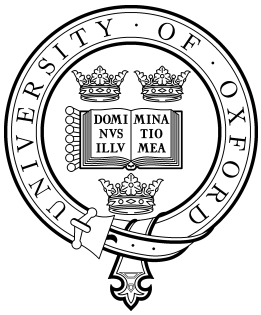
Variational Methods in Materials Science



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A thesis submitted for the degree of
Doctor of Philosophy
in the University of Oxford

Hilary Term 2002

To my grandfather
Georges Cramatte
1917–2001

Abstract

Three problems are being investigated in this thesis. The first two relate to the modelling and analysis of martensitic phase transitions, while the third is concerned with some mathematical tools used in this setting. After a short introduction (Chapter 1) and overviews of the calculus of variations and martensitic phase transformations (Chapter 2), the research part of this thesis is divided into three chapters.

We show in Chapter 3 that for the two wells $\mathrm{SO}(3)U$ and $\mathrm{SO}(3)V$ to be rank-one connected, where the 3×3 symmetric positive definite U and V have the same eigenvalues, it is necessary and sufficient that $\det(U - V) = 0$, a result that does not hold in higher dimensions. Using this criterion and a result of Gurtin, formulæ for the twinning plane and the shearing vector are obtained, which yield an extremely simple condition for the occurrence of so-called compound twins. Our results also provide a simple classification of the twinning mode of the two wells by looking at the crystallographic properties of the eigenvectors of the difference $U - V$. As an illustration, we apply our results to cubic-to-tetragonal, tetragonal-to-monoclinic and cubic-to-monoclinic transitions.

Chapter 4 focuses on the mathematical analysis of biaxial loading experiments in martensite, more particularly on how hysteresis relates to metastability. These experiments were carried out by Chu and James and their mathematical treatment was initiated by Ball, Chu and James. Experimentally it is observed that a homogeneous deformation $y_1(x) = U_1 x$ is the stable state for 'small' loads while $y_2(x) = U_2 x$ is stable for 'large' loads. A model was proposed by Ball, Chu and James which, for a certain intermediate range of loads, predicts crucially that $y_1(x) = U_1 x$ remains metastable (*i.e.*, a local – as opposed to global – minimiser of the energy). This result explains convincingly the hysteresis that is observed experimentally. It is easy to get an upper bound for when metastability finishes. However, it was also noticed that this bound (the Schmid Law) may not be sharp, though this required some geometric conditions on the sample. In this chapter, we rigorously justify the Ball-Chu-James model by means of De Giorgi's Γ-convergence, establish some properties of local minimisers of the (limiting) energy and prove the metastability result mentioned above. An important part of the chapter is then devoted to establishing which geometric conditions are necessary and sufficient for the counter-example to the Schmid Law to apply.

Finally, Chapter 5 investigates the structure of the solutions to the two-well problem. Restricting ourselves to the subset $K = \{H\} \cup \mathrm{SO}(2)V \subset \mathrm{SO}(2)U \cup \mathrm{SO}(2)V$ and assuming the two wells to be compatible, we let T_1 and T_2 denote the two (not necessarily distinct) twins of H on $\mathrm{SO}(2)V$ and ask the following question: if ν_x is a non-trivial gradient Young measure almost everywhere supported on K, does its support necessarily contain a pair of rank-one connected matrices on a set of positive measure? Although we do not provide a solution for the general case, we show that this is true whenever (a) $\nu_x \equiv \nu$ is homogeneous and $\operatorname{supp}\nu \cap \mathrm{SO}(2)V$ is connected, (b) $\nu_x \equiv \nu$ is homogeneous and $T_1 = T_2$ (*i.e.*, when the two wells are trivially rank-one connected) or (c) $\operatorname{supp}\nu_x \subset F$ a.e., for some finite set F. We also establish a more general case provided a strong 'rigidity' conjecture holds.

Acknowledgements

First and foremost, my wholehearted thanks go to my supervisor, John Ball. Over the past three years he has been a continuous source of ideas, suggestions and advice. Working with a man of such broad knowledge, mathematical intuition and scientific rigour has been a marking experience which I shall never forget.

I am also greatly indebted to the Berrow Trust and the Marquis de Amodio for awarding me their scholarship and supporting me financially during my time at Oxford. May they find here the expression of my deepest gratitude. I am also thankful to the TMR Network 'Phase Transitions in Crystals', the London Mathematical Society, Lincoln College, Oxford, and the Isaac Newton Institute, Cambridge for their financial aid which allowed me to attend more conferences than I ever thought I would.

I wish also to thank the past and present members of the group here in Oxford, for answering my questions, no matter how basic they were, for our regular Friday chats in the pub about maths (sometimes) and life in general (more often), and the odd barbecue: Kirill Cherednichenko, Elaine Crooks, Sophia Demoulini, Gero Friesecke, Jan Kristensen, Karsten Matthies, Stéphane Pagano, Roberto Paroni, Anja Schlömerkemper, Ali Taheri and Florian Theil. Elsewhere, I thank Roger Fosdick, Kevin Hane, Richard James, Zhang Kewei, Christian Lexcellent, Mario Pitteri and David Preiss for their useful comments on my talks, my paper, or interesting discussions at various stages of my thesis. And to my undergraduate tutor, Bernard Dacorogna, I am grateful for introducing me to the calculus of variations in the first place and his continuous interest in my work. It is a pleasure to mention my fellow graduate students, past and present, Jonathan Bevan, Kiat Huang, Zamin Iqbal and Mathias Jungen for, amongst other things, mathematical exchanges and cultural activities ranging from a pint of traditional Belgian beer in an Antwerp tavern to the visit of Knossos' splendours. Zam deserves special credit for taking me under his wing upon my arrival on this side of the Channel, making sure I settle well and assuming an elder brother rôle during the first year of my D Phil. We also shared an office during that year which brings me to write about T13. T13 has been so much more than just an office in which my desk happened to be. It has been a place of fun, chat, jokes, bakery tasting, and maths, too. It has been a place of friendship. Thanks thus to Jonathan Woolf (for the week-ends in Cambridge), Richard Thomas (for our nights out watching football and talking about girls), Ivan Smith (for our working and non-working sessions in Blackwell's coffee shop), Zamin Iqbal (for all the above), Louisa Tamplin (for being as cool as it gets), Nathalie Wahl (for bringing an artistic touch to our lives) and Elizabeth Mann (for providing calm and serenity in a sometimes overheated atmosphere). Thanks also go to Tom Fawcett, Manolis Georgoulis and Stelios Koundouros for the cigarette breaks, football in the parks, and discussions in the pub.

An Oxford student's (social) life often revolves mainly around his college and mine was no exception. This page is too short to mention all those people I have met at Lincoln and who have made my years there so enjoyable and unforgettable and an attempt to name them here could only expose a temporary lapse of memory on my part. I thank them all, and will not forget them. Special thanks however go to Alexis Heeb, Jacques Hirsch, and Dave Rhodes for sharing more than their fair part of my ups-and-downs over the years. Elsewhere in Oxford thanks to Pierre Sánchez, a steady source of words of wisdom. I have also a thought for my friends back home in Switzerland who kept in touch despite the daunting obstacle that the Channel sometimes seemed to represent, and amongst which Diego Kuonen deserves a special mention.

I express my deepest gratitude to my parents for offering a listening ear in times of despair, a helpful hand in times of hardship and calling me back every single time throughout these years. I am also sincerely grateful to my late grandfather and to my grandmother for their continuous support, financial or otherwise, throughout my university years. In this thesis, I hope, my family will find my own personal way of saying *Merci*. Thanks finally to Bertrand for nine months of silent, and twenty-seven years of frank and sincere, and rather lively, fraternal friendship.

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1 Introduction

The shape-memory effect is the ability of certain materials to recover, on heating, apparently plastic deformations sustained below a critical temperature. This phenomenon is schematically depicted in Figure 1.1. Consider a single crystal specimen of a given shape (see Figure 1.1a). It is in the austenite phase. Upon cooling the austenite transforms to the martensite. However this happens in such a way that there is no macroscopic change in shape (Figure 1.1b). This is known as *self-accommodation* and was neatly studied by Bhattacharya [35]. When loads are applied to the martensite, it deforms by converting one variant to another and forming a new microstructure (Figure 1.1c). These deformations are macroscopically plastic with strain as large as 10% under very small forces. However, the deformations are recoverable: heating the specimen above the transformation temperature returns each variant of martensite to the unique variant of austenite and the specimen springs back to its original shape. This phenomenon has numerous applications, ranging from microsurgery to ski soles.

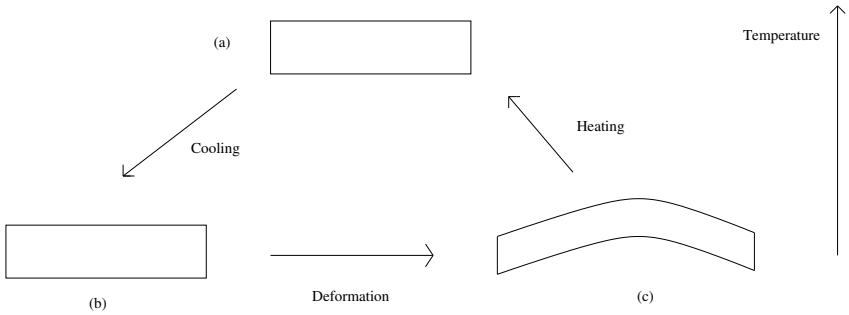


Figure 1.1: The shape-memory effect.

In reality, only certain strains are recoverable: those that can be achieved by the rearrangement of martensitic variants. As a matter of fact, recoverable strains depend dramatically on the type of loading. An important part of this thesis (Chapter 4) is devoted to strains under *load control* (or *dead loads*). We recall that a dead load is a load that remains constant in direction and magnitude per undeformed area as the body deforms. A few remarks on recoverable strains under *displacement control* are made in Chapter 2, although we do not contribute to their study in this thesis.

Mathematically, the problem can be modelled as follows. As is explained in Chapters 2 and 4 we associate to the crystal subjected to a dead load an energy of the type

$$I(y) = \int_\Omega (\varphi(Dy(x)) - \langle T(\sigma), Dy(x)\rangle)\, dx\,, \tag{1.1}$$

which ultimately we seek to minimise. Here Ω is a bounded domain of $\mathbb{R}^3$ (representing the undistorted austenite), $y : \Omega \to \mathbb{R}^3$ is the deformation of the elastic crystal, $\varphi : \mathbb{R}^{3\times 3} \to [0, \infty)$ is the stored-energy density associated to the crystal, and $T : \mathbb{R} \to \mathbb{R}^{3\times 3}$ describes the dead load. We allow T to depend on a loading parameter, σ, because we are interested in the response of the material as the load changes. Finally, $\langle \cdot, \cdot \rangle$ is the Euclidean scalar product in $\mathbb{R}^{3\times 3}$. Because of general symmetry assumptions imposed by solid mechanics (frame indifference, material symmetry), we assume that

$$\varphi^{-1}(0) = \bigcup_{i=1}^{M} \mathrm{SO}(3)U_i\,,$$

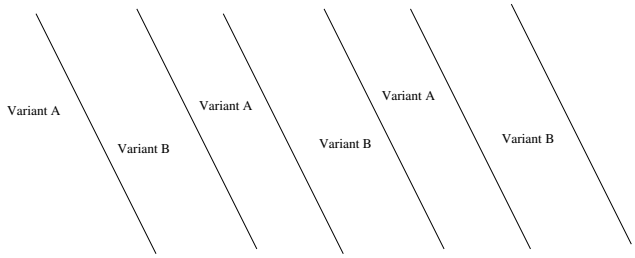


Figure 1.2: A simple laminate.

where the symmetric positive definite U_i have the same eigenvalues. These tensors describe the deformations that transform the higher symmetry parent phase, the austenite, into the lower symmetry martensite phase. We do not include the identity matrix, which represents the austenite, in $\varphi^{-1}(0)$ because we are in the martensite phase, at a temperature θ *below* the critical temperature θ_c at which transformation occurs. In Chapter 2 we explain in greater detail the modelling of martensitic phase transformations as well as overview some mathematical tools to minimise integral functionals.

As alluded to above, the study of (1.1) occupies an important part of this thesis, but before describing this, we concentrate on another problem which also stems from this model and that is dealt with in Chapter 3.

