\alpha, \beta\}), \tag{2.2}$$

where γ_p is given by the optimal profile problem (1.3). (For details about Γ-convergence, introduced by De Giorgi and Franzoni in [9], see for instance [7] and [8].)

The Γ-convergence result is precisely stated in the following theorem.

Theorem 2.1. *Let $G_\varepsilon : W^{1-\frac{1}{p},p}(I) \to \mathbb{R}$ and $G : BV(I, \{\alpha, \beta\}) \to \mathbb{R}$ defined by* (2.1) *and* (2.2).

Then

(i) [Compactness] *Let $(u_\varepsilon) \subset W^{1-\frac{1}{p},p}(I)$ be a sequence such that $G_\varepsilon(u_\varepsilon)$ is bounded. Then (u_ε) is pre-compact in $L^1(I)$ and every cluster point belongs to $BV(I, \{\alpha, \beta\})$.*

(ii) [Lower Bound Inequality] *For every $u \in BV(I, \{\alpha, \beta\})$ and every sequence $(u_\varepsilon) \subset W^{1-\frac{1}{p},p}(I)$ such that $u_\varepsilon \to u$ in $L^1(I)$,*

$$\liminf_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon) \geq G(u).$$

(iii) [Upper Bound Inequality] *For every $u \in BV(I, \{\alpha, \beta\})$ there exists a sequence $(u_\varepsilon) \subset W^{1-\frac{1}{p},p}(I)$ such that $u_\varepsilon \to u$ in $L^1(I)$ and*

$$\limsup_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon) \leq G(u).$$

3. The optimal profile problem

In this section we will study the main features of our functional, namely the scaling property and the optimal profile problem.

It is useful to introduce the *localization* of the functional G_ε. For every open set $J \subseteq I$ and every function $u \in W^{1-\frac{1}{p},p}(J)$ we will denote

$$G_\varepsilon(u,J) := \varepsilon^{p-2} \iint_{J\times J} \left| \frac{u(x)-u(y)}{x-y} \right|^p dxdy + \frac{1}{\varepsilon}\int_J W(u)\,dx.$$

Clearly, $G_\varepsilon(u) = G_\varepsilon(u,I)$, for every $u \in W^{1-\frac{1}{p},p}(I)$.

Given $J \subseteq I$ and $u \in W^{1-\frac{1}{p},p}(J)$ we set $u^{(\varepsilon)}(x) := u(\varepsilon x)$ and $J/\varepsilon := \{x : \varepsilon x \in J\}$. By scaling it is immediately seen that

$$G_\varepsilon(u,J) = G_1(u^{(\varepsilon)}, J/\varepsilon). \tag{3.1}$$

In view of this scaling property it is now natural to consider the following *optimal profile* problem

$$\gamma_p := \inf\left\{ G_1(v,\mathbb{R}) : v \in W^{1-\frac{1}{p},p}_{\mathrm{loc}}(\mathbb{R}),\ \lim_{x\to-\infty} v(x) = \alpha,\ \lim_{x\to+\infty} v(x) = \beta \right\}. \tag{3.2}$$

The constant γ_p represents the minimal cost in the term of the non-scaled energy G_1 for a transition from α to β on the whole real line. By (3.1) γ_p will also give the cost of one jump from α to β.

Using a monotone rearrangement argument, we will prove that the infimum in (3.2) is not trivial and is achieved.

For every $u \in W^{1-\frac{1}{p},p}(J)$, with $J = (a,b)$, the non-decreasing rearrangement u^* of u in J, defined by

$$u^*(a+x) := \sup\{\lambda : |\{t \in (a,b) : u(t) < \lambda\}| \le x\}, \quad \forall x \in (0, b-a), \tag{3.3}$$

satisfies

$$\iint_{J\times J} \left| \frac{u^*(x)-u^*(y)}{x-y} \right|^p dxdy \le \iint_{J\times J} \left| \frac{u(x)-u(y)}{x-y} \right|^p dxdy \tag{3.4}$$

(see for instance [11], Theorem I.1).

Note that, since $\displaystyle\int_J W(u^*)dx = \int_J W(u)dx$, from (3.4) we get

$$G_\varepsilon(u^*,J) \le G_\varepsilon(u,J).$$

This rearrangement result will be also used in the sequel to prove the compactness and the lower bound.

We are now in a position to prove the following proposition.

Proposition 3.1. *The constant γ_p is strictly positive.*

Proof. Fix $\delta > 0$ and fix $v \in W^{1-\frac{1}{p},p}_{\rm loc}(\mathbb{R})$ such that $\lim_{x\to-\infty} v(x) = \alpha$, $\lim_{x\to+\infty} v(x) = \beta$ and $G_1(v,\mathbb{R}) < +\infty$. Let us define

$$I_\alpha := \{x \in \mathbb{R} : v(x) \le \alpha + \delta\} \quad \text{and} \quad I_\beta := \{x \in \mathbb{R} : v(x) \ge \beta - \delta\}\ .$$

Denote by $J_\delta := \mathbb{R} \setminus (I_\alpha \cup I_\beta)$; we notice that, by the asymptotic behavior of v, I_α, I_β and J_δ are not empty and J_δ is bounded, for every fixed $\delta \in (0, (\beta-\alpha)/2)$.

Now, let us consider the truncated function

$$v_\delta(x) := (v(x) \vee (\alpha+\delta)) \wedge (\beta - \delta) \quad \text{for every } x \in \mathbb{R}.$$

It is easy to see that the nonlocal energy decreases under truncation and then it follows that

$$\begin{aligned} G_1(v,\mathbb{R}) &\ge \iint_{\mathbb{R}\times\mathbb{R}} \left|\frac{v_\delta(x)-v_\delta(y)}{x-y}\right|^p dxdy + \int_{\mathbb{R}} W(v)\,dx \\ &\ge \iint_{\mathbb{R}\times\mathbb{R}} \left|\frac{v_\delta(x)-v_\delta(y)}{x-y}\right|^p dxdy + m_\delta |J_\delta|, \end{aligned} \tag{3.5}$$

where

$$m_\delta := \min_{s\in[\alpha+\delta,\beta-\delta]} W(s).$$

Let us define

$$x_\alpha := \min\{x : v(x) > \alpha+\delta\} \quad \text{and} \quad x_\beta := \max\{x : v(x) < \beta-\delta\};$$

since $v_\delta(x) = \alpha+\delta$ for every $x < x_\alpha$ and $v_\delta(x) = \beta-\delta$ for every $x > x_\beta$, for any interval $J \supset [x_\alpha, x_\beta]$ the non-decreasing rearrangement v^*_δ of v_δ in J defined by (3.1) does not depend on J and by (3.4) we have

$$\iint_{\mathbb{R}\times\mathbb{R}} \left|\frac{v_\delta(x)-v_\delta(y)}{x-y}\right|^p dxdy \ge \iint_{J\times J} \left|\frac{v^*_\delta(x)-v^*_\delta(y)}{x-y}\right|^p dxdy$$

and hence

$$\begin{aligned} \iint_{\mathbb{R}\times\mathbb{R}} \left|\frac{v_\delta(x)-v_\delta(y)}{x-y}\right|^p dxdy &\ge \iint_{\mathbb{R}\times\mathbb{R}} \left|\frac{v^*_\delta(x)-v^*_\delta(y)}{x-y}\right|^p dxdy \\ &\ge \int_{-\infty}^{x^*_\alpha}\int_{x^*_\beta}^{+\infty} \left|\frac{v^*_\delta(x)-v^*_\delta(y)}{x-y}\right|^p dxdy, \end{aligned} \tag{3.6}$$

where $x^*_\alpha := \sup\{x : v^*_\delta(x) = \alpha+\delta\}$ and $x^*_\beta := \inf\{x : v^*_\delta(x) = \beta-\delta\}$.

By (3.5) and (3.6), it follows that

$$\begin{aligned} G_1(v,\mathbb{R}) &\ge (\beta-\alpha-2\delta)^p \int_{-\infty}^{x^*_\alpha}\int_{x^*_\beta}^{+\infty} \frac{dxdy}{|x-y|^p} + m_\delta |J_\delta| \\ &= \frac{(\beta-\alpha-2\delta)^p}{(p-1)(p-2)|J_\delta|^{p-2}} + m_\delta |J_\delta|. \end{aligned}$$

Finally, minimizing with respect to $|J_\delta|$, we obtain

$$G_1(v,\mathbb{R}) \geq \frac{(p-1)^{\frac{p-2}{p-1}}}{(p-2)}(\beta-\alpha-2\delta)^{\frac{p}{p-1}} m_\delta^{\frac{p-2}{p-1}} > 0$$

and, by the arbitrariness of v, the proof is complete. □

In order to prove the upper bound it is convenient to introduce an auxiliary optimal profile problem. For every $T>0$, we consider

$$\gamma_p^T := \inf\left\{ G_1(v,\mathbb{R}) : v \in W^{1-\frac{1}{p},p}_{\mathrm{loc}}(\mathbb{R}), v(x)=\alpha \ \forall x \leq -T, v(x)=\beta \ \forall x \geq T \right\}. \tag{3.7}$$

By the compactness of the embedding of $W^{1-\frac{1}{p},p}((-2T,2T))$ in $L^p((-2T,2T))$, it is easy to prove that the minimum in (3.7) is achieved. By truncation and rearrangement it also follows that the minimum can be achieved by a function $\varphi^T \in W^{1-\frac{1}{p},p}_{\mathrm{loc}}(\mathbb{R})$ which is non-decreasing and satisfies $\alpha \leq \varphi^T \leq \beta$.

Proposition 3.2. *The sequence γ_p^T is non-increasing in T and $\lim_{T\to+\infty} \gamma_p^T = \gamma_p$.*

Proof. By the definition of γ_p^T, it immediately follows that γ_p^T is monotone and is greater than or equal to γ_p. Hence, the limit exists and satisfies

$$\lim_{T\to+\infty} \gamma_p^T \geq \gamma_p.$$

It remains to prove the reverse inequality. For every $\mu>0$, let us fix $\psi \in W^{1-\frac{1}{p},p}_{\mathrm{loc}}(\mathbb{R})$ such that

$$\lim_{x\to-\infty} \psi(x) = \alpha, \quad \lim_{x\to+\infty} \psi(x) = \beta \quad \text{and} \quad G_1(\psi,\mathbb{R}) \leq \gamma_p + \mu.$$

Moreover, by truncation we may always assume that $\alpha \leq \psi \leq \beta$.

The idea is to modify ψ in order to construct a function φ which is a good competitor for γ_p^T. To this aim we consider

$$\Psi(x) := \int_{\mathbb{R}} \left| \frac{\psi(x)-\psi(y)}{x-y} \right|^p dy.$$

Since $\Psi \in L^1(\mathbb{R})$ we can choose a sequence $\{T_n\}_{n\in\mathbb{N}}$, with $T_n \to +\infty$, such that

$$\Psi(-T_n) \to 0 \quad \text{and} \quad \Psi(T_n) \to 0 \quad \text{as } n \to +\infty.$$

For every $\delta>0$, due to the asymptotic behavior of ψ, we can find $n_\delta \in \mathbb{N}$ such that

$$\psi(-T_n) \leq \alpha+\delta \quad \text{and} \quad \psi(T_n) \geq \beta-\delta, \quad \forall n \geq n_\delta. \tag{3.8}$$

For every $M>0$, we define a function φ which coincides with ψ in $[-T_n,T_n]$, satisfies $\varphi(x)=\alpha$ if $x<-T_n-M$ and $\varphi(x)=\beta$ if $x>T_n+M$ and it is affine in

$(-T_n - M, -T_n)$ and $(T_n, T_n + M)$. Namely,

$$\varphi(x) := \begin{cases} \alpha & \text{if } x \in (-\infty, -T_n - M], \\ \dfrac{\psi(-T_n) - \alpha}{M}(x + T_n) + \psi(-T_n) & \text{if } x \in (-T_n - M, -T_n), \\ \psi(x) & \text{if } x \in [-T_n, T_n], \\ \dfrac{\beta - \psi(T_n)}{M}(x - T_n) + \psi(T_n) & \text{if } x \in (T_n, T_n + M), \\ \beta & \text{if } x \in [T_n + M, +\infty). \end{cases}$$

Clearly, φ is a good competitor for $\gamma_p^{T_n+M}$. Let us compute its energy, denoting $J_n := (-T_n, T_n)$,

$$\begin{aligned} \gamma_p^{T_n+M} &\leq G_1(\varphi, \mathbb{R}) \\ &= G_1(\psi, J_n) + G_1(\varphi, \mathbb{R} \setminus J_n) + 2\iint_{(\mathbb{R}\setminus J_n)\times J_n} \left|\frac{\varphi(x) - \varphi(y)}{x - y}\right|^p dxdy \\ &\leq \gamma_p + \mu + \iint_{(\mathbb{R}\setminus J_n)\times(\mathbb{R}\setminus J_n)} \left|\frac{\varphi(x) - \varphi(y)}{x - y}\right|^p dxdy + \int_{\mathbb{R}\setminus J_n} W(\varphi)\, dx \\ &\quad + 2\iint_{(\mathbb{R}\setminus J_n)\times J_n} \left|\frac{\varphi(x) - \varphi(y)}{x - y}\right|^p dxdy \\ &= \gamma_p + \mu + I_1 + I_2 + I_3. \end{aligned} \tag{3.9}$$

The first two integrals in the right-hand side of (3.9) can be easily estimated as follows

$$\begin{aligned} I_1 &:= \iint_{(\mathbb{R}\setminus J_n)\times(\mathbb{R}\setminus J_n)} \left|\frac{\varphi(x) - \varphi(y)}{x - y}\right|^p dxdy \\ &\leq (\beta - \alpha)^p \int_{-\infty}^{-T_n} \int_{T_n}^{+\infty} \frac{dxdy}{|x - y|^p} \\ &= \frac{(\beta - \alpha)^p}{(p-1)(p-2)(2T_n)^{p-2}} \end{aligned}$$

and

$$I_2 := \int_{\mathbb{R}/J_n} W(\varphi)\, dx \leq 2M\omega_\delta,$$

where

$$\omega_\delta := \max_{s\in[\alpha,\alpha+\delta]\cup[\beta-\delta,\beta]} W(s). \tag{3.10}$$

Instead, an upper bound for the last integral requires more attention in computation. Let us show it in details.

$$I_3 := 2\int_{-\infty}^{-T_n-M}\int_{-T_n}^{T_n}\left|\frac{\varphi(x)-\varphi(y)}{x-y}\right|^p dxdy + 2\int_{-T_n-M}^{-T_n}\int_{-T_n}^{T_n}\left|\frac{\varphi(x)-\varphi(y)}{x-y}\right|^p dxdy$$
$$+2\int_{T_n+M}^{+\infty}\int_{-T_n}^{T_n}\left|\frac{\varphi(x)-\varphi(y)}{x-y}\right|^p dxdy + 2\int_{T_n}^{T_n+M}\int_{-T_n}^{T_n}\left|\frac{\varphi(x)-\varphi(y)}{x-y}\right|^p dxdy.$$

We have

$$\begin{aligned}2\int_{-\infty}^{-T_n-M}\int_{-T_n}^{T_n}\left|\frac{\varphi(x)-\varphi(y)}{x-y}\right|^p dxdy &= 2\int_{-\infty}^{-T_n-M}\int_{-T_n}^{T_n}\left|\frac{\psi(y)-\alpha}{x-y}\right|^p dxdy\\ &\le 2(\beta-\alpha)^p\int_{-\infty}^{-T_n-M}\int_{-T_n}^{T_n}\frac{dxdy}{|x-y|^p}\\ &= \frac{2(\beta-\alpha)^p}{(p-1)(p-2)M^{p-2}}.\end{aligned}$$

Moreover

$$\begin{aligned}&2\int_{-T_n-M}^{-T_n}\int_{-T_n}^{T_n}\left|\frac{\varphi(x)-\varphi(y)}{x-y}\right|^p dxdy\\ &= 2\int_{-T_n-M}^{-T_n}\int_{-T_n}^{T_n}\frac{\left|\psi(y)-\psi(-T_n)-\frac{\psi(-T_n)-\alpha}{M}(x+T_n)\right|^p}{|x-y|^p}\,dxdy\\ &\le 2^p\int_{-T_n-M}^{-T_n}\Psi(-T_n)dx + 2^p\frac{|\psi(-T_n)-\alpha|^p}{M^p}\int_{-T_n-M}^{-T_n}\int_{-T_n}^{T_n}\left|\frac{x+T_n}{x-y}\right|^p dxdy\\ &\le 2^pM\Psi(-T_n)+\frac{2^{p-1}\delta^p}{(p-1)M^{p-2}},\quad \forall n\ge n_\delta\,,\end{aligned}$$

where we used that

$$\begin{aligned}\int_{-T_n-M}^{-T_n}\int_{-T_n}^{T_n}\frac{|x+T_n|^p}{|x-y|^p}dxdy &= \frac{1}{p-1}\int_{-T_n-M}^{-T_n}\left(|x+T_n|-\frac{|x+T_n|^p}{|T_n-x|^{p-2}}\right)dx\\ &\le \frac{M^2}{2(p-1)}.\end{aligned}$$

Similarly, we can estimate the third and the fourth integrals of I_3 and we get

$$I_3 \le 2^pM(\Psi(-T_n)+\Psi(T_n))+\frac{2^p\delta^p}{(p-1)M^{p-2}}+\frac{4(\beta-\alpha)^p}{(p-1)(p-2)M^{p-2}}.$$

Finally, by (3.9), we obtain

$$\gamma_p^{T_n+M}\le\gamma_p+\mu+r_n+r_\delta+\frac{4(\beta-\alpha)^p}{(p-1)(p-2)M^{p-2}},\quad \forall n\ge n_\delta, \tag{3.11}$$

where

$$r_n := \frac{2(\beta-\alpha)^p}{(p-1)(p-2)(2T_n)^{p-2}} + 2^p M\left(\Psi(-T_n)+\Psi(T_n)\right)$$

and

$$r_\delta := \frac{2^p}{(p-1)M^{p-2}}\delta^p + 2M\omega_\delta.$$

Taking the limit as $n \to +\infty$ and then $\delta \to 0$ and $M \to +\infty$, we get

$$\lim_{T\to+\infty} \gamma_p^T = \lim_{n\to+\infty} \gamma_p^{T_n+M} \le \gamma_p + \mu,$$

which concludes the proof by the arbitrariness of μ. □

Let us conclude this section with the proof of the existence of an *optimal profile*.

