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Geometric Patterns and Microstructures in the study of Material Defects and Composites

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Doctor of Philosophy in Mathematics

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Declaration

I hereby declare that this Thesis is submitted at the University of Sussex only, for the title of Doctor of Philosophy in Mathematics. I also declare that this Thesis was composed by myself, under the supervision of Mariapia Palombaro, and that the work contained therein is my own, except where stated otherwise, such as citations.

Brighton, January 2, 2018,

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(Silvio Fanzon)

Abstract

The main focus of this PhD thesis is the study of *microstructures* and *geometric patterns* in *materials*, in the framework of the *Calculus of Variations.* My PhD research, carried out in collaboration with my supervisor Mariapia Palombaro and Marcello Ponsiglione, led to the production of three papers [21, 22, 23]. Papers [21, 22] have already been published, while [23] is currently in preparation.

This thesis is divided into two main parts. In the first part we present the results obtained in [22, 23]. In these two works *geometric patterns* have to be understood as patterns of *dislocations in crystals.* The second part is devoted to [21], where suitable *microgeometries* are needed as a mean to produce gradients that display critical integrability properties.

Contents

Chapter 1

Introduction

The main focus of this PhD thesis is the study of *microstructures* and *geometric patterns* in *materials*, in the framework of the *Calculus of Variations*. My PhD research, carried out in collaboration with my supervisor M. Palombaro and M. Ponsiglione, led to the production of three papers [21, 22, 23]. Papers [21, 22] have already been published, while [23] is currently in preparation.

This thesis is divided into two main parts. In Part I we present the results obtained in [22, 23]. In these two works *geometric patterns* have to be understood as patterns of *dislocations in crystals*. Part II is devoted to [21], where suitable *microgeometries* are needed as a means to produce gradients that display critical integrability properties.

We will now give a brief overview of Part I. A wide class of materials, such as metals, are *crystalline*, that is, their atoms are arranged in patterns repeated periodically. Ideal crystals consist of superposed layers of crystallographic planes, resulting into a periodic structure replicated throughout the whole material (see Figure 1.1 Left). However, real materials rarely exhibit this long range periodicity. In fact, their periodic atomic structure is disturbed by the presence of *defects*, that are usually classified according to their dimension. One dimensional defects are called *dislocations*, which can be visualised as the boundary lines of crystallographic planes that end within the crystal (see Figure 1.1 Right). *Phase boundaries* and *grain boundaries* are instead two dimensional defects. In certain situations their structure is composed by a *network* of so-called *edge dislocations*. This is for example the case, respectively, of *semi-coherent interfaces* in two-phase materials and of *small*

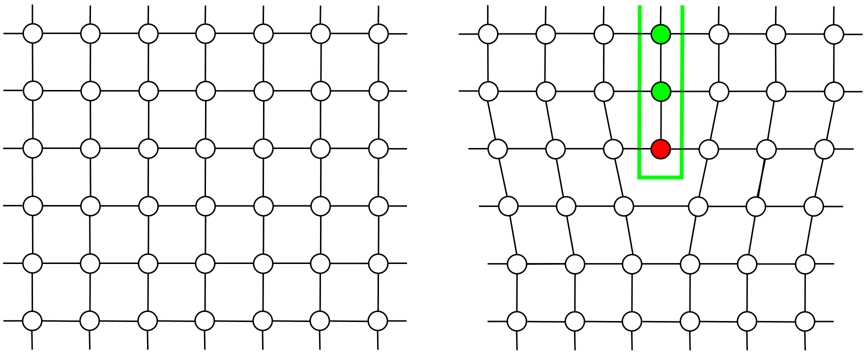


Figure 1.1: Left: cross section of an ideal crystal. Circles are atoms. Lines are atomic bonds. Right: an edge dislocation. The green line of atoms represents a crystallographic plane ending within the crystal. The red atom is an edge dislocation.

angle tilt gran boundaries in single phase materials.

A *semi-coherent interface* forms when two crystalline materials with *different phases*, that is different underlying atomic structures, are joined together at a flat interface. The different atomic structures induce a *mismatch* at the interface. It is well known that when the mismatch is small, it is accommodated by two non parallel arrays of edge dislocations, opportunely spaced (see e.g. [53, Ch 3.4]).

In [22] we analyse a *semi-discrete model* for dislocations at *semi-coherent interfaces*. We consider the case of a flat two dimensional interface between two crystalline materials with different underlying lattice structures Λ^+ and Λ^-. We assume that the lattice Λ^+, lying on top of Λ^-, is a dilation with factor $\alpha > 1$ of a cubic lattice Λ^- of spacing b. The semi-coherent behaviour corresponds to small misfits $\alpha \approx 1$. Since in the reference configuration (where both crystals are in equilibrium) the density of the atoms of Λ^+ is lower than that of Λ^-, in the vicinity of the interface there are many atoms having the "wrong" coordination number, that is, the wrong number of nearest neighbours. Such atoms form line singularities that correspond to edge dislocations. In particular we prove that a *periodic square network* of *edge dislocations* at the interface is optimal in scaling, and we compute the optimal dislocation spacing, which coincides with $\delta = b/(\alpha - 1)$ (see Figure 1.2). Moreover, based on the above analysis, we propose and study a simpler *continuum* variational model to describe this phenomena. The energy functional we consider describes the

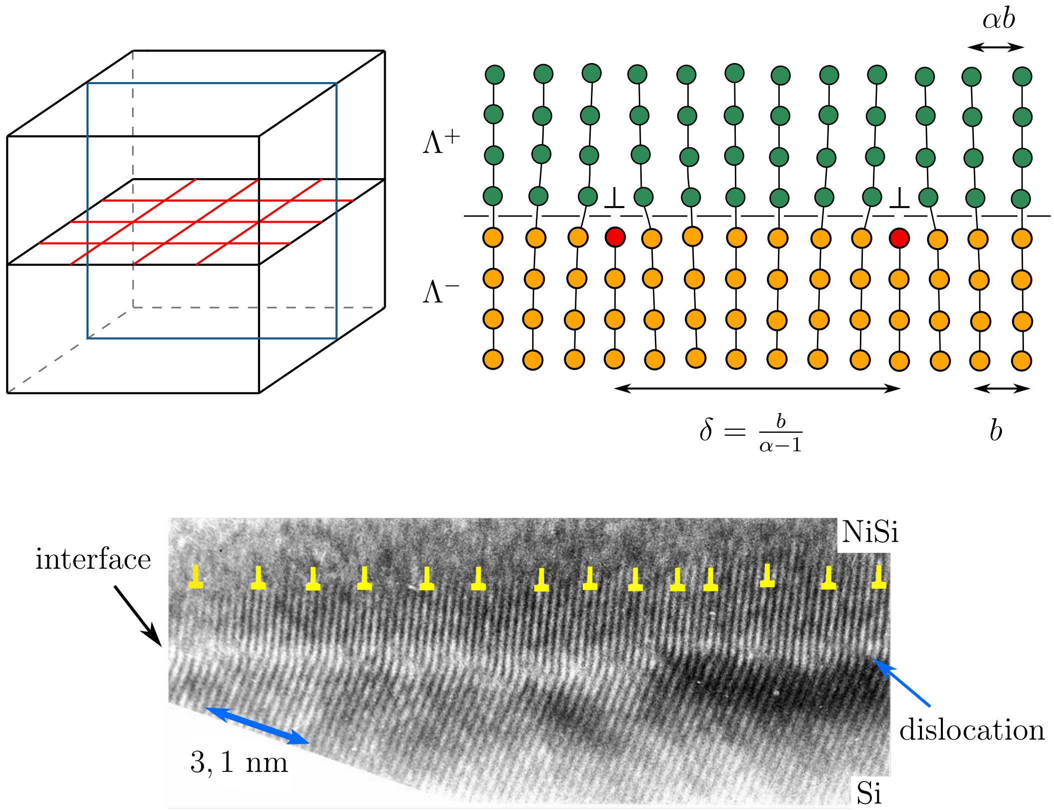


Figure 1.2: Top Left: a schematic picture of the 3D crystal. The red lines at the interface are edge dislocations. The blue square is a 2D slice. Top Right: schematic atomic picture of the 2D slice. Orange and green atoms belong to Λ^- and Λ^+ respectively. The red atoms are edge dislocations (denoted by $\perp$). Bottom: HRTEM picture of a phase boundary between Si (silicon) and NiSi (nickel-silicon). The interface is semi-coherent (light region in the picture), and a periodic network of edge dislocations is observed: the yellow $\perp$ symbols lie vertically above the dislocations, which are located at the interface (image from [26, Section 8.2.1], with permission of the author H. Foell).

competition between two terms: a *surface energy* induced by dislocations and a bulk *elastic energy*, spent to decrease the amount of dislocations needed to compensate the lattice misfit. By means of Γ-convergence, we are able to prove that the former scales like the surface area of the interface and the latter like its diameter. Therefore, for large interfaces, nucleation of dislocations is energetically favourable. Even if we deal with finite elasticity, linearised elasticity naturally emerges in our analysis since the far field strain vanishes as the interface size increases.

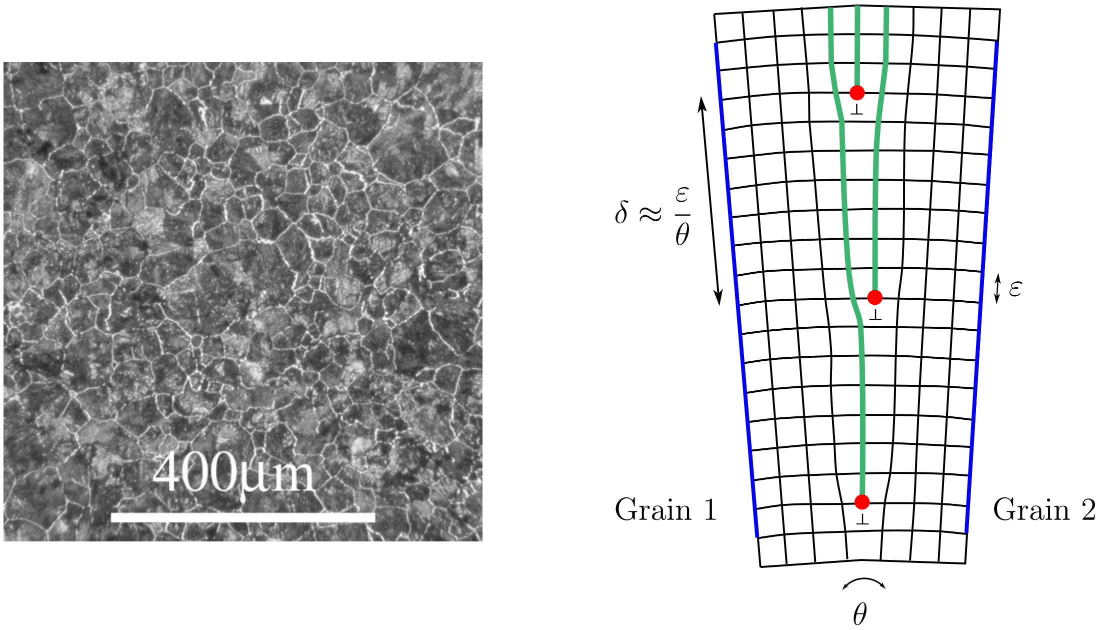


Figure 1.3: Left: section of an iron-carbon alloy. The darker regions are single crystal grains, separated by grain boundaries that are represented by lighter lines (source [59], licensed under CC BY-NC-SA 2.0 UK). Right: schematic picture of a SATGB. The two grains are joined together and the lattice misfit at the interface is accommodated by an array of edge dislocations. The green lines represent lines of atoms ending within the crystal. Their end points inside the crystal are edge dislocations (denoted with $\perp$). The blue lines show the mutual rotation θ between the grains (picture after [54]).

Grain boundaries are two dimensional defects in *single-phase* crystalline materials. A wide class of materials, such as metals, display a polycrystalline behaviour. A *polycrystal* is formed by many individual *crystal grains*, all having the same underlying atomic structure, rotated with respect to each other. The interface that separates two grains with different orientation is called *grain boundary* (see Figure 1.3 Left). Since the grains are mutually rotated, the periodic crystalline structure is disrupted at the interface. As a consequence, grain boundaries are regions of high energy concentration, since the ground state of the energy is given by a single grain.

Let us consider the case of *small angle tilt grain boundaries* (SATGB) in dimension two. In SATBGs, the lattice mismatch between two grains mutually tilted by a small angle θ, is accommodated by a single array of *edge dislocations* at the grain boundary, evenly spaced at distance $\delta \approx \varepsilon/\theta$, where ε is the atomic distance (see [31, Ch 3.4]). In this way, the number of dislocations at a SATGB is of order θ/ε

(see Figure 1.3 Right).

The aim of our paper [23] is to derive by Γ-convergence, as the lattice spacing $\varepsilon \to 0$ and the number of dislocations $N_\varepsilon \to \infty$, a limit energy functional $\mathcal{F}$, whose minimisers display a *polycrystalline behaviour*. We work in the hypothesis of linearised planar elasticity for the material in exam, so that the corresponding variational problem is two dimensional. Dislocations are modelled as point topological defects of the strain fields. The elastic energy is then computed outside the so-called *core region* of radius ε. The energy contribution of a single dislocation core is of order $|\log \varepsilon|$, therefore for a system of N_ε dislocations, the relevant energy regime is

$$E_\varepsilon \approx N_\varepsilon |\log \varepsilon| \,.$$

This scaling was studied in [30] in the critical regime $N_\varepsilon \approx |\log \varepsilon|$. For our analysis we will consider a higher energy regime corresponding to a number of dislocations N_ε such that

$$N_\varepsilon \gg |\log \varepsilon| \,.$$

We will see that this energy regime will account for polycrystals containing grains that are mutually rotated by an *infinitesimal* angle $\theta \approx 0$. To be more specific, we show that the energy functional E_ε, rescaled by $N_\varepsilon |\log \varepsilon|$, Γ-converges as $\varepsilon \to 0$ to a certain functional $\mathcal{F}$, whose dependence on the *elastic* and *plastic* parts of the strain is *decoupled*. Imposing *piecewise constant* Dirichlet boundary conditions on the plastic part of the limit strain, we then show that $\mathcal{F}$ is minimised by strains that are *locally constant* and take values into the set of *antisymmetric matrices*. We call these strains *linearised polycrystals*. This definition is motivated by the fact that *antisymmetric matrices* can be considered as infinitesimal rotations, being the linearisation around the identity of the space of rotations.

Part II of this thesis concerns *composites*. Composites are materials constituted by two or more materials, referred to as *phases*, having different properties. The properties of the resulting composite will depend both on its constituents and on their arrangement. The main difference with the structures considered in Part I, is that composites are non-homogeneous on length scales larger than the atomic scale, but they are homogenous at macroscopic scales.

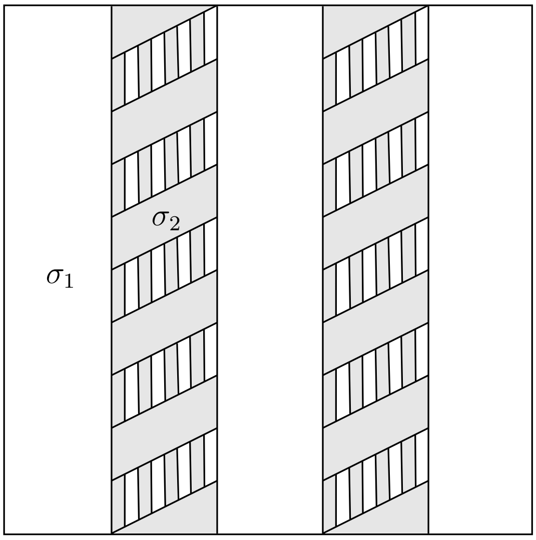


Figure 1.4: A schematic picture of a laminate material. The white portions represent the phase σ_1 while the grey ones represent σ_2.

We focus on the case of composites consisting of two phases having different *electrical conductivities*. The interesting physical question here is to determine how much the electric field can *concentrate*. Mathematically such composites can be modelled by a bounded domain $\Omega \subset \mathbb{R}^2$. The *electric field* $\nabla u \colon \Omega \to \mathbb{R}^2$ then satisfies the equation

$$\operatorname{div}(\sigma \nabla u) = 0\,, \tag{1.1}$$

where σ is a *two-phase conductivity* of the form

$$\sigma = \chi_{E_1}\sigma_1 + \chi_{E_2}\sigma_2\,.$$

Here σ_1, σ_2 are 2×2 constant elliptical matrices and $\{E_1, E_2\}$ is a non trivial measurable partition of Ω. The latter represents the arrangement of the two phases within the composite. Concentration phenomena of the electric field are for example observed when the composite is obtained by layering the phases σ_1 and σ_2 in slices that become thinner and thinner, as displayed in Figure 1.4. These types of structures are called (higher-order) laminates ([41, Ch 9]). The corresponding partition $\{E_1, E_2\}$ defines then a *microgeometry* on Ω, which determines the integrability properties of ∇u.

The study of the integrability properties of ∇u relies on the following fundamental result by Astala [4]: there exist exponents q and p, with $1 < q < 2 < p$, such that if $u \in W^{1,q}(\Omega)$ is a distributional solution to (1.1), then $\nabla u \in L^p_{\text{weak}}(\Omega)$. In

[48] the exponents p and q have been characterised for every pair of elliptic matrices σ_1 and σ_2. More precisely, denoting by $p_{\sigma_1,\sigma_2} \in (2, +\infty)$ and $q_{\sigma_1,\sigma_2} \in (1, 2)$ such exponents, the authors prove that, if $u \in W^{1,q_{\sigma_1,\sigma_2}}(\Omega)$ is a solution to (1.1), then $\nabla u \in L^{p_{\sigma_1,\sigma_2}}_{\text{weak}}(\Omega; \mathbb{R}^2)$. They also show that the upper exponent p_{σ_1,σ_2} is *optimal*, in the sense that there exists a conductivity $\bar{\sigma} \in L^\infty(\Omega; \{\sigma_1, \sigma_2\})$ and a weak solution $u \in W^{1,2}(\Omega)$ to (1.1) with $\sigma = \bar{\sigma}$, satisfying affine boundary conditions and such that $\nabla u \notin L^{p_{\sigma_1,\sigma_2}}(\Omega; \mathbb{R}^2)$.

In [21] we complement the above result by proving the *optimality* of the *lower exponent* q_{σ_1,σ_2}. Precisely, we show that for every arbitrarily small δ, one can find a particular conductivity $\bar{\sigma} \in L^\infty(\Omega; \{\sigma_1, \sigma_2\})$ for which there exists a solution u to (1.1) with $\sigma = \bar{\sigma}$, such that u is affine on $\partial\Omega$ and $\nabla u \in L^{q_{\sigma_1,\sigma_2}-\delta}(\Omega; \mathbb{R}^2)$, but $\nabla u \notin L^{q_{\sigma_1,\sigma_2}}(\Omega; \mathbb{R}^2)$. The existence of such *optimal microgeometries* is achieved by *convex integration methods*, adapting to the present setting the geometric constructions provided in [5] for isotropic conductivities.

This thesis is organised as follows. In Part I we will discuss about geometric patterns of dislocations, presenting our papers [22, 23]. In Chapter 2 we will give a brief review of elasticity theory, introducing rigorously the concept of dislocation (Section 2.1). In Section 2.2 we introduce the variational approach to elasticity, showing how dislocations can be modelled from the mathematical point of view. In Section 2.3 we discuss some important rigidity results. Chapter 3 is dedicated to the presentation of [22], where we introduce and analyse a model for dislocations at semi-coherent interfaces. In Chapter 4 we discuss [23], in which we study a variational model for linearised polycrystals.

Part II is dedicated to the study of microgeometries in composite materials. In Chapter 5 we will present the results obtained in our paper [21]. A fundamental tool to prove such results is convex integration, that we introduce in Section 5.3.1.

The Appendix is dedicated to Calculus of Variations and Geometric Measure Theory, where we collect definitions and results that are useful throughout our analysis. In Section A.1 we introduce the direct method and Γ-convergence. In Section A.2 we define measures and we discuss their main properties, focusing in particular on finite Radon measures. Finally, in Section A.3, we review functions with bounded variation and sets of finite perimeter.

Part I

Geometric Patterns of Dislocations

Chapter 2

Variational approach to Elasticity Theory

Before proceeding with the presentation of the contents of our papers [22, 23], we want to establish the variational formulation of elasticity theory, adopted throughout Part I.

This chapter is structured as follows. In Section 2.1 we will introduce, with a geometrical construction, the concept of dislocation. We will see how two basic types of straight line dislocations, called edge and screw, are sufficient to understand all the possible line defects in a crystal. In Section 2.2 we will lay the mathematical foundations to the variational approach to elasticity theory used in the following chapters. In particular we will define dislocations as line defects of the deformation strain. Finally, in Section 2.3 we will rigorously introduce the concept of microstructure, and recall some well-known rigidity results that will be used in the following analysis.

2.1 Dislocations

In this section we want to rigorously define *dislocations*. As already mentioned in the Introduction, a wide class of materials are *crystalline*, that is, their atoms are arranged in patterns repeated periodically. Ideal crystals consist of superposed layers of crystallographic planes, resulting into a periodic structure replicated throughout the whole material (Figure 2.1c). However, in general, real materials do not exhibit long range periodicity. In fact, their periodic atomic structure is disturbed by the presence of *defects*. One dimensional defects (line defects) are called dislocations (see, e.g., [31, 47, 53, 54]). Dislocations are of fundamental importance in crystals. In fact, dislocations motion represents the microscopic mechanism of plastic deformation ([31, Ch 7]). Another important role of dislocations is decreasing the energy induced by lattice misfits. In this case, dislocations arranged in periodic networks form two dimensional defects, such as semi-coherent interfaces (see Chapter 3) and small angle grain boundaries (Chapter 4)

Dislocations can be generated through a theoretical procedure of cut and displacement within the ideal crystal. Let γ be the boundary, within the crystal, of such cut. When γ is straight, we talk about *straight line* dislocations. If the displacement is orthogonal to γ, this generates an *edge dislocation*, while if it is parallel, it generates a *screw dislocation*. A generic dislocation can be decomposed into edge and screw components, as we will see later in this section.

2.1.1 Edge dislocations

We will now illustrate the theoretical procedure of cut and displacement in the case of edge dislocations. First, cut the ideal crystal along the plane $ABCD$ and then apply a shear in both directions orthogonal to $\gamma := BC$ (see Figure 2.1a). The plane $ABCD$ is called *slip plane*. In this way we displace the top surface of the cut one lattice spacing over the bottom surface, in the direction γ. This displacement results in an extra half plane of atoms $BCEF$ above γ (Figure 2.1b). We define the *dislocation line* as the boundary within the crystal of the slip plane, that is, γ. Every point in the slip plane has been displaced by a vector $\xi \in \mathbb{R}^3$. We say that ξ is the *Burgers vector* of the dislocation. A dislocation can be uniquely identified by the pair (γ, ξ) of dislocation line and Burgers vector. Notice that, for edge dislocations, the Burgers vector is always *orthogonal* to the dislocation line. In Section 2.2 we will see that, if β is the strain that induces that displacement in Figure 2.1b, then the Burgers vector coincides with the circulation of β along any closed path around γ (blue path in Figure 2.1b). If the path does not enclose γ, then the circulation is zero (Figure 2.1a).

Let us analyse the above procedure from the microscopic point of view. Consider

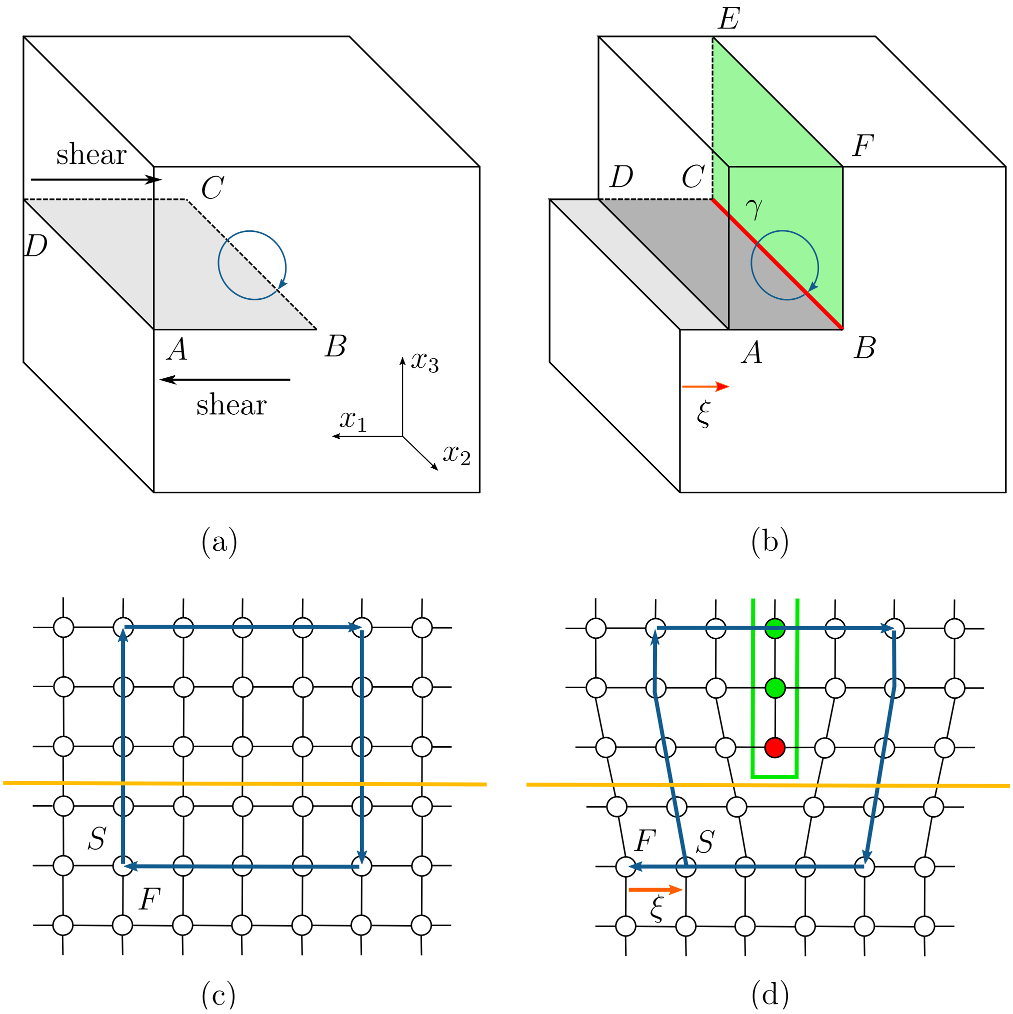


Figure 2.1: (a): ideal crystal cut along $ABCD$. A shear parallel to AB is applied. (b): the top part of $ABCD$ is displaced by ξ, the Burgers vector. The boundary of $ABCD$ is the dislocation line γ. An extra half-plane of atoms $BCEF$ lies on top of γ. (c): atomic cross section of the ideal crystal in (a). Circles are atoms and black lines are atomic bonds. The blue path is the Burgers circuit. (d): cross section of the displaced crystal in (b). The red atom belongs to γ. The green line of atoms belongs to $BCEF$. The closing failure of the Burgers circuit coincides with ξ.

any cross section of the crystal orthogonal to the x_2-axis. The cross sections of Figures 2.1a and 2.1b are represented in Figures 2.1c and 2.1d respectively. The circles represent atoms and the black lines represent atomic bonds (we are assuming that the underlying atomic lattice is cubic). We can obtain the edge dislocation in 2.1b by either repeating the above procedure or by inserting a vertical half-plane of

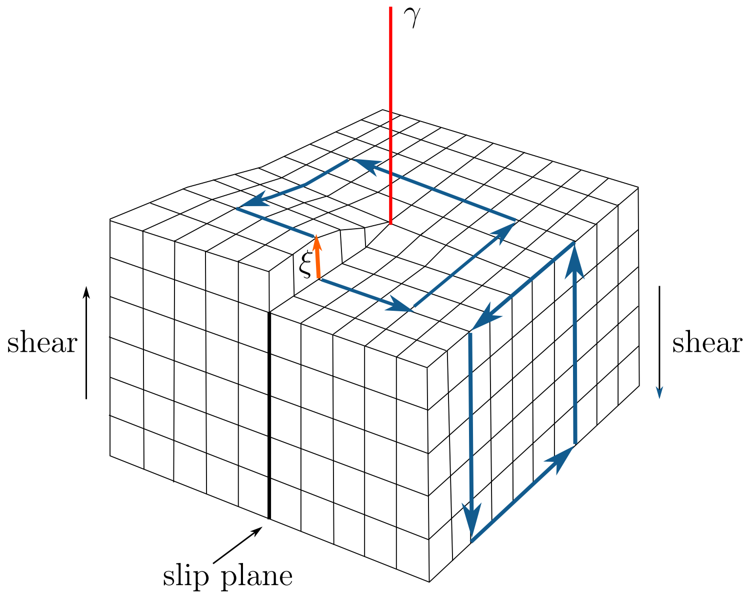


Figure 2.2: The ideal crystal in Figure 2.1a is cut along the plane $ABCD$. A shear parallel to γ is applied, generating a screw dislocation along γ. The blue paths are Burgers circuits. The closing failure of the Burgers circuit around γ defines the Burgers vector ξ, which is parallel to γ.

atoms in the reference configuration in Figure 2.1c. Both procedures yield a line of atoms γ having the "wrong" number of first neighbours (red atom in Figure 2.1d). The Burgers vector can be defined by means of a "discrete" circulation, as follows. Consider a closed path, called *Burgers circuit*, in the reference configuration starting from S and ending at F (as illustrated in Figure 2.1c). This circuit is the discrete analogous of the continuous path displayed in 2.1a. If we follow the same atom to atom path in the deformed configuration (as shown in Figure 2.1d), the circuit fails to close. We define the vector necessary to close the path, i.e. the vector from F to S, as the Burgers vector of the dislocation. Notice that this definition is independent of the path chosen (as long as it includes the dislocation line). The discrete and continuum definitions of dislocation line and Burgers vector coincide.

2.1.2 Screw dislocations

We can generate another type of dislocation by cutting the ideal crystal in Figure 2.1a along the plane $ABCD$ and applying a shear parallel to γ. In this way if one moves along a loop around γ, one never returns to the starting point, but rather one "climbs" by one atomic lattice spacing, as displayed in Figure 2.2. For this

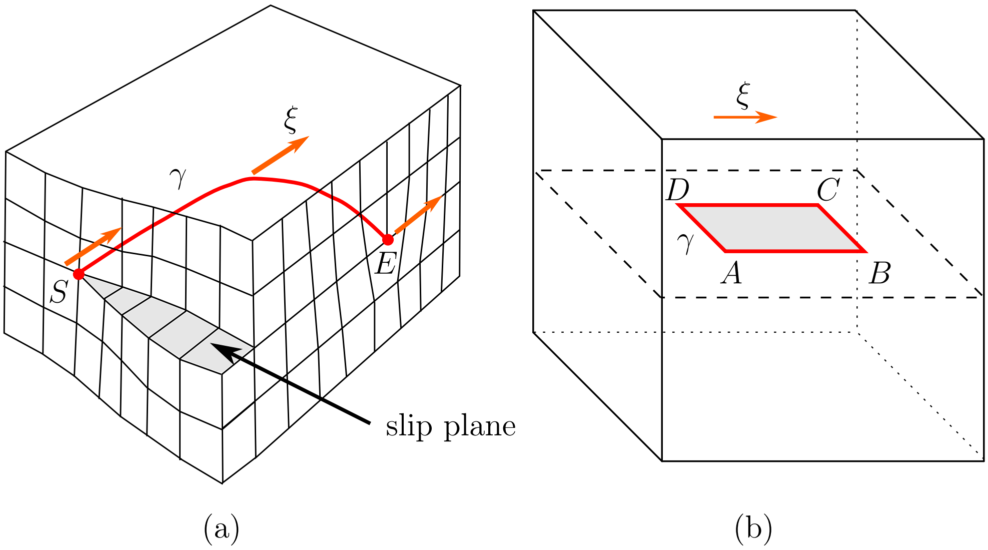


Figure 2.3: (a): curved dislocation line γ, changing from screw dislocation at S to edge dislocation at E. (b): dislocation loop $\gamma \subset \Omega$. Dislocations are of edge type along BC and DA, and of screw type along AB and CD.

reason, this dislocation is called of *screw* type. Formally, by considering a Burgers circuit around γ, the closing failure is given by the vector ξ, which is parallel to the dislocation line γ.

2.1.3 Mixed type dislocations

Through the same procedure of cut and displacement, we can generate other types of line defects. In fact, the boundary γ of the cut can be a generic curve. However, the displacement happens only in one direction, namely the direction of the Burgers vector ξ. For this reason, while the Burgers vector remains constant, the nature of the dislocation can change along γ, and it will depend on the angle formed by the Burgers vector ξ and $\dot{\gamma}(x)$, where $\dot{\gamma}(x)$ is the unit tangent vector to the curve γ at $x \in \mathbb{R}^3$. For example, in Figure 2.3a the dislocation changes from screw type at the point S, to edge type at E and it is a composition of the two in the other points along γ.

By definition of slip plane, its boundary γ cannot end within the crystal. However it is possible to have a *dislocation loop*, as shown in Figure 2.3b. In this case the dislocation is of screw type along the sides AB and CD, since ξ is parallel to these sides, and of edge type along BC and DA, since ξ is orthogonal to these sides.

2.2 Variational approach

2.2.1 Nonlinear elasticity

The main idea behind the variational approach to elasticity is to model an ideal crystal as a nonlinearly elastic continuum. The stress-free reference configuration of the crystal is identified with a bounded domain $\Omega \subset \mathbb{R}^3$. In classical elasticity (see, e.g, [10]) a *deformation* of the crystal is a regular map $v \colon \Omega \to \mathbb{R}^3$. We call $\beta := \nabla v \colon \Omega \to \mathbb{M}^{3\times 3}$ the *deformation strain* associated to v. The nonlinear elastic energy associated to the strain β is defined by

$$E(\beta) := \int_\Omega W(\beta)\, dx\,, \tag{2.1}$$

where $W \colon \mathbb{M}^{3\times 3} \to [0, +\infty)$ is a continuous map, called *stored energy density*. The basic assumption of the variational approach is that any equilibrium configuration will be a minimiser of (2.1).

The underlying crystalline structure enters this approach as properties of W. The assumption that the reference configuration is an equilibrium reads as

$$W(I) = 0\,, \tag{2.2}$$

where I is the identity matrix. Further, we assume that W is *frame indifferent*, i.e.,

$$W(F) = W(RF)\,, \quad \text{for every} \quad F \in \mathbb{M}^{3\times 3},\ R \in SO(3)\,,$$

where $SO(3) := \{R \in \mathbb{M}^{3\times 3} :\ R^T R = I, \det R = 1\}$ is the set of three dimensional rotations. Finally we will make growth assumptions on W. To be more specific, consider the scalar product

$$A : B := \sum_{i,j=1}^{3} a_{ij} b_{ij}$$

on $\mathbb{M}^{3\times 3}$, which induces the norm $|F| := \sqrt{F : F} = \sqrt{\operatorname{Tr} F^T F}$, where $\operatorname{Tr} F$ denotes the trace of F. Define the distance

$$\operatorname{dist}(F, SO(3)) := \min\{|F - R| :\ R \in SO(3)\}\,.$$

We will assume that there exists a positive constant C such that

$$C^{-1} \operatorname{dist}^2(F, SO(3)) \leq W(F) \leq C \operatorname{dist}^2(F, SO(3))\,, \tag{2.3}$$

for every $F \in \mathbb{M}^{3\times 3}$.

2.2.2 Linear elasticity

When the deformation $v\colon \Omega \to \mathbb{R}^3$ is small, we can replace the energy in (2.1) with a linear energy. To make this statement precise, consider the decomposition

$$v = x + \varepsilon u \,.$$

The map $u\colon \Omega \to \mathbb{R}^3$ is called *displacement* and $\varepsilon > 0$ is a small parameter. Here we will assume $u \in W^{1,\infty}(\Omega;\mathbb{R}^3)$, so that ∇u is uniformly bounded. The linear elastic energy associated to $v = x + \varepsilon u$ is computed directly on ∇u and it is defined by

$$E(\nabla u) := \int_\Omega \mathbb{C}\, \nabla u^{\mathrm{sym}} : \nabla u^{\mathrm{sym}}\, dx \,, \tag{2.4}$$

where $\nabla u^{\mathrm{sym}} := (\nabla u + \nabla u^T)/2$ is the symmetric part of the displacement gradient and $\mathbb{C}$ is a fourth order tensor.

The linear energy (2.4) can be deduced, as $\varepsilon \to 0$, from the nonlinear energy defined in (2.1). Indeed, the idea is that $\nabla v = I + \varepsilon \nabla u \to I$ uniformly as $\varepsilon \to 0$, therefore we have

$$\lim_{\varepsilon \to 0} \int_\Omega W(\nabla v)\, dx = \lim_{\varepsilon \to 0} \int_\Omega W(I + \varepsilon \nabla u)\, dx = 0 \,,$$

since $W(I) = 0$. Hence we can linearise W about the equilibrium I. In order to do that, in addition to the hypothesis in Section 2.2.1, assume also that W is C^2 in a neighbourhood of the identity matrix and that the equilibrium is stress-free, namely

$$\partial_F W(I) = 0 \,. \tag{2.5}$$

Notice that, by frame indifference, there exists a map $V\colon \mathbb{M}^{3\times 3}_{\mathrm{sym}} \to [0,+\infty)$ defined by the identity

$$W(F) = V\left(\frac{F^T F - I}{2} \right) \quad \text{for every} \quad F \in \mathbb{M}^{3\times 3} \,. \tag{2.6}$$

Here $\mathbb{M}^{3\times 3}_{\mathrm{sym}}$ denotes the set of 3×3 symmetric matrices. The assumptions on W imply that V is C^2 in a neighbourhood of $E = 0$ and that

$$V(0) = 0 \quad \text{and} \quad \partial_E V(0) = 0 \,. \tag{2.7}$$

Therefore, by Taylor expansion we get

$$V(E) = \frac{1}{2} \mathbb{C} E : E + o(|E|^2) \,, \tag{2.8}$$

for every $E \in \mathbb{M}^{3\times3}_{\rm sym}$, where $\mathbb{C}$ is the fourth order stress-tensor obtained by writing the bilinear form $\partial^2_E V(0) \colon \mathbb{M}^{3\times3}_{\rm sym} \times \mathbb{M}^{3\times3}_{\rm sym} \to \mathbb{R}$ in euclidean coordinates. We note that growth assumptions (2.3) imply that

$$C^{-1}|E|^2 \leq \mathbb{C}E : E \leq C|E|^2 \quad \text{for every} \quad E \in \mathbb{M}^{3\times3}_{\rm sym}\,, \tag{2.9}$$

for some constant $C > 0$ (see, e.g., [15]).

From (2.6) we obtain

$$W(\nabla v) = V\left(\varepsilon \nabla u^{\rm sym} + \frac{\varepsilon^2}{2} C(u)\right)\,, \tag{2.10}$$

where $C(u) := \nabla u^T \nabla u$ is the (right) Cauchy-Green strain tensor. Since ∇u is bounded, we can apply (2.8) to (2.10) and obtain

$$W(\nabla v) = W(I + \varepsilon \nabla u) = \frac{\varepsilon^2}{2} \mathbb{C}\, \nabla u^{\rm sym} : \nabla u^{\rm sym} + o(\varepsilon^2)\,,$$

uniformly in $x \in \Omega$. Therefore

$$\lim_{\varepsilon\to0} \frac{1}{\varepsilon^2} \int_\Omega W(I + \varepsilon\nabla u)\, dx = \int_\Omega \mathbb{C}\, \nabla u^{\rm sym} : \nabla u^{\rm sym}\, dx\,, \tag{2.11}$$

which justifies, at least pointwise, the use of (2.4) for small deformations. It is possible to prove that the limit in (2.11) holds true also for minimisers, by means of Γ-convergence. This result was obtained in [15] and we will present it in more detail in Section 3.4.2, since it will be needed for our analysis.

2.2.3 Line defect model

We now want to introduce dislocations in the nonlinear model described in Section 2.2.1. In this thesis (Chapters 3 and 4) dislocations are defined as line defects of the strain field β (see, e.g., [8, 18, 22, 23, 30, 43]). Indeed this approach is a hybrid between microscopic and continuous description, and it is referred to as *semi-discrete* model. The underlying crystalline structure enters the analysis as a small parameter $\varepsilon > 0$, referred to as *core radius*, which is proportional to the atomic distance. We will assume that dislocation lines are at a distance of 2ε at least. The set of slip directions for the crystal is

$$\mathcal{S} := \{\xi_1, \dots, \xi_s\}$$

where ξ_j are the Burgers vectors, depending on the crystalline lattice. For example, in the case of a cubic lattice, we set $\mathcal{S} := \{e_1, e_2, e_3\}$, the standard basis of $\mathbb{R}^3$.

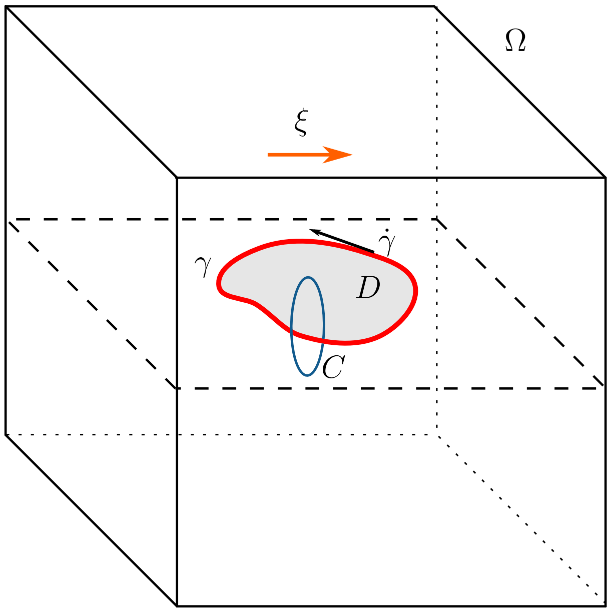


Figure 2.4: Dislocation (γ, ξ) in the reference configuration Ω. D is the flat region enclosed by γ and it represents the slip plane. A strain β generating (γ, ξ) is locally a gradient and it has constant jump equal to ξ through D. C represents a Burgers circuit around γ.

Let $\gamma \subset \Omega$ be a relatively closed Lipschitz curve (that is, $\Omega \setminus \gamma$ is not simply connected), representing a dislocation line. Let $\xi \in \mathcal{S}$ be the Burgers vector associated to γ. A strain $\beta \colon \Omega \to \mathbb{M}^{3\times 3}$ generates the dislocation (γ, ξ) if

$$\operatorname{Curl} \beta = -\xi \otimes \dot{\gamma}\, \mathcal{H}^1 \llcorner \gamma\,, \tag{2.12}$$

in $\mathcal{D}'(\Omega; \mathbb{M}^{3\times 3})$. Here the operator Curl is applied to every row of the matrix β, the tensor product of two vectors $a, b \in \mathbb{R}^3$ is defined as the 3×3 matrix with entries $(a \otimes b)_{ij} := a_i b_j$, and $\mathcal{H}^1 \llcorner \gamma$ is the one dimensional Hausdorff measure restricted to γ. From (2.12), it follows that the circulation of β over any simply connected closed path C around γ is equal to ξ, namely

$$\int_C \beta \cdot t \, d\mathcal{H}^1 = \xi\,. \tag{2.13}$$

To understand the geometrical meaning of (2.12), consider the flat region D enclosed by γ and denote with n the normal unit vector to D (see Figure 2.4). Then there exists a deformation $v \in SBV(\Omega; \mathbb{R}^3)$ such that $\beta = \nabla v$ a.e. in Ω and

$$Dv = \nabla v \, dx + \xi \otimes n \, \mathcal{H}^2 \llcorner D \tag{2.14}$$

in the sense of distributions. Here $SBV(\Omega;\mathbb{R}^3)$ is the set of special functions of bounded variation (see Section A.3 for details), dx is the Lebesgue measure on $\mathbb{R}^3$ and $\mathcal{H}^2 \llcorner D$ is the two dimensional Hausdorff measure restricted to D. Therefore, from (2.14), β can be seen as the elastic part of a deformation which has constant jump equal to ξ across the slip plane D (see [50]).

We remark that, for a strain β satisfying (2.12), the elastic energy defined in (2.1) is not finite, i.e.,

$$E(\beta) = +\infty\,. \tag{2.15}$$

To see this, consider an ε-neighbourhood of γ, that is,

$$I_\varepsilon(\gamma) := \{x \in \mathbb{R}^3 \colon\ \mathrm{dist}(x,\gamma) < \varepsilon\}\,.$$

Fix $\sigma > \varepsilon$ such that $I_\sigma(\gamma) \subset \Omega$. Let $\gamma(s)$ be a parametrisation of γ, and $B_\rho(\gamma(s))$ be the two dimensional disk of radius ρ, centred at $\gamma(s)$, and intersecting D orthogonally. Then, by integrating along γ and using Jensen's inequality and (2.13), we get

$$\begin{aligned}\int_{I_\sigma(\gamma)\setminus I_\varepsilon(\gamma)} |\beta|^2\,dx &= \int_0^l \int_\varepsilon^\sigma \int_{\partial B_\rho(\gamma(s))} |\beta|^2\,d\mathcal{H}^1\,d\rho\,ds \\ &\geq \int_0^l \int_\varepsilon^\sigma \frac{1}{2\pi\rho}\left|\int_{\partial B_\rho(\gamma(s))} \beta\cdot t\,d\mathcal{H}^1\right|^2 d\rho\,ds \\ &= \mathrm{length}(\gamma)\frac{|\xi|^2}{2\pi}\log\frac{\sigma}{\varepsilon}\,.\end{aligned} \tag{2.16}$$

This shows that the energy of a single dislocation diverges logarithmically as the core radius $\varepsilon \to 0$. In particular, we deduce that $\beta \notin L^2(\Omega;\mathbb{M}^{3\times3})$, and also (2.15), which follows from the energy bounds (2.3) and (2.16).

To overcome this problem there are different approaches. One possibility is to truncate the energy at infinity and considering strains in L^p for some $1 < p < 2$. This method is used in Chapter 3, for example. Another option is the so-called *core radius approach*, employed in Chapter 4, which consists in removing an ε-neighbourhood of the dislocation γ from Ω. We will present them in detail below.

Energy truncation

Let $1 < p < 2$. We replace growth condition (2.3) on W with a condition that truncates the energy at infinity, namely we assume that there exists a constant

$C > 0$ such that

$$C^{-1}\left(\operatorname{dist}^2(F, SO(3)) \wedge (|F|^p + 1)\right) \le W(F) \le C\left(\operatorname{dist}^2(F, SO(3)) \wedge (|F|^p + 1)\right) \tag{2.17}$$

for every $F \in \mathbb{M}^{3\times 3}$. The admissible strains inducing the dislocation (γ, ξ) are maps $\beta \in L^p(\Omega; \mathbb{M}^{3\times 3})$ such that (2.12) is satisfied. For such strains $E(\beta)$ is finite, and we can introduce the minimal energy induced by the dislocation (γ, ξ) as

$$E(\gamma, \xi) := \inf\left\{E(\beta) : \beta \in L^p(\Omega; \mathbb{M}^{3\times 3}), \operatorname{Curl}\beta = -\xi \otimes \dot\gamma\, \mathcal{H}^1 \llcorner \gamma\right\}.$$

Core radius approach

Let W satisfy the hypothesis in Section 2.2.1. Given a dislocation (γ, ξ), consider the drilled domain

$$\Omega_\varepsilon(\gamma) := \Omega \setminus I_\varepsilon(\gamma).$$

A strain inducing (γ, ξ) will be a map $\beta \in L^2(\Omega_\varepsilon(\gamma); \mathbb{M}^{3\times 3})$ such that

$$\operatorname{Curl}\beta \llcorner \Omega_\varepsilon(\gamma) = 0 \quad \text{and} \quad \int_C \beta \cdot t\, d\mathcal{H}^1 = \xi, \tag{2.18}$$

for every simply connected path C around γ (the trace is well defined thanks to Theorem 4.1). Notice that we replaced condition (2.12) with (2.18). For such strains we define the elastic energy as

$$E_\varepsilon(\beta) := \int_{\Omega_\varepsilon(\gamma)} W(\beta)\, dx$$

and the minimal energy induced by (γ, ξ) as

$$E_\varepsilon(\gamma, \xi) := \inf\left\{E_\varepsilon(\beta) : \beta \in L^2(\Omega_\varepsilon(\gamma); \mathbb{M}^{3\times 3}) \text{ such that (2.18) holds}\right\}.$$

2.3 Differential inclusions and Rigidity

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain. Consider the following problem: find, and possibly characterise, Lipschitz functions $v\colon \Omega \to \mathbb{R}^3$ such that

$$\nabla v(x) \in K \quad \text{for a.e. } x \text{ in } \Omega \tag{2.19}$$

where $K \subset \mathbb{M}^{3\times 3}$ is a given set of matrices. Condition (2.19) is called a *differential inclusion* and a map v satisfying (2.19) is said to be an *exact solution*.

Differential inclusions of this type arise naturally in applications to Materials Science (see, e.g., [6, 34, 42, 51]). In elasticity theory differential inclusions are useful to model microstructures. Physically a microstructure is any structure that can be observed on a mesoscale. In this case Ω will represent the reference configuration of our material and $v \colon \Omega \to \mathbb{R}^3$ a deformation. As discussed in Section 2.2.1, the energy associated to v is

$$\int_\Omega W(\nabla v)\, dx\,, \tag{2.20}$$

where $W \colon \mathbb{M}^{3\times 3} \to \mathbb{R}$ is the stored energy density. We can normalise W so that $\min W = 0$. Experimentally it is observed that microstructures do not only minimise (2.20), but they minimise the stored energy W pointwise. We are thus led to problem (2.19) where we set $K := W^{-1}(0)$, i.e., K is the set of zero energy affine deformations of the underlying atomic structure of the crystal. The set K will depend on the properties of the material. In the next section we will discuss two significant cases, useful in the following analysis, namely $K = \{A, B\}$ and $K = SO(3)$.

Another application for differential inclusions is to construct gradients that have certain integrability properties. This will be done in Section 5.3.1.

2.3.1 The two-gradient problem

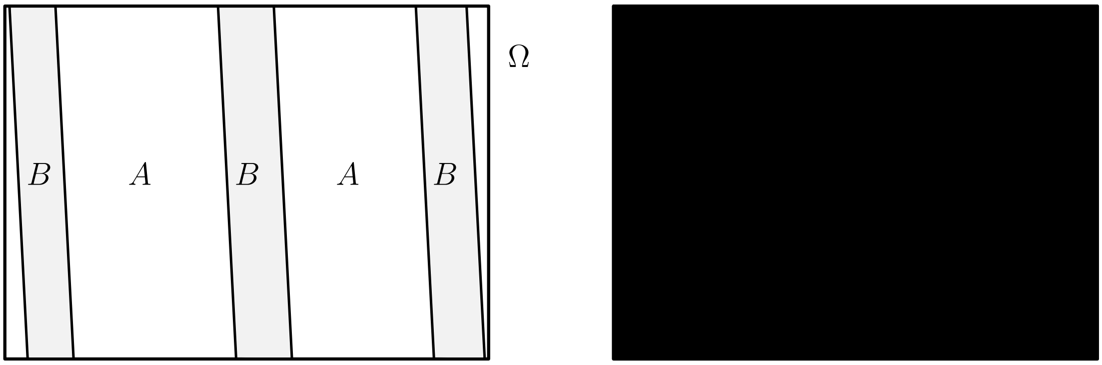
Let $K = \{A, B\}$ for $A, B \in \mathbb{M}^{3\times 3}$ and consider the problem of finding Lipschitz maps $v \colon \Omega \to \mathbb{R}^3$ satisfying

$$\nabla v \in \{A, B\} \quad \text{a.e. in} \quad \Omega\,. \tag{2.21}$$

A trivial solution to (2.21) is given by the constant map $v(x) \equiv Fx$ with $F \in \{A, B\}$. When only constant solutions exist, we say that the problem is *rigid*. However, in some cases it is possible to construct nontrivial solutions (i.e. not constant) to (2.21), by considering *simple laminates*. A simple laminate is a map v for which ∇v is constant on alternating regions delimited by hyperplanes

$$\{x \in \mathbb{R}^3 \colon x \cdot n = c\}\,,$$

for some fixed direction $n \in \mathbb{R}^3$ with $|n| = 1$. The vector n represents the lamination direction (Figure 2.5a). Simple laminates can be used to model microstructures



(a) (b)

Figure 2.5: (a): a simple laminate v in direction n, such that $\nabla v \in \{A, B\}$ a.e. in Ω. (b): atomic resolution micrograph of twinning in Ni-Al alloy (source [42]). This laminate can be modelled by the map v displayed in (a).

observed in real materials, where two phases are mixed in alternating bands (Figure 2.5b). It is possible to model more complicated microstructures as well, by introducing the concept of higher order laminate (see Section 5.3.1).

Since we are requiring that v is Lipschitz, the tangential continuity at the hyperplanes where there is a phase transition from A to B implies that $Ax = Bx$ for every vector $x \in \mathbb{R}^3$ such that $x \cdot n = 0$. Therefore $\operatorname{rank}(B - A) = 1$, with $\ker(B - A) = \{x \in \mathbb{R}^3 \colon x \cdot n = 0\} =: n^\perp$. This implies that

$$B - A = a \otimes n \,, \tag{2.22}$$

with $a := (B - A)n$, since $(a \otimes n)x = (x \cdot n)a$ for $x \in \mathbb{R}^3$. Two matrices $A, B \in \mathbb{M}^{3\times 3}$ such that $\operatorname{rank}(B - A) = 1$ are said to be *rank-one connected*. It turns out that condition (2.22) is both necessary and sufficient for the existence of nontrivial solutions to (2.21), as stated in the following proposition.

Proposition 2.1 ([6], Proposition 1). *Let $\Omega \subset \mathbb{R}^3$ be open, connected and Lipschitz. Let $v \colon \Omega \to \mathbb{R}^3$ be a Lipschitz map that satisfies* (2.21).

(i) Let $\operatorname{rank}(B - A) = 1$, so that $B - A = a \otimes n$ for some $a, n \in \mathbb{R}^3$ with $|n| = 1$. Then the only solutions to (2.21) *are locally simple laminates, i.e., v is locally of the form*

$$v(x) = Ax + a\, h(x \cdot n) + c \,, \tag{2.23}$$

where $h \colon \mathbb{R} \to \mathbb{R}$ is a Lipschitz map such that $h' \in \{0, 1\}$ a.e. in $\mathbb{R}$, and $c \in \mathbb{R}^3$ is a constant. If in addition Ω is convex, then v is globally of the form (2.23).

(ii) Let $\operatorname{rank}(B-A) \geq 2$*. Then* (2.21) *is rigid, that is,* $\nabla v = F$ *a.e. in* Ω*, with* $F \in \{A, B\}$*.*

Moreover, if v *satisfies the affine boundary condition* $v = Fx$ *on* $\partial\Omega$*, then* $v = Fx$ *for every* $x \in \Omega$ *and* $F \in \{A, B\}$*.*

Before proving the proposition, we want to remark that indeed condition (2.23) describes a simple laminate. In fact, if v is of the form (2.23), then

$$\nabla v = A + h'(x \cdot n)\, a \otimes n\,,$$

so that $\nabla v \in \{A, B\}$ a.e. in Ω, since $h' \in \{0, 1\}$ a.e. in $\mathbb{R}$.

Proof. Up to considering $v - Ax$ instead of v, we can assume that $A = 0$. Therefore, if v satisfies (2.21), then $\nabla v = B\chi_E$, for some measurable set $E \subset \Omega$.

Step 1. Let us start with (i). Since $\operatorname{rank}(B) = 1$, after an affine change of variables, we can assume $a = n = e_1$, so that $B = e_1 \otimes e_1$, where e_i is the i-th vector of the standard basis of $\mathbb{R}^3$. Therefore, if we write $v = (v^1, v^2, v^3)$, condition $\nabla v = e_1 \otimes e_1 \chi_E$ reads as

$$\nabla v^1 = e_1 \chi_E\,, \quad \nabla v^2 = 0\,, \quad \nabla v^3 = 0\,.$$

Hence v^2 and v^3 are constant, and v^1 is locally a function of x_1, so that

$$v(x) = e_1 h(x_1) + c\,, \tag{2.24}$$

which is exactly (2.23). If Ω is convex, then (2.24) holds globally, as v^1 is constant on the hyperplanes $\{x \in \mathbb{R}^3 \colon x_1 = \text{const}\}$.

Step 2. We will now prove (ii). Since $\operatorname{rank}(B) \geq 2$, up to an affine change of variables, we can assume that

$$B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ b_1 & b_2 & b_3 \end{pmatrix},$$

for some vector $b \in \mathbb{R}^3$. Since $\nabla v = B\chi_E$,

$$\operatorname{Curl}(B\chi_E) = \operatorname{Curl}(\nabla v) = 0\,.$$

By direct calculation, the first two rows of the above equation read as

$$\operatorname{curl}(e_1\chi_E) = (0, \partial_{x_3}\chi_E, -\partial_{x_2}\chi_E) = 0\,,$$
$$\operatorname{curl}(e_2\chi_E) = (-\partial_{x_3}\chi_E, 0, \partial_{x_1}\chi_E) = 0\,,$$

so that $\nabla\chi_E = 0$ a.e. in Ω. Since Ω is connected, this implies $\chi_E \equiv 0$ a.e. or $\chi_E \equiv 1$ a.e., and the thesis follows.

Step 3. Assume that v satisfies (2.21) and $v = Fx$ on $\partial\Omega$. Integration by parts yields

$$|E|B = \int_\Omega \nabla v\, dx = \int_{\partial\Omega} v \otimes \nu\, d\mathcal{H}^2 = \int_{\partial\Omega} Fx \otimes \nu\, d\mathcal{H}^2 = \int_\Omega F\, dx = |\Omega| F\,,$$

where ν is the outer normal to $\partial\Omega$. Therefore

$$F = \frac{|E|}{|\Omega|} B = (1-\lambda) B\,, \tag{2.25}$$

for $\lambda := 1 - |E|/|\Omega| \in [0,1]$.

Assume that $\operatorname{rank}(B) = 1$ and fix $y \in \partial\Omega$. Then, by (i), we have that

$$v(x) = a\, h(x \cdot n) + c \quad \text{a.e. in} \quad B_r(y) \cap \Omega\,,$$

for some $r > 0$. Since $v = Fx$ on $\partial\Omega$, we can extend v to $\mathbb{R}^3$ by setting $v(x) = Fx$ for every $x \in \mathbb{R}^3 \setminus \Omega$. Therefore we have

$$v(x) = a\, \tilde{h}(x \cdot n) + c \quad \text{a.e. in} \quad B_r(y)\,, \tag{2.26}$$

for some function $\tilde{h}$ such that $\tilde{h}' \in \{0, 1, 1-\lambda\}$. Notice that on the intersection $\{x \cdot n = \text{const}\} \cap (B_r(y) \cap \partial\Omega)$ we have $v = Fx$. Therefore, from (2.26), we deduce that $v = Fx$ on $B_r(y)$. Since $\nabla v \in \{0, B\}$ in $B_r(y) \cap \Omega$, we deduce that $F \in \{0, B\}$. Therefore, from (2.25), we have that either $|E| = 0$ or $|E| = |\Omega|$, and the thesis follows.

If $\operatorname{rank}(B) \geq 2$ then, by (ii), we have $\nabla v = 0$ a.e. or $\nabla v = B$ a.e., which correspond to $|E| = 0$ or $|E| = |\Omega|$ respectively. Hence, by (2.25), $F = 0$ or $F = B$ and the thesis follows. □

2.3.2 The single-well problem

Let $\Omega \subset \mathbb{R}^3$ be open and connected and consider the differential inclusion

$$\nabla v \in SO(3) \quad \text{a.e. in} \quad \Omega \tag{2.27}$$

for some Lipschitz map $v \colon \Omega \to \mathbb{R}^3$. We have the following rigidity theorem.