A microstructure that is commonly observed in martensitic phase transitions (not necessarily in the presence of loads, *i.e.*, when, for example, $T \equiv 0$) is the so-called *simple laminate*. This is a microstructure that involves only two variants of martensite, present alternately in very thin layers (Figure 1.2). For this to be possible the two variants must be *compatible*, in the sense that their difference be of rank one (this comes from the *Hadamard jump condition* recalled later). Therefore, it is important to know which variants of martensite are compatible. In precise terms, given two wells $\mathrm{SO}(3)U$ and $\mathrm{SO}(3)V$, where the symmetric positive definite U and V have the same eigenvalues, we want to know whether there exist two matrices F and G, $F \in \mathrm{SO}(3)U$ and $G \in \mathrm{SO}(3)V$ such that $\mathrm{rank}\,(F-G) = 1$. This question is at the core of the first part of this thesis, Chapter 3. We prove that this holds if and only if $\det(U-V) = 0$. Interestingly, the analogous statement in higher dimensions is false. Then, (relatively) simple formulæ for the vectors a and m such that $F - G = a \otimes m$ are deduced. The main ingredients of the proofs are the following. To get the first result, we establish the identity

$$\det(U^2 - V^2) = h(U,V)\det(U-V)$$

for symmetric matrices that have the same eigenvalues, where $h(U,V) > 0$ if U and V are positive definite. We point out that this identity holds trivially, with $h(U,V) = \det(U+V)$, when U and V commute (which is not true for martensitic variants) since then one has $U^2 - V^2 = (U-V)(U+V)$. The second result is obtained by combining two ingredients: the first is that we can relate U and V in a very simple geometric way, if $\det(U-V) = 0$. Our formulæ then follow from a result of Gurtin [81]. An interesting consequence of our formulæ is that they allow one to deduce the twinning mode of two martensitic variants $\mathrm{SO}(3)U$ and $\mathrm{SO}(3)V$ by looking at the eigenvectors of the difference $U - V$ only. As a straightforward consequence, an easy criterion for the existence of a special, yet very commonly observed, kind of laminate, the *compound twins*, is deduced. Three examples close the first part of this thesis: *cubic-to-tetragonal*, *tetragonal-to-monoclinic* and *cubic-to-monoclinic transitions* (where a simple existence criterion for a rare kind of rank-one connection called *non-generic*

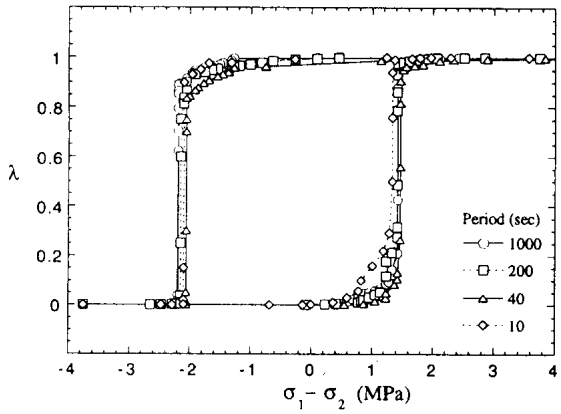


Figure 1.3: Hysteresis loop in biaxial loading experiments.

is obtained). The research contained in this chapter has been published in [76].

Chapter 4 follows the footsteps of Ball, Chu and James [21, 22] on the modelling and mathematical analysis of biaxial loading experiments in martensite and in particular addresses the issue of *hysteresis* as it relates to *metastability*. Let us go back to (1.1), and consider the case where $T(\sigma)$ is of rank two for every σ (this corresponds to biaxial loading, to which we restrict ourselves from now on). Let us vary σ from 0 to 1, say. What is experimentally observed is the following: for small loads, by which we mean for small values of σ, the sample is observed to be homogeneously deformed in a single variant of martensite, variant 1 say. Let us summarise this by saying that for small loads, variant 1 is *stable*. For large loads, it is observed that another variant, 2 say, is stable. Somewhere in the middle, there occurs an exchange of stability, and microstructures combining the two variants can be observed in the sample. (See Figures 4.4 and 4.5 in Chapter 4.) Let us call σ_-, respectively σ_+, the load at which transition occurs when the load is decreased, respectively increased. A plot of the volume fraction λ of variant 2 against σ (written $\sigma_1 - \sigma_2$ for reasons that need not be explained here) is given in Figure 1.3, where a hysteresis loop is clearly observed, because obviously $\sigma_- < \sigma_+$. From this loop the transition stresses can be identified as the value corresponding to $\lambda = 1/2$. For further reference let us write $\sigma_0 = 1/2(\sigma_- + \sigma_+)$.

In [21, 22], Ball et al. argue that the main reason why hysteresis occurs in these experiments is metastability: when loads are increased variant 1 remains metastable after σ_0, up to σ_+, while variant 2 remains metastable after σ_0 (until σ_-) when loads are decreased. If there was no metastability, the transition would occur at σ_0 on the way up as well as on the way down and there would be no hysteresis. An important question is then to estimate σ_+ (an estimate of σ_- then obviously follows, by replacing σ by $1-\sigma$ and interchanging variants 1 and 2).

In the process of estimating the critical load σ_+, an upper bound was first proposed in [21, 22], which the authors showed to be equivalent to a statement otherwise known in the literature as the *Schmid Law*. A natural question thus arises: Is the Schmid Law sharp? By producing an explicit counter-example (in precise terms a three-gradient construction), Ball et al. [21, 22] showed that the Schmid Law is actually not sharp if the sample has an appropriate corner. The main part of Chapter 4 investigates whether this counter-example really requires a special geometry of the sample. We show that these three-gradient constructions do indeed require a corner, at least under some additional assumptions that are typically satisfied in the physical situation. (More precisely, we require that the sample be essentially two-dimensional,

i.e., of the form $\Omega = \omega \times (-h, +h)$ for some $\omega \subset \mathbb{R}^2$ and $h > 0$.) Precise statements are given in Chapter 4, which is organised as follows. After some informal introductory comments, including some words on the experimental setting, we rigorously justify a version of the model proposed by Ball et al. [21, 22] for martensite subjected to biaxial loading. The central tool in our derivation is a (simple) application of Γ-convergence, whose definition we recall in Section 4.2. The limiting model, which we call the *constrained model* following Ball et al. is shown to be equivalent to that introduced by these authors. Essentially, this model consists of minimising the loading term in (1.1) among all maps which satisfy $Dy(x) \in \tilde{K}$ a.e. where $\tilde{K}$ is a set derived from $K = \varphi^{-1}(0)$. ($\tilde{K}$ is in fact the quasiconvex hull of K, which is defined in Chapter 2.) After this we establish some properties of global and local minimisers of the constrained model. In particular we show that for those linear mappings $\bar{y} = Ax$ such that A is a 'strong' extreme point[1] of $\tilde{K}$ the notions of strong and weak local minimisers coincide. In Section 4.3, a version of the *Metastability Theorem* of Ball et al. is proved, explaining rigorously the link between hysteresis and metastability in this theory. The Schmid Law is then shown to provide an upper bound to metastability and we conclude Section 4.3 with the counter-example of Ball et al. in corner-shaped domains. Finally, in Section 4.4 we show that such counter-examples do require the boundary to be singular. Explicit estimates on the singularity are established (Theorem 4.19). Necessary conditions on the geometry of the sample for the counter-example to work are first obtained by building on some reductions that transform the variational problem into a measure-theoretic one and then by a fairly lengthy analysis and some blow-up arguments. Once this is done, these conditions are easily shown to be sufficient, completing the proof. Remarks on some unresolved issues conclude the chapter.

Chapter 5 is not so much concerned with the modelling of martensitic phase transitions as with the mathematical tools used to analyse them. It is an attempt[2] to answer a question which can be described in crude terms as follows. Given a set of matrices, K say, one may ask whether one can construct non-trivial (*i.e.*, non-affine) Lipschitz maps with their gradients lying in K. We have mentioned above the simple laminate construction which clearly shows that the presence of rank-one connections allows one to do precisely this. More generally, one might ask whether sequences of Lipschitz maps whose gradients lie in K but for a set of vanishingly small measure converge to a non-trivial limiting object. In this setting, this limiting object is the *(gradient) Young measure*, the definition of which is recalled in Chapter 2, and non-trivial means not almost everywhere equal to a Dirac mass. While it is known that the absence of rank-one connections in itself does not preclude the existence of non-trivial Lipschitz maps nor that of non-trivial Young measures – two facts which are explained in Chapter 2 – it is known that for a set K of the form

$$K = \mathrm{SO}(2)U \cup \mathrm{SO}(2)V$$

where U and V have equal determinant, this is true. Indeed, if $\mathrm{SO}(2)U$ and $\mathrm{SO}(2)V$ are incompatible, all Lipschitz maps with gradients in K are trivial. So are all Young measures supported on K. On the contrary, if the wells are compatible there exist both non-trivial maps and non-trivial Young measures of these types. However, the structure of these solutions is still unclear. This is the general motivation for our research in this chapter. As a first attempt

[1] The exact hypothesis is that they be *strict exposed points*, a notion we define in Chapter 4. After this research was carried out, Zhang Kewei observed that this result also holds for extreme points, see the remark following Proposition 4.11.

[2] While mathematics is best enjoyed when one solves a problem, one sometimes has to settle for only partial answers, as is the case in this chapter.

we focus on a much simpler problem, where we leave ourselves a minimal number of rank-one connections to play with. More precisely, we take one point on one well, $H \in \mathrm{SO}(2)U$ say, and all of the other well, $\mathrm{SO}(2)V$, and assume that H is rank-one connected to one or two points on $\mathrm{SO}(2)V$. (A point on one well is rank-one connected to either zero, or one, or two points on the other well, as is shown in Chapter 3.) Considering the set $K = \{H\} \cup \mathrm{SO}(2)V$ we ask whether the support of any (non-trivial) gradient Young measure almost everywhere supported on K contains a rank-one connection on a set of positive measure. (There exist non-trivial gradient Young measures whose supports do not contain a rank-one connection almost everywhere, but only on a set of positive measure; such an example is given at the beginning of Chapter 5.) We conjecture that the answer is positive, although we have not succeeded in proving this in general. Nevertheless, we prove the following partial results. Letting ν_x denote a gradient Young measure almost everywhere supported on K, the answer is positive whenever

- $\nu_x \equiv \nu$ is a non-trivial homogeneous gradient Young measure such that $\operatorname{supp}\nu \cap \mathrm{SO}(2)V$ is connected,
- $\nu_x \equiv \nu$ is a non-trivial homogeneous gradient Young measure and $\{H\}$ and $\mathrm{SO}(2)V$ are trivially rank-one connected, that is, there is only one matrix on $\mathrm{SO}(2)V$ compatible with H,
- $\operatorname{supp}\nu_x \subset F$ a.e. for some finite set F.

We deduce that a simple construction that one might think would answer the question negatively is not possible in this context. We also prove a more general result provided a strong rigidity conjecture holds (see Lemma 5.9 and Theorem 5.14). In particular, this conjecture encapsulates the '*exact gradient case*', that every Lipschitz map y such that $Dy \in K$ a.e. but $\{Dy(x)\}$ does not contain any rank-one connection is trivial. We conclude Chapter 5 and indeed this thesis with some ideas which might help solve the general case.

2 Background material

2.1 Introduction

In this chapter we give some background material to this thesis. This is split into two parts. On the one hand we overview some techniques of the multi-dimensional calculus of variations. We also include some basic facts about scalar variational problems for the sake of completeness, even though only vectorial problems are considered in this thesis. Topics covered are existence theorems, relaxation methods, gradient Young measures and generalised convexity conditions of functions and sets. On the other hand, we describe the mathematics of martensitic phase transformations. Beginning with an atomistic setting, we derive a continuum model by means of the Cauchy-Born hypothesis. We then describe some achievements of this theory, in particular its recovering the crystallographic theory of martensite. We also discuss its key hypotheses.

This chapter being an overview, we do not provide proofs, but we give references where they can be found. Also, we do not describe other theories that are used at some stage in this thesis, among which are convex analysis and Γ-convergence. We shall however recall all necessary material when we need it.

2.2 The calculus of variations

A central problem in the calculus of variations consists of minimising an integral of the form

$$I(y) = \int_\Omega \varphi(Dy(x))\,dx\,,$$

over all functions $y : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$, $n \geq 1$, satisfying some given boundary conditions, $y = y_0$ on $\partial\Omega$ say, where $\Omega \subset \mathbb{R}^n$ is open and bounded and $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$ is continuous. We write $\mathbb{R}^{n\times n}$ for the algebra of $n \times n$ matrices with real entries and $Dy(x)$ for the matrix of (weak) partial derivatives of y at x. More general problems can be considered, *e.g.*, when $y : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, $n, m \geq 1$, or when $\varphi = \varphi(x, y, Dy)$ also depends on lower order terms. For the sake of simplicity we restrict ourselves to the case $n = m$ and $\varphi = \varphi(Dy)$ because the problems we are concerned with in this thesis are of this type.

The *direct methods of the calculus of variations*, introduced by Hilbert, Lebesgue and then substantially developed by Tonelli have proved to be one tool to solve this problem, and indeed probably the most successful. Here is the essence of this method. Assuming that $\inf I > -\infty$, take a minimising sequence y^k of I, that is, a sequence such that $I(y^k) \to m = \inf I$ as $k \to \infty$. Assume that:

(*i*) possibly up to a subsequence, y^k converges (in some topology) to a limit y,

(*ii*) I is (sequentially) lower semicontinuous with respect to that topology, *i.e.*, $I(y) \leq \lim I(y^k)$ whenever $y^k \to y$.