Proposition 3.3. *The minimum for γ_p defined by* (3.2) *is achieved by a non-decreasing function φ satisfying $\alpha \le \varphi \le \beta$.*

Proof. Let $T > 0$ and let φ^T be a non-decreasing minimizer for γ_p^T. Since the functions φ^T are monotone and bounded, by Helly's theorem, there exist a subsequence φ^{T_k} of φ^T and a non-decreasing function φ, bounded by α and β, such that φ^{T_k} converges pointwise in $\mathbb{R}$ to φ. By Fatou's lemma and Proposition 3.2 we also have

$$\iint_{\mathbb{R}\times\mathbb{R}} \left|\frac{\varphi(x)-\varphi(y)}{x-y}\right|^p dxdy + \int_{\mathbb{R}} W(\varphi)\,dx \le \lim_{k\to\infty} \gamma_p^{T_k} = \gamma_p\,.$$

This implies that φ is a minimizer for γ_p. □

4. Compactness

The proof of the compactness follows the lines of the proof of Alberti, Bouchitté and Seppecher in [4] and uses the following lemma which gives a (non-optimal) lower bound for G_ε.

Lemma 4.1. *Let $(u_\varepsilon) \subset W^{1-\frac{1}{p},p}(I)$ and let $J \subset I$ be an open interval. For every δ such that $0 < \delta < (\beta-\alpha)/2$, let us define*

$$A_\varepsilon := \{x \in I : u_\varepsilon(x) \le \alpha+\delta\} \quad \text{and} \quad B_\varepsilon := \{x \in I : u_\varepsilon(x) \ge \beta-\delta\}.$$

Let us set

$$a_\varepsilon := \frac{|A_\varepsilon \cap J|}{|J|} \quad \text{and} \quad b_\varepsilon := \frac{|B_\varepsilon \cap J|}{|J|}. \tag{4.1}$$

Then

$$G_\varepsilon(u_\varepsilon, J) \ge \left(\frac{2(\beta-\alpha-2\delta)^p}{(p-1)(p-2)|J|^{p-2}}\left(1-\frac{1}{(1-a_\varepsilon)^{p-2}}-\frac{1}{(1-b_\varepsilon)^{p-2}}\right)\right)\varepsilon^{p-2} + c_\delta, \tag{4.2}$$

where c_δ does not depend on ε.

Proof. Let $x_0, y_0 \in \mathbb{R}$ be such that $J = (x_0, y_0)$; we obtain

$$\begin{aligned} G_\varepsilon(u_\varepsilon, J) &\geq G_\varepsilon(u_\varepsilon^*, J) \\ &\geq 2\varepsilon^{p-2}(\beta-\alpha-2\delta)^p \int_{x_0}^{x_0+a_\varepsilon|J|}\int_{y_0-b_\varepsilon|J|}^{y_0} \frac{dxdy}{|x-y|^p} + \frac{1}{\varepsilon} m_\delta |J|(1-a_\varepsilon-b_\varepsilon) \\ &= \frac{2\varepsilon^{p-2}(\beta-\alpha-2\delta)^p}{(p-1)(p-2)|J|^{p-2}} \left(1 - \frac{1}{(1-a_\varepsilon)^{p-2}} - \frac{1}{(1-b_\varepsilon)^{p-2}} + \frac{1}{(1-a_\varepsilon-b_\varepsilon)^{p-2}}\right) \\ &\quad + \frac{1}{\varepsilon} m_\delta |J|(1-a_\varepsilon-b_\varepsilon), \end{aligned}$$

where u_ε^* denote the non-decreasing rearrangement of u_ε in (x_0, y_0) defined by (3.3) and $m_\delta := \min\{W(s) : \alpha+\delta \leq s \leq \beta-\delta\}$.

Minimizing with respect to $|J|(1-a_\varepsilon-b_\varepsilon)$, we get

$$\begin{aligned} G_\varepsilon(u_\varepsilon, J) \;\geq\; & \varepsilon^{p-2}\left(\frac{2(\beta-\alpha-2\delta)^p}{(p-1)(p-2)|J|^{p-2}}\left(1 - \frac{1}{(1-a_\varepsilon)^{p-2}} - \frac{1}{(1-b_\varepsilon)^{p-2}}\right)\right) \\ & + 2^{\frac{1}{p-1}} \frac{(p-1)^{\frac{p-2}{p-1}}}{p-2} (\beta-\alpha-2\delta)^{\frac{p}{p-1}} m_\delta^{\frac{p-2}{p-1}}, \end{aligned}$$

for every $0 < \delta < (\beta-\alpha)/2$, and hence (4.2) is proved. □

We are now in a position to prove the compactness result (i.e., Theorem 2.1, (i)).

Let $(u_\varepsilon) \subset W^{1-\frac{1}{p},p}(I)$ be a sequence with equi-bounded energy; i.e., a sequence satisfying $\sup_{\varepsilon>0} G_\varepsilon(u_\varepsilon, I) \leq C$. In particular

$$\int_I W(u_\varepsilon)\, dx \leq C\varepsilon$$

and this implies that

$$W(u_\varepsilon) \to 0 \text{ in } L^1(I). \tag{4.3}$$

Thanks to the growth assumption on W, (u_ε) is weakly relatively compact in $L^1(I)$; i.e., there exists $u \in L^1(I)$ such that (up to a subsequences) $u_\varepsilon \rightharpoonup u$ in $L^1(I)$. We have to prove that this convergence is strong in $L^1(I)$ and that $u \in BV(I, \{\alpha, \beta\})$. Let ν_x be the Young measure associated to (u_ε). Since $W \geq 0$, we have

$$\int_I \int_{\mathbb{R}} W(t)\, d\nu_x(t) \leq \liminf_{\varepsilon\to 0} \int_I W(u_\varepsilon)\, dx$$

(see for instance [16], Theorem 16). Hence, by (4.3), it follows that

$$\int_{\mathbb{R}} W(t)\, d\nu_x(t) = 0, \quad \text{a.e. } x \in I,$$

which implies the existence of a function θ on $[0,1]$ such that

$$\nu_x(dt) = \theta(x)\delta_\alpha(dt) + (1-\theta(x))\delta_\beta(dt)\,, \quad x \in I$$

and

$$u(x) = \theta(x)\alpha + (1 - \theta(x))\beta\,, \quad x \in I.$$

It remains to prove that θ belongs to $BV(I, \{0,1\})$. Let us consider the set S of the points where the approximate limits of θ is neither 0 nor 1. For every $N \leq \mathcal{H}^0(S)$ we can find N disjoint intervals $\{J_n\}_{n=1,\dots,N}$ such that $J_n \cap S \neq \emptyset$ and such that the quantities a_ε^n and b_ε^n, defined by (4.1) replacing J by J_n, satisfy

$$a_\varepsilon^n \to a^n \in (0,1) \quad \text{and} \quad b_\varepsilon^n \to b^n \in (0,1) \quad \text{as } \varepsilon \text{ goes to zero.}$$

We can now apply Lemma 4.1 in the interval J_n and, taking the limit as $\varepsilon \to 0$ in the inequality (4.2), we obtain

$$\liminf_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon, J_n) \geq c_\delta.$$

Finally, we use the sub-additivity of $G_\varepsilon(u,\cdot)$ and we get

$$\liminf_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon, I) \geq \sum_{n=1}^{N} \liminf G_\varepsilon(u_\varepsilon, J_n) \geq N c_\delta. \tag{4.4}$$

Since (u_ε) has equi-bounded energy, this implies that S is a finite set. Hence, $\theta \in BV(I, \{0,1\})$ and the proof of the compactness for G_ε is complete.

5. Lower bound inequality

In this section, we prove the Γ-liminf inequality. An optimal lower bound for $G_\varepsilon(u_\varepsilon)$ is a consequence of the following proposition.

Proposition 5.1. *Let J be an open interval of $\mathbb{R}$. Let (u_ε) be a non-decreasing sequence in $W^{1-\frac{1}{p},p}(J)$ and assume that there exist $\bar{a}, \bar{b} \in J$, $\bar{a} < \bar{b}$, such that for every $\delta > 0$ there exists ε_δ such that*

$$u_\varepsilon(\bar{a}) \leq \alpha + \delta \quad \textit{and} \quad u_\varepsilon(\bar{b}) \geq \beta - \delta \quad \forall \varepsilon \leq \varepsilon_\delta.$$

Then

$$\liminf_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon, J) \geq \gamma_p.$$

Proof. Let $J = (a,b)$. It is clearly enough to consider the case

$$\liminf_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon, (a,b)) < +\infty.$$

By a truncation argument, without loss of generality, we may also assume that

$$\alpha \leq u_\varepsilon(x) \leq \beta, \quad \forall x \in (a,b).$$

Let us define

$$U_\varepsilon(x) := \int_a^b \left| \frac{u_\varepsilon(x) - u_\varepsilon(y)}{x - y} \right|^p dy.$$

By the fact that

$$\liminf_{\varepsilon\to 0} \int_a^b U_\varepsilon(x)\, dx$$

is finite, we get that there exist $\tilde{x} \in (a, \bar{a})$ and $\tilde{y} \in (\bar{b}, b)$ such that

$$\liminf_{\varepsilon \to 0} U_\varepsilon(\tilde{x}) \leq C \quad \text{and} \quad \liminf_{\varepsilon \to 0} U_\varepsilon(\tilde{y}) \leq C \quad \text{for some } C > 0. \tag{5.1}$$

Fix $M > 0$. We now extend u_ε in the whole $\mathbb{R}$ as follows

$$\tilde{u}_\epsilon(x) := \begin{cases} \alpha & \text{if } x \in (-\infty, \tilde{x} - M\varepsilon), \\ \dfrac{u_\varepsilon(\tilde{x}) - \alpha}{M\varepsilon}(x - \tilde{x}) + u_\varepsilon(\tilde{x}) & \text{if } x \in [\tilde{x} - M\varepsilon, \tilde{x}], \\ u_\varepsilon(x) & \text{if } x \in (\tilde{x}, \tilde{y}), \\ \dfrac{\beta - u_\varepsilon(\tilde{y})}{M\varepsilon}(x - \tilde{y}) + u_\varepsilon(\tilde{y}) & \text{if } x \in [\tilde{y}, \tilde{y} + M\varepsilon], \\ \beta & \text{if } x \in (\tilde{y} + M\varepsilon, +\infty). \end{cases}$$

Denote $\tilde{J} := (\tilde{x}, \tilde{y}) \subseteq (a, b)$. We have

$$\begin{aligned} G_\varepsilon(u_\varepsilon, \tilde{J}) &\geq \gamma_p - G_\varepsilon(\tilde{u}_\epsilon, \mathbb{R} \setminus \tilde{J}) - 2\varepsilon^{p-2} \iint_{(\mathbb{R}\setminus\tilde{J})\times\tilde{J}} \left| \frac{\tilde{u}_\epsilon(x) - \tilde{u}_\epsilon(y)}{x - y} \right|^p dxdy \\ &= \gamma_p - \varepsilon^{p-2} \iint_{(\mathbb{R}\setminus\tilde{J})\times(\mathbb{R}\setminus\tilde{J})} \left| \frac{\tilde{u}_\epsilon(x) - \tilde{u}_\epsilon(y)}{x - y} \right|^p dxdy - \frac{1}{\varepsilon} \int_{\mathbb{R}\setminus\tilde{J}} W(\tilde{u}_\epsilon)\, dx \\ &\quad -2\varepsilon^{p-2} \iint_{(\mathbb{R}\setminus\tilde{J})\times\tilde{J}} \left| \frac{\tilde{u}_\epsilon(x) - \tilde{u}_\epsilon(y)}{x - y} \right|^p dxdy \\ &= \gamma_p - I_1 - I_2 - I_3. \end{aligned} \tag{5.2}$$

Using the definition of $\tilde{u}_\epsilon$, we easily get

$$\begin{aligned} I_1 &:= \varepsilon^{p-2} \iint_{(\mathbb{R}\setminus\tilde{J})\times(\mathbb{R}\setminus\tilde{J})} \left| \frac{\tilde{u}_\epsilon(x) - \tilde{u}_\epsilon(y)}{x - y} \right|^p dxdy \\ &\leq \varepsilon^{p-2}(\beta - \alpha)^p \iint_{(\mathbb{R}\setminus\tilde{J})\times(\mathbb{R}\setminus\tilde{J})} \frac{dxdy}{|x - y|^p} \\ &= \frac{(\beta - \alpha)^p}{(p-1)(p-2)|\tilde{J}|^{p-2}} \varepsilon^{p-2}. \end{aligned}$$

Moreover, since u_ε is non-decreasing,

$$u_\varepsilon(x) \leq \alpha + \delta \quad \forall\, x \leq \bar{a} \quad \text{and} \quad u_\varepsilon(x) \geq \beta - \delta \quad \forall\, x \geq \bar{b}$$

and, in particular,

$$I_2 := \frac{1}{\varepsilon} \int_{\mathbb{R}\setminus\tilde{J}} W(\tilde{u}_\epsilon)\, dx \leq 2M\omega_\delta,$$

where ω_δ is defined in (3.10).