Proposition 2.2 (Liouville)**.** *Assume that the Lipschitz map* $v\colon \Omega \to \mathbb{R}^3$ *satisfies* (2.27)*. Then* ∇v *is constant and* $v(x) = Qx + b$*, for some* $Q \in SO(3)$ *and* $b \in \mathbb{R}^3$*.*

Proof. This proof can be found in [42]. It is well known (see [39]) that for a Lipschitz map we have

$$\mathrm{div}(\mathrm{cof}\,\nabla v) = 0\,, \tag{2.28}$$

where $\mathrm{cof}\,F$ denotes the cofactor matrix of $F \in \mathbb{M}^{3\times 3}$. Recall that $F^{-1} = \mathrm{cof}\,F/\det F$ whenever $\det F \neq 0$. Hence, for $R \in SO(3)$ we have $\mathrm{cof}\,R = R$. Since $\nabla v \in SO(3)$ a.e., (2.28) implies that v is harmonic in Ω and, in particular, v is smooth. Then we have

$$\frac{1}{2}\Delta|\nabla v|^2 = \nabla v \cdot \Delta\nabla v + |\nabla^2 v|^2 = |\nabla^2 v|^2\,, \tag{2.29}$$

since v is harmonic. For $R \in SO(3)$ we have $|R|^2 = \mathrm{Tr}\,R^T R = 3$. Hence $|\nabla v|^2 = 3$ in Ω and from (2.29) we deduce $|\nabla^2 v| = 0$, which implies $\nabla v \equiv Q$ for some $Q \in SO(3)$. □

In [29] the authors proved a quantitative version of Proposition 2.2, that will be fundamental in the analysis carried out in Chapter 3.

Theorem 2.3 (Geometric Rigidity, [29])**.** *Let* $\Omega \subset \mathbb{R}^3$ *be a bounded Lipschitz domain. There exists a constant* $C > 0$ *depending only on* Ω*, such that the following holds: for every map* $v \in H^1(\Omega;\mathbb{R}^3)$*, there exists an associated constant rotation* $R \in SO(3)$*, such that*

$$\int_\Omega |\nabla v - R|^2\,dx \le C\int_\Omega \mathrm{dist}^2(\nabla v, SO(3))\,dx\,. \tag{2.30}$$

Remark 2.4 (See [29])**.** We remark that the constant C in Theorem 2.3 is invariant under uniform scaling and translation, that is,

$$C(\Omega) = C(\lambda\Omega + c)\,,$$

for every $\lambda > 0$, $c \in \mathbb{R}^3$. The rescaled function $\lambda v((x-c)/\lambda)$ is associated to the same rotation R for v.

Estimate (2.30) is obtained, in [29], by combining Proposition 2.2 and the classic Korn's inequality, stated in the following theorem.

Theorem 2.5 (Korn's inequality, [10]). *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain. There exists a constant $C > 0$ depending only on Ω, such that for every map $u \in H^1(\Omega;\mathbb{R}^3)$ we have*

$$\int_\Omega |\nabla u - A|^2 \, dx \leq C \int_\Omega |\nabla u^{\mathrm{sym}}|^2 \, dx \, , \tag{2.31}$$

where A is the constant antisymmetric matrix defined by

$$A := \frac{1}{|\Omega|} \int_\Omega \nabla u^{\mathrm{skew}} \, dx \, ,$$

with $\nabla u^{\mathrm{sym}} := (\nabla u + \nabla u^T)/2$ and $\nabla u^{\mathrm{skew}} := (\nabla u - \nabla u^T)/2$.

We can see how the rigidity estimate (2.30) is the nonlinear version of Korn's inequality (2.31) by computing the distance from $SO(3)$ for a deformation of the form $v = x + \varepsilon u$, with $\varepsilon > 0$ small. Notice that the tangent space of $SO(3)$ about the identity is given by the space of antisymmetric matrices $\mathbb{M}^{3\times3}_{\mathrm{skew}}$, hence we have

$$\mathrm{dist}(F, SO(3)) = |F^{\mathrm{sym}} - I| + O(|F - I|^2) \, .$$

Applying the above identity to $\nabla v = I + \varepsilon \nabla u$ yields

$$\mathrm{dist}(\nabla v, SO(3)) = \varepsilon |\nabla u^{\mathrm{sym}}| + o(\varepsilon^2) \, .$$

Chapter 3

A variational model for dislocations at semi-coherent interfaces

3.1 Introduction

In this chapter we present the results obtained in our paper [22], in which we propose and analyse a variational model describing dislocations at semi-coherent interfaces. We focus on flat two dimensional interfaces between two crystalline materials with different underlying lattice structures Λ^+ and Λ^-. Specifically, we assume that the lattice Λ^+ (lying on top of Λ^-) is a dilation with factor $\alpha > 1$ of Λ^-. We are interested in semi-coherent interfaces, corresponding to small misfits $\alpha \approx 1$.

Since in the reference configuration (where both crystals are in equilibrium) the density of the atoms of Λ^+ is lower than that of Λ^-, in the vicinity of the interface there are many atoms having the "wrong" coordination number, namely, the wrong number of nearest neighbours (see Figure 3.1 Left). Such atoms form line singularities (relatively closed paths lying on the interface), which correspond to edge dislocations (see Section 2.1 for more details on dislocations). The crystal can reduce the number of such dislocations through a compression strain acting on Λ^+ near the interface, at the price of storing some far field elastic energy. A deformation that coincides with $x \mapsto \alpha^{-1}x$ near the interface would provide a defect-free perfect match between the crystal lattices (Figure 3.1 Right). In fact, the true deformed configuration is the result of a balance (Figure 3.1 Centre) between the elastic energy spent to match the crystal structures and the dislocation energy spent to release the

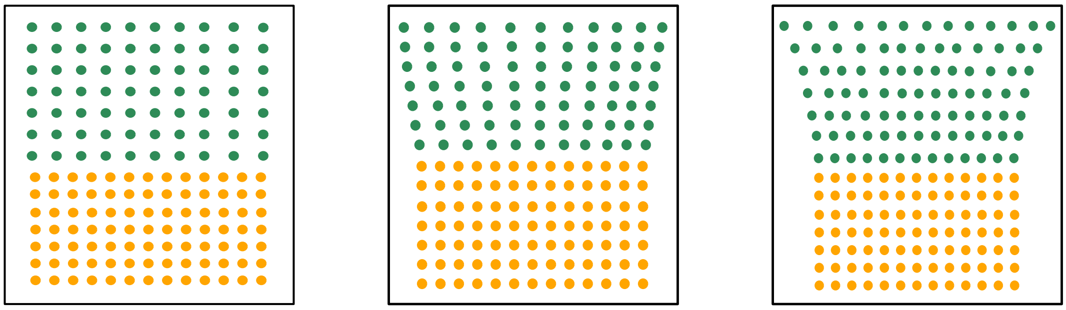


Figure 3.1: Left: a bulk stress-free configuration. Right: a defect-free configuration. Centre: a schematic picture of a true energy minimiser; the density of atoms on the top and on the bottom of the interface is almost the same, giving rise to a semi-coherent interface.

far field elastic energy, with the former scaling (for defect free configurations) like the volume of the body and the latter like the surface area of the interface.

This is why the common perspective of the scientific community working on this problem has been to understand which configurations of dislocations minimise the elastic stored energy, and much effort has been devoted to describe those configurations for which the dislocation energy contribution is predominant, and the far field elastic energy is negligible ([55], [32]). As a matter of fact, for large crystals, periodic patterns of edge dislocations are observed at interfaces, as displayed, for example, in Figure 3.2 (see [19, 53]).

In [22], we propose a simple variational model to analyse the competition between surface and elastic energy. We show that, for large interfaces, the dislocation energy of minimisers scales like the area of the interface, while the elastic far field energy like its diameter.

The proposed model is not purely discrete; indeed it is a continuum model that stems from some heuristic considerations and some rigorous computations done in the framework of the so called semi-discrete theory of dislocations.

In single crystals, the energy induced by straight edge dislocations has a logarithmic tail (see (2.16)), which diverges as the ratio between the crystal size and the atomic distance tends to $+\infty$. The Γ-convergence analysis for these systems as the atomic distance tends to zero has been recently done in [17], [13] showing that dipoles as well as isolated dislocations do not contribute to decrease the elastic en-

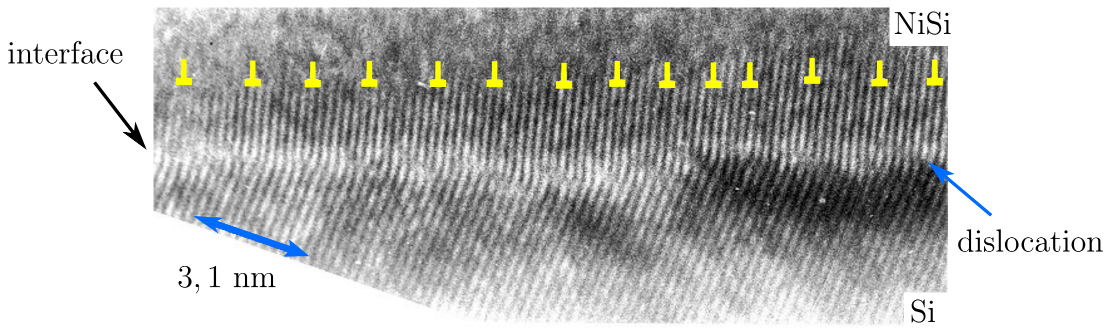


Figure 3.2: HRTEM picture of the interface between Si (silicon) and NiSi (nickel-silicon). The interface is semi-coherent (light region in the picture), and a periodic network of edge dislocations is observed: the yellow $\perp$ symbols lie vertically above the dislocations, which are located at the interface (image from [26, Section 8.2.1], with permission of the author H. Foell).

ergy, so that in single crystals only the so called *geometrically necessary dislocations* are good competitors in the energy minimisation (see Section A.1.2 for details on Γ-convergence).

Quite different is the case of polycrystals treated in our paper [22], where dislocations contribute to decrease the elastic energy. The first rigorous variational justification of dislocation nucleation in heterostructured nanowires was obtained by Müller and Palombaro [43] in the context of nonlinear elasticity. The model proposed in [43] was later generalised to a discrete to continuum setting in [36, 37] (see also [2] for recent advancements in the microscopic setting). A variational model for misfit dislocations in elastic thin films, in connection with epitaxial growth, has been recently proposed in [28] (we refer the readers interested in the mathematical theory of epitaxy to the lecture notes [38]). Finally, a rigorous derivation of a small angle grain boundary has been obtained in the recent paper [35].

In Section 3.2 we set and analyse the problem in the semi-discrete framework, which provides the theoretical background for the proposed continuum model. In the semi-discrete model, the reference configuration of the hyper-elastic body is the cylindrical region $\Omega_r := S_r \times (-hr, hr)$, where $r, h > 0$ and $S_r := [-r/2, r/2]^2$. The interface $S_r \times \{0\}$ separates the two regions of the body, $\Omega_r^- := S_r \times (-hr, 0)$ and $\Omega_r^+ := S_r \times (0, hr)$, with underlying crystal structures Λ^- and Λ^+ respectively. We will refer to Ω_r^- and Ω_r^+ as the underlayer and overlayer, respectively. We assume that the material equilibrium is the identity I in Ω_r^- (implying that the underlayer is already in equilibrium) and αI in Ω_r^+, where $\alpha > 1$ measures the misfit between the two lattice parameters. Notice that the identical deformation of Ω_r, which corresponds to a dislocation-free configuration, is not stress-free, since the overlayer is not in equilibrium. Furthermore, in order to simplify the analysis, we assume that Ω_r^- is rigid, so that only Ω_r^+ is subjected to deformations.

We assume that deformations try to minimise a stored elastic energy (in Ω_r^+), whose density is described by a nonlinear frame indifferent function $W\colon \mathbb{M}^{3\times 3} \to [0, +\infty)$. In classical finite elasticity (see Section 2.2.1), W acts on deformation gradients $\beta := \nabla v$. In this framework dislocations are introduced as line defects of the strain: more precisely, we allow the strain field β to have a non vanishing curl, concentrated on dislocation lines at the interface S_r (see Section 2.2.3). Therefore, the admissible strains are maps $\beta \in L^p(\Omega_r; \mathbb{M}^{3\times 3})$ (where $1 < p < 2$ is fixed, according to the growth assumptions on W, see (3.7)) that satisfy

$$\operatorname{Curl} \beta = \sum_i -\xi_i \otimes \dot{\gamma}_i \, \mathcal{H}^1 \llcorner \gamma_i \tag{3.1}$$

in the sense of measures and such that $\beta = I$ in Ω_r^-. Here $\{\gamma_i\}$ is a finite collection of closed curves, and $\xi_i \in \mathbb{R}^3$ denotes the *Burgers vector*, which is constant on each γ_i. The Burgers vector belongs to the set of slip directions, which is a given material property of the crystal. We assume that the Burgers vectors are given by

$$\mathcal{S} := \{b e_1, b e_2\} \tag{3.2}$$

where $b > 0$ represents the lattice spacing of Λ^-. We then define the set of slip directions

$$\mathbb{S} := \operatorname{Span}_{\mathbb{Z}} \mathcal{S} \,, \tag{3.3}$$

which coincides with the set of Burgers vectors for multiple dislocations. We also suppose that the dislocation curves γ_i have support on the grid

$$\mathcal{G} := \Big[\big((b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z}) \big) \cap S_r \Big] \times \{0\} \,. \tag{3.4}$$

Notice that this choice is consistent with the cubic crystal structure, and that b is independent of r, i.e., independent of the size of the body.

In Section 3.2 we study the asymptotic behaviour of minimisers of the elastic energy functional with respect to all possible pairs of compatible (i.e., satisfying

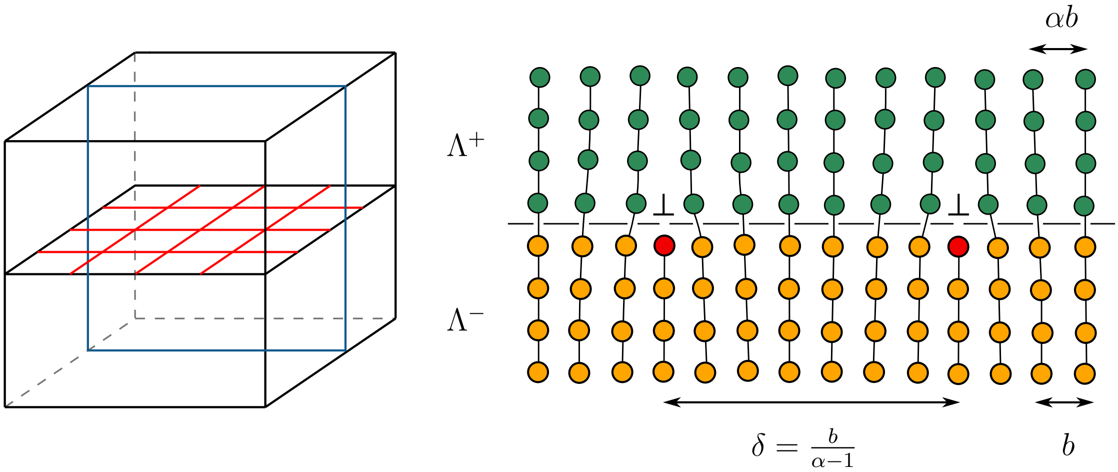


Figure 3.3: Left: schematic picture of the 3D crystal. The red lines at the interface are edge dislocations. The blue square is a 2D slice. Right: schematic atomic picture of the 2D slice. Orange and green atoms belong to Λ^- and Λ^+ respectively. The red atoms are edge dislocations (denoted by $\perp$).

(3.1)) strains and dislocations, refining the analysis first done in [43]. In Proposition 3.2 we show that, as $r \to +\infty$, the elastic energy of minimisers per unit area of the interface tends to a given surface energy density E_α. As a consequence, we show that there exists a critical r^* such that, for larger size of the interface, dislocations are energetically favourable (see Theorem 3.5). The proof of these results is based on an explicit construction of an array of dislocations (see Figure 3.3) and of admissible fields, which is optimal in the energy scaling (see Proposition 3.6). While we could guess that the dislocation configuration is somehow optimal, the strains that we consider as energy competitors are surely not, so that our construction does not provide the sharp formula for the surface energy density E_α, which depends on the specific form of the elastic energy density W. Indeed, the main problem raised in our paper [22] concerns the identification of the sharp energy density E_α and of the corresponding optimal geometries for the dislocations net. Less ambitious is the question about the optimal spacing between the dislocation lines. As already explained, by scaling arguments the optimal geometry of dislocations should release the far field elastic energy as much as possible. This consideration leads us to construct and analyse a net of dislocations with spacing $\frac{b}{\alpha-1}$. One of the main goals of this paper is to show that, for large interfaces, such density of dislocations is optimal in energy. In order to prove this fact, in Section 3.4, we propose and analyse a simplified continuous model for dislocations at semi-coherent interfaces, describing in particular heterogeneous nanowires.

Although we deal with a continuum model, our approach is built on the analysis developed in the first part of [22], and it is consistent with the discrete analysis developed in [36, 37]. In this model we work with actual gradient fields far from the interface, where the curl of the strain is now a diffuse measure, in contrast with (3.1). Dislocations nucleation is taken into account by introducing a free parameter into the total energy and eventually optimising over it. Specifically, we assume that the underlayer occupies the cylindrical region Ω_R^- (which is fixed), while the reference configuration of the overlayer is Ω_r^+, where $r = \theta R$ and $\theta \in (0,1)$ is a free parameter in the total energy functional. The class of admissible deformation maps is defined by

$$\mathcal{ADM}_{\theta,R} := \left\{ v \in W^{1,2}(\Omega_r^+;\mathbb{R}^3) : \ v(x) = \frac{1}{\theta}\, x \ \text{ on } S_r \right\}. \tag{3.5}$$

In this way $v(S_r) = S_R$ for all $v \in \mathcal{ADM}_{\theta,R}$, so that there is a perfect match between the two layers at the interface. In view of the analysis performed in the semi-discrete setting, the area of $S_R \setminus S_r$ divided by b can be interpreted as the total dislocation length. This suggests to introduce the plastic energy defined by

$$E_R^{pl}(\theta) := \sigma r^2(\theta^{-2} - 1) = \sigma R^2(1 - \theta^2).$$

Here $\sigma > 0$ is a given material constant of the crystal, which multiplied by b represents the energy cost of dislocations per unit length. In principle, σ could be derived starting from the surface energy density E_α introduced in Proposition 3.2, yielding in the limit of vanishing misfit $\sigma = \lim_{\alpha\to 1} \frac{E_\alpha}{\alpha^2 - 1}$ (see (4.124)). Alternatively, assuming isotropy, σ can be expressed in terms of the Lamé moduli of the linearised elastic tensor corresponding to W and of the (unknown) chemical core energy density γ^{ch} induced by dislocations (see (3.26) in Section 3.3). The latter contribution is implicitly taken into account by the nonlinear energy density W in finite elasticity.

Based on the previous considerations, our goal is to study the total energy functional defined by

$$E_{\alpha,R}^{tot}(\theta, v) := E_{\alpha,R}^{el}(\theta, v) + E_R^{pl}(\theta) = \int_{\Omega_r^+} W(\nabla v(x))\, dx + \sigma R^2(1-\theta^2),$$

for $v \in \mathcal{ADM}_{\theta,R}$. Set

$$E_{\alpha,R}^{el}(\theta) := \inf\left\{ E_{\alpha,R}^{el}(\theta, v) : \ v \in \mathcal{ADM}_{\theta,R} \right\}, \qquad E_{\alpha,R}^{tot}(\theta) := E_{\alpha,R}^{el}(\theta) + E_R^{pl}(\theta).$$

Notice that if $\theta = 1$, then no dislocation energy is present, i.e., $E^{tot}_{\alpha,R}(1) = E^{el}_{\alpha,R}(1)$. Instead, if $\theta = \alpha^{-1}$ no elastic energy is stored (since $v(x) := \alpha x$ is admissible and $W(\alpha I) = 0$).

The remaining and main part of [22] is devoted to the analysis of minimisers of $E^{tot}_{\alpha,R}$, as $R \to +\infty$. In Theorem 3.13 we show that the optimal θ_R tends to α^{-1} from below, corresponding to the average spacing $\frac{b}{\alpha-1}$ between the dislocation lines. In particular, the dislocation energy spent to release the bulk energy is predominant, but still $\theta_R \neq \alpha^{-1}$, so that also a far field bulk energy is present (see Figure 3.1).

In order to compute the optimal θ_R, we perform a Taylor expansion (through a Γ-convergence analysis) of the plastic and elastic part of the energy, proving in particular that the first scales like R^2, while the second like R. Prefactors in such energy expansions are computed, depending only on α, σ and on the fourth-order tensor obtained by linearising W.

In conclusion, the proposed energy functional provides a simple prototypical variational model to describe the competition between the dislocation energy concentrated in the vicinity of the interface between materials with different crystal structures, and the far field elastic energy. This model fits into the class of free boundary problems, since the overlayer is a variable in the minimisation problem, though only through a scalar parameter representing its size. Our formulation is quite specific, dealing with two lattices where one is a small dilation of the other. Therefore, it is meant to model semi-coherent interfaces between two different lattices, for example in heterostructured nanowires. Nevertheless, our approach seems flexible enough to be adapted to more general situations, to model epitaxial crystal growth (where the surface energy of the free external boundary in contact with air should be added to the energy functional), and to more general interfaces, such as grain boundaries, where the misfit in the crystal structures is due to mutual rotations between the grains instead of dilations of the lattice parameters.

3.2 A line defect model

3.2.1 Description of the model

We introduce a semi-discrete model for dislocations, which are described as line defects of the strain.

Let $\Omega_1 = S_1 \times (-h, h)$ be the reference configuration of a cylindrical hyper-elastic body. Here $h > 0$ is a fixed height and $S_1 = \{(x_1, x_2, 0) \in \mathbb{R}^3 : \ |x_1|, |x_2| < 1/2\}$ is a square of side one centred at the origin, separating parts of the body with underlying crystal structures Λ^- and $\Lambda^+ := \alpha\Lambda^-$, with $\alpha > 1$. For any given $r > 0$, we will consider scaled versions of the body $\Omega_r := r\Omega_1$ and $S_r := rS_1$.

Set $\Omega_r^- := S_r \times (-hr, 0)$ and $\Omega_r^+ := S_r \times (0, hr)$. We assume that the material equilibrium is the identity I in Ω_r^- (which means that the material is already in equilibrium in Ω_r^-) and αI in Ω_r^+. We are interested in small misfits, which generate so called semi-coherent interfaces; therefore, we will deal with $\alpha \approx 1$. More specifically, we assume that the lattice distances of Λ^- and Λ^+ are commensurable, and in particular that $\alpha := 1 + 1/n$ for some given $n \in \mathbb{N}$. Moreover, in order to simplify the analysis, we assume that Ω_r^- is rigid, namely, that the admissible deformations coincide with the identical deformation in Ω_r^-.

According to the hypothesis of hyper-elasticity, we assume that the crystal tries to minimise a stored elastic energy (in Ω_r^+), whose density is described by a function $W \colon \mathbb{M}^{3\times3} \to [0, +\infty)$. As discussed in Section 2.2.1, we require that W is continuous and frame indifferent, i.e.,

$$W(F) = W(R\,F) \qquad \text{for every} \quad F \in \mathbb{M}^{3\times3},\ R \in SO(3)\,. \tag{3.6}$$

Moreover, we suppose that there exist $p \in (1, 2)$ and constants $C_1, C_2 > 0$, such that W satisfies the following growth conditions:

$$C_1 \left(\operatorname{dist}^2(F, \alpha SO(3)) \wedge (|F|^p + 1) \right) \leq W(F) \leq C_2 \left(\operatorname{dist}^2(F, \alpha SO(3)) \wedge (|F|^p + 1) \right) \tag{3.7}$$

for every $F \in \mathbb{M}^{3\times3}$. Here the condition $p > 1$ prevents the formation of cracks in the body, while $p < 2$ guarantees that dislocations induce finite core energy, as explained below.

In absence of dislocations, the deformed configuration of the body can be described by a sufficiently smooth deformation $v : \Omega_r^+ \to \mathbb{R}^3$. The corresponding elastic energy is given by

$$E^{el}(v) := \int_{\Omega_r^+} W(\nabla v)\, dx. \tag{3.8}$$

The field ∇v is referred to as the deformation strain.

We now explain how to introduce dislocations in the present model. As in [43], dislocations are described by deformation strains whose curl is not free, but concentrated on lines lying on the interface S_r between Ω_r^- and Ω_r^+.

Assume for the time being that the dislocation line $\gamma \subset S_r$ is a Lipschitz, relatively closed curve in S_r. The latter condition implies that $\Omega_r \setminus \gamma$ is not simply connected. Therefore, the strain is a map $\beta \in L^p(\Omega_r; \mathbb{M}^{3\times 3})$ that satisfies

$$\operatorname{Curl} \beta = -\xi_\gamma \otimes \dot{\gamma}\, \mathcal{H}^1 \llcorner \gamma \tag{3.9}$$

in the sense of distributions and $\beta = I$ in Ω_r^-. The vector $\xi_\gamma \in \mathbb{R}^3$ denotes the Burgers vector, which is constant on γ, and together with the dislocation line γ, uniquely characterises the dislocation (see Figure 3.4 Left). From (3.9) one can deduce that in the vicinity of γ

$$|\beta(x)| \sim \frac{1}{\operatorname{dist}(x, \gamma)}, \tag{3.10}$$

which implies that the L^2 norm of β in a cylindrical neighbourhood of γ diverges logarithmically (see (2.16)). This is exactly why we consider energy densities W which grow slower than quadratic at infinity.

The Burgers vector belongs to the class of slip directions, which is a given material property of the crystal. As a further simplification, we assume that the slip directions are given by $\mathbb{S} := \operatorname{Span}_{\mathbb{Z}}\{be_1, be_2\}$, where $b > 0$ represents the lattice spacing of the lower crystal Ω_r^-.

If $\omega \subset \Omega_r \setminus \gamma$ is a simply connected region, then (3.9) implies that $\operatorname{Curl} \beta = 0$ in $\mathcal{D}'(\omega, \mathbb{M}^{3\times 3})$ and therefore there exists $v \in W^{1,p}(\omega; \mathbb{R}^3)$ such that $\beta = \nabla v$ a.e. in ω. Thus, any vector field β satisfying (3.9) is locally the gradient of a Sobolev map. In particular, if Σ is a sufficiently smooth surface having γ as its boundary, then one can find $v \in SBV_{\text{loc}}(\Omega_r; \mathbb{R}^3)$ (see A.3 for more details on BV functions) such that

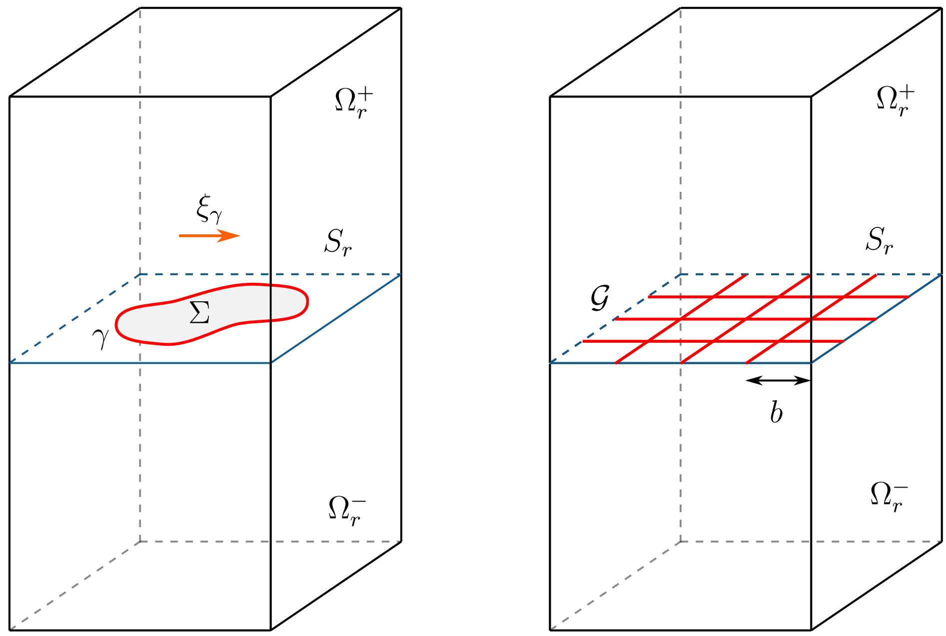


Figure 3.4: Reference configuration $\Omega_r := \Omega_r^- \cup S_r \cup \Omega_r^+$. Left: dislocation (γ, ξ_γ) at the interface S_r. Note that $\partial\Sigma = \gamma$. Right: admissible dislocation curves lie on the grid $\mathcal{G} \subset S_r$.

$\beta = \nabla v$, $v = x$ in Ω_r^- and its distributional gradient satisfies

$$Dv = \nabla v \, dx + \xi_\gamma \otimes \nu \, \mathcal{H}^2 \llcorner \Sigma \,,$$

where ν is the unit normal to Σ. That is, $\beta = \nabla v$ is the absolutely continuous part of the distributional gradient of v. As customary (see [50]), we interpret β as the elastic part of the deformation v, so that the elastic energy induced by v is given by

$$E^{el}(v) := \int_{\Omega_r^+} W(\beta) \, dx.$$

From now on we will assume that the dislocation curves have support in the grid $\mathcal{G} := (b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z}) \subset S_r$ (see Figure 3.4 Right). Moreover, we will consider multiple dislocation curves. More precisely, we denote by

$$\mathcal{AD} := \{(\Gamma, B) : \; \Gamma = \{\gamma_i\}, \, \gamma_i \in \mathcal{G}, \, B = \{\xi_i\}, \, \xi_i \in \mathbb{S}, \text{ finite collections}\} \tag{3.11}$$

the class of all admissible dislocations. Notice that each dislocation curve can be decomposed into "minimal components", i.e., we can always assume that $\gamma_i = \partial Q_i$, where Q_i is a square of size b with sides contained in the grid $(b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z})$. Given an admissible pair (Γ, B), we denote by $\xi \otimes \dot\gamma(x)$ the field that coincides with

$\xi_i \otimes \dot\gamma_i(x)$ if x belongs to a single curve γ_i, and with $\xi_i \otimes \dot\gamma_i(x) + \xi_j \otimes \dot\gamma_j(x)$ if x belongs to two different curves γ_i and γ_j. The set of admissible deformation strains $\mathcal{AS}(\Gamma, B)$ associated with a given admissible dislocation (Γ, B) is then defined by

$$\mathcal{AS}(\Gamma, B) := \left\{\beta \in L^p_{\rm loc}(\Omega_r; \mathbb{M}^{3\times3})\colon \beta = I \text{ in } \Omega_r^-,\, \operatorname{Curl}\beta = -\xi \otimes \dot\gamma\, \mathcal{H}^1 \llcorner \Gamma\right\}, \quad (3.12)$$

where, abusing notation, we identify Γ with the union of the supports of γ_i. We define the minimal energy induced by the pair (Γ, B) as

$$E_{\alpha,r}(\Gamma, B) := \inf\left\{\int_{\Omega_r^+} W(\beta)\, dx : \beta \in \mathcal{AS}(\Gamma, B)\right\}, \quad (3.13)$$

and the minimal energy induced by the lattice misfit as

$$E_{\alpha,r} := \min\left\{E_{\alpha,r}(\Gamma, B) : \ (\Gamma, B) \in \mathcal{AD}\right\}. \quad (3.14)$$

Notice that, by the growth assumptions (3.7) on W and by (3.10), the minimum problem in (3.14) involves only dislocations with Burgers vectors in a bounded set (and thus in a finite set), so that the existence of a minimiser is trivial. We denote by $E_{\alpha,r}(\emptyset)$ the minimal elastic energy induced by curl free strains. Notice that $E_{\alpha,r}(\Gamma, B) = E_{\alpha,r}(\emptyset)$ whenever $\Gamma \cap S_r = \emptyset$.

For the sake of computational simplicity, whenever it is convenient we will assume

$$\frac{r(\alpha - 1)}{2b} \in \mathbb{N}. \quad (3.15)$$

Recalling that $\alpha = 1 + \frac{1}{n}$, assumption (3.15) implies that $\frac{r}{2b} \in \mathbb{N}$.

3.2.2 Scaling properties of the energies

The next proposition, proved in [43, Proposition 3.2], states that the quantities defined by (3.13) and (3.14) are strictly positive.

Proposition 3.1. *For all $r > 0$ one has $E_{\alpha,r} > 0$. Moreover, $E_{\alpha,r}(\emptyset) = r^3\, E_{\alpha,1}(\emptyset)$, with $E_{\alpha,1}(\emptyset) > 0$.*

Proposition 3.1 asserts that $E_{\alpha,r}(\emptyset)$ grows cubically in r. We will show that the energy (3.13) grows quadratically in r, by suitably introducing dislocations on S_r. In fact we will introduce dislocations on the boundary of many (of the order of $(r(\alpha - 1)/b)^2$) squares.

Proposition 3.2. *There exists* $0 < E_\alpha < +\infty$ *such that*

$$\lim_{r\to+\infty} \frac{E_{\alpha,r}}{r^2} = E_\alpha. \tag{3.16}$$

Proof. For the sake of computational simplicity, we assume that (3.15) holds, so that $r/2 \in b\mathbb{N}$ (see Remark 3.3 to deal with the general case). We first show that the limit exists. Let $m, n \in \mathbb{N}$ with $n > m$, and let j be the integer part of $\frac{n}{m}$, $R := nb$, $r := mb$. Then, there are j^2 disjoint squares of size r in S_R, so there are j^2 disjoint sets equivalent to Ω_r (up to horizontal translations) in Ω_R. By minimality, $E_{\alpha,r}$ is smaller than the energy stored in each of such domains, so that

$$\frac{E_{\alpha,r}}{r^2} \leq \frac{E_{\alpha,R}}{r^2 j^2} = \frac{E_{\alpha,R}}{R^2 + q(r)}\,, \tag{3.17}$$

where $q(r) := -\big[(\frac{R}{r} - j)^2 + 2j(\frac{R}{r} - j)\big]r^2 = o(R^2)$. Since this inequality holds true for all $r, R \in b\mathbb{N}$ with $r \leq R$, we deduce that

$$\liminf_{n\to+\infty} \frac{E_{\alpha,bn}}{(bn)^2} = \limsup_{n\to+\infty} \frac{E_{\alpha,bn}}{(bn)^2} = \lim_{n\to+\infty} \frac{E_{\alpha,bn}}{(bn)^2} =: E_\alpha.$$

In order to establish that $E_\alpha > 0$, it suffices to plug $r = 1$ in (3.17), and to recall that $E_{\alpha,1} > 0$, by Proposition 3.2.

Next we show that $E_\alpha < +\infty$. For this purpose, we will exhibit a sequence of deformations and associated dislocations for which the energy grows at most quadratically in r. The construction uses some ideas introduced in [44] and [43]. Let $\delta := \frac{b}{(\alpha-1)} = nb$ and recall that by (3.15) we have $r/\delta \in \mathbb{N}$. Denote by Q_i, $i = 1, \ldots, q$, the squares of side δ with vertices in the lattice $S_r \cap \delta\mathbb{Z}^2$, and let x_i be the centre of each Q_i. Since the side of S_r is r, we have that $q = (r/\delta)^2$.

We will define a deformation $v\colon \Omega_r \to \mathbb{R}^3$ such that $v = x$ in Ω_r^-, $v = \alpha x$ if $x_3 > \delta$ and the transition from x to αx is distributed into constant jumps across the squares Q_i's. In this way the energy will be concentrated in a δ-neighbourhood of the interface S_r and the contribution to the energy will come mostly from dislocations.

To this end, let C_i^1 and C_i^2 be the pyramids of base Q_i and vertices $x_i + \delta/2\, e_3$ and $x_i + \delta e_3$ respectively (see Figure 3.5 Left). Define a displacement $u\colon \Omega_r \to \mathbb{R}^3$ such that

$$u(x) = \begin{cases} (\alpha - 1)x & \text{if } x \in \Omega_r^+ \setminus \cup_{i=1}^q C_i^2\,, \\ 0 & \text{if } x \in \Omega_r^-\,. \end{cases}$$

We complete the above definition by setting $u := u_i$ in C_i^2, where u_i is the unique solution of the minimum problem

$$m_{\delta,p,(\alpha-1)I} := \min\left\{\int_{C_i^2} |\nabla w|^p \,:\, w \in W^{1,p}_{loc}(\mathbb{R}^3_+;\mathbb{R}^3),\, w \equiv (\alpha-1)x_i \text{ in } C_i^1, \right. \tag{3.18}$$
$$\left. w(x) = (\alpha-1)x \text{ in } \mathbb{R}^3_+ \setminus C_i^2 \right\},$$

where $\mathbb{R}^3_+ := \mathbb{R}^3 \cap \{x_3 > 0\}$. Notice that $m_{\delta,p,(\alpha-1)I}$ is independent of i and that u is well defined; indeed if Q_i and Q_j are adjacent squares, i.e.,

$$Q_j = Q_i \mp \delta e_s \qquad \text{for some} \quad s \in \{1,2\},$$

then

$$u_j(x) = u_i(x \pm \delta e_s) \mp (\alpha-1)\delta e_s \quad \text{for every} \quad x \in Q_j \times [0,+\infty].$$

Moreover, in Proposition 3.6 we will show that $0 < m_{\delta,p,(\alpha-1)I} < +\infty$ and

$$m_{\delta,p,(\alpha-1)I} = \delta^3(\alpha-1)^p\, m_{1,p,I}\,. \tag{3.19}$$

Set $v(x) := x + u(x)$. Notice that the deformation v has constant jump equal to $(\alpha-1)x_i$ across Q_i. Therefore, if Q_i and Q_j are adjacent and we set $\gamma_{ij} := Q_i \cap Q_j$, we have that γ_{ij} is a dislocation line with Burgers vector $\xi_{ij} = (\alpha-1)(x_j - x_i)$ (see Figure 3.5 Right). By construction $\gamma_{i,j}$ lies in the grid $(b\mathbb{Z}\times\mathbb{R}) \cup (\mathbb{R}\times b\mathbb{Z})$. Moreover, since $\delta = b/(\alpha-1)$ and $x_j - x_i = \pm\delta e_s$, with $s \in \{0,1\}$, we have that $\xi_{ij} \in \pm b\{e_1, e_2\}$. Therefore, setting $\Gamma := \{\gamma_{ij}\}$ and $B := \{\xi_{ij}\}$, we have that $(\Gamma, B) \in \mathcal{AD}$ and $\nabla v \in \mathcal{AS}(\Gamma, B)$.

We are left to estimate from above the elastic energy of v. Recalling that $W(\alpha I) = 0$, the growth condition (3.7) and (3.19), we get

$$\begin{aligned}\int_{\Omega_r^+} W(\nabla v)\,dx &= \sum_{i=1}^q \int_{C_i^2} W(\nabla v)\,dx \le C\sum_{i=1}^q \int_{C_i^2} (|\nabla v|^p + 1)\,dx \\ &\le Cq\left|C_i^2\right| + q\delta^3(\alpha-1)^p\, m_{1,p,I} = q\delta^3\left(C + (\alpha-1)^p\, m_{1,p,I}\right).\end{aligned}$$

Writing $q = r^2/\delta^2$ and $\delta = b/(\alpha-1)$ yields

$$\int_{\Omega_r^+} W(\nabla v) \le r^2 b\left[(\alpha-1)^{p-1}\, m_{1,p,I} + (\alpha-1)^{-1}C\right]. \tag{3.20}$$

□

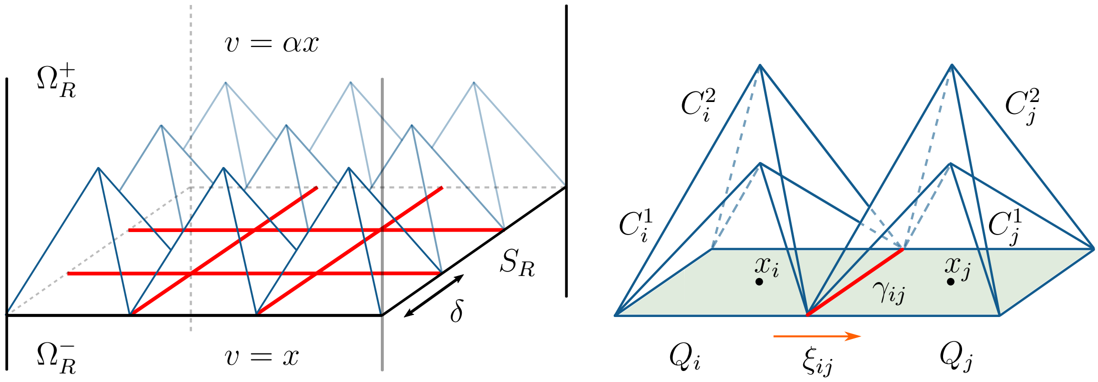


Figure 3.5: The double pyramid construction. Left: the jump from x to αx is divided into constant jumps across the pyramids lying on top of the squares Q_i at the interface. Right: detail of two adjacent double pyramids. The deformation v induces the dislocation line γ_{ij}, with Burgers vector $\xi_{ij} = \delta e_2$ (in this particular example).

Remark 3.3. In the case when (3.15) does not hold, it suffices to observe that

$$E_{\alpha,[\frac{r}{2\delta}]2\delta} \leq E_{\alpha,r} \leq E_{\alpha,[\frac{r}{2\delta}]2\delta+2\delta} \quad \text{and} \quad \lim_{r\to\infty} \frac{([\frac{r}{2\delta}]2\delta)^2}{r^2} = \lim_{r\to\infty} \frac{([\frac{r}{2\delta}]2\delta + 2\delta)^2}{r^2} = 1,$$

where $[a]$ denotes the integer part of a. The above inequalities follow from the fact that if $r_1 < r_2$, then the restriction to Ω_{r_1} of any test function for E_{α,r_2} provides a test function for E_{α,r_1}.

Remark 3.4. The proof of the asymptotic behaviour of the energy described by Proposition 3.2 strongly relies on the assumption made on the admissible dislocation lines. In fact, local lower bounds of the energy can be easily obtained in a neighbourhood of the dislocation lines, as long as these are sufficiently regular and well separated.

As a corollary of Propositions 3.1 and 3.2 we obtain the following theorem, asserting that nucleation of dislocations is energetically convenient for sufficiently large values of r.

Theorem 3.5. *There exists a threshold r^* such that, for every $r > r^*$,*

$$E_{\alpha,r} < E_{\alpha,r}(\emptyset).$$

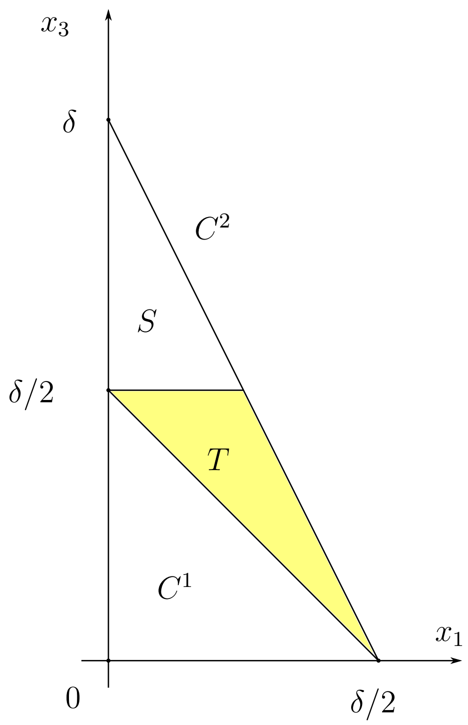


Figure 3.6: Section $\varphi = 0$ of the double pyramid.

3.2.3 Double pyramid construction

Fix $\delta > 0$ and let C^1 and C^2 be the pyramids with common base the square $(-\delta/2, \delta/2)^2 \times \{0\}$ and heights $\delta/2$ and δ respectively. Note that $C^1 \subset C^2$. Set $S := C^2 \cap \{\delta/2 < x_3 < \delta\}$ and $T := (C^2 \setminus C^1) \cap \{0 < x_3 < \delta/2\}$. See Figure 3.6 for a cross section of this construction in cylindrical coordinates.

Let $A \in \mathbb{M}^{3\times3}$ with $A \neq 0$, and consider the following minimisation problem

$$m_{\delta,p,A} := \inf \Big\{ \int_{C^2} |\nabla w|^p \, dx : \ w \in W^{1,p}_{loc}(\mathbb{R}^3_+; \mathbb{R}^3), w \equiv 0 \text{ in } C^1, \\ w \equiv Ax \text{ in } \mathbb{R}^3_+ \setminus C^2 \Big\}, \tag{3.21}$$

where $\mathbb{R}^3_+ := \mathbb{R}^3 \cap \{x_3 > 0\}$.

Proposition 3.6. *The following facts hold true:*

(i) For every $1 < p < 2$, there exists a minimiser of problem (3.21) *and the minimal value $m_{1,p,A}$ is strictly positive;*

(ii) $m_{1,2,A} = +\infty$;

(iii) for all positive δ and λ we have $m_{\delta,p,\lambda A} = \delta^3 \lambda^p m_{1,p,A}$.

Proof. Property (iii) holds because if w is a competitor for $m_{\delta,p,\lambda A}$, then $\tilde{w}(x) := w(\delta x)/\lambda\delta$ is a competitor for $m_{1,p,A}$.

As far as (i) is concerned, first remark that $m_{1,p,A} > 0$. Indeed, arguing by contradiction, assume that $m_{1,p,A} = 0$. Then, by the direct method of the calculus of variations (see Section A.1.1), we would have a minimiser w satisfying $\nabla w \equiv 0$ in C^2 and $\nabla w \equiv A$ in $\mathbb{R}^3_+ \setminus C^2$, which provides a contradiction since this is only possible when $A = 0$. In fact, since w is regular, we have tangential continuity of ∇w at $\partial C^2 \cap \mathbb{R}^3_+$. This implies $Ax = 0$ for every vector x tangent to $\partial C^2 \cap \mathbb{R}^3_+$. Therefore $A = 0$.

Now, we will prove that $m_{1,p,A} < +\infty$ by exhibiting an admissible deformation w with finite energy. In order to simplify the computations, we will show it in the case when C^1 and C^2 are the cones with base the disk of diameter 1 and centre the origin, and heights 1/2 and 1 respectively. The estimate in the case of two pyramids can be proved in the same way, with minor changes. Introduce the cylindrical coordinates $x_1 = \rho\cos\varphi$, $x_2 = \rho\sin\varphi$ and $x_3 = z$, with $\rho > 0$ and $\varphi \in [0, 2\pi)$. Set $w := 0$ in C^1 and $w(x) := Ax$ in $\mathbb{R}^3_+ \setminus C^2$. First we extend w to S (Figure 3.6). To this end, for all $\bar{\varphi} \in [0, 2\pi)$ we define w in the triangle $S_{\bar{\varphi}} := S \cap \{\varphi = \bar{\varphi}\}$ by linear interpolation of the values of w at the three vertices of $S_{\bar{\varphi}}$. Notice that w is Lipschitz continuous in S. Next, we extend w to $T := C^2 \setminus (S \cup C^1)$. For this purpose, for all $\bar{\varphi} \in [0, 2\pi)$ and $\bar{z} \in (0, \frac{1}{2})$ consider the segment $L_{\bar{\varphi},\bar{z}} := T \cap \{\varphi = \bar{\varphi}\} \cap \{z = \bar{z}\}$, and define w on $L_{\bar{\varphi},\bar{z}}$ by linear interpolation of the values of w on the two extreme points of $L_{\bar{\varphi},\bar{z}}$.

We will now estimate the L^p norm of ∇w in C^2. Since w is piecewise Lipschitz in $C^2 \setminus T$, we only have to compute the energy in T. By construction we have that

$$|\nabla w(x, y, z)| \leq \frac{c}{z} \qquad \text{for all } (x, y, z) \in T, \tag{3.22}$$

where c is a suitable positive constant depending only on A. A straightforward computation yields $m_{1,p,A} \leq C(p, A)$ with the constant C depending only on A and p, and diverging as $p \to 2^-$.

Finally, let us prove (ii), i.e., that $m_{1,2,A} = +\infty$. For every admissible function w and all $0 < \varepsilon < 1/2$, by Jensen's inequality we have

$$\int_{T\cap\{\varepsilon<z<\frac{1}{2}\}} |\nabla w|^2 \, dx \geq \int_{T\cap\{\varepsilon<z<\frac{1}{2}\}} \left|\frac{\partial w}{\partial \rho}\right|^2 dx \geq c \int_{\varepsilon}^{\frac{1}{2}} \frac{1}{s} \left(\int_{T\cap\{z=s\}} \frac{\partial w}{\partial \rho} \, d\rho \right)^2 ds \geq c \log \frac{1}{\varepsilon}.$$

Taking the limit as $\varepsilon \to 0$ in the above inequality yields $\int_{C^2} |\nabla w|^2 = +\infty$. □

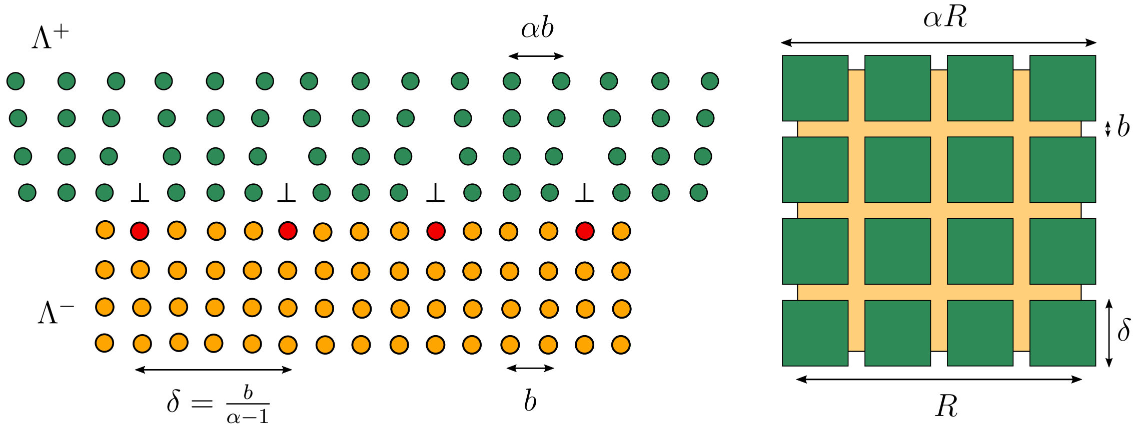


Figure 3.7: Left: a discrete vertical section of the crystal, deformed through the map v constructed in the proof of Proposition 3.2. The red atoms are edge dislocations. Right: view from above of the interface, deformed through the map v. The green squares represent the deformed overlayer. Dislocation lines lie in the gaps between the green squares. The orange square represents the underlayer.

3.3 Some considerations on the proposed model

In this section we discuss some features and limits of the semi-discrete model presented in Section 3.2, in connection with modelling epitaxial growth, heterostructured nanowires and grain boundaries. Such limits of the theory will be overcome in the continuous model discussed and analysed in detail in the next section. In this respect, the semi-discrete model is somehow meant as a theoretical background to derive material constants, and in particular the energy per unit dislocation length and interface area, that will be involved in the continuous model discussed in Section 3.4.

In the construction illustrated in the proof of Proposition 3.2, $v(S_r)$ is the union of disjoint squares of size δ, separated by strips of width b; dislocation lines lie in the middle of such strips (see Figure 3.7). Note that some lines of atoms (in the deformed configuration) fall outside of S_r, suggesting that the chosen reference configuration is not convenient to describe heterostructured nanowires, or epitaxial growth.

In fact, this is not the physical configuration we are interested in modelling and analysing. In order to prevent unphysical configurations like in Figure 3.7, where some lines of atoms fall outside of S_r, in the next section we will rather modify our

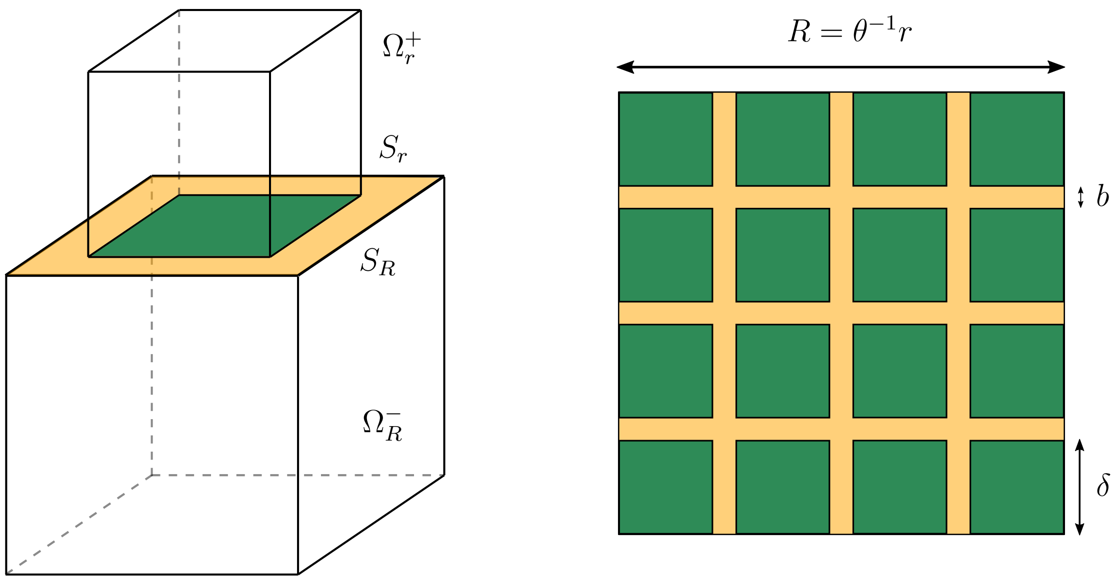


Figure 3.8: Left: the new reference configuration $\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+$. The orange square is S_R, the green S_r. The area of $S_R \backslash S_r$ represents the dislocation energy. Right: view from above of the interface between S_r and S_R. Here S_r is deformed through the map v obtained by adapting the proof of Proposition 3.2, with $\delta = \frac{b}{\theta^{-1}-1}$, to the new reference configuration. The total dislocation length is given, in first approximation, by the area of the orange region, divided by b.

point of view: we will deal with a reference configuration $\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+$ with $r := \theta R$ for some $0 < \theta < 1$ (see Figure 3.8 Left), enforcing that $v(S_r) = S_R$, thus describing a perfect match between the two parts of the crystal, as in Figure 3.3. The new parameter θ represents the ratio between the size of S_r and that of its deformed counterpart $v(S_r)$. Optimisation over θ corresponds to “getting rid” of unnecessary atoms at the interface and will yield (see (3.68)) $\theta \approx \alpha^{-1}$ in the limit $R \to \infty$.

In this context it is quite natural to measure the dislocation length in the deformed configuration $v(\Omega_r^+)$. In the construction made in the proof of Proposition 3.2, the number of dislocation straight-lines is of the order $\frac{2r}{\delta}$, where $\delta = \frac{b}{\alpha-1}$. Mimicking the same construction in the new reference configuration $\Omega_{R,r}$, in order to enforce $v(S_r) = S_R$, now we have to choose $\delta = \frac{b}{\theta^{-1}-1}$. The total length L of dislocations (in the deformed configuration) is then of the order $L = \frac{2r^2}{b}(\theta^{-2} - \theta^{-1})$. The above formula can be obtained alternatively as follows. Let $\tilde{L}$ be the total length of dislocations in the reference configuration. Then, $b\tilde{L}$ coincides with the total variation of μ, the curl of the deformation strain, which is a measure concentrated on S_r (see Section A.2 for more details on measure theory). By a direct computation the total variation $|\mu|(S_r)$ is given by $r^2 2\left(\theta^{-1}-1\right)$. Therefore,

$$L = \theta^{-1}\tilde{L} = \frac{\theta^{-1}}{b} r^2 2\left(\theta^{-1}-1\right) = \frac{2r^2}{b}(\theta^{-2}-\theta^{-1}).$$

We are interested in small misfits $\theta^{-1} \approx 1$. Therefore, $(\theta^{-2}-\theta^{-1}) \approx \frac{1}{2}(\theta^{-2}-1)$, so that the total length of dislocations is of the order

$$L = \frac{1}{b} r^2(\theta^{-2}-1) = \frac{1}{b} \text{ Area Gap},$$

where Area Gap, in a continuous modelling of the crystal, represents the difference between the area of the base of the deformed configuration $v(S_r)$ of Ω_r^+, and the area of the base of the reference configuration, namely the area of S_r (see Figure 3.8).

We do not claim that our constructions are optimal in energy. Nevertheless, we believe that, as r, $R \to \infty$, the optimal configuration of dislocations exhibits some periodicity. As a matter of fact, in Proposition 3.2 we have proved that

$$E_{\alpha,r} \approx r^2 E_\alpha = \sigma_{\alpha,\theta} \text{ Area Gap} \qquad \text{as } r \to +\infty, \tag{3.23}$$

for

$$\sigma_{\alpha,\theta} := \frac{E_\alpha}{\theta^{-2}-1}.$$

In view of the considerations above, this reflects that the energy is proportional to the total dislocation length. In particular, as $r \to \infty$ and $\alpha \to 1^+$, we expect that $E_{\alpha,r}$ be minimised by a periodic configuration of more and more dilute and well separated dislocations. Taking this into account, we expect that

$$\lim_{\alpha \to 1^+} \frac{E_\alpha}{\alpha^2 - 1} = \lim_{\alpha \to 1^+} \sigma_{\alpha,\alpha^{-1}} =: \sigma, \tag{3.24}$$

for some $0 < \sigma < \infty$, where $b\sigma$ represents the self energy of a single dislocation line per unit length.

Let us compare the nonlinear energy induced by dislocations with the solid framework of linearised elasticity. It is well known that the energy per unit (edge dislocation) length in a single crystal of size r is given by $b^2 \frac{\mu}{4\pi(1-\nu)} \ln(\frac{r}{b})$ (see, e.g., [33, 47]), where μ is the shear modulus and ν is Poisson's ratio. Based on the heuristic observation that the periodicity of the lattice is restored on lines at the interface which are equidistant from two consecutive edge dislocations, one could exploit this formula, with r replaced by the average distance $\delta = \frac{b}{\alpha-1}$ between dislocations. Moreover, due to the fact that Ω_R^- is rigid, the stress and the corresponding energy are concentrated on half disks around each dislocation (in fact, half cylinders around the dislocation lines). A purely dimensional argument yields that the resulting strain is twice the one induced by the dislocations in a purely elastic single crystal; the corresponding elastic energy density, being quadratic, should be multiplied by 4, but it is concentrated on half domain (the half cylinders). The resulting energy is then twice the energy induced by the dislocations in a purely elastic crystal. These heuristic arguments lead us to consider the following energy per unit dislocation length:

$$\gamma^{lin} := b^2 \frac{\mu}{2\pi(1-\nu)} \ln\left(\frac{1}{\alpha-1}\right). \tag{3.25}$$

To such energy, a chemical core energy γ^{ch} per unit dislocation length should be added. Notice that this contribution is already present in our nonlinear formulation, and it is stored in the region where $|\nabla v|$ is large, and the energy density $W(\nabla v)$ behaves like $|\nabla v|^p$. We deduce that, for small misfits,

$$(\gamma^{lin} + \gamma^{ch}) \frac{1}{b} \text{ Area Gap } \approx E_{\alpha,r} \approx \sigma \text{ Area Gap},$$

which yields the following expression for σ:

$$\sigma = b \frac{\mu}{2\pi(1-\nu)} \ln\left(\frac{1}{\alpha-1}\right) + \frac{1}{b}\gamma^{ch}. \tag{3.26}$$

Finally, we notice that $\sigma(\alpha^2-1)$ is nothing but the energy per unit surface area, so that the total energy is given by

$$E_{\alpha,r} \approx r^2(\alpha^2-1)\left(b\frac{\mu}{2\pi(1-\nu)} \ln\left(\frac{1}{\alpha-1}\right) + \frac{1}{b}\gamma^{ch}\right).$$

3.4 A simplified continuous model for dislocations

Based on the analysis and the considerations on the semi-discrete model discussed in Section 3.3, here we want to propose a simplified and more realistic model for dislocations at interfaces. Instead of working with SBV functions with piece-wise constant jumps at the interface, we allow only for regular jumps but we introduce a penalisation to the elastic energy, which represents the dislocation energy.