Then, we at once conclude that

$$m \leq I(y) \leq \liminf_{k\to\infty} I(y^k) = m\,,$$

so that y *is a global minimiser of* I and we have solved our problem. We now need to introduce the function space X over which we wish to solve our problem. A reasonable[3] function space

[3]This is a subtle point. The infimum of I generally depends upon the space of competing functions (this is the so-called *Lavrentiev phenomenon*). See [31, 43, 102, 105].

ought to be complete under integral-type norms. Thus, spaces of smooth functions, C^1 say, are to be excluded. We thus take X to be a Sobolev space. Recall that for $1 \leq p < \infty$ the Sobolev space $W^{1,p}(\Omega)$ is defined as the space of (equivalence classes of) functions $y : \Omega \to \mathbb{R}$ such that

$$\int_\Omega |y(x)|^p \, dx < \infty \ \text{ and } \ \int_\Omega |Dy(x)|^p \, dx < \infty \,,$$

where Dy denotes the weak (or distributional) derivative of y, and here and throughout this thesis, $|\xi|$ denotes the Euclidean norm of $\xi \in \mathbb{R}^N$ for any N (it being understood, for example, that $\mathbb{R}^{n\times n} \cong \mathbb{R}^{n^2}$). It should be clear from the context what N equals in each case. When $p = \infty$, $y \in W^{1,\infty}(\Omega)$ if

$$\operatorname{ess\,sup} y < \infty \ \text{ and } \ \operatorname{ess\,sup} Dy < \infty \,.$$

Recall that $\operatorname{ess\,sup} y = \inf\{C > 0 : |y| \leq C \text{ a.e. in } \Omega\}$. In other words, for $1 \leq p \leq \infty$, $y \in W^{1,p}(\Omega)$ if and only if $y \in L^p(\Omega)$ and its weak derivative $Dy \in L^p$. See Adams [2] or Brézis [42] for more on these spaces. Furthermore, $L^p(\Omega, \mathbb{R}^n)$ (respectively $W^{1,p}(\Omega, \mathbb{R}^n)$) denotes the space of those mappings whose components lie in $L^p(\Omega)$ (respectively in $W^{1,p}(\Omega)$).

As regards Property (i) we recall that although Sobolev spaces do not enjoy 'good' compactness properties when endowed with their strong topology, their *weak*[4] (*weak-*$*$ if $p = \infty$) topology is well-behaved if $p > 1$, because $W^{1,p}(\Omega)$ is reflexive if $1 < p < \infty$ while $W^{1,1}(\Omega)$ is separable. Thus, a bounded sequence in $W^{1,p}$, $p > 1$, always has a weakly (weakly-$*$ if $p = \infty$) convergent subsequence. (We write '$\rightharpoonup$' ('$\overset{*}{\rightharpoonup}$' if $p = \infty$) to denote weak convergence.) Hence, if we impose some coercivity condition on φ, *e.g.*,

$$\varphi(\xi) \geq -\alpha_1 + \alpha_2 |\xi|^p \,, \ \text{ for all } \xi \in \mathbb{R}^{n\times n}, \tag{2.1}$$

for some $\alpha_1 > 0$, $\alpha_2 > 0$, $p > 1$, and $\varphi(\xi) \to \infty$ as $|\xi| \to \infty$, if $p = \infty$, then Property (i) will be fulfilled.

Achieving Property (ii) is unsurprisingly much less trivial. This is not surprising since the weaker the topology we choose, the harder it is to obtain semicontinuity (because the more convergent sequences there are). As it turns out, we need to distinguish two cases, as the condition ensuring (sequential) weak lower semicontinuity when $n = 1$ differs from that in the case $n > 1$. Throughout this thesis, we mean sequential weak lower semicontinuity whenever we speak of weak lower semicontinuity.

The scalar case

If $n = 1$, then it has been known since the work of Tonelli that the crucial condition ensuring weak lower semicontinuity is the *convexity* of φ.

(2.1) Theorem (Tonelli). *Assume that $\varphi \geq 0$ is convex. Then the functional I is weakly (weakly-$*$ if $p = \infty$) lower semicontinuous on $W^{1,p}(\Omega)$ for all $p \geq 1$. Conversely, if I is*

[4] Let X be a Banach space and let X^* denote its dual. A sequence $x^k \in X$ *converges weakly* if there exists $x \in X$ such that

$$\langle x^k, x^* \rangle \to \langle x, x^* \rangle \ \text{ as } k \to \infty,$$

for every $x^* \in X^*$ and where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between X and X^*. Similarly, a sequence $x_k^* \in X^*$ *converges weakly-*$*$ if there exists $x^* \in X^*$ such that

$$\langle x, x_k^* \rangle \to \langle x, x^* \rangle \ \text{ as } k \to \infty,$$

for every $x \in X$. Recall that if $1 \leq p < \infty$, $(L^p)^* = L^{p'}$ where $\frac{1}{p} + \frac{1}{p'} = 1$.

weakly-∗ lower semicontinuous on $W^{1,\infty}(\Omega)$ *(in particular, if* I *is weakly lower semicontinuous on* $W^{1,p}(\Omega)$*), then* φ *is convex.*

Remark. Various authors contributed to the study of scalar problems of the calculus of variations: Tonelli [151], Serrin [135], De Giorgi [60], Ekeland and Témam [65], Marcellini and Sbordone [109] to name but a few. As stated, Theorem 2.1 and its proof can be found in Buttazzo, Giaquinta and Hildebrandt [43] (sufficiency) and Dacorogna [54] (necessity).

Combining this theorem and the above coercivity condition, we obtain the existence of a global minimiser of I. Let[5] $1 < p < \infty$, $y_0 \in W^{1,p}(\Omega)$ and

$$\mathscr{A} = \{y \in W^{1,p}(\Omega) \,:\, y = y_0 \text{ on } \partial\Omega\}\,,$$

where the boundary condition is understood in the sense of trace. An equivalent way of expressing the boundary condition is that $y \in y_0 + W_0^{1,p}(\Omega)$, where $W_0^{1,p}(\Omega)$ is the closure of $\mathscr{C}_0^\infty(\Omega)$ (smooth, compactly supported functions) in the $W^{1,p}$ norm. Then, we have

(2.2) Theorem. *Assume that* φ *is convex and satisfies* (2.1)*. Assume also that there exists* $\tilde{y} \in \mathscr{A}$ *such that* $I(\tilde{y}) < \infty$*. Then* I *attains its minimum on* $\mathscr{A}$*.*

Remark. Here as well as when $n > 1$, we concentrate on the case $p < \infty$ for simplicity, but similar results may easily be obtained when $p = \infty$.

Although convexity of φ remains sufficient to imply weak lower semicontinuity when $n > 1$, it is far from being necessary.

The vectorial case

The case $n > 1$ is much harder. In his fundamental paper [113] (see also his book [114]), C. B. Morrey introduces the notion of *quasiconvexity* which turns out to be the correct condition ensuring weak lower semicontinuity in higher dimensions.

(2.3) Definition. *A continuous function* $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$ *is* quasiconvex *if*

$$\varphi(\xi) \le \frac{1}{\mathscr{L}^n(D)} \int_D \varphi(\xi + Dy(x))\,dx\,, \tag{2.2}$$

for every bounded domain $D \subset \mathbb{R}^n$*, for every* $\xi \in \mathbb{R}^{n\times n}$ *and every* $y \in \mathscr{C}_0^\infty(D, \mathbb{R}^n)$*. Here* $\mathscr{L}^n$ *denotes the* n*-dimensional Lebesgue measure and* $\mathscr{C}_0^\infty$ *denotes the space of compactly supported, infinitely differentiable mappings.*

Remarks. It can be shown that quasiconvexity does not depend on the domain D; if (2.2) holds for one bounded domain D, then it holds for all such sets. Also, when $n = 1$, we shall see later that quasiconvexity reduces to convexity. However, if $n > 1$, quasiconvexity is a weaker condition (take for example $\varphi(\xi) = \det\xi$, which although quasiconvex is not convex). It should finally be noted that deciding whether a given function is quasiconvex can prove extremely difficult, since it is neither a pointwise, nor local [101], condition. Other, more tractable, notions of convexity have therefore been introduced (one necessary, the other one

[5] The case $p = 1$ is not covered here, nor in the corresponding result in the vectorial case, Theorem 2.5 below. Minimal surfaces problems are of this type, for example. See *e.g.*, [65, 80, 114] for more on this issue.

sufficient) and we shall mention them later, but for the time being we focus on the properties of quasiconvex functions.

We now are in a position to state the semicontinuity result.

(2.4) Theorem. *Assume $|\varphi(\xi)| \le a(|\xi|)$ for every $\xi \in \mathbb{R}^{n\times n}$ where a is an increasing function. If I is weakly-$*$ lower semicontinuous on $W^{1,\infty}(\Omega,\mathbb{R}^n)$ (in particular, if I is weakly lower semicontinuous on $W^{1,p}(\Omega,\mathbb{R}^n)$), then φ is quasiconvex. Conversely, assume that φ is quasiconvex and satisfies the following growth condition for some $1 \le p \le \infty$:*

- *when $p = \infty$,*
$$|\varphi(\xi)| \le a(|\xi|)\,, \quad \text{for all } \xi \in \mathbb{R}^{n\times n},$$
for some continuous and increasing function a,
- *when $1 < p < \infty$,*
$$-\alpha(1+|\xi|^q) \le \varphi(\xi) \le \alpha(1+|\xi|^p)\,, \quad \text{for all } \xi \in \mathbb{R}^{n\times n},$$
for some $\alpha > 0$, $1 \le q < p$,
- *when $p = 1$,*
$$|\varphi(\xi)| \le \alpha(1+|\xi|)\,, \quad \text{for all } \xi \in \mathbb{R}^{n\times n},$$
for some $\alpha > 0$.

Then, I is weakly (weakly-$*$ if $p = \infty$) lower semicontinuous on $W^{1,p}(\Omega,\mathbb{R}^n)$.

Remark. This theorem is essentially due to Morrey [113, 114], and has been refined by Meyers [112], Acerbi and Fusco [1] and Marcellini [107]. See also Dacorogna [54] and the references quoted above for more lower semicontinuity results, *e.g.*, for integrands depending on lower order terms.

Combining this theorem with an appropriate coercivity condition, we get the existence of minimisers of I.

(2.5) Theorem. *Let $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$ be continuous and satisfy*
$$-\alpha_1 + \alpha_2|\xi|^p \le \varphi(\xi) \le \alpha_1(1+|\xi|^p)\,, \quad \text{for all } \xi \in \mathbb{R}^{n\times n},$$
for some $\alpha_1 > 0$, $\alpha_2 > 0$ and $1 < p < \infty$. Let $y_0 \in W^{1,p}(\Omega,\mathbb{R}^n)$ be given. Then I admits a global minimiser in the class
$$\mathscr{A} = \{y \in W^{1,p}(\Omega,\mathbb{R}^n) \,:\, y = y_0 \text{ on } \partial\Omega\}\,.$$

So far so good. We set ourselves a problem and produced a method to solve it, provided three requirements on the integrand φ are satisfied (we concentrate on the vectorial case in this discussion):

(*i*) coercivity, $\varphi(\xi) \ge -\alpha_1 + \alpha_2|\xi|^p$,

(*ii*) growth condition, $\varphi(\xi) \le \alpha_1(1+|\xi|^p)$,

(*iii*) quasiconvexity.

Let us look at each of these separately. Property (*i*) is absolutely vital: without it, we do not know that we can extract a convergent subsequence from a minimising sequence, and we cannot apply the direct methods. Also, this hypothesis is compatible with those imposed by the models we are concerned with in this thesis.

As for the second, however, it is incompatible with the natural condition that $\varphi(\xi) \to \infty$ as $\det \xi \to 0^+$, precluding the interpenetration of matter. On similar grounds, φ should take the value ∞ for all deformation gradients with negative determinant. Note, in this respect, that we only defined quasiconvexity for finite-valued functions. It is not clear how to define quasiconvexity for functions allowed to take infinite values. (We use one possible definition in Chapter 5 in this thesis.) In a celebrated paper, Ball [13] proposed a strengthened convexity condition that he called *polyconvexity* that allows for infinite-valued functions and requires less stringent growth conditions, and obtained existence results in this case. We define polyconvex functions later on in this chapter. In particular Ball was able to deal with the constraint $\varphi(\xi) \to \infty$ as $\det \xi \to 0^+$. In the context of martensitic phase transitions, this constraint can also be handled. See for example Ball and James [28]. However, in this thesis, we assume such a growth condition **despite** its physical shortcomings, see Chapter 4.

Finally, regarding the quasiconvexity assumption, it so happens that in the problems we are concerned with, it is not satisfied (see Section 2.3 below). When this happens, then minimisers might not exist and the infimum of I might not be attained. How should we proceed in this case? There are two possibilities. Both build upon the idea of introducing a *generalised problem* which admits a solution, and view the latter as a generalised minimiser of the original problem.

(a) We replace the non-quasiconvex integrand φ by the largest quasiconvex function smaller than, or equal to, φ. This new function is denoted by φ^{qc} and called the *quasiconvex hull* of φ. Introducing the new variational problem

$$\min\ I^{qc}(y) = \int_\Omega \varphi^{qc}(Dy(x))\,dx\,,$$

we obtain the existence of a minimiser of I^{qc} (by smoothly applying the direct methods) which is interpreted as a generalised minimiser of I. This procedure is called *relaxation* and we will give more details on this shortly. It is perhaps worth pointing out that physically, relaxation corresponds to the passage from a *micro-* to a *macro-energy*.