Finally, using the fact that $u_\varepsilon(\tilde{x}) \le \alpha + \delta$ and $u_\varepsilon(\tilde{y}) \ge \beta - \delta$, we can estimate the third integral

$$I_3 := 2\varepsilon^{p-2}\iint_{(\mathbb{R}\setminus\tilde{J})\times\tilde{J}} \left|\frac{\tilde{u}_\epsilon(x)-\tilde{u}_\epsilon(y)}{x-y}\right|^p dxdy = 2\varepsilon^{p-2}\int_{-\infty}^{\tilde{x}-M\varepsilon}\int_{\tilde{x}}^{\tilde{y}} \left|\frac{\tilde{u}_\epsilon(x)-\tilde{u}_\epsilon(y)}{x-y}\right|^p dxdy$$
$$+2\varepsilon^{p-2}\int_{\tilde{x}-M\varepsilon}^{\tilde{x}}\int_{\tilde{x}}^{\tilde{y}} \left|\frac{\tilde{u}_\epsilon(x)-\tilde{u}_\epsilon(y)}{x-y}\right|^p dxdy + 2\varepsilon^{p-2}\int_{\tilde{y}+M\varepsilon}^{+\infty}\int_{\tilde{x}}^{\tilde{y}} \left|\frac{\tilde{u}_\epsilon(x)-\tilde{u}_\epsilon(y)}{x-y}\right|^p dxdy$$
$$+2\varepsilon^{p-2}\int_{\tilde{y}}^{\tilde{y}+M\varepsilon}\int_{\tilde{x}}^{\tilde{y}} \left|\frac{\tilde{u}_\epsilon(x)-\tilde{u}_\epsilon(y)}{x-y}\right|^p dxdy. \tag{5.3}$$

We have

$$\begin{aligned} 2\varepsilon^{p-2}\int_{-\infty}^{\tilde{x}-M\varepsilon}\int_{\tilde{x}}^{\tilde{y}} \left|\frac{\tilde{u}_\epsilon(x)-\tilde{u}_\epsilon(y)}{x-y}\right|^p dxdy &\le 2\varepsilon^{p-2}(\beta-\alpha)^p\int_{-\infty}^{\tilde{x}-M\varepsilon}\int_{\tilde{x}}^{\tilde{y}} \frac{dxdy}{|x-y|^p} \\ &\le \frac{2(\beta-\alpha)^p}{(p-1)(p-2)M^{p-2}}. \end{aligned}$$

Moreover,

$$\begin{aligned} &2\varepsilon^{p-2}\int_{\tilde{x}-M\varepsilon}^{\tilde{x}}\int_{\tilde{x}}^{\tilde{y}} \left|\frac{\tilde{u}_\epsilon(x)-\tilde{u}_\epsilon(y)}{x-y}\right|^p dxdy \\ &\quad= 2\varepsilon^{p-2}\int_{\tilde{x}-M\varepsilon}^{\tilde{x}}\int_{\tilde{x}}^{\tilde{y}} \frac{|u_\varepsilon(y)-u_\varepsilon(\tilde{x})-\frac{u_\varepsilon(\tilde{x})-\alpha}{M\varepsilon}(x-\tilde{x})|^p}{|x-y|^p} dxdy \\ &\quad\le 2^p\varepsilon^{p-2}\int_{\tilde{x}-M\varepsilon}^{\tilde{x}} U_\varepsilon(\tilde{x})dx + 2^p\frac{|u_\varepsilon(\tilde{x})-\alpha|^p}{M^p\varepsilon^2}\int_{\tilde{x}-M\varepsilon}^{\tilde{x}}\int_{\tilde{x}}^{\tilde{y}} \frac{|\tilde{x}-x|^p}{|x-y|^p} dxdy \\ &\quad\le 2^p\varepsilon^{p-1}MU_\varepsilon(\tilde{x}) + \frac{2^{p-1}\delta^p}{(p-1)M^{p-2}}, \quad \forall\ \varepsilon \le \varepsilon_\delta, \end{aligned}$$

where we used that

$$\begin{aligned} \int_{\tilde{x}-M\varepsilon}^{\tilde{x}}\int_{\tilde{x}}^{\tilde{y}} \frac{|\tilde{x}-x|^p}{|x-y|^p} dxdy &= \frac{1}{(p-1)}\int_{\tilde{x}-M\varepsilon}^{\tilde{x}} \left(|x-\tilde{x}| - \frac{|x-\tilde{x}|^p}{|\tilde{y}-x|^{p-1}}\right) dx \\ &\le \frac{(M\varepsilon)^2}{2(p-1)}. \end{aligned}$$

Similarly, we can estimate the third and the fourth integrals of I_3 and we get

$$I_3 \le 2^p M(U_\varepsilon(\tilde{x}) + U_\varepsilon(\tilde{y}))\varepsilon^{p-1} + \frac{2^p\delta^p}{(p-1)M^{p-2}} + \frac{4(\beta-\alpha)^p}{(p-1)(p-2)M^{p-2}}, \quad \forall\ \varepsilon \le \varepsilon_\delta.$$

Hence, by (5.2), we obtain

$$G_\varepsilon(u_\varepsilon,\tilde{J}) \;\geq\; \gamma_p - \left(\frac{(\beta-\alpha)^p}{(p-1)(p-2)|\tilde{J}|^{p-2}} + 2^p M(U_\varepsilon(\tilde{x})+U_\varepsilon(\tilde{y}))\varepsilon\right)\varepsilon^{p-2} - r_\delta$$
$$-\frac{4(\beta-\alpha)^p}{(p-1)(p-2)M^{p-2}}\,, \quad \forall\ \varepsilon\leq\varepsilon_\delta\,,$$

with

$$r_\delta := \frac{2^p\delta^p}{(p-1)M^{p-2}}\delta^p + 2M\omega_\delta$$

vanishing as $\delta\to 0$.Thus, by (5.1) and taking the liminf as $\varepsilon\to 0$ and then as $\delta\to 0$, we get

$$\liminf_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon,\tilde{J}) \geq \gamma_p - \frac{4(\beta-\alpha)^p}{(p-1)(p-2)M^{p-2}},$$

which conclude the proof by the arbitrariness of M. □

Remark 5.2. Clearly an analogue proposition holds in the case of u_ε non-increasing satisfying the hypotheses with $\bar{a}>\bar{b}$.

In order to conclude, let us first observe that, thanks to the compactness result for G_ε, we may assume that the sequence (u_ε) converges in $L^1(I)$ to some $u\in BV(I,\{\alpha,\beta\})$. Hence, the jump set Su is finite and we can find $N:=\mathcal{H}^0(Su)$ disjoint subintervals $\{I_i\}_{i=1,\dots,N}$ such that $Su\cap I_i\neq\emptyset$, for every $i=1,\dots,N$.

Now, let us consider the monotone rearrangement $u^*_{\varepsilon,i}$ of u_ε in I_i. The rearrangement $u^*_{\varepsilon,i}$ is non-decreasing if u is non-decreasing in I_i and non-increasing otherwise. With this choice clearly $u^*_{\varepsilon,i}$ converges to u in $L^1(I_i)$ and thus it satisfies the assumptions of Proposition 5.1 (see also Remark 5.2) with J replaced by I_i. Then, for every $i=1,\dots,N$, we may conclude that

$$\liminf_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon,I_i) \geq \liminf_{\varepsilon\to 0} G_\varepsilon(u^*_{\varepsilon,i},I_i) \geq \gamma_p.$$

Finally, using the sub-additivity of $G_\varepsilon(u_\varepsilon,\cdot)$, we get

$$\liminf_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon,I) \geq \liminf_{\varepsilon\to 0}\sum_{i=1}^N G_\varepsilon(u_\varepsilon,I_i) \geq N\gamma_p = \gamma_p\mathcal{H}^0(Su)$$

and hence the lower bound stated by Theorem 2.1, (ii), is proved. □

6. Upper bound inequality

In this section, we conclude the proof of the Theorem 2.1, proving the limsup inequality. Let us first construct an optimal sequence for u of the form

$$u(x)=\begin{cases}\alpha, & \text{if } x\leq x_0,\\ \beta, & \text{if } x>x_0.\end{cases}$$

Let $T > 0$ be fixed and let $\varphi^T \in W^{1-\frac{1}{p},p}_{\rm loc}(\mathbb{R})$ be the minimizer for γ_p^T defined by (3.7); i.e.,

$$\varphi^T(x) = \alpha \quad \forall\, x \le -T, \quad \varphi^T(x) = \beta \quad \forall\, x \ge T \quad \text{and} \quad G_1(\varphi, \mathbb{R}) = \gamma_p^T.$$

Let us define, for every $\varepsilon > 0, u_\varepsilon(x) := \varphi^T\left(\dfrac{x - x_0}{\varepsilon}\right)$, for every $x \in I$. We have

$$u_\varepsilon \to u \text{ in } L^1(I)$$

and

$$\begin{aligned} G_\varepsilon(u_\varepsilon) &= \varepsilon^{p-2} \iint_{I\times I} \left| \frac{\varphi^T\left(\frac{x-x_0}{\varepsilon}\right) - \varphi^T\left(\frac{y-x_0}{\varepsilon}\right)}{x-y} \right|^p dxdy + \frac{1}{\varepsilon}\int_I W\left(\varphi^T\left(\frac{x-x_0}{\varepsilon}\right)\right) dx \\ &= G_1(\varphi^T, (I-x_0)/\varepsilon) \le G_1(\varphi^T, \mathbb{R}) = \gamma_p^T. \end{aligned} \tag{6.1}$$

By Proposition 3.2 we get

$$\lim_{T\to+\infty} \limsup_{\varepsilon\to 0} G_\varepsilon(u_\varepsilon) \le \gamma_p.$$

Then by a diagonalization argument we can construct a sequence $\tilde{u}_\epsilon$ converging to u in $L^1(I)$, which satisfies

$$\limsup_{\varepsilon\to 0} G_\varepsilon(\tilde{u}_\epsilon) \le \gamma_p.$$

The optimal sequence for an arbitrary $u \in BV(I, \{\alpha, \beta\})$ can be easily obtained gluing the sequences constructed above for each single jump of u and taking into account that, thanks to the scaling ε^{p-2}, the long range interactions between two different recovery sequences decay as $\varepsilon \to 0$.

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Smooth and Creased Equilibria for Elastic-plastic Plates and Beams

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Abstract. We show that minimizers of elastic-plastic energies dependent on jump integrals are smooth provided a smallness condition is fulfilled by the load. We examine also the structure of extremals when this smallness condition is violated.

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1. Introduction

The problem of modelling elastic-plastic plates and beams has been widely studied in the literature ([12], [7], [6]). In last years several results in the derivation of these models by variational limits of thin 3D elastic plastic plates has been achieved in [8], [9], [10]. The resulting functional contains a *volume* term which is responsible of the elastic energy released in the deformation and a *surface* term which represents the cost of formation of free *plastic hinges*: plasticity occurs along free *yield lines* whose location satisfies a variational principle ([8], [9], [10]).
Here we deal with the consistency of these models: in particular it would be quite natural to expect that if external loads are small then solutions have no creases, while it should be possible exhibiting a threshold and a transverse load with total mass above this threshold such that the corresponding solution has at least one plastic hinge.
This fact, at least in the case of beams, is strictly related to the structure of the Green function of the operator d^4/dx^4 and to the best constant in *Poincarè inequality* (see Lemma 3.1). However when load distribution is symmetric with respect to the center of the beam then the solution is always regular provided

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a safe load condition is satisfied, say total mass of load is less than 8 times the yielding constant normalized by the length of the beam.
We can prove that, for generic transverse load acting on elastic-plastic plates or beams, the behavior of the material remains elastic as long as the maximum stress does not exceed a critical value (see Theorem 2.2 and Theorem 3.7) while, beyond this value we can exhibit examples undergoing formation of (no more than two) plastic hinges, at least in the case of beams (see Theorem 4.1). Here we mention only the case of homogeneous Dirichlet boundary conditions; detailed proofs for homogeneous and non homogeneous boundary data are given in [11].

2. Regular minimizers for clamped elastic-plastic plates

Let $\Sigma \subset \mathbb{R}^2$ be an open bounded set with Lipschitz boundary, $\mu > 0, \beta > 0, \gamma > 0$ and $\lambda \in \mathbb{R}$ be given constants such that $3\lambda + 2\mu > 0$ and σ be a finite Radon measure such that $\sigma = f\,dx + \sigma_s$, $\operatorname{spt} f \subset \overline{\Sigma}, \operatorname{spt} \sigma_s \subset\subset \Sigma$.
According to the variational model derived in [9], we study the functional

$$\begin{aligned} \mathcal{P}(w) = \quad & \frac{2}{3}\mu \int_\Sigma (|\nabla^2 w|^2 + \frac{\lambda}{\lambda + 2\mu} |\Delta_a w|^2)\, dx \\ & + \beta\, \mathcal{H}^1(S_{\nabla w}) + \gamma \int_{S_{\nabla w}} \left| \left[\frac{\partial w}{\partial \nu_{\nabla w}} \right] \right| d\mathcal{H}^1 - \int_\Sigma w\, d\sigma \end{aligned} \tag{2.1}$$

to be minimized among scalar functions $w \in SBH(\mathbb{R}^2)$ such that $\operatorname{spt} w \subset \overline{\Sigma}$.

Here $SBH(\mathbb{R}^2)$ is the space of $W^{1,1}(\mathbb{R}^2)$ functions whose Hessian is a (matrix valued) measure without Cantor part and $\mathcal{H}^1$ is the one-dimensional Hausdorff measure. If $w \in SBH(\mathbb{R}^2)$, then $S_{\nabla w}$ denotes the set of jump points of ∇w, $\nu_{\nabla w}$ its normal unit vector, $\nabla^2 w$ denotes the absolutely continuous part of $D^2 w$ and $\Delta_a w$ the absolutely continuous part of Δw, that is $\Delta_a w = \operatorname{Tr} \nabla^2 w$. The total variation in $\mathbb{R}$ of σ will be denoted with $|\sigma|_T$.

We remark explicitly that, in general, a minimizer of $\mathcal{P}$ exists whenever a smallness condition on the total mass of σ is satisfied, namely the following result holds (see [2], [3], [4], [5], [9]):

Theorem 2.1. *Assume that*

$$|\sigma|_T < 4\gamma. \qquad \textbf{(safe load condition)} \tag{2.2}$$

Then $\mathcal{P}$ achieves a finite minimum.

Our analysis shows that when the maximum stress does not exceed a critical value depending on the material, then the behavior of the material itself remains elastic (see [11] for a detailed proof).

Theorem 2.2. *Let u be the unique solution of*

$$u \in H^2(\mathbb{R}^2)\,, \qquad u \equiv 0 \ \textit{in}\ \mathbb{R}^2 \setminus \overline{\Sigma}\,, \qquad \Delta^2 u \ = \ \frac{3(\lambda+2\mu)}{8\mu(\lambda+\mu)}\,\sigma \quad \textit{in}\ \Sigma\,. \tag{2.3}$$

If

$$\left\| D^2 u \ + \ \frac{\lambda}{\lambda+2\mu}\,(\Delta u)\,\mathbb{I} \right\|_{L^\infty(\Sigma)} \ \leq \ \frac{3\gamma}{4\mu} \tag{2.4}$$

then u is the unique minimizer of $\mathcal{P}$.

We notice that standard estimates on the solution of (2.3) show that when $|\sigma|_T$ is sufficiently small then (2.4) is satisfied.

3. The clamped elastic-plastic beam

Analogous properties can be proved for beams; moreover, in dimension one a lot of additional information about creased solution can be stated. We summarize the main results in the present and in the next section, where the following assumptions are always understood: $L > 0\,,\ \beta > 0\,, \gamma > 0$ are given constants and $\sigma = f\,dx + \sigma_s$ is a Radon measure in $\mathbb{R}$ such that $\operatorname{spt} f \subset [0, L]$ and $\operatorname{spt} \sigma_s \subset\subset (0, L)$.
According with the beam model obtained in [8] and [10] we want to minimize the functional

$$\mathcal{F}(w) \ = \ \frac{1}{2}\int_{\mathbb{R}} |\ddot{w}|^2 \ dx - \int_{\mathbb{R}} w\, d\sigma \ + \beta\, \sharp(S_{\dot{w}}) \ + \ \gamma \sum_{S_{\dot{w}}} |[\dot{w}]| \tag{3.1}$$

among scalar functions w such that $w \in SBH(\mathbb{R})$, $\operatorname{spt} w \subset [0, L]$.
Here and in the following: $\sharp$ is the counting measure; if $v \in L^1_{loc}(\mathbb{R})$ then $v', \dot{v}$ denote respectively the distributional derivative of v and its absolutely continuous part; $SBH(\mathbb{R})$ denotes the space of $W^{1,1}(\mathbb{R})$ functions such that $v'' = (v')'$ is a finite Radon measure without Cantor part; for every $v \in SBH(\mathbb{R})$, $\dot{v} \equiv v'$ holds true, $S_{\dot{v}}$ is the set of jump points of $\dot{v}$ and $\ddot{v}$ denotes the absolutely continuous part of $v'' = (\dot{v})'$.

3.1. Existence of minimizers

Analogously to the case of elastic-plastic plates, existence of minimizers of (3.1) depends upon an estimate of the embedding constant: in this special case we have the following sharp result for the optimal embedding constant.

Lemma 3.1. (*Poincaré inequality* [11]) *Let $z \in SBH(\mathbb{R})$ with $\operatorname{spt} z \subset [0, L]$. Then*

$$\|z\|_{L^\infty} \leq \frac{L}{8}|z''|_T$$

and we notice that equality holds when $z(x) = \frac{L}{2} - |x - \frac{L}{2}|$ for $x \in [0, L]$.

Starting from the above Poincaré inequality we can prove that a smallness condition (safe load condition) on $|\sigma|_T$ entails the existence of minimizers.