3.4.1 The simplified energy functional

Fix $\alpha > 1$, $R > 0$, $\theta \in [\alpha^{-1}, 1]$ and set $r := \theta R$. Let $\Omega_R^- := S_R \times (-hR, 0)$, where $S_R \subset \mathbb{R}^2$ is the square of side length R centred at the origin and $h > 0$ a fixed height. Define now the reference configuration (see Figure 3.9),

$$\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+.$$

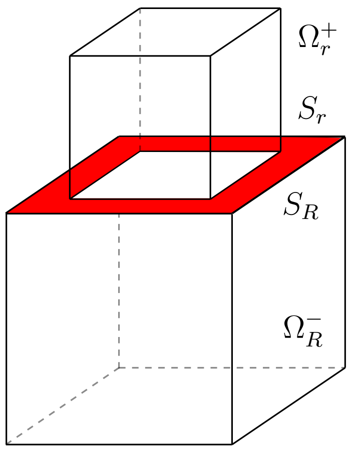


Figure 3.9: The reference configuration $\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+$. The red area $S_R \setminus S_r$ is proportional to the dislocation energy.

As in Section 3.2 we will suppose that Ω_R^- is rigid and that Ω_r^+ is in equilibrium with αI. We assume that there exists an energy density $W \colon \mathbb{M}^{3\times 3} \to [0, +\infty)$ that is continuous, C^2 in a neighbourhood of $\alpha SO(3)$ and frame indifferent (see (3.6)). Furthermore we suppose that

$$W(\alpha I) = 0 \tag{3.27}$$

and that for every $F \in \mathbb{M}^{3\times 3}$

$$C \ \mathrm{dist}^2(F, \alpha SO(3)) \leq W(F) \tag{3.28}$$

for some constant $C > 0$. Here we assume that W grows more than quadratically, since the energy density describes now only the bulk elastic energy stored in the crystal, i.e., the strain is actually curl-free, while the core dislocation energy is taken into account by an additional plastic term, defined in (3.30) below. In fact one could also consider weaker growth conditions away from the well (see [1]); however we will stick to (3.28) for simplicity. The class of admissible deformation maps is defined by

$$\mathcal{ADM}_{\theta,R} := \left\{ v \in W^{1,2}(\Omega_r^+;\mathbb{R}^3) :\ v(x) = \frac{1}{\theta}\, x \ \text{ on } S_r \right\}. \tag{3.29}$$

In this way $v(S_r) = S_R$ for all $v \in \mathcal{ADM}_{\theta,R}$. A deformation $v \in \mathcal{ADM}_{\theta,R}$ stores an elastic energy

$$E^{el}_{\alpha,R}(\theta, v) := \int_{\Omega_r^+} W(\nabla v)\, dx\,.$$

To this energy we add a dislocation energy $E^{pl}_R(\theta)$ proportional to the area of $S_R \setminus S_r$, representing the total dislocation length,

$$E^{pl}_R(\theta) := \sigma r^2(\theta^{-2} - 1) = \sigma R^2(1 - \theta^2). \tag{3.30}$$

Here $\sigma > 0$ is a given constant, which in our model is a material property of the crystal, representing (multiplied by b) the energy cost of dislocations per unit length. In principle, σ could be derived starting from the semi-discrete model discussed in Section 3.2 (see Section 3.3). Assuming isotropic linearised elasticity, a possible choice is to set σ according to (4.124) (where the Lamé coefficients are obtained from W by linearisation), so that $b\sigma$ represents the energy induced by a single dislocation line per unit length. We are thus led to study the energy functional

$$E^{tot}_{\alpha,R}(\theta, v) := E^{el}_{\alpha,R}(\theta, v) + E^{pl}_R(\theta) = \int_{\Omega_r^+} W(\nabla v)\, dx + \sigma R^2(1 - \theta^2).$$

We further define

$$E^{el}_{\alpha,R}(\theta) := \inf\left\{ E^{el}_{\alpha,R}(\theta, v) :\ v \in \mathcal{ADM}_{\theta,R} \right\}, \qquad E^{tot}_{\alpha,R}(\theta) := E^{el}_{\alpha,R}(\theta) + E^{pl}_R(\theta). \tag{3.31}$$

As explained in the Introduction (Section 3.1), the case $\theta = 1$ corresponds to a dislocation free configuration, i.e., $E^{tot}_{\alpha,R}(1) = E^{el}_{\alpha,R}(1)$. Instead, if $\theta = \alpha^{-1}$ no elastic energy is stored, since $v(x) := \alpha x$ is admissible and $W(\alpha I) = 0$. In order to simplify notation we set $E^{el}_\alpha(\theta) := E^{el}_{\alpha,\frac{1}{\theta}}(\theta)$, which corresponds to the minimum energy in the unit cylinder, i.e., with $r = 1$.

Proposition 3.7. *The elastic energy $E^{el}_{\alpha,R}(\theta)$ satisfies:*

(i) $E^{el}_{\alpha,R}(\theta) = R^3\theta^3 E^{el}_\alpha(\theta)$*;*

(ii) $E^{el}_\alpha(\theta) > 0$ *if and only if* $\theta > \alpha^{-1}$*.*

Proof. Property (i) follows by noticing that if v is in $\mathcal{ADM}_{\theta,R}$, then $\tilde{v}(x) := v(R\theta x)/R\theta$ is in $\mathcal{ADM}_{\theta,\frac{1}{\theta}}$. For the second property, we have to prove that $E^{el}_{\alpha}(\theta) = 0$ if and only if $\theta = \alpha^{-1}$. We already pointed out that $E^{el}_{\alpha}(\alpha^{-1}) = 0$. Suppose that $E^{el}_{\alpha}(\theta) = 0$. Then there exists a sequence $v_n \in H^1(\Omega_1^+;\mathbb{R}^3)$ such that $v_n = \theta^{-1}x$ on S_1, and

$$\int_{\Omega_1^+} W(\nabla v_n)\, dx \to 0 \qquad \text{as } n \to \infty\,. \tag{3.32}$$

The Rigidity Theorem 3.9, the growth assumption (3.28) and the compactness of $SO(3)$ in combination with (3.32) imply that there exists a fixed rotation $\mathcal{R} \in SO(3)$ such that (up to subsequences)

$$\int_{\Omega_1^+} |\nabla v_n - \alpha\mathcal{R}|^2 \; dx \to 0 \qquad \text{as } n \to \infty\,.$$

Setting $\zeta_n := (1/\left|\Omega_1^+\right|)\int_{\Omega_1^+}(v_n(x) - \alpha\mathcal{R}x)\, dx$, from the Poincaré inequality and the trace theorem we deduce that

$$\int_{S_1} |v_n - \alpha\mathcal{R}x - \zeta_n|^2 \; d\mathcal{H}^2(x) \to 0 \qquad \text{as } n \to \infty\,. \tag{3.33}$$

Since $v_n = \theta^{-1}x$ on S_1, (3.48) yields

$$(\theta^{-1}I - \alpha\mathcal{R})x - \zeta_n \to 0 \qquad \text{in } L^2(S_1)\,. \tag{3.34}$$

By plugging $x = 0$ in (3.34) we get $\zeta_n \to 0$, so that

$$(\theta^{-1}I - \alpha\mathcal{R})x = 0 \quad \text{for every} \quad x \in S_1\,.$$

Therefore

$$\operatorname{rank}(\theta^{-1}I - \alpha\mathcal{R}) \leq 1\,, \tag{3.35}$$

(see Section 2.3), which is possible if and only if $\mathcal{R} = I$ and $\theta = \alpha^{-1}$. □

In analogy with Theorem 3.5, we find that for R sufficiently large, configurations with dislocations are energetically preferred.

Theorem 3.8. *There exists a threshold R^* such that, for every $R > R^*$*

$$\inf_{\theta\in[\alpha^{-1},1)} E^{tot}_{\alpha,R}(\theta) < E^{tot}_{\alpha,R}(1) = E^{el}_{\alpha,R}(1)\,. \tag{3.36}$$

Proof. The left hand side of (3.36) can grow at most quadratically in R, indeed

$$\inf_{\theta\in[\alpha^{-1},1)} E^{tot}_{\alpha,R}(\theta) \leq E^{tot}_{\alpha,R}(\alpha^{-1}) = \sigma R^2\left(1 - \frac{1}{\alpha^2}\right)\,.$$

In contrast, by Proposition 3.7, the right hand side $E^{tot}_{\alpha,R}(1)$ grows cubically in R. □

The minimal energy induced by the lattice misfit is given by

$$E^{tot}_{\alpha,R} := \inf_{\theta\in[\alpha^{-1},1]} E^{tot}_{\alpha,R}(\theta)\,. \tag{3.37}$$

One can show that $E^{tot}_{\alpha,R}(\cdot)$ is continuous, so that the infimum is in fact a minimum. Our goal is to study the asymptotic behaviour of $E^{tot}_{\alpha,R}$ as $R\to\infty$. In Theorem 3.13 we will write $E^{tot}_{\alpha,R}$ as an expansion in powers of R.

3.4.2 An overview of the Rigidity Estimate and Linearisation

First, we recall the Rigidity Estimate from [29] (see also Section 2.3.2). In this section, $U\subset\mathbb{R}^3$ will be a Lipschitz bounded domain.

Theorem 3.9 (Rigidity Estimate, [29])**.** *There exists a constant $C>0$ depending only on the domain U such that the following holds: for every $v\in H^1(U;\mathbb{R}^3)$ there exists a constant rotation $R\in SO(3)$ such that*

$$\int_U |\nabla v(x)-\alpha R|^2\,dx \le C\int_U \operatorname{dist}^2(\nabla v(x);\alpha SO(3))\,dx\,. \tag{3.38}$$

In order to compute the Taylor expansion of $E^{tot}_{\alpha,R}$ defined in (3.37), we will linearise the elastic energy as in [15] (see also Section 2.11). Therefore, following [15], we will make further assumptions on W. First, assume that the equilibrium αI is stress free, i.e.,

$$\partial_F W(\alpha I)=0\,. \tag{3.39}$$

By frame indifference there exists a function $V\colon\mathbb{M}^{3\times3}_{\mathrm{sym}}\to[0,+\infty]$, such that

$$W(F)=V\left(\frac{1}{2}\left(F^TF-\alpha^2 I\right)\right)\qquad\text{for every}\quad F\in\mathbb{M}^{3\times3}. \tag{3.40}$$

Here $\mathbb{M}^{3\times3}_{\mathrm{sym}}$ is the set of 3×3 symmetric matrices and F^T is the transpose of F. The regularity assumptions on W (see Section 3.4.1) imply that $V(E)$ is of class C^2 in a neighbourhood of $E=0$. From (3.27), (3.39) and (3.40) it follows that $V(0)=0$ and $\partial_E V(0)=0$. Moreover, by (3.28), there exist γ, $\delta>0$ such that

$$\partial^2_E V(E)[T,T]\ge\gamma\,|T|^2\qquad\text{if }|E|<\delta\text{ and }T\in\mathbb{M}^{3\times3}_{\mathrm{sym}}\,, \tag{3.41}$$

as shown, for example, in [15]. By Taylor expansion we find

$$V(E)=\frac{1}{2}\partial^2_E V(0)[E,E]+o(|E|^2)\,. \tag{3.42}$$

Let $v \in W^{1,\infty}(U;\mathbb{R}^3)$ and write $v = \alpha x + \varepsilon u$. Then from (3.40),

$$W(\nabla v) = V\left(\alpha\varepsilon \nabla u^{\mathrm{sym}} + \frac{\varepsilon^2}{2} C(u)\right),$$

where $\nabla u^{\mathrm{sym}} := (\nabla u + \nabla u^T)/2$ and $C(u) := \nabla u^T \nabla u$. By (3.42) we get

$$W(\nabla v) = \frac{\varepsilon^2}{2} \mathbb{C} \nabla u^{\mathrm{sym}} : \nabla u^{\mathrm{sym}} + o(\varepsilon^2), \tag{3.43}$$

where $\mathbb{C}$ is the fourth order stress tensor obtained by writing the bilinear form

$$\alpha^2 \partial_E^2 V(0) \colon \mathbb{M}^{3\times 3}_{\mathrm{sym}} \times \mathbb{M}^{3\times 3}_{\mathrm{sym}} \to \mathbb{R}$$

in euclidean coordinates. Notice that, by (3.41), the tensor $\mathbb{C}$ satisfies the growth condition

$$C|E|^2 \leq \mathbb{C}E : E \quad \text{for every} \quad E \in \mathbb{M}^{3\times 3}_{\mathrm{sym}}, \tag{3.44}$$

for some positive constant C. Equation (3.43) is uniform in x, since ∇v is bounded. Hence

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} \int_U W(\alpha I + \varepsilon \nabla u)\, dx = \frac{1}{2} \int_U \mathbb{C} \nabla u^{\mathrm{sym}} : \nabla u^{\mathrm{sym}}\, dx.$$

In [15] it is proved that the above convergence holds also for minimisers, by means of Γ-convergence (see Section A.2 for details on Γ-convergence). Specifically, let $\Sigma \subset \partial U$ be closed and such that $\mathcal{H}^2(\Sigma) > 0$. Introduce the space

$$H^1_{x,\Sigma}(U;\mathbb{R}^3) := \left\{ u \in H^1(U;\mathbb{R}^3) :\ u(x) = x \text{ on } \Sigma \right\}$$

and, for $u \in H^1_{x,\Sigma}(U;\mathbb{R}^3)$, define the functionals

$$G_\varepsilon(u) := \frac{1}{\varepsilon^2} \int_U W(\alpha I + \varepsilon \nabla u)\, dx \qquad \text{and} \qquad G(u) := \frac{1}{2} \int_U \mathbb{C} \nabla u^{\mathrm{sym}} : \nabla u^{\mathrm{sym}}\, dx.$$

We can now recall [15, Theorem 2.1]:

Theorem 3.10 (Linearization). *We have that $G_\varepsilon \xrightarrow{\Gamma} G$ with respect to the weak topology on $H^1(U;\mathbb{R}^3)$. In particular, if $\{u_\varepsilon\} \subset H^1_{x,\Sigma}(U;\mathbb{R}^3)$ is a minimising sequence, i.e.,*

$$\inf_{H^1_{x,\Sigma}(U;\mathbb{R}^3)} G_\varepsilon = G_\varepsilon(u_\varepsilon) + o(1),$$

then u_ε converges weakly to the unique solution u_0 of

$$\min_{H^1_{x,\Sigma}(U;\mathbb{R}^3)} G.$$

Moreover we have

$$\inf_{H^1_{x,\Sigma}(U;\mathbb{R}^3)} G_\varepsilon \to \min_{H^1_{x,\Sigma}(U;\mathbb{R}^3)} G \quad \text{as} \quad \varepsilon \to 0. \tag{3.45}$$

3.4.3 Taylor expansion of the energy

We can now carry on our analysis. We say that $\theta_R \in [\alpha^{-1}, 1]$ is a minimising sequence for the energy $E^{tot}_{\alpha,R}$ defined in (3.37) if

$$E^{tot}_{\alpha,R} = E^{tot}_{\alpha,R}(\theta_R) + o(1)\,,$$

where $o(1) \to 0$ as $R \to +\infty$.

Proposition 3.11. *Let θ_R be a minimising sequence for $E^{tot}_{\alpha,R}$. Then*

(i) $E^{el}_{\alpha}(\theta_R) \to 0$ as $R \to +\infty$;

(ii) $\theta_R \to \alpha^{-1}$ as $R \to +\infty$.

Proof. By Proposition 3.7 we have (for R large enough)

$$R^3\theta_R^3 E^{el}_{\alpha}(\theta_R) = E^{el}_{\alpha,R}(\theta_R) \leq E^{tot}_{\alpha,R}(\theta_R) \leq E^{tot}_{\alpha,R}(\alpha^{-1}) + 1 = \sigma R^2\left(1 - \frac{1}{\alpha^2}\right) + 1\,,$$

which proves (i), since $\theta_R \geq \alpha^{-1} > 0$.

Let us now prove (ii). From (i), we know that there exists a sequence $\{v_R\}$ in $H^1(\Omega_1^+;\mathbb{R}^3)$ such that $v_R = \theta_R^{-1}\,x$ on S_1 and

$$\int_{\Omega_1^+} W(\nabla v_R)\,dx \to 0 \quad \text{ as } \quad R \to +\infty\,. \tag{3.46}$$

We will show that $\theta_R \to \alpha^{-1}$, and also that we have full rigidity, namely $v_R \to \alpha x$ in $H^1(\Omega_1^+;\mathbb{R}^3)$.

Indeed, as in the proof of Proposition 3.7, by combining the Rigidity Theorem 3.9, the growth assumption (3.28), the compactness of $SO(3)$ and (3.46), we have that there exists a fixed rotation $\mathcal{R} \in SO(3)$ such that, up to subsequences,

$$\int_{\Omega_1^+} |\nabla v_R - \alpha\mathcal{R}|^2\,dx \to 0 \quad \text{as} \quad R \to \infty\,. \tag{3.47}$$

Set $\zeta_R := 1/\left|\Omega_1^+\right| \int_{\Omega_1^+}(v_R - \alpha\mathcal{R}x)\,dx$. From the Poincaré and trace inequalities we then deduce

$$\int_{\Omega_1^+} |v_R - \alpha\mathcal{R}x - \zeta_R|^2\,dx \to 0\,, \tag{3.48}$$

$$\int_{S_1} |v_R - \alpha\mathcal{R}x - \zeta_R|^2\,d\mathcal{H}^2(x) \to 0\,, \tag{3.49}$$

as $R \to \infty$. Since $v_R = \theta_R^{-1} x$ on S_1, from (3.49) we have that, up to subsequences,

$$\left(\theta_R^{-1} I - \alpha \mathcal{R}\right) x - \zeta_R \to 0 \quad \text{on} \quad S_1 \,. \tag{3.50}$$

In particular, choosing $x = 0$ in (3.50), yields $\zeta_R \to 0$. Since θ_R is bounded we can then assume $\theta_R \to \theta$ to get

$$\left(\theta^{-1} I - \alpha \mathcal{R}\right) x = 0 \quad \text{on} \quad S_1 \,.$$

As in the proof of Proposition 3.7, we conclude that $\mathcal{R} = I$ and $\theta = \alpha^{-1}$. Since the limit of θ_R does not depend on the subsequence selected, the thesis holds.

Moreover, notice that if we use $\zeta_R \to 0$ and $\mathcal{R} = I$ in (3.47)-(3.48) we get that $v_R \to \alpha x$ in $H^1(\Omega_1^+; \mathbb{R}^3)$. □

For $v \in H^1(\Omega_1^+; \mathbb{R}^3)$ such that $v = \theta^{-1} x$ on S_1, we can write

$$v = \alpha x + \left(\frac{1}{\theta} - \alpha\right) u$$

where $u \in H^1(\Omega_1^+; \mathbb{R}^3)$ is such that $u = x$ on S_1. If we set $\Sigma = S_1$ we can apply Theorem 3.10 to the functional $E_\alpha^{el}(\theta)$ to obtain the following Corollary.

Corollary 3.12. *If* $\theta \to \alpha^{-1}$ *then*

$$\frac{1}{\left(\theta^{-1} - \alpha\right)^2} E_\alpha^{el}(\theta) \longrightarrow C^{el}, \tag{3.51}$$

where

$$C^{el} := \min \left\{ \frac{1}{2} \int_{\Omega_1^+} \mathbb{C} \nabla u^{\text{sym}} : \nabla u^{\text{sym}} \, dx : \; u \in H^1(\Omega_1^+; \mathbb{R}^3), \, u = x \textit{ on } S_1 \right\} . \tag{3.52}$$

Moreover $C^{el} > 0$.

Proof. We only need to prove that $C^{el} > 0$, since the rest of the statement follows from Theorem 3.10. Let u be the unique (regular) solution to (3.52). Assume by contradiction that $C^{el} = 0$, that is,

$$\int_{\Omega_1^+} \mathbb{C} \nabla u^{\text{sym}} : \nabla u^{\text{sym}} \, dx = 0 \,. \tag{3.53}$$

Then, by Korn's inequality (see Theorem 2.31), growth condition (3.44), and (3.53), there exists a constant antisymmetric matrix $A \in \mathbb{M}^{3\times 3}_{\text{skew}}$ such that

$$\int_{\Omega_1^+} |\nabla u - A|^2 \, dx = 0 \,,$$

which implies $\nabla u = A$ a.e. in Ω_1^+. Since $u = x$ on S_1, we can extend u to Ω_1^-, so that

$$\nabla u = A \quad \text{in} \quad \Omega_1^+ , \qquad \nabla u = I \quad \text{in} \quad \Omega_1^- . \tag{3.54}$$

As seen in Section 2.3.1, condition (3.54) implies that $\operatorname{rank}(A - I) = 1$. However this is a contradiction, since one can readily check that $A - I$ is invertible for every $A \in \mathbb{M}^{3\times 3}_{\text{skew}}$. Therefore $C^{el} > 0$. □

From Proposition 3.11 we know that, if $\{\theta_R\}$ is a minimising sequence, then $\theta_R \to \alpha^{-1}$. We can then linearise the elastic energy along the sequence θ_R:

$$\begin{aligned} E^{el}_{\alpha,R}(\theta_R) &= R^3\theta_R^3\, E^{el}_{\alpha}(\theta_R) = R^3\theta_R^3(\theta_R^{-1} - \alpha)^2 \, \frac{1}{(\theta_R^{-1} - \alpha)^2} \, E^{el}_{\alpha}(\theta_R) \\ &\overset{(3.51)}{=} R^3\theta_R^3(\theta_R^{-1} - \alpha)^2 (C^{el} + \varepsilon_R) = k^{el}_R R^3 \theta_R \,(\alpha\theta_R - 1)^2, \end{aligned}$$

where $\varepsilon_R \to 0$ as $R \to +\infty$ and $k^{el}_R := C^{el} + \varepsilon_R$. Since $C^{el} > 0$, $k^{el}_R > 0$ for R sufficiently large (and in fact for all R). We are thus led to define the family of polynomials

$$P^{tot}_{k,R}(\theta) := P^{el}_{k,R}(\theta) + E^{pl}_R(\theta), \tag{3.55}$$

where $k, R > 0$ are positive parameters and $P^{el}_{k,R}(\theta) := kR^3\theta(\alpha\theta - 1)^2$. In this way we can write

$$E^{tot}_{\alpha,R}(\theta_R) = P^{tot}_{k^{el}_R,R}(\theta_R) . \tag{3.56}$$

By optimising $P^{tot}_{k,R}$ with respect to θ, we deduce the asymptotic behavior of $E^{tot}_{\alpha,R}$. Set

$$\mathcal{E}^{el}(R) := \frac{\sigma^2}{\alpha^3 C^{el}}\, R \qquad \text{and} \qquad \mathcal{E}^{pl}(R) := \sigma R^2 \left(1 - \frac{1}{\alpha^2}\right) - 2\frac{\sigma^2}{\alpha^3 C^{el}} R .$$

Theorem 3.13. *Let θ_R be a minimising sequence for $E^{tot}_{\alpha,R}$. We have*

$$\theta_R = \frac{1}{\alpha}\Big(1 + \frac{\sigma}{\alpha C^{el}} \frac{1}{R} + o\Big(\frac{1}{R}\Big)\Big) , \tag{3.57}$$

where $\frac{o(t)}{t} \to 0$ as $t \to 0$. Moreover,

$$E^{el}_{\alpha,R}(\theta_R) = \mathcal{E}^{el}(R) + o(R), \quad E^{pl}_R(\theta_R) = \mathcal{E}^{pl}(R) + o(R), \tag{3.58}$$

where $\frac{o(R)}{R} \to 0$ as $R \to +\infty$. In particular, we have

$$E^{tot}_{\alpha,R} = \mathcal{E}^{el}(R) + \mathcal{E}^{pl}(R) + o(R).$$

Proof. First we show that for every $k > 0$ and R large enough there exists a unique minimizer $\theta_{k,R}$ of $P^{tot}_{k,R}$ in $[\alpha^{-1}, 1]$, with $\theta_{k,R} \to \alpha^{-1}$ as $R \to +\infty$. To this purpose, we compute the derivative of $P^{tot}_{k,R}$ with respect to θ

$$(P^{tot}_{k,R})'(\theta) = R^2 \left\{(3\alpha^2 kR)\theta^2 - 2(2\alpha kR + \sigma)\theta + kR\right\}.$$

One can check that it vanishes at

$$\theta_{\pm}(R) = \frac{1}{3\alpha}\left\{2 + \frac{c}{R} \pm f(R)\right\}, \tag{3.59}$$

where

$$f(R) := \sqrt{1 + \frac{4c}{R} + \frac{c^2}{R^2}} \qquad \text{and} \qquad c := \frac{\sigma}{\alpha k}. \tag{3.60}$$

Since $f(R) > 1$ we have $\theta_+(R) > \alpha^{-1}$. Moreover, $f(R) \to 1$, and thus $\theta_+(R) \to \alpha^{-1}$, as $R \to +\infty$. Hence $\theta_+(R) \in [\alpha^{-1}, 1]$ for R large enough. Also note that $\theta_-(R) < \alpha^{-1}$ for R sufficiently large. The second derivative is given by

$$(P^{tot}_{k,R})''(\theta) = R^2 \left\{(6\alpha^2 kR)\theta - 2(2\alpha kR + \sigma)\right\},$$

which can be checked to be nonnegative at $\theta_+(R)$

$$(P^{tot}_{k,R})''(\theta_+(R)) = 2\alpha kR^3 f(R) \geq 0.$$

This proves that $\theta_{k,R} := \theta_+(R)$ is the unique minimizer of $P^{tot}_{k,R}$ in $[\alpha^{-1}, 1]$, for R sufficiently large. Moreover from (3.59) we conclude that $\theta_{k,R} \to \alpha^{-1}$ as $R \to +\infty$.

Evaluating $P^{el}_{k,R}$ and E^{pl}_R at $\theta = \theta_{k,R}$ we find

$$P^{el}_{k,R}(\theta_{k,R}) = \frac{2}{27\alpha^4 k^2}\{2\sigma^3 + 2\alpha k\sigma^2(3 + f(R))R + \left(2\alpha^2 k^2 \sigma f\right) R^2 + \alpha^3 k^3 (1 - f(R))R^3\}, \tag{3.61}$$

$$E^{pl}_R(\theta_{k,R}) = \sigma R^2(1 - \theta^2_{k,R}). \tag{3.62}$$

In order to show (3.57) and (3.58) we perform a Taylor expansion in (3.60) and (3.59). Using $\sqrt{1+x} = 1 + x/2 - x^2/8 + x^3/16 + o(x^3)$ we compute

$$f(R) = 1 + 2\left(\frac{\sigma}{\alpha k}\right)\frac{1}{R} - \frac{3}{2}\left(\frac{\sigma^2}{\alpha^2 k^2}\right)\frac{1}{R^2} + 3\left(\frac{\sigma^3}{\alpha^3 k^3}\right)\frac{1}{R^3} + o\left(\frac{1}{R^3}\right). \tag{3.63}$$

Plugging (3.63) into (3.59) and recalling that $k^{el}_R \to C^{el}$ as $R \to +\infty$, we deduce (3.57).

Using (3.63) we can expand the terms in (3.61) to get

$$2\alpha k\sigma^2(3+f(R))R = (8\alpha k\sigma^2)R + 4\sigma^3 + o\left(R\right) , \tag{3.64}$$

$$\left(2\alpha^2k^2\sigma f\right) R^2 = (2\alpha^2k^2\sigma)R^2 + (4\alpha k\sigma^2)R - 3\sigma^3 + o\left(R\right) , \tag{3.65}$$

$$\alpha^3k^3(1-f(R))R^3 = -(2\alpha^2k^2\sigma)R^2 + \frac{3}{2}(\alpha k\sigma^2)R - 3\sigma^3 + o\left(R\right) . \tag{3.66}$$

Recalling that $k_R^{el} \to C^{el}$ as $R \to +\infty$, plugging (3.64)-(3.66) into (3.61) yields the first equation in (3.58). Next we compute

$$\theta_{k,R}^2 = \frac{1}{9\alpha^2}\left\{5 + 4f(R) + 2c(4+f(R))\frac{1}{R} + \frac{2c}{R^2}\right\} . \tag{3.67}$$

Plugging (3.63) into (3.67) gives

$$\theta_{k,R}^2 = \frac{1}{\alpha^2}\left\{1 + \frac{2c}{R} + o\left(\frac{1}{R^3}\right)\right\} . \tag{3.68}$$

The second relation in (3.58) follows by inserting (3.68) into (3.62), using again $k_R^{el} \to C^{el}$ as $R \to +\infty$.

□

Remark 3.14. The analysis developed in this section can be applied to different crystal configurations. For instance, consider two concentric wires N_{int} and N_{ext}. Specifically, the external wire can be represented by $(S_{2R} \setminus S_R) \times (0, hR)$ and the internal by $S_{\theta R} \times (0, hR)$ with $\theta \in [\alpha^{-1}, 1]$. Here $h > 0$ is a fixed height and αI is the equilibrium of N_{int}, with $\alpha > 1$. The external wire is already in equilibrium. The admissible deformations of N_{int} are maps $v \colon N_{\text{int}} \to \mathbb{R}^3$ such that $v = \theta^{-1}x$ on the lateral boundary of N_{int}, so that it matches the internal lateral boundary of N_{ext}. The total energy is given by the sum of an elastic term and a plastic term, the latter proportional to the reference surface mismatch between the lateral boundaries of the nanowires:

$$E^{tot}(v,\theta) = \int W(\nabla v)\, dx + \sigma h R^2(1-\theta) . \tag{3.69}$$

If $\theta = 1$ the two wires coincide and the energy is entirely elastic. If $\theta = \alpha^{-1}$ then the elastic energy has minimum zero and E^{tot} is purely dislocation energy. If $\theta \in (\alpha^{-1}, 1)$ then none of the two contributions is zero and we are in a mixed case. For such physical system we can carry on the same analysis as before, up to very minor changes.

3.5 Conclusions and perspectives

In [22] we have proposed a simple continuous model for dislocations at semi-coherent interfaces. Our analysis seems flexible enough to describe different interfaces and crystalline configurations. Here we discuss the main achievements of our paper, possible extensions to other physical systems, and future perspectives.

In Section 3.2 we have analysed a line tension model for dislocations at semi-coherent interfaces, in the context of nonlinear elasticity. Within this model, we have shown that there exists a critical size of the crystal such that dislocations become energetically more favorable than purely elastic deformations (see Theorem 3.5). More precisely, we have shown that the energy induced by dislocations scales like the surface area of the interface, while the purely elastic energy scales like the volume of the crystal. This is compatible with the experimental observation that dislocations form periodic networks at the interface. In fact, the proof of Proposition 3.2 is based on the fact that, if a net of dislocations is optimal on an interface S_r of size r, then cutting and pasting such a geometry on S_{4r} one constructs a good periodic energy competitor for a larger interface. A more challenging question is whether the optimal geometry of dislocations is periodic in the microscopic scale b. Although we have not given a rigorous proof of this fact, we have shown an explicit construction of a periodic array of dislocations spaced at distance $\frac{b}{\alpha-1}$, that is optimal in the scaling of the energy.

Then, in Section 3.4, we have proposed a simpler and more specific continuous model for dislocations, describing, to some extent, dislocations at phase boundaries, in heterostructured wires and in epitaxial crystal growth. In such a model the area of the reference configuration of the overlayer is a free parameter, while in the deformed configuration there is a perfect match between the underlayer and the overlayer.

The variational formulation is very basic, depending only on three parameters: the diameter of the underlayer, the misfit between the lattice parameters, and the free boundary, described by a single parameter: the area gap between the reference underlayer and overlayer, tuning the amount of dislocations at the interface.

The proposed variational model is rich enough to describe the size effects already discussed, and allows us to refine the analysis of the energy minimisers. Indeed, we have shown that, in the limit $R \to +\infty$, the surface energy induced by dislocations is predominant (scaling like R^2), while the volume elastic energy represents a lower order term (scaling like R). Since the elastic energy is vanishing (Proposition 3.11), we can perform a linearization: the asymptotic behaviour of the total energy functional is explicit, depending only on the material parameters in the energy functional, and on the linearised elastic tensor (see Theorem 3.13). The only unknown parameter in our formulation is σ, which roughly speaking (multiplied by b) represents the energy per unit dislocation length (while $\sigma(\alpha^2 - 1)$ represents the energy per unit area of the interface). We have proposed some explicit formula for σ, depending only on the elastic tensor and on a core energy parameter γ^{ch}, describing the core (chemical) energy per unit dislocation length (see (3.26)).

Summarising, [22] proposes a basic variational model describing the competition between the plastic energy spent at interfaces, and the corresponding release of bulk energy. In this variational formulation, the size of the interface of the overlayer is a free parameter. In this respect, our model fits into the class of so called free boundary problems.

The proposed energy is built upon some heuristic arguments, supported by formal mathematical derivations based on the semi-discrete theory of dislocations.

While the paper focuses on a specific configuration, the method seems flexible to be extended to several crystalline structures and to different physical contexts, such as grain boundaries, where the misfit between the crystal lattices are described by rotations rather than dilations (see [35]), and epitaxial growth, where the total energy should be completed by adding the surface energy induced by the exterior boundary of the overlayer (see [38]).

Chapter 4

Linearised polycrystals from a 2D system of edge dislocations

4.1 Introduction

In this chapter we present the results obtained in [23], where we derive polycrystalline structures starting from a two-dimensional system of edge dislocations (see Section 2.1 for more information on dislocations).

Many solids in nature exhibit a polycrystalline structure. A *single phase polycrystal* is formed by many individual crystal grains, having the same underlying periodic atomic structure, but rotated with respect to each other. The region that separates two grains with different orientation is called *grain boundary*. Since the grains are mutually rotated, the periodic crystalline structure is disrupted at grain boundaries. As a consequence, grain boundaries are regions of high energy concentration.

Polycrystalline structures, which a priori may seem energetically not convenient, arise from the crystallisation of a melt. As the temperature decreases, crystallisation starts from a number of points within the melt. These single grains grow until they meet. Since their orientation is generally different, the grains are not able to arrange in a single crystal and grain boundaries appear as local minimisers of the energy, in fact as metastable configurations. After crystallisation there is a grain growth phase, when the solid tries to minimise the energy by reducing boundary area. This process happens by atomic diffusion within the material, and it is thermally activated (see

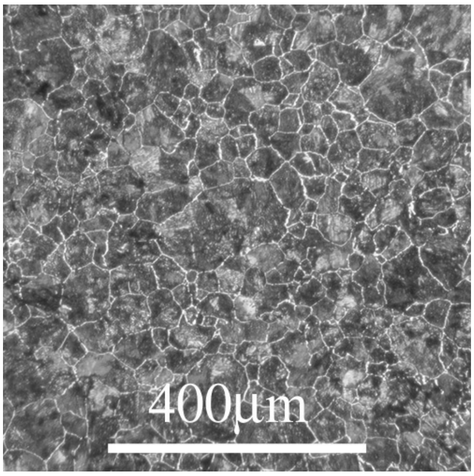


Figure 4.1: Section of an iron-carbon alloy. The darker regions are single crystal grains, separated by grain boundaries that are represented by lighter lines (source [59], licensed under CC BY-NC-SA 2.0 UK).

[31, Ch 5.7], [9]). On a mesoscopic scale a polycrystal resembles the structure in Figure 4.1.

The purpose of [23] is to describe, and to some extent to predict, polycrystalline structures by variational principles. To this purpose, we first derive by Γ-convergence, as the lattice spacing of the crystal tends to zero, a total energy functional depending on the strain and on the dislocation density. Then, we focus on the ground states of this energy, neglecting the fundamental mechanisms driving the formation and evolution of grain boundaries. The main feature of [23] is that grain boundaries and the corresponding grain orientations are not introduced as internal variables of the energy; actually, they spontaneously arise only as a result of energy minimisation under suitable boundary conditions.

Let us start our discussion by considering the case of two dimensional small angle tilt grain boundaries (abbreviated in SATGB from now on). The atomic structure for SATGBs is well understood (see [31, Ch 3.4], [55]). In fact, the lattice mismatch between two grains mutually tilted by a small angle θ is accommodated by a single array of edge dislocations at the grain boundary, evenly spaced at distance $\delta \approx \varepsilon/\theta$, where ε represents the atomic lattice spacing. Therefore the number of dislocations at a SATGB is of order θ/ε (see Figure 4.2). The elastic energy for SATGBs is given

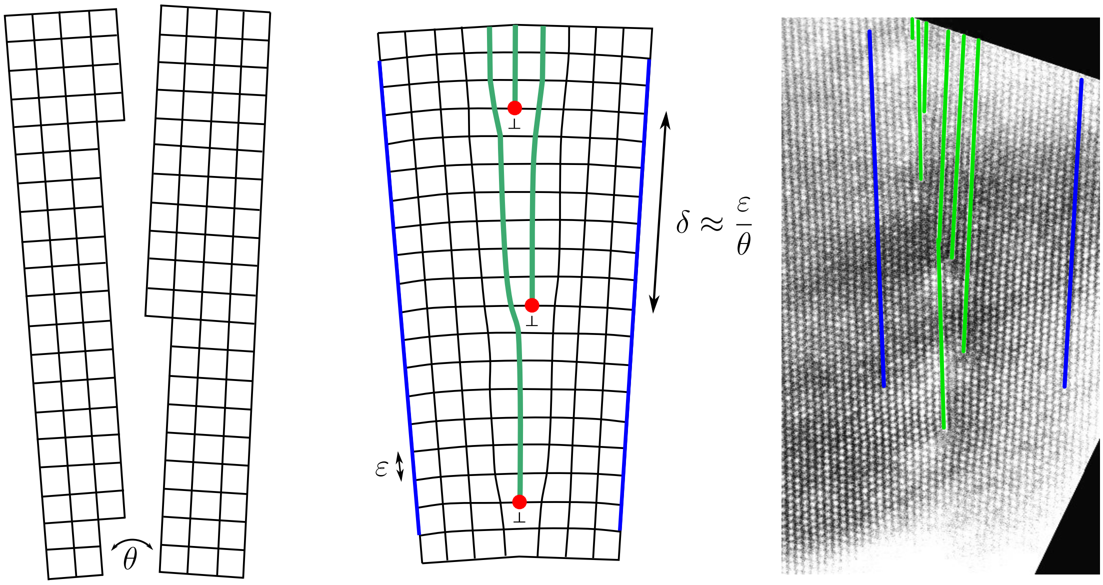


Figure 4.2: Left: schematic picture of two grains mutually rotated by an angle θ. Centre: schematic picture of a SATGB. The two grains are joined together and the lattice misfit is accommodated by an array of edge dislocations spaced with δ and denoted with red dots (pictures after [54]). Right: HRTEM of a SATGB in silicon. The green lines represent lines of atoms ending within the crystal. Their end points inside the crystal are edge dislocations, which correspond to the red atoms in the central picture. The blue lines show the mutual rotation between the grains (image from [26, Section 7.2.2] with permission of the author H. Foell).

by the celebrated Read-Shockley formula introduced in [55]

$$\text{Elastic Energy} = \mathrm{E}_0\theta(\mathrm{A} + |\log\theta|)\,, \tag{4.1}$$

where E_0 and A are positive constants depending only on the material. Recently Lauteri and Luckhaus in [35] derived the Read-Shockley formula by scaling arguments starting from a nonlinear elastic energy.

In [23] we will deal with lower energy regimes, deriving by Γ-convergence, as the lattice spacing $\varepsilon \to 0$ and the number of dislocations $N_\varepsilon \to \infty$, some limit energy functional $\mathcal{F}$ that could be seen as a linearised version of the Read-Shockley formula. We will work in the setting of linearised planar elasticity of [30] and in particular we will require good separation of the dislocation cores. Such good separation hypothesis will in turn imply that the number of dislocations at grain boundaries is of order

$$N_\varepsilon \ll \frac{\theta}{\varepsilon}\,. \tag{4.2}$$

This low density of dislocations is compatible with the low energy regime we deal with. More precisely, as a consequence of our energy bounds, there are not enough dislocations to accommodate small rotations θ between grains, but rather we can have rotations of an infinitesimal angle $\theta \approx 0$, that is, antisymmetric matrices. It is in this respect that our analysis represents the linearised counterpart of the celebrated Read-Shockley formula: grains are micro-rotated by infinitesimal angles and the corresponding ground states can be seen as linearised polycrystals, whose energy is linear with respect to the number of dislocations at grain boundaries.

We will now briefly introduce the setting of our problem, following [30]. In linearised planar elasticity, the reference configuration is a bounded domain $\Omega \subset \mathbb{R}^2$, representing a horizontal section of an infinite cylindrical crystal $\Omega \times \mathbb{R}$. A displacement is a regular map $u\colon \Omega \to \mathbb{R}^2$ and the stored energy density $W\colon \mathbb{M}^{2\times 2} \to [0,+\infty)$ is defined by

$$W(F) := \frac{1}{2}\mathbb{C}F : F\,,$$

where $\mathbb{C}$ is the fourth order stress tensor, that satisfies

$$c^{-1}|F^{\rm sym}|^2 \le \mathbb{C}F : F \le c|F^{\rm sym}|^2 \quad \text{for every} \quad F \in \mathbb{M}^{2\times 2}\,.$$

Here $F^{\rm sym} := (F + F^T)/2$ and c is some positive constant (see Section 2.2.2 for details on linear elasticity). The energy density W acts on gradient strain fields $\beta := \nabla u$ and the elastic energy induced by β is defined as

$$\int_\Omega W(\beta)\,dx\,.$$

Following the discrete dislocation model, dislocations are introduced as point defects of the strain β (see [8, 18, 30] and Section 2.2.3). More specifically, a straight dislocation line γ orthogonal to the cross section Ω is identified with the point $x_0 = \gamma \cap \Omega$. We then require

$$\operatorname{Curl}\beta = \xi\,\delta_{x_0}\,, \tag{4.3}$$

in the sense of distributions. Here $\xi := (\xi_1, \xi_2, 0)$ is the Burgers vector, orthogonal to γ, so that (γ, ξ) defines an edge dislocation. Therefore, also (x_0, ξ) represents an

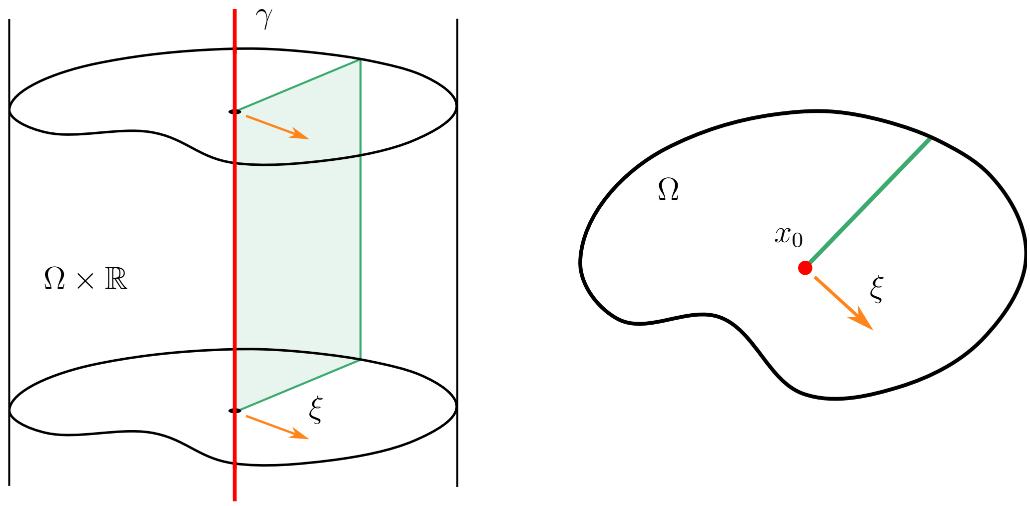


Figure 4.3: Left: cylindrical domain $\Omega \times \mathbb{R}$. The dislocation (γ, ξ) is of edge type. The green plane represents the extra half-plane of atoms corresponding to γ. Right: section Ω of the cylindrical domain in the left picture. The red point $x_0 = \gamma \cap \Omega$ represents the section of the dislocation line, so that (x_0, ξ) is an edge dislocation. The green line is the intersection of the extra half-plane of atoms in the left picture with Ω.

edge dislocation (see Figure 4.3). By proceeding as in the proof of Proposition 4.9, it is immediate to check that (4.3) implies

$$\int_{B_\sigma(x_0)\setminus B_\varepsilon(x_0)} W(\beta)\, dx \geq c \log \frac{\sigma}{\varepsilon}\,, \quad \text{for every} \quad \sigma > \varepsilon > 0\,.$$

From the above inequality we deduce that, as $\varepsilon \to 0$, the energy diverges logarithmically in neighbourhoods of x_0. To overcome this problem we adopt the so-called core radius approach (see also Section 2.2.3). Namely, we remove from Ω the ball $B_\varepsilon(x)$, called the *core region*, where ε is proportional to the underlying lattice spacing, and we replace (4.3) with the circulation condition

$$\int_{\partial B_\varepsilon(x_0)} \beta \cdot t\, ds = \xi\,.$$

In the above formula t is the unit tangent vector to $\partial B_\varepsilon(x_0)$ and ds in the 1 - dimensional Hausdorff measure. A generic distribution of N dislocations will therefore be identified with the points $\{x_i\}_{i=1}^N$. To each x_i we associate a corresponding Burgers vector ξ_i, belonging to a finite set $\mathcal{S} \subset \mathbb{R}^2$ of admissible Burgers vectors, which depends on the underlying crystalline structure. Clearly the Burgers vector scales like ε; for example for a square lattice we have $\mathcal{S} = \varepsilon\{\pm e_1, \pm e_2\}$. From now on we

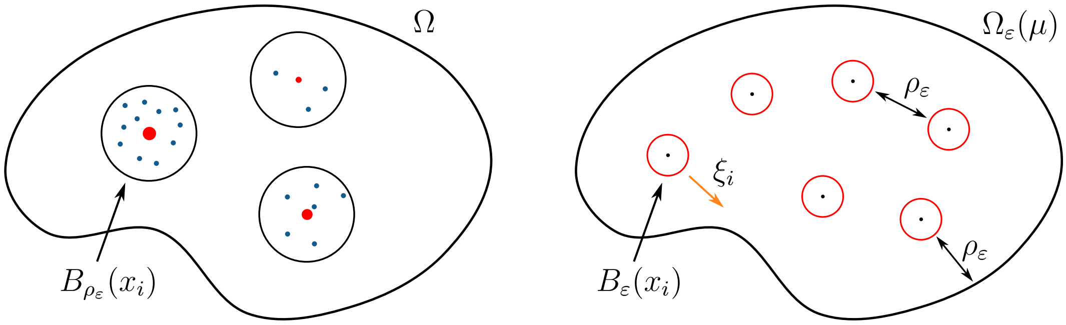


Figure 4.4: Left: clusters of dislocations (blue points) inside balls $B_{\rho_\varepsilon}(x_i)$ are identified with a single dislocation $\xi_i\,\delta_{x_i}$ centred at x_i (red point). The size of the point denoting x_i in the picture is proportional to the magnitude of the total Burgers vector in the cluster. Right: the drilled domain $\Omega_\varepsilon(\mu)$. Balls of radius ε, centred at the dislocation points x_i, are removed from Ω. A circulation condition on the strain is assigned on each $\partial B_\varepsilon(x_i)$.

will always renormalise the Burgers vectors, scaling them by ε^{-1}, so that $\mathcal{S}$ becomes a fixed set independent of the lattice spacing. Since the energy is quadratic with respect to the Burgers vector, our energy is in turn scaled by ε^{-2}. Following [30], we make a technical hypothesis of good separation for the dislocation cores, by introducing a small scale $\rho_\varepsilon \gg \varepsilon$, called hard core radius. Any cluster of dislocations contained in a ball $B_{\rho_\varepsilon}(x_0) \subset \Omega$ will be identified with a multiple dislocation $\xi\,\delta_{x_0}$, where ξ is the sum of the Burgers vectors corresponding to the dislocations in the cluster (see Figure 4.4 Left). Therefore $\xi \in \mathbb{S} := \mathrm{Span}_{\mathbb{Z}}\,\mathcal{S}$, where $\mathbb{S}$ represents the set of multiple Burgers vectors. Under this assumption, a generic distribution of dislocations is identified with a measure

$$\mu = \sum_{i=1}^{N} \xi_i\,\delta_{x_i}\,, \quad \xi_i \in \mathbb{S}\,,$$

with $|x_i - x_j| \geq 2\rho_\varepsilon$ and $\mathrm{dist}(x_k, \partial\Omega) > \rho_\varepsilon$. Denote with $\Omega_\varepsilon(\mu) := \Omega \setminus \bigcup_i B_\varepsilon(x_i)$ the drilled domain (see Figure 4.4 Right). The admissible strains associated to μ are matrix fields $\beta \in L^2(\Omega_\varepsilon(\mu); \mathbb{M}^{2\times 2})$ such that $\mathrm{Curl}\,\beta \llcorner \Omega_\varepsilon(\mu) = 0$ and

$$\int_{\partial B_\varepsilon(x_i)} \beta \cdot t\, ds = \xi_i\,, \quad \text{for every} \quad i = 1, \dots, N\,. \tag{4.4}$$

The elastic energy corresponding to (μ, β) is defined as

$$E_\varepsilon(\mu, \beta) := \int_{\Omega_\varepsilon(\mu)} W(\beta)\, dx\,. \tag{4.5}$$

The energy induced by the dislocation μ is given by minimising (4.5) over the set of strains satisfying (4.4). This energy is always positive if $\mu \neq 0$, due to (4.4).

The energy contribution of a single dislocation core is of order $|\log \varepsilon|$ (see Proposition 4.10). Therefore for a system of N_ε dislocations, with $N_\varepsilon \to \infty$ as $\varepsilon \to 0$, the relevant energy regime is

$$E_\varepsilon \approx N_\varepsilon |\log \varepsilon| \,.$$

This scaling was already studied in [30] in the critical regime $N_\varepsilon \approx |\log \varepsilon|$, where the authors characterise the Γ-limit of E_ε, rescaled by $|\log \varepsilon|^2$. We will later discuss how this compares to our Γ-convergence result.

For our analysis we will consider a higher energy regime corresponding to

$$N_\varepsilon \gg |\log \varepsilon| \,.$$

We will see that this energy regime will account for grain boundaries that are mutually rotated by an *infinitesimal* angle $\theta \approx 0$. To be more specific, one can split the contribution of E_ε into

$$E_\varepsilon(\mu, \beta) = E_\varepsilon^{\text{inter}}(\mu, \beta) + E_\varepsilon^{\text{self}}(\mu, \beta) \,,$$

where $E_\varepsilon^{\text{self}}$ is the self-energy computed in the hard core region $\cup_i B_{\rho_\varepsilon}(x_i)$ while $E_\varepsilon^{\text{inter}}$ is the interaction energy calculated outside the hard core region. In Theorem 4.17 we will prove that the Γ-limit as $\varepsilon \to 0$ of the rescaled functionals E_ε, with respect to the strains and the dislocation measures, is of the form

$$\mathcal{F}(\mu, S, A) = \int_\Omega W(S)\, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| \,. \tag{4.6}$$

The first term of $\mathcal{F}$ comes from the interaction energy. It represents the elastic energy of the symmetric field S, which is the weak limit of the symmetric part of the strains rescaled by $\sqrt{N_\varepsilon |\log \varepsilon|}$. Instead, the antisymmetric part of the strain, rescaled by N_ε, weakly converges to an antisymmetric field A. Therefore, since $N_\varepsilon \gg |\log \varepsilon|$, the symmetric part of the strain is of lower order with respect to the antisymmetric part.

The second term of $\mathcal{F}$ is the plastic energy. The density function φ is positively 1-homogeneous and it can be defined as the relaxation of a cell-problem formula. To be more specific, we can define (see Proposition 4.12) the self-energy $\psi \colon \mathbb{R}^2 \to [0, \infty)$

induced by a single dislocation $\xi\,\delta_0$ centred at the origin as

$$\psi(\xi) := \lim_{\varepsilon\to 0} \min \left\{ \frac{1}{|\log\varepsilon|} \int_{C_\varepsilon} W(\beta)\,dx : \ \beta \in L^2(C_\varepsilon;\mathbb{M}^{2\times 2}) , \right.$$

$$\left. \operatorname{Curl}\beta \llcorner C_\varepsilon = 0 \, , \ \int_{\partial B_\varepsilon(0)} \beta \cdot t\,ds = \xi \right\} ,$$

where $C_\varepsilon := B_1(0) \setminus B_\varepsilon(0)$. Then the density φ is defined as the relaxation of ψ on the set of Burgers vectors $\mathbb{S}$

$$\varphi(\xi) := \min \left\{ \sum_{i=1}^{M} \lambda_i \psi(\xi_i) : \ \sum_{i=1}^{M} \lambda_i \xi_i = \xi \, , \ M \in \mathbb{N}, \, \lambda_i \geq 0 \, , \ \xi_i \in \mathbb{S} \right\} .$$

The measure μ in (4.4) is the weak-$*$ limit of the dislocation measures rescaled by N_ε, and $d\mu/d|\mu|$ represents the Radon-Nikodym derivative of μ with respect to $|\mu|$ (see Section A.2.4). Notice that the antisymmetric part of the strain is of the same order N_ε, whereas the symmetric part is of lower order. As a consequence, the compatibility condition (4.4) reads as $\operatorname{Curl} A = \mu$ in the limit. This implies that the *elastic* and *plastic* terms in $\mathcal{F}$ are *decoupled*. Indeed this is the main difference with the critical regime $N_\varepsilon \approx |\log\varepsilon|$ studied in [30], where the contribution of the symmetric and antisymmetric part of the strain, as well as the dislocation measure, have the same order $|\log\varepsilon|$. This results into the coupling in [30] of the two terms of the energy, through the condition $\operatorname{curl}\beta = \mu$ where $\beta = S + A$.

Next we focus on the study of the Γ-limit $\mathcal{F}$. Precisely, we impose *piecewise constant* Dirichlet boundary conditions on A, and we show that $\mathcal{F}$ is minimised by strains that are *locally constant* and take values into the set of *antisymmetric matrices*. More precisely, there is a Caccioppoli partition of Ω with sets of finite perimeter where the antisymmetric strain is constant. Such sets are nothing but the grains of the polycrystal, while the corresponding constant antisymmetric matrices represents their orientation. We call these configurations *linearised polycrystals*. This definition is motivated by the fact that *antisymmetric matrices* can be considered as infinitesimal rotations, being the linearisation about the identity of the space of rotations. The proof of this result is based on the simple observation that the variational problem is equivalent to minimise some anisotropic total variation of a scalar function, which is locally constant on $\partial\Omega$. By coarea formula, it is easy to show that there always exists a piece-wise constant minimiser.

This chapter is organised as follows. In Section 4.2 we introduce the rigorous mathematical setting of the problem. In Section 4.3 we recall some results from [30] that will be useful for the Γ-convergence analysis of the rescaled energy E_ε. The main Γ-convergence result will be proved in Section 4.4. In Section 4.5 we will add Dirichlet type boundary conditions to the Γ-convergence analysis done in the previous section. Finally, in Section 4.6 we will show that the plastic part of $\mathcal{F}$ is minimised by linearised polycrystals, by prescribing piecewise constant boundary conditions on the antisymmetric part of the limit strain.

4.2 Setting of the problem

Let $\Omega \subset \mathbb{R}^2$ be a bounded open domain with Lipschitz boundary. The set Ω represents a horizontal section of an infinite cylindrical crystal $\Omega \times \mathbb{R}$. Define as $\mathcal{S} := \{b_1, \dots, b_s\}$ the class of Burgers vectors. We will assume that $\mathcal{S}$ contains at least two linearly independent vectors so that $\operatorname{Span}_{\mathbb{R}} \mathcal{S} = \mathbb{R}^2$. We then define the set of slip directions

$$\mathbb{S} := \operatorname{Span}_{\mathbb{Z}} \mathcal{S} \,,$$

that coincides with the set of Burgers vectors for multiple dislocations. A dislocation, of edge type, can be identified with a point $x_i \in \Omega$ and a vector $\xi_i \in \mathbb{S}$.

Let $\varepsilon > 0$ be the interatomic distance for the crystal and N_ε be the number of dislocations present in the crystal at a scale ε. As in [30], we introduce a hard core radius ρ_ε such that

(i) $\lim_{\varepsilon \to 0} \rho_\varepsilon / \varepsilon^s = \infty$ for every fixed $0 < s < 1$,

(ii) $\lim_{\varepsilon \to 0} N_\varepsilon \rho_\varepsilon^2 = 0$.

The first condition implies that the hard core region contains almost all the-self energy (see Proposition 4.13), while the second one guarantees that the area of the hard core region tends to zero. The above conditions are compatible if

$$N_\varepsilon \varepsilon^s \to 0 \,, \quad \text{for every fixed} \quad s > 0 \,. \tag{4.7}$$

The class of admissible dislocations is defined by

$$\begin{aligned}\mathcal{AD}_\varepsilon(\Omega) := \Big\{\mu \in & \mathcal{M}(\Omega;\mathbb{R}^2) : \ \mu = \sum_{i=1}^{M} \xi_i \delta_{x_i} \,, \ M \in \mathbb{N}, \ \xi_i \in \mathbb{S} \,, \\ & B_{\rho_\varepsilon}(x_i) \subset \Omega \,, \ |x_j - x_k| \geq 2\rho_\varepsilon \,, \ \text{for every } i \text{ and } \ j \neq k \Big\} \,.\end{aligned} \tag{4.8}$$

Here $\mathcal{M}(\Omega;\mathbb{R}^2)$ denotes the space of $\mathbb{R}^2$ valued Radon measures on Ω and $B_r(x)$ is the ball of radius r centred at $x \in \mathbb{R}^2$ (see Section A.2 for more details on measures). For a given $\mu \in \mathcal{AD}_\varepsilon(\Omega)$ and $r > 0$ define

$$\Omega_r(\mu) := \Omega \setminus \bigcup_{x_i \in \operatorname{supp}(\mu)} \overline{B_r(x_i)} \,. \tag{4.9}$$

The class of admissible strains associated with $\mu = \sum_{i=1}^{M} \xi_i \delta_{x_i} \in \mathcal{AD}_\varepsilon(\Omega)$ is given by the maps $\beta \in L^2(\Omega_\varepsilon(\mu);\mathbb{R}^2)$ such that

$$\operatorname{Curl} \beta \llcorner \Omega_\varepsilon(\mu) = 0 \,, \qquad \int_{\partial B_\varepsilon(x_i)} \beta \cdot t \, ds = \xi_i \quad \text{for every} \quad i = 1, \dots, M \,.$$

The identity $\operatorname{Curl} \beta = 0$ is intended in the sense of distributions, where

$$\operatorname{Curl} \beta := (\partial_1 \beta_{12} - \partial_2 \beta_{11}, \partial_1 \beta_{22} - \partial_2 \beta_{21}) \,.$$

The integrand $\beta \cdot t$ is intended in the sense of traces (see Remark 4.2 in Section 4.3.1), and t is the unit tangent vector to $\partial B_\varepsilon(x_i)$, obtained by a clock-wise rotation of $\pi/2$ of the inner normal ν to $B_\varepsilon(x)$, that is $t := J\nu$ with

$$J := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \,. \tag{4.10}$$

In the following it will be useful to extend the admissible strains to the whole Ω. Therefore, for a dislocation measure $\mu = \sum_{i=1}^{M} \xi_i \delta_{x_i} \in \mathcal{AD}_\varepsilon(\Omega)$, we introduce the class $\mathcal{AS}_\varepsilon(\mu)$ of admissible strains as

$$\begin{aligned}\mathcal{AS}_\varepsilon(\mu) := \Big\{ & \beta \in L^2(\Omega;\mathbb{M}^{2\times 2}) : \ \beta \equiv 0 \text{ in } \Omega \setminus \Omega_\varepsilon(\mu) \,, \ \operatorname{Curl} \beta = 0 \text{ in } \Omega_\varepsilon(\mu) \,, \\ & \int_{\partial B_\varepsilon(x_i)} \beta \cdot t \, ds = \xi_i \,, \ \int_{\Omega_\varepsilon(\mu)} \beta^{\text{skew}} \, dx = 0 \,, \ \text{for every } i = 1, \dots, M \Big\} \,.\end{aligned} \tag{4.11}$$

Here $F^{\text{skew}} := (F - F^T)/2$. The last condition in (4.11) is not restrictive and will guarantee the existence of the minimising strain.

The energy associated to an admissible pair (μ, β) with $\mu \in \mathcal{AD}_\varepsilon(\Omega)$ and $\beta \in \mathcal{AS}_\varepsilon(\mu)$ is defined by

$$E_\varepsilon(\mu, \beta) := \int_{\Omega_\varepsilon(\mu)} W(\beta)\, dx = \int_\Omega W(\beta)\, dx\,,$$

where

$$W(F) := \frac{1}{2}\mathbb{C}F : F$$

is the strain energy density. The elasticity tensor $\mathbb{C}$ satisfies

$$c^{-1}|F^{\rm sym}|^2 \le W(F) \le c|F^{\rm sym}|^2 \qquad \text{for every} \quad F \in \mathbb{M}^{2\times 2}\,, \tag{4.12}$$

where $c > 0$ is a given constant.