(b) Instead of changing the integrand we extend the set of admissible functions to a set of admissible measures. More precisely, we use the gradient Young measures which are well-tailored tools to represent limits of nonlinear functions of weakly convergent sequences. We then introduce the generalised variational problem

$$\min\ I^{YM}(\nu) = \int_\Omega \langle \varphi, \nu_x \rangle\,dx\,,$$

over gradient Young measures $\nu = (\nu_x)_{x\in\Omega}$ and where $\langle \varphi, \nu_x \rangle$ denotes the action of the measure ν_x on the function φ. We show below that even if φ does not satisfy a convexity condition, a minimiser exists in this bigger class, which is again considered as a generalised minimiser of I. We also explain the relation between the relaxation methods and the Young measures approach.[6]

[6]Strictly speaking the Young measures approach is also a relaxation method, albeit in a different topology. However, to help distinguish between the two, we only use this terminology once.

Relaxation methods

We concentrate here on the vectorial case $n > 1$ but the theorem we state covers the scalar case, too (see the remarks after Theorem 2.6). Let $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$ be continuous. Then

$$\varphi^{qc} = \sup\{\psi \le \varphi \ : \ \psi \ \text{ quasiconvex}\}$$

is called the *quasiconvex hull* (or *quasiconvexification*) of φ. The following characterisation is due to Dacorogna [53, 54]:

$$\varphi^{qc}(\xi) = \inf\Big\{ \frac{1}{\mathscr{L}^n(D)} \int_D \varphi(\xi + Dy(x))\, dx \ : \ y \in \mathscr{C}_0^\infty(D, \mathbb{R}^n)\Big\}, \tag{2.3}$$

where $D \subset \mathbb{R}^n$ is a bounded domain. In fact, the infimum in (2.3) does not depend on the choice of D. We mention in passing a recent result of Ball, Kirchheim and Kristensen [29] that φ^{qc} is $\mathscr{C}^1$ if φ is. With this definition at hand, we can state the relaxation result.

(2.6) Theorem. *Let $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$ satisfy*

$$-\alpha_1 + \alpha_2|\xi|^p \le \varphi(\xi) \le \alpha_1(1 + |\xi|^p)\ , \quad \text{for all } \xi \in \mathbb{R}^{n\times n},$$

for some $\alpha_1 > 0$, $\alpha_2 > 0$ and $p > 1$. Let us consider the two variational problems

$$\inf\Big\{ I(y) = \int_\Omega \varphi(Dy(x))\, dx \ : \ \ y \in y_0 + W_0^{1,p}(\Omega, \mathbb{R}^n)\Big\}, \tag{$\mathscr{P}$}$$

$$\inf\Big\{ I^{qc}(y) = \int_\Omega \varphi^{qc}(Dy(x))\, dx \ : \ \ y \in y_0 + W_0^{1,p}(\Omega, \mathbb{R}^n)\Big\}, \tag{$\mathscr{P}^{qc}$}$$

where φ^{qc} stands for the quasiconvex hull of φ. Then,

$$\min(\mathscr{P}^{qc}) = \inf(\mathscr{P}).$$

Furthermore, if $\bar{y}$ is a solution of $(\mathscr{P}^{qc})$, there exists a minimising sequence y^k for $(\mathscr{P})$ such that $y^k \rightharpoonup \bar{y}$ in $W^{1,p}$ and $I(y^k) \to I^{qc}(\bar{y})$ as $k \to \infty$. Conversely, since every minimising sequence y^k of $(\mathscr{P})$ is also one of $(\mathscr{P}^{qc})$, up to a subsequence, y^k converges weakly to a solution of $(\mathscr{P}^{qc})$.

Remarks. When $n = 1$, we mentioned earlier that quasiconvexity reduces to the usual convexity, and so $\varphi^{qc} = \varphi^c$, the convex hull of φ, in this case. Thus, this theorem also encapsulates the scalar case. The history of Theorem 2.6 is two-fold. The scalar case dates back to Young [156] (see also [32, 33, 65, 108]). As for the vectorial case, it was first proved by Dacorogna [52, 53] (see also [1]).

We now describe a second way to tackle non-convex variational problems, consisting of enlarging the set of competing functions without changing the integrand.

Young measures

The Young measures, introduced by L.C.Young[7] [156], turn out to be useful tools in order to answer the following question. Take a weakly (but not in general strongly!) convergent

[7] It is fair to mention at this point that Tartar and Di Perna were the first to use Young measures in partial differential equations, triggering their application to other areas of analysis.

sequence in L^p, z^k say, and denote its limit by z. Given a continuous function ψ, we would like to compute the (weak) limit of the sequence $\psi(z^k)$. Except in some exceptional cases, the weak limit is not $\psi(z)$. (This obviously is the case, however, if ψ is linear. If $z^k = Dy^k$ for some y^k, we will see later that there are nonlinear ψ which have this remarkable weak continuity property; see the remarks after Theorem 2.14.) The Young measures allow us precisely to compute the weak limit of $\psi(z^k)$: they are a family of probability measures ν_x such that if $\psi(y^k)$ converges weakly, then the weak limit is the function

$$\bar{\psi}(x) = \int \psi(\xi)\, d\nu_x(\xi) = \langle \psi, \nu_x \rangle \,.$$

We now recall the basic existence theorem for Young measures, see [15, 116, 120, 148].

(2.7) Theorem. *Let $\Omega \subset \mathbb{R}^n$ be a bounded measurable set and let $z^k : \Omega \to \mathbb{R}^N$ be a sequence of measurable functions such that*

$$\sup \int_\Omega a(|z^k(x)|)\, dx < \infty \,, \tag{2.4}$$

where $a : [0,\infty) \to [0,\infty)$ is a continuous nondecreasing function such that $a(t) \to \infty$ as $t \to \infty$. Then, there exists a subsequence, not relabelled, and a family of probability measures $\{\nu_x\}_{x\in\Omega}$ on $\mathbb{R}^N$, depending measurably on $x \in \Omega$, with the following property. Given any measurable $E \subset \Omega$ and a continuous function $\psi : \mathbb{R}^N \to \mathbb{R}$ such that the sequence $\psi(z^k)$ is weakly convergent in $L^1(E)$, the weak limit is the function

$$\bar{\psi}(x) = \langle \psi, \nu_x \rangle = \int_{\mathbb{R}^N} \psi(\xi)\, d\nu_x(\xi) \,.$$

We say that $(\nu_x)_{x\in\Omega}$ is the Young measure *associated to (a subsequence of) z^k and that (up to a subsequence) z^k* generates *$(\nu_x)_{x\in\Omega}$.*

Remarks.

- We often speak of a measure when we really mean a family of measures (or a parametrised measure). We hope this is not too confusing. Also, we say that a Young measure is *trivial* if it is equal to a Dirac mass, *i.e.*, $\nu_x = \delta_{z(x)}$ a.e. for some measurable function z.

- Note that condition (2.4) is a kind of equi-integrability condition (in fact closer to the De La Vallée-Poussin criterion). Thus, if z^k is equi-integrable, it satisfies (2.4). In particular, taking $a(t) = t^p$ we see that a uniformly bounded sequence in L^p has a subsequence with an associated Young measure.

- In fact, the existence of a Young measure is guaranteed under weaker assumptions than those stated in Theorem 2.7 (but then, the associated Young measure may only be a sub-probability measure, for example), see *e.g.*, [15, 116, 120] for more general statements.

- In this thesis, we will always consider sequences z^k that in addition converge in measure to a compact set $K \subset \mathbb{R}^N$, *i.e.*, such that $\mathscr{L}^n(\{x \in \Omega : z^k(x) \notin \mathcal{U}\}) \to 0$ as $k \to \infty$ for all open sets $\mathcal{U} \supset K$. When this holds, the associated Young measure is supported on K almost everywhere: $\operatorname{supp} \nu_x \subset K$ a.e. $x \in \Omega$.

- Suppose z^k is uniformly bounded in $L^p(\Omega,\mathbb{R}^N)$, $1 \le p < \infty$ and that z^k generates a Young measure $(\nu_x)_{x\in\Omega}$ that is a Dirac mass, *i.e.*, $\nu_x = \delta_{z(x)}$ a.e. $x \in \Omega$. Then, $z^k \to z$ strongly in $L^q(\Omega,\mathbb{R}^n)$ for all $1 \le q < p$. More generally, $z^k \to z$ in measure[8] if and only if $\nu_x = \delta_{z(x)}$ a.e. $x \in \Omega$. Obviously, it is always true that if z^k generates a Young measure $(\nu_x)_{x\in\Omega}$ and in addition $z^k \rightharpoonup z$ in L^p, then $z = \langle \mathrm{id}, \nu_x\rangle$ a.e. where $\mathrm{id} : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ is the identity mapping $\mathrm{id}(\xi) = \xi$. In other words, the weak limit of the generating sequence is the centre of mass of the associated Young measure.

- *(Probabilistic interpretation)* It was shown in [15] that the Young measure ν_x gives the limiting local probability distribution of the values taken by z^k in a limitingly small ball around x. More precisely, letting $B(x,r)$ denote the ball centred at x of radius r, define a probability distribution $\nu^k_{x,r}$ by picking points $x' \in B(x,r)$ uniformly at random and observing the values of $z^k(x')$. Thus, for a measurable $E \subset \mathbb{R}^N$,

$$\nu^k_{x,r}(E) = \frac{\mathscr{L}^n(\{x' \in B(x,r) \,:\, z^k(x') \in E\})}{\mathscr{L}^n(B(x,r))}\,.$$

  Then,

$$\nu_x = \lim_{r\to 0}\lim_{k\to\infty} \nu^k_{x,r}\,,$$

  the limits being weak-$*$ limits of measures (*i.e.*, $\langle \phi, \nu^k\rangle \to \langle \phi, \nu\rangle$ for all $\phi \in \mathscr{C}(\mathbb{R}^N)$ with $\phi(\xi) \to 0$ as $|\xi| \to \infty$).

- In effect, any measure on $\mathbb{R}^N$ can arise as the Young measure generated by a sequence. A smaller class of Young measures is that of $W^{1,p}$– *gradient Young measures*, which are generated by a weakly (weakly-$*$ if $p = \infty$) convergent sequence of gradients, $z^k = Dy^k$ for some $y^k \in W^{1,p}(\Omega,\mathbb{R}^n)$, $1 \le p \le \infty$. (Hence a gradient Young measure is a probability measure supported on $\mathbb{R}^{n\times n}$.) This constraint naturally yields some restrictions on the Young measure, and not every probability measure is a gradient Young measure. The following characterisation is due to Kinderlehrer and Pedregal [94, 95]. We start with the case $p = \infty$, which is simpler and which we are concerned with in this thesis.

(2.8) Theorem. *Let $\Omega \subset \mathbb{R}^n$ be open and bounded. A family $(\nu_x)_{x\in\Omega}$ of probability measures on $\mathbb{R}^{n\times n}$ depending measurably on x (* i.e., *$x \to \nu_x(E)$ is measurable for every E) is a $W^{1,\infty}$– gradient Young measure if and only if*

(i) its centre of mass $\bar\nu_x = \langle id, \nu_x\rangle$ is a gradient: there exists $y \in W^{1,\infty}(\Omega,\mathbb{R}^n)$ such that $\bar\nu_x = Dy(x)$ a.e.

(ii) Jensen's inequality holds for every quasiconvex function, i.e.,

$$\langle \psi, \nu_x\rangle \ge \psi(\langle id, \nu_x\rangle) \quad a.e. \tag{2.5}$$

for every quasiconvex function $\psi : \mathbb{R}^{n\times n} \to \mathbb{R}$,

[8] Recall that $z^k \to z$ *in measure* if, for all $\varepsilon > 0$,

$$\lim_{k\to\infty} \mathscr{L}^n(\{x \in \Omega \,:\, |z^k(x) - z(x)| \ge \varepsilon\}) = 0\,.$$

(iii) there exists a compact set $K \subset \mathbb{R}^{n\times n}$ *such that* $\operatorname{supp}\nu_x \subset K$ *a.e.*

We now turn to the case $1 \le p < \infty$.