Lemma 3.2. *Assume that*

$$|\sigma|_T \ < \ \frac{8\,\gamma}{L} \qquad \textbf{(safe load condition)} \tag{3.2}$$

then $\mathcal{F}$ achieves a finite minimum.

Proof. By Lemma 3.1, (3.2) and Young inequality we get

$$\begin{aligned} \left|\int_{\mathbb{R}} w\,d\sigma\right| \ &\le \ \frac{L}{8}|\sigma|_T|w''|_T \le \frac{L}{8}|\sigma|_T \sum_{S_{\dot w}} |[\dot w]| + \gamma\int_0^L |\ddot w|\,dx \le \\ &\le \frac{L}{8}|\sigma|_T \sum_{S_{\dot w}} |[\dot w]| + \frac{1}{4}\int_0^L |\ddot w|^2\,dx + \gamma^2 L \end{aligned} \tag{3.3}$$

for every $w \in SBH(0,L)$ such that $\operatorname{spt} w \subset [0,L]$. Hence

$$\mathcal{F}(w) \ge \frac{1}{4}\int_0^L |\ddot w|^2\,dx + \beta\,\sharp(S_{\dot w}) + \left(\gamma - \frac{L}{8}|\sigma|_T\right)\sum_{S_{\dot w}} |[\dot w]| - \gamma^2 L$$

and existence of minimizers follows by (3.2) with a standard compactness and l.s.c argument (see [1], [3], [4], [8], [9]). □

Evaluation of the first variation of $\mathcal{F}$ yields (see [11]) the following statement.

Theorem 3.3. (*Euler equations*) *Let $w \in argmin\mathcal{F}$. Then*

$$\begin{aligned} &\text{(i)} && (\ddot w)'' = \sigma && \text{in } (0,L) \\ &\text{(ii)} && \ddot w_- = \gamma\,\operatorname{sign}([\dot w]) && \text{in } S_{\dot w} \cap (0,L] \\ &\text{(iii)} && \ddot w_+ = \gamma\,\operatorname{sign}([\dot w]) && \text{in } S_{\dot w} \cap [0,L)\,. \end{aligned}$$

In particular $\ddot w \in BH(0,L)$, hence $\ddot w$ is continuous in $[0,L]$ and $w'''' = \sigma$ in $(0,L) \setminus S_{\dot w}$.
We notice that if $\sigma_s \equiv 0$ then $\dddot w_- \ = \ \dddot w_+$ on the whole $(0,L)$.

Remark 3.4. We notice that if $w \in \operatorname{argmin}\mathcal{F}$ and $S_{\dot w} = \emptyset$, then $w(0) = w(L) = w'(0) = w'(L))$, $\ddot w = w''$ and condition i) of Theorem (3.3) entails $w'''' = \sigma$ in $(0,L)$: hence $w \equiv u$, say it is the solution of (3.4).

Another important consequence of Euler equations is the following statement.

Lemma 3.5. (*Compliance identity*) *Assume that w satisfies conditions* (i), (ii), (iii) *of Theorem* 3.3. *Then*

$$\mathcal{F}(w) \ = \ -\frac{1}{2}\int_0^L |\ddot w|^2\,dx \ + \ \beta\,\sharp\,(S_{\dot w}).$$

Proof. By i) we have $(\ddot{w})'' = \sigma$. By ii) iii) $\ddot{w}$ is continuous in $(0, L)$. By taking into account $\operatorname{spt}\sigma_s \subset\subset (0, L)$, $\operatorname{spt} w \subset [0, L]$ and $w'' = \ddot{w} + \sum_{S_{\dot{w}}} [\dot{w}]\, d\sharp\llcorner S_{\dot{w}}$ we get

$$\int_{\mathbb{R}} w\, d\sigma = \int_0^L w\, d\sigma = \int_0^L (\ddot{w})'' w = -\int_0^L (\ddot{w})' w' = \int_0^L \ddot{w}\, w'' = \int_0^L |\ddot{w}|^2 + \sum_{S_{\dot{w}}} \ddot{w}\, [\dot{w}]\,.$$

Recalling that $\ddot{w} = \gamma \operatorname{sign}[\dot{w}]$

$$\int_0^L w\, d\sigma \;=\; \int_0^L |\ddot{w}|^2\, dx \;+\; \gamma \sum_{S_{\dot{w}}} |[\dot{w}]|$$

and the thesis follows by the definition of $\mathcal{F}$. □

3.2. Green function and regular minimizers

An argument analogous to the one used in the proof of Theorem 1.2 leads to the following theorem about regular minimizers ([11]).

Theorem 3.6. *Let $u \in H^2(\mathbb{R})$, $u \equiv 0$ in $\mathbb{R} \setminus (0, L)$ such that*

$$\begin{cases} u'''' = \sigma \text{ in } (0, L) \\ u(0) = u(L) = u'(0) = u'(L) = 0\,. \end{cases} \tag{3.4}$$

If

$$\|u''\|_{L^\infty(0,L)} \le \gamma \qquad \textbf{(stress regularity condition)}\,, \tag{3.5}$$

then u is the unique minimizer of $\mathcal{F}$.

From now on any solution of (3.4) which is also a minimizer of $\mathcal{F}$ is called a *smooth minimizer* of $\mathcal{F}$.

Let $\mathcal{G}(x, y)$ be the Green function of the operator d^4/dx^4 in $(0, L)$, say

$$\begin{cases} \mathcal{G}_{xxxx}(\cdot\,, y) = \delta_y \;\text{ in } (0, L)\,, \\ \\ \mathcal{G}(0, y) = \mathcal{G}_x(0, y) = \mathcal{G}(L, y) = \mathcal{G}_x(L, y) = 0\,. \end{cases} \tag{3.6}$$

Then the solution of (3.4) is given by

$$u(x) \;=\; \int_0^L \mathcal{G}(x, y)\, d\sigma(y)\,. \tag{3.7}$$

By setting $P_3(y) = L^{-3}\,(3L - 2y)\, y^2$, $P_1(y) = L^{-1} y$, and

$$J_3(x, y) = \begin{cases} P_3(y) & \text{if } 0 \le y \le x \le L, \\ -P_3(L - y) & \text{if } 0 \le x < y \le L, \end{cases} \tag{3.8}$$

$$J_1(x, y) = \begin{cases} P_1(y) & \text{if } 0 \le y \le x \le L, \\ -P_1(L - y) & \text{if } 0 \le x < y \le L, \end{cases} \tag{3.9}$$

we have $J_3(x,\cdot) \in C([0,L]-\{x\})$, moreover $J_3(x,\cdot)$ is a bounded Borel function for every $x \in [0,L]$. Therefore

$$u'''(x) \;=\; \int_0^L J_3(x,y)\, d\sigma(y) \quad \text{for a.e. } x \in [0,L] \tag{3.10}$$

$$u''(x) \;=\; \int_0^L J_1(x,y) \left(\int_0^L J_3(x,\tau)\, d\sigma(\tau) \right) dy \tag{3.11}$$

for every $x \in [0,L]$ and direct calculations show that

$$u''(x) \;=\; \int_0^L K(x,y)\, d\sigma(y) \tag{3.12}$$

where

$$K(x,y) = \frac{1}{2}(2x-L)P_3(y) - \frac{1}{2L}y^2 + (y-x)^+. \tag{3.13}$$

By using (3.12), (3.13) and Hölder inequality we get the following theorem.

Theorem 3.7. *Let u be the unique solution of problem* (3.4)*, then*

$$\|u''\|_{L^\infty} \;\le\; \frac{4L}{27}\; |\sigma|_T. \tag{3.14}$$

Remark 3.8. By considering the special case $\sigma = \delta_{\frac{2L}{3}}$ we get

$$u''(x) = \frac{1}{2}(2x-L)P_3(\frac{2L}{3}) - \frac{2L}{9} + (\frac{2L}{3} - x)^+\,, \tag{3.15}$$

hence, $\sigma = \delta_{\frac{2L}{3}}$ entails the equality in (3.14):

$$\|u''\|_\infty = \frac{4L}{27}. \tag{3.16}$$

Therefore the constant $\dfrac{4L}{27}$ in (3.14) is the best possible.

A straightforward consequence of Theorems 3.7 and 3.6 is the following statement.

Theorem 3.9. *If*

$$|\sigma|_T \le\; \frac{27\,\gamma}{4\,L} \qquad \textbf{(load regularity condition)} \tag{3.17}$$

then u is a smooth minimizer of $\mathcal{F}$ and is also the unique minimizer of $\mathcal{F}$.

Theorem 3.10. *Assume* (3.2) *holds true, $\sigma \ge 0$ (or $\sigma \le 0$) and*

$$\sigma(x) \;=\; \sigma(L-x) \tag{3.18}$$

Then $\mathcal{F}$ has a unique and smooth minimizer which coincides with the solution of problem (3.4)*.*

Proof. Let u be the unique solution of (3.4). Then

$$J_3\left(\frac{L}{2}-\tau,y\right)=-J_3\left(\frac{L}{2}+\tau,L-y\right)\qquad\forall\tau\in[0,L/2]\,.$$

By taking into account (3.18), Green representation (3.10) yields for a.e. $\tau\in[0,\frac{L}{2}]$

$$u'''\left(\frac{L}{2}-\tau\right)=\int_0^L J_3\left(\frac{L}{2}-\tau,y\right)\,d\sigma(y) \tag{3.19}$$

$$=-\int_0^L J_3\left(\frac{L}{2}+\tau,L-y\right)d\nu(y)\;=-\int_0^L J_3\left(\frac{L}{2}+\tau,y\right)d\sigma(y)=-u'''\left(\frac{L}{2}+\tau\right).$$

Hence u'' is convex (resp. concave) and symmetric with respect to $x=L/2$. Therefore $\|u''\|_{L^\infty}=\max\{|u''(L)|,|u''(\frac{L}{2})|\}$ and (3.12) entails

$$u''(L)=\int_0^L K(L,y)\,d\sigma(y)=\frac{1}{L^2}\int_0^L y^2(L-y)\,d\sigma(y) \tag{3.20}$$

$$u''\left(\frac{L}{2}\right)=\int_0^L K\left(\frac{L}{2},y\right)\,d\sigma(y)=\int_0^L\left(-\frac{y^2}{2L}+\left(y-\frac{L}{2}\right)^+\right)\,d\sigma(y). \tag{3.21}$$

Hence

$$\|u''\|_{L^\infty}\le\frac{L}{8}|\sigma|_T \tag{3.22}$$

and recalling (3.2) and Theorem 3.6 the thesis follows. □

4. Existence and properties of creased minimizers

We have shown in Lemma 3.2 that a minimizer of $\mathcal{F}$ exists provided $|\sigma|_T<8\gamma/L$, while in Theorem 3.9 we have proven that, whenever $|\sigma|_T\le\frac{27\gamma}{4L}<\frac{8\gamma}{L}$, this minimizer is smooth and coincides with the unique solution of (3.4).

We emphasize that the gap between the safe load condition (3.2) and the load regularity condition (3.15) is so small that, at a first glance one could think that no creased minimizer exists. Actually finding explicit examples of creased minimizers is a quite hard task, but the difficulty may be circumvented by exploiting the estimate (3.20).

Here we show an explicit example of of load ,whose total mass belongs to $(\frac{27\gamma}{4L},\frac{8\gamma}{L})$, such that the corresponding minimizers of $\mathcal{F}$ are not solutions of (3.4), say they are not smooth minimizers.

4.1. An example of creased minimizer

We choose

$$\sigma\;=\;\frac{k\,\gamma}{L}\,\delta_{2L/3}\qquad\text{where}\;\;\frac{27}{4}<k<8\,. \tag{4.1}$$

Then

$$\frac{27\,\gamma}{4L}<|\sigma|_T=\frac{k\,\gamma}{L}<\frac{8\,\gamma}{L}$$

and the safe load condition is satisfied but condition (3.17) is violated.

Let u the solution of (3.4): we want to show that if in addition

$$0 < \beta < \frac{L}{4}\,(\ddot{u}(L)-\gamma)^2$$

then there exists $w \in SBH(\mathbb{R}),\ w \equiv 0$ outside $(0,L)$ such that $\mathcal{F}(w) < \mathcal{F}(u)$. We first observe that by (4.1) and (3.20) we get

$$u''(L) = \frac{1}{L^2}\int_0^L \tau^2(L-\tau)\,d\sigma(\tau) = \frac{4k\gamma}{27} > \gamma. \tag{4.2}$$

Let now v be solution of

$$\begin{cases} v'''' = 0 & \text{in } (0,L) \\ v(0) = v'(0) = v(L) = 0, & v''(L) = \gamma - u''(L), \end{cases}$$

explicitly

$$v(x) = \frac{\gamma - u''(L)}{4L}\,x^2(x-L)\,, \qquad v'(L) = \frac{L}{4}(\gamma - u''(L)).$$

Then $w = u + v$ is a solution of

$$\begin{cases} w'''' = f & (0,L) \\ w(0) = w'(0) = w(L) = 0; \quad \ddot{w}(L) = \gamma \end{cases}$$

If we define $w \equiv 0$ in $\mathbb{R} \setminus (0,L)$ then $S_{\dot{w}} = \{L\}$, $[\dot{w}](L) = \dfrac{L}{4}(u''(L)-\gamma) > 0$, $\ddot{w}(L) = \gamma = \gamma\,\mathrm{sign}([w](L))$. Hence all Euler equations in Theorem 3.3 are fulfilled. Then by taking into account $u(0) = u(L) = \dot{u}(0) = \dot{u}(L) = 0 = v(0) = \dot{v}(0) = v(L)$ and $\dddot{v} \equiv$ constant, the compliance identity (Lemma 3.5) gives:

$$\mathcal{F}(w) = \beta - \frac{1}{2}\int_0^L |\ddot{w}|^2 = \beta - \frac{1}{2}\int_0^L |\ddot{u}|^2 - \int_0^L \ddot{u}\,\ddot{v} - \frac{1}{2}\int_0^L |\ddot{v}|^2$$

$$= \beta - \frac{1}{2}\int_0^L |\ddot{u}|^2 - (\dot{u}\,\ddot{v})\Big|_0^L + \int_0^L \dot{u}\,\dddot{v} - \frac{1}{2}(\dot{v}\,\ddot{v})\Big|_0^L + \frac{1}{2}\int_0^L \dot{v}\,\dddot{v}$$

$$= \beta - \frac{1}{2}\int_0^L |\ddot{u}|^2 - \frac{1}{2}\dot{v}(L)\,\ddot{v}(L)$$

$$= -\frac{1}{2}\int_0^L |\ddot{u}|^2 + \beta - \frac{L}{4}(\ddot{u}(L)-\gamma)^2 < -\frac{1}{2}\int_0^L |\ddot{u}|^2 = \mathcal{F}(u).$$

4.2. Structure of creased minimizers

We conclude our analysis by showing that the number of creases can be estimated independently of data β, γ, L, σ.

Theorem 4.1. *If* $v \in \operatorname{argmin}\mathcal{F}$ *then* $\sharp(S_{\dot{v}}) \le 2$.