Notice that for any $\mu \in \mathcal{AD}_\varepsilon(\Omega)$ the minimum problem

$$\min\left\{\int_{\Omega_\varepsilon(\mu)} W(\beta)\, dx :\ \beta \in \mathcal{AS}_\varepsilon(\mu)\right\} \tag{4.13}$$

has a unique solution. This can be seen by removing a finite number of cuts L from $\Omega_\varepsilon(\mu)$ so that $\Omega_\varepsilon(\mu) \setminus L$ becomes simply connected and there exists a displacement gradient such that $\nabla u = \beta$ in $\Omega_\varepsilon(\mu) \setminus L$. Then we can apply the classic Korn inequality (Theorem 4.4) to ∇u, and conclude by using the direct method of calculus of variations (Theorem A.1). Details for this argument can be found in the proof of Proposition 4.11, in the case when $\mu = \xi\delta_0$.

In the following we will assume that we are in the supercritical regime

$$N_\varepsilon \gg |\log \varepsilon|\,. \tag{4.14}$$

As already discussed, the relevant scaling for the asymptotic study of E_ε is given by $N_\varepsilon|\log \varepsilon|$. Therefore we introduce the scaled energy functional defined on $\mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2})$ as

$$\mathcal{F}_\varepsilon(\mu,\beta) := \begin{cases} \dfrac{1}{N_\varepsilon|\log\varepsilon|}\, E_\varepsilon(\mu,\beta) & \text{if } \mu \in \mathcal{AD}_\varepsilon(\Omega)\,,\ \beta \in \mathcal{AS}_\varepsilon(\mu)\,, \\ +\infty & \text{otherwise.} \end{cases} \tag{4.15}$$

4.3 Preliminaries

In this section we will recall some useful results, mainly from [30], that will be needed in the following Γ-convergence analysis.

4.3.1 Remarks on the distributional Curl

Let $\Omega \subset \mathbb{R}^2$ be a Lipschitz bounded domain. For $\beta \in L^2(\Omega; \mathbb{M}^{2\times 2})$ we define the distribution $\operatorname{Curl}\beta \in \mathcal{D}'(\Omega; \mathbb{R}^2)$ as

$$\operatorname{Curl}\beta := (\partial_1 \beta_{12} - \partial_2 \beta_{11}, \partial_1 \beta_{22} - \partial_2 \beta_{21}) . \tag{4.16}$$

Introduce the space of L^2 strains with L^2 Curl as

$$H(\operatorname{Curl}, \Omega) := \left\{ \beta \in L^2(\Omega; \mathbb{M}^{2\times 2}) \colon \operatorname{Curl}\beta \in L^2(\Omega; \mathbb{R}^2) \right\} ,$$

which is a Hilbert space with the norm $(\|\beta\|_{L^2} + \|\operatorname{Curl}\beta\|_{L^2})^{\frac{1}{2}}$. We denote by $H_0(\operatorname{Curl}, \Omega)$ the closure of $C_c^\infty(\Omega; \mathbb{M}^{2\times 2})$ in $H(\operatorname{Curl}, \Omega)$. Also set

$$C^\infty(\overline{\Omega}; \mathbb{M}^{2\times 2}) := \left\{ \varphi \chi_\Omega \colon \varphi \in C^\infty(\mathbb{R}^2; \mathbb{M}^{2\times 2}) \right\} .$$

Recall that $H^{-1/2}(\partial\Omega; \mathbb{R}^2)$ is defined as the dual of the space

$$H^{1/2}(\partial\Omega; \mathbb{R}^2) := \left\{ v \in L^2(\partial\Omega; \mathbb{R}^2) \colon \|v\|_{H^{1/2}} < \infty \right\} ,$$

where $\|\cdot\|_{H^{1/2}}$ is the norm

$$\|v\|_{H^{1/2}} := \int_{\partial\Omega} |v(x)|^2 \, dx + \iint_{\partial\Omega\times\partial\Omega} \frac{|v(x) - v(y)|^2}{|x-y|^2} \, dx \, dy .$$

For the space $H(\operatorname{Curl}, \Omega)$ we have the following trace theorem (see [16, Theorem 2, p. 204]).

Theorem 4.1 (Trace theorem for $H(\operatorname{Curl}, \Omega)$)**.** *Let $\Omega \subset \mathbb{R}^2$ be a Lipschitz bounded domain. Then $C^\infty(\overline{\Omega}; \mathbb{M}^{2\times 2})$ is dense in $H(\operatorname{Curl}, \Omega)$. Moreover, there exists a continuous linear map*

$$T \colon H(\operatorname{Curl}, \Omega) \to H^{-1/2}(\partial\Omega; \mathbb{R}^2) ,$$

called trace map, such that

$$T(\varphi) = (\varphi \cdot t)|_{\partial\Omega} \quad \textit{for every} \quad \varphi \in C^\infty(\overline{\Omega}; \mathbb{M}^{2\times 2}) ,$$

where t is the unit tangent vector to $\partial\Omega$. Furthermore, the kernel of T is such that $\ker T = H_0(\operatorname{Curl}, \Omega)$. *For $\beta \in H(\operatorname{Curl}, \Omega)$ we will denote $T(\beta) = (\beta \cdot t)|_{\partial\Omega}$.*

Remark 4.2 (Trace of admissible strains)**.** Let $\mu \in \mathcal{AD}_\varepsilon(\Omega)$ and $\beta \in L^2(\Omega_\varepsilon(\mu); \mathbb{M}^{2\times 2})$ such that $\operatorname{Curl}\beta \llcorner \Omega_\varepsilon(\mu) = 0$. This implies that $\beta \in H(\operatorname{Curl}, \Omega_\varepsilon(\mu))$ and therefore the trace $\beta \cdot t$ on each $\partial B_\varepsilon(x_i)$ is well defined by Theorem 4.1.

Remark 4.3 (Curl of admissible strains)**.** Let $\mu \in \mathcal{AD}_\varepsilon(\Omega)$ and $\beta \in \mathcal{AS}_\varepsilon(\mu)$. We want to make some considerations on $\operatorname{Curl}\beta$ (see [30, Remark 1]). Recalling definition (4.16), we can define the scalar distribution

$$\operatorname{curl}\beta_{(i)} := \frac{\partial}{\partial x_1}\beta_{i2} - \frac{\partial}{\partial x_2}\beta_{i1}\,,$$

where $\beta_{(i)}$ denotes the i-th row of β. This means that for any test function φ in $C_c^\infty(\Omega)$, we can write

$$\langle \operatorname{curl}\beta_{(i)}, \varphi\rangle = \int_\Omega \beta_{(i)} \cdot J\nabla\varphi\, dx\,, \tag{4.17}$$

where J is the clock-wise rotation of $\pi/2$, as defined in (4.10). Notice that, if $\beta_{(i)} \in L^2(\Omega;\mathbb{R}^2)$, then (4.17) implies that $\operatorname{curl}\beta_{(i)}$ is well defined also for $\varphi \in H_0^1(\Omega)$ and acts continuously on it. Therefore

$$\operatorname{Curl}\beta \in H^{-1}(\Omega;\mathbb{R}^2) \quad \text{for every} \quad \beta \in \mathcal{AS}_\varepsilon(\mu)\,,$$

where $H^{-1}(\Omega;\mathbb{R}^2)$ denotes the dual of the space $H_0^1(\Omega;\mathbb{R}^2)$.

Further, if $\mu = \sum_{i=1}^M \xi_i\,\delta_{x_i} \in \mathcal{AD}_\varepsilon(\Omega)$, then the circulation condition

$$\int_{\partial B_\varepsilon(x_i)} \beta \cdot t\, ds = \xi_i\,, \quad \text{for every} \quad i = 1,\dots,M\,,$$

can be written as

$$\langle \operatorname{Curl}\beta, \varphi\rangle = \sum_{i=1}^M \xi_i\, c_i\,,$$

for every $\varphi \in H_0^1(\Omega)$ such that $\varphi \equiv c_i$ in $B_\varepsilon(x_i)$. If in addition $\varphi \in C_0(\Omega) \cap H_0^1(\Omega)$, then

$$\langle \operatorname{Curl}\beta, \varphi\rangle = \int_\Omega \varphi\, d\mu\,.$$

4.3.2 Korn type inequalities

In this section we will recall some Korn type inequalities useful in the following analysis. Let us start by stating the classic Korn inequality in two-dimensions.

Theorem 4.4 (Korn's inequality, [10])**.** *Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain. There exists a constant $C > 0$ depending only on Ω, such that for every map $u \in H^1(\Omega;\mathbb{R}^2)$ we have*

$$\int_\Omega |\nabla u - A|^2\, dx \le C\int_\Omega |\nabla u^{\mathrm{sym}}|^2\, dx\,, \tag{4.18}$$

where A *is the constant* 2×2 *antisymmetric matrix defined by*

$$A := \frac{1}{|\Omega|}\int_\Omega \nabla u^{\mathrm{skew}}\,dx\,,$$

with $\nabla u^{\mathrm{sym}} := (\nabla u + \nabla u^T)/2$ *and* $\nabla u^{\mathrm{skew}} := (\nabla u - \nabla u^T)/2$.

Remark 4.5 (Korn's constant)**.** As stated in the above theorem, the constant in (4.18) depends only on the domain Ω. Moreover C is invariant under uniform scaling and translation, that is,

$$C(\Omega) = C(\lambda\Omega + c)$$

for every $\lambda > 0$, $c \in \mathbb{R}^2$. The rescaled function $\lambda u((x-c)/\lambda)$ is obviously associated to the same antisymmetric matrix A, since

$$A = \frac{1}{|\Omega|}\int_\Omega \nabla u^{\mathrm{skew}}\,dx = \frac{1}{|\lambda\Omega + c|}\int_{\lambda\Omega+c} \nabla u^{\mathrm{skew}}\,dy\,.$$

Remark 4.6 (Annular domains with a cut)**.** Let $\mu \in \mathcal{AD}_\varepsilon(\Omega)$ and $\beta \in \mathcal{AS}_\varepsilon(\mu)$. We want to estimate from below the energy of β in annuli $B_{r_2}(x_i) \setminus B_{r_1}(x_i)$ for $0 < r_1 < r_2$ sufficiently small, and $x_i \in \operatorname{supp}\mu$. Notice that β is not a gradient in $B_{r_2}(x_i) \setminus B_{r_1}(x_i)$, so we cannot use the classic Korn inequality (4.18) to estimate the energy. However, by removing a cut $L_{r_1,r_2} := \{x_i\} \times (r_1, r_2)$ from $B_{r_2}(x_i) \setminus B_{r_1}(x_i)$, we can find a displacement u such that $\nabla u = \beta$ in $(B_{r_2}(x_i) \setminus B_{r_1}(x_i)) \setminus L_{r_1,r_2}$. To such gradient we can apply (4.18). The question is to understand the behaviour of the constant C in (4.18) in terms of r_1 and r_2.

In the case of an annular domain $B_{r_2}(x_i) \setminus B_{r_1}(x_i)$, the constant C can be computed explicitly and it can be shown that $C = C(r_1/r_2)$, that is, C depends only on the ratio of the radii (see [14]). Moreover we have that $C(r_1/r_2) \to \infty$ if $r_1/r_2 \to 1$, that is, Korn's constant explodes on thin annuli.

It turns out that this is true also for annular domains with a cut, as proved in [57, Proposition 3.3]. Let us now consider a domain $(B_1(0) \setminus B_\varepsilon(0)) \setminus L_\varepsilon$, with $L_\varepsilon := \{0\} \times (\varepsilon, 1)$ and $0 < \varepsilon < 1$. From the above discussion, a priori, Korn's constant is a function of ε, and $C(\varepsilon) \to \infty$ as $\varepsilon \to 1$. However if ε is such that $0 < \varepsilon < \delta$, for some fixed $\delta < 1$, then it can be shown ([57, Proposition 3.3]) that C is uniform in ε. We will summarise these results in the following theorem.

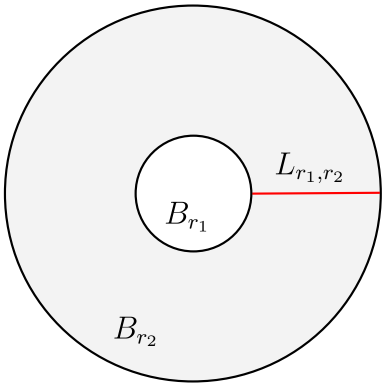


Figure 4.5: Annular domain with a cut $(B_{r_2} \setminus B_{r_1}) \setminus L_{r_1,r_2}$.

Theorem 4.7. *Consider the annulus $B_{r_2} \setminus B_{r_1}$, with $0 < r_1 < r_2$, where B_r is the ball of radius r centred at the origin. Set $L_{r_1,r_2} := \{0\} \times (r_1, r_2)$. There exists a constant $C > 0$, depending only on the ratio r_1/r_2, with the following property: for every $u \in H^1((B_{r_2} \setminus B_{r_1}) \setminus L_{r_1,r_2}; \mathbb{R}^2)$, we have*

$$\int_{(B_{r_2}\setminus B_{r_1})\setminus L_{r_1,r_2}} |\nabla u - A|^2 \, dx \le C \int_{(B_{r_2}\setminus B_{r_1})\setminus L_{r_1,r_2}} |\nabla u^{\mathrm{sym}}|^2 \, dx \,, \tag{4.19}$$

where $A := 1/|B_{r_2} \setminus B_{r_1}| \int_{(B_{r_2}\setminus B_{r_1})\setminus L_{r_1,r_2}} \nabla u^{\mathrm{skew}} \, dx$.

Moreover, let $0 < \varepsilon < 1/2$ and $r_1 = \varepsilon$, $r_2 = 1$. Then the constant in (4.19) *is uniform in ε.*

Theorem 4.7 holds true also for strains $\beta \in \mathcal{AS}_\varepsilon(\mu_\varepsilon)$ in the case when the number of dislocations is uniformly bounded, that is, if $\sup_\varepsilon |\mu_\varepsilon|(\Omega) < \infty$. On the other hand, when the number of dislocations $N_\varepsilon \to \infty$ as $\varepsilon \to 0$, the contribution from $|\mu_\varepsilon|(\Omega)$ has to be taken into account in the right hand side of (4.19), in order to obtain a uniform estimate. This leads us to the following generalised Korn inequality, first proved in [30, Theorem 11].

Theorem 4.8 (Generalised Korn inequality)**.** *There exists a constant $C > 0$, depending only on Ω, with the following property: for every $\beta \in L^1(\Omega; \mathbb{M}^{2\times 2})$ with*

$$\operatorname{Curl} \beta = \mu \in \mathcal{M}(\Omega; \mathbb{R}^2) \,,$$

we have

$$\int_\Omega |\beta - A|^2 \, dx \le C \left(\int_\Omega |\beta^{\mathrm{sym}}|^2 \, dx + |\mu|(\Omega)^2 \right) \,, \tag{4.20}$$

where A is the constant 2×2 antisymmetric matrix defined by

$$A := \int_\Omega \beta^{\mathrm{skew}} \, dx \,.$$

4.3.3 Cell formula for the self-energy

In this section we want to rigorously define the density function φ appearing in the Γ-limit $\mathcal{F}$ defined in (4.6). In order to do so, following [30, Section 4], we will introduce the self-energy $\psi(\xi)$ stored in the core region of a single dislocation $\xi\,\delta_0$ centred at the origin.

Let us start by defining, for every $\xi \in \mathbb{R}^2$ and $0 < r_1 < r_2$, the space

$$\mathcal{AS}_{r_1,r_2}(\xi) := \left\{ \beta \in L^2(B_{r_2} \setminus B_{r_1}; \mathbb{M}^{2\times 2}) : \ \mathrm{Curl}\,\beta = 0, \int_{\partial B_{r_1}} \beta \cdot t\, ds = \xi \right\}, \quad (4.21)$$

where B_r is the ball of radius r centred at the origin. For strains belonging to such class, we have the following bound from below of the energy (see [30, Remark 3]).

Proposition 4.9. *Let $0 < r_1 < r_2$ and $\xi \in \mathbb{R}$. There exists a constant $c > 0$ depending only on the ratio r_1/r_2, such that, for every $\beta \in AS_{r_1,r_2}(\xi)$,*

$$\int_{B_{r_2}\setminus B_{r_1}} |\beta^{\mathrm{sym}}|^2\, dx \geq c|\xi|^2 \log \frac{r_2}{r_1}\,. \quad (4.22)$$

Moreover, let $0 < \varepsilon < 1/2$ and $r_1 := \varepsilon$, $r_2 := 1$. Then the constant in (4.22) is uniform in ε.

Proof. Let $\beta \in AS_{r_1,r_2}(\xi)$. By introducing a cut $L_{r_1,r_2} := \{0\} \times (r_1, r_2)$ and considering $(B_{r_2} \setminus B_{r_1}) \setminus L_{r_1,r_2}$, the domain becomes simply connected (see Figure 4.5). Since $\mathrm{Curl}\,\beta = 0$, there exists a displacement $u \in H^1((B_{r_2} \setminus B_{r_1}) \setminus L_{r_1,r_2}; \mathbb{R}^2)$ such that $\nabla u = \beta$. Therefore we can apply Theorem 4.7 to obtain an antisymmetric matrix $A \in \mathbb{M}^{2\times 2}_{\mathrm{skew}}$ such that

$$\int_{B_{r_2}\setminus B_{r_1}} |\beta - A|^2\, dx \leq C \int_{B_{r_2}\setminus B_{r_1}} |\beta^{\mathrm{sym}}|^2\, dx\,.$$

Notice that the constant $C > 0$ comes from (4.19) and it depends only on the ratio r_1/r_2. By Jensen's inequality and by recalling that $\beta \in AS_{r_1,r_2}(\xi)$, we have

$$\begin{aligned}\int_{B_{r_2}\setminus B_{r_1}} |\beta - A|^2\ dx &\geq \int_{r_1}^{r_2} \int_{\partial B_\rho} |(\beta - A)\cdot t|^2\, ds\, d\rho \\ &\geq \int_{r_1}^{r_2} \frac{1}{2\pi\rho} \left| \int_{\partial B_\rho} (\beta - A)\cdot t\, ds \right|^2 d\rho \\ &= \int_{r_1}^{r_2} \frac{1}{2\pi\rho} \left| \int_{\partial B_\rho} \beta\cdot t\, ds \right|^2 d\rho = \frac{|\xi|^2}{2\pi} \int_{r_1}^{r_2} \frac{1}{\rho}\, d\rho = \frac{|\xi|^2}{2\pi} \log\frac{r_2}{r_1}\,,\end{aligned}$$

where $\int_{\partial B_\rho} A\cdot t\, ds = 0$, since A is constant. The rest of the statement follows directly from the second part of Theorem 4.7. $\square$

Let $C_\varepsilon := B_1 \setminus B_\varepsilon$, with $0 < \varepsilon < 1$, and introduce $\psi_\varepsilon \colon \mathbb{R}^2 \to \mathbb{R}$ through the cell problem

$$\psi_\varepsilon(\xi) := \frac{1}{|\log \varepsilon|} \min \left\{ \int_{C_\varepsilon} W(\beta)\, dx : \ \beta \in \mathcal{AS}_{\varepsilon,1}(\xi) \right\} . \tag{4.23}$$

Remark 4.10 (Heuristic for the scaling)**.** There exists a constant $c > 0$, such that, for every $0 < \varepsilon < 1/2$ and $\xi \in \mathbb{R}^2$, we have

$$c^{-1}|\xi|^2 \leq \psi_\varepsilon(\xi) \leq c|\xi|^2 . \tag{4.24}$$

Indeed $\psi_\varepsilon \geq c^{-1}|\xi|^2$ follows directly from Proposition 4.9, with c uniform in ε. For the upper bound, consider the strain

$$K_\xi(x) := \frac{1}{2\pi}\, \xi \otimes J \frac{x}{|x|^2} ,$$

where J is the clock-wise rotation of $\pi/2$. It is immediate to check that $\operatorname{Curl} K_\xi = \xi\, \delta_0$ in $\mathcal{D}'(\mathbb{R}^2;\mathbb{R}^2)$. Therefore $K_\xi \in \mathcal{AS}_{\varepsilon,1}(\xi)$. Moreover the energy is such that

$$\int_{C_\varepsilon} |K_\xi|^2\, dx \leq c|\xi|^2 \int_{C_\varepsilon} \frac{1}{|x|^2}\, dx = c|\xi|^2 |\log \varepsilon| ,$$

where C does not depend on ε. Therefore the upper bound in (4.24) follows directly from the energy bounds (4.12).

Indeed it is possible to prove that the scaling in (4.24) is optimal. In order to do so, let us first prove that (4.23) admits a minimiser for each fixed $0 < \varepsilon < 1$.

Proposition 4.11. *For every fixed $0 < \varepsilon < 1$ and $\xi \in \mathbb{R}^2$, there exists a unique solution $\beta_\varepsilon = \beta_\varepsilon(\xi)$ to (4.23), such that $\int_\Omega \beta_\varepsilon^{\mathrm{skew}} = 0$.*

Proof. This is a simple application of the direct method of the calculus of variations (see Theorem A.1) in combination with Korn's inequality (Theorem 4.4). Fix $0 < \varepsilon < 1$ and let β_n be a minimising sequence, that is, $\beta_n \in \mathcal{AS}_{\varepsilon,1}(\xi)$ and

$$\lim_{n\to\infty} \int_{C_\varepsilon} W(\beta_n)\, dx = I_\varepsilon := \inf_{\beta \in \mathcal{AS}_{\varepsilon,1}(\xi)} \int_{C_\varepsilon} W(\beta)\, dx . \tag{4.25}$$

By Remark 4.10 we have $I_\varepsilon < \infty$. Up to a translation by an antisymmetric matrix, we can assume that β_n is such that $\int_{C_\varepsilon} \beta_n^{\mathrm{skew}}\, dx = 0$, without changing the energy, since W depends only on the symmetric part of the strain. Let $L_\varepsilon := \{0\} \times (\varepsilon, 1)$. Since $\operatorname{Curl} \beta = 0$ and $C_\varepsilon \setminus L_\varepsilon$ is simply connected, there exists $u_n \in H^1(C_\varepsilon \setminus L_\varepsilon; \mathbb{R}^2)$ such that $\nabla u_n = \beta_n$. Therefore, by applying the classic Korn inequality, we have

$$\int_{C_\varepsilon} |\beta_n|^2\, dx \leq C \int_{C_\varepsilon} |\beta_n^{\mathrm{sym}}|^2\, dx ,$$

for some $C > 0$. By the energy bounds (4.12) and by (4.25) we conclude that the sequence β_n is uniformly bounded in $L^2(C_\varepsilon; \mathbb{M}^{2\times 2})$. Therefore $\beta_n \rightharpoonup \beta$, up to subsequences (not relabelled). Notice that $\beta \in \mathcal{AS}_{\varepsilon,1}(\xi)$ and $\int_{C_\varepsilon} \beta^{\text{skew}}\, dx = 0$. Furthermore, our energy is weakly lower semicontinuous, that is,

$$\int_{C_\varepsilon} W(\beta)\, dx \leq \liminf_{n\to\infty} \int_{C_\varepsilon} W(\beta_n)\, dx\,, \tag{4.26}$$

whenever $\beta_n \rightharpoonup \beta$. Indeed, by the energy bounds (4.12), we have

$$\int_{C_\varepsilon} W(\beta_n)\, dx + \int_{C_\varepsilon} W(\beta)\, dx - 2\int_{C_\varepsilon} \mathbb{C}\beta_n : \beta\, dx = \int_{C_\varepsilon} W(\beta_n - \beta)\, dx \geq 0$$

so that (4.26) follows. Since our minimising sequence is such that $\beta_n \rightharpoonup \beta$, from (4.25)-(4.26) we conclude that β is a minimiser. Moreover $\int_{C_\varepsilon} \beta^{\text{skew}}\, dx = 0$. To prove the uniqueness, assume that β_1 and β_2 are two minimisers such that $\int_{C_\varepsilon} \beta_1^{\text{skew}}\, dx = \int_{C_\varepsilon} \beta_1^{\text{skew}}\, dx = 0$. Consider $\beta := (\beta_1 + \beta_2)/2$. Notice that $\beta \in \mathcal{AS}_{\varepsilon,1}(\xi)$ and $\int_{C_\varepsilon} \beta^{\text{skew}}\, dx = 0$. By minimality we have

$$\int_{C_\varepsilon} W(\beta_1)\, dx + \int_{C_\varepsilon} W(\beta_2)\, dx \leq 2\int_{C_\varepsilon} W(\beta)\, dx\,.$$

By rearranging the above inequality, we obtain

$$\int_{C_\varepsilon} W(\beta_1 - \beta_2)\, dx \leq 0\,.$$

Note that $\int_{C_\varepsilon} (\beta_1 - \beta_2)^{\text{skew}}\, dx = 0$, therefore, by Korn's inequality and the energy bounds (4.12), we get

$$\int_{C_\varepsilon} |\beta_1 - \beta_2|^2\, dx \leq c\int_{C_\varepsilon} |\beta_1^{\text{sym}} - \beta_2^{\text{sym}}|^2\, dx \leq c\int_{C_\varepsilon} W(\beta_1 - \beta_2)\, dx \leq 0$$

so that $\beta_1 = \beta_2$ a.e. in C_ε. □

It is easy to check that the minimiser $\beta_\varepsilon(\xi)$ of Proposition 4.11 satisfies the boundary value problem

$$\begin{cases} \operatorname{Div} \mathbb{C}\beta_\varepsilon(\xi) = 0 & \text{in } C_\varepsilon, \\ \mathbb{C}\beta_\varepsilon(\xi)\cdot\nu = 0 & \text{on } \partial C_\varepsilon, \end{cases}$$

where ν is the inner normal to ∂C_ε. Also, consider the strain $\beta_0(\xi) \colon \mathbb{R}^2 \to \mathbb{M}^{2\times 2}$ that solves in the sense of distributions

$$\begin{cases} \operatorname{Div} \mathbb{C}\beta_0(\xi) = 0 & \text{in } \mathbb{R}^2, \\ \operatorname{Curl} \beta_0(\xi) = \xi\, \delta_0 & \text{in } \mathbb{R}^2. \end{cases}$$

The following results holds true (see [30, Corollary 6]).

Proposition 4.12 (Self-energy)**.** *There exists a constant $C > 0$ such that for every $\xi \in \mathbb{R}^2$,*

$$\psi_\varepsilon(\xi) \leq \frac{1}{|\log \varepsilon|} \int_{C_\varepsilon} W(\beta_0(\xi))\, dx \leq \psi_\varepsilon(\xi) + \frac{C|\xi|^2}{|\log \varepsilon|}\,. \tag{4.27}$$

In particular, for every $\xi \in \mathbb{R}^2$, we have that

$$\lim_{\varepsilon \to 0} \psi_\varepsilon(\xi) = \psi(\xi)\,,$$

pointwise, where the map $\psi \colon \mathbb{R}^2 \to \mathbb{R}$ is the self-energy defined by

$$\psi(\xi) := \lim_{\varepsilon \to 0} \frac{1}{|\log \varepsilon|} \int_{C_\varepsilon} W(\beta_0(\xi))\, dx\,. \tag{4.28}$$

Moreover,

$$|\psi_\varepsilon(\xi) - \psi(\xi)| \leq \frac{C|\xi|^2}{|\log \varepsilon|}\,.$$

Also, by definition of ψ and (4.24), (4.27)*, there exists a constant $c > 0$ such that*

$$c^{-1}|\xi|^2 \leq \psi(\xi) \leq c|\xi|^2\,, \tag{4.29}$$

for every $\xi \in \mathbb{R}^2$.

We now want to show that the self-energy $\psi(\xi)$ is indeed concentrated in the hardcore region $B_{\rho_\varepsilon} \setminus B_\varepsilon$ of the dislocation $\xi\,\delta_0$, whenever $|\log \rho_\varepsilon| \ll |\log \varepsilon|$. To this end, define the map $\bar{\psi}_\varepsilon \colon \mathbb{R}^2 \to \mathbb{R}$ as

$$\bar{\psi}_\varepsilon(\xi) := \frac{1}{|\log \varepsilon|} \min \left\{ \int_{B_{\rho_\varepsilon} \setminus B_\varepsilon} W(\beta)\, dx :\ \beta \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\xi) \right\}, \tag{4.30}$$

for $\xi \in \mathbb{R}^2$. It will also be useful to introduce $\tilde{\psi}_\varepsilon \colon \mathbb{R}^2 \to \mathbb{R}$ as

$$\tilde{\psi}_\varepsilon(\xi) := \frac{1}{|\log \varepsilon|} \min \left\{ \int_{B_{\rho_\varepsilon} \setminus B_\varepsilon} W(\beta)\, dx :\ \beta \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\xi),\ \beta \cdot t = \hat{\beta} \cdot t \ \text{ on } \ \partial B_\varepsilon \cup \partial B_{\rho_\varepsilon} \right\}, \tag{4.31}$$

where $\hat{\beta} \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\xi)$, is such that

$$|\hat{\beta}(x)| \leq K \frac{|\xi|}{|x|}\,, \tag{4.32}$$

for some positive constant K. By (4.12), and proceeding as in the proof of Proposition 4.11, it is immediate to see that problems (4.30)-(4.31) are well posed. The following results holds (see [30, Remark 7, Proposition 8]).

Proposition 4.13. *Assume that $\rho_\varepsilon > 0$ is such that $\log \rho_\varepsilon / \log \varepsilon \to 0$ as $\varepsilon \to 0$. Then $\bar{\psi}_\varepsilon(\xi) = \psi_\varepsilon(\xi)(1 + o(\varepsilon))$ and $\tilde{\psi}_\varepsilon(\xi) = \psi_\varepsilon(\xi)(1 + o(\varepsilon))$, with $o(\varepsilon) \to 0$ as $\varepsilon \to 0$ uniformly with respect to $\xi \in \mathbb{R}^2$. In particular*

$$\lim_{\varepsilon \to 0} \bar{\psi}_\varepsilon(\xi) = \lim_{\varepsilon \to 0} \tilde{\psi}_\varepsilon(\xi) = \psi(\xi)$$

pointwise, where ψ is the self-energy defined in (4.28).

We can now define the density $\varphi \colon \mathbb{R}^2 \to [0, +\infty)$ as a relaxation of the self-energy map ψ,

$$\varphi(\xi) := \inf \left\{ \sum_{k=1}^{N} \lambda_k \psi(\xi_k) : \sum_{k=1}^{N} \lambda_k \xi_k = \xi,\ N \in \mathbb{N},\ \lambda_k \geq 0,\ \xi_k \in \mathbb{S} \right\}. \tag{4.33}$$

Proposition 4.14. *The function φ defined in* (4.33) *is convex and positively* 1-*homogeneous, that is*

$$\varphi(\lambda \xi) = \lambda \varphi(\xi), \quad \text{for every } \xi \in \mathbb{R}^2,\ \lambda > 0\,.$$

Moreover there exists a constant $c > 0$ such that

$$c^{-1}|\xi| \leq \varphi(\xi) \leq c|\xi|\,, \tag{4.34}$$

for every $\xi \in \mathbb{R}^2$. In particular, the infimum in (4.33) *is actually a minimum.*

Proof. Convexity and homogeneity are immediate to check. As for (4.34), note that φ is continuous (φ being convex). Therefore by homogeneity, for every $\xi \neq 0$, we have $\varphi(\xi) = |\xi| \varphi(\xi/|\xi|)$. Hence (4.34) follows, since φ admits minimum and maximum on $\{\xi \in \mathbb{R}^2 \colon |\xi| = 1\}$. Finally, the fact that the minimum is attained follows from the direct method of the calculus of variations, by using (4.34) and the fact that φ is continuous. □

4.4 Γ-convergence analysis for the regime $N_\varepsilon \gg |\log \varepsilon|$

In this section we will study, by means of Γ-convergence, the behaviour as $\varepsilon \to 0$ of the functionals $\mathcal{F}_\varepsilon \colon \mathcal{M}(\Omega; \mathbb{R}^2) \times L^2(\Omega; \mathbb{M}^{2\times 2}) \to \mathbb{R}$ defined in (4.15), in the energy regime $N_\varepsilon \gg |\log \varepsilon|$. In Theorem 4.17 we will prove that the Γ-limit for the sequence

$\mathcal{F}_\varepsilon$ is given by the functional $\mathcal{F}\colon \mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}}) \to \mathbb{R}$ defined as

$$\mathcal{F}(\mu,S,A) := \begin{cases} \displaystyle\int_\Omega W(S)\,dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| & \text{if } \mu\in H^{-1}(\Omega;\mathbb{R}^2),\ \operatorname{Curl} A = \mu, \\ +\infty & \text{otherwise}, \end{cases} \tag{4.35}$$

where φ is the energy density introduced in (4.33). The topology under which the Γ-convergence result holds is given by the following definition.

Definition 4.15. We say that the sequence $(\mu_\varepsilon,\beta_\varepsilon)\in\mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2})$ is converging to a triplet $(\mu,S,A)\in\mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$ if

$$\frac{\mu_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu \quad \text{in} \quad \mathcal{M}(\Omega;\mathbb{R}^2)\,, \tag{4.36}$$

$$\frac{\beta_\varepsilon^{\mathrm{sym}}}{\sqrt{N_\varepsilon|\log\varepsilon|}} \rightharpoonup S \qquad \text{and} \qquad \frac{\beta_\varepsilon^{\mathrm{skew}}}{N_\varepsilon} \rightharpoonup A \quad \text{weakly in} \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,. \tag{4.37}$$

Remark 4.16. The topology introduced in Definition 4.15 is metrisable, hence we will can apply the fundamental theorem of Γ-convergence given in Appendix A.2.

Theorem 4.17. *The following* Γ*-convergence result holds with respect to the topology of Definition 4.15.*

(i) (Compactness) *Let* $\varepsilon_n\to 0$ *and assume that* $(\mu_n,\beta_n)\in\mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2})$ *is such that* $\sup_n \mathcal{F}_{\varepsilon_n}(\mu_n,\beta_n)\le E$*, for some positive constant* E*. Then there exists* $(\mu,S,A)\in\mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$ *such that, up to subsequences (not relabelled),* (μ_n,β_n) *converges to* (μ,S,A) *in the sense of Definition 4.15. Moreover* $\mu\in H^{-1}(\Omega;\mathbb{R}^2)$ *and* $\operatorname{Curl} A=\mu$.

(i) (Γ-convergence) *The functionals* $\mathcal{F}_\varepsilon$ *defined in* (4.15) Γ*-converge to the functional* $\mathcal{F}$ *defined in* (4.35)*, with respect to the convergence of Definition 4.15. Specifically, for every*

$$(\mu,S,A)\in(H^{-1}(\Omega;\mathbb{R}^2)\cap\mathcal{M}(\Omega;\mathbb{R}^2))\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$$

such that $\operatorname{Curl}\mu = A$ *we have:*

- (Γ-liminf inequality) *for all sequences* $(\mu_\varepsilon,\beta_\varepsilon)\in\mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2})$ *converging to* (μ,S,A) *in the sense of Definition 4.15,*

$$\mathcal{F}(\mu,S,A)\le\liminf_{\varepsilon\to 0}\mathcal{F}_\varepsilon(\mu_\varepsilon,\beta_\varepsilon)\,.$$

- (Γ-limsup inequality) *there exists a recovery sequence* $(\mu_\varepsilon, \beta_\varepsilon)$ *belonging to* $\mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times 2})$*, such that* $(\mu_\varepsilon, \beta_\varepsilon)$ *converges to* (μ, S, A) *in the sense of Definition 4.15, and*

$$\limsup_{\varepsilon\to 0} \mathcal{F}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon) \le \mathcal{F}(\mu, S, A)\,.$$

4.4.1 Compactness

We will prove the compactness statement in Theorem 4.17. Assume that (μ_n, β_n) is a sequence in $\mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times 2})$ such that

$$\sup_n \mathcal{F}_{\varepsilon_n}(\mu_n, \beta_n) \le E\,. \tag{4.38}$$

The proof is divided into four parts.

Part 1. Compactness of the rescaled measures.

Let $\mu_n := \sum_{i=1}^{M_n} \xi_{n,i}\delta_{x_{n,i}} \in \mathcal{AD}_{\varepsilon_n}(\Omega)$. We show that the total variation of μ_n/N_{ε_n} is uniformly bounded, i.e., there exists $C > 0$ such that

$$\frac{1}{N_{\varepsilon_n}}|\mu_n|(\Omega) = \frac{1}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}|\xi_{n,i}| \le C\,, \tag{4.39}$$

for every $n \in \mathbb{N}$. Since the function $y \mapsto \beta_n(x_{n,i} + y)$ belongs to $\mathcal{AS}_{\varepsilon_n,\rho_{\varepsilon_n}}(\xi_{n,i})$, we have

$$\begin{aligned} E \ge \mathcal{F}_{\varepsilon_n}(\mu_n, \beta_n) &\ge \frac{1}{N_{\varepsilon_n}|\log\varepsilon_n|}\sum_{i=1}^{M_n}\int_{B_{\rho_{\varepsilon_n}}(x_{n,i})\setminus B_{\varepsilon_n}(x_{n,i})} W(\beta_n)\,dx \\ &= \frac{1}{N_{\varepsilon_n}|\log\varepsilon_n|}\sum_{i=1}^{M_n}\int_{B_{\rho_{\varepsilon_n}}(0)\setminus B_{\varepsilon_n}(0)} W(\beta_n(x_{n,i}+y))\,dy \ge \frac{1}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}\bar{\psi}_{\varepsilon_n}(\xi_{n,i})\,, \end{aligned}$$

where $\bar{\psi}_\varepsilon$ is defined in (4.30). Let ψ be the self-energy defined in (4.28) and set $c := \frac{1}{2}\min_{|\xi|=1}\psi(\xi)$. Notice that $c > 0$, by (4.29). By Proposition 4.13, $\bar{\psi}_\varepsilon \to \psi$ pointwise as $\varepsilon \to 0$, therefore for sufficiently large n, we have $\bar{\psi}_{\varepsilon_n}(\xi) \ge c$ for every $\xi \in \mathbb{R}^2$ with $|\xi| = 1$. Hence,

$$\begin{aligned} \frac{1}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}\bar{\psi}_{\varepsilon_n}(\xi_{n,i}) &= \frac{1}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}|\xi_{n,i}|^2\,\bar{\psi}_{\varepsilon_n}\left(\frac{\xi_{n,i}}{|\xi_{n,i}|}\right) \ge \frac{c}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}|\xi_{n,i}|^2 \\ &\ge \frac{c}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}|\xi_{n,i}| = c\,\frac{|\mu_n|(\Omega)}{N_{\varepsilon_n}}\,. \end{aligned}$$

The last inequality follows from the fact that the vectors $\xi_{n,i}$ are bounded away from zero. By putting together the above estimates, we conclude (4.36).

Part 2. Compactness of the rescaled β_n^{sym}.

This follows immediately by the bounds on the energy (4.12). Indeed by (4.38),

$$CN_{\varepsilon_n}|\log\varepsilon_n| \geq CE_{\varepsilon_n}(\mu_n,\beta_n) \geq C\int_\Omega |\beta_n^{\text{sym}}|^2\,dx\,, \tag{4.40}$$

and the weak compactness of $\beta_n^{\text{sym}}/\sqrt{N_{\varepsilon_n}|\log\varepsilon_n|}$ in $L^2(\Omega;\mathbb{M}^{2\times 2})$ follows.

Part 3. Compactness of the rescaled β_n^{skew}.

Now that the bounds (4.39)-(4.40) are established, the idea is to apply the generalised Korn inequality of Theorem 4.8, in order to obtain a uniform upper bound for $\beta_n^{\text{skew}}/N_{\varepsilon_n}$ in $L^2(\Omega;\mathbb{M}^{2\times 2})$. To do that, we need a control over $|\operatorname{Curl}\beta_n|(\Omega)$. In fact, even if β_n is related to μ_n by circulation compatibility conditions, the relationship between $|\operatorname{Curl}\beta_n|(\Omega)$ and $|\mu_n|(\Omega)$ is not clear. In order to obtain a bound for $|\operatorname{Curl}\beta_n|(\Omega)$ in terms of $|\mu_n|(\Omega)$, we will define new strains $\tilde\beta_n$ that have the same order of energy of β_n and that satisfy $|\operatorname{Curl}\tilde\beta_n|(\Omega) = |\mu_n|(\Omega)$.

Recall that $\mu_n = \sum_{i=1}^{M_n}\xi_{i,n}\delta_{x_{i,n}}$. Define the annuli $C_{i,n} := B_{2\varepsilon_n}(x_{i,n})\setminus B_{\varepsilon_n}(x_{i,n})$ and the functions $K_{i,n}\colon C_{i,n}\to\mathbb{M}^{2\times 2}$ by

$$K_{i,n}(x) := \frac{1}{2\pi}\xi_{i,n}\otimes J\frac{x-x_{i,n}}{|x-x_{i,n}|^2}\,,$$

where J is the clock-wise rotation of $\pi/2$. It is immediate to check that

$$\int_{C_{i,n}} |K_{i,n}|^2\,dx = C|\xi_{i,n}|^2\,,$$

where the constant $C>0$ does not depend on ε_n. By Proposition 4.9 we also have

$$\int_{C_{i,n}} |\beta_n^{\text{sym}}|^2\,dx \geq C|\xi_{i,n}|^2\,,$$

where, again, the constant $C>0$ does not depend on ε_n. Therefore

$$\int_{C_{i,n}} |K_{i,n}|^2\,dx \leq C\int_{C_{i,n}} |\beta_n^{\text{sym}}|^2\,dx\,. \tag{4.41}$$

Note that $\operatorname{Curl}K_{i,n} = \xi_{i,n}\delta_{x_{i,n}}$ in $\mathcal{D}'(\mathbb{R}^2;\mathbb{R}^2)$, hence $\operatorname{Curl}(\beta_n - K_{i,n}) = 0$ in $C_{i,n}$. Moreover $\int_{\partial B_{\varepsilon_n}(x_{i,n})}(\beta_n - K_{i,n})\cdot t\,ds = 0$, therefore there exists $v_{i,n}\in H^1(C_{i,n};\mathbb{R}^2)$ such that $\nabla v_{i,n} = \beta_n - K_{i,n}$ in $C_{i,n}$. By (4.41),

$$\int_{C_{i,n}} |\nabla v_{i,n}^{\text{sym}}|^2\,dx \leq C\int_{C_{i,n}} |\beta_n^{\text{sym}}|^2\,dx\,.$$

By applying the classic Korn inequality (Theorem 4.4) we get

$$\int_{C_{i,n}} |\nabla v_{i,n} - A_{i,n}|^2\, dx \le C \int_{C_{i,n}} |\nabla v_{i,n}^{\rm sym}|^2\, dx \le C \int_{C_{i,n}} |\beta_n^{\rm sym}|^2\, dx\,,$$

for some constant matrix $A_{i,n} \in \mathbb{M}^{2\times 2}_{\rm skew}$ and some uniform constant $C > 0$. By standard extension methods, there exists $u_{i,n} \in H^1(B_{2\varepsilon_n}(x_{i,n}); \mathbb{R}^2)$ such that $\nabla u_{i,n} = \nabla v_{i,n} - A_{i,n}$ in $C_{i,n}$ and

$$\int_{B_{2\varepsilon_n}(x_{i,n})} |\nabla u_{i,n}|^2\, dx \le C \int_{C_{i,n}} |\nabla v_{i,n} - A_{i,n}|^2\, dx \le C \int_{C_{i,n}} |\beta_n^{\rm sym}|^2\, dx\,. \tag{4.42}$$

Define $\tilde\beta_n \colon \Omega \to \mathbb{M}^{2\times 2}$ by setting

$$\tilde\beta_n(x) := \begin{cases} \beta_n(x) & \text{if } x \in \Omega_{\varepsilon_n}(\mu_n)\,, \\ \nabla u_{i,n}(x) + A_{i,n} & \text{if } x \in B_{\varepsilon_n}(x_{i,n})\,. \end{cases}$$

From (4.40) and (4.42), we have

$$\begin{aligned} \int_\Omega |\tilde\beta_n^{\rm sym}|^2\, dx &= \int_{\Omega_{\varepsilon_n}(\mu_n)} |\beta_n^{\rm sym}|^2\, dx + \sum_{i=1}^{M_n} \int_{B_{\varepsilon_n}(x_{i,n})} |\nabla u_{i,n}^{\rm sym}|^2\, dx \\ &\le C \int_\Omega |\beta_n^{\rm sym}|^2\, dx \le C N_{\varepsilon_n} |\log \varepsilon_n|\,. \end{aligned}$$

Moreover by construction $\operatorname{Curl} \tilde\beta_n$ is concentrated on $\partial B_{\varepsilon_n}(x_{i,n})$ and we have $|\operatorname{Curl} \tilde\beta_n|(\Omega) = |\mu_n|(\Omega)$. Therefore we can apply the generalised Korn inequality of Theorem 4.8 to get

$$\begin{aligned} \int_\Omega |\tilde\beta_n - \tilde A_n|^2\, dx &\le C \left(\int_\Omega |\tilde\beta_n^{\rm sym}|^2\, dx + (|\mu_n|(\Omega))^2 \right) \\ &\le C \left(N_{\varepsilon_n} |\log \varepsilon_n| + N_{\varepsilon_n}^2 \right) \le C N_{\varepsilon_n}^2\,, \end{aligned}$$

where $\tilde A_n := \frac{1}{|\Omega|} \int_\Omega \tilde\beta_n^{\rm skew} \in \mathbb{M}^{2\times 2}_{\rm skew}$. The last inequality follows from the assumption $|\log \varepsilon_n| \ll N_{\varepsilon_n}$. Now recall that by hypothesis the average of β_n is a symmetric matrix and $\beta_n \equiv 0$ in $\Omega \setminus \Omega_{\varepsilon_n}(\mu_n)$. Therefore, since symmetric and skew matrices are orthogonal, we have

$$\int_{\Omega_{\varepsilon_n}(\mu_n)} \beta_n \colon \tilde A_n\, dx = \int_\Omega \beta_n\, dx \colon \tilde A_n = 0\,.$$

Hence $|\beta_n - \tilde A_n|^2 = |\beta_n|^2 + |\tilde A_n|^2$, so that

$$\int_{\Omega_{\varepsilon_n}(\mu_n)} |\beta_n|^2\, dx \le \int_{\Omega_{\varepsilon_n}(\mu_n)} |\beta_n - \tilde A_n|^2\, dx \le \int_\Omega |\tilde\beta_n - \tilde A_n|^2\, dx \le C N_{\varepsilon_n}^2\,,$$

which yields the desired compactness for $\beta_n^{\rm skew}/N_{\varepsilon_n}$ in $L^2(\Omega; \mathbb{M}^{2\times 2})$.

Part 4. $\mu \in H^{-1}(\Omega;\mathbb{R}^2)$ and $\operatorname{Curl} A = \mu$.

Recall that $\mu_n = \sum_{i=1}^{M_n} \xi_{n,i}\delta_{x_{n,i}} \in \mathcal{AD}_{\varepsilon_n}(\Omega)$ and $\beta_n \in \mathcal{AS}_{\varepsilon_n}(\mu_n)$. Let $\varphi \in C_0^1(\Omega)$ and $\varphi_n \in H_0^1(\Omega)$ be a sequence converging to φ uniformly and strongly in $H_0^1(\Omega)$, and such that

$$\varphi_n \equiv \varphi(x_{n,i}) \quad \text{in} \quad B_{\varepsilon_n}(x_{n,i})\,.$$

By Remark 4.3, we then have

$$\int_\Omega \varphi_n \, d\mu_n = \langle \operatorname{Curl} \beta_n, \varphi_n \rangle = \int_\Omega \beta_n J \nabla \varphi_n \, dx\,.$$

Hence, by invoking (4.14), (4.36) and (4.37), we have

$$\begin{aligned}\int_\Omega \varphi \, d\mu &= \lim_{n\to\infty} \frac{1}{N_{\varepsilon_n}} \int_\Omega \varphi_n \, d\mu_n = \lim_{n\to\infty} \frac{1}{N_{\varepsilon_n}} \langle \operatorname{Curl} \beta_n, \varphi_n \rangle \\ &= \lim_{n\to\infty} \frac{1}{N_{\varepsilon_n}} \int_\Omega \beta_n J\nabla\varphi_n \, dx = \int_\Omega A\, J\nabla\varphi \, dx = \langle \operatorname{Curl} A, \varphi\rangle\,.\end{aligned}$$

From this we conclude that $\operatorname{Curl} A = \mu$. Moreover, since $A \in L^2(\Omega;\mathbb{M}^{2\times 2})$, then by definition $\operatorname{Curl} A \in H^{-1}(\Omega;\mathbb{R}^2)$. Hence also $\mu \in H^{-1}(\Omega;\mathbb{R}^2)$.

4.4.2 Γ-liminf inequality

We now want to prove the Γ-liminf inequality of Theorem 4.17. Let $\mu_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$, $\beta_\varepsilon \in \mathcal{AS}_\varepsilon(\mu_\varepsilon)$ and

$$(\mu, S, A) \in (H^{-1}(\Omega;\mathbb{R}^2) \cap \mathcal{M}(\Omega;\mathbb{R}^2)) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}}) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})\,,$$

such that $\operatorname{Curl} A = \mu$. Assume that $(\mu_\varepsilon, \beta_\varepsilon)$ converges to (μ, S, A) in the sense of Definition 4.15. We need to show that

$$\liminf_{\varepsilon\to 0} \mathcal{F}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon) \geq \mathcal{F}(\mu, S, A)\,. \tag{4.43}$$

In order to do so, we decompose the energy in

$$\frac{1}{N_\varepsilon |\log\varepsilon|} \int_\Omega W(\beta_\varepsilon)\, dx = \frac{1}{N_\varepsilon |\log\varepsilon|} \int_{\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\, dx + \frac{1}{N_\varepsilon |\log\varepsilon|} \int_{\Omega \setminus \Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\, dx \tag{4.44}$$

and study the two contributions separately.

Recall that $\mu_\varepsilon = \sum_{i=1}^{M_\varepsilon} \xi_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$. Since we are assuming that $\mu_\varepsilon / N_\varepsilon \stackrel{*}{\rightharpoonup} \mu$, this implies that $|\mu_\varepsilon|(\Omega)/N_\varepsilon$ is uniformly bounded, hence $M_\varepsilon \leq C N_\varepsilon$ for some uniform constant $C > 0$. Moreover $N_\varepsilon \rho_\varepsilon^2 \to 0$ by hypothesis, therefore $\chi_{\Omega_{\rho_\varepsilon}} \to 1$ in $L^1(\Omega)$, as

$$\int_\Omega |\chi_{\Omega_{\rho_\varepsilon}} - 1|\, dx = \sum_{i=1}^{M_\varepsilon} |B_{\rho_\varepsilon}(x_{\varepsilon,i})| = \pi \rho_\varepsilon^2 M_\varepsilon \leq C \rho_\varepsilon^2 N_\varepsilon\,.$$

Since $\beta_\varepsilon^{\text{sym}}/\sqrt{N_\varepsilon|\log\varepsilon|} \rightharpoonup S$, we deduce that

$$\frac{\beta_\varepsilon^{\text{sym}}\chi_{\Omega_{\rho_\varepsilon}}}{\sqrt{N_\varepsilon|\log\varepsilon|}} \rightharpoonup S \quad \text{weakly in} \quad L^2(\Omega;\mathbb{M}^{2\times 2}).$$

Hence, by weak lower semicontinuity,

$$\begin{aligned}\liminf_{\varepsilon\to 0}\frac{1}{N_\varepsilon|\log\varepsilon|}\int_{\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\,dx &= \liminf_{\varepsilon\to 0}\int_\Omega W\left(\frac{\beta_\varepsilon^{\text{sym}}\chi_{\Omega_{\rho_\varepsilon}}}{\sqrt{N_\varepsilon|\log\varepsilon|}}\right)dx\\ &\geq \int_\Omega W(S)\,dx\,.\end{aligned}$$

Let us consider the second integral in (4.44). By Proposition 4.13 and definition (4.33), we have

$$\begin{aligned}\frac{1}{|\log\varepsilon|}\int_{\Omega\setminus\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\,dx &= \sum_{i=1}^{M_\varepsilon}\frac{1}{|\log\varepsilon|}\int_{B_{\rho_\varepsilon}(x_{\varepsilon,i})} W(\beta_\varepsilon)\,dx \geq \sum_{i=1}^{M_\varepsilon}\bar{\psi}_\varepsilon(\xi_{\varepsilon,i})\\ &= (1+o(\varepsilon))\sum_{i=1}^{M_\varepsilon}\psi(\xi_{\varepsilon,i}) \geq (1+o(\varepsilon))\sum_{i=1}^{M_\varepsilon}\varphi(\xi_{\varepsilon,i})\\ &= (1+o(\varepsilon))\int_\Omega \varphi\left(\frac{d\mu_\varepsilon}{d|\mu_\varepsilon|}\right)d|\mu_\varepsilon|,\end{aligned}$$

where $o(\varepsilon)\to 0$ as $\varepsilon\to 0$, and last equality follows from the properties of φ. Since φ is convex and 1-homogeneous, by Reshetnyak's Theorem (see (A.5) in Theorem A.17), we have

$$\begin{aligned}\liminf_{\varepsilon\to 0}\frac{1}{N_\varepsilon|\log\varepsilon|}\int_{\Omega\setminus\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\,dx &\geq \liminf_{\varepsilon\to 0}\frac{1}{N_\varepsilon}\int_\Omega\varphi\left(\frac{d\mu_\varepsilon}{d|\mu_\varepsilon|}\right)d|\mu_\varepsilon|\\ &\geq \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right)d|\mu|\,,\end{aligned}$$

and (4.43) follows.

4.4.3 Γ-limsup inequality

In this section we prove the Γ-limsup inequality of Theorem 4.17. Before proceeding, we need the following technical Lemma to construct the recovery sequence for the measure μ. Let us first introduce some notation. For a sequence of atomic measures of the form $\nu_\varepsilon := \sum_{i=1}^{M_\varepsilon}\alpha_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$ and a sequence $r_\varepsilon\to 0$, we define the corresponding diffused measures

$$\tilde{\nu}_\varepsilon^{r_\varepsilon} := \frac{1}{\pi r_\varepsilon^2}\sum_{i=1}^{M_\varepsilon}\alpha_{i,\varepsilon}\,\mathcal{H}^2\llcorner B_{r_\varepsilon}(x_{i,\varepsilon})\,,\quad \hat{\nu}_\varepsilon^{r_\varepsilon} := \frac{1}{2\pi r_\varepsilon}\sum_{i=1}^{M_\varepsilon}\alpha_{i,\varepsilon}\,\mathcal{H}^1\llcorner \partial B_{r_\varepsilon}(x_{i,\varepsilon})\,. \tag{4.45}$$

For $x_{\varepsilon,i} \in \operatorname{supp} \nu_\varepsilon$, define the functions $\tilde{K}^{\alpha_{\varepsilon,i}}_{\varepsilon,i}$, $\hat{K}^{\alpha_{\varepsilon,i}}_{\varepsilon,i} : B_{r_\varepsilon}(x_{\varepsilon,i}) \to \mathbb{M}^{2\times 2}$ as

$$\tilde{K}^{\alpha_{\varepsilon,i}}_{\varepsilon,i}(x) := \frac{1}{2\pi r_\varepsilon^2}\, \alpha_{\varepsilon,i} \otimes J(x - x_{\varepsilon,i})\,, \quad \hat{K}^{\alpha_{\varepsilon,i}}_{\varepsilon,i}(x) := \frac{1}{2\pi}\, \alpha_{\varepsilon,i} \otimes J\frac{x - x_{\varepsilon,i}}{|x - x_{\varepsilon,i}|^2}\,, \tag{4.46}$$

where J is the clock-wise rotation of $\pi/2$. Finally define $\tilde{K}^{\nu_\varepsilon}_\varepsilon$, $\hat{K}^{\nu_\varepsilon}_\varepsilon : \Omega \to \mathbb{M}^{2\times 2}$ as

$$\tilde{K}^{\nu_\varepsilon}_\varepsilon := \sum_{i=1}^{M_\varepsilon} \tilde{K}^{\alpha_{\varepsilon,i}}_{\varepsilon,i} \chi_{B_{r_\varepsilon}(x_{\varepsilon,i})}\,, \quad \hat{K}^{\nu_\varepsilon}_\varepsilon := \sum_{i=1}^{M_\varepsilon} \hat{K}^{\alpha_{\varepsilon,i}}_{\varepsilon,i} \chi_{B_{r_\varepsilon}(x_{\varepsilon,i})}\,. \tag{4.47}$$

It is easy to show that

$$\operatorname{Curl} \tilde{K}^{\nu_\varepsilon}_\varepsilon = \tilde{\nu}^{r_\varepsilon}_\varepsilon - \hat{\nu}^{r_\varepsilon}_\varepsilon\,, \quad \operatorname{Curl} \hat{K}^{\nu_\varepsilon}_\varepsilon = \nu_\varepsilon - \hat{\nu}^{r_\varepsilon}_\varepsilon\,. \tag{4.48}$$

Lemma 4.18. *Let $N_\varepsilon \to \infty$ be such that (4.7) holds. Let $\xi := \sum_{k=1}^M \lambda_k \xi_k$ with $\xi_k \in \mathbb{S}$, $\lambda_k \geq 0$, $\Lambda := \sum_{k=1}^M \lambda_k$, $\mu := \xi\, dx$. Let $g \colon \Omega \to \mathbb{R}^2$ be a continuous function and set $\sigma := g(x)\, dx$. Define $r_\varepsilon := C/\sqrt{N_\varepsilon}$, for $C := \max\{\Lambda, \|g\|_{L^\infty}\}$.*

Then there exist sequences $\sigma_\varepsilon = \sum_{i=1}^{M_\varepsilon} g_{\varepsilon,i} \delta_{x_{\varepsilon,i}}$ and $\mu_\varepsilon = \sum_{k=1}^M \xi_k \mu^k_\varepsilon$, with $\mu^k_\varepsilon = \sum_{l=1}^{M^k_\varepsilon} \delta_{x_{\varepsilon,l}}$, such that $\mu_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$, $|g_{\varepsilon,i}| \leq C$, $B_{r_\varepsilon}(x_{\varepsilon,i}) \subset \Omega$, $|x_{\varepsilon,j} - x_{\varepsilon,k}| \geq 2r_\varepsilon$ for every $j \neq k$. Moreover

$$\frac{|\mu^k_\varepsilon|}{N_\varepsilon} \overset{*}{\rightharpoonup} \lambda_k\, dx \quad in \quad \mathcal{M}(\Omega;\mathbb{R})\,, \qquad \frac{\mu_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu \quad in \quad \mathcal{M}(\Omega;\mathbb{R}^2)\,, \tag{4.49}$$

$$\frac{\tilde{\mu}^{r_\varepsilon}_\varepsilon}{N_\varepsilon} \to \mu \quad in \quad H^{-1}(\Omega;\mathbb{R}^2)\,, \tag{4.50}$$

$$\frac{\sigma_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \sigma \quad in \quad \mathcal{M}(\Omega;\mathbb{R}^2)\,, \qquad \frac{\tilde{\sigma}^{r_\varepsilon}_\varepsilon}{N_\varepsilon} \to \sigma \quad in \quad H^{-1}(\Omega;\mathbb{R}^2)\,, \tag{4.51}$$

where the measures $\tilde{\mu}^{r_\varepsilon}_\varepsilon$, $\tilde{\sigma}^{r_\varepsilon}_\varepsilon$ are defined according to (4.45).

Proof. This proof is similar to the one of [30, Lemma 14].

Step 1. The case $M = 1$ and $\mu = \xi\, dx$ with $\xi \in \mathbb{S}$.

We cover $\mathbb{R}^2$ with squares of side length $2r_\varepsilon$, and plug a mass $\xi\, \delta_{x_{\varepsilon,i}}$ at the centre of each square contained in Ω (see Figure 4.6). We can then define the measure $\mu_\varepsilon := \sum_{i=1}^{M_\varepsilon} \xi\, \delta_{x_{\varepsilon,i}}$ where $M_\varepsilon \approx N_\varepsilon$. In this way $\mu_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$. Notice that the density of $\mu - \frac{\tilde{\mu}_\varepsilon}{N_\varepsilon}$ converges to zero weakly in $L^2(\Omega;\mathbb{R}^2)$, so that (4.49) is verified. Since the embedding of L^2 in H^{-1} is compact, also (4.50) follows.