(2.9) Theorem. *A family* $(\nu_x)_{x\in\Omega}$ *of probability measures on* $\mathbb{R}^{n\times n}$ *depending measurably on* x *is a* $W^{1,p}$*– gradient Young measure if and only if*

(i) there exists $y \in W^{1,p}(\Omega,\mathbb{R}^n)$ *such that* $\bar{\nu}_x = Dy(x)$ *a.e.*

(ii) Jensen's inequality holds for every quasiconvex function $\psi : \mathbb{R}^{n\times n} \to \mathbb{R}$ *that satisfies the growth condition*

$$\psi(\xi) \le \alpha(1 + |\xi|^p)\,,$$

(iii) ν_x *has finite* p^{th} *moment,*

$$\int_\Omega \int_{\mathbb{R}^{n\times n}} |\xi|^p \, d\nu_x(\xi)dx < \infty\,.$$

- A gradient Young measure is called *homogeneous* if it constant a.e. (as a map $x \to \nu_x$). In other words, a gradient Young measure is homogeneous if it does not depend on $x \in \Omega$. Kinderlehrer and Pedregal [94, 95] showed that if $(\nu_x)_{x\in\Omega}$ is a $W^{1,p}$– gradient Young measure, then for almost every $a \in \Omega$, the probability measure $\nu = \nu_a$ is a homogeneous $W^{1,p}$– gradient Young measure (the *Localisation Principle*).
- We conclude these remarks by quoting a result of Zhang [159], to the effect that if Dy^k is bounded in L^p, $p > 1$, and has a Young measure $(\nu_x)_{x\in\Omega}$ with $\operatorname{supp}\nu_x \subset K$ a.e. for some compact set K, then there exists $\tilde{y}^k$ with $D\tilde{y}^k$ bounded in L^∞ having the same Young measure $(\nu_x)_{x\in\Omega}$. In other words, a $W^{1,p}$– gradient Young measure with compact support is a $W^{1,\infty}$– gradient Young measure. We refer to this result as *Zhang's Lemma.*

We are now in a position to explain the use of Young measures in non-convex variational problems. We focus here on the vectorial case $n > 1$ (although similar results exist for the scalar case). Recall that we seek to minimise a functional of the form

$$\inf\Big\{ I(y) = \int_\Omega \varphi(Dy(x))\,dx \;:\; y \in y_0 + W_0^{1,p}(\Omega,\mathbb{R}^n)\Big\}\,, \tag{$\mathscr{P}$}$$

that we introduced the relaxed problem

$$\inf\Big\{ I^{qc}(y) = \int_\Omega \varphi^{qc}(Dy(x))\,dx \;:\; y \in y_0 + W_0^{1,p}(\Omega,\mathbb{R}^n)\Big\}\,, \tag{$\mathscr{P}^{qc}$}$$

and assumed that φ satisfies

$$-\alpha_1 + \alpha_2|\xi|^p \le \varphi(\xi) \le \alpha_1(1 + |\xi|^p)\,,\ \text{ for all } \xi \in \mathbb{R}^{n\times n},$$

for some $\alpha_1 > 0$, $\alpha_2 > 0$ and $p > 1$. Let us define

$$I^{YM}(\nu) = \int_\Omega \langle \varphi, \nu_x\rangle\,dx\,,$$

where $\nu = (\nu_x)_{x\in\Omega}$ is a $W^{1,p}$– gradient Young measure generated by a sequence $y^k \in y_0 + W_0^{1,p}(\Omega,\mathbb{R}^n)$, subject to the compatibility condition that there exist $y \in y_0 + W_0^{1,p}(\Omega,\mathbb{R}^n)$ such that

$$Dy(x) = \langle id, \nu_x \rangle \,.$$

We say that such a ν is *admissible* for I^{YM}, and consider the problem

$$\inf \left\{ I^{YM}(\nu) = \int_\Omega \langle \varphi, \nu_x \rangle \, dx \ : \ \nu \ \text{admissible} \right\}. \qquad (\mathscr{P}^{YM})$$

We have the following results linking $(\mathscr{P})$, $(\mathscr{P}^{qc})$ and $(\mathscr{P}^{YM})$ (see *e.g.*, Pedregal [120]).

(2.10) Theorem. *We have*

$$\min (\mathscr{P}^{YM}) = \min (\mathscr{P}^{\,qc}) = \inf (\mathscr{P}) \,.$$

Furthermore, if $\nu = (\nu_x)_{x\in\Omega}$ is a minimiser of I^{YM}, then the mapping $y \in y_0 + W_0^{1,p}(\Omega,\mathbb{R}^n)$ such that $Dy(x) = \bar{\nu}_x$ a.e. is a minimiser of I^{qc} and

$$\varphi^{qc}(Dy(x)) = \langle \varphi, \nu_x \rangle \ \ a.e.$$

Conversely, if y is a minimiser of I^{qc} and $(\nu_x)_{x\in\Omega}$ is an admissible Young measure such that $\bar{\nu}_x = Dy(x)$ a.e. and

$$\varphi^{qc}(Dy(x)) = \langle \varphi, \nu_x \rangle \ \ a.e.$$

then (ν_x) is a minimiser of I^{YM}. In particular,

$$\operatorname{supp} \nu_x \subset \{\xi \in \mathbb{R}^{n\times n} \ : \ \varphi(\xi) = \varphi^{qc}(\xi)\} \ \ a.e.$$

Remark. In particular, we see that if y^k is a minimising sequence of $(\mathscr{P})$, then up to a subsequence, Dy^k generates a gradient Young measure which is a solution of $(\mathscr{P}^{YM})$.

We mentioned earlier that quasiconvexity being very hard to check in practice, other notions of convexity had been introduced. We recall them now.

Generalised convexity conditions for functions

We start with the following

(2.11) Definition. *A function $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R} \cup \{\infty\}$ is* rank-one convex *if*

$$\varphi(\lambda\xi + (1-\lambda)\eta) \le \lambda\varphi(\xi) + (1-\lambda)\varphi(\eta) \,,$$

for every $0 \le \lambda \le 1$ and every $\xi, \eta \in \mathbb{R}^{n\times n}$ such that $\operatorname{rank}(\xi - \eta) = 1$.

Remarks. In other words, a function is rank-one convex if it is convex along rank-one lines. A weaker notion is separate convexity, requiring convexity only along those (rank-one) lines parallel to the co-ordinate axes. If $\varphi \in \mathscr{C}^2(\mathbb{R}^{n\times n})$ (*i.e.*, finite-valued and twice continuously differentiable), φ is rank-one convex if and only if it satisfies the *Legendre-Hadamard condition*:

$$\sum_{i,j,k,l=1}^{n} \frac{\partial^2 \varphi(\xi)}{\partial \xi_{ij} \partial \xi_{kl}} a_i a_j m_k m_l \ge 0 \,,$$

for all $\xi = (\xi_{ij}) \in \mathbb{R}^{n\times n}$, $a = (a_i), m = (m_i) \in \mathbb{R}^n$. In other words, φ is rank-one convex if $D^2\varphi(a \otimes m, a \otimes m) \geq 0$ for all rank-one matrices $a \otimes m$. Suitably strengthened this is the usual inequality ensuring that the Euler-Lagrange equations (associated to a variational problem with integrand φ) be elliptic.

The next definition, due to Ball [13] simply means that a function is *polyconvex* if it is a convex function of the minors. As noted by Ball, polyconvexity is equivalent to a condition shown by Morrey to be sufficient for quasiconvexity, see [13, 114].

(2.12) Definition. *A function $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R} \cup \{\infty\}$ is* polyconvex *is there exists a convex function $g : \mathbb{R}^{n^2} \times \mathbb{R}^{\binom{n}{2}^2} \times \ldots \times \mathbb{R}^{\binom{n}{n-1}^2} \times \mathbb{R} \to \mathbb{R} \cup \{\infty\}$ such that*

$$\varphi(\xi) = g(T(\xi)),$$

where $T : \mathbb{R}^{n\times n} \to \mathbb{R}^{n^2} \times \mathbb{R}^{\binom{n}{2}^2} \times \ldots \times \mathbb{R}^{\binom{n}{n-1}^2} \times \mathbb{R}$ is defined by

$$T(\xi) = (\xi, \operatorname{adj}_2(\xi), \ldots, \operatorname{adj}_{n-1}(\xi), \det \xi),$$

and where $\operatorname{adj}_s(\xi) \in \mathbb{R}^{\binom{n}{s}^2}$ stands for the matrix of all $s \times s$ minors (subdeterminants) of ξ, $2 \leq s \leq n-1$. To shorten notation, we sometimes write $\tau(n) = \sum_{i=1}^{n} \sigma(s)$, where $\sigma(s) = \binom{n}{s}^2$, so that $g : \mathbb{R}^{\tau(n)} \to \mathbb{R} \cup \{\infty\}$.

Remarks. It is worth realising that in the definition of polyconvexity, the function g need not be unique. As pointed out earlier, an important feature of polyconvexity is that variational integrals with polyconvex integrands can be proved to be weakly lower semicontinuous under less stringent growth conditions than those with quasiconvex integrands, thereby providing existence results in nonlinear elasticity, as first realised by Ball [13].

Let us point out that in the preceding definitions, the functions are allowed to take the value ∞ which was not the case when we defined quasiconvexity. The following relations are due to Morrey [113, 114] and Ball [13]. If $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$, then

$$\varphi \text{ convex} \quad \Rightarrow \quad \varphi \text{ polyconvex} \quad \Rightarrow \quad \varphi \text{ quasiconvex} \quad \Rightarrow \quad \varphi \text{ rank-one convex}, \tag{2.6}$$

while if $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R} \cup \{\infty\}$, we have

$$\varphi \text{ convex} \quad \Rightarrow \quad \varphi \text{ polyconvex} \quad \Rightarrow \quad \varphi \text{ rank-one convex}.$$

In particular, if φ is real-valued and convex, polyconvex, quasiconvex, or rank-one convex, it is locally Lipschitz (and thus continuous), because so is a separately convex function, see [54].

If $n = 1$, then all notions are equivalent, because rank-one convexity then trivially implies convexity. The reverse implications are all false (except that it is still an open problem whether a rank-one convex function is quasiconvex when $n = 2$): see

- Šveràk [142], Müller [115], Alibert and Dacorogna [4] (see also [57]), Zhang [159] for examples of quasiconvex, non-polyconvex functions,
- Šveràk's remarkable article [144] for an example of a rank-one convex, non-quasiconvex quartic polynomial,

- Aubert [5] (or indeed Chapter 5 in this thesis) for an example of an infinite-valued rank-one convex, non-polyconvex function.

Let us mention two examples.

Example. For $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$ that are quadratic (such as in the classical Dirichlet integral), $\varphi(\xi) = \langle M\xi, \xi\rangle$ for[9] some symmetric positive definite $M \in \mathbb{R}^{n^2\times n^2}$, we have:

- φ is rank-one convex if and only if it is quasiconvex. This is due to Van Hove [152, 153].
- If $n = 2$, then

$$\varphi \text{ polyconvex} \quad \Leftrightarrow \quad \varphi \text{ quasiconvex} \quad \Leftrightarrow \quad \varphi \text{ rank-one convex.}$$

  This has received considerable attention, and among those who contributed are Albert [3], Reid [127], Mac Shane [104], Hestenes and Mac Shane [86], Terpstra [150], Serre [134], Marcellini [106].

- If $n \geq 3$, then in general,

$$\varphi \text{ rank-one convex} \quad \not\Rightarrow \quad \varphi \text{ polyconvex.}$$

  This dates back to Terpstra [150] and much later, Serre [134] (see also Ball [14]).

Example. We quote an example due to Dacorogna and Marcellini [57] (see [4] for properties (i) and (iii) below): let $\gamma \in \mathbb{R}$ and define $\varphi : \mathbb{R}^{2\times 2} \to \mathbb{R}$ by

$$\varphi_\gamma(\xi) = |\xi|^2(|\xi|^2 - 2\gamma \det \xi)\,.$$

Then,

(i) φ_γ is convex if and only if $|\gamma| \leq 2\sqrt{2}/3$,

(ii) φ_γ is polyconvex if and only if $|\gamma| \leq 1$,

(iii) there exists $\varepsilon > 0$ such that φ_γ is quasiconvex if and only if $|\gamma| \leq 1 + \varepsilon$,

(iv) φ_γ is rank-one convex if and only if $|\gamma| \leq 2/\sqrt{3}$.

The constant ε in (iii) is not known, but numerical experiments suggest that $1 + \varepsilon = 2/\sqrt{3}$, see [55, 56].

By analogy with the relation between affine and convex functions, we introduce the following

(2.13) Definition. *A function $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$ is* quasiaffine *(*polyaffine, rank-one affine *respectively) if φ and $-\varphi$ are quasiconvex (polyconvex, rank-one convex respectively). A quasiaffine function is sometimes called a* null Lagrangian.

[9] Here, $\langle\cdot,\cdot\rangle$ stands for the scalar product in $\mathbb{R}^{n^2\times n^2}$. In this thesis, we constantly write $\langle\cdot,\cdot\rangle$ to denote the scalar product in $\mathbb{R}^N$, whatever N. It should be clear from the context what we are taking the inner product of.

A theorem of Ball [13] asserts that

(2.14) Theorem. *Let $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$. Then,*

$$\varphi \text{ polyaffine} \quad \Leftrightarrow \quad \varphi \text{ quasiaffine} \quad \Leftrightarrow \quad \varphi \text{ rank-one affine.}$$

Moreover, this holds if and only if there exists $\beta \in \mathbb{R}^{\tau(n)}$ such that

$$\varphi(\xi) = \varphi(0) + \langle \beta, T(\xi)\rangle \,,$$

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

Remarks. When $n = 2$, the only quasiaffine functions are thus of the form

$$\varphi(\xi) = \varphi(0) + \langle \beta, \xi\rangle + \gamma \det \xi \,,$$

while for $n = 3$,

$$\varphi(\xi) = \varphi(0) + \langle \beta, \xi\rangle + \langle \gamma, \operatorname{cof} \xi\rangle + \delta \det \xi \,,$$

where $\operatorname{cof} \xi$ is the cofactor matrix of ξ.

As alluded to earlier, quasiaffine functions enjoy remarkable weak continuity properties, as shown by Reshetnyak [128, 129, 130] and Ball [11, 12, 13] (see also [23]). If $p \geq n$ (to simplify) $\varphi : \mathbb{R}^{n\times n} \to \mathbb{R}$ is weakly continuous, *i.e.*,

$$\varphi(Dy^k) \to \varphi(Dy) \text{ in } \mathscr{D}'(\Omega) \,,$$

whenever $y^k \rightharpoonup y$ in $W^{1,p}(\Omega, \mathbb{R}^n)$ ($y^k \overset{*}{\rightharpoonup} y$ if $p = \infty$) if and only if φ is quasiaffine. Here 'in $\mathscr{D}'(\Omega)$' means 'in distributions'. There being (fully) nonlinear weakly continuous functions is a remarkable feature of the vectorial nature of the problem: if $n = 1$, the only weakly continuous functions are affine.