Proof. Assume by contradiction that $w \in \operatorname{argmin}\mathcal{F}$ and $x_1 < x_2 < x_3$ are three distinct points in $S_{\dot w}$. Then we can modify w by eliminating one of them and reducing at the same time the energy. Set

$$\lambda = \frac{x_2 - x_1}{x_3 - x_1}, \qquad \varepsilon_0 = \min\left\{ |[\dot w](x_1)|\,,\ \frac{1-\lambda}{\lambda}\,|[\dot w](x_3)| \right\} \tag{4.3}$$

For every $0 < \varepsilon \le \varepsilon_0$ we define a function $w_\varepsilon \in SBH(\mathbb{R})$ such that $w_\varepsilon(0_-) = 0$ and

$$w'_\varepsilon = \dot w_\varepsilon \;=\; \dot w - \varepsilon\,\operatorname{sign}([\dot w](x_1))\,\chi_{[x_1,x_2)} + \frac{\lambda\,\varepsilon\,\operatorname{sign}([\dot w](x_1))}{1-\lambda}\,\chi_{[x_2,x_3]}, \tag{4.4}$$

hence w_ε is different from w only outside $[x_1, x_3]$, moreover

$$\int_0^L \dot w_\varepsilon = \int_0^L \dot w = 0, \qquad \operatorname{spt} w \subset [0, L],$$
$$[\dot w_\varepsilon](x_2) \;=\; \frac{\varepsilon}{1-\lambda}\operatorname{sign}[\dot w](x_1) + [\dot w](x_2).$$

At first we assume $\varepsilon_0 = |[\dot w](x_1)|$. Then

$$[\dot w_{\varepsilon_0}](x_1) = 0,$$

and either $[\dot w_{\varepsilon_0}](x_2)\,[\dot w](x_2) \ge 0$ or $[\dot w_{\varepsilon_0}](x_2)\,[\dot w](x_2) < 0$.
In the first case w_{ε_0} fulfills all the Euler equations in Theorem 3.3 (since the sign of all survived jumps are preserved by (4.3)) and $\ddot w_{\varepsilon_0} = \ddot w$, $\sharp(S_{\dot w_{\varepsilon_0}}) \le 2 < 3 = \sharp(S_{\dot w})$. Hence $\mathcal{F}(w_{\varepsilon_0}) < \mathcal{F}(w)$ by the compliance identity.
In the second case since $[\dot w_\varepsilon](x_2)]$ and $[\dot w](x_2)$ has the same (resp. opposite) sign for $\varepsilon = 0$ (respectively $\varepsilon = \varepsilon_0$) we can choose $\overline{\varepsilon} \in (0, \varepsilon_0]$ such that

$$[\dot w_{\overline{\varepsilon}}](x_2) \;=\; \frac{\overline{\varepsilon}}{1-\lambda}\operatorname{sign}[\dot w](x_1) + [\dot w](x_2) = 0$$

then, by (4.3) $w_{\overline{\varepsilon}}$ fulfills all conditions in Theorem 3.3 and $\ddot w_{\varepsilon_0} = \ddot w$, $\sharp(S_{\dot w_{\varepsilon_0}}) \le 2 < 3 = \sharp(S_{\dot w})$. Hence $\mathcal{F}(w_{\varepsilon_0}) < \mathcal{F}(w)$ by the compliance identity.
Eventually, still assuming (4.3), we examine the case

$$\varepsilon_0 = \frac{1-\lambda}{\lambda}\,|[w](x_3)|$$

and we define a function $\omega_\varepsilon \in SBH(\mathbb{R})$ such that $\omega_\varepsilon(0_-) = 0$ and

$$\omega'_\varepsilon \;=\; \dot\omega_\varepsilon \;=\; \dot w \,-\, \varepsilon\,\operatorname{sign}([\dot w](x_3))\,\chi_{[x_1,x_2]} \,+\, \frac{\lambda\,\varepsilon\,\operatorname{sign}([\dot w](x_3))}{1-\lambda}\,\chi_{[x_2,x_3]}\,. \tag{4.5}$$

Then

$$\int_0^L \dot\omega_\varepsilon = \int_0^L \dot w = 0, \qquad \operatorname{spt} w \subset [0, L],$$
$$[\dot\omega_\varepsilon](x_2) \;=\; \frac{\varepsilon}{1-\lambda}\operatorname{sign}[\dot w](x_3) + [\dot w](x_2),$$

and

$$[\dot\omega_{\varepsilon_0}](x_3) = 0\,.$$

so we can proceed as above by interchanging x_1 and x_3. □

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On Concentrated Contact Interactions

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Abstract. Three examples of equilibrium problems are presented where *concentrated contact interactions* arise to guarantee partwise equilibrium. In the first example, a concentrated force is applied at the boundary of a half plane, and the stress field has an integrable singularity at the point where the force is applied. Suturing two such stress fields so as to have a mirror-symmetric stress field in the whole plane produces a second example of concentrated contact interactions. For a third example, a concentrated couple is applied at the boundary of a half plane, and the standard stress field has a nonintegrable singularity at the point where the couple is applied, whereas the associated hyperstress field, although still singular, is integrable.

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1. Introduction

In continuum mechanics, both a body and its environment and adjacent body parts are presumed to have *distance* and *contact interactions*, collectively inducing in the body a state of *stress*. In the classical case of *simple* material bodies, a pair $\big((\boldsymbol{d},\boldsymbol{c}),\boldsymbol{S}\big)$ is considered, formed by distance and contact *force fields* $\boldsymbol{d}$ and $\boldsymbol{c}$ and a *stress field* $\boldsymbol{S}$ over Ω, the region the body occupies; such a pair is called *weakly balanced* whenever the *force working* (*distance*+*contact*) *equals the stress working*, i.e., whenever

$$\int_\Omega \boldsymbol{d}\cdot\boldsymbol{v}+\int_{\partial\Omega}\boldsymbol{c}\cdot\boldsymbol{v}=\int_\Omega \boldsymbol{S}\cdot\nabla\boldsymbol{v},\quad \text{for all smooth test fields } \boldsymbol{v}. \tag{1.1}$$

The standard differential identity

$$\int_\Omega \boldsymbol{S}\cdot\nabla\boldsymbol{v}=\int_\Omega(-\operatorname{Div}\boldsymbol{S})\cdot\boldsymbol{v}+\int_{\partial\Omega}(\boldsymbol{S}\boldsymbol{n})\cdot\boldsymbol{v} \tag{1.2}$$

allows us to regard $(-\mathrm{Div}\,\boldsymbol{S}, \boldsymbol{S}\boldsymbol{n})$ as a pair $(\boldsymbol{d}_{\boldsymbol{S}}, \boldsymbol{c}_{\boldsymbol{S}})$ of distance and contact force fields associated to a given stress field $\boldsymbol{S}$. Accordingly, we may interpret the weak-balance condition (1.1) as the requirement that, in a distributional sense to be made precise, both $\boldsymbol{d}_{\boldsymbol{S}}$ must equal $\boldsymbol{d}$ and $\boldsymbol{c}_{\boldsymbol{S}}$ must equal $\boldsymbol{c}$:

$$\begin{aligned} \boldsymbol{d}_{\boldsymbol{S}} = -\mathrm{Div}\,\boldsymbol{S} &= \boldsymbol{d} \quad \text{in } \Omega, \\ \boldsymbol{c}_{\boldsymbol{S}} = \boldsymbol{S}\boldsymbol{n} &= \boldsymbol{c} \quad \text{in } \partial\Omega. \end{aligned} \tag{1.3}$$

It is implicit in the formal structure of such notions that, whenever they are to be formulated within a fairly general and precise mathematical setting, recourse to concepts and tools from geometric measure theory is in order. Basically, the stress fields of interest must be locally integrable and have both a locally integrable divergence at interior points of Ω and a meaningful trace at almost every point of $\partial\Omega$. A considerable amount of work has been done as to characterizing larger and larger classes of admissible stress fields under reasonable assumptions on the smoothness of $\partial\Omega$: L^∞ vector fields with divergence measure [1, 2, 3]; L^p vector fields with divergence in L^p [4, 5]; L^1 vector fields with divergence measure [6, 7]; and, finally, vector fields which are measures and have divergence measure [8, 9]. So far, the body has been taken to occupy a region of *finite perimeter*, or smoother;[1] moreover, the regularity requirements for the applied distance and contact force fields have not been specified, since in the light of any mathematically precise version of (1.1) and (1.2) they can be regarded as subservient to, in fact, dictated by those for the stress field. Conversely, building on experience gained since long from specific problems in classical elasticity, one expects that singular stress fields are needed to weakly balance such irregular load fields as a concentrated force, be it applied at an interior or at a boundary point. Yet, the fact that *concentrated loads may induce concentrated contact interactions* was noticed only very recently [10]. Not only that, and perhaps more surprisingly, *in the presence of certain singular stress fields being weakly balanced for everywhere null applied loads, contact interactions between adjacent body parts may turn out to be concentrated* [10].

The occurrence of concentrated contact interactions calls for some rethinking of certain strongholds of continuum mechanics, such as Cauchy's Tetrahedron Theorem. In this paper, which follows closely the lines of thought I developed in [10], I firstly reconsider a basic example there discussed in greater detail, in which a concentrated force is applied at the boundary of a half plane and the accompanying equilibrium stress field has an integrable singularity at the point where the load is applied. Then, I elaborate on another example given in [10], obtained by suture of two mirror-symmetric problems of the previous type. Finally, I briefly discuss a new example, the case of a concentrated couple applied at the boundary

[1] Classically, a body's periphery is assigned the geometrical nature of an orientable differentiable manifold of codimension 1. An exhaustive treatment of fractal bodies or of bodies with a fractal boundary is still wanted.

of a half-plane, in which the equilibrium ordinary stress has a *nonintegrable* singularity but the equilibrium *hyperstress* is instead integrable, an indication that a nonclassical reformulation of the problem is in order.

2. The Flamant stress field in a half-plane

Nothing of importance is lost if we confine attention to two space dimensions. We then consider a partial two-dimensional version of a problem solved in 1892 by the French mechanist Alfred-Aimé Flamant [11], and study the equilibrium stress field associated to a concentrated load applied to a half-plane.[2]

With reference to Figure 1, let a concentrated force $\boldsymbol{f} = f\boldsymbol{e}_1$ be applied at point o of the half-plane

$$\mathcal{H}^+ := \{x \,|\, (x-o)\cdot \boldsymbol{e}_3 = 0,\ \ (x-o)\cdot \boldsymbol{e}_1 \geq 0\},$$

and let the distance force field $\boldsymbol{d}$ be identically null in $\mathcal{H}^+$. For $\boldsymbol{r} := x - o$ the

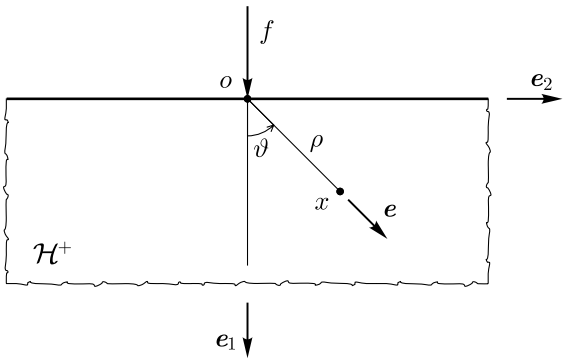

FIGURE 1. The Flamant half-plane.

position vector of point $x \in \mathcal{H}^+$ with respect to o, let $\rho := |\boldsymbol{r}|$, $\boldsymbol{e} := \rho^{-1}\boldsymbol{r}$ and $\vartheta := \arcsin((\boldsymbol{e}_1 \times \boldsymbol{e})\cdot \boldsymbol{e}_3)$, whence

$$\boldsymbol{e}(\vartheta) := \cos\vartheta\, \boldsymbol{e}_1 + \sin\vartheta\, \boldsymbol{e}_2.$$

The *Flamant stress field* in $\mathcal{H}^+$ has the form

$$\boldsymbol{S}_F(\rho,\vartheta) = -\frac{2f}{\pi\rho}\cos\vartheta\, \boldsymbol{e}(\vartheta)\otimes\boldsymbol{e}(\vartheta), \quad \text{for } \rho\in(0,+\infty),\ \vartheta\in[-\pi/2,+\pi/2]. \tag{2.1}$$

[2]Flamant solved the equilibrium problem in terms of displacements for a linearly elastic, isotropic body occupying a half space and being acted upon by a perpendicular *line load* of constant magnitude per unit length and infinitely long support. The case of a *concentrated load* perpendicular to a half space had been considered by Boussinesq in 1878 [12]. Both Boussinesq's and Flamant's are relatively easy problems in three-dimensional elasticity, the first because of its inherent central symmetry, the second because it admits a plane-strain solution; their two-dimensional versions cohalesce.

2.1. Distance and contact force fields associated to the Flamant stress

We now determine $(\boldsymbol{d}_{\boldsymbol{S}_F}, \boldsymbol{c}_{\boldsymbol{S}_F})$, the pair of distance and contact force fields associated to $\boldsymbol{S}_F$.

To begin with, it is easy to show that

$$\boldsymbol{d}_{\boldsymbol{S}_F} = -\mathrm{Div}\, \boldsymbol{S}_{\boldsymbol{F}} \equiv \boldsymbol{0} \quad \text{in the interior of } \mathcal{H}^+. \tag{2.2}$$

Thus, the Flamant stress satisfies the standard pointwise condition of force balance $(1.3)_1$; it remains for us to show in what sense $\boldsymbol{S}_F$ satisfies the accompanying traction boundary condition $(1.3)_2$, for the half-space $\mathcal{H}^+$ and for its parts.

For any fixed $\rho > 0$, we consider a half-disk $\mathcal{S}_\rho$ of radius ρ about o, whose oriented contour is the union of the half-circle

$$\mathcal{C}_\rho := \{x \,|\, x - o = \rho \boldsymbol{e}(\vartheta),\, \vartheta \in [-\pi/2, +\pi/2]\}$$

and the segment

$$\mathcal{I}_\rho := \{x \,|\, x - o = \sigma \boldsymbol{e}_2,\, \sigma \in [+\rho, -\rho]\}$$

(Figure 2). It follows from (2.1) that the contact force $\boldsymbol{c}_{\boldsymbol{S}_F} = \boldsymbol{S}_F \boldsymbol{n}$ over $\partial\mathcal{S}_\rho$ is null

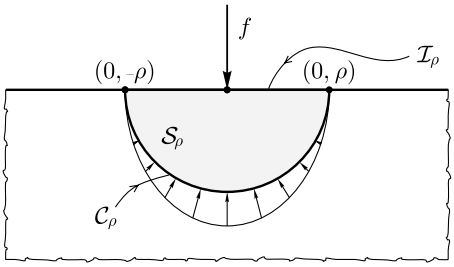

FIGURE 2. Forces, concentrated and diffused, applied at the periphery $\mathcal{C}_\rho \cup \mathcal{I}_\rho$ of a half-disk $\mathcal{S}_\rho$.

at points of $\mathcal{I}_\rho \setminus \{o\}$, and is

$$\boldsymbol{S}_F \boldsymbol{e} = -\frac{2f}{\pi\rho} \cos\vartheta\, \boldsymbol{e} \tag{2.3}$$

at points of $\mathcal{C}_\rho$; the latter relation implies that

$$\int_{\mathcal{C}_\rho} \boldsymbol{S}_F \boldsymbol{e} = -\boldsymbol{f}. \tag{2.4}$$

If we interpret the force $\boldsymbol{f}$ concentrated at o as a *Dirac contact force* $\boldsymbol{c}_\rho$ applied over the segment $\mathcal{I}_\rho$:

$$\boldsymbol{f} = \int_{\mathcal{I}_\rho} \boldsymbol{c}_\rho, \quad \boldsymbol{c}_\rho(x) := \delta(x - o)\boldsymbol{f},\ x \in \mathcal{I}_\rho. \tag{2.5}$$

then relation (2.4) becomes:

$$\int_{\mathcal{C}_\rho} \boldsymbol{S}_F \boldsymbol{e} + \int_{\mathcal{I}_\rho} \boldsymbol{c}_\rho = \boldsymbol{0}, \tag{2.6}$$

and expresses the *force balance* for the part $\mathcal{S}_\rho$, whatever $\rho > 0$. Moreover, since the Flamant stress field is divergenceless over $\mathcal{S}_\rho$, we have that

$$\boldsymbol{0} = \int_{\mathcal{S}_\rho} \mathrm{Div}\, \boldsymbol{S}_F = \int_{\mathcal{C}_\rho} \boldsymbol{S}_F \boldsymbol{e} - \int_{\mathcal{I}_\rho} \boldsymbol{S}_F \boldsymbol{e}_1 \quad \Rightarrow \quad \int_{\mathcal{I}_\rho} (\boldsymbol{c}_\rho + \boldsymbol{S}_F \boldsymbol{e}_1) = \boldsymbol{0}. \tag{2.7}$$

Thus, over the straight line bounding $\mathcal{H}^+$,

$$\boldsymbol{c}_{\boldsymbol{S}_F} = \boldsymbol{c}_\rho; \tag{2.8}$$

in words, the contact force is an area vector-measure, concentrated at the point o where the external force $\boldsymbol{f}$ is applied.

2.2. Flux and divergence measures associated to the Flamant stress

A stress field $\boldsymbol{S}$ is said to have *divergence measure* in Ω if

$$\int_\Omega (-\mathrm{Div}\, \boldsymbol{S}) \cdot \boldsymbol{v} = \int_\Omega \boldsymbol{d} \cdot \boldsymbol{v} \quad \text{for all smooth test fields } \boldsymbol{v}, \tag{2.9}$$

with $\boldsymbol{d}$ a *volume vector-measure*; and it is said to have *flux measure* over $\partial\Omega$ if

$$\int_{\partial\Omega} \boldsymbol{S}^T \boldsymbol{v} \cdot \boldsymbol{n} = \int_{\partial\Omega} \boldsymbol{c} \cdot \boldsymbol{v} \quad \text{for all smooth test fields } \boldsymbol{v}, \tag{2.10}$$

for $\boldsymbol{c}$ an *area vector-measure* (the vector field $\boldsymbol{S}^T \boldsymbol{v}$ is the *stress flux* associated to the pseudo-velocity field $\boldsymbol{v}$).