Step 2. The general case $M > 1$.

We can approximate $\mu = \xi\, dx$ with periodic locally constant measures coinciding with $\xi_k\, dx$ on portions of Ω having volume fraction λ_k/Λ. In every region where the

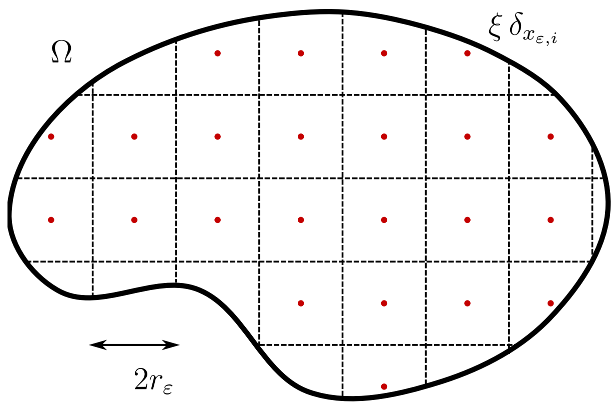


Figure 4.6: Approximating $\mu = \xi\,dx$ with Dirac masses $\xi\,\delta_{x_{\varepsilon,i}}$, represented by red dots, on a square lattice of size $2r_\varepsilon$.

approximating measure is constant, we apply the above construction. In this way we obtain a measure μ_ε supported at points $x_{\varepsilon,i}$ and such that (4.49)-(4.50) hold.

Now set $g_{\varepsilon,i} := g(x_{\varepsilon,i})$ and define the measure $\sigma_\varepsilon := \sum_{i=1}^{M_\varepsilon} g_{\varepsilon,i}\,\delta_{x_{\varepsilon,i}}$, which trivially satisfies (4.51). □

We are now ready to prove the Γ-limsup inequality of Theorem 4.17.

Proof of Γ*-limsup inequality of Theorem 4.17.* Let

$$(\mu, S, A) \in (H^{-1}(\Omega;\mathbb{R}^2) \cap \mathcal{M}(\Omega;\mathbb{R}^2)) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}}) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})\,,$$

with $\operatorname{Curl} A = \mu$. We will construct a recovery sequence in three steps.

Step 1. The case $\mu = \xi\,dx$ and $S \in C^1(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})$.

Assume that $\xi \in \mathbb{R}^2$ and set $\mu := \xi\,dx$. Let $S \in C^1(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})$ and $A \in L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$, with $\operatorname{Curl} A = \mu$. We will construct a recovery sequence $\mu_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$, $\beta_\varepsilon \in \mathcal{AS}_\varepsilon(\mu_\varepsilon)$, such that $(\mu_\varepsilon, \beta_\varepsilon)$ converges to (μ, S, A) in the sense of Definition 4.15 and

$$\limsup_{\varepsilon\to 0} \frac{1}{N_\varepsilon|\log\varepsilon|}\int_\Omega W(\beta_\varepsilon)\,dx \le \int_\Omega (W(S) + \varphi(\xi))\,dx\,. \tag{4.52}$$

By Proposition 4.14, there exist $\lambda_k \ge 0$, $\xi_k \in \mathbb{S}$, $M \in \mathbb{N}$, such that $\xi = \sum_{k=1}^M \lambda_k \xi_k$ and

$$\varphi(\xi) = \sum_{k=1}^M \lambda_k \psi(\xi_k)\,, \tag{4.53}$$

where φ is the self-energy defined in (4.33). Set $\sigma := \operatorname{Curl} S$. Since $S \in C^1(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})$, then $\sigma = g(x)\,dx$ for some continuous function $g\colon \Omega \to \mathbb{R}^2$. Let $\mu_\varepsilon := \sum_{i=1}^{M_\varepsilon} \xi_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$, $\sigma_\varepsilon := \sum_{i=1}^{M_\varepsilon} g_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$ and $r_\varepsilon := C/\sqrt{N_\varepsilon}$ be the sequences given by Lemma 4.18. Since by assumption $N_\varepsilon \rho_\varepsilon^2 \to 0$, we have $r_\varepsilon \gg \rho_\varepsilon$. Hence $\mu_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$. By (4.49), μ_ε is a recovery sequence for μ.

It will be useful to introduce the perturbed measure η_ε, where

$$\eta_\varepsilon := \mu_\varepsilon - \sqrt{\frac{|\log \varepsilon|}{N_\varepsilon}}\, \sigma_\varepsilon = \sum_{i=1}^{M_\varepsilon} \zeta_{\varepsilon,i} \delta_{x_{\varepsilon,i}}\,, \quad \zeta_{\varepsilon,i} := \xi_{\varepsilon,i} - \sqrt{\frac{|\log \varepsilon|}{N_\varepsilon}}\, g_{\varepsilon,i}\,. \tag{4.54}$$

Moreover let $\tilde{\eta}_\varepsilon^{r_\varepsilon}, \hat{\eta}_\varepsilon^{r_\varepsilon}, \tilde{\sigma}_\varepsilon^{r_\varepsilon}, \hat{\sigma}_\varepsilon^{r_\varepsilon}$ be defined according to (4.45). Remark that

$$\frac{\eta_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu \quad \text{in} \quad \mathcal{M}(\Omega;\mathbb{R}^2)\,, \quad \frac{\tilde{\eta}_\varepsilon^{r_\varepsilon}}{N_\varepsilon} \to \mu \quad \text{in} \quad H^{-1}(\Omega;\mathbb{R}^2)\,, \tag{4.55}$$

by Lemma 4.18 and the hypothesis $N_\varepsilon \gg |\log \varepsilon|$.

Notice that $\hat{K}_{\varepsilon,i}^{\zeta_{\varepsilon,i}} \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\zeta_{\varepsilon,i})$ and it satisfies (4.32). Therefore, by Proposition 4.13, there exist strains $\hat{A}_{\varepsilon,i}$ such that

(i) $\hat{A}_{\varepsilon,i} \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\zeta_{\varepsilon,i})$,

(ii) $\hat{A}_{\varepsilon,i} \cdot t = \hat{K}_{\varepsilon,i}^{\zeta_{\varepsilon,i}} \cdot t$ on $\partial B_\varepsilon(x_{\varepsilon,i}) \cup \partial B_{\rho_\varepsilon(x_{\varepsilon,i})}$,

and

$$\frac{1}{|\log \varepsilon|} \int_{B_{\rho_\varepsilon}(x_{\varepsilon,i}) \setminus B_\varepsilon(x_{\varepsilon,i})} W(\hat{A}_{\varepsilon,i})\, dx = \psi(\xi_{\varepsilon,i})(1 + o(\varepsilon)) \tag{4.56}$$

since $N_\varepsilon \gg |\log \varepsilon|$ by (4.14). Now extend $\hat{A}_{\varepsilon,i}$ to be $\hat{K}_{\varepsilon,i}^{\zeta_{\varepsilon,i}}$ in $B_{r_\varepsilon}(x_{\varepsilon,i}) \setminus B_{\rho_\varepsilon}(x_{\varepsilon,i})$ and zero in $\Omega \setminus (B_{r_\varepsilon}(x_{\varepsilon,i}) \setminus B_\varepsilon(x_{\varepsilon,i}))$. Set

$$\hat{S}_\varepsilon := \sum_{i=1}^{M_\varepsilon} \hat{K}_\varepsilon^{g_{\varepsilon,i}} \chi_{B_{r_\varepsilon}(x_{\varepsilon,i}) \setminus B_\varepsilon(x_{\varepsilon,i})}\,, \quad \hat{A}_\varepsilon := \sum_{i=1}^{M_\varepsilon} \hat{A}_{\varepsilon,i}\,. \tag{4.57}$$

Hence

$$\operatorname{Curl} \hat{S}_\varepsilon = -\hat{\sigma}_\varepsilon^{r_\varepsilon} + \hat{\sigma}_\varepsilon^{\varepsilon}\,, \quad \operatorname{Curl} \hat{A}_\varepsilon = -\hat{\eta}_\varepsilon^{r_\varepsilon} + \hat{\eta}_\varepsilon^{\varepsilon}\,, \tag{4.58}$$

recalling definition (4.45). Define $Q_\varepsilon := \nabla u_\varepsilon\, J$, where u_ε is solution of

$$\begin{cases} -\Delta u_\varepsilon = \sqrt{N_\varepsilon |\log \varepsilon|}\, \sigma - \sqrt{\dfrac{|\log \varepsilon|}{N_\varepsilon}}\, \tilde{\sigma}_\varepsilon^{r_\varepsilon} & \text{in} \quad \Omega\,, \\ u_\varepsilon \in H_0^1(\Omega;\mathbb{R}^2)\,. \end{cases} \tag{4.59}$$

In this way,

$$\operatorname{Curl} Q_\varepsilon = -\sqrt{N_\varepsilon |\log \varepsilon|}\, \sigma + \sqrt{\frac{|\log \varepsilon|}{N_\varepsilon}}\, \tilde{\sigma}_\varepsilon^{r_\varepsilon}\,. \tag{4.60}$$

By (4.51) and standard elliptic estimates, we have

$$\frac{Q_\varepsilon}{\sqrt{N_\varepsilon |\log \varepsilon|}} \to 0 \quad \text{in} \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,. \tag{4.61}$$

Consider the measure $F_\varepsilon := -N_\varepsilon\mu + \tilde{\eta}_\varepsilon^{r_\varepsilon}$. There exists a positive constant C depending only on Λ and $\|g\|_{L^\infty(\Omega;\mathbb{R}^2)}$, such that

$$\|\mathrm{Div}\, F_\varepsilon\|_{H^{-1}(\Omega)} \leq C\sqrt{N_\varepsilon}\,. \tag{4.62}$$

In fact, if $\varphi \in H^1_0(\Omega)$ is a test function,

$$\begin{aligned} < \mathrm{Div}\, F_\varepsilon, \varphi > &= -\frac{1}{\pi r_\varepsilon^2}\sum_{i=1}^{M_\varepsilon}\int_{B_{r_\varepsilon}(x_{\varepsilon,i})} \zeta_{\varepsilon,i}\cdot\nabla\varphi\,dx \leq \frac{C}{r_\varepsilon^2}\sum_{i=1}^{M_\varepsilon}\int_{B_{r_\varepsilon}(x_{\varepsilon,i})}|\nabla\varphi|\,dx \\ &\leq \frac{C}{r_\varepsilon^2}\sum_{i=1}^{M_\varepsilon}\|\nabla\varphi\|_{L^2(B_{r_\varepsilon}(x_{\varepsilon,i}))}\,|B_{r_\varepsilon}(x_{\varepsilon,i})|^{1/2} \leq \frac{C}{r_\varepsilon}\,\|\varphi\|_{H^1_0(\Omega)}\,, \end{aligned}$$

by Hölder's inequality. Denote with t the unit tangent vector to $\partial\Omega$, defined by $t := J\nu$, where ν is the inner normal to Ω. By Helmholtz decomposition (see, e.g. [58, Theorem 4.2, Part 1]), there exist sequences $f_\varepsilon, h_\varepsilon$ in $H^1(\Omega)$, with $h_\varepsilon\cdot t = 0$ on $\partial\Omega$, and such that

$$\nabla f_\varepsilon + J\nabla h_\varepsilon = F_\varepsilon \quad \text{in} \quad H^{-1}(\Omega)\,, \tag{4.63}$$

$$\|f_\varepsilon\|_{H^1(\Omega)} \leq C\,\|\mathrm{Div}\,F_\varepsilon\|_{H^{-1}(\Omega)}\,, \quad \|h_\varepsilon\|_{H^1(\Omega)} \leq C\,\|F_\varepsilon\|_{H^{-1}(\Omega;\mathbb{R}^2)}\,. \tag{4.64}$$

Define

$$R_\varepsilon := \begin{pmatrix} f_\varepsilon & h_\varepsilon \\ -h_\varepsilon & f_\varepsilon \end{pmatrix}, \tag{4.65}$$

so that, by (4.63), (4.55), (4.62),

$$\mathrm{Curl}\, R_\varepsilon = -N_\varepsilon\mu + \tilde{\eta}_\varepsilon^{r_\varepsilon}\,, \tag{4.66}$$

$$\frac{R_\varepsilon^{\mathrm{sym}}}{\sqrt{N_\varepsilon|\log\varepsilon|}},\ \frac{R_\varepsilon^{\mathrm{skew}}}{N_\varepsilon} \to 0 \quad \text{in} \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,. \tag{4.67}$$

Note that by construction one has

$$\frac{(Q_\varepsilon + R_\varepsilon)\cdot t}{\sqrt{N_\varepsilon|\log\varepsilon|}} \to 0 \quad \text{strongly in} \quad H^{-1/2}(\partial\Omega)\,. \tag{4.68}$$

Indeed, the trace of $Q_\varepsilon + R_\varepsilon$ is well defined in $H^{-1/2}(\partial\Omega)$ by Theorem 4.1, since $\mathrm{Curl}(Q_\varepsilon + R_\varepsilon)$ is absolutely continuous with respect to the Lebsegue measure, by (4.60) and (4.66).

We can now define the candidate recovery sequence as

$$\beta_\varepsilon := (S_\varepsilon + A_\varepsilon)\,\chi_{\Omega_\varepsilon(\mu_\varepsilon)}\,,$$

where

$$S_\varepsilon := \sqrt{N_\varepsilon\,|\log\varepsilon|}\,S + \sqrt{\frac{|\log\varepsilon|}{N_\varepsilon}}\,\hat{S}_\varepsilon - \sqrt{\frac{|\log\varepsilon|}{N_\varepsilon}}\,\tilde{K}_\varepsilon^{\sigma_\varepsilon} + Q_\varepsilon\,, \tag{4.69}$$

$$A_\varepsilon := N_\varepsilon A + \hat{A}_\varepsilon - \tilde{K}_\varepsilon^{\eta_\varepsilon} + R_\varepsilon\,. \tag{4.70}$$

By definition and (4.58), (4.48), (4.60), (4.66), it is immediate to check that

$$\operatorname{Curl} S_\varepsilon = \sqrt{\frac{|\log\varepsilon|}{N_\varepsilon}}\,\hat{\sigma}_\varepsilon^\varepsilon\,, \quad \operatorname{Curl} A_\varepsilon = \hat{\eta}_\varepsilon^\varepsilon \quad \text{in } \Omega\,.$$

From this, and the definition of η_ε in (4.54), we deduce

$$\operatorname{Curl}\beta_\varepsilon = \hat{\mu}_\varepsilon^\varepsilon \quad \text{in } \Omega\,,$$

so that

$$\operatorname{Curl}\beta_\varepsilon \llcorner \Omega_\varepsilon(\mu_\varepsilon) = 0\,,$$

and the circulation condition $\int_{\partial B_\varepsilon(x_{\varepsilon,i})} \beta_\varepsilon \cdot t\, ds = \xi_{\varepsilon,i}$ is satisfied for every point $x_{\varepsilon,i} \in \operatorname{supp}\mu_\varepsilon$. Hence $\beta_\varepsilon \in \mathcal{AS}_\varepsilon(\mu_\varepsilon)$.

In order for $(\mu_\varepsilon, \beta_\varepsilon)$ to be the desired recovery sequence, we need to prove that

$$\frac{\beta_\varepsilon^{\text{sym}}}{\sqrt{N_\varepsilon|\log\varepsilon|}} \rightharpoonup S \qquad \text{weakly in } \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,, \tag{4.71}$$

$$\frac{\beta_\varepsilon^{\text{skew}}}{N_\varepsilon} \rightharpoonup A \qquad \text{weakly in } \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,, \tag{4.72}$$

$$\lim_{\varepsilon\to 0} \frac{1}{N_\varepsilon|\log\varepsilon|}\int_\Omega W(\beta_\varepsilon)\,dx = \int_\Omega (W(S) + \varphi(\xi))\,dx\,. \tag{4.73}$$

Notice that

$$\frac{\hat{S}_\varepsilon}{\sqrt{N_\varepsilon\,|\log\varepsilon|}}, \; \frac{\hat{A}_\varepsilon}{\sqrt{N_\varepsilon\,|\log\varepsilon|}} \rightharpoonup 0 \quad \text{weakly in} \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,, \tag{4.74}$$

$$\frac{\tilde{K}_\varepsilon^{\sigma_\varepsilon}}{\sqrt{N_\varepsilon\,|\log\varepsilon|}}, \; \frac{\tilde{K}_\varepsilon^{\eta_\varepsilon}}{\sqrt{N_\varepsilon\,|\log\varepsilon|}} \to 0 \quad \text{strongly in} \quad L^2(\Omega;\mathbb{M}^{2\times 2})\;. \tag{4.75}$$

Indeed by definition one has

$$\begin{aligned}\int_{\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} \frac{|\hat{A}_\varepsilon|^2}{N_\varepsilon|\log\varepsilon|}\,dx &= \frac{1}{N_\varepsilon|\log\varepsilon|}\sum_{i=1}^{M_\varepsilon}\int_{B_{r_\varepsilon}(x_{\varepsilon,i})\setminus B_{\rho_\varepsilon}(x_{\varepsilon,i})} |\hat{K}_{\varepsilon,i}^{\zeta_{\varepsilon,i}}|^2\,dx \\ &\le \frac{C}{N_\varepsilon|\log\varepsilon|}\sum_{i=1}^{M_\varepsilon}\int_{B_{r_\varepsilon}(x_{\varepsilon,i})\setminus B_{\rho_\varepsilon}(x_{\varepsilon,i})} |x - x_{\varepsilon,i}|^{-2}\,dx \\ &\le C\,\frac{M_\varepsilon(\log r_\varepsilon - \log\rho_\varepsilon)}{N_\varepsilon|\log\varepsilon|} \to 0\,,\end{aligned} \tag{4.76}$$

as $\varepsilon \to 0$. By (4.76), (4.49), (4.56), (4.53), we have

$$
\begin{aligned}
\lim_{\varepsilon\to 0}\frac{1}{N_\varepsilon|\log\varepsilon|}\int_\Omega W(\hat{A}_\varepsilon)\,dx &= \lim_{\varepsilon\to 0}\frac{1}{N_\varepsilon|\log\varepsilon|}\int_{\Omega\setminus\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\hat{A}_\varepsilon)\,dx \\
&= \lim_{\varepsilon\to 0}\frac{1}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon}\psi(\xi_{\varepsilon,i})(1+o(\varepsilon)) = \lim_{\varepsilon\to 0}\frac{1}{N_\varepsilon}\sum_{k=1}^{M}|\mu_\varepsilon^k|(\Omega)\,\psi(\xi_k)(1+o(\varepsilon)) \\
&= |\Omega|\sum_{k=1}^{M}\lambda_k\psi(\xi_k) = \int_\Omega \varphi(\xi)\,dx\,.
\end{aligned}
\tag{4.77}
$$

From (4.12), (4.76), (4.77) we conclude (4.74), since $\hat{A}_\varepsilon/\sqrt{N_\varepsilon|\log\varepsilon|}$ is bounded in $L^2(\Omega;\mathbb{M}^{2\times 2})$ and its energy is concentrated in the hard core region. Similarly, we have that

$$
\begin{aligned}
\int_\Omega \frac{|\hat{S}_\varepsilon|^2}{N_\varepsilon|\log\varepsilon|}\,dx &\leq C\,\frac{M_\varepsilon(\log r_\varepsilon - \log\varepsilon)}{N_\varepsilon|\log\varepsilon|} \leq C\,, \\
\int_{\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} \frac{|\hat{S}_\varepsilon|^2}{N_\varepsilon|\log\varepsilon|}\,dx &\leq C\,\frac{M_\varepsilon(\log r_\varepsilon - \log\rho_\varepsilon)}{N_\varepsilon|\log\varepsilon|} \to 0\,,
\end{aligned}
$$

as $\varepsilon \to 0$ and (4.74) follows. As for (4.75), one can readily see that

$$
\int_\Omega \frac{|\tilde{K}_\varepsilon^{\sigma_\varepsilon}|^2}{N_\varepsilon|\log\varepsilon|}\,dx \leq \frac{C}{N_\varepsilon|\log\varepsilon|}\sum_{i=1}^{M_\varepsilon}\frac{1}{r_\varepsilon^4}\int_{B_{r_\varepsilon}(x_{\varepsilon,i})}|x-x_{\varepsilon,i}|^2\,dx = C\,\frac{M_\varepsilon}{N_\varepsilon|\log\varepsilon|} \to 0
$$

as $\varepsilon \to 0$. The statement for $\tilde{K}_\varepsilon^{\eta_\varepsilon}$ can be proved in a similar way. Therefore (4.71), (4.72) follow from the hypothesis $N_\varepsilon \gg |\log\varepsilon|$ and (5.55), (4.67), (4.74), (4.75). Moreover,

$$
\lim_{\varepsilon\to 0}\frac{1}{N_\varepsilon|\log\varepsilon|}\int_\Omega W(\beta_\varepsilon)\,dx = \lim_{\varepsilon\to 0}\frac{1}{N_\varepsilon|\log\varepsilon|}\int_\Omega W(\sqrt{N_\varepsilon|\log\varepsilon|}\,S + \hat{A}_\varepsilon)\,dx\,.
$$

Since $\hat{A}_\varepsilon/\sqrt{N_\varepsilon|\log\varepsilon|} \rightharpoonup 0$ in $L^2(\Omega;\mathbb{M}^{2\times 2})$, by (4.77) we conclude (4.73).

Step 2. The case $\mu = \sum_{l=1}^{L}\chi_{\Omega_l}\xi_l\,dx$ and $S \in C^1(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})$.

Assume that μ is locally constant, i.e., $\mu = \sum_{l=1}^{L}\chi_{\Omega_l}\xi_l\,dx$, with $\xi_l \in \mathbb{R}^2$ and $\Omega_l \subset \Omega$ are Lipschitz pairwise disjoint domains such that $|\Omega\setminus\cup_{l=1}^{L}\Omega_l| = 0$. We will construct the recovery sequence by combining the previous step with classical localisation arguments of Γ-convergence.

Let $S_l := S \llcorner \Omega_l$, $A_l := A \llcorner \Omega_l$, $\mu_l := \mu \llcorner \Omega_l = \xi_l\,dx$. Denote by $(\mu_{l,\varepsilon}, \beta_{l,\varepsilon})$ the recovery sequence for (μ_l, S_l, A_l) given by Step 1. We can now define $\mu_\varepsilon \in \mathcal{M}(\Omega;\mathbb{R}^2)$ and $\bar{\beta}_\varepsilon\colon \Omega \to \mathbb{M}^{2\times 2}$ as

$$
\bar{\beta}_\varepsilon := \sum_{l=1}^{L}\chi_{\Omega_l}\,\beta_{l,\varepsilon}\,, \quad \mu_\varepsilon := \sum_{l=1}^{L}\mu_{l,\varepsilon}\,.
$$

By construction $\mu_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$ and $\bar{\beta}_\varepsilon$ satisfies the circulation condition on every $\partial B_\varepsilon(x_\varepsilon)$, with $x_\varepsilon \in \operatorname{supp}\mu_\varepsilon$. Also notice that on each set Ω_l belonging to the partition of Ω, we have

$$\operatorname{Curl}\bar{\beta}_\varepsilon \llcorner \Omega_l(\mu_\varepsilon) = 0\,.$$

However $\operatorname{Curl}\bar{\beta}_\varepsilon$ could concentrate on the intersection region between two elements of the partition $\{\Omega_l\}_{l=1}^L$. To overcome this problem, it is sufficient to notice that by construction

$$\left\| \frac{\operatorname{Curl}\bar{\beta}_\varepsilon \llcorner \Omega_\varepsilon(\mu_\varepsilon)}{\sqrt{N_\varepsilon|\log\varepsilon|}} \right\|_{H^{-1}(\Omega;\mathbb{R}^2)} \leq \sum_{l=1}^{L} \left\| \frac{Q_{l,\varepsilon} + R_{l,\varepsilon}}{\sqrt{N_\varepsilon|\log\varepsilon|}} \right\|_{H^{-1/2}(\partial\Omega_l)}\,,$$

so that

$$\frac{\operatorname{Curl}\bar{\beta}_\varepsilon \llcorner \Omega_\varepsilon(\mu_\varepsilon)}{\sqrt{N_\varepsilon|\log\varepsilon|}} \to 0 \quad \text{strongly in} \quad H^{-1}(\Omega;\mathbb{R}^2)\,,$$

by (4.68). Hence we can add a vanishing perturbation to $\bar{\beta}_\varepsilon$ (on the scale $\sqrt{N_\varepsilon|\log\varepsilon|}$), in order to obtain the desired recovery sequence $\beta_\varepsilon \in \mathcal{AS}_\varepsilon(\mu_\varepsilon)$.

Step 3. *The general case.*

Let (μ, S, A) be in the domain of the Γ-limit $\mathcal{F}$. We can easily adapt the proof given in [30, Theorem 12, Step 3] to our case. By standard density arguments of Γ-convergence, it is sufficient to find sequences (μ_n, S_n, A_n) such that

$$\begin{gathered} \mu_n \text{ is locally constant as in Step 2}\,, \\ S_n \in C^1(\Omega;\mathbb{M}^{2\times 2}_{\text{sym}})\,,\ A_n \in L^2(\Omega;\mathbb{M}^{2\times 2}_{\text{skew}})\,, \quad \text{with} \quad \operatorname{Curl} A_n = \mu_n, \end{gathered} \tag{4.78}$$

and that

$$\beta_n \to \beta \ \text{ in } \ L^2(\Omega;\mathbb{M}^{2\times 2})\,, \quad \mu_n \overset{*}{\rightharpoonup} \mu \ \text{ in } \ \mathcal{M}(\Omega;\mathbb{R}^2)\,, \quad |\mu_n|(\Omega) \to |\mu|(\Omega)\,, \tag{4.79}$$

where $\beta_n := S_n + A_n$. In this way (μ_n, S_n, A_n) is admissible for $\mathcal{F}$ and the topology defined by (4.79) is stronger than the one given in Definition 4.15. Moreover, under (4.79) we have

$$\lim_{n\to\infty} \mathcal{F}(\mu_n, \beta_n) = \mathcal{F}(\mu, S, A)\,. \tag{4.80}$$

Indeed, since $\beta_n \to \beta$ strongly in $L^2(\Omega;\mathbb{M}^{2\times 2})$, then

$$\lim_{n\to\infty} \int_\Omega W(S_n)\,dx = \int_\Omega W(S)\,dx\,.$$

Also, $|\mu_n|(\Omega) \to |\mu|(\Omega)$ implies

$$\lim_{n\to\infty} \int_\Omega \varphi\left(\frac{d\mu_n}{d|\mu_n|}\right) d|\mu_n| = \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| \,,$$

by Reshetnyak Theorem (see (A.6) in Theorem A.17), so that (4.80) is proved. Therefore the thesis will follow from (4.79)-(4.80), since by Step 2 there exists a recovery sequence for (S_n, A_n, μ_n).

Let us then proceed to the construction of the sequence (β_n, μ_n) satisfying properties (4.78)-(4.79). By standard reflection arguments we can extend A to an antisymmetric field A_U defined in a neighbourhood U of Ω, such that $\operatorname{Curl} A_U = \mu_U$ is a measure on U, with $|\mu_U|(\partial\Omega) = 0$. Let ρ_h be a sequence of mollifiers (see Section A.2.3) and set

$$f_h := A_U * \rho_h \llcorner \Omega \qquad g_h := \mu_U * \rho_h \llcorner \Omega \,.$$

For sufficiently large h one has $\operatorname{Curl} f_h = g_h$. Furthermore

$$f_h \to A \text{ in } L^2(\Omega;\mathbb{M}^{2\times 2}) \,, \quad g_h\, dx \overset{*}{\rightharpoonup} \mu \text{ in } \mathcal{M}(\Omega;\mathbb{R}^2) \,, \quad |g_h|\, dx(\Omega) \to |\mu|(\Omega) \,. \tag{4.81}$$

Now consider locally constant functions $g_{h,k}$, such that

$$\|g_{h,k} - g_h\|_{L^\infty(\Omega;\mathbb{R}^2)} \to 0 \text{ as } k \to \infty \,, \quad \text{and} \quad \int_\Omega (g_{h,k} - g_h)\, dx = 0 \,. \tag{4.82}$$

Let $r_{h,k}$ be a solution to

$$\begin{cases} \operatorname{Curl} r_{h,k} = g_{h,k} - g_h & \text{in } \Omega \,, \\ \operatorname{Div} r_{h,k} = 0 & \text{in } \Omega \,, \\ r_{h,k} \cdot t = 0 & \text{on } \partial\Omega \,. \end{cases} \tag{4.83}$$

By standard elliptic estimates

$$\|r_{h,k}\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} \le C \, \|g_{h,k} - g_h\|_{L^2(\Omega;\mathbb{R}^2)} \,. \tag{4.84}$$

Now set $f_{h,k} := f_h + r_{h,k}$ so that by (4.82)-(4.84) one has

$$f_{h,k} \to f_h \text{ in } L^2(\Omega;\mathbb{M}^{2\times 2}) \text{ as } k \to \infty \,, \quad \text{and} \quad \operatorname{Curl} f_{h,k} = g_{h,k} \,. \tag{4.85}$$

By means of a diagonal argument, we can define sequences μ_n and A_n such that $\operatorname{Curl} A_n = \mu_n$ and

$$A_n \to A \text{ in } L^2(\Omega;\mathbb{M}^{2\times 2}) \,, \quad \mu_n \overset{*}{\rightharpoonup} \mu \text{ in } \mathcal{M}(\Omega;\mathbb{R}^2) \,, \quad \text{and} \quad |\mu_n|(\Omega) \to |\mu|(\Omega) \,. \tag{4.86}$$

Next, we can approximate S in $L^2(\Omega;\mathbb{M}^{2\times2}_{\mathrm{sym}})$ with a sequence $S_n \in C^1(\Omega;\mathbb{M}^{2\times2}_{\mathrm{sym}})$ and set $\beta_n := S_n + A_n$. In this way (4.79) follows from (4.86). □

4.5 Γ-convergence analysis with Dirichlet-type boundary conditions

The aim of this section is to add a Dirichlet type boundary condition to the Γ-convergence statement of Theorem 4.17. Fix a boundary condition

$$(\sigma, g_S, g_A) \in (H^{-1}(\Omega;\mathbb{R}^2) \cap \mathcal{M}(\Omega;\mathbb{R}^2)) \times L^2(\Omega;\mathbb{M}^{2\times2}_{\mathrm{sym}}) \times L^2(\Omega;\mathbb{M}^{2\times2}_{\mathrm{skew}}), \tag{4.87}$$

such that

$$\sigma = \operatorname{Curl} g_A . \tag{4.88}$$

Also fix $\sigma_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$ and $g_\varepsilon \in \mathcal{AS}_\varepsilon(\sigma_\varepsilon)$ such that $(\sigma_\varepsilon, g_\varepsilon)$ converges to (σ, g_S, g_A) in the sense of Definition 4.15. Such a sequence exists thanks to Theorem 4.17, for example.

The set of dislocations compatible with the boundary data is defined as

$$\mathcal{AD}^{g_\varepsilon}_\varepsilon(\Omega) := \left\{ \mu \in \mathcal{AD}_\varepsilon(\Omega) : \ \mu(\Omega) = \int_{\partial\Omega} g_\varepsilon \cdot t \, ds \right\} , \tag{4.89}$$

where t is the unit tangent to $\partial\Omega$, defined as $t := J\nu$ with ν the inner unit normal to Ω. For a dislocation measure $\mu \in \mathcal{AD}^{g_\varepsilon}_\varepsilon(\Omega)$, the set of admissible strains are defined as

$$\mathcal{AS}^{g_\varepsilon}_\varepsilon(\mu) := \{ \beta \in \mathcal{AS}_\varepsilon(\mu) : \ \beta \cdot t = g_\varepsilon \cdot t \ \text{ on } \ \partial\Omega \} .$$

The rescaled energy functional $\mathcal{F}^{g_\varepsilon}_\varepsilon : \mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times2}) \to \mathbb{R}$ is defined by

$$\mathcal{F}^{g_\varepsilon}_\varepsilon(\mu,\beta) := \begin{cases} \dfrac{1}{N_\varepsilon |\log\varepsilon|} E_\varepsilon(\mu,\beta) & \text{if } \mu \in \mathcal{AD}^{g_\varepsilon}_\varepsilon(\Omega) \, , \, \beta \in \mathcal{AS}^{g_\varepsilon}_\varepsilon(\mu) \, , \\ +\infty & \text{otherwise.} \end{cases} \tag{4.90}$$

The candidate Γ-limit is the functional

$$\mathcal{F}^g \colon (H^{-1}(\Omega;\mathbb{R}^2) \cap \mathcal{M}(\Omega;\mathbb{R}^2)) \times L^2(\Omega;\mathbb{M}^{2\times2}_{\mathrm{sym}}) \times L^2(\Omega;\mathbb{M}^{2\times2}_{\mathrm{skew}}) \to \mathbb{R} ,$$

defined by

$$\mathcal{F}^g(\mu,S,A) := \int_\Omega W(S)\,dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| + \int_{\partial\Omega} \varphi((g_A - A)\cdot t)\,ds , \tag{4.91}$$

if $\operatorname{Curl} A = \mu$ and $\mathcal{F}^g(\mu, S, A) := \infty$ otherwise. Here ds coincides with $\mathcal{H}^1 \llcorner \partial\Omega$. The boundary term appearing in the definition of $\mathcal{F}^g$ is intended in the sense of traces of BV functions (see Theorem A.56). Indeed, since A and g_A are antisymmetric, there exist $u, a \in L^2(\Omega)$ such that

$$A = \begin{pmatrix} 0 & u \\ -u & 0 \end{pmatrix}, \quad g_A = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix},$$

a.e. in Ω. Notice that $\operatorname{Curl} A = Du$ and $\operatorname{Curl} g_A = Da$ in the sense of distributions. Therefore, conditions $\operatorname{Curl} A, \operatorname{Curl} g_A \in \mathcal{M}(\Omega; \mathbb{R}^2)$ imply that $a, u \in BV(\Omega)$. Hence a and u admit traces on $\partial\Omega$ that belong to $L^1(\partial\Omega; \mathbb{R}^2)$. By noting that

$$\int_{\partial\Omega} \varphi((g_A - A) \cdot t)\, ds = \int_{\partial\Omega} \varphi((u - a)\nu)\, ds\,,$$

where ν is the inner normal to Ω, we conclude that the definition of $\mathcal{F}^g$ is well-posed.

We are now ready to state the Γ-convergence result with boundary condition.

Theorem 4.19. *The following Γ-convergence statement holds with respect to the convergence of Definition 4.15.*

(i) (Compactness) *Let $\varepsilon_n \to 0$ and assume that $(\mu_n, \beta_n) \in \mathcal{M}(\Omega; \mathbb{R}^2) \times L^2(\Omega; \mathbb{M}^{2\times 2})$ is such that $\sup_n \mathcal{F}^{g_{\varepsilon_n}}_{\varepsilon_n}(\mu_n, \beta_n) \leq E$, for some positive constant E. Then there exists $(\mu, S, A) \in (H^{-1}(\Omega; \mathbb{R}^2) \cap \mathcal{M}(\Omega; \mathbb{R}^2)) \times L^2(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{sym}}) \times L^2(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{skew}})$ such that (μ_n, β_n) converges to (μ, S, A) in the sense of Definition 4.15. Moreover $\mu \in H^{-1}(\Omega; \mathbb{R}^2)$ and* $\operatorname{Curl} A = \mu$.

(ii) (Γ-convergence) *The energy functionals $\mathcal{F}^{g_\varepsilon}_\varepsilon$ defined in* (4.90) *Γ-converge with respect to the convergence of Definition 4.15 to the functional $\mathcal{F}^g$ defined in* (4.91). *To be more precise, for every*

$$(\mu, S, A) \in (H^{-1}(\Omega; \mathbb{R}^2) \cap \mathcal{M}(\Omega; \mathbb{R}^2)) \times L^2(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{sym}}) \times L^2(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{skew}})$$

such that $\operatorname{Curl} \mu = A$, *then:*

- (Γ-liminf inequality) *for every sequence $(\mu_\varepsilon, \beta_\varepsilon) \in \mathcal{M}(\Omega; \mathbb{R}^2) \times L^2(\Omega; \mathbb{M}^{2\times 2})$ converging to (μ, S, A) in the sense of Definition 4.15, we have*

$$\mathcal{F}^g(\mu, S, A) \leq \liminf_{\varepsilon \to 0} \mathcal{F}^{g_\varepsilon}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon)\,.$$

- (Γ-limsup inequality) *there exists a recovery sequence* $(\mu_\varepsilon, \beta_\varepsilon)$ *belonging to* $\mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times 2})$ *such that* $(\mu_\varepsilon, \beta_\varepsilon)$ *converges to* (μ, S, A) *in the sense of Definition 4.15, and*

$$\limsup_{\varepsilon\to 0} \mathcal{F}^{g_\varepsilon}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon) \le \mathcal{F}^g(\mu, S, A)\,.$$

The compactness statement follows immediately from the compactness of Theorem 4.17, since $\mathcal{F}^{g_\varepsilon}_\varepsilon(\mu,\beta) = \mathcal{F}_\varepsilon(\mu,\beta)$ for $\mu \in \mathcal{AD}^{g_\varepsilon}_\varepsilon(\Omega)$ and $\beta \in \mathcal{AS}^{g_\varepsilon}_\varepsilon(\mu)$. Let us proceed with the proof of the Γ-convergence result.

Proof of Γ-lim sup *inequality of Theorem 4.19.* Let (μ, S, A) be given in the domain of the Γ-limit $\mathcal{F}^g$. We will construct a recovery sequence in two steps, relying on Theorem 4.17.

Step 1. Approximation of the boundary values.

For $\delta > 0$ fixed, set $\omega_\delta := \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) > \delta\}$, so that $\omega_\delta \subset\subset \Omega$. Define $S_\delta \in L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})$ and $A_\delta \in L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$ as

$$A_\delta := \begin{cases} A & \text{in } \omega_\delta\,, \\ g_A & \text{in } \Omega\setminus\omega_\delta\,, \end{cases} \qquad S_\delta := \begin{cases} S & \text{in } \omega_\delta\,, \\ g_S & \text{in } \Omega\setminus\omega_\delta\,. \end{cases} \tag{4.92}$$

Further, let $\mu_\delta \in \mathcal{M}(\Omega;\mathbb{R}^2)$ be such that

$$\mu_\delta := \mu \llcorner \omega_\delta + \sigma \llcorner (\Omega\setminus\omega_\delta) + (g_A - A)\cdot t\; \mathcal{H}^1 \llcorner \partial\omega_\delta\,. \tag{4.93}$$

Notice that

$$\operatorname{Curl} A_\delta = \mu_\delta \quad \text{ and } \quad \mu_\delta \in H^{-1}(\Omega;\mathbb{R}^2)\,, \tag{4.94}$$

therefore $(\mu_\delta, S_\delta, A_\delta)$ belongs to the domain of the functional $\mathcal{F}$. Indeed, by using cutoff functions, it is immediate to check that for every $\psi \in H^1_0(\Omega)$ and $i = 1, 2$,

$$\langle \operatorname{Curl} A^{(i)}_\delta, \psi\rangle = \int_{\omega_\delta} A^{(i)}\cdot J\nabla\psi\,dx + \int_{\Omega\setminus\omega_\delta} g^{(i)}_A \cdot J\nabla\psi\,dx + \int_{\partial\omega_\delta} (g^{(i)}_A - A^{(i)})\cdot t\;\psi\;ds\,.$$

Recalling that $\operatorname{Curl} A = \mu$ and $\operatorname{Curl} g_A = \sigma$, we obtain (4.94). Also note that

$$S_\delta \to S\,,\; A_\delta \to A \;\text{ in }\; L^2(\Omega;\mathbb{M}^{2\times 2})\,,\; \mu_\delta \overset{*}{\rightharpoonup} \mu \;\text{ in }\; \mathcal{M}(\Omega;\mathbb{R}^2)\,,\; |\mu_\delta|(\Omega) \to |\mu|(\Omega)\,, \tag{4.95}$$

as $\delta \to 0$. Therefore, by Reshetnyak's Theorem (see (A.6) in Theorem A.17), we have

$$\lim_{\delta \to 0} \mathcal{F}(\mu_\delta, S_\delta, A_\delta) = \mathcal{F}^g(\mu, S, A) . \tag{4.96}$$

It will now be sufficient to construct dislocation measures $\mu^{g_\varepsilon}_{\delta,\varepsilon} \in \mathcal{AD}^{g_\varepsilon}_\varepsilon(\Omega)$ and strains $\beta^{g_\varepsilon}_{\delta,\varepsilon} \in \mathcal{AS}^{g_\varepsilon}_\varepsilon(\mu^{g_\varepsilon}_{\delta,\varepsilon})$, such that $(\mu^{g_\varepsilon}_{\delta,\varepsilon}, \beta^{g_\varepsilon}_{\delta,\varepsilon})$ converges to $(\mu_\delta, S_\delta, A_\delta)$ in the sense of Definition 4.15 and that

$$\lim_{\varepsilon \to 0} \mathcal{F}^{g_\varepsilon}_\varepsilon(\mu^{g_\varepsilon}_{\delta,\varepsilon}, \beta^{g_\varepsilon}_{\delta,\varepsilon}) = \mathcal{F}(\mu_\delta, S_\delta, A_\delta) . \tag{4.97}$$

Indeed, by taking a diagonal sequence $(\mu^{g_\varepsilon}_{\delta_\varepsilon,\varepsilon}, \beta^{g_\varepsilon}_{\delta_\varepsilon,\varepsilon})$ and using (4.95), (4.96), the thesis will follow.

Step 2. Recovery sequence for strains satisfying the boundary condition.

Let us now proceed to construct the sequence $(\mu^{g_\varepsilon}_{\delta,\varepsilon}, \beta^{g_\varepsilon}_{\delta,\varepsilon})$ as stated in the previous step. From Theorem 4.17, there exist sequences $\mu_{\delta,\varepsilon} = \sum_{i=1}^{M_\varepsilon} \xi_{\varepsilon,i}\, \delta_{x_{\varepsilon,i}} \in \mathcal{AD}_\varepsilon(\Omega)$ and $\beta_{\delta,\varepsilon} \in \mathcal{AS}_\varepsilon(\mu_{\delta,\varepsilon})$ such that $(\mu_{\delta,\varepsilon}, \beta_{\delta,\varepsilon})$ converges to $(\mu_\delta, S_\delta, A_\delta)$ in the sense of Definition 4.15 and

$$\lim_{\varepsilon \to 0} \mathcal{F}_\varepsilon(\mu_{\delta,\varepsilon}, \beta_{\delta,\varepsilon}) = \mathcal{F}(\mu_\delta, S_\delta, A_\delta) . \tag{4.98}$$

The idea is to modify $(\mu_{\delta,\varepsilon}, \beta_{\delta,\varepsilon})$ so that it becomes admissible for the boundary condition g. Introduce the vector

$$\xi_\varepsilon := \int_{\partial\Omega} (g_\varepsilon - \beta_{\delta,\varepsilon}) \cdot t \; ds .$$

By construction one has $\xi_\varepsilon \in \mathbb{S}$ and

$$\frac{\xi_\varepsilon}{N_\varepsilon} \to 0 \quad \text{as} \quad \varepsilon \to 0 . \tag{4.99}$$

Since $\xi_\varepsilon \in \mathbb{S}$, we have

$$\xi_\varepsilon = \sum_{j=1}^{s} \lambda_{\varepsilon,j} b_j , \quad \text{with } \lambda_{\varepsilon,j} \in \mathbb{Z}_+, \ b_j \in \mathcal{S}_\pm ,$$

where for convenience we define $\mathcal{S}_\pm := \{\pm b_1, \dots, \pm b_s\}$ for $b_i \in \mathcal{S}$. It will be also convenient to write $\xi_\varepsilon = \sum_{i=1}^{\Lambda_\varepsilon} b_{\varepsilon,i}$ with $b_{\varepsilon,i} \in \mathcal{S}_\pm$ and $\Lambda_\varepsilon := \sum_{j=1}^{s} \lambda_{\varepsilon,j}$. Notice that (4.99) implies that

$$\frac{\Lambda_\varepsilon}{N_\varepsilon} \to 0 \quad \text{as} \quad \varepsilon \to 0 . \tag{4.100}$$

Since the number of masses in $\mu_{\delta,\varepsilon}$ is such that $M_\varepsilon \le C N_\varepsilon$ and $\Lambda_\varepsilon \ll N_\varepsilon$, it is possible to choose a collection of distinct points $\{y_{\varepsilon,i}\}_{i=1}^{\Lambda_\varepsilon} \subset \Omega$, possibly intersecting $\operatorname{supp}\mu_{\delta,\varepsilon}$, such that

$$|y_{\varepsilon,i} - y_{\varepsilon,j}| > r_\varepsilon\,, \quad \operatorname{dist}(y_{\varepsilon,k}, \partial\Omega) > r_\varepsilon\,, \tag{4.101}$$

where $r_\varepsilon := C/\sqrt{N_\varepsilon}$ for some constant $C > 0$. Define the measures

$$\nu_\varepsilon := \sum_{i=1}^{\Lambda_\varepsilon} b_{\varepsilon,i}\, \delta_{y_{\varepsilon,i}}\,, \qquad \mu_{\delta,\varepsilon}^{g_\varepsilon} := \mu_{\delta,\varepsilon} + \nu_\varepsilon\,,$$

and notice that by construction we have $\mu_{\delta,\varepsilon}^{g_\varepsilon} \in \mathcal{AS}_\varepsilon^{g_\varepsilon}(\Omega)$ and

$$\frac{\mu_{\delta,\varepsilon}^{g_\varepsilon}}{N_\varepsilon} \stackrel{*}{\rightharpoonup} \mu_\delta \quad \text{in} \quad \mathcal{M}(\Omega;\mathbb{R}^2)\,. \tag{4.102}$$

Introduce

$$\tilde{K}_\varepsilon^{\nu_\varepsilon} := \sum_{i=1}^{\Lambda_\varepsilon} \tilde{K}_{\varepsilon,i}^{b_{\varepsilon,i}}\, \chi_{B_{r_\varepsilon}(x_{\varepsilon,i})}\,, \qquad \hat{K}_\varepsilon^{\nu_\varepsilon} := \sum_{i=1}^{\Lambda_\varepsilon} \hat{K}_{\varepsilon,i}^{b_{\varepsilon,i}}\, \chi_{B_{r_\varepsilon}(x_{\varepsilon,i})\setminus B_\varepsilon(x_{\varepsilon,i})}\,, \tag{4.103}$$

so that

$$\operatorname{Curl} \tilde{K}_\varepsilon^{\nu_\varepsilon} = \tilde{\nu}_\varepsilon^{r_\varepsilon} - \hat{\nu}_\varepsilon^{r_\varepsilon}\,, \qquad \operatorname{Curl} \hat{K}_\varepsilon^{\nu_\varepsilon} = \hat{\nu}_\varepsilon^{\varepsilon} - \hat{\nu}_\varepsilon^{r_\varepsilon}\,, \tag{4.104}$$

recalling notations (4.45), (4.46). Notice that

$$\frac{\hat{K}_\varepsilon^{\nu_\varepsilon}}{\sqrt{N_\varepsilon\,|\log\varepsilon|}}, \frac{\tilde{K}_\varepsilon^{\nu_\varepsilon}}{\sqrt{N_\varepsilon\,|\log\varepsilon|}} \to 0 \quad \text{strongly in} \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,. \tag{4.105}$$

Indeed, by definition (4.103), it is straightforward to check that

$$\int_\Omega \frac{|\hat{K}_\varepsilon^{\nu_\varepsilon}|^2}{N_\varepsilon|\log\varepsilon|}\,dx \le C\,\frac{\Lambda_\varepsilon(\log r_\varepsilon - \log\varepsilon)}{N_\varepsilon|\log\varepsilon|} \to 0\,,$$
$$\int_\Omega \frac{|\tilde{K}_\varepsilon^{\nu_\varepsilon}|^2}{N_\varepsilon|\log\varepsilon|}\,dx \le C\,\frac{\Lambda_\varepsilon}{N_\varepsilon|\log\varepsilon|} \to 0\,,$$

as $\varepsilon \to 0$, by (4.100). Here $C > 0$ is a constant depending only on the set of Burgers vectors $\mathcal{S}$. From (4.100), it is immediate to show that

$$\frac{\tilde{\nu}_\varepsilon^{r_\varepsilon}}{N_\varepsilon} \to 0 \quad \text{in} \quad H^{-1}(\Omega;\mathbb{R}^2)\,. \tag{4.106}$$

Moreover, by proceeding as in (4.62), we have that

$$\|\operatorname{Div} \tilde{\nu}_\varepsilon^{r_\varepsilon}\|_{H^{-1}(\Omega)} \le \frac{C}{r_\varepsilon} = C\sqrt{N_\varepsilon}\,. \tag{4.107}$$

By Helmholtz decomposition, there exist sequences $f_\varepsilon, h_\varepsilon \in H^1(\Omega)$, with $h_\varepsilon \cdot t = 0$ on $\partial\Omega$ and such that

$$\nabla f_\varepsilon + J\nabla h_\varepsilon = \tilde{\nu}_\varepsilon^{r_\varepsilon} \quad \text{in} \quad H^{-1}(\Omega)\,, \tag{4.108}$$

$$\|f_\varepsilon\|_{H^1(\Omega)} \leq C\,\|\operatorname{Div}\tilde{\nu}_\varepsilon^{r_\varepsilon}\|_{H^{-1}(\Omega)}\,, \quad \|h_\varepsilon\|_{H^1(\Omega)} \leq C\,\|\tilde{\nu}_\varepsilon^{r_\varepsilon}\|_{H^{-1}(\Omega;\mathbb{R}^2)}\,. \tag{4.109}$$

Define

$$R_\varepsilon := \begin{pmatrix} f_\varepsilon & h_\varepsilon \\ -h_\varepsilon & f_\varepsilon \end{pmatrix} \tag{4.110}$$

so that

$$\operatorname{Curl} R_\varepsilon = \tilde{\nu}_\varepsilon^{r_\varepsilon}\,. \tag{4.111}$$

Moreover, by (4.106),(4.107) and (4.109),

$$\frac{R_\varepsilon^{\mathrm{sym}}}{\sqrt{N_\varepsilon|\log\varepsilon|}},\ \frac{R_\varepsilon^{\mathrm{skew}}}{N_\varepsilon} \to 0 \quad \text{in} \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,. \tag{4.112}$$

We can now define

$$\overline{\beta}_{\delta,\varepsilon} := \left(\beta_{\delta,\varepsilon} + \hat{K}_\varepsilon^{\nu_\varepsilon} - \tilde{K}_\varepsilon^{\nu_\varepsilon} + R_\varepsilon\right)\chi_{\Omega_\varepsilon(\mu_{\delta,\varepsilon}^{g_\varepsilon})}\,.$$

Recalling that $\operatorname{Curl}\beta_{\delta,\varepsilon} \llcorner \Omega_\varepsilon(\mu_{\delta,\varepsilon}) = 0$ and from (4.104), (4.111) we have

$$\operatorname{Curl}\overline{\beta}_{\delta,\varepsilon} \llcorner \Omega_\varepsilon(\mu_{\delta,\varepsilon}^{g_\varepsilon}) = 0\,.$$

Moreover, by construction, $\overline{\beta}_{\delta,\varepsilon}$ satisfies the circulation condition on $\cup_{i=1}^{N_\varepsilon}\partial B_\varepsilon(x_{\varepsilon,i}) \cup \cup_{i=1}^{\Lambda_\varepsilon}\partial B_\varepsilon(y_{\varepsilon,i})$ and

$$\int_{\partial\Omega} \overline{\beta}_{\delta,\varepsilon}\cdot t\; ds = \int_{\partial\Omega} g_\varepsilon \cdot t\; ds\,. \tag{4.113}$$

Let $u_{\delta,\varepsilon}$ be the solution to

$$\min\left\{ \int_{\Omega\setminus\omega_{\rho_\varepsilon}} W(\beta)\,dx :\ \beta \in L^2(\Omega\setminus\omega_{\rho_\varepsilon};\mathbb{R}^2)\,,\ \operatorname{Curl}\beta = 0\,,\right.$$
$$\left. \beta\cdot t = \overline{\beta}_{\delta,\varepsilon}\cdot t \ \text{ on } \ \partial\omega_{\rho_\varepsilon}\,,\ \beta\cdot t = g_\varepsilon\cdot t \ \text{ on } \ \partial\Omega \right\},$$

which exists by (4.113), and define

$$\beta_{\delta,\varepsilon}^{g_\varepsilon} := \overline{\beta}_{\delta,\varepsilon}\chi_{\omega_{\rho_\varepsilon}} + \nabla u_{\delta,\varepsilon}\,\chi_{\Omega\setminus\omega_{\rho_\varepsilon}}\,. \tag{4.114}$$

By construction, we have $\beta_{\delta,\varepsilon}^{g_\varepsilon} \in \mathcal{AS}_\varepsilon^{g_\varepsilon}(\mu_{\delta,\varepsilon}^{g_\varepsilon})$. From (4.102), (4.105) and (4.112), we have that $(\mu_{\delta,\varepsilon}^{g_\varepsilon}, \beta_{\delta,\varepsilon}^{g_\varepsilon})$ converges to $(\mu_\delta, S_\delta, A_\delta)$ in the sense of Definition 4.15. Moreover (4.105) and (4.112) imply that

$$\mathcal{F}_\varepsilon^{g_\varepsilon}(\mu_{\delta,\varepsilon}^{g_\varepsilon}, \beta_{\delta,\varepsilon}^{g_\varepsilon}) = \mathcal{F}_\varepsilon(\mu_{\delta,\varepsilon}, \beta_{\delta,\varepsilon}) + o(1)\,,$$

therefore (4.97) follows from (4.98).

□

Proof of Γ-lim inf *inequality of Theorem 4.19.* Let $(\mu_\varepsilon, \beta_\varepsilon)$ with $\mu_\varepsilon \in \mathcal{AD}^{g_\varepsilon}_\varepsilon(\Omega)$ and $\beta_\varepsilon \in \mathcal{AS}^{g_\varepsilon}_\varepsilon(\mu_\varepsilon)$ be convergent, in the sense of Definition 4.15, to (μ, S, A) in the domain of the Γ-limit. By combining an extension argument with the Γ-lim inf inequality in Theorem 4.17 we will show that

$$\mathcal{F}^g(\mu, S, A) \leq \liminf_{\varepsilon \to 0} \mathcal{F}^{g_\varepsilon}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon)\,. \tag{4.115}$$

Fix $\delta > 0$ and define $U_\delta := \{x \in \mathbb{R}^2 : \ \mathrm{dist}(x, \Omega) < \delta\}$. By standard reflexion arguments one can extend g_S and g_A to $\tilde{g}_S \in L^2(U_\delta; \mathbb{M}^{2\times2}_{\mathrm{sym}}), \tilde{g}_A \in L^2(U_\delta; \mathbb{M}^{2\times2}_{\mathrm{skew}})$ respectively, in such a way that $\mathrm{Curl}\, \tilde{g}_S$ and $\tilde{\sigma} := \mathrm{Curl}\, \tilde{g}_A$ are measures on U_δ satisfying $|\mathrm{Curl}\, \tilde{g}_S|(\partial\Omega) = |\tilde{\sigma}|(\partial\Omega) = 0$. By proceeding as in the previous proof, we can construct a recovery sequence $(\tilde{\sigma}_\varepsilon, \tilde{g}_\varepsilon)$ such that

- $\tilde{\sigma}_\varepsilon \in \mathcal{AD}_\varepsilon(U_\delta \setminus \Omega)$ and $\tilde{g}_\varepsilon \in \mathcal{AS}_\varepsilon(\tilde{\sigma}_\varepsilon)$,
- $\tilde{g}_\varepsilon \cdot t = g_\varepsilon \cdot t$ a.e. on $\partial\Omega$,
- $(\tilde{\sigma}_\varepsilon, \tilde{g}_\varepsilon)$ converges to $(\tilde{\sigma}, \tilde{g}_S, \tilde{g}_A)$ in the sense of Definition 4.15 in U_δ,

and that

$$\lim_{\varepsilon \to 0} \frac{1}{N_\varepsilon |\log \varepsilon|} \int_{U_\delta \setminus \Omega} W(\tilde{g}_\varepsilon)\, dx = \int_{U_\delta \setminus \Omega} W(\tilde{g}_S)\, dx + \int_{U_\delta \setminus \Omega} \varphi\left(\frac{d\tilde{\sigma}}{d|\tilde{\sigma}|}\right) d|\tilde{\sigma}|\,. \tag{4.116}$$

Notice that in (4.116) there is no contribution from the boundary, since $\tilde{g}_\varepsilon \cdot t = g_\varepsilon \cdot t$ a.e. on $\partial\Omega$.

Define strains on U_δ

$$\tilde{\beta}_\varepsilon = \begin{cases} \beta_\varepsilon & \text{in } \Omega\,, \\ \tilde{g}_\varepsilon & \text{in } U_\delta \setminus \Omega\,, \end{cases} \qquad \tilde{S} := \begin{cases} S & \text{in } \Omega\,, \\ \tilde{g}_S & \text{in } U_\delta \setminus \Omega\,, \end{cases} \qquad \tilde{A} := \begin{cases} A & \text{in } \Omega\,, \\ \tilde{g}_A & \text{in } U_\delta \setminus \Omega\,, \end{cases}$$

and also measures

$$\tilde{\mu}_\varepsilon := \mu_\varepsilon \llcorner \Omega + \tilde{\sigma}_\varepsilon \llcorner (U_\delta \setminus \Omega)\,,$$
$$\tilde{\mu} := \mu \llcorner \Omega + \tilde{\sigma} \llcorner (U_\delta \setminus \Omega) + (g_A - A) \cdot t\, \mathcal{H}^1 \llcorner \partial\Omega\,.$$

Notice that by definition $\tilde{\mu}_\varepsilon \in \mathcal{AD}_\varepsilon(U_\delta)$ and $\tilde{\beta}_\varepsilon \in \mathcal{AS}_\varepsilon(\tilde{\mu}_\varepsilon)$. Moreover, by using cutoff functions, one can check that $\tilde{\mu}_\varepsilon / N_\varepsilon \overset{*}{\rightharpoonup} \tilde{\mu}$ in $\mathcal{M}(U_\delta; \mathbb{R}^2)$, $\mathrm{Curl}\, \tilde{A} = \tilde{\mu}$ and

$\tilde{\mu} \in H^{-1}(U_\delta;\mathbb{R}^2)$. Therefore $(\tilde{\mu}_\varepsilon, \tilde{\beta}_\varepsilon)$ converges to $(\tilde{\mu}, \tilde{S}, \tilde{A})$ in U_δ in the sense of Definition 4.15. By the Γ-liminf inequality of Theorem 4.17 we have

$$\liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon |\log\varepsilon|} \int_{U_\delta} W(\tilde{\beta}_\varepsilon)\,dx \geq \int_{U_\delta} W(\tilde{S})\,dx + \int_{U_\delta} \varphi\left(\frac{d\tilde{\mu}}{d|\tilde{\mu}|}\right) d|\tilde{\mu}|\,. \tag{4.117}$$

By definition and by (4.116) we have

$$\begin{aligned}\liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon |\log\varepsilon|} \int_{U_\delta} W(\tilde{\beta}_\varepsilon)\,dx = &\liminf_{\varepsilon\to 0} \mathcal{F}_\varepsilon^{g_\varepsilon}(\mu_\varepsilon, \beta_\varepsilon) + \\ &+ \int_{U_\delta\setminus\Omega} W(\tilde{g}_S)\,dx + \int_{U_\delta\setminus\Omega} \varphi\left(\frac{d\tilde{\sigma}}{d|\tilde{\sigma}|}\right) d|\tilde{\sigma}|\,.\end{aligned} \tag{4.118}$$

Also note that, by computing the Radon-Nikodym derivative of $\tilde{\mu}$, we have

$$\begin{aligned}\int_{U_\delta} W(\tilde{S})\,dx + \int_{U_\delta} \varphi\left(\frac{d\tilde{\mu}}{d|\tilde{\mu}|}\right) d|\tilde{\mu}| = &\mathcal{F}^g(\mu, S, A) + \\ &+ \int_{U_\delta\setminus\Omega} W(\tilde{g}_S)\,dx + \int_{U_\delta\setminus\Omega} \varphi\left(\frac{d\tilde{\sigma}}{d|\tilde{\sigma}|}\right) d|\tilde{\sigma}|\,.\end{aligned} \tag{4.119}$$

By putting together (4.117)-(4.119), we obtain (4.115). □

4.6 Linearised polycrystals as minimisers of the Γ-limit

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with Lipschitz boundary. Let $k \in \mathbb{N}$ be fixed and let $\{U_i\}_{i=1}^k$ be a Caccioppoli partition of Ω (see Definition A.41). Moreover fix $m_1, \dots, m_k \in \mathbb{R}_+$ with $m_i < m_{i+1}$, and define the piecewise constant function $a \in BV(\Omega)$ as

$$a := \sum_{i=1}^k m_i \chi_{U_i}\,, \tag{4.120}$$

(Definition A.42). In particular, (4.120) implies that $a \in L^\infty(\Omega)$ and $Da \in \mathcal{M}(\Omega;\mathbb{R}^2)$. We can now define the piecewise constant boundary condition $g_A \in L^\infty(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$ as

$$g_A := \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix}. \tag{4.121}$$

Notice that $g_A \in L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$ and $\operatorname{Curl} g_A = Da$, therefore $\operatorname{Curl} g_A \in H^{-1}(\Omega;\mathbb{R}^2) \cap \mathcal{M}(\Omega;\mathbb{R}^2)$. In this way g_A is an admissible boundary condition for $\mathcal{F}^g$, as required in (4.87)-(4.88).