We now turn to generalised convexity conditions for sets.

Semiconvex hulls of sets

Let us start with a short review on the various ways one can define the convex hull of a set. We concentrate on convex (and later semiconvex) hulls of *compact* sets $K \subset \mathbb{R}^{n\times n}$. Obviously, one traditionally defines the convex hull K^c of K as the smallest convex set containing K. By Carathéodory's Theorem,[10] this can be explicitly computed by taking all possible convex combinations of at most $n^2 + 1$ points in K. From this angle, it is not clear, however, how to generalise this approach to the polyconvex, quasiconvex or rank-one convex equivalents. On the other hand, there are (at least) three characterisations of the convex hull which appear more flexible and thus better equipped in that respect.

- *As the zero set of convex functions.* One can prove that

$$K^c = \{\xi \in \mathbb{R}^{n\times n} : \ \varphi(\xi) = 0 \ \ \forall\, \varphi : \mathbb{R}^{n\times n} \to \mathbb{R} \text{ convex with } \varphi \geq 0 \text{ and } \varphi|_K = 0\} \,.$$

[10] A classical theorem in convex analysis, Carathéodory's Theorem states that the convex hull of a set $A \subset \mathbb{R}^N$ consists of all possible convex combinations of at most $N + 1$ points in A, see [131].

- *As the set of centres of mass of probability measures.* Denoting by $\mathscr{P}(\mathbb{R}^{n\times n})$ the set of all probability measures on $\mathbb{R}^{n\times n}$, we have

$$K^c = \{\bar{\nu} \,:\, \nu \in \mathscr{P}(\mathbb{R}^{n\times n}) \text{ such that } \operatorname{supp}\nu \subset K\}\,.$$

- *As the set of weak limits.* Tartar [148] showed that if $z^k \in L^\infty(\Omega,\mathbb{R}^n)$ is weakly-$*$ convergent to z and $z^k \to K$ in measure, then $z \in K^c$ a.e. Conversely, if $z \in K^c$ a.e. then there exists a sequence $z^k \in L^\infty(\Omega,\mathbb{R}^n)$ converging weakly-$*$ to z in L^∞.

With the first of these different characterisations at hand, we now easily see how to define the corresponding definitions involving polyconvexity, quasiconvexity and rank-one convexity. We will also see that all three views above apply to quasiconvexity, but this is not completely the case neither for polyconvexity nor for rank-one convexity.

(2.15) Definition. *Let $K \subset \mathbb{R}^{n\times n}$ be compact. The* quasiconvex hull *of K, denoted by K^{qc}, is defined by*

$$K^{qc} = \{\xi \in \mathbb{R}^{n\times n} \,:\, \varphi(\xi) = 0 \text{ for every quasiconvex } \varphi \text{ with } \varphi \geq 0 \text{ and } \varphi|_K = 0\}\,. \tag{2.7}$$

The rank-one convex hull K^{rc} *(*polyconvex hull K^{pc} *respectively) of K is defined analogously, by taking rank-one convex functions (polyconvex functions respectively) in* (2.7)*. Sometimes, we use the terminology* polyconvexification*, (*quasiconvexification, rank-one convexification *respectively) instead of polyconvex hull (quasiconvex hull, rank-one convex hull respectively).*

Remarks. Some authors refer to the rank-one convex hull as the *functional rank-one convex hull* but we shall not use this designation.

If K is open rather than compact, a condition like (2.7) will give the *closed* convex and polyconvex hulls (provided the correct test functions are considered, of course). To obtain *open* hulls, we need to consider finite- and infinite-valued functions. Note however, that for the rank-one convex hull, this is not the case: including infinite-valued, rank-one convex φ in (2.7) does not amount to taking the closure of the set obtained by considering only finite-valued rank-one convex functions. In fact, allowing infinite-valued rank-one convex functions in (2.7) defines yet another semiconvex hull, the *lamination convex hull*, the definition of which we shall give shortly. Since we have not defined quasiconvexity for infinite-valued functions, this remark does not apply to the quasiconvex hull. We simply observe that the above definition always delivers a closed quasiconvex hull. In finishing this remark, K reverts to its denoting a compact set of $\mathbb{R}^{n\times n}$ as everywhere else in this thesis.

(2.16) Definition. *A set $U \subset \mathbb{R}^{n\times n}$ is called* lamination convex *if whenever $\xi,\eta \in U$ and* $\operatorname{rank}(\xi-\eta) = 1$*, then $\lambda\xi + (1-\lambda)\eta \in U$ for all $0 \leq \lambda \leq 1$. We define the* lamination convex hull *of a compact set $K \subset \mathbb{R}^{n\times n}$, K^{lc}, to be the smallest lamination convex set containing K.*

Remarks. Some authors call the lamination convex hull the *set-theoretic rank-one convex hull*, but this terminology will not be used in this thesis. We notice that the lamination convex hull of a compact set need not be compact, see [100].

The following implications are a straightforward consequence of the corresponding implications for functions, see (2.6):

$$K \subset K^{lc} \subset K^{rc} \subset K^{qc} \subset K^{pc} \subset K^c\,.$$

We now give several characterisations of the different semiconvex hulls that have just been defined. We refer to [116] (unless stated otherwise) for the proofs.

- We start with the quasiconvex hull. We may see K^{qc} as a set of
  - *Centres of mass of gradient Young measures.* We have
    $$K^{qc} = \{\bar{\nu} \,:\, \nu \text{ homogeneous } W^{1,\infty}\text{- gradient Young measure supported on } K\}\,.$$
    This is an immediate consequence of Kinderlehrer and Pedregal's characterisation of $W^{1,\infty}$– gradient Young measures, Theorem 2.8.
  - *Weak-$*$ limits of gradients.* Equally, if $y^k \in W^{1,\infty}(\Omega,\mathbb{R}^n)$ is such that $Dy^k \to K$ in measure and $Dy^k \overset{*}{\rightharpoonup} Dy$ in L^∞ for some $y \in W^{1,\infty}(\Omega,\mathbb{R}^n)$, then $Dy \in K^{qc}$ a.e. Conversely, if $Dy \in K^{qc}$ a.e. then there exists $y^k \in W^{1,\infty}(\Omega,\mathbb{R}^n)$ such that $Dy^k \overset{*}{\rightharpoonup} Dy$ in L^∞ and $Dy^k \to K$ in measure.
  - *Linear boundary conditions* $\xi \in \mathbb{R}^{n\times n}$ such that there exists a bounded sequence $y^k \in W^{1,\infty}(\Omega,\mathbb{R}^n)$ such that
    $$\begin{cases} Dy^k \to K \text{ in measure in } \Omega, \\ y^k = \xi x \text{ on } \partial\Omega. \end{cases}$$
- We now turn to polyconvexity.
  - The polyconvex hull being the closest to the ordinary convex hull, classical results for the latter can easily be adapted to the former. For example, Carathéodory's Theorem [131] for convex sets yields
    $$K^{pc} = \Big\{\xi \in \mathbb{R}^{n\times n} : T(\xi) = \sum_{i=1}^{\tau(n)+1} \lambda_i T(\xi_i)\,, \xi_i \in K, \lambda_i \geq 0\,,\ \sum_{i=1}^{\tau(n)+1} \lambda_i = 1\Big\}\,,$$
    see Definition 2.12 for the notation and [58] for a proof. Another basic property of the polyconvex hull is that it is the intersection of a convex set with a non-convex constraint. More precisely, letting $\hat{K} = \{T(\xi) \,:\, \xi \in K\}$, then
    $$K^{pc} = \{\xi \in \mathbb{R}^{n\times n} \,:\, T(\xi) \in (\hat{K})^c\}\,.$$
  - In order to give an expression of K^{pc} in terms of probability measures, let us introduce the following classes of measures. Looking back at (2.5), we know that every homogeneous $W^{1,\infty}$– gradient Young measure satisfies Jensen's inequality for all quasiconvex functions. In particular, it satisfies Jensen's inequality for all polyconvex functions. Let us write $\mathscr{M}^{pc}(K)$ ($\mathscr{M}^{qc}(K)$, $\mathscr{M}^{rc}(K)$ respectively) for the set of all probability measures supported on K satisfying Jensen's inequality for polyconvex (quasiconvex, rank-one convex respectively) functions. (We have just explained that $\mathscr{M}^{qc}(K) \subset \mathscr{M}^{pc}(K)$. Similarly, $\mathscr{M}^{rc}(K) \subset \mathscr{M}^{qc}(K)$). One can prove[11] that $\nu \in \mathscr{M}^{pc}(K)$ if and only if
    $$M(\bar{\nu}) = \langle M, \nu\rangle\,,$$

[11] This basically comes from the fact that in the same way as a convex function is the pointwise supremum of all its affine minorants, see [65], one can show that a polyconvex (finite-valued) function is the pointwise supremum of its quasiaffine minorants. See [13, 54]. Then, passing to the limit in the minors relations, we get Jensen's inequality for polyconvex functions, as desired.

for every minor M of order s, $1 \leq s \leq n$, *i.e.*, ν satisfies Jensen's *equality* for all quasiaffine functions. These are the so-called *minors relations*. For short,

$$\mathscr{M}^{pc}(K) = \{\nu \,:\, \nu \text{ satisfies the minors relations}\}\,.$$

Then,

$$K^{pc} = \{\bar{\nu} \,:\, \nu \in \mathscr{M}^{pc}(K)\}\,.$$

- A homogeneous gradient Young measure that satisfies Jensen's inequality, not only for all quasiconvex, but for all rank-one convex functions is called a *laminate*. Thus, the set of all laminates supported on K is precisely $\mathscr{M}^{rc}(K)$. (Pedregal [120] proved that the set of laminates is the weak closure (in the sense of measures) of measures produced from sequences generated by layering rank-one connected gradients.) Then,

$$K^{rc} = \{\bar{\nu} \,:\, \nu \in \mathscr{M}^{rc}(K)\}\,.$$

- We notice that there is no explicit description of the polyconvex and rank-one convex hulls in terms of weak limits of sequences. Only quasiconvexity shares this property with convexity.

- Finally, the lamination convex hull can be obtained by inductively adding rank-one segments, *i.e.*,

$$K^{lc} = \bigcup_{i=1}^{\infty} K^{(i)},\ K^{(1)} = K\,, \tag{2.8}$$

and $K^{(i+1)} = K^{(i)} \cup \{\lambda\xi + (1-\lambda)\eta \,:\, \xi, \eta \in K^{(i)}, \operatorname{rank}(\xi - \eta) \leq 1,\ 0 \leq \lambda \leq 1\}$.

We refer to [63, 160, 162, 161] for more on these generalised convex hulls. Let us now mention some examples of sets and their semiconvex hulls. We point out that in practice they are extremely hard to compute and only relatively simple cases can at present be handled. We start with some finite sets.

- If $K = \{A, B\} \in \mathbb{R}^{n\times n}$ consists of two matrices, it has been shown by Ball and James [27] that

$$K^{lc} = K^{qc} = K^{pc} = \begin{cases} K = \{A, B\} & \text{if } \operatorname{rank}(A-B) > 1 \\ [A, B] & \text{if } \operatorname{rank}(A-B) \leq 1 \end{cases}.$$

Here $[A, B] = \{\lambda A + (1-\lambda)B \,:\, 0 \leq \lambda \leq 1\}$. We say that two matrices A, B are *rank-one connected* (or *compatible*) if $\operatorname{rank}(A-B) \leq 1$. Rank-one connections play an essential rôle here because they precisely constitute the simplest jump discontinuity for Sobolev functions: the gradient of a $W^{1,\infty}$ mapping can take the two constant values A and B on either side of a hyperplane if and only if $\operatorname{rank}(A-B) = 1$ and the plane is the kernel of $A-B$ (the *Hadamard jump condition*). Hence, if A and B are compatible we can construct a sequence of rapidly oscillating mappings whose gradients converge weakly to a convex combination of A and B. Thus the quasiconvex hull of A and B is not trivial. On the other hand, if $\operatorname{rank}(A-B) > 1$, then the quasiconvex hull is trivial. Thus, a sufficient condition for a set K to support non-trivial gradient Young measures is that K contain at least one rank-one connection. Is it necessary? This question was first asked by Tartar [148], who conjectured that the answer was positive. As we shall see shortly this is not the case.

- If $K = \{A_1, A_2, A_3\}$, the quasiconvex hull has been computed by Šveràk [141, 143] and Zhang [158]. First of all, if K does not contain any rank-one connections, then $K^{qc} = K$. Moreover, any gradient Young measure supported on K is not only trivial, but homogeneous, that is $\nu_x \equiv \delta_{A_i}$ for some i. We point out that although this set seems fairly simple, the proof required to show that its quasiconvex hull is trivial is anything but trivial. (Šveràk produced two proofs: one using deep, non-standard regularity results for the Monge-Ampère equation [141], the other using clever quasiconvex functions that he constructed [143].) We observe that even without rank-one connections, K^{pc} may be non-trivial, as is well-known [147]. We come across an example of this fact in Chapter 5 in this thesis. If there are rank-one connections, then K^{qc} is not trivial. The exact form of K^{qc} depends on where the rank-one connections are. For example, if there are two rank-one connections, A_1 and A_2 on the one hand and $\lambda A_1 + (1-\lambda)A_2$ and A_3 for some $0 < \lambda < 1$ on the other, the quasiconvex hull equals

$$K^{qc} = K^{lc} = K^{pc} = [A_1, A_2] \cup [\lambda A_1 + (1-\lambda)A_2, A_3]\,.$$

  As a matter of fact, Young measures supported on a set K with these rank-one connections are thoroughly studied in Chapter 4, Section 4.4 below.