In the last part of the previous subsection we have shown that *the Flamant stress field $\boldsymbol{S}_F$ has flux measure over $\partial\mathcal{H}^+$*. Suppose now that $\boldsymbol{S}_F$ is continuously extended to null in the upper half-plane $\mathcal{H}^-$, and let $\widetilde{\boldsymbol{S}}_F$ denote such extended field over the whole plane $\mathcal{H} = \mathcal{H}^+ \cup \mathcal{H}^-$. Then, it is not difficult to show that *the extended Flamant stress field $\widetilde{\boldsymbol{S}}_F$ has divergence measure in $\mathcal{H}$*, with

$$-\mathrm{Div}\, \widetilde{\boldsymbol{S}}_F = \delta(x - o)\boldsymbol{f}, \quad x \in \mathcal{H}. \tag{2.11}$$

To interpret this result as a consequence of a force balance, we consider a disk-shaped part $\mathcal{D}_\rho$ of $\mathcal{H}$, of center o and radius ρ, and imagine it as subject to an external *distance force* $\boldsymbol{f}$ applied at o, balanced by diffused tractions being identically null over $\partial\mathcal{D}_\rho \cap \mathcal{H}^-$ and equal to $\boldsymbol{S}_F \boldsymbol{e}$ over $\partial\mathcal{D}_\rho \cap \mathcal{H}^+$.

To sum up, if we apply the balance format (1.1) to the parts $\mathcal{S}_\rho$ of $\mathcal{H}^+$ and $\mathcal{D}_\rho$ of $\mathcal{H}$, we find that

$$\int_{\mathcal{S}\rho} \boldsymbol{S}_F \cdot \nabla \boldsymbol{v} - \int_{\mathcal{C}_\rho} \boldsymbol{S}_F \boldsymbol{e} \cdot \boldsymbol{v} = \boldsymbol{f} \cdot \boldsymbol{v}(o) = \int_{\mathcal{D}\rho} \widetilde{\boldsymbol{S}}_F \cdot \nabla \boldsymbol{v} - \int_{\mathcal{C}_\rho} \boldsymbol{S}_F \boldsymbol{e} \cdot \boldsymbol{v}.^3 \tag{2.12}$$

[3]Note that, by definition,

$$\int_{\partial\mathcal{D}_\rho} \widetilde{\boldsymbol{S}}_F \boldsymbol{n} \cdot \boldsymbol{v} = \int_{\mathcal{C}_\rho} \boldsymbol{S}_F \boldsymbol{e} \cdot \boldsymbol{v}.$$

In the case of $\mathcal{S}_\rho$ and $\boldsymbol{S}_F$, we may write

$$\boldsymbol{f}\cdot\boldsymbol{v}(o)=\int_{\mathcal{I}_\rho}\boldsymbol{S}_F^T\boldsymbol{v}\cdot\boldsymbol{n}=\text{the contact working of }\boldsymbol{S}_F\text{ over }\mathcal{I}_\rho;\tag{2.13}$$

in the case of $\mathcal{D}_\rho$ and $\widetilde{\boldsymbol{S}}_F$,

$$\boldsymbol{f}\cdot\boldsymbol{v}(o)=\int_{\mathcal{D}_\rho}(-\operatorname{Div}\widetilde{\boldsymbol{S}}_F)\cdot\boldsymbol{v}=\text{the distance working of }\widetilde{\boldsymbol{S}}_F\text{ over }\mathcal{D}_\rho.\tag{2.14}$$

2.3. Concentrated contact interactions

Consider now the quarter-disk $\mathcal{P}_\rho$ sketched in Figure 3. When part $\mathcal{P}_\rho$ is ideally cut

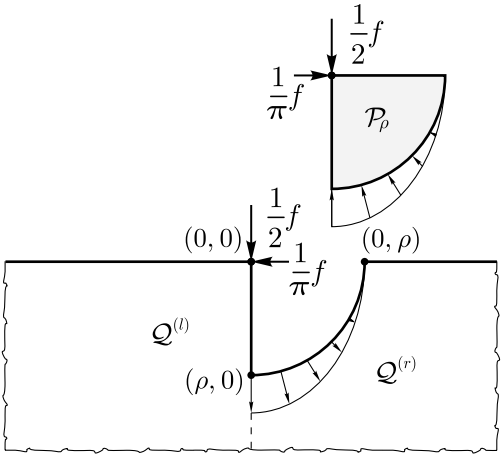

FIGURE 3. Forces, concentrated and diffused, applied at the periphery of a quarter-disk $\mathcal{P}_\rho$.

away from the rest of $\mathcal{H}^+$, then it must be in equilibrium under the action of: (i) the concentrated force $1/2\,f\,\boldsymbol{e}_1$; (ii) the diffused contact force $\boldsymbol{S}_F\boldsymbol{e}$ exerted by the right adjacent part $\mathcal{Q}^{(r)}$, which, in view of (2.3), is equipollent to the concentrated force

$$\int_{\frac{1}{2}\mathcal{C}_\rho}\boldsymbol{S}_F\boldsymbol{e}=-\frac{1}{2}f\,\boldsymbol{e}_1-\frac{1}{\pi}f\,\boldsymbol{e}_2,\tag{2.15}$$

applied at o; (iii) the contact action exerted by the left adjacent part $\mathcal{Q}^{(l)}$. Now, the diffused contact force $-\boldsymbol{S}_F\boldsymbol{e}_2$ exerted by $\mathcal{Q}^{(l)}$ on $\mathcal{P}_\rho$ is everywhere null along their common boundary:

$$\boldsymbol{S}_F(\sigma,0)\boldsymbol{e}_2\equiv 0\quad\text{for}\quad\sigma\in[0,\rho]\,,\tag{2.16}$$

just as their internal contact interaction is before the cut. Then, to guarantee the free-body equilibrium of $\mathcal{P}_\rho$, we are driven to admit that the cut operation brings

into evidence an internal *concentrated contact interaction*

$$\hat{\boldsymbol{f}}(\mathcal{P}_\rho, \mathcal{Q}^{(l)}) = -\hat{\boldsymbol{f}}(\mathcal{Q}^{(l)}, \mathcal{P}_\rho) = \frac{1}{\pi} f\, \boldsymbol{e}_2 \tag{2.17}$$

at point o.[4]

It can be shown that this result is neither dependent on the parameter ρ nor on whichever curve from point $(\rho, 0)$ to point $(0, \rho)$ we pick to bound part $\mathcal{P}_\rho$. Thus, the concentrated contact force arising at point o is a *local effect*, in the sense that it is a manifestation of the interaction between any two adjacent body parts having the segment $\mathcal{I}_\rho$ as a common boundary, whatever $\rho > 0$.

3. Sutured Flamant stress fields in a plane

The previous example intimates that a concentrated contact interaction may arise when an ideal cut is made through a body point where an external concentrated force is applied. We now give an example of concentrated contact interaction brought into the open by an ideal cut through a focal point of a given balanced stress field, such as the stress field in the whole plane which results from 'suturing' two mirror-symmetric Flamant stress fields (Figure 4), namely,

$$\overline{\boldsymbol{S}}_F(\rho, \vartheta) = -\frac{2f}{\pi\rho} |\cos\vartheta|\, \boldsymbol{e}(\vartheta) \otimes \boldsymbol{e}(\vartheta), \quad \text{for } \rho \in (0, +\infty),\ \vartheta \in [-\pi/2, +3\pi/2]. \tag{3.1}$$

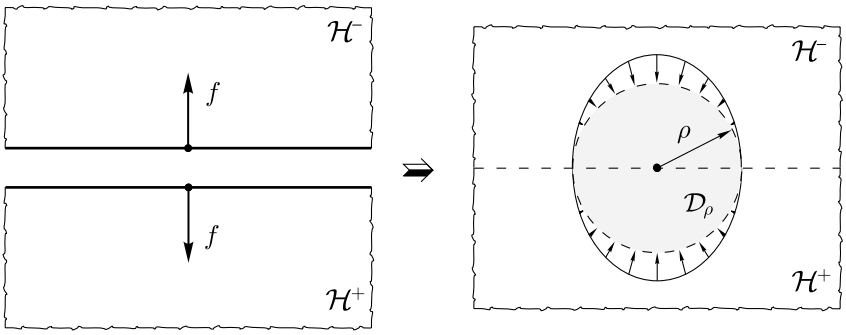

FIGURE 4. Diffused forces applied at the periphery of a disk $\mathcal{D}_\rho$ being a centered circular part of two sutured mirror-symmetric Flamant half-planes.

In this example, no concentrated loads are in sight, and the stress is identically null along the suture line; the disk $\mathcal{D}_\rho$, if isolated from the rest by means of an ideal

[4]Here $\hat{\boldsymbol{f}}(\mathcal{A}, \mathcal{B})$ denotes the total contact force exerted by part $\mathcal{B}$ over part $\mathcal{A}$ over their common boundary.

cut, would be in equilibrium under the sketched distribution of Flamant boundary tractions

$$\overline{\boldsymbol{S}}_F \boldsymbol{e} = -\frac{2f}{\pi\rho}|\cos\vartheta\,|\,\boldsymbol{e}. \tag{3.2}$$

However, were the two half-disks composing $\mathcal{D}_\rho$ separated by a further ideal cut along the suture line, then their individual equilibrium would require concentrated contact interactions, in fact, the mirror-symmetric concentrated forces of the two Flamant problems we begun our construction with. More generally, the only contact force on the half-plane

$$\mathcal{H}^-(\vartheta) := \{x\,|\,(x-o)\cdot\boldsymbol{e}_3 = 0,\ \ (x-o)\cdot\boldsymbol{e}'(\vartheta) \le 0,\ \ \boldsymbol{e}'(\vartheta) = -\sin\vartheta\boldsymbol{e}_1 + \cos\vartheta\boldsymbol{e}_2\}$$

is the Dirac force

$$\boldsymbol{c}_\rho(x,\vartheta) = \delta(x-o)\boldsymbol{g}(\vartheta), \quad \boldsymbol{g}(\vartheta) = \frac{2f}{\pi}\big((\vartheta+\sin\vartheta\cos\vartheta)\boldsymbol{e}_1 - \cos^2\vartheta)\boldsymbol{e}_2\big), \tag{3.3}$$

concentrated at the origin of the interval

$$\mathcal{I}_\rho(\vartheta) := \{x\,|\,x-o = \sigma\boldsymbol{e}(\vartheta),\ \sigma\in[+\rho,-\rho]\},\ \text{ whatever }\ \rho>0.$$

Interestingly, at variance with the previous example, the concentrated interaction now arises at an interior point, not at an end point, of the common boundary with the adjacent part applying it to the part of interest. We are entitled to mimic the last equation in (2.7), and write

$$\int_{\mathcal{I}_\rho(\vartheta)} (\boldsymbol{c}_\rho(\vartheta) - \overline{\boldsymbol{S}}_F\boldsymbol{e}'(\vartheta)) = \boldsymbol{0}, \tag{3.4}$$

or rather, in the manner of (2.8),

$$\boldsymbol{c}_{\overline{\boldsymbol{S}}_F}(\vartheta) = \boldsymbol{c}_\rho(\vartheta), \quad \vartheta\in[-\pi/2,+3\pi/2]. \tag{3.5}$$

Remark 3.1. At a singular point o for the stress field the standard relationships between contact forces and stress, which are the essence of the celebrated Tetrahedron Theorem of Cauchy, do not hold: neither there is a tensor $\underline{\boldsymbol{S}}(o)$ such that the contact force $\boldsymbol{c}(o;\boldsymbol{n})$ on an oriented half-plane through o of normal $\boldsymbol{n}$ is given by

$$\boldsymbol{c}(o;\boldsymbol{n}) = \underline{\boldsymbol{S}}(o)\boldsymbol{n} \tag{3.6}$$

nor, given the contact forces $\boldsymbol{c}(o;\boldsymbol{n}_\alpha)$, $\alpha=1,2$, on two mutually orthogonal oriented half-planes, the tensor

$$\overline{\boldsymbol{S}}(o) := \boldsymbol{c}(o;\boldsymbol{n}_1)\otimes\boldsymbol{n}_1 + \boldsymbol{c}(o;\boldsymbol{n}_2)\otimes\boldsymbol{n}_2 \tag{3.7}$$

would restitute $\boldsymbol{c}(o;\boldsymbol{n})$ when applied to $\boldsymbol{n}$, as specified by (3.6). To see this in the case of the stress field (3.1), take

$$\boldsymbol{n} = \boldsymbol{e}'(\vartheta) \quad \text{and} \quad \boldsymbol{c}(o;\boldsymbol{n}) = \boldsymbol{g}(\vartheta).$$

With this, the closest one can get to (3.6) is by setting

$$\boldsymbol{g}(\vartheta) = \underline{\boldsymbol{S}}(o;\vartheta)\boldsymbol{e}'(\vartheta),\ \text{ with }\ \underline{\boldsymbol{S}}(o;\vartheta) := -\frac{2f}{\pi}\Big(\big(\frac{\vartheta}{\sin\vartheta}+\cos\vartheta\big)\boldsymbol{e}_1\otimes\boldsymbol{e}_1 + \cos\vartheta\boldsymbol{e}_2\otimes\boldsymbol{e}_2\Big).$$

Moreover, with the recipe (3.7) we easily construct

$$\overline{\boldsymbol{S}}(o) = \boldsymbol{g}(0) \otimes \boldsymbol{e}'(0) + \boldsymbol{g}(\frac{\pi}{2}) \otimes \boldsymbol{e}'(\frac{\pi}{2}) = -f\Big(\boldsymbol{e}_1 \otimes \boldsymbol{e}_1 + \frac{2}{\pi}\boldsymbol{e}_2 \otimes \boldsymbol{e}_2\Big),$$

but

$$\overline{\boldsymbol{S}}(o)\boldsymbol{e}'(\vartheta) \neq \boldsymbol{g}(\vartheta),$$

except for $\vartheta = 0$ and $\vartheta = \pi/2$.

4. Concentrated couple applied at the boundary of a half-plane

Recall, as a premiss, that a couple $\boldsymbol{m}$ applied over the boundary of a body occupying a region Ω enters a weak-balance condition of type (1.1) through an integral having the following alternative forms:

$$\int_{\partial\Omega} \boldsymbol{m} \cdot \boldsymbol{w} = 2 \int_{\partial\Omega} \boldsymbol{M} \cdot \boldsymbol{W}, \tag{4.1}$$

where the *spin* $\boldsymbol{w}$ is defined to be the vector uniquely associated to $\boldsymbol{W} := \mathrm{skw}(\nabla \boldsymbol{v})$, the skew part of the velocity gradient, and where, likewise, $\boldsymbol{M}$ denotes the skew tensor uniquely associated to $\boldsymbol{m}$. As we shall quickly see, if a concentrated couple is applied to the boundary of a simple material body, whose only stress response to loading consists in developing a standard stress field, then such an anomalous situation is denounced mathematically by the occurrence of a nonintegrable equilibrium stress. However, if the same problem is set within the framework of an equilibrium theory for *nonsimple* material bodies (the class of second-grade material bodies, which is next in complication to the simple class, suffices), then this mathematical difficulty does not occur, because the body may now develop an *integrable hyperstress field*, in addition to, or in the place of, a standard stress field.[5]

A couple $\boldsymbol{m} = m\boldsymbol{e}_3$ applied at point o of the half-plane $\mathcal{H}^+$ can be regarded as the limit for $\varepsilon \to 0$ of a pair of concentrated forces $\mp(m/2\varepsilon)\boldsymbol{e}_1$ applied at points $o \pm \varepsilon \boldsymbol{e}_2$. Thus, the equilibrium standard stress field can almost be read off the Flamant stress (2.1), and is found to have the following form:

$$\boldsymbol{C}_F(\rho, \vartheta) = -\frac{2m}{\pi}\rho^{-2}\big(g(\vartheta)\boldsymbol{e}(\vartheta) \otimes \boldsymbol{e}(\vartheta)\big)', \quad g(\vartheta) = \cos^2\vartheta. \tag{4.2}$$

Remarkably, in spite of the nonintegrable singularity at the origin, this stress field gives rise to tractions that allow for partwise balance of both a centered half-disk $\mathcal{S}_\rho$ and a quarter disk $\mathcal{P}_\rho$.[6] But, a tensorial distribution whose divergence

[5] These matters will be treated in greater detail in [13].