We want to minimise the Γ-limit (4.91) with boundary condition g_A prescribed by (4.120)-(4.121). Since the elastic energy and plastic energy are decoupled in $\mathcal{F}^g$, and there is no boundary condition fixed on the elastic part of the strain S, we have

$$\inf \mathcal{F}^g(\operatorname{Curl} A, S, A) = \inf \mathcal{F}^g(\operatorname{Curl} A, 0, A)\,.$$

Therefore it is sufficient to study

$$\begin{aligned}\inf \Bigg\{ \int_\Omega \varphi(\operatorname{Curl} A) + \int_{\partial\Omega} \varphi((g_A - A)\cdot t)\, ds :\ A \in L^2(\Omega; \mathbb{M}^{2\times 2}_{\text{skew}}),& \\ \operatorname{Curl} A \in H^{-1}(\Omega;\mathbb{R}^2) \cap \mathcal{M}(\Omega;\mathbb{R}^2) \Bigg\}\,,&\end{aligned} \tag{4.122}$$

where t is the unit tangent to $\partial\Omega$ defined as the $\pi/2$ clock-wise rotation of the inner normal ν to Ω, $\varphi\colon \mathbb{R}^2 \to [0,\infty)$ is the density defined in (4.33), and

$$\int_\Omega \varphi(\mu) := \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|$$

is the anisotropic φ-total variation for a measure $\mu \in \mathcal{M}(\Omega;\mathbb{R}^2)$ (see Section A.3.6 for details), which is well defined, since φ satisfies the properties given in Proposition 4.14.

For $A \in L^2(\Omega; \mathbb{M}^{2\times 2}_{\text{skew}})$, we have that

$$A = \begin{pmatrix} 0 & u \\ -u & 0 \end{pmatrix}\,, \tag{4.123}$$

for some $u \in L^2(\Omega)$. Moreover $\operatorname{Curl} A = Du$, therefore condition $\operatorname{Curl} A \in \mathcal{M}(\Omega;\mathbb{R}^2)$ implies $u \in BV(\Omega)$. Also notice that

$$\int_{\partial\Omega} \varphi((g_A - A)\cdot t)\, ds = \int_{\partial\Omega} \varphi((u-a)\nu)\, ds\,,$$

where a is the piecewise constant function (4.120). We claim that (4.122) is equivalent to the following minimisation problem

$$\inf \left\{ \int_\Omega \varphi(Du) + \int_{\partial\Omega} \varphi((u-a)\nu)\, ds :\ u \in BV(\Omega) \right\}\,. \tag{4.124}$$

Indeed, we already showed that if A is a competitor for (4.122), then the function u, given by (4.123), belongs to $BV(\Omega)$, and it is a competitor for (4.124). Conversely, assume that $u \in BV(\Omega)$ and define A through (4.123). Since $u \in BV(\Omega)$, then $\operatorname{Curl} A = Du \in \mathcal{M}(\Omega;\mathbb{R}^2)$. Moreover, recall that the immersion $BV(\Omega) \hookrightarrow L^2(\Omega)$ is continuous (see Remark A.31), therefore $u \in L^2(\Omega)$, which implies $A \in L^2(\Omega; \mathbb{M}^{2\times 2})$, so that $\operatorname{Curl} A \in H^{-1}(\Omega; \mathbb{R}^2)$. This shows that (4.122) and (4.124) are equivalent.

The main result of this section is that, given the piecewise constant boundary condition a defined in (4.120), there exists a piecewise constant minimiser $\tilde{u}$ to (4.124). In our model the function $\tilde{u}$ corresponds to a linearised polycrystal.

Theorem 4.20. *There exists a locally constant minimiser $\tilde{u} \in BV(\Omega)$ to (4.124), i.e.,*

$$\tilde{u} = \sum_{i=1}^{k} m_i \chi_{\Omega_i}$$

where $\{\Omega_i\}_{i=1}^k$ is a Caccioppoli partition of Ω, and the values m_i are the ones of (4.120).

The proof of this theorem relies on the anisotropic coarea formula. For the readers convenience we briefly recall it here (more details can be found in Section A.3.6). For $E \subset \Omega$ of finite perimeter, the anisotropic φ-perimeter of E in Ω is defined as

$$\operatorname{Per}_\varphi(E, \Omega) := \int_\Omega \varphi(D\chi_E)\,.$$

Since φ is convex and positively 1-homogenous, the anisotropic coarea formula holds true for every $u \in BV(\Omega)$:

$$\int_\Omega \varphi(Du) = \int_{-\infty}^{\infty} \operatorname{Per}_\varphi(E_t, \Omega)\, dt\,, \tag{4.125}$$

where E_t is the level set $E_t := \{x \in \Omega :\ u(x) > t\}$, defined for every $t \in \mathbb{R}$.

Proof of Theorem 4.20.

Step 1. Equivalent minimisation problem.

We start by rewriting (4.124) as a boundary value problem in BV. Let $\Omega' := \{x \in \mathbb{R}^2 :\ \operatorname{dist}(x, \partial\Omega) < 1\}$, so that $\Omega \subset\subset \Omega'$. Consider a piecewise constant extension $\tilde{a} \in BV(\Omega')$ of the function $a \in BV(\Omega)$ defined in (4.120), that is,

$$\tilde{a} = \sum_{i=1}^{k} m_i\, \chi_{U_i'}\,,$$

where $\{U_i'\}_{i=1}^k$ is a Caccioppoli partition of Ω', agreeing with $\{U_i\}_{i=1}^k$ on Ω. This is possible thanks to Theorem A.53, since the extension can be chosen such that

$|D\tilde{a}|(\partial\Omega) = 0$, that is, we are not creating any jump on $\partial\Omega$. Consider the new minimisation problem

$$I := \inf \left\{ \int_{\Omega'} \varphi(Du) : \ u \in BV(\Omega'), \ u = \tilde{a} \text{ a.e. in } \Omega' \setminus \Omega \right\} . \tag{4.126}$$

Finding a solution to (4.126) is equivalent to finding a solution to (4.124). Indeed, if $u \in BV(\Omega')$ is such that $u = \tilde{a}$ in $\Omega' \setminus \Omega$ then by Corollary A.58 we have

$$Du = Du \llcorner \Omega + (u^\Omega - a^\Omega)\, \nu\, \mathcal{H}^1 \llcorner \partial\Omega + D\tilde{a} \llcorner (\Omega' \setminus \Omega) , \tag{4.127}$$

where $u^\Omega, a^\Omega \in L^1(\partial\Omega)$ are the traces of u and a on $\partial\Omega$, given by Theorem A.56. Notice that we can use a^Ω in (4.127) because the extension $\tilde{a}$ is such that $|D\tilde{a}|(\partial\Omega) = 0$, hence by Theorem A.54 we have $\tilde{a}^+_{\partial\Omega} = \tilde{a}^-_{\partial\Omega} = a^\Omega$ $\mathcal{H}^{n-1}$-a.e. in $\partial\Omega$.

Step 2. Existence of a minimiser for (4.126).

Let $u_j \in BV(\Omega')$ be a minimising sequence for (4.126), that is $u_j = \tilde{a}$ a.e. on $\Omega' \setminus \Omega$ and

$$\lim_{j\to\infty} \int_{\Omega'} \varphi(Du_j) = I . \tag{4.128}$$

By the Poincaré inequality given in Theorem A.29, and the bound (4.34), there exists a constant $C > 0$ such that

$$\int_{\Omega'} |u_j| \, dx \leq C \, |Du_j|(\Omega') \leq C \int_{\Omega'} \varphi(Du_j) .$$

In particular, from (4.128), we deduce that $\sup_j \|u_j\|_{BV(\Omega')} < \infty$. By compactness Theorem A.27, there exists $\tilde{u} \in BV(\Omega')$ such that, up to subsequences, $u_j \to \tilde{u}$ in $L^1(\Omega')$ and $Du_j \overset{*}{\rightharpoonup} D\tilde{u}$ weakly in $\mathcal{M}(\Omega'; \mathbb{R}^2)$. Since $u_j = \tilde{a}$ a.e. on $\Omega' \setminus \Omega$, the strong convergence in L^1 implies that (up to subsequences) $u_j \to \tilde{u}$ a.e. in Ω', so that $\tilde{u} = \tilde{a}$ a.e. in $\Omega' \setminus \Omega$. From Reshetnyak's Theorem (see (A.5) in Theorem A.17) we conclude that

$$\int_{\Omega'} \varphi(D\tilde{u}) \leq \liminf_{j\to\infty} \int_{\Omega'} \varphi(Du_j) = I ,$$

so that $\tilde{u}$ is a minimiser for (4.126).

Step 3. Existence of a piecewise constant minimiser for (4.124).

Let u be a minimiser for (4.126). By a standard truncation argument we can assume that $m_1 \leq u \leq m_k$ a.e. on Ω'. Formula (4.125) then reads

$$\int_{\Omega'} \varphi(Du) = \sum_{i=1}^{k-1} \int_{m_i}^{m_{i+1}} \mathrm{Per}_\varphi(E_t, \Omega') \, dt , \tag{4.129}$$

where $E_t := \{x \in \Omega' \colon u(x) > t\}$ for $t \in \mathbb{R}$. By the mean value theorem, for every $i = 1, \ldots, k-1$, there exists a Lebesgue value $t_i \in (m_i, m_{i+1})$ such that

$$\int_{m_i}^{m_{i+1}} \mathrm{Per}_\varphi(E_t, \Omega')\, dt \geq (m_{i+1} - m_i)\, \mathrm{Per}_\varphi(E_{t_i}, \Omega')\,. \tag{4.130}$$

We define the piecewise constant function

$$\tilde{u}(x) := \begin{cases} m_1 & \text{if } x \in \Omega' \setminus E_{t_1}\,, \\ m_2 & \text{if } x \in E_{t_1} \setminus E_{m_2}\,, \\ m_i & \text{if } x \in E_{m_i} \setminus E_{t_i}\,, \\ m_{i+1} & \text{if } x \in E_{t_i} \setminus E_{m_{i+1}}\,, \end{cases}$$

where $i = 2, \ldots, k-1$ and recalling that $E_{m_k} = \emptyset$ set theoretically. Since the sets E_t have finite perimeter in Ω', by Theorem A.55 we have that $\tilde{u} \in BV(\Omega')$. Moreover, by construction, $\tilde{u} = \tilde{a}$ on $\Omega' \setminus \Omega$, so that $\tilde{u}$ is a piecewise constant competitor for (4.126). It is immediate to compute that

$$D\tilde{u} = \sum_{i=1}^{k-1} (m_{i+1} - m_i)\, \nu_{E_{t_i}}\, \mathcal{H}^1 \llcorner \partial^* E_{t_i}\,,$$

so that

$$\begin{aligned} \int_{\Omega'} \varphi(D\tilde{u}) &= \sum_{i=1}^{k-1} (m_{i+1} - m_i) \int_{\partial^* E_{t_i}} \varphi(\nu_{E_{t_i}})\, d\mathcal{H}^1 \\ &= \sum_{i=1}^{k-1} (m_{i+1} - m_i)\, \mathrm{Per}_\varphi(E_{t_i}, \Omega')\,. \end{aligned} \tag{4.131}$$

By minimality of u and (4.129)-(4.131) we conclude that $\tilde{u}$ is a locally constant minimiser for (4.126). Hence $\tilde{u}|_\Omega$ is a locally constant minimiser for (4.124). □

4.7 Conclusions and perspectives

In this chapter we presented our paper [23]. The aim of [23] is to describe polycrystalline structures from the variational point of view. Grain boundaries and the corresponding grain orientations are not introduced as internal variables of the energy, but they spontaneously arise as a result of energy minimisation, under suitable boundary conditions.

We work under the hypothesis of linear planar elasticity of [30], with the reference configuration $\Omega \subset \mathbb{R}^2$ representing a section of an infinite cylindrical crystal. The elastic energy functional depends on the lattice spacing ε of the crystal and we allow N_ε edge dislocations in the reference configuration, with $N_\varepsilon \to \infty$ as $\varepsilon \to 0$. Each dislocation contributes by a factor $|\log \varepsilon|$ to the elastic energy, so that the natural rescaling for the energy functional is $N_\varepsilon |\log \varepsilon|$. We work in the energy regime

$$N_\varepsilon \gg |\log \varepsilon| \,,$$

which accounts for grain boundaries that are mutually rotated by an infinitesimal angle $\theta \approx 0$. Further, we assume good separation of the dislocation cores, which will imply the bound $N_\varepsilon \ll 1/\varepsilon$ on the number of dislocations. However this bound is compatible with our energy regime.

After rescaling the elastic energy of such system of dislocations and sending the lattice spacing ε to zero, in Theorem 4.17 we obtain a macroscopic energy functional of the form

$$\mathcal{F}(\mu, S, A) = \int_\Omega \mathbb{C} S : S \, dx + \int_\Omega \varphi \left(\frac{d\mu}{d|\mu|} \right) d|\mu| \,,$$

where $\mathbb{C}$ is the linear elasticity tensor and φ is a positively 1-homogeneous density function, defined through a suitable cell-problem. The elastic energy is computed on S, that represents the elastic part of the macroscopic strain. The plastic energy depends only on the dislocation measure μ, which is coupled to the plastic part A of the macroscopic strain through the relation $\mu = \operatorname{Curl} A$. The contributions of elastic energy and plastic energy are decoupled in the Γ-limit $\mathcal{F}$, due to the fact that S and A live on different scales: $\sqrt{N_\varepsilon |\log \varepsilon|}$ and N_ε, respectively.

Indeed this is the main difference with the energy regime $N_\varepsilon \approx |\log \varepsilon|$ studied in [30], where S and A live on the same scale $|\log \varepsilon|$. In their work the authors deduce a macroscopic energy that has the same structure of $\mathcal{F}$, but in which the contributions of elastic energy and plastic energy are coupled by the relation $\mu = \operatorname{Curl} \beta$, where $\beta = S + A$ represents the whole macroscopic strain.

Once the Γ-limit $\mathcal{F}$ is obtained, we impose a piecewise constant Dirichlet boundary condition on A, and minimise $\mathcal{F}$ under such constraint. In Theorem 4.20 we prove that $\mathcal{F}$ admits piecewise constant minimisers, of the form

$$\hat{A} = \sum_{i=1}^{k} A_i \, \chi_{\Omega_i} \,,$$

where the A_is are antisymmetric matrices and $\{\Omega_i\}$ is a Caccioppoli partition of Ω. We interpret $\hat{A}$ as a linearised polycrystal, with Ω_i representing a single grain having orientation A_i. This interpretation is motivated by the fact that antisymmetric matrices can be considered as infinitesimal rotations. The (linear) energy corresponding to $\hat{A}$ can be seen as a linearised version of the Read-Shockley formula for small angle tilt grain boundaries, i.e.,

$$E = E_0\,\theta(1 + |\log\theta|)\,, \tag{4.132}$$

where $E_0 > 0$ is a constant depending only on the material and θ is the angle formed by two grains. Indeed, the Read-Shockley formula is obtained in [55] by computing the elastic energy for an evenly spaced array of $1/\varepsilon$ dislocations at the grain boundaries. Our energy regime accounts only for $N_\varepsilon \ll 1/\varepsilon$ dislocations, therefore we do not have enough dislocations to cause rotations between grains. Nevertheless we still observe polycrystalline structures, but the rotation angle between grains is infinitesimal.

Recently Lauteri and Luckhaus [35] obtained, by scaling arguments, the Read-Shockley formula (4.132) starting from a non-linear energy. It would be interesting to understand if our Γ-limit can be deduced from their model as the angle θ between grains tends to zero.

Another natural question is whether the minimiser $\hat{A}$ is unique, or at least if all the minimisers are piece-wise constant. We suspect that in general, by enforcing piece-wise constant boundary conditions, all minimisers are piece-wise constant. However it is not clear how to obtain this rigidity result.

One more question is deducing our Γ-limit $\mathcal{F}$ by starting from a nonlinear energy computed on small deformations $v = x + \varepsilon u$, in the energy regime $N_\varepsilon \gg |\log\varepsilon|$. A similar analysis was already performed in [45], where the authors derive the Γ-limit obtained in [30] starting from a nonlinear energy, under the assumption that $N_\varepsilon \approx |\log\varepsilon|$. It seems possible to adapt the techniques used in [45] to our case. This research direction is currently under investigation by the authors.

A further step forward in our analysis should be the following: in this paper the formation of polycrystalline structure is driven by boundary conditions; it would be interesting to replace them by forcing terms. For instance, bulk forces in competition with the surface energy at grain boundaries should result in polycrystals exhibiting some intrinsic length scale. This is the case of semi-coherent interfaces, separated by periodic nets of dislocations (see [22]).

Part II

Microgeometries in Composites

Chapter 5

Critical lower integrability for solutions to elliptic equations

5.1 Introduction

In this chapter we will present the results obtained in [21]. Let $\Omega \subset \mathbb{R}^2$ be a bounded open domain and let $\sigma \in L^\infty(\Omega; \mathbb{M}^{2\times 2})$ be *uniformly elliptic*, i.e.,

$$\sigma\xi \cdot \xi \geq \lambda |\xi|^2 \text{ for every } \xi \in \mathbb{R}^2 \text{ and for a.e. } x \in \Omega,$$

for some $\lambda > 0$. We study the gradient integrability of distributional solutions $u \in W^{1,1}(\Omega)$ to

$$\operatorname{div}(\sigma \nabla u) = 0 \quad \text{in} \quad \Omega, \tag{5.1}$$

in the case when $\sigma \in L^\infty(\Omega; \{\sigma_1, \sigma_2\})$, that is,

$$\sigma = \chi_{E_1}\sigma_1 + \chi_{E_2}\sigma_2\,, \tag{5.2}$$

where σ_1, σ_2 are 2×2 constant elliptic matrices, and $\{E_1, E_2\}$ is a measurable partition of Ω.

As already discussed in the Introduction, Ω represents a two-dimensional section of a composite material obtained by mixing two materials with different *electric conductivities* σ_1 and σ_2. The function σ defined by (5.2) is called a *two-phase conductivity*. The partition $\{E_1, E_2\}$ represents the arrangement of the two phases within the composite. Under these assumptions, the *electric field* ∇u will then solve (5.1). We are interested in studying the integrability properties of ∇u, that are determined by the geometry induced by $\{E_1, E_2\}$ on Ω.

The study of the integrability properties of ∇u relies on this fundamental result by Astala [4]: there exist exponents q and p, with $1 < q < 2 < p$, such that if $u \in W^{1,q}(\Omega)$ is solution to (5.1), then $\nabla u \in L^p_{\text{weak}}(\Omega; \mathbb{R}^2)$ (see Section 5.3.3 for more details on weak L^p spaces). In [48] the optimal exponents p and q have been characterised for every pair of elliptic matrices σ_1 and σ_2. Denoting by p_{σ_1,σ_2} and q_{σ_1,σ_2} such exponents, whose precise formulas are recalled in Section 5.2, we summarise the result of [48] in the following theorem.

Theorem 5.1. *[48, Theorem 1.4 and Proposition 4.2] Let $\sigma_1, \sigma_2 \in \mathbb{M}^{2\times 2}$ be elliptic.*

(i) If $\sigma \in L^\infty(\Omega; \{\sigma_1, \sigma_2\})$ and $u \in W^{1,q_{\sigma_1,\sigma_2}}(\Omega)$ solves (5.1), then $\nabla u \in L^{p_{\sigma_1,\sigma_2}}_{\text{weak}}(\Omega; \mathbb{R}^2)$.

(ii) There exists $\bar\sigma \in L^\infty(\Omega; \{\sigma_1, \sigma_2\})$ and a weak solution $\bar u \in W^{1,2}(\Omega)$ to (5.1) with $\sigma = \bar\sigma$, satisfying affine boundary conditions and such that $\nabla \bar u \notin L^{p_{\sigma_1,\sigma_2}}(\Omega; \mathbb{R}^2)$.

Theorem 5.1 proves the optimality of the upper exponent p_{σ_1,σ_2}. The objective of our paper [21] is to complement this result by proving the optimality of the lower exponent q_{σ_1,σ_2}. As shown in [48] (and recalled in Section 5.2), there is no loss of generality in assuming that

$$\sigma_1 = \operatorname{diag}(1/K, 1/S_1), \quad \sigma_2 = \operatorname{diag}(K, S_2), \tag{5.3}$$

with

$$K > 1 \qquad \text{and} \qquad \frac{1}{K} \le S_j \le K\,, \quad j = 1, 2\,. \tag{5.4}$$

Thus it suffices to show optimality for this class of coefficients, for which the exponents p_{σ_1,σ_2} and q_{σ_1,σ_2} read as

$$q_{\sigma_1,\sigma_2} = \frac{2K}{K+1}, \quad p_{\sigma_1,\sigma_2} = \frac{2K}{K-1}. \tag{5.5}$$

Our main result is the following.

Theorem 5.2. *Let σ_1, σ_2 be defined by (5.3) for some $K > 1$ and $S_1, S_2 \in [1/K, K]$. There exist coefficients $\sigma_n \in L^\infty(\Omega; \{\sigma_1; \sigma_2\})$, exponents $p_n \in \left[1, \frac{2K}{K+1}\right]$, functions $u_n \in W^{1,1}(\Omega)$ such that*

$$
\begin{cases} \operatorname{div}(\sigma_n \nabla u_n) = 0 & in \quad \Omega\,, \\ u_n(x) = x_1 & on \quad \partial\Omega\,, \end{cases} \tag{5.6}
$$

$$
\nabla u_n \in L^{p_n}_{\mathrm{weak}}(\Omega;\mathbb{R}^2), \quad p_n \to \frac{2K}{K+1}, \tag{5.7}
$$

$$
\nabla u_n \notin L^{\frac{2K}{K+1}}(\Omega;\mathbb{R}^2). \tag{5.8}
$$

In particular $u_n \in W^{1,q}(\Omega)$ *for every* $q < p_n$*, but* $\int_\Omega |\nabla u_n|^{\frac{2K}{K+1}}\,dx = \infty$.

Theorem 5.2 was proved in [5] in the case of isotropic coefficients, namely for $\sigma_1 = \frac{1}{K}I$ and $\sigma_2 = KI$. More precisely, in [5] the authors obtain a slightly stronger result by constructing a single coefficient $\sigma \in \{KI, \frac{1}{K}I\}$ and a single function u that satisfies the associated elliptic equation and is such that $\nabla u \in L^{\frac{2K}{K+1}}_{\mathrm{weak}}(\Omega;\mathbb{R}^2)$, but $\nabla u \notin L^{\frac{2K}{K+1}}(\Omega;\mathbb{R}^2)$. We follow the method developed in [5], which relies on convex integration as used in [46], and provides an explicit construction of the sequence u_n. The adaptation of such method to the present context turns out to be non-trivial due to the anisotropy of the coefficients (see Remark 5.14). It is not clear how to modify the construction in order to get a stronger result as in [5].

Convex integration is a method to solve differential inclusions of the form

$$
\nabla f(x) \in T \quad \text{a.e. in} \quad \Omega\,, \tag{5.9}
$$

where $f\colon \Omega \to \mathbb{R}^2$ and $T \subset \mathbb{M}^{2\times 2}$ is a fixed closed set of matrices. In order to prove Theorem 5.2 we first rewrite (5.1) as a differential inclusion, defining an appropriate set T (see Lemma 5.6), and then proceed by convex integration. The functions u and f will be integrable with the same exponent. Adapting the constructions of [5], in Lemma 5.12 we construct a sequence of laminates (see Definition 5.4) with the desired integrability properties. These are called *staircase laminates*, and will be supported in an appropriate set. The next step is to construct, for every small $\delta > 0$, a piecewise affine function f that solves the differential inclusion (5.9) up to an arbitrarily small L^∞ error, and such that

$$
\nabla f \in L^p_{\mathrm{weak}}(\Omega;\mathbb{M}^{2\times 2})\,, \quad p \in \left(\frac{2K}{K+1} - \delta, \frac{2K}{K+1}\right]\,, \quad \nabla f \notin L^{\frac{2K}{K+1}}(\Omega;\mathbb{M}^{2\times 2})\,.
$$

This is done in Proposition 5.15, by repeatedly applying Lemma 5.12 and Proposition 5.5. Loosely speaking, the idea of the proof is that, thanks to Proposition 5.5, we are able to construct f in a way that ∇f is close to the points of the support of the laminate given by Lemma 5.12. Therefore ∇f behaves asymptotically like the staircase laminate. Finally, in Theorem 5.16, we remove the L^∞ error introduced in Proposition 5.15, by means of a standard argument, obtaining the sequence u_n of Theorem 5.2.

5.2 Connection with the Beltrami equation and explicit formulas for the optimal exponents

For the reader's convenience we recall in this section how to reduce to the case (5.3) starting from any pair of matrices σ_1, σ_2. We will also give the explicit formulas for p_{σ_1,σ_2} and q_{σ_1,σ_2}.

It is well-known that a solution $u \in W^{1,q}_{loc}(\Omega)$, $q \geq 1$, to the elliptic equation (5.1) can be regarded as the real part of a complex map $f : \Omega \to \mathbb{C}$ which is a $W^{1,q}_{loc}(\Omega; \mathbb{C})$ solution to a *Beltrami equation*. Precisely, if v is such that

$$R^T_{\frac{\pi}{2}} \nabla v = \sigma \nabla u, \quad R_{\frac{\pi}{2}} := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{5.10}$$

then $f := u + iv$ solves the equation

$$f_{\bar{z}} = \mu\, f_z + \nu\, \overline{f_z} \quad \text{a.e. in } \Omega\,, \tag{5.11}$$

where the so called complex dilatations μ and ν, both belonging to $L^\infty(\Omega; \mathbb{C})$, are given by

$$\mu = \frac{\sigma_{22} - \sigma_{11} - i(\sigma_{12} + \sigma_{21})}{1 + \mathrm{Tr}\ \sigma + \det \sigma}\,, \quad \nu = \frac{1 - \det \sigma + i(\sigma_{12} - \sigma_{21})}{1 + \mathrm{Tr}\ \sigma + \det \sigma}\,, \tag{5.12}$$

and satisfy the ellipticity condition

$$\| |\mu| + |\nu| \|_{L^\infty} < 1\,. \tag{5.13}$$

The ellipticity (5.13) is often expressed in a different form. Indeed, it implies that there exists $0 \leq k < 1$ such that $\| |\mu| + |\nu| \|_{L^\infty} \leq k < 1$ or equivalently that

$$\| |\mu| + |\nu| \|_{L^\infty} \leq \frac{K-1}{K+1}\,, \tag{5.14}$$

for some $K > 1$. Let us recall that weak solutions to (5.11), (5.14) are called K-quasiregular mappings. Furthermore, we can express σ as a function of μ, ν by inverting the algebraic system (5.12),

$$\sigma = \begin{pmatrix} \frac{|1-\mu|^2-|\nu|^2}{|1+\nu|^2-|\mu|^2} & \frac{2\Im(\nu-\mu)}{|1+\nu|^2-|\mu|^2} \\ \\ \frac{-2\Im(\nu+\mu)}{|1+\nu|^2-|\mu|^2} & \frac{|1+\mu|^2-|\nu|^2}{|1+\nu|^2-|\mu|^2} \end{pmatrix}. \tag{5.15}$$

Conversely, if f solves (5.11) with $\mu, \nu \in L^\infty(\Omega, \mathbb{C})$ satisfying (5.13), then its real part is a solution to the elliptic equation (5.1) with σ defined by (5.15). Notice that ∇f and ∇u enjoy the same integrability properties. Assume now that $\sigma : \Omega \to \{\sigma_1, \sigma_2\}$ is a two-phase elliptic coefficient and f is solution to (5.11)-(5.12). Abusing notation, we identify Ω with a subset of $\mathbb{R}^2$ and $f = u + iv$ with the real mapping $f = (u, v) : \Omega \to \mathbb{R}^2$. Then, as shown in [48], one can find matrices $A, B \in SL(2)$ (with $SL(2)$ denoting the set of invertible matrices with determinant equal to one) depending only on σ_1 and σ_2, such that, setting

$$\tilde{f}(x) := A^{-1} f(Bx), \tag{5.16}$$

one has that the function $\tilde{f}$ solves the new Beltrami equation

$$\tilde{f}_{\bar{z}} = \tilde{\mu}\, f_z + \tilde{\nu}\, \overline{\tilde{f}_z} \quad \text{a.e. in } B^{-1}(\Omega),$$

and the corresponding $\tilde{\sigma} : B(\Omega) \to \{\tilde{\sigma}_1, \tilde{\sigma}_2\}$ defined by (5.15) is of the form (5.3):

$$\tilde{\sigma}_1 = \operatorname{diag}(1/K, 1/S_1), \quad \tilde{\sigma}_2 = \operatorname{diag}(K, S_2), \quad K > 1, \quad S_1, S_2 \in [1/K, K].$$

The results in [4] and [52] imply that if $\tilde{f} \in W^{1,q}$, with $q \geq \frac{2K}{K+1}$, then $\nabla \tilde{f} \in L^{\frac{2K}{K-1}}_{\text{weak}}$; in particular, $\tilde{f} \in W^{1,p}$ for each $p < \frac{2K}{K-1}$. Clearly $\nabla \tilde{f}$ enjoys the same integrability properties as ∇f and ∇u.

Finally, we recall the formula for K which will yield the optimal exponents. Denote by D_1 and D_2 the determinant of the symmetric part of σ_1 and σ_2 respectively,

$$D_i := \det\left(\frac{\sigma_i + \sigma_i^T}{2}\right), \quad i = 1, 2,$$

and by $(\sigma_i)_{jk}$ the jk-entry of σ_i. Set

$$m := \frac{1}{\sqrt{D_1 D_2}}\left[(\sigma_2)_{11}(\sigma_1)_{22} + (\sigma_1)_{11}(\sigma_2)_{22} - \frac{1}{2}\Big((\sigma_2)_{12} + (\sigma_2)_{21}\Big)\Big((\sigma_1)_{12} + (\sigma_1)_{21}\Big)\right],$$

$$n := \frac{1}{\sqrt{D_1 D_2}}\left[\det \sigma_1 + \det \sigma_2 - \frac{1}{2}\Big((\sigma_1)_{21} - (\sigma_1)_{12}\Big)\Big((\sigma_2)_{21} - (\sigma_2)_{12}\Big)\right].$$

Then

$$K = \left(\frac{m + \sqrt{m^2 - 4}}{2} \right)^{\frac{1}{2}} \left(\frac{n + \sqrt{n^2 - 4}}{2} \right)^{\frac{1}{2}} . \tag{5.17}$$

Thus, for any pair of elliptic matrices $\sigma_1, \sigma_2 \in \mathbb{M}^{2\times 2}$, the explicit formula for the optimal exponents p_{σ_1,σ_2} and q_{σ_1,σ_2} are obtained by plugging (5.17) into (5.5).

5.3 Preliminaries

5.3.1 Convex integration

We denote by $\mathcal{M}(\mathbb{M}^{2\times 2})$ the set of signed Radon measures on $\mathbb{M}^{2\times 2}$ having finite mass. We refer to Section A.2 for more details. By Riesz's representation theorem (see Theorem A.8) we can identify $\mathcal{M}(\mathbb{M}^{2\times 2})$ with the dual of the space $C_0(\mathbb{M}^{m\times n})$, i.e, the space of continuous functions $f\colon \mathbb{M}^{m\times n} \to \mathbb{R}$ that vanish at infinity. Given $\nu \in \mathcal{M}(\mathbb{M}^{2\times 2})$ we define its *barycenter* as

$$\overline{\nu} := \int_{\mathbb{M}^{2\times 2}} A \, d\nu(A) .$$

We say that a map $f \in C(\overline{\Omega}; \mathbb{R}^2)$ is *piecewise affine* if there exists a countable family of pairwise disjoint open subsets $\Omega_i \subset \Omega$ with $|\partial\Omega_i| = 0$ and

$$\left| \Omega \setminus \bigcup_{i=1}^{\infty} \Omega_i \right| = 0 ,$$

such that f is affine on each Ω_i. Let $A, B \in \mathbb{M}^{2\times 2}$ and consider the following problem: find a piecewise affine Lipschitz map $f\colon \Omega \to \mathbb{R}^2$ such that

$$\begin{cases} \nabla f \in \{A, B\} & \text{a.e. in } \Omega , \\ f(x) = Cx & \text{on } \partial\Omega , \end{cases} \tag{5.18}$$

where $C := \lambda A + (1-\lambda)B$, for some $\lambda \in [0,1]$. We have already discussed this problem in Section 2.3 and saw that the boundary condition $f(x) = Cx$ on $\partial\Omega$ always forces rigidity, that is $f \equiv Cx$ on Ω (see Proposition 2.1). In this section we want to discuss the problem of *approximate solutions* to (5.18), that is, find a sequence of piecewise affine Lipschitz maps $f_n\colon \Omega \to \mathbb{R}^2$ such that

$$\begin{cases} \operatorname{dist}(\nabla f_n, \{A, B\}) \to 0 & \text{a.e. in } \Omega , \\ f_n(x) = Cx & \text{on } \partial\Omega . \end{cases} \tag{5.19}$$

We recall that the matrices A and B are said to be *rank-one connected* if

$$\mathrm{rank}(B - A) = 1\,.$$

In this case it is possible to construct non-trivial solutions to (5.19) by means of convex integration, as stated in the following proposition (see [42, Lemma 5.1]).

Proposition 5.3. *Let* $A, B \in \mathbb{M}^{2\times 2}$ *be such that* $\mathrm{rank}(B - A) = 1$ *and assume that* $C = \lambda A + (1-\lambda)B$ *for some* $\lambda \in (0,1)$. *Let* $\Omega \subset \mathbb{R}^2$ *be a bounded open set and* $0 < \delta < |A - B|/2$. *There exists a piecewise affine Lipschitz map* $f \colon \Omega \to \mathbb{R}^2$ *such that*

(i) $f(x) = Cx$ *on* $\partial\Omega$,

(ii) $[f - Cx]_{C^0(\overline{\Omega})} < \delta$,

(iii) $|\{x \in \Omega : \ |\nabla f(x) - A| < \delta\}| = \lambda|\Omega|$,

(iv) $|\{x \in \Omega : \ |\nabla f(x) - B| < \delta\}| = (1-\lambda)|\Omega|$,

(v) $\mathrm{dist}(\nabla f, \{A, B\}) < \delta$ *a.e. in* Ω.

In particular, there exists a sequence of piecewise affine Lipschitz maps $f_n \colon \Omega \to \mathbb{R}^2$ *satisfying* (5.19).

We remark that this result holds for matrices in $\mathbb{M}^{m\times n}$ with C^α approximation, for a fixed $\alpha \in (0,1)$ (see [5, Lemma 2.1]). However we choose to present the case of $\mathbb{M}^{2\times 2}$ with C^0 approximation, as the proof is simpler and gives all the geometric ideas necessary to build such functions.

Proof. The proof is divided into two steps. First we build a function $\tilde{f}$ that satisfies (i)-(v) in a particular domain W. Then, by means of the Vitali covering theorem, we scale and replicate $\tilde{f}$ throughout the whole Ω.

Note that, by an affine change of variables, we can assume that $C = 0$ and $B - A = a \otimes e_2$ for some $a \in \mathbb{R}^2$ with $|a| = 1$. Therefore

$$\lambda A + (1-\lambda)B = 0, \quad A = -(1-\lambda)a \otimes e_2, \quad B = \lambda a \otimes e_2\,.$$

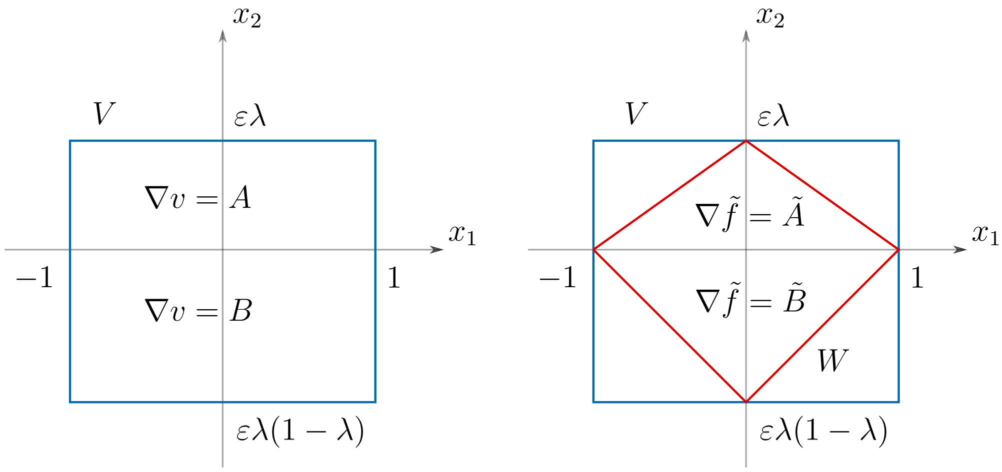


Figure 5.1: Left: the blue square represents V. The map v satisfies (ii)-(v) in V, but v does not vanish on the vertical sides of V. Right: the red polytope represents W. The map $\tilde{f}$ satisfies (i)-(v) in W.

Step 1. Let $\varepsilon > 0$ be such that $\varepsilon\lambda(1-\lambda) < \delta$ and define

$$V := (-1, 1) \times (\varepsilon(\lambda - 1), \varepsilon\lambda)\,,$$

and the scalar function

$$s(t) := \varepsilon\lambda(1-\lambda) + \begin{cases} -(1-\lambda)t & \text{if } t \geq 0\,, \\ \lambda t & \text{if } t < 0\,. \end{cases}$$

Also define the piecewise affine Lipschitz map $v\colon V \to \mathbb{R}^2$ as $v(x) := as(x_2)$, so that, explicitly,

$$v(x) := \varepsilon\lambda(1-\lambda)a + \begin{cases} -(1-\lambda)ax_2 & \text{if } x_2 \geq 0\,, \\ \lambda a x_2 & \text{if } x_2 < 0\,. \end{cases}$$

Therefore $\nabla v \in \{A, B\}$, since $\nabla v = A$ if $x_2 \geq 0$ and $\nabla v = B$ if $x_2 < 0$. Also note that

$$|\{x \in V \colon \nabla v = A\}| = \lambda |V|\,, \quad |\{x \in V \colon \nabla v = B\}| = (1-\lambda)|V|\,,$$

because $|V| = 2\varepsilon$. Moreover $|v| \leq \varepsilon\lambda(1-\lambda) < \delta$. Hence, v satisfies (ii)-(v) with $\Omega = V$. However v does not satisfy (i), since $v = 0$ for $x_2 = \varepsilon(\lambda - 1)$ and $x_2 = \varepsilon\lambda$, (see left picture in Figure 5.1), but v does not vanish on the whole ∂V. Therefore, the idea is to suitably perturb v so that also (i) holds.

To this end, define the piecewise affine map $h\colon \mathbb{R}^2 \to \mathbb{R}$ as $h(x) := \varepsilon\lambda(1-\lambda)|x_1|$ and $w\colon V \to \mathbb{R}$ as $w(x) := s(x_2) - h(x)$. Finally, define $\tilde{f}\colon V \to \mathbb{R}^2$ as

$$\tilde{f}(x) := aw(x) = v(x) - ah(x)\,. \tag{5.20}$$

It is clear that $\tilde{f}$ is piecewise affine Lipschitz. Set

$$W := \{x \in V\colon w(x) > 0\}\,, \tag{5.21}$$

so that by continuity $\tilde{f} = 0$ on ∂W. Notice that W is a polytope contained in V, as displayed in the right picture in Figure 5.1. Therefore $\tilde{f}$ satisfies (i) in W. Also notice that $|\tilde{f}| < \delta$ so that (ii) holds as well. Define $W^+ := W \cap \{x \geq 0\}$, $W^- := W \cap \{x < 0\}$ and remark that

$$|W^+| = \lambda|W| \quad \text{and} \quad |W^-| = (1-\lambda)|W|. \tag{5.22}$$

By direct calculation,

$$\nabla\tilde{f}(x) = \chi_{W^+}\tilde{A} + \chi_{W^-}\tilde{B}\,,$$

where

$$\tilde{A} := A - \operatorname{sign}(x_1)\,\varepsilon\lambda(1-\lambda)a \otimes e_1\,, \quad \tilde{B} := B - \operatorname{sign}(x_1)\,\varepsilon\lambda(1-\lambda)a \otimes e_1\,,$$

so that $\tilde{A}$ and $\tilde{B}$ lie in a δ-neighbourhood of A and B respectively. Hence

$$\{x \in \Omega\colon |\nabla\tilde{f}(x) - A| < \delta\} = W^+\,, \quad \{x \in \Omega\colon |\nabla\tilde{f}(x) - A| < \delta\} = W^+$$

and (iii)-(iv) follow by (5.22). Notice that, since $\delta < |B-A|/2 = 1/2$, also (v) follows.

Step 2. Let W be as in (5.21). By the Vitali covering theorem, there exist points $b_i \in \mathbb{R}^2$ and $0 < r_i < 1$, $i \in \mathbb{N}$, such that the sets

$$\Omega_i := b_i + r_i W$$

are pairwise disjoint and satisfy

$$\left|\Omega \setminus \bigcup_i \Omega_i\right| = 0\,.$$

Define the function $f\colon \Omega \to \mathbb{R}^2$ as

$$f(x) := r_i\tilde{f}\left(\frac{x-b_i}{r_i}\right) \quad \text{for} \quad x \in \Omega_i\,,$$

where $\tilde{f}$ is as in (5.20). Clearly f is piecewise affine Lipschitz and $f = 0$ on $\partial\Omega$, since $\tilde{f} = 0$ on ∂W. Moreover $|f| < \delta$ because $r_i < 1$ and $|\tilde{f}| < \delta$. Finally,

$$\nabla f(x) = \nabla \tilde{f}\left(\frac{x - b_i}{r_i}\right) \quad \text{for} \quad x \in \Omega_i \,,$$

therefore we have

$$\nabla f = \chi_{\Omega^+}\tilde{A} + \chi_{\Omega^-}\tilde{B} \,,$$

where $\Omega^+ := \cup_i \Omega_i^+$, $\Omega^- := \cup_i \Omega_i^-$, with $\Omega_i^+ := b_i + r_i W^+, \Omega_i^- := b_i + r_i W^-$. Hence

$$\{x \in \Omega \colon |\nabla f - A| < \delta\} = \Omega^+ \,, \quad \{x \in \Omega \colon |\nabla f - B| < \delta\} = \Omega^- \,,$$

and (iii)-(v) follow from (5.22). □

It is convenient to interpret Proposition 5.3 from the point of view of the gradient distribution of the map f. In order to do that, denote with $\mathcal{L}^2_\Omega$ the two dimensional normalised Lebesgue measure restricted to Ω, so that $\mathcal{L}^2_\Omega(U) = |U \cap \Omega|/|\Omega|$ for every Borel set $U \subset \mathbb{R}^2$. For a Lipschitz map $f \colon \Omega \to \mathbb{R}^2$ we can define the push-forward measure $\nabla f_\#(\mathcal{L}^2_\Omega)$ on $\mathbb{M}^{2\times 2}$ as

$$\nabla f_\#(\mathcal{L}^2_\Omega)(V) := \mathcal{L}^2_\Omega((\nabla f)^{-1}(V)) \quad \text{for every Borel set } V \subset \mathbb{M}^{2\times 2} \,.$$

The measure $\nabla f_\#(\mathcal{L}^2_\Omega)$ is called the *gradient distribution* of f (see e.g. [24]). Now let f_n be the sequence given by Proposition 5.3, where we set $\delta_n := 1/n$. As a corollary of the proof, it is immediate to see that

$$\nu_n := (\nabla f_n)_\#(\mathcal{L}^2_\Omega) = \lambda \delta_{\tilde{A}_n} + (1-\lambda)\delta_{\tilde{B}_n}$$

with $\operatorname{rank}(\tilde{B}_n - \tilde{A}_n) = 1$ and $\tilde{A}_n \to A$, $\tilde{B}_n \to B$. The measures ν_n encode all the relevant properties of f_n, including the boundary condition $f_n = Cx$, as $\bar{\nu}_n = \lambda \tilde{A}_n + (1-\lambda)\tilde{B}_n = C$, and the oscillating behaviour of ∇f_n, since

$$\nu_n \overset{*}{\rightharpoonup} \nu := \lambda \delta_A + (1-\lambda)\delta_B \text{ weakly in } \mathcal{M}(\mathbb{M}^{2\times 2}) \,. \tag{5.23}$$

Moreover we have

$$\frac{1}{|\Omega|}\int_\Omega |\nabla f_n|^p \, dx = \int_{\mathbb{M}^{2\times 2}} |\lambda|^p \, d\nu_n(\lambda) \,, \tag{5.24}$$

so also the integrability properties of ∇f_n can be described through ν_n. A probability measure ν of the form (5.23), with $\operatorname{rank}(B - A) = 1$ and $\lambda \in [0,1]$, is called a *laminate of first order* (see also [42, 46, 51, 34]).

Since Proposition 5.3 yields piecewise affine maps, we can iterate the construction by modifying f in the sets where it is affine. For example we could decompose B as

$$B = \lambda' C_1 + (1-\lambda')C_2\,,$$

with $\lambda' \in (0,1)$ and $\mathrm{rank}(C_2 - C_1) = 1$. Then in the open set

$$\{x \in \Omega : \, |\nabla f(x) - B| < \delta\}\,,$$

we can replace f with a piecewise affine map (by applying Proposition 5.3) whose gradient oscillates on a much smaller scale, say δ^2, between neighbourhoods of C_1 and C_2. Therefore we will have

$$|\{x \in \Omega : \, |\nabla f(x) - C_1| < \delta\}| = (1-\lambda)\lambda'|\Omega|\,,$$
$$|\{x \in \Omega : \, |\nabla f(x) - C_2| < \delta\}| = (1-\lambda)(1-\lambda')|\Omega|\,.$$

The gradient distribution of the new map f is therefore given by replacing δ_B in (5.23) with the new laminate of first order $\lambda'\delta_{C_1} + (1-\lambda')\delta_{C_2}$, obtaining

$$\nu' := \lambda\delta_A + (1-\lambda)(\lambda'\delta_{C_1} + (1-\lambda')\delta_{C_2})\,.$$

Notice that ν' is still a probability measure and $\bar{\nu}' = \bar{\nu} = C$. This iterative procedure motivates the following definition.

Definition 5.4. The family of *laminates of finite order* $\mathcal{L}(\mathbb{M}^{2\times 2})$ is the smallest family of probability measures in $\mathcal{M}(\mathbb{M}^{2\times 2})$ satisfying the following conditions:

(i) $\delta_A \in \mathcal{L}(\mathbb{M}^{2\times 2})$ for every $A \in \mathbb{M}^{2\times 2}$;

(ii) assume that $\sum_{i=1}^N \lambda_i\delta_{A_i} \in \mathcal{L}(\mathbb{M}^{2\times 2})$ and $A_1 = \lambda B + (1-\lambda)C$ with $\lambda \in [0,1]$ and $\mathrm{rank}(B - C) = 1$. Then the probability measure

$$\lambda_1(\lambda\delta_B + (1-\lambda)\delta_C) + \sum_{i=2}^N \lambda_i\delta_{A_i}$$

is also contained in $\mathcal{L}(\mathbb{M}^{2\times 2})$.

The process of obtaining new measures via (ii) is called *splitting*.

By repeatedly applying the iterative argument stated above, we can obtain, given a laminate of finite order ν, a piecewise affine function f satisfying the piecewise affine boundary condition $f(x) = \bar{\nu}x$ on $\partial\Omega$, and whose gradient distribution is given by ν. More precisely, we can prove the following result (that we state with C^α approximation. See [5, Proposition 2.3] for a proof).

Proposition 5.5. *Let $\nu = \sum_{i=1}^N \alpha_i \delta_{A_i} \in \mathcal{L}(\mathbb{M}^{2\times 2})$ be a laminate of finite order with barycenter $\overline{\nu} = A$, that is $A = \sum_{i=1}^N \alpha_i A_i$ with $\sum_{i=1}^N \alpha_i = 1$. Let $\Omega \subset \mathbb{R}^2$ be a bounded open set, $\alpha \in (0,1)$ and $0 < \delta < \min |A_i - A_j|/2$. Then there exists a piecewise affine Lipschitz map $f \colon \Omega \to \mathbb{R}^2$ such that*

(i) $f(x) = Ax$ *on* $\partial\Omega$,

(ii) $[f - A]_{C^\alpha(\overline{\Omega})} < \delta$,

(iii) $|\{x \in \Omega : \ |\nabla f(x) - A_i| < \delta\}| = \alpha_i |\Omega|$,

(iv) $\operatorname{dist}(\nabla f, \operatorname{supp} \nu) < \delta$ *a.e. in* Ω.

5.3.2 Conformal coordinates

For every real matrix $A \in \mathbb{M}^{2\times 2}$,

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix},$$

we write $A = (a_+, a_-)$, where $a_+, a_- \in \mathbb{C}$ denote its conformal coordinates. By identifying any vector $v = (x, y) \in \mathbb{R}^2$ with the complex number $v = x + iy$, conformal coordinates are defined by the identity

$$Av = a_+ v + a_- \overline{v} \, . \tag{5.25}$$

Here $\overline{v}$ denotes the complex conjugation. From (5.25) we have the relations

$$a_+ = \frac{a_{11} + a_{22}}{2} + i\,\frac{a_{21} - a_{12}}{2}\,, \qquad a_- = \frac{a_{11} - a_{22}}{2} + i\,\frac{a_{21} + a_{12}}{2}\,, \tag{5.26}$$

and, conversely,

$$\begin{aligned} a_{11} &= \Re a_+ + \Re a_- \,, & a_{12} &= -\Im a_+ + \Im a_- \,, \\ a_{21} &= \Im a_+ + \Im a_- \,, & a_{22} &= \Re a_+ - \Re a_- \,. \end{aligned} \tag{5.27}$$

Here $\Re z$ and $\Im z$ denote the real and imaginary part of $z \in \mathbb{C}$ respectively. We recall that

$$AB = (a_+ b_+ + a_- \overline{b}_-, a_+ b_- + a_- \overline{b}_+)\,, \tag{5.28}$$

and $\operatorname{Tr} A = 2\Re a_+$. Moreover

$$\begin{aligned} \det(A) &= |a_+|^2 - |a_-|^2 \,, \\ |A|^2 &= 2\,|a_+|^2 + 2\,|a_-|^2 \,, \\ \|A\| &= |a_+| + |a_-| \,, \end{aligned} \tag{5.29}$$

where $|A|$ and $\|A\|$ denote the Hilbert-Schmidt and the operator norm, respectively.

We also define the second complex dilatation of the map A as

$$\mu_A := \frac{a_-}{\overline{a}_+} \,, \tag{5.30}$$

and the distortion

$$K(A) := \left| \frac{1 + |\mu_A|}{1 - |\mu_A|} \right| = \frac{\|A\|^2}{|\det(A)|} \,. \tag{5.31}$$

The last two quantities measure how far A is from being conformal. Following the notation introduced in [5], we define

$$E_\Delta := \{A = (a, \mu\,\overline{a}) : \; a \in \mathbb{C}, \; \mu \in \Delta\} \tag{5.32}$$

for a set $\Delta \subset \mathbb{C} \cup \{\infty\}$; namely, E_Δ is the set of matrices with the second complex dilatation belonging to Δ. In particular E_0 and E_∞ denote the set of conformal and anti-conformal matrices respectively. From (5.28) we have that E_Δ is invariant under precomposition by conformal matrices, that is

$$E_\Delta = E_\Delta A \qquad \text{for every} \qquad A \in E_0 \setminus \{0\} \,. \tag{5.33}$$

5.3.3 Weak L^p spaces

We recall the definition of weak L^p spaces. Let $f \colon \Omega \to \mathbb{R}^2$ be a Lebesgue measurable function. Define the distribution function of f as

$$\lambda_f \colon (0, \infty) \to [0, \infty] \quad \text{with} \quad \lambda_f(t) := |\{x \in \Omega : \; |f(x)| > t\}| \,.$$

Let $1 \leq p < \infty$, then the following formula holds (see e.g. [27, Ch 6.4])

$$\int_\Omega |f(x)|^p \, dx = p \int_0^\infty t^{p-1} \lambda_f(t) \, dt \,. \tag{5.34}$$

Define the quantity

$$[f]_p := \left(\sup_{t>0} t^p \lambda_f(t) \right)^{1/p}$$

and the weak L^p space as

$$L^p_{\text{weak}}(\Omega;\mathbb{R}^2) := \left\{ f\colon \Omega \to \mathbb{R}^2 : \ f \ \text{ measurable}, \ [f]_p < \infty \right\} .$$

L^p_{weak} is a topological vector space and by Chebyshev's inequality we have $[f]_p \leq \|f\|_{L^p}$. In particular this implies $L^p \subset L^p_{\text{weak}}$. Moreover $L^p_{\text{weak}} \subset L^q$ for every $q < p$.

5.4 Proof of Theorem 5.2

For the rest of this chapter, σ_1 and σ_2 are as in (5.3)-(5.4) and $\Omega \subset \mathbb{R}^2$ is a bounded domain. We start by rewriting (5.1) as a differential inclusion. To this end, define the sets

$$T_1 := \left\{ \begin{pmatrix} x & -y \\ S_1^{-1}\, y & K^{-1}\, x \end{pmatrix} \ : \ x, y \in \mathbb{R} \right\} , \quad T_2 := \left\{ \begin{pmatrix} x & -y \\ S_2\, y & K\, x \end{pmatrix} \ : \ x, y \in \mathbb{R} \right\} . \tag{5.35}$$

Lemma 5.6. *Let $\sigma \in L^\infty(\Omega; \{\sigma_1, \sigma_2\})$. A function $u \in W^{1,1}(\Omega)$ is a distributional solution to (5.1) if and only if there exists a stream function $v \in W^{1,1}(\Omega)$ such that $f := (u, v)\colon \Omega \to \mathbb{R}^2$ satisfies*

$$\nabla f \in T_1 \cup T_2 \quad \textit{a.e. in} \ \ \Omega \, . \tag{5.36}$$

Proof. Since Ω is simply connected, the field $\sigma \nabla u$ is divergence free if and only if

$$\sigma \nabla u = R_{\frac{\pi}{2}} \nabla v \quad \text{a.e. in } \Omega \, , \tag{5.37}$$

for some $v \in W^{1,1}(\Omega)$. If we set $f := (u, v)$, it is immediate to check that (5.36) holds. Conversely, if $f = (f^1, f^2)$ is such that $\nabla f \in T_1 \cup T_2$, define

$$E_1 := \{ x \in \Omega : \ \nabla f(x) \in T_1 \} , \quad E_2 := \{ x \in \Omega : \ \nabla f(x) \in T_2 \} ,$$

and set $u := f^1$, $v := f^2$, $\sigma := \sigma_1 \, \chi_{E_1} + \sigma_2 \, \chi_{E_2}$. With these definitions (5.37) holds, and u satisfies (5.1). □

In order to solve the differential inclusion (5.36), it is convenient to use (5.26) and write our target sets in conformal coordinates:

$$T_1 = \{ (a, d_1(\overline{a})) \ : \ a \in \mathbb{C} \} , \qquad T_2 = \{ (a, -d_2(\overline{a})) \ : \ a \in \mathbb{C} \} , \tag{5.38}$$

where the operators $d_j\colon \mathbb{C} \to \mathbb{C}$ are defined as

$$d_j(a) := k\,\Re a + i\,s_j\,\Im a\,, \quad \text{with} \quad k := \frac{K-1}{K+1} \quad \text{and} \quad s_j := \frac{S_j - 1}{S_j + 1}\,. \tag{5.39}$$

Conditions (5.4) imply

$$0 < k < 1 \quad \text{and} \quad -k \le s_j \le k \quad \text{for} \quad j = 1, 2\,. \tag{5.40}$$

Introduce the quantities

$$s := \frac{s_1 + s_2}{2} = \frac{S_1 S_2 - 1}{(1 + S_1)(1 + S_2)} \tag{5.41}$$

$$S := \frac{1 + s}{1 - s} = \frac{S_1 + S_2 + 2S_1 S_2}{2 + S_1 + S_2}\,. \tag{5.42}$$

By (5.40) we have

$$-k \le s \le k \qquad \text{and} \qquad \frac{1}{K} \le S \le K\,. \tag{5.43}$$

We distinguish three cases.

1. Case $s > 0$ **(corresponding to** $S > 1$**).** We study this case in Section 5.5, where we generalise the methods used in [5, Section 3.2]. Observe that this case includes the one studied in [5]. Indeed, for $s = k$ one has that $s_1 = s_2 = k$ and the target sets (5.38) become

$$T_1 = E_k = \{(a, k\overline{a}) \,:\, a \in \mathbb{C}\}\,, \qquad T_2 = E_{-k} = \{(a, -k\overline{a}) \,:\, a \in \mathbb{C}\}\,,$$

where $E_{\pm k}$ are defined in (5.32). We remark that, in this particular case, the construction provided in Section 5 coincides with the one given in [5, Section 3.2].

2. Case $s < 0$ **(corresponding to** $S < 1$**).** This case can be reduced to the previous one. Indeed, if we introduce $\hat{s}_j := -s_j$, $\hat{s} := (\hat{s}_1 + \hat{s}_2)/2 > 0$ and the operators $\hat{d}_j(a) := k\,\Re a + i\,\hat{s}_j\,\Im a$ then the target sets (5.38) read as

$$T_1 = \{(a, \hat{d}_1(a)) :\, a \in \mathbb{C}\}, \qquad T_2 = \{(a, -\hat{d}_2(a)) :\, a \in \mathbb{C}\}.$$

This is the same as the previous case, since the absence of the conjugation does not affect the geometric properties relevant to the constructions of Section 5.5.

We notice that this case includes $s = -k$ for which the target sets become

$$T_1 = \{(a, ka) \,:\, a \in \mathbb{C}\}\,, \qquad T_2 = \{(a, -ka) \,:\, a \in \mathbb{C}\}\,.$$

We remark that in this case, (5.36) coincides with the classical Beltrami equation (see also [5, Remark 3.21]).

3. ***Case*** $s = 0$ **(corresponding to** $s_1 = -s_2$**,** $S_1 = 1/S_2$**)** This is a degenerate case, in the sense that the constructions provided in Section 5 for $s > 0$ are not well defined. Nonetheless, Theorem 5.2 still holds true. In fact, as already pointed out in [48, Section A.3], by an affine change of variables, the existence of a solution can be deduced by [5, Lemma 4.1,Theorem 4.14], where the authors prove the optimality of the lower critical exponent $\frac{2K}{K+1}$ for the solution of a system in non-divergence form. We remark that in this case Theorem 5.2 actually holds in the stronger sense of exact solutions, namely, there exists $u \in W^{1,1}(\Omega)$ solution to (5.6) and such that

$$\nabla u \in L^{\frac{2K}{K+1}}_{\mathrm{weak}}(\Omega;\mathbb{R}^2)\,, \quad \nabla u \notin L^{\frac{2K}{K+1}}(\Omega;\mathbb{R}^2)\,.$$

5.5 The case $s > 0$

In the present section we prove Theorem 5.2 under the hypothesis that the average s is positive, namely that

$$\begin{aligned} &0 < k < 1 \ \text{ and } \ -s_2 < s_1 \le s_2\,, \ \text{ with } \ 0 < s_2 \le k\,, \ \text{or} \\ &0 < k < 1 \ \text{ and } \ -s_1 < s_2 \le s_1\,, \ \text{ with } \ 0 < s_1 \le k\,. \end{aligned} \tag{5.44}$$

From (5.44), recalling definitions (5.39), (5.41), (5.42), we have

$$0 < s \le k\,, \qquad 1 < S \le K\,, \tag{5.45}$$

$$1/S_2 < S_1 \le S_2\,, \quad 1 < S_2 \le K\,, \quad \text{or} \quad 1/S_1 < S_2 \le S_1\,, \quad 1 < S_1 \le K\,. \tag{5.46}$$

In order to prove Theorem 5.2, we will solve the differential inclusion (5.36) by adapting the convex integration program developed in [5, Section 3.2] to the present context. As already pointed out in Section 5.1, the anisotropy of the coefficients σ_1, σ_2 poses some technical difficulties in the construction of the so-called staircase laminate, needed to obtain the desired approximate solutions. In fact, the anisotropy of σ_1, σ_2 translates into the lack of conformal invariance (in the sense of (5.33)) of the target sets (5.38), while the constructions provided in [5] heavily rely on the conformal invariance of the target set $E_{\{-k,k\}}$. We point out that the lack of conformal invariance was a source of difficulty in [48] as well, for the proof of the optimality of the upper exponent.