- If $K = \{A_1, A_2, A_3, A_4\}$, K^{qc} need not be trivial, even if K contains no rank-one connections. There is an example[12] of four incompatible matrices whose quasiconvex hull is not trivial, see Figure 2.1. The idea here is to borrow four additional matrices, J_1, J_2, J_3 and J_4 in Figure 2.1, which offer rank-one connections with the A_i, build a sequence of gradients that use them in small proportions and them remove them successively to end up with a Young measure supported only on $\{A_1, A_2, A_3, A_4\}$. See [39] for a detailed exposition of this construction, sometimes referred to as a *Tartar square*. Obviously, K^{lc} is trivial in this case. Sets of four matrices are extensively studied in

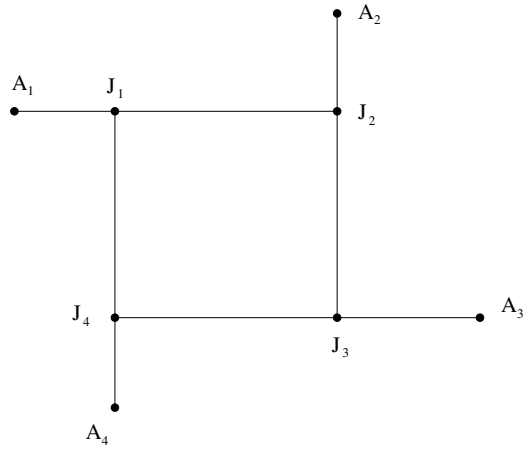


Figure 2.1: A set of four incompatible matrices whose quasiconvex hull is not trivial. Solid lines are rank-one connections. Notice that J_1 is compatible with A_1 and J_2, that J_2 is on the rank-one line joining A_2 and J_3 which itself is on that joining A_3 and J_4. In turn, J_4 is compatible with A_4 and J_1.

[12] It seems that this example has been discovered independently by many authors in different contexts. The most accurate historical review in that respect is due to Müller [116] who quotes Scheffer [133], Aumann and Hart [6], Casadio-Tarabusi [46] and Tartar [149]. See also [39, 116].

[48, 49]. In particular Chlebìk and Kirchheim show that even if the quasiconvex hull is not trivial, the *exact gradient* problem has no non-trivial solutions: every Lipschitz map y such that $Dy \in K$ a.e. is affine. This however is false for five or more matrices, see Kirchheim and Preiss [96].

We now turn to sets motivated by the modelling of phase transitions in crystals, see Section 2.3. Some of these, and indeed those of interest to us in this thesis, are of the form

$$K = \bigcup_{i=1}^{M} \mathrm{SO}(n)U_i\,,$$

where $\det U_i > 0$ for $i = 1, \ldots, M$. (In fact, all the U_i have the same eigenvalues and in particular, the same determinant.)

- *The one-well problem.* We start with the simplest case, when $M = 1$. Then one can show that there are no rank-one connections within the well (see Chapter 3 for a proof of this fact) and it has been proved that $K^{qc} = K$ in this case, whatever the dimension n. Moreover, any gradient Young measure supported on K is homogeneous. See [16, 28, 93, 116].

- *The two-well problem.* The situation becomes more complicated in this case.

  - In two dimensions, that is if $n = 2$, it is known that if the two wells are not compatible (*i.e.*, that there are no rank-one connections between them) then the quasiconvex hull is trivial (see [38, 39, 110, 145, 146] – in [38, 39, 146], this is proved for an arbitrary number of wells, not just two). In fact, any gradient Young measure supported on two incompatible wells is trivial and homogeneous, [110, 145]. On the other hand, if there exists a rank-one connection between the two wells, the quasiconvex hull is not trivial. The hull was completely characterised by Šveràk in [146]; if the two wells have equal determinant, 1 say, the quasiconvex hull corresponds to the intersection of the convex hull with the constraint $\det = 1$. See also [38].
  - In three dimensions, the quasiconvex hull was computed by Ball and James [28] in the case when the two wells have equal determinants and are non-trivially rank-one connected (each point in each well is rank-one connected to exactly two points on the other, see Chapter 3 where the existence of rank-one connections between two wells is investigated). We use their formula in the proof of Lemma 4.17 in Chapter 4 below. In fact they proved that K^{pc} and K^{lc} coincide and that $K^{lc} = K^{(2)}$ in (2.8). To our knowledge, nothing is known if the wells do not have the same determinant. If the two wells are incompatible, the question is still open. The best results are due to Dolzmann, Kirchheim, Müller and Šveràk [64] who have shown that
    - K^{rc} is always trivial.
    - K^{qc} is trivial if the two wells are not too 'far apart' (see [64] for details) because so is K^{pc}. However, if not, then the polyconvex hull may be non-trivial, and then it is not clear what happens with the quasiconvex hull.

    See also [110, 111, 146] for earlier work on this problem.

- For three or more wells in three dimensions hardly anything is known. This is a huge and unwelcome obstacle, for most interesting phase transitions do involve three wells or more (*e.g.*, cubic-to-tetragonal, when $M = 3$ or cubic-to-orthorhombic, when $M = 6$ and with which we are concerned in Chapter 4). We mention that Friesecke has a formula for the polyconvex hull of three non-trivially rank-one connected wells of equal determinant [77]. However, the quasiconvex hull remains unknown.

We conclude this section by noting that in the examples above, all the wells were assumed to have positive determinant. This is of paramount importance: if the sign of the determinants is not constant, then even in two dimensions two incompatible wells can support a non-trivial gradient Young measure, see [47].

2.3 Martensitic phase transitions in elastic crystals

A martensitic transformation is a solid-to-solid phase transformation observed in various crystalline solids (*e.g.*, metals, alloys, ceramics and even biological systems). We mentioned earlier the example of the shape-memory effect, but martensitic transformations are involved in many other phenomena of practical interest, the oldest and most significant of which is strengthening steel. They are named after the German microscopist, Adolf Martens, who in the 1890s was the first to observe many patterns at the micron scale in steel. In these transitions, the lattice structure of the crystal changes abruptly at some temperature: there is a loss of symmetry between the high symmetry, (most often) high temperature phase called *austenite* and the low symmetry, (most often) low temperature phase called *martensite*. Essential features of these transformations are that they are *first-order* (or discontinuous) and *diffusionless*. In other words, the change of symmetry between the parent phase, the austenite, and the product phase, the martensite is sudden and a graph of lattice parameters vs. temperature shows a marked discontinuity. Furthermore, there is no diffusion of atoms during this transformation. Another striking feature of these transformations is the occurrence of very fine geometric patterns, or *microstructures*, that can be seen on scales that vary from material to material but that can be as small as a few atomic spacings. To give an example, the scale of the micrographs showed in Figures 4.4 and 4.5 in Chapter 4 in this thesis is of the order of the millimetre.

Before embarking upon describing the model we use in this thesis we should like to point out that our presentation is by no means exhaustive. We follow the ideas of Ball and James [25, 27, 28] as presented in their papers or in those of other authors that are closely related [35, 36, 37, 83, 90, 103, 116, 121, 126]. Also, we should mention that this approach is influenced by earlier work by Ericksen, among others, [66, 68, 70, 74, 75, 91, 93] to which the reader is referred for further details. We see[13] a crystal as a Bravais lattice $\mathscr{L}(e_i)$, *i.e.*, an infinite set of points in three-dimensional space generated by the translation of a single point o through integer multiples of three linearly independent lattice vectors $\{e_1, e_2, e_3\}$, which define a *unit cell*. Without loss of generality, we assume that o is the origin. For later use, we introduce the symmetry group

$$\mathscr{G} = \{M = (m_{ij}) \in \mathbb{R}^{3\times 3} : \det M = \pm 1 \ , \ m_{ij} \in \mathbb{Z}\} \, ,$$

[13] If this representation seems obvious, it is then worth mentioning that more complicated structures do exist in Nature (*e.g.*, *multi-lattices*, which cannot be represented in this way, see [126]) but we do not consider them here.

consisting of those deformations that map the lattice back onto itself. Furthermore, we define the *(Laue) point group*

$$\mathscr{P} = \mathscr{G}(\mathscr{L}) \cap \mathrm{SO}(3)\,.$$

Notice that a key difference between $\mathscr{G}$ and $\mathscr{P}$ is that the former contains large shears that leave the lattice invariant whereas the latter crucially does not. In all examples we encounter in this thesis, $\mathscr{P}$ is a (not necessarily proper) subgroup of the *cubic point group* consisting of those 24 rotations mapping a unit cube back into itself. We assume that the *free energy density* of the lattice $\mathscr{L}(e_i)$ at a temperature θ is given by $\hat{\phi} = \hat{\phi}(e_i, \theta)$. We require that the energy density satisfy two properties.

(i) (*Frame-indifference*) We assume that a rigid rotation of the lattice, or a change of frame, does not change the energy density,

$$\hat{\phi}(Re_i, \theta) = \hat{\phi}(e_i, \theta)\,, \quad \text{for all } R \in \mathrm{SO}(3).$$

(ii) (*Material symmetry*) We assume that the energy density does not depend on the choice of lattice vectors,

$$\hat{\phi}(e_i M) = \hat{\phi}(e_i)\,, \quad \text{for all } M \in \mathscr{G}.$$

Since we want to exclude large lattice-preserving shears (more associated with plasticity than the elastic viewpoint adopted here) we restrict the requirement (ii) to the point group $\mathscr{P}$. Why this can be done is rather subtle and uses the notion of an Ericksen-Pitteri neighbourhood [66, 122]. We refer to [28] for more on this. In order to pass from this lattice point of view to a continuum theory, we invoke the *Cauchy-Born hypothesis* [68].[14] The idea is the following. Imagine that at each point x in a reference configuration Ω there is a Bravais lattice with lattice vectors $\{e_i^o(x)\}$. Now suppose that the solid undergoes a deformation $y(x)$ (due to a change in temperature, for instance). Letting $F(x) = Dy(x)$ denote the deformation gradient and $e_i(x)$ the lattice vectors of the deformed lattice, the Cauchy-Born hypothesis states that

$$e_i(x) = F(x)e_i^o(x)\,.$$

In other words, the lattice vectors behave like 'material filaments'. We are now ready to state our continuum theory. Let $\Theta \subset \mathbb{R}$ be an interval of temperatures containing the critical temperature θ_c at which the martensitic transformation occurs and let us take the undistorted austenite at $\theta = \theta_c$ as our reference configuration, which we denote by Ω. Hence, e_i^o are taken to be the lattice vectors, and $\mathcal{P}$ the point group, of the austenite. We define a continuum free energy density $\varphi = \varphi(F, \theta)$ depending on the change of shape and the temperature by setting

$$\varphi(F, \theta) = \hat{\phi}(Fe_i^o, \theta)\,.$$

Having defined φ from $\hat{\phi}$, the former inherits properties from the latter:

(i) (*Frame-indifference*) $\varphi(RF, \theta) = \varphi(F, \theta)$ for all $R \in \mathrm{SO}(3)$.

(ii) (*Material symmetry*) $\varphi(FQ) = \varphi(F)$ for all $Q \in \mathscr{P}$.

[14] It is important to realise that it is a *hypothesis* as opposed to a *rule*: Friesecke and Theil [79] recently showed that in a simple example, the Cauchy-Born hypothesis does not necessarily hold in a rigorously derived continuum model.