[6] In the half-disk case, in addition to the *Dirac couple*

$$\boldsymbol{m} = \int_{\mathcal{I}_\rho} \boldsymbol{m}_\rho, \quad \boldsymbol{m}_\rho(x) := \delta(x - o)\boldsymbol{m},\ x \in \mathcal{I}_\rho,$$

applied to the segment $\mathcal{I}_\rho$, a diffused contact force

$$\boldsymbol{C}_F\boldsymbol{e} = -\frac{2m}{\pi}\rho^{-2}(g\boldsymbol{e})'$$

equals the concentrated couple $\boldsymbol{m}$ remains to be found. It can be shown that such distribution is represented by the locally integrable tensor field

$$\boldsymbol{C} := \boldsymbol{X}\boldsymbol{C}_F = -\frac{2m}{\pi}\rho^{-1}g(\vartheta)\boldsymbol{e}_3 \otimes \boldsymbol{e}(\vartheta), \quad \boldsymbol{X} = \rho\boldsymbol{E}(\vartheta), \tag{4.3}$$

where $\boldsymbol{E}$ is the skew tensor uniquely associated to the unit vector $\boldsymbol{e}$. More importantly, it can also be shown that there is another equivalent tensorial distribution, represented by the third-order hyperstress field $\mathbb{T}$ over the half-plane $\mathcal{H}^+$ defined by

$$\mathbb{T} := -\frac{2m}{\pi}\rho^{-1}g(\vartheta)(\boldsymbol{e}_1 \otimes \boldsymbol{e}_2 - \boldsymbol{e}_2 \otimes \boldsymbol{e}_1) \otimes \boldsymbol{e}(\vartheta), \tag{4.4}$$

and such that

$$-\mathrm{Div}\,\mathbb{T} = \boldsymbol{M} \quad \text{in a distributional sense.} \tag{4.5}$$

Finally, let $\widetilde{\mathbb{T}}$ denote the null extension of $\mathbb{T}$ to all of the plane $\mathcal{H}$. Then, within the framework of the equilibrium theory for second-grade material bodies, the weak-balance conditions for the the parts $\mathcal{S}_\rho$ of $\mathcal{H}^+$ and $\mathcal{D}_\rho$ of $\mathcal{H}$ may be jointly written as

$$\int_{\mathcal{S}_\rho} \mathbb{T}\cdot\nabla\boldsymbol{V} - \int_{\mathcal{C}_\rho} \mathbb{T}\boldsymbol{e}\cdot\boldsymbol{V} = \boldsymbol{M}\cdot\boldsymbol{V}(o) = \int_{\mathcal{D}_\rho} \widetilde{\mathbb{T}}\cdot\nabla\boldsymbol{V} - \int_{\mathcal{C}_\rho} \mathbb{T}\boldsymbol{e}\cdot\boldsymbol{V}. \tag{4.6}$$

In the case of $\mathcal{S}_\rho$ and $\mathbb{T}$,

$$\boldsymbol{M}\cdot\boldsymbol{V}(o) = \int_{\mathcal{I}_\rho} \mathbb{T}\boldsymbol{n}\cdot\boldsymbol{V} = \text{the contact working of } \mathbb{T} \text{ over } \mathcal{I}_\rho; \tag{4.7}$$

in the case of $\mathcal{D}_\rho$ and $\widetilde{\mathbb{T}}$,

$$\boldsymbol{M}\cdot\boldsymbol{V}(o) = \int_{\mathcal{D}_\rho} (-\mathrm{Div}\,\widetilde{\mathbb{T}})\cdot\boldsymbol{V} = \text{the distance working of } \widetilde{\mathbb{T}} \text{ over } \mathcal{D}_\rho. \tag{4.8}$$

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is applied to the points of $\mathcal{C}_\rho$; both forces and torques are balanced:

$$\text{(force balance)} \qquad \int_{\partial\mathcal{P}_\rho} \boldsymbol{C}_F e = -\frac{2m}{\pi}\rho^{-1}\int_{-\pi/2}^{+\pi/2} (g\boldsymbol{e})'\,d\vartheta = \boldsymbol{0};$$

$$\text{(torque balance)} \qquad \int_{\partial\mathcal{P}_\rho} (x-o)\times\boldsymbol{C}_F\boldsymbol{e} = -\frac{2m}{\pi}\int_{-\pi/2}^{+\pi/2} \boldsymbol{e}\times(g\boldsymbol{e})'\,d\vartheta + \boldsymbol{m} = \boldsymbol{0}.$$

In the quarter-disk case, in addition to the concentrated couple $1/2\,\boldsymbol{m}$ and the diffused contact force $\boldsymbol{C}_F\boldsymbol{e}$ exerted by the right adjacent part $\mathcal{Q}^{(r)}$ on the pertinent part of $\mathcal{C}_\rho$, a nonvanishing diffused traction is now exerted on $\mathcal{P}_\rho$ by the adjacent part $\mathcal{Q}^{(l)}$ on the left, namely,

$$-\boldsymbol{C}_F(\sigma,0)\boldsymbol{e}_2 = \frac{2m}{\pi}\sigma^{-2}\boldsymbol{e}_1 \quad \text{for} \quad \sigma\in[0,\rho]\,;$$

most unusually, such contact interaction becomes unbounded as $\sigma\to 0$.

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Discontinuous Hysteresis and P.D.E.s

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Abstract. Hysteresis can be represented via *hysteresis operators.* Some basic models of discontinuous hysteresis are here reviewed: the *relay operator,* the *Preisach model,* and their vector extensions. In view of the analysis of related problems at the P.D.E.s, a weak formulation is also provided. The conservation law

$$\frac{\partial}{\partial t}[u + \mathcal{F}(u)] + \frac{\partial u}{\partial x} = f \qquad \text{in } \mathbf{R}\times]0,T[$$

is then briefly discussed, $\mathcal{F}$ being a discontinuous hysteresis operator.

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1. Hysteresis

Hysteresis operators. Hysteresis occurs in ferromagnetism, ferroelectricity, plasticity, pseudo-elasticity, superconductivity, phase transitions, porous media filtration, and in several other phenomena.

For instance, let us consider a homogeneous isotropic toroidal specimen of a magnetic material, wound it uniformly with an electrically conducting coil, and let a current flow along the latter. By Ampère's law, this induces a magnetic field $\vec{H}$ along the axis of the torus, which in turn determines a parallel magnetization $\vec{M}$; in this setting the intensity of both fields is of course uniform. The dependence between the components H and M is outlined in Fig. 1.

In a time interval $[0,T]$ this relation can then be represented in the form

$$\vec{M}(t) = [\mathcal{F}(\vec{H})](t) \qquad \forall t \in [0,T], \tag{1.1}$$

where $\mathcal{F}$ is a *hysteresis operator.* By this we mean that:

(i) $\mathcal{F}$ has *memory.* Indeed at each instant t, $\vec{M}(t)$ depends not only on $\vec{H}(t)$ (at the same instant t), but also on the history of $\vec{H}$ in the time interval $[0,t]$ and on the initial value $\vec{M}(0)$ (that we omitted in the formula $\vec{M} = \mathcal{F}(\vec{H})$). In more advanced models the initial value may include internal variables, too.

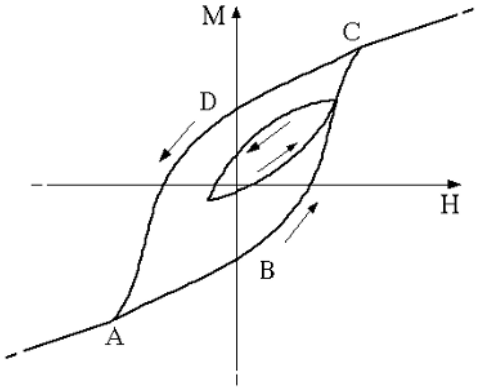

FIGURE 1. Hysteresis dynamics, for a univariate system.

(ii) $\mathcal{F}$ is *rate-independent.* This means that the path of the pair $(\vec{H}(t), \vec{M}(t))$ is invariant w.r.t. any increasing homeomorphism $\varphi : [0,T] \to [0,T]$, that is,

$$\mathcal{F}(\vec{H} \circ \varphi) = \mathcal{F}(\vec{H}) \circ \varphi \qquad \text{in } [0,T].$$

In other terms, if $\mathcal{F}$ maps $\vec{H}$ to $\vec{M}$, then it also maps $\vec{H} \circ \varphi$ to $\vec{M} \circ \varphi$. In particular, if $\vec{H}$ is periodic, then the $\vec{M}$ vs. $\vec{H}$ relation does not depend on the frequency.

The latter property distinguishes hysteresis from other memory phenomena. In ferromagnetic materials it is fulfilled within a good degree of approximation, provided that the time rate of $\vec{H}$ is not too large. For high frequencies a relaxation dynamics should however be considered.

For univariate systems $\mathcal{F}$ may be represented either by the *Preisach model* (here reviewed in Sect. 2), or by one of its generalizations, or by other hysteresis models.

Hysteresis operators are essentially due to the late M.A. Krasnosel'skiĭ, see, e.g., the pioneering monograph he wrote with A.V. Pokrovskiĭ [16]. These operators provide a rather general framework, in which more specific models may be formulated: this notion may be regarded as one of the terms that may be used to describe hysteresis. This concept may look rather obvious for systems characterized only by time-dependence; space-distributed systems instead look more problematic in this respect. In that case it seems natural to regard the space-variable x as a parameter, and to extend (1.1) by setting

$$\vec{M}(x,t) = [\mathcal{F}(\vec{H}(x,\cdot)](t) \qquad \forall t \in [0,T]. \tag{1.2}$$

(where by $\vec{H}(x,\cdot)$ we denote the time-function $t \mapsto \vec{H}(x,t)$). However this formulation is more compromising than it might look, for it excludes that at any point $\vec{M}$ may be influenced *via the constitutive law* by the past behavior of $\vec{H}$ at another point. Of course (1.2) must be coupled with another equation (typically a P.D.E.) to close the problem, and this may (actually, will) account for space interactions.

Nevertheless the absence of any interaction of that sort in (1.2) is an assumption that might be questioned. In any case relations of this are not the only analytic way to represent the hysteresis behavior, and we shall illustrate a different approach.

Quasilinear hyperbolic P.D.E.s with hysteresis. In this note we review some basic models of discontinuous hysteresis: the *relay operator,* the Preisach model, and their vector extensions. We also provide a weak formulation, which is convenient for the analysis of related problems at the P.D.E.s. We then discuss how the equation

$$\frac{\partial}{\partial t}[u + \mathcal{F}(u)] + \frac{\partial u}{\partial x} = f \qquad \text{in } \mathbf{R}\times]0,T[\tag{1.3}$$

may be related to an analogous equation, in which the hysteresis relation $w = u + \mathcal{F}(u)$ is replaced by $u = \varphi(w)$ for a nonmonotone function φ. We also deal with some related equations.

The conservation law (1.3) may model transport with adsorption and desorption, cf. [27]. Well-posedness for this equation was proved in Chap. VIII of [30] for an either continuous or discontinuous hysteresis operator $\mathcal{F}$, in the framework of the theory of nonlinear semigroups in Banach spaces. More recently in [34] somehow stronger results were derived via the weak formulation of discontinuous hysteresis that we outline in the next section.

In [31], [33] this formulation was applied to second-order quasilinear hyperbolic equations with (either continuous or discontinuous) hysteresis in several space dimensions:

$$\frac{\partial^2}{\partial t^2}[u + \mathcal{F}(u)] - \Delta u = f \qquad \text{in } \Omega\times]0,T[\ (\Omega \subset \mathbf{R}^N). \tag{1.4}$$

A different approach to these equations in a single dimension of space was used by Krejčí in several works, see, e.g., [17], [18], Chaps. III,IV of [19] and references therein.

Bibliographic note. The notion of hysteresis operator is essentially due to the late M.A. Krasnosel'skiĭ, who set it at the basis of the pioneering research on hysteresis he carried out with a group of Russian analysts. These results were then illustrated in the monograph [16]. Since then research in this field has been progressing, see, e.g., the monographs [5], [19], [30] and [1], [9], [15], [21] for mathematically- and physically-oriented approaches, respectively. See also the proceedings [3], [4], [29]. The recent volume [2] gathers a wide spectrum of contributions, covering mathematical and applicative aspects.

A different approach to hysteresis was recently proposed for quasistationary evolution by Levitas, Mielke, Theil [24]–[26] and others for a number of phenomena, as well as by Francfort and Marigo [12] and by Dal Maso and Toader [7] to represent brittle fracture. Their formulation consists in coupling the energy balance with a stability condition; there are some similarities between this model and the relay operator of the next section, although these approaches are quite at variance. Recently Evans also expressed a new point of view in [10], [11].

2. Discontinuous hysteresis and the Preisach model

In this section we review a basic example of discontinuous hysteresis operator, the so-called (delayed) *relay operator.* A more detailed presentation may be found, e.g., in Chap. VI of [30].

Scalar relay. Let us fix any pair $\rho := (\rho_1, \rho_2) \in \mathbf{R}^2$ with $\rho_1 < \rho_2$, and assume that two scalar functions $u(t)$ and $w(t)$ are related as it is outlined in Fig. 2(b). More precisely, for any $u \in C^0([0,T])$ and any $\xi \in [-1,1]$, we set $w \in k_\rho(u,\xi)$ if and only if w is measurable in $]0,T[$,

$$w(0) := \begin{cases} -1 & \text{if } u(0) < \rho_1 \\ \xi & \text{if } \rho_1 \le u(0) \le \rho_2, \\ 1 & \text{if } u(0) > \rho_2, \end{cases} \tag{2.1}$$

and, for any $t \in]0,T]$,

$$w(t) \in \begin{cases} \{-1\} & \text{if } u(t) < \rho_1, \\ [-1,1] & \text{if } \rho_1 \le u(t) \le \rho_2, \\ \{1\} & \text{if } u(t) > \rho_2, \end{cases} \tag{2.2}$$

$$\begin{cases} \text{if } u(t) = \rho_1, & \text{then } w \text{ is nonincreasing in a neighbourhood of } t, \\ \text{if } u(t) = \rho_2, & \text{then } w \text{ is nondecreasing in a neighbourhood of } t, \\ \text{if } u(t) \ne \rho_1, \rho_2, & \text{then } w \text{ is constant in a neighbourhood of } t. \end{cases} \tag{2.3}$$

Because of the latter condition, it is easy to see that $w \in BV(0,T)$ whenever $u \in C^0([0,T])$. Thus (2.1)–(2.3) define a multivalued mapping

$$k_\rho : C^0([0,T]) \times [-1,1] \to BV(0,T) : (u,\xi) \mapsto w, \tag{2.4}$$

that we name *completed relay operator,* Fig. 2(b). We use this denomination because k_ρ is the closure (w.r.t. suitable topologies that here we do not specify) of the relay operator of Fig. 2(a).

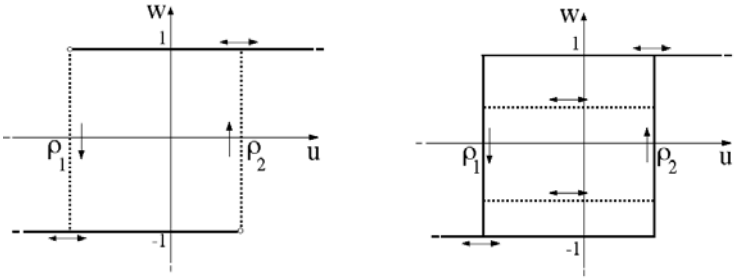

FIGURE 2. The relay operator and its completion are represented in part (a) and (b), respect.