This section is divided as follows. In Section 5.5.1 we establish some geometric properties of rank-one lines in $\mathbb{M}^{2\times 2}$, that will be used in Section 5.5.2 for the construction of the staircase laminate. For every sufficiently small $\delta > 0$, such laminate allows us to define (in Proposition 5.15) a *piecewise affine* map f that solves the differential inclusion (5.36) up to an arbitrarily small L^∞ error. Moreover f will have the desired integrability properties (see (5.103)), that is,

$$\nabla f \in L^p_{\text{weak}}(\Omega; \mathbb{M}^{2\times 2}), \quad p \in \left(\frac{2K}{K+1} - \delta, \frac{2K}{K+1} \right], \quad \nabla f \notin L^{\frac{2K}{K+1}}(\Omega; \mathbb{M}^{2\times 2}).$$

Finally, in Theorem 5.16, we remove the L^∞ error introduced in Proposition 5.15, by means of a standard argument (see, e.g., [48, Theorem A.2]).

Throughout this section $c_K > 1$ will denote various constants depending on K, S_1 and S_2, whose precise value may change from place to place. The complex conjugation is denoted by $J := (0, 1)$ in conformal coordinates, i.e., $Jz = \overline{z}$ for $z \in \mathbb{C}$. Moreover, $R_\theta := (e^{i\theta}, 0) \in SO(2)$ denotes the counter clockwise rotation of angle $\theta \in (-\pi, \pi]$. Define the argument function

$$\arg z := \theta, \quad \text{where} \quad z = |z|e^{i\theta}, \quad \text{with} \quad \theta \in (-\pi, \pi].$$

Abusing notation we write $\arg R_\theta = \theta$. For $A = (a, b) \in \mathbb{M}^{2\times 2} \setminus \{0\}$ we set

$$\theta_A := -\arg(b - d_1(\overline{a})). \tag{5.47}$$

5.5.1 Properties of rank-one lines

In this section we will establish some geometric properties of rank-one lines in $\mathbb{M}^{2\times 2}$. Lemmas 5.8, 5.9 are generalisations of [5, Lemmas 3.14, 3.15] to our target sets (5.38). In Lemmas 5.10, 5.11 we will study certain rank-one lines connecting T to E_∞, that will be used in Section 5.5.2 to construct the staircase laminate.

Lemma 5.7. *Let $Q \in T_j$ with $j \in \{1, 2\}$ and T_j as in* (5.38). *Then*

$$\det Q > 0 \quad \textit{for} \quad Q \neq 0, \tag{5.48}$$

$$|s_j| \leq |\mu_Q| \leq k, \tag{5.49}$$

$$\max\{S_j, 1/S_j\} \leq K(Q) \leq K, \tag{5.50}$$

where μ_Q and $K(Q)$ are defined in (5.30) *and* (5.31) *respectively.*

Proof. Let $Q = (q, d_1(\overline{q})) \in T_1$. By (5.40) we have $|s_1||q| \leq |d_1(q)| \leq k|q|$ which readily implies (5.49) and

$$(1 - k^2)\,|q|^2 \leq \det(Q) \leq (1 - s_1^2)\,|q|^2 .$$

The last inequality implies (5.48). Finally $K(Q)$ is increasing with respect to $|\mu_Q| \in (0,1)$, therefore (5.50) follows from (5.49). The proof is analogous if $Q \in T_2$. $\square$

Lemma 5.8. *Let $A, B \in \mathbb{M}^{2\times 2}$ with $\det B \neq 0$ and $\det(B-A) = 0$, then*

$$|B| \leq \sqrt{2}\, K(B)\, |A|\,. \tag{5.51}$$

In particular, if $A \in \mathbb{M}^{2\times 2}$ and $Q \in T_j$, $j \in \{1,2\}$, are such that $\det(A-Q) = 0$, then

$$\operatorname{dist}(A, T_j) \leq |A - Q| \leq (1 + \sqrt{2}K)\operatorname{dist}(A, T_j)\,.$$

Proof. The first part of the statement is exactly like in [5, Lemma 3.14]. For the second part, one can easily adapt the proof of [5, Lemma 3.14] to the present context taking into account (5.48) and (5.50). For the reader's convenience we recall the argument. Let $A \in \mathbb{M}^{2\times 2}, Q \in T_1$ and $Q_0 \in T_1$ such that $\operatorname{dist}(A, T_1) = |A - Q_0|$. By (5.48), we can apply the first part of the lemma to $A - Q_0$ and $Q - Q_0$ to get

$$|Q - Q_0| \leq \sqrt{2}K(Q - Q_0)|A - Q_0| \leq \sqrt{2}K|A - Q_0|\,,$$

where the last inequality follows from (5.50), since $Q - Q_0 \in T_1$. Therefore

$$|A - Q| \leq |A - Q_0| + |Q - Q_0| \leq (1 + \sqrt{2}K)|A - Q_0| = (1 + \sqrt{2}K)\operatorname{dist}(A, T_1)\,.$$

The proof for T_2 is analogous. $\square$

Lemma 5.9. *Every $A = (a, b) \in \mathbb{M}^{2\times 2} \setminus \{0\}$ lies on a rank-one segment connecting T_1 and E_∞. Precisely, there exist matrices $Q \in T_1 \setminus \{0\}$ and $P \in E_\infty \setminus \{0\}$, with $\det(P - Q) = 0$, such that $A \in [Q, P]$. We have $P = tJR_{\theta_A}$ for some $t > 0$ and θ_A as in (5.47). Moreover, there exists a constant $c_K > 1$, depending only on K, S_1, S_2, such that*

$$\frac{1}{c_K}\,|A| \leq |P - Q|\,, |P|\,, |Q| \leq c_K\,|A|\,. \tag{5.52}$$

Proof. The proof can be deduced straightforwardly from the one of [5, Lemma 3.15]. We decompose any $A = (a, b)$ as

$$A = (a, d_1(\overline{a})) + \frac{1}{t}(0, tb - td_1(\overline{a})) = Q + \frac{1}{t}P_t\,,$$

with $Q \in T_1$ and $P_t \in E_\infty$. The matrices Q and P_t are rank-one connected if and only if $|a| = |d_1(\overline{a}) + t(b - d_1(\overline{a}))|$. Since $\det Q > 0$ for $Q \neq 0$, it is easy to see that there exists only one $t_0 > 0$ such that the last identity is satisfied. We then set $\rho := 1 + 1/t_0$ so that

$$A = \frac{1}{\rho}(\rho\, Q) + \frac{1}{t_0\rho}(\rho\, P_{t_0}).$$

The latter is the desired decomposition, since $\rho\, Q \in T_1$, $\rho P_{t_0} \in E_\infty$ are rank-one connected, $\rho > 0$ and $\rho^{-1} + (t_0\rho)^{-1} = 1$. Also notice that $\rho P_{t_0} = \rho t_0 |b - d_1(\overline{a})| J R_{\theta_A}$ as stated.

Finally let us prove (5.52). Note that

$$\operatorname{dist}(A, T_1) + \operatorname{dist}(A, E_\infty) \leq |A - P| + |A - Q| = |P - Q|.$$

By the linear independence of T_1 and E_∞, we get

$$\frac{1}{c_K}|A| \leq |P - Q|.$$

Using Lemma 5.8, (5.48) and (5.50) we obtain

$$|P| \leq c_K|A|, \quad |Q| \leq c_K|A|, \quad |Q| \leq c_K|P|, \quad |P| \leq c_K|Q|.$$

By the triangle inequality,

$$|P - Q| \leq |P| + |Q| \leq (1 + c_K)\min(|P|, |Q|),$$

and (5.52) follows. □

We now turn our attention to the study of rank-one connections between the target set T and E_∞.

Lemma 5.10. *Let $R = (r, 0)$ with $|r| = 1$ and $a \in \mathbb{C} \setminus \{0\}$. For $j \in \{1, 2\}$ define*

$$Q_1(a) := \lambda_1(a, d_1(\overline{a})) \in T_1, \quad Q_2(a) := \lambda_2(-a, d_2(\overline{a})) \in T_2,$$

$$\lambda_j(a) := \frac{1}{\sqrt{B_j^2(a) + A_j(a)} + B_j(a)}, \tag{5.53}$$

$$\begin{cases} A_j(a) := \det(a, d_j(a)) = |a|^2 - |d_j(a)|^2, \\ B_j(a) := \Re\,(\overline{r}\, d_j(a)). \end{cases} \tag{5.54}$$

Then $\lambda_j > 0$, $A_j > 0$ and $\det(Q_j - JR) = 0$. Moreover there exists a constant $c_K > 1$ depending only on K, S_1, S_2 such that

$$\frac{1}{c_K} \leq |Q_j(a)| \leq c_K, \tag{5.55}$$

for every $a \in \mathbb{C} \setminus \{0\}$ and $R \in SO(2)$.

Proof. Condition $\det(Q_j - JR) = 0$ is equivalent to $|\lambda_j a| = |\lambda_j d_j(\overline{a}) - \overline{r}|$, that is

$$A_j(a)\lambda_j^2 + 2B_j(a)\lambda_j - 1 = 0 \tag{5.56}$$

with A_j, B_j defined by (5.54). Notice that $A_j > 0$ by (5.48). Therefore λ_j defined in (5.53) solves (5.56) and satisfies $\lambda_j > 0$.

We will now prove (5.55). Since $a \neq 0$, we can write $a = t\omega$ for some $t > 0$ and $\omega \in \mathbb{C}$, with $|\omega| = 1$. We have $A_j(a) = t^2 A_j(\omega)$ and $B_j(a) = tB_j(\omega)$ so that $\lambda_j(a) = \lambda_j(\omega)/t$. Hence

$$Q_1(a) = \lambda_1(\omega)(\omega, d_1(\overline{\omega}))\,, \quad Q_2(a) = \lambda_2(\omega)(-\omega, d_2(\overline{\omega}))\,. \tag{5.57}$$

Since λ_j is continuous and positive in $(\mathbb{C} \setminus \{0\}) \times SO(2)$, (5.55) follows from (5.57). □

Notation. Let $\theta \in (-\pi, \pi]$. For $R_\theta = (e^{i\theta}, 0) \in SO(2)$, define $x := \cos\theta, y := \sin\theta$ and

$$a(R_\theta) := \frac{x}{k} + i\,\frac{y}{s}\,, \tag{5.58}$$

where s is defined in (5.41). Identifying $SO(2)$ with the interval $(-\pi, \pi]$, for $j = 1, 2$, we introduce the function

$$\lambda_j \colon (-\pi, \pi] \to (0, +\infty) \qquad \text{defined by} \qquad \lambda_j(R_\theta) := \lambda_j(a(R_\theta)) \tag{5.59}$$

with $\lambda_j(a(R_\theta))$ as in (5.53). Furthermore, for $n \in \mathbb{N}$ set

$$M_j(R_\theta) := \frac{\lambda_j}{\dfrac{\lambda_1 + \lambda_2}{2} - \lambda_1\lambda_2}\,, \quad l(R_\theta) := \frac{M_1 + M_2}{2} - 1\,, \quad m := \min_{\theta \in (-\pi,\pi]} \frac{M_2}{2 - M_2}$$
$$L(R_\theta) := \frac{1+l}{1-l}\,, \quad \beta_n(R_\theta) := 1 - \frac{1+l}{n}\,, \quad p(R_\theta) := \frac{2L}{L+1}\,. \tag{5.60}$$

Lemma 5.11. *For $j = 1, 2$, the functions*

$$\lambda_j \colon (-\pi, \pi] \to \left[\frac{s}{1+s_j}, \frac{k}{1+k}\right]\,, \qquad l \colon (-\pi, \pi] \to [s, k]\,,$$
$$L \colon (-\pi, \pi] \to [S, K]\,, \qquad p \colon (-\pi, \pi] \to \left[\frac{2S}{S+1}, \frac{2K}{K+1}\right]\,,$$

are even, surjective and their periodic extension is C^1. Furthermore, they are strictly decreasing in $(0, \pi/2)$ and strictly increasing in $(\pi/2, \pi)$, with maximum at $\theta = 0, \pi$

and minimum at $\theta = \pi/2$. Finally

$$0 < M_j < 2\,, \qquad m > 0\,, \tag{5.61}$$

$$\prod_{j=1}^{n} \beta_j(R_\theta) = \frac{1}{n^{p(R_\theta)}} + O\left(\frac{1}{n}\right)\,, \tag{5.62}$$

where $O(1/n) \to 0$ as $n \to \infty$ uniformly for $\theta \in (-\pi, \pi]$.

Proof. Let us consider λ_j first. By definitions (5.54), (5.58) and by recalling that $x^2 + y^2 = 1$, we may regard A_j, B_j and λ_j as functions of $x \in [-1, 1]$. In particular,

$$A_j(x) = \left(\frac{1-k^2}{k^2} - \frac{1-s_j^2}{s^2}\right)x^2 + \frac{1-s_j^2}{s^2}\,, \quad B_j(x) = \left(1 - \frac{s_j}{s}\right)x^2 + \frac{s_j}{s}\,. \tag{5.63}$$

By symmetry we can restrict to $x \in [0, 1]$. We have three cases:

1. *Case $s_1 = s_2$.* Since $s_1 = s_2 = s$, from (5.63) we compute

$$\lambda_1(x) = \lambda_2(x) = \left(1 + \sqrt{\left(\frac{1}{k^2} - \frac{1}{s^2}\right)x^2 + \frac{1}{s^2}}\right)^{-1}.$$

By (5.44),(5.45) this is a strictly increasing function in $[0, 1]$, and the rest of the thesis for λ_j readily follows.

2. *Case $s_1 < s_2$.* By (5.44) we have

$$-\, s_2 < s_1 < s \qquad \text{and} \qquad 0 < s < s_2\,. \tag{5.64}$$

Relations (5.63) and (5.64) imply that

$$A_j'(0) = 0\,, \quad A_j'(x) < 0\,, \quad \text{for} \quad x \in (0, 1]\,, \tag{5.65}$$

$$B_1'(0) = 0\,, \quad B_1'(x) > 0\,, \quad \text{for} \quad x \in (0, 1]\,, \tag{5.66}$$

$$B_2'(0) = 0\,, \quad B_2'(x) < 0\,, \quad \text{for} \quad x \in (0, 1]\,. \tag{5.67}$$

We claim that

$$\lambda_j'(0) = 0\,, \quad \lambda_j'(x) > 0\,, \quad \text{for} \quad x \in (0, 1]\,. \tag{5.68}$$

Before proving (5.68), notice that $\lambda_j(0) = \dfrac{s}{1+s_j}$ and $\lambda_j(1) = \dfrac{k}{1+k}$, therefore the surjectivity of λ_j will follow from (5.68). Let us now prove (5.68). For $j = 2$ condition (5.68) is an immediate consequence of the definition of λ_2 and (5.65), (5.67). For $j = 1$ we have

$$\lambda_1'(x) = -\frac{1}{\lambda_1^2}\left(\frac{A_1' + 2B_1B_1'}{2\sqrt{B_1^2 + A_1}} + B_1'\right) \tag{5.69}$$

and we immediately see that $\lambda_1'(0) = 0$ by (5.65) and (5.66). Assume now that $x \in (0,1]$. By (5.66) and (5.69), the claim (5.68) is equivalent to

$$A_1'^2 + 4A_1'B_1B_1' - 4A_1B_1'^2 > 0\,, \qquad \text{for} \qquad x \in (0,1]\,.$$

After simplifications, the above inequality is equivalent to

$$\frac{4f(s_1,s_2)}{k^4(s_1+s_2)^4}\,x^2 > 0\,, \qquad \text{for} \qquad x \in (0,1]\,, \tag{5.70}$$

where $f(s_1,s_2) = abcd$, with

$$a = -2k + (1+k)s_1 + (1-k)s_2\,, \qquad b = 2k + (1+k)s_1 + (1-k)s_2\,,$$
$$c = -2k - (1-k)s_1 - (1+k)s_2\,, \qquad d = 2k - (1-k)s_1 - (1+k)s_2\,.$$

We have that $a, c < 0$ since $s_1 < s_2$ and $b, d > 0$ since $s_1 > -s_2$. Hence (5.70) follows.

3. Case $s_2 < s_1$. In particular we have

$$-s_1 < s_2 < s \qquad \text{and} \qquad 0 < s < s_1\,. \tag{5.71}$$

This is similar to the previous case. Indeed (5.65) is still true, but for B_j we have

$$B_1'(0) = 0\,, \quad B_1'(x) < 0\,, \qquad \text{for} \qquad x \in (0,1]\,, \tag{5.72}$$
$$B_2'(0) = 0\,, \quad B_2'(x) > 0\,, \qquad \text{for} \qquad x \in (0,1]\,. \tag{5.73}$$

This implies (5.68) with $j = 1$. Similarly to the previous case, we can see that (5.68) for $j = 2$ is equivalent to

$$\frac{4f(s_2,s_1)}{k^4(s_1+s_2)^4}\,x^2 > 0\,, \qquad \text{for} \qquad x \in (0,1]\,. \tag{5.74}$$

Notice that f is symmetric, therefore (5.74) is a consequence of (5.70).

We will now turn our attention to the function l. Notice that

$$l = \frac{1}{1-H} - 1\,, \quad \text{where} \quad H := \frac{2\lambda_1\lambda_2}{\lambda_1+\lambda_2} = 2\left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)^{-1} \tag{5.75}$$

is the harmonic mean of λ_1 and λ_2. Therefore H is differentiable and even. By direct computation we have

$$H' = 2\,\frac{\lambda_1'\lambda_2^2 + \lambda_1^2\lambda_2'}{(\lambda_1+\lambda_2)^2}\,.$$

Since $\lambda_j > 0$, by (5.68) we have

$$H'(0) = 0\,, \quad H'(x) > 0\,, \quad \text{for} \quad x \in (0,1]\,. \tag{5.76}$$

Moreover $H(0) = \dfrac{s}{1+s}$ and $H(1) = \dfrac{k}{1+k}$. Then from (5.75) we deduce $l(0) = s, l(1) = k$ and the rest of the statement for l.

The statements for L and p follow directly from the properties of l and from the fact that $t \to \dfrac{1+t}{1-t}$, $t \to \dfrac{2t}{t+1}$ are C^1 and strictly increasing for $0 < t < 1$ and $t > 1$, respectively.

Next we prove (5.61). By (5.44) and the properties of λ_j, we have in particular

$$0 < \lambda_j < \frac{1}{2}\,, \quad 0 < H < \frac{1}{2}\,, \tag{5.77}$$

where H is defined in (5.75). Since $\lambda_j > 0$, the inequality $M_j > 0$ is equivalent to $H < 1$, which holds by (5.77). The inequality $M_2 < 2$ is instead equivalent to $\lambda_1(1 - 2\lambda_2) > 0$, which is again true by (5.77). The case $M_1 < 2$ is similar. Finally $m > 0$ follows from $0 < M_2 < 2$ and the continuity of λ_j.

Lastly we prove (5.62). By definition we have $1 + l = \dfrac{2L}{L+1} = p$. By taking the logarithm of $\prod_{j=1}^n \beta_j(R_\theta)$, we see that there exists a constant $c > 0$, depending only on K, S_1, S_2, such that

$$\left| \log \left(\prod_{j=1}^n \beta_j(R_\theta) \right) + p(R_\theta) \log n \right| < c\,, \quad \text{for every} \quad \theta \in (-\pi, \pi]\,. \tag{5.78}$$

Estimate (5.78) is uniform because β_j and p are π-periodic and uniformly continuous.

□

5.5.2 Weak staircase laminate

We are now ready to construct a staircase laminate in the same fashion as [5, Lemma 3.17]. We remark that the construction of this type of laminates, first introduced in [24], has also been used in [11] and [12] in connection with the problem of regularity for rank-one convex functions and in [25] and [49] for constructing Sobolev homeomorphisms with gradients of law rank.

The steps of our staircase will be the sets

$$\mathcal{S}_n := nJSO(2) = \left\{ (0, ne^{i\theta}) :\ \theta \in (-\pi, \pi] \right\}\,, \quad n \geq 1\,.$$

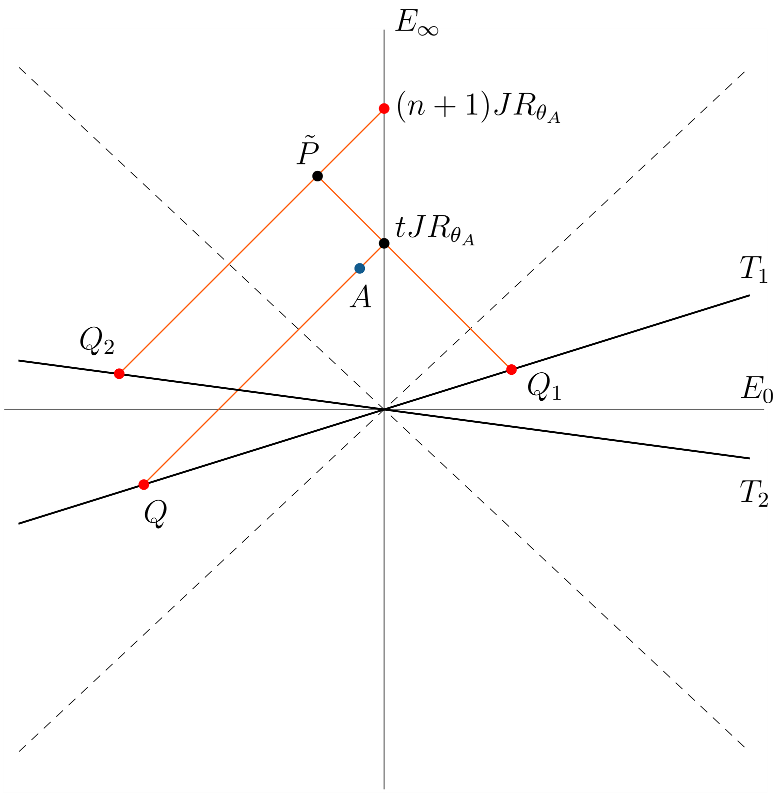


Figure 5.2: Weak staircase laminate. The horizontal axis represents conformal maps E_0, while the vertical axis represents anticonformal maps E_∞. The lines T_1 and T_2 are the target sets. The blue dot is the barycentre of the staircase laminate ν_A, while the red dots are the points of its support. Finally, the orange lines are rank-one connections.

For $0 < \delta < \pi/2$ we introduce the set

$$E_\infty^\delta := \{(0, z) \in E_\infty : \, |\arg z| < \delta\} , \qquad \mathcal{S}_n^\delta := \mathcal{S}_n \cap E_\infty^\delta .$$

Lemma 5.12. *Let $0 < \delta < \pi/4$ and $0 < \rho < \min\{m, \frac{1}{2}\}$, with $m > 0$ defined in (5.60). There exists a constant $c_K > 1$ depending only on K, S_1, S_2, such that for every $A = (a, b) \in \mathbb{M}^{2\times 2}$ satisfying*

$$\operatorname{dist}(A, \mathcal{S}_n) < \rho , \tag{5.79}$$

there exists a laminate of third order ν_A, such that:

(i) $\overline{\nu}_A = A$,

(ii) $\operatorname{supp} \nu_A \subset T \cup \mathcal{S}_{n+1}$,

(iii) $\operatorname{supp}\nu_A \subset \{\xi \in \mathbb{M}^{2\times 2} : \, c_K^{-1} n < |\xi| < c_K\, n\}$,

(iv) $\operatorname{supp}\nu_A \cap \mathcal{S}_{n+1} = \{(n+1)JR\}$, *with* $R = R_{\theta_A}$ *as in* (5.47).

Moreover

$$\left(1 - c_K\,\frac{\rho}{n}\right)\beta_n(R) \leq \nu_A(\mathcal{S}_{n+1}) \leq \left(1 + c_K\,\frac{\rho}{n}\right)\beta_{n+2}(R)\,, \tag{5.80}$$

where β_n *is defined in* (5.60). *If in addition* $n \geq 2$ *and*

$$\operatorname{dist}(A, \mathcal{S}_n^\delta) < \rho\,, \tag{5.81}$$

then

$$|\arg R| = |\theta_A| < \delta + \rho\,. \tag{5.82}$$

In particular $\operatorname{supp}\nu_A \subset T \cup \mathcal{S}_{n+1}^{\delta+\rho}$.

Proof. Let us start by defining ν_A. From Lemma 5.9 there exist $c_K > 1$ and non zero matrices $Q \in T_1$, $P \in E_\infty$, such that $\det(P - Q) = 0$,

$$A = \mu_1 Q + (1 - \mu_1)P\,, \quad \text{for some} \quad \mu_1 \in [0,1]\,, \tag{5.83}$$

$$\frac{1}{c_K}\,|A| \leq |P - Q|\,, |P|\,, |Q| \leq c_K\,|A|\,. \tag{5.84}$$

Moreover $P = tJR$ with $R = R_{\theta_A} = (r, 0)$ as in (5.47) and $t > 0$. We will estimate t. By (5.79), there exists $\tilde{R} \in SO(2)$ such that $|A - nJ\tilde{R}| < \rho$. Applying Lemma 5.8 to $A - nJ\tilde{R}$ and $P - nJ\tilde{R}$ yields

$$|P - nJ\tilde{R}| < \sqrt{2}\rho\,, \tag{5.85}$$

since $P - nJ\tilde{R} \in E_\infty$. Hence from (5.85) we get

$$|t - n| < \rho\,, \tag{5.86}$$

since $|JR| = |J\tilde{R}| = \sqrt{2}$. We also have

$$\mu_1 = \frac{|A - Q|}{|P - Q|} \geq 1 - \frac{|P - A|}{|P - Q|} \geq 1 - c_K\frac{\rho}{n}\,, \tag{5.87}$$

since $|P - A| < 3\rho$ and $|P - Q| > n/c_K$, by (5.81), (5.84), (5.85).

Next we split P in order to “climb” one step of the staircase (see Figure 5.2). Define $x := \cos\theta_A, y := \sin\theta_A$ and

$$a := \frac{x}{k} + i\,\frac{y}{s}\,,$$

as in (5.58). Moreover set

$$Q_1 := \lambda_1(a, d_1(\overline{a}))\,, \quad Q_2 := \lambda_2(-a, d_2(\overline{a}))\,.$$

Here λ_1, λ_2 are chosen as in (5.53), so that $Q_j \in T_j$ and, by Lemma 5.10, $\det(Q_j - JR) = 0$. Furthermore, set

$$\begin{cases} \mu_2 := \dfrac{M_2 - (t-n)M_2}{2n + M_2 + (t-n)(2-M_2)}\,, \\ \mu_3 := \dfrac{M_1 - (t-n)M_1}{2(n+1)}\,, \end{cases} \tag{5.88}$$

with M_j as in (5.60). With the above choices we have

$$\begin{cases} tJR = \mu_2 t Q_1 + (1-\mu_2)\tilde{P}\,, \\ \tilde{P} = \mu_3(n+1)Q_2 + (1-\mu_3)(n+1)JR\,, \end{cases} \tag{5.89}$$

and $\mu_2, \mu_3 \in [0,1]$ by (5.61). In order to check (5.89), we solve the first equation in $\tilde{P}$ to get

$$\gamma_2 tJR + (1-\gamma_2)tQ_1 = \gamma_3(n+1)Q_2 + (1-\gamma_3)(n+1)JR\,, \tag{5.90}$$

with $\mu_2 = 1 - 1/\gamma_2$ and $\mu_3 = \gamma_3$. Equating the first conformal coordinate of both sides of (5.90) yields

$$\gamma_2 = 1 + \gamma_3\,\frac{n+1}{t}\frac{\lambda_2}{\lambda_1}\,. \tag{5.91}$$

Substituting (5.91) in the second component of (5.90) gives us

$$\gamma_3\left(\lambda_1 + \lambda_2 - \lambda_1\lambda_2\left(d_1(a) + d_2(a)\right) r^{-1}\right) = \frac{1-(t-n)}{n+1}\,\lambda_1\,. \tag{5.92}$$

By (5.58), $d_1(a) + d_2(a) = 2r$ and equation (5.92) yields

$$\gamma_3 = \frac{1-(t-n)}{n+1}\,\frac{\lambda_1}{\lambda_1 + \lambda_2 - 2\lambda_1\lambda_2} = \frac{1-(t-n)}{2(n+1)}\,M_1\,. \tag{5.93}$$

Equations (5.91) and (5.93) give us (5.88). Therefore, by (5.83) and (5.89), the measure

$$\nu_A := \mu_1\delta_Q + (1-\mu_1)\left(\mu_2\delta_{tQ_1} + (1-\mu_2)\left(\mu_3\delta_{(n+1)Q_2} + (1-\mu_3)\delta_{(n+1)JR}\right)\right)$$

defines a laminate of third order with barycenter A, supported in $T_1 \cup T_2 \cup \mathcal{S}_{n+1}$ and such that $\operatorname{supp}\nu_A \cap \mathcal{S}_{n+1} = \{(n+1)JR\}$ with $R = R_{\theta_A}$. Moreover

$$\operatorname{supp}\nu_A \subset \{\xi \in \mathbb{M}^{2\times 2} :\, c_K^{-1} n < |\xi| < c_K\, n\}\,,$$

since $c_K^{-1} n < |Q| < c_K n$ by (5.79),(5.84) and

$$c_K^{-1} n < |tQ_1|, |(n+1)Q_2| < c_K n$$

by (5.86), (5.55). Next we prove (5.80) by estimating

$$\nu_A(\mathcal{S}_{n+1}) = \mu_1(1-\mu_2)(1-\mu_3)\,. \tag{5.94}$$

Notice that $\nu_A(\mathcal{S}_{n+1})$ depends on R. For small ρ, we have

$$\mu_2 = \frac{M_2}{2n} + \rho\, O\left(\frac{1}{n}\right)\,, \quad \mu_3 = \frac{M_1}{2n} + \rho\, O\left(\frac{1}{n}\right)\,,$$

so that

$$(1-\mu_2)(1-\mu_3) = 1 - \frac{M_1+M_2}{2n} + \rho\, O\left(\frac{1}{n^2}\right) = 1 - \frac{1+l}{n} + \rho\, O\left(\frac{1}{n^2}\right)\,,$$

with l as in (5.60). Although this gives the right asymptotic, we will need to estimate (5.94) for every $n \in \mathbb{N}$. By direct calculation

$$(1-\mu_2)(1-\mu_3) = \frac{n+(t-n)}{n+1}\,\frac{2n+2-M_1+(t-n)M_1}{2n+M_2+(t-n)(2-M_2)}\,,$$

so that

$$(1-\mu_2)(1-\mu_3) = \left(1+\frac{t-n}{n}\right)\left(1-\frac{1}{n+1}\right)\left(1-\frac{2l\,(1-(t-n))}{2n+M_2+(t-n)(2-M_2)}\right)\,. \tag{5.95}$$

Let us bound (5.95) from above. Recall that $t-n < \rho < 1$ and $2-M_2 > 0$, by (5.61), so the denominator of the third factor in (5.95) is bounded from above by $2(n+1)$ and

$$\begin{aligned}(1-\mu_2)(1-\mu_3) &\le \left(1+\frac{\rho}{n}\right)\left(1-\frac{1}{n+1}\right)\left(1-\frac{l}{n+1}+l\,\frac{\rho}{n+1}\right)\\ &\le \left(1+c_K\,\frac{\rho}{n}\right)\left(1-\frac{1}{n+1}\right)\left(1-\frac{l}{n+1}\right)\,,\end{aligned} \tag{5.96}$$

where $c_K > 1$ is such that

$$l\,\frac{\rho}{n+1}\left(1+\frac{\rho}{n}\right) \le (c_K-1)\,\frac{\rho}{n}\left(1-\frac{l}{n+1}\right)\,.$$

Moreover

$$\left(1-\frac{1}{n+1}\right)\left(1-\frac{l}{n+1}\right) = 1-\frac{1+l}{n+1}+\frac{l}{(n+1)^2} \le 1-\frac{1+l}{n+2} = \beta_{n+2}(R)\,. \tag{5.97}$$

The upper bound in (5.80) follows from (5.96) and (5.97).

Let us now bound (5.95) from below. We can estimate from below the denominator in the third factor of (5.95) with $2n$, since $t - n > -\rho$ by (5.86) and the assumption that $\rho < m$ with m as in (5.60). Therefore

$$\begin{aligned}(1-\mu_2)(1-\mu_3) &\geq \left(1-\frac{\rho}{n}\right)\left(1-\frac{1}{n+1}\right)\left(1-\frac{l}{n}-l\,\frac{\rho}{n}\right)\\ &\geq \left(1-c_K\,\frac{\rho}{n}\right)\left(1-\frac{1}{n+1}\right)\left(1-\frac{l}{n}\right),\end{aligned} \tag{5.98}$$

if we choose $c_K > 1$ such that

$$\left(1-\frac{\rho}{n}\right) l \leq (c_K-1)\left(1-\frac{l}{n}\right).$$

Finally

$$\left(1-\frac{1}{n+1}\right)\left(1-\frac{l}{n}\right) \geq 1-\frac{1+l}{n} = \beta_n(R). \tag{5.99}$$

The lower bound in (5.80) follows from (5.98) and (5.99).

Finally, the last part of the statement follows from a simple geometrical argument, recalling that $\arg R = \theta_A = -\arg(b - d_1(\overline{a}))$ and using hypothesis (5.81). □

Remark 5.13. By iteratively applying Lemma 5.12, one can obtain, for every $R_\theta \in SO(2)$, a sequence of laminates of finite order $\nu_n \in \mathcal{L}(\mathbb{M}^{2\times 2})$ that satisfies $\overline{\nu}_n = JR_\theta$, $\operatorname{supp}\nu_n \subset T_1 \cup T_2 \cup \mathcal{S}_{n+1}$, and

$$\lim_{n\to\infty} \int_{\mathbb{M}^{2\times 2}} |\lambda|^{p(R_\theta)}\, d\nu_n(\lambda) = \infty, \tag{5.100}$$

where $p(R_\theta) \in \left[\frac{2S}{S+1}, \frac{2K}{K+1}\right]$ is the function defined in (5.60). Indeed, setting $A = JR_\theta$ and iterating the construction of Lemma 5.12, yields $\nu_n \in \mathcal{L}(\mathbb{M}^{2\times 2})$ such that $\overline{\nu}_n = JR_\theta$ and $\operatorname{supp}\nu_n \subset T_1 \cup T_2 \cup \mathcal{S}_{n+1}$. Notice that ν_n contains the term

$$\prod_{j=1}^{n}(1-\mu_2^j)(1-\mu_3^j)\delta_{(n+1)JR_\theta},$$

with μ_2^j, μ_3^j as defined in (5.88). Therefore, using (5.62) and (5.80) (with $\rho = 0$), we obtain

$$\prod_{j=1}^{n}(1-\mu_2^j)(1-\mu_3^j) \approx \prod_{j=1}^{n}\beta_j(R_\theta) \approx \frac{1}{n^{p(R_\theta)}} \tag{5.101}$$

which implies (5.100).

In particular, by applying Proposition 5.5 to ν_n, and by a diagonal argument, we can obtain a sequence $f_n \colon \Omega \to \mathbb{R}^2$ of piecewise affine Lipschitz functions such that $f_n(x) = JR_\theta x$ on $\partial\Omega$ and

$$\lim_{n\to\infty} \int_\Omega |\nabla f_n|^{p(R_\theta)}\, dx = \infty \tag{5.102}$$

by (5.24) and (5.100).

Remark 5.14. In the isotropic case $S = K$, the laminate ν_A provided by Lemma 5.12 coincides with the one in [5, Lemma 3.16]. In particular, the growth condition (5.80) is independent of the initial point A, and it reads as

$$\left(1 - c_K \frac{\rho}{n}\right) \beta_n(I) \le \nu_A(\mathcal{S}_{n+1}) \le \left(1 + c_K \frac{\rho}{n}\right) \beta_{n+2}(I)\,, \quad \beta_n(I) = 1 - \frac{1+k}{n}\,.$$

Moreover, by Remark 5.13, for every $R_\theta \in SO(2)$, JR_θ is the centre of mass of a sequence of laminates of finite order such that (5.100) holds with $p(R_\theta) \equiv \frac{2K}{K+1}$, which gives the desired growth rate.

In contrast, in the anisotropic case $1 < S < K$, the growth rate of the laminates explicitly depends on the argument of the barycenter JR_θ. The desired growth rate corresponds to $\theta = 0$, that is, the centre of mass has to be J.

In constructing approximate solutions with the desired integrability properties, it is then crucial to be able to select rotations whose angle lies in an arbitrarily small neighbourhood of $\theta = 0$.

We now proceed to show the existence of a *piecewise affine* map f that solves the differential inclusion (5.36) up to an arbitrarily small L^∞ error. Such map will have the integrability properties given by (5.103).

Proposition 5.15. *Let $\Omega \subset \mathbb{R}^2$ be an open bounded domain. Let $K > 1$, $\alpha \in (0,1)$, $\varepsilon > 0$, $0 < \delta_0 < \frac{2K}{K+1} - \frac{2S}{S+1}$, $\gamma > 0$. There exist a constant $c_{K,\delta_0} > 1$, depending only on K, S_1, S_2, δ_0, and a piecewise affine map $f \in W^{1,1}(\Omega;\mathbb{R}^2) \cap C^\alpha(\overline{\Omega};\mathbb{R}^2)$, such that*

(i) $f(x) = Jx$ *on* $\partial\Omega$,

(ii) $[f - Jx]_{C^\alpha(\overline{\Omega})} < \varepsilon$,

(iii) $\operatorname{dist}(\nabla f(x), T) < \gamma$ *a.e. in* Ω.

Moreover

$$\frac{1}{c_{K,\delta_0}} t^{-\frac{2K}{K+1}} < \frac{|\{x \in \Omega : \ |\nabla f(x)| > t\}|}{|\Omega|} < c_{K,\delta_0}\, t^{-p}\,, \tag{5.103}$$

where $p \in \left(\frac{2K}{K+1} - \delta_0, \frac{2K}{K+1}\right]$. *That is,* $\nabla f \in L^p_{\text{weak}}(\Omega; \mathbb{M}^{2\times 2})$ *and* $\nabla f \notin L^{\frac{2K}{K+1}}(\Omega; \mathbb{M}^{2\times 2})$. *In particular* $f \in W^{1,q}(\Omega; \mathbb{R}^2)$ *for every* $q < p$, *but* $\int_\Omega |\nabla f(x)|^{\frac{2K}{K+1}}\, dx = \infty$.

Proof. By Lemma 5.11 the function $p \colon (-\pi, \pi] \to \left[\frac{2S}{S+1}, \frac{2K}{K+1}\right]$ is uniformly continuous. Let $\alpha \colon [0,\infty] \to [0,\infty]$ be its modulus of continuity. Fix $0 < \delta < \pi/4$ such that

$$\alpha(\delta) < \delta_0\,. \tag{5.104}$$

Let $\{\rho_n\}$ be a strictly decreasing positive sequence satisfying

$$\rho_1 < \frac{1}{4}\min\{m, c_K^{-1}, \operatorname{dist}(\mathcal{S}_1, T), \gamma\}\,, \quad \rho_n < \frac{\delta}{4}\, 2^{-n}\,, \tag{5.105}$$

where $m > 0$ and $c_K > 1$ are the constants from Lemma 5.12. Define $\{\delta_n\}$ as

$$\delta_1 := 0 \quad \text{and} \quad \delta_n := \sum_{j=1}^{n-1} \rho_n \ \text{ for } \ n \geq 2\,. \tag{5.106}$$

In particular from (5.105),(5.106) it follows that

$$\delta_n < \frac{\delta}{2}\,, \qquad \text{for every} \ \ n \in \mathbb{N}\,. \tag{5.107}$$

Step 1. Similarly to the proof of [5, Proposition 3.17], by repeatedly combining Lemma 5.12 and Proposition 5.5, we will prove the following statement:

Claim. There exist sequences of piecewise constant functions $\tau_n \colon \Omega \to (0,\infty)$ and piecewise affine Lipschitz mappings $f_n \colon \Omega \to \mathbb{R}^2$, such that

(a) $f_n(x) = Jx$ on $\partial\Omega$,

(b) $[f_n - Jx]_{C^\alpha(\overline{\Omega})} < (1 - 2^{-n})\varepsilon$,

(c) $\operatorname{dist}(\nabla f_n(x), T \cup \mathcal{S}_n^{\delta_n}) < \tau_n(x)$ a.e. in Ω,

(d) $\tau_n(x) = \rho_n$ in Ω_n,

where

$$\Omega_n := \{x \in \Omega : \ \operatorname{dist}(\nabla f_n(x), T) \geq \rho_n\}\,.$$

Moreover

$$\prod_{j=1}^{n-1}\left(1 - c_K\frac{\rho_j}{j}\right)\beta_j(R_0) \leq \frac{|\Omega_n|}{|\Omega|} \leq \prod_{j=1}^{n-1}\left(1 + c_K\frac{\rho_j}{j}\right)\beta_{j+2}(R_\delta)\,. \tag{5.108}$$

Proof of claim. We proceed by induction. Set $f_1(x) := Jx$ and $\tau_1(x) := \rho_1$ for every $x \in \Omega$. Since $J \in \mathcal{S}_1^0$, then f_1 satisfies (a)-(c). Also, $\rho_1 < \operatorname{dist}(T, \mathcal{S}_1)/4$ by (5.105), so $\Omega_1 = \Omega$ and (d), (5.108) follow.

Assume now that f_n and τ_n satisfy the inductive hypothesis. We will first define f_{n+1} by modifying f_n on the set Ω_n. Since f_n is piecewise affine we have a decomposition of Ω_n into pairwise disjoint open subsets $\Omega_{n,i}$ such that

$$\left|\Omega_n \setminus \bigcup_{i=1}^{\infty}\Omega_{n,i}\right| = 0\,, \tag{5.109}$$

with $f_n(x) = A_i x + b_i$ in $\Omega_{n,i}$, for some $A_i \in \mathbb{M}^{2\times 2}$ and $b_i \in \mathbb{R}^2$. Moreover

$$\operatorname{dist}(A_i, \mathcal{S}_n^{\delta_n}) < \rho_n \tag{5.110}$$

by (c) and (d). Since (5.110) and (5.105) hold, we can invoke Lemma 5.12 to obtain a laminate ν_{A_i} and a rotation $R^i = R_{\theta_{A_i}}$ satisfying, in particular, $\overline{\nu}_{A_i} = A_i$,

$$|\arg R^i| = |\theta_{A_i}| < \delta_{n+1}\,, \tag{5.111}$$

$$\operatorname{supp}\nu_{A_i} \subset T \cup \mathcal{S}_{n+1}^{\delta_{n+1}}\,, \tag{5.112}$$

since $\delta_{n+1} = \delta_n + \rho_n$ by (5.106). By applying Proposition 5.5 to ν_{A_i} and by taking into account (5.112), we obtain a piecewise affine Lipschitz mapping $g_i\colon \Omega_{n,i} \to \mathbb{R}^2$, such that

(e) $g_i(x) = A_i x + b_i$ on $\partial\Omega_{n,i}$,

(f) $[g_i - f_n]_{C^\alpha(\overline{\Omega_{n,i}})} < 2^{-(n+1+i)}\varepsilon$,

(g) $c_K^{-1} n < |\nabla g_i(x)| < c_K n$ a.e. in $\Omega_{n,i}$,

(h) $\operatorname{dist}(\nabla g_i(x), T \cup \mathcal{S}_{n+1}^{\delta_{n+1}}) < \rho_{n+1}$ a.e. in $\Omega_{n,i}$.

Moreover

$$\left(1 - c_K\frac{\rho_n}{n}\right)\beta_n(R^i) \le \frac{|\omega_{n,i}|}{|\Omega_{n,i}|} \le \left(1 + c_K\frac{\rho_n}{n}\right)\beta_{n+2}(R^i)\,, \tag{5.113}$$

with

$$\omega_{n,i} := \left|\left\{x \in \Omega_{n,i} : \ \operatorname{dist}(\nabla g_i(x), \mathcal{S}_{n+1}^{\delta_{n+1}}) < \rho_{n+1}\right\}\right|\,.$$

Set

$$f_{n+1}(x) := \begin{cases} f_n(x) & \text{if } x \in \Omega \smallsetminus \Omega_n\,, \\ g_i(x) & \text{if } x \in \Omega_{n,i}\,. \end{cases}$$

Since Ω_{n+1} is well defined, we can also introduce

$$\tau_{n+1}(x) := \begin{cases} \tau_n(x) & \text{for } x \in \Omega \smallsetminus \Omega_{n+1}\,, \\ \rho_{n+1} & \text{for } x \in \Omega_{n+1}\,, \end{cases}$$

so that (d) holds. From (e) we have $f_{n+1}(x) = Jx$ on $\partial\Omega$. From (f) we get $[f_{n+1} - f_n]_{C^\alpha(\overline{\Omega})} < 2^{-(n+1)}\varepsilon$ so that (b) follows. (c) is a direct consequence of (d), (h), and the fact that ρ_n is strictly decreasing. Finally let us prove (5.108). First notice that the sets $\omega_{n,i}$ are pairwise disjoint. By (5.105), in particular we have $\rho_{n+1} < \operatorname{dist}(T, \mathcal{S}_1)/4$, so that

$$\left|\Omega_{n+1} \smallsetminus \bigcup_{i=1}^{\infty}\omega_{n,i}\right| = 0\,. \tag{5.114}$$

By (5.111) and (5.107) we have $|\arg R^i| < \delta$. Then by the properties of β_n (see Lemma 5.11),

$$\beta_n(R^i) \ge \beta_n(R_0) \quad \text{and} \quad \beta_{n+2}(R^i) \le \beta_{n+2}(R_\delta)\,. \tag{5.115}$$

Using (5.115), (5.109), (5.114) in (5.108) yields

$$|\Omega_n|\left(1 - c_K\frac{\rho_n}{n}\right)\beta_j(R_0) \le |\Omega_{n+1}| \le |\Omega_n|\left(1 + c_K\frac{\rho_n}{n}\right)\beta_{j+2}(R_\delta)\,,$$

and (5.108) follows.

Step 2. Notice that on $\Omega \smallsetminus \Omega_n$ we have that $\nabla f_{n+1} = \nabla f_n$ almost everywhere, so $\Omega_{n+1} \subset \Omega_n$. Therefore $\{f_n\}$ is obtained by modification on a nested sequence of open sets, satisfying

$$\prod_{j=1}^{n-1}\left(1 - c_K\frac{\rho_j}{j}\right)\beta_j(R_0) \le \frac{|\Omega_n|}{|\Omega|} \le \prod_{j=1}^{n-1}\left(1 + c_K\frac{\rho_j}{j}\right)\beta_{j+2}(R_\delta)\,.$$

By (5.105) we have $\rho_n < \min\{2^{-n}\,\delta, c_K^{-1}\}/4$, so that

$$\prod_{j=1}^{\infty}\left(1 - c_K\frac{\rho_j}{j}\right) = c_1\,, \quad \prod_{j=1}^{\infty}\left(1 + c_K\frac{\rho_j}{j}\right) = c_2\,,$$

with $0 < c_1 < c_2 < \infty$, depending only on K, S_1, S_2, δ (and hence on δ_0, by (5.104)). Moreover, from Lemma 5.11,

$$\prod_{j=1}^{n}\beta_j(R_\theta) = n^{-p(R_\theta)} + O\left(\frac{1}{n}\right)\,, \qquad \text{uniformly in} \quad (-\pi,\pi]\,.$$

Therefore, there exists a constant $c_{K,\delta_0} > 1$ depending only on K, S_1, S_2, δ_0, such that

$$\frac{1}{c_{K,\delta_0}}\,n^{-\frac{2K}{K+1}} \le |\Omega_n| \le c_{K,\delta_0}\,n^{-p_{\delta_0}}\,, \tag{5.116}$$

since $p(R_0) = \dfrac{2K}{K+1}$. Here $p_{\delta_0} := p(R_\delta)$. Notice that, by (5.104), $p_{\delta_0} \in \left(\frac{2K}{K+1} - \delta_0, \frac{2K}{K+1}\right]$, since p is strictly decreasing in $[0,\pi/2]$.

From (5.116), in particular we deduce $|\Omega_n| \to 0$. Therefore $f_n \to f$ almost everywhere in Ω, with f piecewise affine. Furthermore f satisfies (i)-(iii) by construction.

We are left to estimate the distribution function of ∇f. By (g) we have that

$$|\nabla f(x)| > \frac{n}{c_{K,\delta_0}} \quad \text{in} \quad \Omega_n \qquad \text{and} \qquad |\nabla f(x)| < c_{K,\delta_0}\,n \quad \text{in} \quad \Omega\smallsetminus\Omega_n\,.$$

For a fixed $t > c_{K,\delta_0}$, let $n_1 := [c_{K,\delta_0}t]$ and $n_2 := [c_{K,\delta_0}^{-1}t]$, where $[\cdot]$ denotes the integer part function. Therefore

$$\Omega_{n_1+1} \subset \{x \in \Omega : \, |\nabla f(x)| > t\} \subset \Omega_{n_2}$$

and (5.103) follows from (5.116), with $p = p_{\delta_0}$. Lastly, (5.103) implies that ∇f_n is uniformly bounded in L^1, so that $f \in W^{1,1}(\Omega;\mathbb{R}^2)$ by dominated convergence. □

We remark that the constant c_{K,δ_0} in (5.103) is monotonically increasing as a function of δ_0, that is $c_{K,\delta_1} \le c_{K,\delta_2}$ if $\delta_1 \le \delta_2$.

We now proceed with the construction of exact solutions to (5.36). We will follow a standard argument (see, e.g., [24, Remark 6.3], [48, Thoerem A.2]).

Theorem 5.16. *Let σ_1, σ_2 be defined by* (5.3) *for some K, S_1, S_2 as in* (5.46) *and S as in* (5.42). *There exist coefficients $\sigma_n \in L^\infty(\Omega; \{\sigma_1,\sigma_2\})$, exponents $p_n \in$*

$\left[\frac{2S}{S+1}, \frac{2K}{K+1}\right]$, *functions* $u_n \in W^{1,1}(\Omega)$, *such that*

$$\begin{cases} \operatorname{div}(\sigma_n \nabla u_n) = 0 & \textit{in} \quad \Omega\,, \\ u_n(x) = x_1 & \textit{on} \quad \partial\Omega\,, \end{cases} \tag{5.117}$$

$$\nabla u_n \in L^{p_n}_{\text{weak}}(\Omega;\mathbb{R}^2), \quad p_n \to \frac{2K}{K+1}, \tag{5.118}$$

$$\nabla u_n \notin L^{\frac{2K}{K+1}}(\Omega;\mathbb{R}^2). \tag{5.119}$$

In particular $u_n \in W^{1,q}(\Omega)$ *for every* $q < p_n$, *but* $\int_\Omega |\nabla u_n|^{\frac{2K}{K+1}}\,dx = \infty$.

Proof. By Proposition 5.15 there exist sequences $f_n \in W^{1,1}(\Omega;\mathbb{R}^2) \cap C^\alpha(\overline{\Omega};\mathbb{R}^2)$, $\gamma_n \searrow 0$, $p_n \in \left[\frac{2S}{S+1}, \frac{2K}{K+1}\right]$, such that, $f_n(x) = Jx$ on $\partial\Omega$,

$$\operatorname{dist}(\nabla f_n, T_1 \cup T_2) < \gamma_n \quad \text{a.e. in} \quad \Omega\,, \tag{5.120}$$

$$\nabla f_n \in L^{p_n}_{\text{weak}}(\Omega;\mathbb{M}^{2\times 2})\,, \quad p_n \to \frac{2K}{K+1}\,, \quad \nabla f_n \notin L^{\frac{2K}{K+1}}(\Omega;\mathbb{M}^{2\times 2})\,. \tag{5.121}$$

In euclidean coordinates, condition (5.120) implies that

$$\begin{pmatrix} \nabla f_n^1 \\ \nabla f_n^2 \end{pmatrix} = \begin{pmatrix} E_n \\ R_{\frac{\pi}{2}} \sigma_n E_n \end{pmatrix} + \begin{pmatrix} a_n \\ b_n \end{pmatrix} \quad \text{a.e. in} \quad \Omega \tag{5.122}$$

with $f_n = (f_n^1, f_n^2)$, $\sigma_n := \sigma_1 \chi_{\{\nabla f \in T_1\}} + \sigma_2 \chi_{\{\nabla f \in T_2\}}$, $E_n \colon \Omega \to \mathbb{R}^2$, $R_{\frac{\pi}{2}} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and

$$a_n, b_n \to 0 \qquad \text{in} \qquad L^\infty(\Omega;\mathbb{R}^2)\,. \tag{5.123}$$

The boundary condition $f_n = Jx$ reads $f_n^1 = x_1$ and $f_n^2 = -x_2$. We set $u_n := f_n^1 + v_n$, where $v_n \in H_0^1(\Omega)$ is the unique solution to

$$\operatorname{div}(\sigma_n \nabla v) = -\operatorname{div}(\sigma_n a_n - R^T_{\frac{\pi}{2}} b_n)\,.$$

Notice that v_n is uniformly bounded in H^1 by (5.123). Since (5.122) holds, it is immediate to check that $\operatorname{div}(\sigma_n \nabla u_n) = \operatorname{div}(R^T_{\frac{\pi}{2}} \nabla f_n^2) = 0$, so that u_n is a solution of (5.117). Finally, the regularity thesis (5.118), (5.119), follows from the definition of u_n and the fact that $v_n \in H_0^1(\Omega)$ and f_n^1 satisfies (5.121) with $1 < p_n < 2$. $\square$

5.6 Conclusions and perspectives

In this chapter we presented the results obtained in [21]. In that paper we addressed the analysis of the critical integrability of distributional solutions to

$$\operatorname{div}(\sigma\nabla u) = 0 \quad \text{in} \quad \Omega\,,$$

in dimension two, when $\sigma \in \{\sigma_1, \sigma_2\}$ for two elliptic matrices σ_1, σ_2. In [48] the authors characterise critical exponents q_{σ_1,σ_2} and p_{σ_1,σ_2}, and prove the optimality of the upper critical exponent p_{σ_1,σ_2}, as stated in Theorem 5.1. In our paper [21] we complemented the analysis in [48] by proving the optimality of the lower critical exponent p_{σ_1,σ_2} in Theorem 5.2.

At present it is still not clear how to modify the proofs of our results in order to obtain a stronger result as in [5], namely, to obtain a single map $u \in W^{1,1}(\Omega)$ that satisfies (5.6) and such that $\nabla u \in L^{\frac{2K}{K+1}}_{\text{weak}}(\Omega)$ but

$$\int_B |\nabla u|^{\frac{2K}{K+1}}\, dx = +\infty$$

for every ball $B \subset \Omega$. A suitable modification of the staircase laminate we construct in Lemma 5.12 might be required.

Another interesting open problem is the extension of these results to the case of three (or more) phases, i.e., $\sigma \in L^\infty(\Omega; \{\sigma_1, \sigma_2, \sigma_3\})$. In this context a characterisation for the lower and upper critical exponents $q_{\sigma_1,\sigma_2,\sigma_3}$ and $p_{\sigma_1,\sigma_2,\sigma_3}$ is not known. A first step in this direction would be to extend the results in [48] in order to compute $q_{\sigma_1,\sigma_2,\sigma_3}$ and $p_{\sigma_1,\sigma_2,\sigma_3}$ as functions of the ellipticity constant of σ and subsequently prove the analog of Theorems 5.1, 5.2.

Finally, a more ambitious goal is to understand the problem in dimension $d \geq 3$, even in the simple case of two isotropic phases, i.e., $\sigma \in \{KI, K^{-1}I\}$, for $K > 1$. A fundamental tool employed in the analysis of the two-dimensional case was the celebrated Astala's Theorem in [4]. An analog of such result is missing in higher dimension.

Appendix A

Calculus of Variations and Geometric Measure Theory

A.1 Direct methods of the Calculus of Variations

A.1.1 Direct method

Let $(X, \|\cdot\|)$ be a reflexive and separable Banach space and $S \subseteq X$ be a closed and convex subspace. Consider a functional $\mathcal{F}\colon X \to [-\infty, +\infty]$. We are concerned with the existence of solutions to the problem

$$\inf \{\mathcal{F}(x),\, x \in S\} \,. \tag{A.1}$$

We say that $\mathcal{F}$ is *sequentially weakly lower semicontinuous* (swls) if for any sequence $x_n \rightharpoonup x$ (with respect to the weak topology of X) we have $\mathcal{F}(x) \leq \liminf_{n\to\infty} \mathcal{F}(x_n)$. We say that $\mathcal{F}$ is *coercive* on S if

$$\lim_{\substack{\|x\|_X \to +\infty \\ x \in S}} \mathcal{F}(x) = +\infty \,.$$

Theorem A.1 (Direct method)**.** *Assume that $\mathcal{F}$ is swls and coercive on S. Then there exists a solution to* (A.1)*. If in addition $\mathcal{F}$ is strictly convex on S, the solution is unique.*

An example of application of the direct method can be found in the proof of Proposition 4.11.

A.1.2 Γ-convergence

In this section (X, τ) will be a topological space. In some applications one is lead to study a family of minimisation problems depending on a continuous parameter $\varepsilon > 0$

$$\min \{\mathcal{F}_\varepsilon(x) : \; x \in X\} \;, \tag{A.2}$$

where $\mathcal{F}_\varepsilon \colon X \to [-\infty, +\infty]$. Sometimes it can be difficult to study (A.2) directly, but it is possible to guess an asymptotic behaviour for the minimisers and get rid of the parameter ε, by defining a limiting problem

$$\min \{\mathcal{F}(x) : \; x \in X\} \;, \tag{A.3}$$

for some functional $\mathcal{F} \colon X \to [-\infty, +\infty]$. The idea is to define a notion of convergence of functionals, which is stable from the variational point of view. This means that if x_ε are solutions to (A.2) such that $x_\varepsilon \to x$, then the following properties should hold true:

- x is solution to (A.3),
- $\mathcal{F}_\varepsilon(x_\varepsilon) \to \mathcal{F}(x)$.

We will make this statement precise by introducing Γ-convergence in Definition A.2. Such definition will satisfy the above properties, as stated in Theorem A.4.

An example of application of Γ-convergence is the author's work [23] (discussed in Chapter 4). In this paper the family (A.2) describes a mesoscopic theory for defects in a crystal and the limiting problem (A.3) can be physically interpreted as a macroscopic model for the defects.

Γ-convergence can be used also in the opposite direction. An example of this procedure are *dimension reduction* problems, as in [43, 44, 29]. Another example of application of Γ-convergence is the derivation of linearised elasticity starting from nonlinear elasticity, as done in [15] (see Section 3.4.2 for more details).

Definition A.2 (Γ-convergence)**.** We say that a sequence $\mathcal{F}_\varepsilon \colon X \to [-\infty, +\infty]$ Γ-converge to $\mathcal{F} \colon X \to [-\infty, +\infty]$ in X (as $\varepsilon \to 0$) if for all $x \in X$ we have:

(i) (Γ-*liminf* inequality) for every sequence x_ε such that $x_\varepsilon \to x$,

$$\mathcal{F}(x) \leq \liminf_{\varepsilon \to 0} \mathcal{F}_\varepsilon(x_\varepsilon) \,,$$

(ii) (Γ-*limsup* inequality) there exists a sequence x_ε (called *recovery sequence*) such that $x_\varepsilon \to x$ and

$$\limsup_{\varepsilon \to 0} \mathcal{F}_\varepsilon(x_\varepsilon) \leq \mathcal{F}(x)\,.$$

$\mathcal{F}$ is called the Γ-limit of $\mathcal{F}_\varepsilon$ and we write $\mathcal{F}_\varepsilon \xrightarrow{\Gamma} \mathcal{F}$.

We remark that the above definition can also be stated pointwise, i.e., we say that $\mathcal{F}_\varepsilon$ Γ-converge at $x_0 \in X$ to $\mathcal{F}(x_0)$ if $(i), (ii)$ hold for x_0. Also notice that if (i) holds for every $x \in X$ then (ii) is equivalent to

(iii) there exists a recovery sequence $x_\varepsilon \to x$ such that

$$\mathcal{F}(x) = \lim_{\varepsilon \to 0} \mathcal{F}_\varepsilon(x_\varepsilon)\,.$$

Before proceeding to state the main theorem for Γ-convergence, we introduce a compactness property that will guarantee convergence of minimising sequences.

Definition A.3 (Equi-coercivity)**.** A family of functionals $\mathcal{F}_\varepsilon \colon X \to [-\infty, +\infty]$ is *equi-coercive* if for every sequence $x_\varepsilon \in X$ such that

$$\sup_{\varepsilon} \mathcal{F}_\varepsilon(x_\varepsilon) \leq C$$

for some $C > 0$, we have that $x_\varepsilon \to x$, up to subsequences.

Theorem A.4 (See Theorem 1.21 in [7])**.** *Let $\mathcal{F}_\varepsilon, \mathcal{F} \colon X \to [-\infty, +\infty]$ and assume*

(i) (Compactness)*: the functionals $\mathcal{F}_\varepsilon$ are equi-coercive,*

(ii) (Γ-convergence)*: $\mathcal{F}_\varepsilon$ Γ-converge to $\mathcal{F}$.*

Then $\mathcal{F}$ admits minimum on X and

$$\lim_{\varepsilon \to 0} \inf_X \mathcal{F}_\varepsilon = \min_X \mathcal{F}\,.$$

If x_ε is a sequence of almost minimisers for $\mathcal{F}_\varepsilon$, that is, $\lim_{\varepsilon \to 0} \mathcal{F}_\varepsilon(x_\varepsilon) = \lim_{\varepsilon \to 0} \inf_X \mathcal{F}_\varepsilon$, then x_ε is precompact and any accumulation point of x_ε is a minimiser for $\mathcal{F}$ on X.

In view of Theorem A.4, the prototypical Γ-convergence result will involve proving both compactness and Γ-convergence for the functionals $\mathcal{F}_\varepsilon$ with respect to the *same* topology on the ambient space X. This implies that the choice of topology will play a crucial role, since one needs to balance between having many open sets (for the compactness) and few open sets (for the Γ-convergence). Moreover the topology also influences the structure of the Γ-limit $\mathcal{F}$.

A.2 Measure theory

In this section we want to recall the main definitions and notation in measure theory used throughout this thesis. We will also recall the main properties needed. We will mainly follow the approach of [3], which the reader can refer to for further clarification.

Throughout this section, X will coincide either with $\mathbb{R}^n$, or with an open bounded subset $\Omega \subset \mathbb{R}^n$. We will denote by τ the topology induced by the euclidean norm on X.

A.2.1 Radon measures

Let $\mathcal{A}$ be a collection of subsets of X. We say that $\mathcal{A}$ is a *σ-algebra* on X if $\emptyset \in \mathcal{A}$, $X \setminus U \in \mathcal{A}$ and $\bigcup_{i\in\mathbb{N}} U_i \in \mathcal{A}$ for every set $U \in \mathcal{A}$ and every sequence $\{U_i\} \subset \mathcal{A}$. The pair $(X, \mathcal{A})$ is called a *measure space.* We denote by $\mathcal{B}(X)$ the *σ-algebra of Borel*, that is, the smallest σ-algebra on X containing the open sets of the topology τ. We will now introduce the notion of positive measure.

Definition A.5 (Positive measures)**.** Let $(X, \mathcal{A})$ be a measure space and let $\mu \colon \mathcal{A} \to [0, \infty]$. We say that μ is a *positive measure* if $\mu(\emptyset) = 0$ and μ is σ-additive, that is,

$$\mu\left(\bigcup_{i=1}^{\infty} U_i\right) = \sum_{i=1}^{\infty} \mu(U_i)\,,$$

for every sequence U_i of pairwise disjoint elements of $\mathcal{A}$. We say that the positive measure μ is *finite* if $\mu(X) < \infty$. We say that a set $E \subset X$ is *μ-negligible* if there exists $U \in \mathcal{A}$ such that $E \subset U$ and $\mu(U) = 0$. We say that a property depending on points of X holds μ-a.e. if the set where it fails is μ-negligible.

We now define vector valued measures.

Definition A.6 (Real and vector measures)**.** Let $(X, \mathcal{A})$ be a measure space and let $m \in \mathbb{N}$, $m \geq 1$. We say that $\mu \colon \mathcal{A} \to \mathbb{R}^m$ is a *measure* if $\mu(\emptyset) = 0$ and for every sequence $\{U_i\}$ of pairwise disjoint elements of $\mathcal{A}$

$$\mu\left(\bigcup_{i=1}^{\infty} U_i\right) = \sum_{i=1}^{\infty} \mu(U_i)\,.$$

If $m > 1$ we say that μ is a *vector measure*. If $m = 1$ we say that μ is a *real measure*.

Notice that positive measures are not a particular case of real measures, because positive measures are allowed to be unbounded, while real measures must be finite.

For a measure $\mu\colon \mathcal{A} \to \mathbb{R}^m$ we define its *total variation* $|\mu|$ as the measure

$$|\mu|(U) := \sup \left\{ \sum_{i=1}^{\infty} |\mu(U_i)| \,:\, U_i \in \mathcal{A} \text{ pairwise disjoint, } U = \bigcup_{i=1}^{\infty} U_i \right\} ,$$

for every $U \in \mathcal{A}$. Since μ is a measure, we have that $|\mu|$ is a positive finite measure (see [3, Theorem 1.6]).

Definition A.7 (Regularity of measures)**.** Consider the measure space $(X, \mathcal{B}(X))$. Then:

(i) a positive measure on $(X, \mathcal{B}(X))$ is called a *Borel measure*. If a Borel measure is finite on compact sets, it is said to be a *positive Radon measure*.

(ii) if $\mu\colon \mathcal{B}(X) \to \mathbb{R}^m$ is a measure, we say that it is a *finite Radon measure*. The space of finite $\mathbb{R}^m$-valued Radon measures is denoted by $\mathcal{M}(X; \mathbb{R}^m)$.

For a positive measure μ on X we define its *support* as the set

$$\operatorname{supp} \mu := \overline{\{x \in X \,:\, \mu(U) > 0 \text{ for every neighbourhood } U \text{ of } x\}}$$

If μ is a real or vector measure, then we define $\operatorname{supp} \mu := \operatorname{supp} |\mu|$.

For a measure μ on $(X, \mathcal{A})$ and a fixed set $A \in \mathcal{A}$ we define the *restriction* of μ to A as the measure $\mu \llcorner A$ defined as

$$(\mu \llcorner A)(U) := \mu(U \cap A) \quad \text{for all} \quad U \in \mathcal{A} \,.$$

If μ is a Borel (respectively Radon) measure and A is a Borel set, then also $\mu \llcorner A$ is Borel (respectively Radon). Finally, if $u\colon X \to \mathbb{R}$, we say that u is μ-measurable if $\{x \in X \,:\, u(x) > t\} \in \mathcal{A}$ for every $t \in \mathbb{R}$. For $1 \leq p \leq \infty$ the spaces $L^p(X, \mu)$ are defined as usual (see for example [3, Chapter 1]). Also we set $L^p(X, \mu; \mathbb{R}^m) := [L^p(X, \mu)]^m$, product of vector spaces.

A.2.2 Duality with continuous functions

Let $C_c(X)$ be the vector space of real continuous functions on X with compact support. We endow $C_c(X)$ with the norm $\|u\|_\infty := \sup\{|u(x)|,\, x \in X\}$. Denote as

$C_0(X)$ the completion of $C_c(X)$ with respect to such norm, so that $(C_0(X), \|\cdot\|_\infty)$ is a Banach space. Notice that $C_0(\mathbb{R}^n)$ coincides with the space of real continuous functions on $\mathbb{R}^n$ vanishing at infinity. We will also define $C_c(X;\mathbb{R}^m) := [C_c(X)]^m$ and $C_0(X;\mathbb{R}^m) := [C_0(X)]^m$, products of vector spaces, for $m \in \mathbb{N}, m > 1$.

Theorem A.8 (Riesz (Remark 1.57 in [3]))**.** *The dual of $C_0(X;\mathbb{R}^m)$ is the space $\mathcal{M}(X;\mathbb{R}^m)$ of finite $\mathbb{R}^m$-valued Radon measures on X, under the pairing*

$$\langle \mu, u \rangle := \sum_{i=1}^{m} \int_X u_i \, d\mu_i \, .$$

Moreover, $|\mu|(X)$ is the dual norm.

Definition A.9 (Weak-$*$ convergence.)**.** For $\mu \in \mathcal{M}(X;\mathbb{R}^m)$ and a sequence μ_j belonging to $\mathcal{M}(X;\mathbb{R}^m)$, we say that μ_j weakly-$*$ converges to μ, in symbols $\mu_j \overset{*}{\rightharpoonup} \mu$, if

$$\lim_{j\to\infty} \int_X u \, d\mu_j = \int_X u \, d\mu \, ,$$

for every $u \in C_0(X)$.

Example A.10 (Dirac masses)**.** For a point $x \in \Omega$ we define the Dirac measure $\delta_x \in \mathcal{M}(\Omega)$ as $\delta_x(U) = 1$ if $x \in U$ and $\delta_x(U) = 0$ if $x \notin U$. Label as x_k the points of $(\mathbb{Z}/j) \times (\mathbb{Z}/j)$ lying in Ω and define the sequence of measures $\mu_j := M_j^{-1} \sum_{k=1}^{M_j} \delta_{x_k}$, where $M_j \approx 1/j^2$ is the number of such points. We have that $\mu_j \overset{*}{\rightharpoonup} \mathcal{L}^2 \llcorner \Omega$.

Thanks to the Riesz duality Theorem, we have the following compactness result.

Theorem A.11 (Weak-$*$ compactness (Theorem 1.59 in [3]))**.** *If $\{\mu_j\} \subset \mathcal{M}(X;\mathbb{R}^m)$ is such that* $\sup_j |\mu_j|(X) < \infty$*, then (up to subsequences) $\mu_j \overset{*}{\rightharpoonup} \mu$ for some μ belonging to $\mathcal{M}(X;\mathbb{R}^m)$. Moreover the norm map $\mu \mapsto |\mu|(X)$ is lower semicontinuous with respect to the weak-$*$ convergence.*

A.2.3 Regularisation of Radon measures

Define $B_r(x) := \{y \in \mathbb{R}^n : |y - x| < r\}$. We recall that a *regularising kernel* is a function $\rho \in C_c^\infty(\mathbb{R}^N)$ such that $\rho(x) \geq 0$, $\rho(x) = \rho(-x)$ for any x, $\operatorname{supp} \rho \subset B_1(0)$, $\int_{\mathbb{R}^n} \rho \, dx = 1$. For $\varepsilon \in (0, 1)$ we define the family of *mollifiers* as $\rho_\varepsilon(x) := \varepsilon^{-n}\rho(x/\varepsilon)$. Let $1 \leq p < \infty$ and $f \in L^p(\Omega)$. The *convolution* of f with ρ_ε is the map

$$(f * \rho_\varepsilon)(x) := \int_\Omega \rho_\varepsilon(x - y) f(y) \, dy$$

for $x \in U_\varepsilon := \{x \in \Omega : \ \mathrm{dist}(x, \partial\Omega) < \varepsilon\}$. We have $f * \rho_\varepsilon \in C^\infty(U_\varepsilon)$ and $f * \rho_\varepsilon \to f$ in $L^p(A)$ for every $A \subset\subset \Omega$.

If $\mu \in \mathcal{M}(\Omega; \mathbb{R}^m)$ we define the function $\mu * \rho_\varepsilon \colon U_\varepsilon \to \mathbb{R}^m$ as

$$(\mu * \rho_\varepsilon)(x) := \int_\Omega \rho_\varepsilon(x - y)\, d\mu(y)\,.$$

Theorem A.12 (see Theorem 2.2 in [3]). *Let $\mu \in \mathcal{M}(\Omega; \mathbb{R}^m)$. Then $\mu * \rho_\varepsilon$ belongs to $C^\infty(U_\varepsilon; \mathbb{R}^m)$. Moreover the measures $\mu_\varepsilon := \mu * \rho_\varepsilon\, dx$ are such that*

$$\mu_\varepsilon \overset{*}{\rightharpoonup} \mu \quad \text{in } \mathcal{M}(A; \mathbb{R}^m) \quad \text{and} \quad |\mu_\varepsilon| \overset{*}{\rightharpoonup} |\mu| \quad \text{in } \mathcal{M}(A)\,,$$

for any fixed $A \subset\subset \Omega$.

A.2.4 Differentiation of measures

We refer to [40, Section 5.2] for this section.

Definition A.13 (Absolute continuity and singlularity). Let $\mu, \nu \in \mathcal{M}(X)$ and $\sigma, \eta \in \mathcal{M}(X; \mathbb{R}^m)$. We say that:

(i) ν is *absolutely continuous* with respect to μ, in symbols $\nu \ll \mu$, if for every $U \in \mathcal{B}(X)$ such that $\mu(U) = 0$ we have $\nu(U) = 0$,

(ii) μ and ν are *mutually singular*, in symbols $\mu \perp \nu$, if there exists $U \in \mathcal{B}(X)$ such that $\mu(U) = \nu(X \setminus U) = 0$,

(iii) σ is *absolutely continuous* with respect to μ if $|\sigma| \ll \mu$,

(iv) σ and η are *mutually singular* if $|\sigma| \perp |\eta|$.

Theorem A.14 (Radon-Nikodym (see Corollary 5.11 in [40])). *Let $\mu \in \mathcal{M}(X; \mathbb{R}^m)$ and $\nu \in \mathcal{M}(X)$. Then there exists a unique pair of measures $\mu^a, \mu^s \in \mathcal{M}(X; \mathbb{R}^m)$ such that*

$$\mu = \mu^a + \mu^s\,, \quad \text{with} \quad \mu^a \ll \nu,\ \mu^s \perp \nu\,.$$

Moreover there exists a unique function $f \in L^1_{\mathrm{loc}}(X, \mu; \mathbb{R}^m)$ such that

$$\mu^a = f\,\nu\,.$$

The function f is denoted as $d\mu/d\nu$ and it is such that

$$\frac{d\mu}{d\nu}(x) = \lim_{r \to 0^+} \frac{\mu(B_r(x))}{\nu(B_r(x))} \tag{A.4}$$

for ν-a.e. $x \in X$.

For $\mu \in \mathcal{M}(X;\mathbb{R}^m)$ we clearly have $|\mu| \ll \mu$. Therefore, as a corollary of the Radon-Nikodym Theorem we have the so called *polar decomposition* of μ.

Corollary A.15 (Polar decomposition (Corollary 1.29 in [3]))**.** *Let $\mu \in \mathcal{M}(X;\mathbb{R}^m)$. Then there exists a unique S^{m-1}-valued function $d\mu/d|\mu| \in L^1_{\mathrm{loc}}(X,|\mu|;\mathbb{R}^m)$ such that $\mu = d\mu/d|\mu|\,|\mu|$. Furthermore $d\mu/d|\mu|$ can be computed by using formula* (A.4) *for $|\mu|$-a.e. $x \in X$.*

Example A.16. As an example, for the measure $\mu := \xi\,\delta_{x_0}$ with $x_0 \in X, \xi \in \mathbb{R}^m \setminus \{0\}$ we have

$$\frac{d\mu}{d|\mu|}(x) = \begin{cases} \dfrac{\xi}{|\xi|} & \text{for } x = x_0, \\ +\infty & \text{otherwise,} \end{cases}$$

since $|\mu| = |\xi|\,\delta_{x_0}$. If instead $\mu := f\,dx$ for some $f \in L^p_{\mathrm{loc}}(X;\mathbb{R}^m)$, then $d\mu/dx = f$.

Consider a function $\varphi\colon \mathbb{R}^m \to [0,\infty]$ and define the functional $H\colon \mathcal{M}(X;\mathbb{R}^m) \to [0,\infty]$ as

$$H(\mu) := \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right)\,d|\mu|\,.$$

We are interested in the properties of such functional, first studied in [56].

First notice that if $\varphi\colon \mathbb{R}^m \to [0,\infty]$ is convex and positively 1-homogeneous, that is, $\varphi(\lambda\xi) = \lambda\varphi(\xi)$ for every $\lambda > 0$, $\xi \in \mathbb{R}^m$, then also H is convex and positively 1-homogeneous. We have the following theorems (see [3, Theorems 2.38, 2.39]).

Theorem A.17 (Reshetnyak)**.** *Let $\varphi\colon \mathbb{R}^m \to [0,\infty]$ be convex and positively* 1-*homogeneous and consider the sequence $\mu_j \in \mathcal{M}(X;\mathbb{R}^m)$. The following statements hold:*

(i) (Reshetnyak lower semicontinuity) *if $\mu_j \overset{*}{\rightharpoonup} \mu$, then*

$$H(\mu) \le \liminf_{j\to\infty} H(\mu_j)\,, \tag{A.5}$$

(ii) (Reshetnyak continuity) *if $|\mu_j|(\Omega) \to |\mu|(\Omega)$, then*

$$\lim_{j\to\infty} H(\mu_j) = H(\mu)\,. \tag{A.6}$$

A.3 Functions with bounded variation

We refer to [3], [20], [40] for this appendix on BV functions. Throughout this section $n, m \geq 1$ and $\Omega \subset \mathbb{R}^n$ is a bounded domain with Lipschitz boundary. For a map u in $L^1(\Omega; \mathbb{R}^m)$ we denote as $Du \in \mathcal{D}'(\Omega; \mathbb{M}^{m\times n})$ its distributional derivative. The entries of Du are given by $(Du)_{ij} = \partial u_i / \partial x_j$, which coincides with the j-th distributional partial derivative of u_i, where $u = (u_1, \dots, u_m)$.

Definition A.18 (BV functions)**.** Let $u \in L^1(\Omega)$. We say that u has *bounded variation* in Ω if its distributional gradient is a vector valued finite Radon measure on Ω, that is, if $Du \in \mathcal{M}(\Omega; \mathbb{R}^n)$. This means

$$\int_\Omega u \operatorname{div} \varphi \, dx = - \int_\Omega \varphi \cdot d\, Du \,,$$

for all $\varphi \in C^1_c(\Omega; \mathbb{R}^n)$. The space of functions of bounded variation is denoted as $BV(\Omega)$.

Analogously we can introduce vector valued functions with bounded variation. If $u \in L^1(\Omega; \mathbb{R}^m)$, we say that $u \in BV(\Omega; \mathbb{R}^m)$ if $Du \in \mathcal{M}(\Omega; \mathbb{M}^{m\times n})$, that is, if

$$\int_\Omega u \cdot \operatorname{Div} \varphi \, dx = - \int_\Omega \varphi : d\, Du \,,$$

for every $\varphi \in C^1_c(\Omega; \mathbb{M}^{m\times n})$. Here we denote $\operatorname{Div} \varphi := (\operatorname{div} f_1, \dots, \operatorname{div} f_m)$ where $f = (f_1, \dots, f_m)$.

Example A.19 (Sobolev functions have bounded variation)**.** The Sobolev space $W^{1,1}(\Omega; \mathbb{R}^m)$ is contained in $BV(\Omega; \mathbb{R}^m)$, since for $u \in W^{1,1}(\Omega; \mathbb{R}^m)$ we have $Du = \nabla u \, \mathcal{L}^n$, where ∇u is the weak derivative of u. Notice that the inclusion is strict: indeed if $\Omega := (-1, 1) \subset \mathbb{R}$ and $u := \chi_{(0,1)}$, then $Du = \delta_0$, so that $u \in BV(-1, 1)$, but $u \notin W^{1,1}(-1, 1)$.

Proposition A.20 (See Proposition 3.2 in [3])**.** *Let $u \in BV(\Omega; \mathbb{R}^m)$ be such that $Du = 0$. Then $u = c$ a.e. in Ω, where $c \in \mathbb{R}^m$ is a constant.*

It is useful to introduce the concept of variation for a BV function u in Ω.

Definition A.21 (Variation)**.** Let $u \in L^1(\Omega; \mathbb{R}^m)$. The variation $V(u, \Omega)$ of u in Ω is defined as

$$V(u, \Omega) := \sup \left\{ \int_\Omega u \cdot \operatorname{Div} \varphi \, dx : \ \varphi \in C^1_c(\Omega; \mathbb{M}^{m\times n}), \ \|\varphi\|_{L^\infty(\Omega)} \leq 1 \right\} .$$

For BV functions the variation enjoys the following properties (see Proposition [3, Proposition 3.6]).

Proposition A.22. *Let $u \in L^1(\Omega;\mathbb{R}^m)$. Then $u \in BV(\Omega;\mathbb{R}^m)$ if and only if $V(u,\Omega) < \infty$. In addition $V(u,\Omega) = |Du|(\Omega)$, where $|Du|(\Omega)$ denotes the total variation of the measure Du. Furthermore the map $u \mapsto |Du|(\Omega)$, defined for $u \in BV(\Omega;\mathbb{R}^m)$, is lower semicontinuous with respect to the $L^1(\Omega;\mathbb{R}^m)$ topology, that is*

$$|Du|(\Omega) \le \liminf_{j\to\infty} |Du_j|(\Omega)$$

for every sequence u_j belonging to $BV(\Omega;\mathbb{R}^m)$ and such that $u_j \to u$ in $L^1(\Omega;\mathbb{R}^m)$.

In view of the above proposition, we will call $|Du|(\Omega)$ the *variation* of u in Ω.

A.3.1 Topologies on BV

For $u \in BV(\Omega;\mathbb{R}^m)$ we define the norm

$$\|u\|_{BV} := \int_\Omega |u|\,dx + |Du|(\Omega)\,.$$

Notice that $BV(\Omega;\mathbb{R}^m)$ equipped with such norm is a Banach space. However the BV norm is too strong for many applications, therefore we introduce two weaker topologies on BV, induced by the so-called weak-$*$ convergence and strict convergence.

Definition A.23 (Weak-$*$ convergence)**.** Let $u_j, u \in BV(\Omega;\mathbb{R}^m)$. We say that u_j weakly-$*$ converges to u in $BV(\Omega;\mathbb{R}^m)$ if $u_j \to u$ in $L^1(\Omega;\mathbb{R}^m)$ and $Du_j \overset{*}{\rightharpoonup} Du$ in $\mathcal{M}(\Omega;\mathbb{M}^{m\times n})$, that is

$$\lim_{j\to\infty} \int_\Omega \varphi\,d\,Du_j = \int_\Omega \varphi\,d\,Du\,,$$

for every $\varphi \in C_0(\Omega)$.

The following proposition characterises weak-$*$ convergence in BV (see [3, Proposition 3.13]).

Proposition A.24 (Characterisation of weak-$*$ convergence)**.** *Let $u_j \in BV(\Omega;\mathbb{R}^m)$. Then u_j weakly-$*$ converges to u in $BV(\Omega;\mathbb{R}^m)$ if and only if $\sup_j \|u_j\|_{BV} < \infty$ and $u_j \to u$ in $L^1(\Omega;\mathbb{R}^m)$.*

Definition A.25 (Strict convergence)**.** Let $u_j, u \in BV(\Omega;\mathbb{R}^m)$. We say that u_j strictly converges to u in $BV(\Omega;\mathbb{R}^m)$ if $u_j \to u$ in $L^1(\Omega;\mathbb{R}^m)$ and

$$\lim_{j\to\infty} |Du_j|(\Omega) = |Du|(\Omega)\,.$$

Notice that strict convergence implies weak-$*$ convergence by Proposition A.24. However the converse is not true. For example $u_j(x) := \sin(jx)/j$ weakly-$*$ converges to 0 in $BV(0,2\pi)$, but $|Du_j|((0,2\pi)) = 4$.

Let us turn our attention to density of smooth functions in BV. Indeed, we have the inclusions

$$C^\infty(\Omega;\mathbb{R}^m) \subset W^{1,1}(\Omega;\mathbb{R}^m) \subset BV(\Omega;\mathbb{R}^m)\,.$$

For $u \in C^\infty(\Omega;\mathbb{R}^m)$, we have

$$|Du|(\Omega) = \int_\Omega |\nabla u|\, dx\,,$$

therefore the closure of $C^\infty(\Omega;\mathbb{R}^m)$ in $BV(\Omega;\mathbb{R}^m)$ with respect to the BV norm coincides with $W^{1,1}(\Omega;\mathbb{R}^m)$. However, $C^\infty(\Omega;\mathbb{R}^m)$ is dense in $BV(\Omega;\mathbb{R}^m)$ with respect to the strict convergence, as stated in the following theorem (see [3, Theorem 3.9]).

Theorem A.26 (Density of smooth functions)**.** *Let $u \in L^1(\Omega;\mathbb{R}^m)$. Then u belongs to $BV(\Omega;\mathbb{R}^m)$ if and only if there exists a sequence u_j belonging to $C^\infty(\Omega;\mathbb{R}^m)$ and such that $u_j \to u$ strictly in $BV(\Omega;\mathbb{R}^m)$, that is, $u_j \to u$ in $L^1(\Omega;\mathbb{R}^m)$ and*

$$\lim_{j\to\infty} \int_\Omega |\nabla u_j|\, dx = |Du|(\Omega)\,.$$

The following theorem provides us with a compactness criterion in BV (see [3, Theorem 3.23]).

Theorem A.27 (Compactness in BV)**.** *Let u_j be a sequence in $BV(\Omega;\mathbb{R}^m)$ and assume that u_j is uniformly bounded in BV norm, i.e.,*

$$\sup\left\{\int_\Omega |u_j|\, dx + |Du_j|(\Omega) :\ j \in \mathbb{N}\right\} < \infty\,.$$

Then there exist a subsequence of u_j (not relabelled) and a function $u \in BV(\Omega;\mathbb{R}^m)$, such that $u_j \to u$ weakly-$*$ in BV, that is $u_j \to u$ in $L^1(\Omega;\mathbb{R}^m)$ and $Du_j \overset{*}{\rightharpoonup} Du$ in $\mathcal{M}(\Omega;\mathbb{M}^{m\times n})$.

A.3.2 Embedding theorems for BV

In this section we will be concerned with embedding theorems for the space $BV(\Omega)$. We start by recalling the classic Poincaré inequality in BV (see [3, Theorem 3.44]).

Theorem A.28 (Poincaré inequality)**.** *Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain. Then there exists a positive constant C, depending only on Ω, such that for every $u \in BV(\Omega)$,*

$$\int_\Omega |u - u_\Omega| \, dx \leq C \, |Du|(\Omega) \, . \tag{A.7}$$

Here the scalar $u_\Omega := 1/|\Omega| \int_\Omega u \, dx$ is the average of u in Ω.

For our applications in Chapter 4, we will need a version of (A.7) for BV functions satisfying a Dirichlet type condition in a region of the domain Ω having positive measure. The precise statement is given in the following theorem.

Theorem A.29 (Poincaré inequality with boundary data)**.** *Let $\Omega \subset \mathbb{R}^n$ be a bounded open domain and let $\Omega' := \{x \in \mathbb{R}^n \colon \operatorname{dist}(x, \Omega) < 1\}$. Fix boundary data $g \in BV(\Omega')$. Then there exists a constant $C > 0$, depending only on Ω' and g, with the following property: for every $u \in BV(\Omega')$ such that $u = g$ a.e. in $\Omega' \setminus \Omega$ we have*

$$\int_{\Omega'} |u| \, dx \leq C \, |Du|(\Omega') \, . \tag{A.8}$$

The proof of this Poincaré type inequality in BV can be easily obtained by applying a standard argument (see for example the proof of Theorem 3.44 in [3]).

Proof. **Step 1.** We first prove inequality (A.8) in the case $g \equiv 0$ in Ω', showing that it holds for some constant $C > 0$ depending only on Ω'. By contradiction, assume that (A.8) is false. Then there exists a sequence $u_j \in BV(\Omega')$ such that $u_j = 0$ a.e. on $\Omega' \setminus \Omega$, and

$$\int_{\Omega'} |u_j| \, dx \geq j \, |Du_j|(\Omega') \, , \quad \text{for every} \quad j \in \mathbb{N}. \tag{A.9}$$

Since the quantities appearing in (A.9) are 1-homogeneous and $u_j = 0$ in $\Omega' \setminus \Omega$, we can rescale u_j so that

$$\int_{\Omega'} |u_j| \, dx = 1 \, , \quad \text{for every} \quad j \in \mathbb{N}. \tag{A.10}$$

Hence (A.9) reads as

$$|Du_j|(\Omega') \leq \frac{1}{j} \, , \quad \text{for every} \quad j \in \mathbb{N} \, . \tag{A.11}$$

From (A.10)-(A.11) we deduce that $\|u_j\|_{BV(\Omega')}$ is uniformly bounded, so that (Theorem A.27) there exists $u \in BV(\Omega')$ such that $u_j \to u$ in $L^1(\Omega')$. From (A.10), u satisfies

$$\int_{\Omega'} |u| \, dx = 1 \, . \tag{A.12}$$

Moreover by the lower semicontinuity of the BV norm with respect to the L^1 convergence (Proposition A.22), from (A.11) we deduce $|Du|(\Omega') = 0$. Since Ω' is connected, Proposition A.20 implies that $u = c$ a.e. in Ω', for some constant $c \in \mathbb{R}$. Since $u = 0$ in $\Omega' \setminus \Omega$, this implies that $u = c = 0$ a.e. in Ω', which contradicts (A.12).

Step 2. Let now $u \in BV(\Omega')$ be such that $u = g$ on $\Omega' \setminus \Omega$. We can conclude our proof by appling the inequality obtained in Step 1 to the function $u - g$,

$$\begin{aligned}\int_{\Omega'} |u| \, dx &\leq \int_{\Omega'} |u - g| \, dx + \int_{\Omega'} |g| \, dx \\ &\leq C(\Omega') \, |D(u - g)|(\Omega') + C(g) \leq C(\Omega', g) \, |Du|(\Omega') \, .\end{aligned}$$

□

We conclude this section with a Sobolev type inequality for $BV(\Omega)$. To this end, let $1 \leq p \leq n$, where n is the dimension of the ambient space, and define the critical exponent

$$p^* := \begin{cases} \dfrac{Np}{N-p} \, , & \text{if} \quad p < n \, , \\ \infty \, , & \text{otherwise.} \end{cases}$$

We have the following embedding theorem (see [3, Theorem 3.49]).

Theorem A.30. *Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with Lipschitz boundary. Then the embedding $BV(\Omega) \hookrightarrow L^{1^*}(\Omega)$ is continuous, that is, there exists a positive constant C depending only on Ω and on the dimension n, such that*

$$\|u\|_{L^{1^*}(\Omega)} \leq C \, \|u\|_{BV(\Omega)} \, ,$$

for every $u \in BV(\Omega)$.

Remark A.31 (Embedding in two-dimensions)**.** Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain. Then Theorem A.30 asserts that the embedding

$$BV(\Omega) \hookrightarrow L^2(\Omega) \, ,$$

is continuous, since $1^* = 2$ in this case.

A.3.3 Sets of finite perimeter

In this section we will introduce the notion of set of finite perimeter, and investigate the main properties. For $E \subset \mathbb{R}^n$ we denote as χ_E its characteristic function.

Definition A.32 (Sets of finite perimeter)**.** Let $E \subset \mathbb{R}^n$ be an $\mathcal{L}^n$-measurable set. For any open set $\Omega \subset \mathbb{R}^n$, we define the perimeter of E in Ω as

$$\mathrm{Per}(E, \Omega) := \sup \left\{ \int_E \operatorname{div} \varphi \, dx : \ \varphi \in C_c^1(\Omega; \mathbb{R}^n) \, , \ \|\varphi\|_{L^\infty(\Omega)} \leq 1 \right\} . \tag{A.13}$$

We say that E has finite perimeter in Ω if $\mathrm{Per}(E, \Omega) < \infty$.

Example A.33 (Regular sets have finite perimeter)**.** Let $\Omega \subset \mathbb{R}^n$ be open , and let $E \subset \mathbb{R}^n$ be a bounded set with C^1 boundary. Hence $\mathcal{H}^{n-1}(\partial E \cap \Omega) < \infty$. Then E has finite perimeter in Ω, and

$$\mathrm{Per}(E, \Omega) = \mathcal{H}^{n-1}(\partial E \cap \Omega) \, , \tag{A.14}$$

that is, the notion of perimeter given in (A.13) coincides with the usual perimeter of E in Ω. To show this claim, it is sufficient to recall that by the Gauss-Green theorem we have

$$\int_E \operatorname{div} \varphi \, dx = - \int_{\Omega \cap \partial E} \varphi \cdot \nu_E \, d\mathcal{H}^{n-1} \quad \text{for every} \quad \varphi \in C_c^1(\Omega; \mathbb{R}^n) \, ,$$

where ν_E is the inner unit normal to E. By using this formula in definition (A.13) it is immediate to show (A.14).

There is a connection between sets of finite perimeter and BV functions, which we will highlight in the following theorem (see [3, Theorem 3.36]).

Theorem A.34. *Let $E \subset \mathbb{R}^n$ be an $\mathcal{L}^n$-measurable set, and let $\Omega \subset \mathbb{R}^n$ be open. We have that E has finite perimeter in Ω if and only if $\chi_E \in BV(\Omega)$. Moreover* $\mathrm{Per}(E, \Omega) = |D\chi_E|(\Omega)$*, and the following generalised Gauss-Green formula holds*

$$\int_E \operatorname{div} \varphi \, dx = - \int_\Omega \varphi \cdot \nu_E \, d\, |D\chi_E| \quad \textit{for every} \quad \varphi \in C_c^1(\Omega; \mathbb{R}^n) \, , \tag{A.15}$$

where $D\chi_E = \nu_E \, |D\chi_E|$ is the polar decomposition of $D\chi_E$, that is, ν_E is the Radon-Nikodym derivative of $D\chi_E$ with respect to $|D\chi_E|$, and it coincides with

$$\nu_E(x) = \lim_{r \to 0^+} \frac{D\chi_E(B_r(x))}{|D\chi_E|(B_r(x))} \, , \tag{A.16}$$

for $|D\chi_E|$-a.e. point $x \in \Omega$.

Notice that, where it is defined, $|\nu_E(x)| = 1$, so that it can be interpreted as a measure theoretic inner normal to E. It is possible to make the Gauss-Green formula (A.15) more precise, by introducing notions of measure theoretic boundary for sets of finite perimeter. To be more precise, we will introduce the reduced boundary $\mathcal{F}E$ and the essential boundary $\partial^* E$. The main feature of these sets is that they are manifolds of dimension $n-1$, they agree $\mathcal{H}^{n-1}$-a.e. (see Theorem A.39) and

$$\mathrm{Per}(E, \Omega) = \mathcal{H}^{n-1}(\mathcal{F}E \cap \Omega) = \mathcal{H}^{n-1}(\partial^* E \cap \Omega)\,.$$

Moreover, for regular sets E, we have that $\mathcal{F}E$ and $\partial^* E$ coincide with the topological boundary ∂E. Let us start with the definition of reduced boundary.

Definition A.35 (Reduced boundary)**.** Let $E \subset \mathbb{R}^n$ be an $\mathcal{L}^n$-measurable set, and let $\Omega \subset \mathbb{R}^n$ be open. Assume that $\mathrm{Per}(E, \Omega) < \infty$. The reduced boundary of E is defined as the set of points

$$\mathcal{F}E := \{x \in \mathrm{supp}\,|D\chi_E| \cap \Omega :\ \nu_E(x) \text{ exists}\}\,,$$

where ν_E is the derivative defined in (A.16). The function

$$\nu_E \colon \mathcal{F}E \to S^{n-1}$$

is called the generalised inner unit normal to E.

Let us introduce a notion of regularity for $\mathcal{H}^k$-measurable sets.

Definition A.36 (Rectifiable set)**.** Let $E \subset \mathbb{R}^n$ be an $\mathcal{H}^k$-measurable set. We say that E is countably k-rectifiable if it is locally the graph of Lipschitz functions, that is, if there exists a sequence of Lipschitz functions $f_j \colon \mathbb{R}^k \to \mathbb{R}^n$ such that

$$E \subset \bigcup_{j=1}^{\infty} f_j(\mathbb{R}^k)\,.$$

The main properties of the reduced boundary for sets of finite perimeter are summarised in the following statement (see [3, Theorem 3.59]).

Theorem A.37 (De Giorgi)**.** *Let $E \subset \mathbb{R}^n$ be an $\mathcal{L}^n$-measurable set. Then $\mathcal{F}E$ is countably $(n-1)$-rectifiable and*

$$D\chi_E = \nu_E\, \mathcal{H}^{n-1} \llcorner \mathcal{F}E\,, \quad |D\chi_E| = \mathcal{H}^{n-1} \llcorner \mathcal{F}E\,.$$

In particular if E *has finite perimeter in* Ω*, then*

$$\mathrm{Per}(E,\Omega) = \mathcal{H}^{n-1}(\mathcal{F}E \cap \Omega)\,.$$

Moreover the Gauss-Green formula (A.15) *reads as*

$$\int_E \operatorname{div} \varphi \, dx = -\int_{\mathcal{F}E\cap\Omega} \varphi \cdot \nu_E \, d\mathcal{H}^{n-1} \quad \textit{for every} \quad \varphi \in C^1_c(\Omega;\mathbb{R}^n)\,. \tag{A.17}$$

Let us analyse the density properties of sets of finite perimeter. For an $\mathcal{L}^n$-measurable set $E \subset \mathbb{R}^n$ we denote by E^t, for $t \in [0,1]$, the set of points where E has density t, that is,

$$E^t := \left\{ x \in \mathbb{R}^n : \lim_{r\to 0^+} \frac{|E \cap B_r(x)|}{|B_r(x)|} = t \right\}.$$

The sets E^1 and E^0 can be considered, respectively, as the measure theoretic interior and exterior of E. This interpretation motivates the following definition of essential boundary.

Definition A.38 (Essential boundary)**.** Let $E \subset \mathbb{R}^n$ be an $\mathcal{L}^n$-measurable set. The essential boundary of E is the set

$$\partial^* E := \mathbb{R}^n \setminus (E^0 \cup E^1)\,,$$

that is, $\partial^* E$ is the set of points where the density of E is neither 1 nor 0.

The relation between the definitions of reduced boundary and essential boundary are made clear in the following theorem (see [3, Theorem 3.61]).

Theorem A.39 (Federer)**.** *Let* $\Omega \subset \mathbb{R}^n$ *be open and let* $E \subset \Omega$ *be such that* E *has finite perimeter in* Ω*. Then*

$$\mathcal{F}E \subset E^{1/2} \subset \partial^* E \quad \textit{and} \quad \mathcal{H}^{n-1}(\partial^* E \setminus \mathcal{F}E) = 0\,,$$

that is, the definitions of boundary $\mathcal{F}E, E^{1/2}, \partial^* E$ *agree* $\mathcal{H}^{n-1}$*-a.e. This implies that* $\mathcal{F}E$ *can be replaced by* $E^{1/2}$ *or* $\partial^* E$ *in the Gauss-Green formula* (A.17)*, and the perimeter of* E *in* Ω *can be computed as*

$$\mathrm{Per}(E,\Omega) = \mathcal{H}^{n-1}(\mathcal{F}E \cap \Omega) = \mathcal{H}^{n-1}(E^{1/2} \cap \Omega) = \mathcal{H}^{n-1}(\partial^* E \cap \Omega)\,.$$

In particular E *has density either* 0 *or* $1/2$ *or* 1 *at* $\mathcal{H}^{n-1}$*-a.e. point* $x \in \Omega$*.*

Example A.40. If $E \subset \mathbb{R}^n$ is a bounded set with Lipschitz boundary, then E has finite perimeter in $\mathbb{R}^n$ and $|D\chi_E| = \mathcal{H}^{n-1} \llcorner \partial E$, that is, the definitions of boundary $\mathcal{F}E, E^{1/2}, \partial^* E$ agree with the topological boundary ∂E (see [3, Proposition 3.62]).

We now define partitions of a set $\Omega \subset \mathbb{R}^n$ in sets of finite perimeter.

Definition A.41 (Caccioppoli partitions)**.** Let $\Omega \subset \mathbb{R}^n$ be an open set. Let $I \subset \mathbb{N}$ and consider a partition $\{E_i\}_{i\in I}$ of Ω. We say that $\{E_i\}_{i\in I}$ is a Caccioppoli partition if

$$\sum_{i\in I} \mathrm{Per}(E_i, \Omega) < \infty\,.$$

As a consequence of Theorem A.39, if $\{E_i\}_{i\in I}$ is a finite Caccioppoli partition of Ω, then $\mathcal{H}^{n-1}$-a.e. point of Ω belongs to exactly one element E_i of the partition, or belongs to the intersection of two (and only two) sets $\mathcal{F}E_i$.

We can now define piecewise constant BV functions.

Definition A.42 (Piecewise constant BV functions)**.** Let $u \in BV(\Omega; \mathbb{R}^m)$. We say that u is piecewise constant in Ω if there exists a Caccioppoli partition $\{E_i\}_{i\in I}$ of Ω and a function $m\colon I \to \mathbb{R}^m$ such that

$$u = \sum_{i\in I} m(i)\, \chi_{E_i}\,.$$

We conclude this section with the statement of the coarea formula. To be more specific, let $u \in BV(\Omega)$. The coarea formula gives a relation between $|Du|(\Omega)$ and the perimeters of its level sets, defined for each $t \in \mathbb{R}$ as

$$E_t := \{x \in \Omega : \; u(x) > t\}\,.$$

The precise statement is given by the following theorem (see [3, Theorem 3.40]).

Theorem A.43 (Coarea formula in BV)**.** *Let $u \in BV(\Omega)$. Then the mapping*

$$t \mapsto \mathrm{Per}(E_t, \Omega)\,,$$

for $t \in \mathbb{R}$, is $\mathcal{L}^1$-measurable. Moreover the set E_t has finite perimeter in Ω for a.e. $t \in \mathbb{R}$, and

$$|Du|(\Omega) = \int_{-\infty}^{\infty} \mathrm{Per}(E_t, \Omega)\, dt\,. \tag{A.18}$$

A.3.4 Fine properties of BV functions and the space SBV

In this section $\Omega \subset \mathbb{R}^n$ is an open bounded set, and $n \geq 2$. We want to analyse local properties of BV functions, to arrive to the decomposition of the derivative Du given in Corollary A.51. Let us start with the definition of approximate limit.

Definition A.44 (Approximate limit)**.** Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $u \in L^1(\Omega; \mathbb{R}^m)$. We say that u has an approximate limit at $x \in \Omega$ if there exists a point $z \in \mathbb{R}^m$ such that

$$\lim_{r \to 0^+} \frac{1}{|B_r(x)|} \int_{B_r(x)} |u(x) - z| \, dx = 0 \,. \tag{A.19}$$

We define the set of approximate discontinuity of u as

$$S_u := \{x \in \Omega \colon \text{(A.19) does not hold}\} \,.$$

For $x \in \Omega \setminus S_u$ the point z given by (A.19) is called approximate limit of u at x, and it is denoted by $\tilde{u}(x)$, while x is called a Lebesgue point.

For L^1 functions we have that the set of approximate discontinuity has Lebesgue measure zero (see [20, Theorem 1, Section 1.7]).

Theorem A.45 (Lebesgue-Besicovitch)**.** *Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $u \in L^1(\Omega; \mathbb{R}^m)$. Then $\mathcal{L}^n(S_u) = 0$ and $u = \tilde{u}$ a.e. in Ω.*

Let us introduce also the notion of approximate jump points, where the function jumps from a value a to a value b along a direction ν. For $r > 0$, $x \in \mathbb{R}^n$ and $\nu \in S^{n-1}$, denote the two halves of $B_r(x)$ obtained by intersecting $B_r(x)$ with the hyperplane $\{y \in \mathbb{R}^n : \ (y - x) \cdot \nu = 0\}$ as

$$B_r^+(x, \nu) := \{y \in B_r(x) \colon (y - x) \cdot \nu > 0\} \,, \ B_r^-(x, \nu) := \{y \in B_r(x) \colon (y - x) \cdot \nu < 0\} \,.$$

We are now ready to give the definition of approximate jump point.

Definition A.46 (Approximate jump points)**.** Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $u \in L^1(\Omega; \mathbb{R}^m)$. We say that a point $x \in \Omega$ is an approximate jump point of u if there exist values $a, b \in \mathbb{R}^m$ with $a \neq b$, and a direction $\nu \in S^{n-1}$, such that

$$\lim_{r \to 0^+} \frac{1}{|B_r^+(x, \nu)|} \int_{B_r^+(x,\nu)} |u(y) - a| \, dy = 0 \,,$$
$$\lim_{r \to 0^-} \frac{1}{|B_r^-(x, \nu)|} \int_{B_r^-(x,\nu)} |u(y) - b| \, dy = 0 \,.$$

The triplet (a, b, ν) is denoted as $(u^+(x), u^-(x), \nu_u(x))$. The set of approximate jump point of u is denoted by J_u. Notice that by definition $J_u \subset S_u$.

Example A.47 (Characteristic functions)**.** Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $E \subset \Omega$ be a set of finite perimeter in Ω. Set $u := \chi_E$. Then the sets S_u and J_u coincide $\mathcal{H}^{n-1}$-a.e. with the essential boundary $\partial^* E$. Moreover the triplet $(u^+(x), u^-(x), \nu_u(x))$ coincides with $(1, 0, \nu_E(x))$ $\mathcal{H}^{n-1}$-a.e. in J_u, where $\nu_E(x)$ is the inner normal of E at $x \in \partial^* E$.

Finally let us introduce the notion of approximate differentiability.

Definition A.48 (Approximate differentiability)**.** Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $u \in L^1(\Omega; \mathbb{R}^m)$. Let $x \in \Omega \setminus S_u$. We say that u is approximately differentiable at x if the exists a matrix $L \in \mathbb{M}^{m \times n}$ such that

$$\lim_{r \to 0^+} \frac{1}{|B_r(x)|} \int_{B_r(x)} \frac{|u(y) - \tilde{u}(x) - L(y - x)|}{r} \, dy = 0 \, .$$

The matrix L is called approximate differential of u at x and we denote it by $\nabla u(x)$. The set of approximate differentiability points of u is denoted by $\mathcal{D}_u$.

For BV functions the sets of approximate discontinuity and approximate jump points have the following properties. (see [3, Theorem 3.78]).

Theorem A.49 (Jump points of BV functions)**.** *Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $u \in BV(\Omega; \mathbb{R}^m)$. The discontinuity set S_u is countably $(n-1)$-rectifiable and $\mathcal{H}^{n-1}(S_u \setminus J_u) = 0$. Moreover*

$$Du \llcorner J_u = (u^+ - u^-) \otimes \nu_u \, \mathcal{H}^{n-1} \llcorner J_u \, .$$

Let us introduce some notation. For $u \in BV(\Omega; \mathbb{R}^m)$ let

$$Du = D^a u + D^s u$$

be the Radon-Nikodym decomposition of the measure Du in absolutely continuous part $D^a u$ and singular part $D^s u$, with respect to $\mathcal{L}^n$ (see Theorem A.14). Recall that the density of $D^a u$ with respect to $\mathcal{L}^n$ is given by the Radon-Nikodym derivative of Du with respect to $\mathcal{L}^n$. The following theorem states that such density coincides $\mathcal{L}^n$-a.e. with the approximate differential ∇u (see [3, Theorem 3.83]).

Theorem A.50 (Approximate differentiability for BV functions)**.** *Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $u \in BV(\Omega; \mathbb{R}^m)$. Then u is approximately differentiable at $\mathcal{L}^n$-a.e. point of Ω. Moreover,*

$$D^a u = \nabla u \, \mathcal{L}^n \, .$$

We are now ready to give the decomposition result for the derivative of BV functions. The measures

$$D^j u := D^s u \llcorner J_u \, , \quad D^c u := D^s u \llcorner (\Omega \setminus S_u)$$

are called, respectively, the jump part of the derivative and the Cantor part of the derivative. As a consequence of Theorems A.49, A.50, and the fact that Du is zero on $S_u \setminus J_u$, we have the following.

Corollary A.51 (Decomposition of derivative)**.** *Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $u \in BV(\Omega; \mathbb{R}^m)$. Then*

$$Du = D^a u + D^s u = D^a u + D^j u + D^c u \, ,$$

with

$$D^a u = \nabla u \, \mathcal{L}^n \, , \quad D^j u = (u^+ - u^-) \otimes \nu_u \; \mathcal{H}^{n-1} \llcorner J_u \, .$$

Finally let us give the definition of special functions with bounded variation.

Definition A.52 (SBV)**.** Let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $u \in BV(\Omega; \mathbb{R}^m)$. We say that u is a special function with bounded variation if the Cantor part of the derivative is zero, that is, if

$$Du = D^a u + D^j u = \nabla u \, \mathcal{L}^n + (u^+ - u^-) \otimes \nu_u \; \mathcal{H}^{n-1} \llcorner J_u \, .$$

The space of special functions with bounded variation is denoted by $SBV(\Omega; \mathbb{R}^m)$.

A.3.5 Extensions and traces of BV functions

Let us start by stating the extension theorem for BV functions (see [3, Proposition 3.21]).

Theorem A.53 (Extension for BV)**.** *Let $\Omega \subset \mathbb{R}^n$ be a bounded open set with Lipschitz boundary, and let A be an open set such that $\overline{\Omega} \subset A$. Then there exists a linear continuous extension operator*

$$E\colon BV(\Omega;\mathbb{R}^m) \to BV(\mathbb{R}^n;\mathbb{R}^m)\,,$$

such that

(i) $Eu = 0$ *a.e. in* $\mathbb{R}^n \setminus A$ *for any* $BV(\Omega;\mathbb{R}^m)$,

(ii) $|DEu|(\partial\Omega) = 0$ *for any* $BV(\Omega;\mathbb{R}^m)$,

(iii) for any $1 \leq p \leq \infty$, *the restriction of* E *to* $W^{1,p}(\Omega;\mathbb{R}^m)$ *induces a linear continuous map between* $W^{1,p}(\Omega;\mathbb{R}^m)$ *and* $W^{1,p}(\mathbb{R}^n;\mathbb{R}^m)$.

We want to briefly comment on the properties of the extension operator E. As stated in the theorem, E depends on the set $A \supset \overline{\Omega}$ chosen. Indeed property (i) means that the extension Eu belongs to $BV(A;\mathbb{R}^m)$. Property (ii) ensures that we are not creating any jump at the boundary $\partial\Omega$ (see Section A.3.4). Finally property (iii) ensures that we can use the same extension operator for Sobolev functions belonging to $W^{1,p}(\Omega;\mathbb{R}^m) \subset BV(\Omega;\mathbb{R}^m)$.

Let us now discuss traces of BV functions, starting with the case of traces defined on a countably $(n-1)$-rectifiable set $\Gamma \subset \Omega$ (see [3, Theorem 3.77]).

Theorem A.54 (Traces on interior rectifiable sets)**.** *Let $\Omega \subset \mathbb{R}^n$ be open and bounded, and let $u \in BV(\Omega;\mathbb{R}^m)$. Assume that $\Gamma \subset \Omega$ is a countably $(n-1)$-rectifiable set oriented by ν. Then for $\mathcal{H}^{n-1}$-a.e. $x \in \Gamma$, there exist values $u_\Gamma^+(x), u_\Gamma^-(x) \in \mathbb{R}^m$, such that*

$$Du \llcorner \Gamma = (u_\Gamma^+ - u_\Gamma^-) \otimes \nu\, \mathcal{H}^{n-1} \llcorner \Gamma\,.$$

The previous theorem allows us to study functions obtained by cutting and pasting BV functions. Indeed, if we consider $u, v \in BV(\Omega;\mathbb{R}^m)$, and we fix a set of finite perimeter $E \subset \Omega$, then we can define

$$w := u\,\chi_E + v\,\chi_{\Omega\setminus E}\,.$$

By Theorem A.37, we know that $\partial^* E$ is $(n-1)$-rectifiable and it is oriented by the inner normal ν_E, so that we can apply the above theorem to study the properties of w (see [3, Theorem 3.84] for a proof).

Theorem A.55 (Cut and paste). *Let $\Omega \subset \mathbb{R}^n$ be open and bounded, $u, v \in BV(\Omega;\mathbb{R}^m)$, and E be a set of finite perimeter in Ω, with $\partial^* E$ oriented by ν_E. Set $w := u\,\chi_E + v\,\chi_{\Omega\setminus E}$. Let $u^+_{\partial^* E}(x), v^-_{\partial^* E}(x) \in \mathbb{R}^m$ be given by Theorem A.54, for $\mathcal{H}^{n-1}$-a.e. $x \in \partial^* E$. Then:*

$$w \in BV(\Omega;\mathbb{R}^m) \quad \textit{if and only if} \quad \int_{\partial^* E} |u^+_{\partial^* E} - v^-_{\partial^* E}|\, d\mathcal{H}^{n-1} < \infty .$$

If $w \in BV(\Omega;\mathbb{R}^m)$, its derivative is given by

$$Dw = Du \llcorner E^1 + (u^+_{\partial^* E} - v^-_{\partial^* E}) \otimes \nu_E\, \mathcal{H}^{n-1} \llcorner \partial^* E + Dv \llcorner E^0 .$$

Let us now turn our attention to boundary traces for BV functions. The main theorem is the following (see [3, Theorems 3.87, 3.88]).

Theorem A.56 (Boundary traces). *Let $\Omega \subset \mathbb{R}^n$ be an open bounded set with Lipschitz boundary, and $u \in BV(\Omega;\mathbb{R}^m)$. For $\mathcal{H}^{n-1}$-a.e. $x \in \partial\Omega$ there exists $u^\Omega(x) \in \mathbb{R}^m$ such that*

$$\lim_{r\to 0^+} \frac{1}{|B_r(x)|} \int_{\Omega \cap B_r(x)} |u(y) - u^\Omega(x)|\, dy = 0 .$$

Moreover there exists a constant $C > 0$ depending only on Ω such that

$$\left\| u^\Omega \right\|_{L^1(\partial\Omega)} \leq C\, \|u\|_{BV(\Omega)} ,$$

for every $u \in BV(\Omega;\mathbb{R}^m)$. In this way the trace operator

$$T \colon BV(\Omega;\mathbb{R}^m) \to L^1(\partial\Omega;\mathbb{R}^m) ,$$

defined by $Tu := u^\Omega$, is linear and continuous. The trace operator is also continuous with respect to the strict convergence on $BV(\Omega;\mathbb{R}^m)$.

If we denote by $\bar{u}$ the extension of u to 0 out of Ω, that is $\bar{u} := u\,\chi_\Omega$, then $\bar{u} \in BV(\mathbb{R}^n;\mathbb{R}^m)$ and

$$D\bar{u} = Du \llcorner \Omega + Tu \otimes \nu_\Omega\, \mathcal{H}^{n-1} \llcorner \partial\Omega ,$$

where ν_Ω is the inner normal to Ω.

Remark A.57 (Definition of traces by density). We remark that the restriction to $W^{1,1}(\Omega;\mathbb{R}^m)$ of trace operator T defined in Theorem A.56 coincides with the usual trace operator for Sobolev functions (see, e.g., [39]). In particular T coincides with the extension by density of the restriction to $\partial\Omega$ of functions belonging to $C^\infty(\overline{\Omega};\mathbb{R}^m)$. Indeed, by Theorem A.26, given $u \in BV(\Omega;\mathbb{R}^m)$, there exists a sequence $u_j \in C^\infty(\overline{\Omega};\mathbb{R}^m)$ such that $u_j \to u$ with respect to the strict convergence. Since by Theorem A.56 the operator T is continuous with respect to the strict convergence, we have that

$$Tu = \lim_{j\to\infty} u_j|_{\partial\Omega}$$

where the limit is in the sense of the strong convergence in $L^1(\partial\Omega;\mathbb{R}^m)$.

Finally, we give the following useful corollary (see [3, Corollary 3.89]).

Corollary A.58. *Let $\Omega \subset \mathbb{R}^n$ be an open bounded set with Lipschitz boundary, and $u \in BV(\Omega;\mathbb{R}^m)$, $v \in (\mathbb{R}^n \setminus \overline{\Omega};\mathbb{R}^m)$. Define the function*

$$w := u\,\chi_\Omega + v\,\chi_{\mathbb{R}^n\setminus\overline{\Omega}}\,.$$

Let Tu and Tv denote the traces of u and v with respect to Ω and $\mathbb{R}^n \setminus \overline{\Omega}$. Then $w \in BV(\mathbb{R}^n;\mathbb{R}^m)$ and

$$Dw = Du \llcorner \Omega + (Tu - Tv) \otimes \nu_\Omega\, \mathcal{H}^{n-1} \llcorner \partial\Omega + Dv \llcorner (\mathbb{R}^n \setminus \overline{\Omega})\,.$$

A.3.6 Anisotropic coarea formula

In this section $\varphi\colon \mathbb{R}^n \to [0,\infty]$ is a convex, positively 1-homogeneous function satisfying

$$c^{-1}|\xi| \le \varphi(\xi) \le c|\xi|\,, \qquad \text{for every} \quad \xi \in \mathbb{R}^n\,, \tag{A.20}$$

for some positive constant c. For a function $u \in BV(\Omega)$ its anisotropic φ-variation is defined as follows

$$\int_\Omega \varphi(Du) := \int_\Omega \varphi\left(\frac{d\,Du}{d\,|Du|}\right) d\,|Du|\,,$$

which is well posed, since we are assuming (A.20). Note that when $\varphi \equiv 1$, the φ-variation coincides with the usual variation $|Du|(\Omega)$. We now want to introduce a notion of anisotropic φ-perimeter. Let $E \subset \mathbb{R}^n$ be a set of finite perimeter in Ω, that is, $\chi_E \in BV(\Omega)$. We can define the anisotropic perimeter of E in Ω as

$$\mathrm{Per}_\varphi(E,\Omega) := \int_\Omega \varphi(D\chi_E)\,.$$

Recall that for every set of finite perimeter one has

$$\mathrm{Per}_\varphi(E,\Omega) = \int_{\partial^* E\cap\Omega} \varphi(\nu_E)\, d\mathcal{H}^{n-1}$$

where $\partial^* E$ is the essential boundary of E and $\nu_E \colon \partial^* E \to S^{n-1}$ denotes the inner unit normal to E, as defined in (A.16). Indeed for $\varphi \equiv 1$ we have $\mathrm{Per}_1(E, \Omega) = \mathcal{H}^{n-1}(\partial^* E \cap \Omega) = \mathrm{Per}(E, \Omega)$.

The following density result holds.

Proposition A.59. *Let $u \in BV(\Omega)$. Then there exists a sequence u_j belonging to $C^\infty(\Omega)$ such that $u_j \to u$ in $L^1(\Omega)$ and $\int_\Omega \varphi(Du_j) \to \int_\Omega \varphi(Du)$.*

Proof. By the density Theorem A.26 there exists a sequence $u_j \in C^\infty(\Omega)$ such that $u_j \to u$ in $L^1(\Omega)$ and $|Du_j|(\Omega) \to |Du|(\Omega)$. Then by Reshetnyak's continuity theorem (see (A.6) in Theorem A.17) we conclude that also $\int_\Omega \varphi(Du_j) \to \int_\Omega \varphi(Du)$. □

We now want to establish an anisotropic coarea formula that relates the φ-variation of a function $u \in BV(\Omega)$ to the φ-perimeter of its level sets E_t defined as $E_t := \{x \in \Omega : \ f(x) > t\}$ for $t \in \mathbb{R}$.

Theorem A.60 (Anisotropic coarea formula)**.** *Let $u \in BV(\Omega)$. Then the mapping*

$$t \mapsto \mathrm{Per}_\varphi(E_t, \Omega)\,,$$

for $t \in \mathbb{R}$, is $\mathcal{L}^1$-measurable. Moreover $\mathrm{Per}_\varphi(E_t, \Omega) < \infty$ *for a.e. $t \in \mathbb{R}$, and*

$$\int_\Omega \varphi(Df) = \int_{-\infty}^{\infty} \mathrm{Per}_\varphi(E_t, \Omega)\, dt\,. \tag{A.21}$$

Idea of the proof. It is easy to prove (A.21) for regular functions. Then the proof in the general case follows by invoking the density result of Proposition A.59. □

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