Weak formulation. Now we reformulate the conditions (2.2) and (2.3) as inequalities. It is easy to see that (2.2) is equivalent to

$$\begin{aligned}&(w(t)-\eta)(u(t)-\xi)\geq 0\\&\forall(\xi,\eta)\in\big(]-\infty,\rho_1]\times\{-1\}\big)\cup\big([\rho_2,+\infty[\times\{1\}\big),\forall t\in\,]0,T].\end{aligned}\tag{2.5}$$

Moreover, as $dw=(dw)^+-(dw)^-$ and $|\,dw|=(dw)^++(dw)^-$, (2.3) is equivalent to

$$\begin{aligned}\int_0^t u\,dw&=\int_0^t\rho_2\,(dw)^+-\int_0^t\rho_1\,(dw)^-\\&=\frac{\rho_2+\rho_1}{2}\int_0^t dw+\frac{\rho_2-\rho_1}{2}\int_0^t|dw|\\&=\frac{\rho_2+\rho_1}{2}[w(t)-w(0)]+\frac{\rho_2-\rho_1}{2}\int_0^t|dw|=:\Psi_\rho(w;[0,t])\end{aligned}\tag{2.6}$$

for any $t\in\,]0,T]$ (these are Stieltjes integrals); cf. [31].

Notice that $\Psi_\rho(w;[0,t])$ depends on $w|_{[0,t]}$, thus also $w(0)$. It is easy to see that (2.2) entails that

$$u\,dw\leq\rho_2\,(dw)^+-\rho_1\,(dw)^-,\qquad\text{whence}\qquad\int_0^t u\,dw\leq\Psi_\rho(w;[0,t]),$$

independently from the dynamics. The opposite inequality is then equivalent to (2.6). Therefore the system (2.2) and (2.3) is equivalent to (2.5) coupled with

$$\int_0^t u\,dw\geq\Psi_\rho(w;[0,t])\qquad\forall t\in\,]0,T].\tag{2.7}$$

Vector relay. Let us set

$$\mathcal{P}:=\{\rho:=(\rho_1,\rho_2)\in\mathbf{R}^2:\rho_1<\rho_2\},\qquad S^2:=\{\vec\theta\in\mathbf{R}^3:|\vec\theta|=1\}.$$

For any $(\rho,\vec\theta)\in\mathcal{P}\times S^2$, along the lines of [8],[23] and Sect. IV.5 of [30], we introduce the multivalued (*completed*) *vector-relay operator:*

$$\vec k_{(\rho,\vec\theta)}:C^0([0,T])^3\times[-1,1]\to L^\infty(0,T)^3:(\vec u,\xi)\mapsto k_\rho(\vec u\cdot\vec\theta,\xi)\vec\theta.\tag{2.8}$$

The component of the input $\vec u$ in the direction $\vec\theta$ is here assumed as input of the scalar relay k_ρ; the output is then multiplied by the unit vector $\vec\theta$.

The characterization (2.5) and (2.7) of the scalar relay is easily extended to vectors. For any $(\rho,\vec\theta)\in\mathcal{P}\times S^2$ and any $(\vec u,\xi)\in C^0([0,T])^3\times[-1,1]$, $\vec w\in\vec k_{(\rho,\vec\theta)}(\vec u,\xi)$ if and only if $\vec w(t):=w(t)\vec\theta$ for any t, and

$$w(0)=\begin{cases}-1 & \text{if } \vec u(0)\cdot\vec\theta<\rho_1,\\ \xi & \text{if } \rho_1\leq\vec u(0)\cdot\vec\theta\leq\rho_2.\\ 1 & \text{if } \vec u(0)\cdot\vec\theta>\rho_2,\end{cases}\tag{2.9}$$

$$\begin{aligned}&(w(t)-\eta)(\vec{u}(t)\cdot\vec{\theta}-\xi)\geq 0\\&\forall(\xi,\eta)\in\big(]-\infty,\rho_1]\times\{-1\}\big)\cup\big([\rho_2,+\infty[\times\{1\}\big),\forall t\in]0,T],\end{aligned}\tag{2.10}$$

$$\int_0^t \vec{u}\cdot\vec{\theta}\,dw\geq\Psi_\rho(w;[0,t])\qquad\forall t\in]0,T].\tag{2.11}$$

Preisach model. This model was proposed by the physicist F. Preisach [28] in 1935 to represent scalar ferromagnetism, and was then also applied to model other hysteresis phenomena. Here we introduce the corresponding hysteresis operator. First, let us denote by $\mathcal{R}$ the family of Borel measurable functions $\mathcal{P}\to[-1,1]$, and by $\xi=\{\xi_\rho\}$ any element of $\mathcal{R}$. To any finite Borel measure μ over $\mathcal{P}$ we then associate the multivalued operator

$$\begin{aligned}&\mathcal{K}_\mu:C^0([0,T])\times\mathcal{R}\to L^\infty(0,T),\\&[\mathcal{K}_\mu(u,\xi)](t):=\int_{\mathcal{P}}[k_\rho(u,\xi_\rho)](t)\,d\mu(\rho)\qquad\forall t\in[0,T],\end{aligned}\tag{2.12}$$

that we name (completed) *Preisach operator.* Clearly this is a hysteresis operator. This representation may be regarded as a sort of *spectral resolution* of the operator itself.

Theorem 2.1. [6] *Let μ be a finite Borel measure over $\mathcal{P}$ and $\xi\in\mathcal{R}$. Then:*

$$\mathcal{K}_\mu(u,\xi)\in C^0([0,T])\qquad\forall u\in C^0([0,T])\tag{2.13}$$

if and only if (*setting $\mu:=0$ outside $\mathcal{P}$*)

$$|\mu|(\mathbf{R}\times\{r\})=|\mu|(\{r\}\times\mathbf{R})=0\qquad\forall r\in\mathbf{R}.\tag{2.14}$$

Moreover, whenever $\mathcal{K}_\mu(\cdot,\xi)$ operates from $C^0([0,T])$ to itself, it is also continuous in this space.

Under appropriate conditions on the Preisach measure μ, $\mathcal{K}_\mu(\cdot,\xi)$ operates in the Sobolev spaces $W^{1,p}(0,T)$ $(1\leq p\leq+\infty)$, or in the Hölder spaces $C^{0,\nu}([0,T])$ $(0<\nu\leq1)$, or in $C^0([0,T])\cap BV(0,T)$, see [6]. Other conditions on μ guarantee the existence of the inverse operator $\mathcal{K}_\mu^{-1}$, and yield its continuity.

Vector Preisach model. The Preisach model can be extended to vectors by integrating a family of vector relays w.r.t. a finite Borel measure ν over $\mathcal{P}\times S^2$. Let us denote by $\tilde{\mathcal{R}}$ the family of Borel measurable functions $\mathcal{P}\times S^2\to[-1,1]$, and by $\xi=\{\xi_{\rho,\vec{\theta}}\}$ any element of $\tilde{\mathcal{R}}$. We then define the multivalued (completed) vector Preisach operator as follows:

$$\begin{aligned}&\vec{\mathcal{K}}_\nu:C^0([0,T])^3\times\tilde{\mathcal{R}}\to L^\infty(0,T)^3,\\&\Big[\vec{\mathcal{K}}_\mu(\vec{u},\xi)\Big](t):=\iint_{\mathcal{P}\times S^2}\Big[\vec{k}_\rho(\vec{u}\cdot\vec{\theta},\xi_{\rho,\vec{\theta}})\Big](t)\,d\nu(\rho,\vec{\theta})\qquad\forall t\in[0,T].\end{aligned}\tag{2.15}$$

In alternative, at the expense of some generality, one might also use the following procedure:

(i) project the input onto any direction $\vec{\theta}$;
(ii) apply to it a scalar Preisach operator, which may depend on $\vec{\theta}$;
(iii) average these outputs with respect to a prescribed weight function, $\gamma(\vec{\theta})$.

The above operators can also be extended to space-distributed systems, by inserting the variable $x \in \Omega$ as a parameter.

3. On First-order P.D.E. with discontinuous hysteresis

A discontinuous hysteresis relation $w = \mathcal{F}(u)$ may represent the limit behavior of the time-relaxation dynamics associated to a nonmonotone relation. However if the variables u and w are also coupled by another equation, in particular by a P.D.E., the situation may be less clear. Difficulties may appear especially if the hysteresis operator occurs in the principal part of the P.D.E., as it is the case for the conservation law

$$\frac{\partial}{\partial t}[u + \mathcal{F}(u)] + \frac{\partial u}{\partial x} = f \qquad \text{in } \mathbf{R}\times]0, T[. \tag{3.1}$$

For $\mathcal{F}$ equal to a relay operator, well-posedness for the corresponding Cauchy problem was proved in [34], by means of the weak formulation of the relay that we just outlined; that result may easily be extended to $\mathcal{F}$ equal to a Preisach operator. Well-posedness of a weak formulation in the framework of the theory of accretive operators was also proved in Chap. VIII of [30].

In view of introducing a different equation, let $\varphi : \mathbf{R} \to \mathbf{R}$ be a noninvertible, Lipschitz-continuous function, as it is outlined in Fig. 3(a).

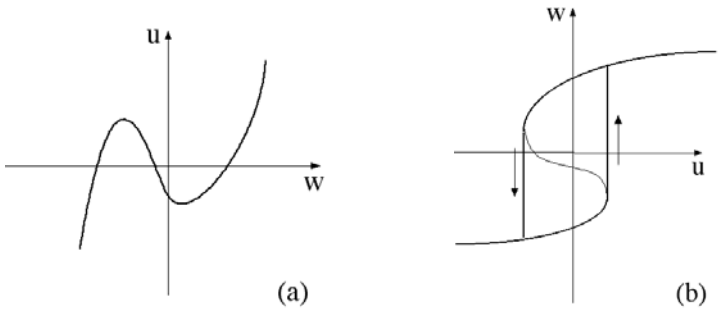

FIGURE 3. Nonmonotone relation in part (a); associated hysteresis loop in part (b).

The Cauchy problem for the semilinear system

$$\begin{cases} \dfrac{\partial w}{\partial t} + \dfrac{\partial u}{\partial x} - \eta \Delta w = f \\ u = \varphi(w) \end{cases} \qquad \text{in } \mathbf{R}\times]0,T[\ \ (\eta : \text{constant} > 0) \tag{3.2}$$

is well posed in natural function spaces, for any $T > 0$. After Kružkov [20] it is known that as $\eta \to 0$ the solution $w = w_\eta$ converges to the entropic solution of the first-order quasilinear equation

$$\frac{\partial w}{\partial t} + \frac{\partial \varphi(w)}{\partial x} = f \qquad \text{in } \mathbf{R}\times]0,T[. \tag{3.3}$$

An open question. The quasilinear system

$$\begin{cases} \dfrac{\partial w}{\partial t} + \dfrac{\partial u}{\partial x} - \eta \Delta u = f \\ u = \varphi(w) \end{cases} \qquad \text{in } \mathbf{R}\times]0,T[\ \ (\eta : \text{constant} > 0) \tag{3.4}$$

is less standard then (3.2) and looks rather challenging. In order to get some understanding of this setting, let us replace the nonmonotone condition $(3.4)_2$ by a relaxation dynamics, and consider the system

$$\begin{cases} \dfrac{\partial w}{\partial t} + \dfrac{\partial u}{\partial x} - \eta \Delta u = f \\ u = \varphi(w) + \lambda \dfrac{\partial w}{\partial t} \end{cases} \qquad \text{in } \mathbf{R}\times]0,T[\ \ (\eta, \lambda : \text{constants} > 0). \tag{3.5}$$

Let us see that this problem is well posed for any $\lambda > 0$. If in the argument of φ we replace w by some function v, a unique solution pair (u, w) is determined. By eliminating $\partial w/\partial t$ we then get

$$u - \varphi(v) + \lambda \frac{\partial u}{\partial x} - \lambda \eta \Delta u = \lambda f \qquad \text{in } \mathbf{R}\times]0,T[.$$

Adding initial- and boundary-conditions, this construction defines a Lipschitz-continuous operator $A : v \mapsto u$ in $L^2(\mathbf{R}\times]0,T[)$. The equation $A(v) = \varphi(v) + \lambda \partial w/\partial t$ then determines an operator $B : v \mapsto w$ in $L^2(\mathbf{R}\times]0,T[)$. It is easy to see that for T small enough B is contracting; hence it has a fixed-point, which solves (3.5) for small times. Reiterating the argument stepwise, existence of a solution for large times follows.

For a moment let us consider the relaxation dynamics $(3.5)_2$ independently of the equation $(3.5)_1$, and pass to the limit as $\lambda \to 0$. If it is assumed that the evolution of the variable w is pointwise controlled by that of u via $(3.4)_2$, it is known that the dependence of w on u exhibits hysteresis, as it is outlined in Fig. 3(b) (see, e.g., Chap. XI of [30]); accordingly, we write

$$w = \mathcal{F}(u), \quad \mathcal{F} \text{ being a discontinuous hysteresis operator.} \tag{3.6}$$

But if u and w are also coupled via the equation $(3.4)_1$, the feedback of w on u might modify this picture. Actually the analysis of the behavior of the system (3.5) as $\lambda \to 0$ seems to exhibit the same difficulties as the direct study of (3.4).

An alternative approach. On account of the drawback we just indicated, a different formulation was introduced in [32] for a similar problem. On the basis of a heuristic argument, the relation $u = \varphi(w)$ was replaced by (3.6), for instance with $\mathcal{F} = \alpha + k_\rho$, where α is a nondecreasing and continuous real function and k_ρ is a completed relay operator. Now we apply that approach to the equation (3.1), replacing α by the identity for the sake of simplicity. One can show that, up to a subsequence, as $\eta \to 0$ the solution of the system

$$\begin{cases} \dfrac{\partial w}{\partial t} + \dfrac{\partial u}{\partial x} - \eta \Delta u = f \\ w \in u + k_\rho(u) \end{cases} \qquad \text{in } \mathbf{R}\times]0,T[\ \ (\eta : \text{constant} > 0) \tag{3.7}$$

tends to one of

$$\begin{cases} \dfrac{\partial w}{\partial t} + \dfrac{\partial u}{\partial x} = f \\ w \in u + k_\rho(u) \end{cases} \qquad \text{in } \mathbf{R}\times]0,T[. \tag{3.8}$$

More precisely, for any $\eta > 0$ let (u_η, w_η) be the solution of the Cauchy problem for (3.7). Then there exists a pair (u, w) such that, as $\eta \to 0$ along a suitable sequence,

$$\begin{aligned} &u_\eta \to u \quad \text{strongly in } L^1(\mathbf{R}\times]0,T[), \\ &w_\eta \to w \quad \text{weakly in } L^1(\mathbf{R}\times]0,T[); \end{aligned} \tag{3.9}$$

moreover (u, w) is a solution of the analogous Cauchy problem for the system (3.8). This may be shown as follows. First multiplying the equation $(3.7)_1$ by u_η, a uniform-in-η estimates for u_η in $L^\infty(0,T;L^2(\mathbf{R}))$ is obtained. In view of deriving further a priori estimates, let us approximate the sign graph by a sequence $\{s_j\}$ of smooth functions, apply the time-increment operator δ to $(3.7)_1$, and multiply it by $s_j(\delta u_\eta)$ for any $j \in \mathbf{N}$. A remarkable inequality due to Hilpert [14] yields

$$\delta k_\rho(u_\eta) s_j(\delta u_\eta) \geq |\delta k_\rho(u_\eta)|. \tag{3.10}$$

This yields uniform-in-η estimates for δu_η and $\delta k_\rho(u_\eta)$ in $L^1(\mathbf{R}\times]0,T[)$. A comparison in the approximate equation then yields a uniform estimate for $\partial u_\eta/\partial x$ in the same space. Therefore (3.9) holds for suitable u, w, and we can perform the limit procedure; see [34] for details.

As an alternative approximation technique, one might also insert a time-relaxation in $(3.8)_2$:

$$\begin{cases} \dfrac{\partial w}{\partial t} + \dfrac{\partial u}{\partial x} = f \\ w \in u + k_\rho\Big(u - \lambda \dfrac{\partial w}{\partial t}\Big) \end{cases} \qquad \text{in } \mathbf{R}\times]0,T[\ \ (\lambda : \text{constant} > 0). \tag{3.11}$$

As λ vanishes, the associated Cauchy problem converges to that of (3.8) in this case, too.

A further question. The following equation arises in modelling traffic flow, see, e.g., [13]:

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial w}{\partial x} = f & \text{in } \mathbf{R}\times]0,T[, \\ u = \varphi(w) \end{cases} \tag{3.12}$$

with $\varphi : \mathbf{R} \to \mathbf{R}$ a nonmonotone. In alternative, one might also consider the system

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial w}{\partial x} = f & \text{in } \mathbf{R}\times]0,T[. \\ w \in u + k_\rho(u) \end{cases} \tag{3.13}$$

It is not clear whether and how the two latter systems might be related each other; moreover, for either equation it is not obvious that the associated Cauchy problem has a solution.

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