We also assume φ to be bounded from below with respect to F for each $\theta \in \Theta$ and so, by adding a suitable function of θ we may assume that

$$\min_F \varphi(F,\theta) = 0\,.$$

Let

$$K(\theta) = \{F\,:\,\varphi(F,\theta) = 0\}\,.$$

By frame-indifference and material symmetry,

$$RK(\theta)Q = K(\theta)\,, \tag{2.9}$$

for every $R \in \mathrm{SO}(3)$ and $Q \in \mathscr{P}$. Since we want to model a phase transition and therefore, an exchange of stability at $\theta = \theta_c$, we assume that for $\theta \geq \theta_c$, $\varphi(\alpha(\theta)\mathbb{I},\theta) \leq \varphi(F,\theta)$ for all F and for some function $\alpha = \alpha(\theta)$ (describing the thermal expansion of the austenite) with $\alpha(\theta_c) = 1$, whereas for $\theta \leq \theta_c$ we assume that there exists a tensor $U(\theta) \neq \alpha(\theta)\mathbb{I}$ that minimises $\varphi(\cdot,\theta)$. Thus, while above θ_c (a scalar multiple of) the identity matrix minimises the energy, below θ_c, the minimiser is the matrix $U(\theta)$ which represents the deformation transforming the austenitic lattice into the martensitic lattice. Taking into account (2.9), we thus have assumed that[15]

$$K(\theta) = \begin{cases} \alpha(\theta)\,\mathrm{SO}(3) & \text{for } \theta > \theta_c\,, \\ \mathrm{SO}(3) \cup \bigcup_{i=1}^{M} \mathrm{SO}(3)U_i(\theta_c) & \text{at } \theta = \theta_c\,, \\ \bigcup_{i=1}^{M} \mathrm{SO}(3)U_i(\theta) & \text{for } \theta < \theta_c\,, \end{cases} \tag{2.10}$$

where the $U_i(\theta)$, $1 \leq i \leq M$ are the distinct symmetric positive definite matrices of the form $R^tU(\theta)R$, $R \in \mathscr{P}$. (A simple way of defining first and second order transitions is to say that the transformation is first order if $U_i(\theta_c) \neq \mathbb{I}$ and second order if $U_i(\theta_c) = \mathbb{I}$.) We assume that M is independent of θ. We say that each U_i describes a different *variant* of martensite, and we call a set of the form $\mathrm{SO}(3)U_i$ a *(martensitic) well*. One can show, see [28], that if $\mathscr{P}^m$ is the point group of the martensite, then $\mathscr{P}^m$ is a subgroup of $\mathscr{P}$ and that the number M is given by the formula

$$M = \frac{\text{order of } \mathscr{P}}{\text{order of } \mathscr{P}^m}\,. \tag{2.11}$$

For example, in the case of a cubic-to-tetragonal transformation, we may take

$$U(\theta) = U_1(\theta) = \mathrm{diag}\,(\eta_2, \eta_1, \eta_1)\,, \tag{2.12}$$

where $\eta_1(\theta), \eta_2(\theta) > 0$ and then we find that $M = 3$ and

$$U_2(\theta) = \mathrm{diag}\,(\eta_1, \eta_2, \eta_1)\,,\ U_3(\theta) = \mathrm{diag}\,(\eta_1, \eta_1, \eta_2)\,. \tag{2.13}$$

In this thesis, we also consider cubic-to-orthorhombic (Chapter 4), cubic-to-monoclinic and tetragonal-to-monoclinic transitions (Chapter 3). We refer to the corresponding chapters for the form of K in each case. We may then take the *total free energy* associated to the deformation $y : \Omega \to \mathbb{R}^3$ to be

$$I_\theta(y) = \int_\Omega \varphi(Dy(x)),\theta)\,dx.$$

[15] We mention in passing that using $\mathscr{P}$ instead of $\mathscr{G}$ in (2.9) has important consequences. For example, with $\mathscr{G}$, one would have an infinite number of wells and the analysis would then be very different. We do not elaborate this point further but refer the reader to *e.g.*, [74, 75] instead.

For mathematical definiteness, we assume furthermore that $\Omega \subset \mathbb{R}^3$ is a bounded domain (open, connected set) and that $\varphi(\cdot,\theta) : \mathbb{R}^{3\times 3} \to [0,\infty)$ is continuous and satisfies

$$-\alpha_1 + \alpha_2|\xi|^p \leq \varphi(\xi,\theta) \leq \alpha_1(1+|\xi|^p)\,, \quad \text{for all } \xi \in \mathbb{R}^{3\times 3}, \tag{2.14}$$

for some $\alpha_1 > 0$, $\alpha_2 > 0$ and $1 < p < \infty$.

Remark. The assumption (2.14) is made here for the sake of simplicity since it is the variational framework we have been describing in this chapter and that we are concerned with in Chapter 4 below. As pointed out above the growth condition is incompatible with the requirement that $\varphi(\xi,\theta) \to \infty$ as $\det\xi \to 0^+$. However, this growth condition can be dropped and this constraint successfully handled, see Ball and James [28].

We finally assume some boundary conditions, $y = y_0$ on $\partial\Omega$, say, for some given $y_0 \in W^{1,p}(\Omega,\mathbb{R}^3)$, where p is as in (2.14) and seek to minimise I_θ over

$$\mathscr{A} = y_0 + W_0^{1,p}(\Omega,\mathbb{R}^3)\,.$$

Let us assume that

$$m = \inf_{\mathscr{A}} I_\theta = 0\,. \tag{2.15}$$

We shall make a few comments on this hypothesis shortly.

Most often, $K(\theta)$ contains rank-one connections, *i.e.* pairs of rank-one connected matrices. Typically, when a rotation of angle π is 'lost' in the transformation (*i.e.*, a rotation of angle π belonging to $\mathscr{P}$ is not in $\mathscr{P}^m$) the existence of rank-one connections between some martensitic wells is guaranteed (see Chapter 3). If this is the case, φ cannot be rank-one convex, since it is zero at two matrices whose difference is rank-one but positive on the segment joining them. Hence φ is not quasiconvex and I_θ may not admit global minimisers. However, we deduce from the preceding section that a Young measure $(\nu_x)_{x\in\Omega}$ associated to a (subsequence of a) minimising sequence (at the temperature θ) exists and satisfies

$$\operatorname{supp}\nu_x \subset K(\theta) \ \text{ a.e. } x \in \Omega.$$

This is the key hypothesis behind the ideas of Ball and James [28]: *the formation of microstructure in the material is due to non-attainment of the energy.* Within this model, we thus identify microstructure and (non-trivial) gradient Young measures. In this framework, we also say that $\bar\nu_x$ is the *macroscopic deformation gradient.* Before going any further we make two remarks.

- First, the assumption (2.15) is a strong one, but covers some important cases of physical interest. Let us restrict ourselves to linear boundary conditions, $y_0 = Ax$, say. Then, $m = 0$ if and only if there exists a minimising sequence y^k such that $y^k = Ax$ on $\partial\Omega$ and $Dy^k \to K(\theta)$ in measure. Using the language of the preceding section, we may conclude that $m = 0$ if and only if $A \in K(\theta)^{qc}$. (This set is the set of recoverable strains under displacement control described in the Introduction.) As pointed out earlier, we do not know much about the quasiconvex hull of sets with multi-wells structure. Of course, we have seen (the one-well problem) that $K(\theta)^{qc} = K(\theta)$ for $\theta > \theta_c$, but for $\theta \leq \theta_c$, the question remains largely open. The two-well problem has been solved, which corresponds to a set $K(\theta)$ at $\theta < \theta_c$ for an orthorhombic-to-monoclinic transformation, but it is not yet possible to handle the case $\theta < \theta_c$ for a cubic-to-tetragonal transition, for example.

- Secondly, it is an open problem[16] to determine (assuming (2.15) holds) for which bound-

[16] We follow Ball's captivating paper [10] here.

ary conditions the minimum of I_θ is attained, and for which it is not. As Ball writes, '*a solution of this problem (...) would help clarify the validity of the hypothesis of Ball and James* [28] *that the formation of microstructure is associated with non-attainment of minimum energy*'. When $K(\theta)$ consists of two (three-dimensional) rank-one connected wells, Ball and Carstensen [20] proved that if $A \in K(\theta)^{qc} \setminus K(\theta)$, then the infimum of I_θ subject to the boundary conditions $y_0(x) = Ax$ is not attained. However, in the corresponding two-dimensional case, the answer is different, see [58, 117]. A solution to this problem, which is tightly related to solving differential inclusions, seems as yet far away.

In spite of these two remarks, the achievements of this model should not be overlooked. We mention some now. Their common idea is to choose a microstructure and see (a) whether the material is able to realise it, and if so (b) predict its exact geometry. We remind the reader that the only input in this model is the coefficients of the matrices U_i in (2.10) which may be computed from crystallographic data (the *lattice parameters*) and the knowledge of which transformation is being studied (*i.e.*, symmetry groups of the austenite and of the martensite).

- (*Twinning in martensite*) Looking for which variants can participate in a simple laminate (see the Introduction), in this model one does not need to know the twinning modes *a priori*; instead they are obtained as a result. We do not elaborate further this issue which is thoroughly studied in Chapter 3 in this thesis.

- (*Austenite-martensite interfaces*) Although there are in general no rank-one connections between the austenite and any martensitic well, Ball and James [27] showed that austenite-finely twinned martensite interfaces were possible in this framework.[17] Consider a cubic-to-tetragonal transition at $\theta = \theta_c$ (to simplify) and drop θ from the notation. Thus, the variants are as in (2.12)–(2.13). We want to find a rank-one connection between the austenite (the identity matrix, say) and a convex combination of two rank-one connected matrices, one on each of two martensitic wells. In other words, one has to solve

$$\begin{aligned} U_j + a \otimes m &= QU_i\,, \\ \mathbb{I} + b \otimes p &= \lambda QU_i + (1-\lambda)U_j\,, \end{aligned} \tag{2.16}$$

  for $Q \in \mathrm{SO}(3)$, $a, b, m, p \in \mathbb{R}^3$ and $0 \leq \lambda \leq 1$. These equations are exactly those obtained via the *crystallographic* (or *phenomenological*) *theory of martensite* due independently to Wechsler, Lieberman and Read [154] and to Bowles and MacKenzie [40], a popular and highly-regarded theory among material scientists. That this model encapsulates the crystallographic theory has undoubtedly been a major publicity and some experimentalists do now refer to this model alongside the crystallographic theory in their papers. In this model (2.16) is derived as follows. Considering a planar interface $\{\langle x, m\rangle = \text{const}\}$ (it can be shown that the interface is necessarily planar) we try and choose the normal m in such a way that there exists a minimising sequence y^k such that $Dy^k \to \mathbb{I}$ in measure on $\{\langle x, m\rangle > \text{const}\}$ while $Dy^k \to \{A, B\}$ in measure

[17] The austenite is compatible with a variant of martensite only in very rare instances: when the middle eigenvalue of the martensitic variant equals one, see [27] or the remarks following Corollary 3.8 in Chapter 3 below. These exact austenite-martensite interfaces are very scarcely observed, but there are two examples when this happens: Ti-Ni-Cu and Ti-29 at.% Ta. The latter was specially obtained by Bywater and Christian [44] by carefully adjusting the concentration of tantalum during preparation of the alloy so that this condition be satisfied.

on $\{\langle x, m\rangle < \text{const}\}$. Then it is shown that for this to be possible, (2.16) must hold, and one recovers the crystallographic theory. Notice that $(2.16)_2$ is a compatibility condition for the macroscopic gradient. Another way of phrasing (2.16) is

$$\mathbb{I} + b \otimes p = \lambda A + (1-\lambda)B \tag{2.17}$$

for some $A, B \in \mathrm{SO}(3)U_i \cup \mathrm{SO}(3)U_j$, $b, p \in \mathbb{R}^3$ and $0 \leq \lambda \leq 1$. Ball and James proved in [27] that (2.16) has a solution if and only if the parameters η_1 and η_2 satisfy

$$\eta_1^2 + \eta_2^2 \leq 2 \quad \text{if} \quad \eta_1\eta_2 \leq 1\,, \quad \eta_1^{-2} + \eta_2^{-2} \leq 2 \quad \text{if} \quad \eta_1\eta_2 \geq 1\,. \tag{2.18}$$

The different vectors p solving (2.16), known as *habit planes*, can be explicitly computed. As was previously known, one finds 24 different solutions, and they match experimental data. Another interesting development of this theory is the prediction of *non-classical austenite-martensite interfaces*, as carried out by Ball and Carstensen [18, 19, 20]. Instead of solving (2.17) one tries to solve the more general problem

$$\mathbb{I} + b \otimes p \in K^{qc}\,.$$

Thanks to a little miracle[18] it is possible to prove that non-classical interfaces are possible if and only if

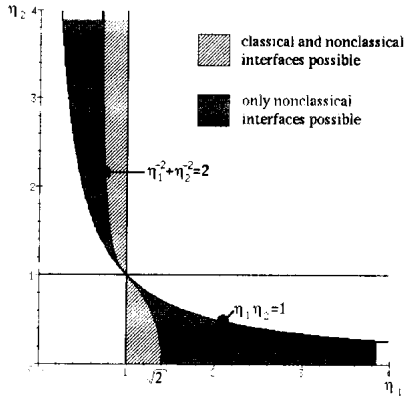


Figure 2.2: Lattice parameters allowing classical and non-classical austenite-martensite interfaces [20].

$$\eta_1 \leq \eta_1^{-1} \leq \eta_2 \quad \text{if} \quad \eta_1 \leq \eta_2\,, \quad \eta_2 \leq \eta_1^{-1} \leq \eta_1 \quad \text{if} \quad \eta_1 \geq \eta_2\,. \tag{2.19}$$

Experimentally, non-classical interfaces are hard to observe, probably because condition (2.19) is hard to achieve whenever η_1 and η_2 are close to 1 which is typically the case in experiments, see Figure 2.2. However, it seems that non-classical interfaces have been observed in cubic-to-orthorhombic materials (we recall that we have assumed a cubic-to-tetragonal transition in this discussion), see [18, 19, 20].

- Other microstructures can be accurately predicted using this theory. We do not describe them but simply quote some examples and indicate relevant bibliographical references.

[18] The miracle is that one has $\mathbb{I} + b \otimes p \in K^{qc}$ if and only if $\mathbb{I} + b \otimes p \in K^{pc}$. This given, conditions so that $\mathbb{I} + b \otimes p \in K^{pc}$ can be obtained. Interestingly enough this can be done without using a formula for K^{pc}!

- Wedge-like microstructures are very commonly observed. These were neatly analysed by Bhattacharya in [34]. He predicted that for this microstructure to be possible, the lattice parameters must satisfy very stringent conditions, which were found to match experimental data remarkably closely.
- For parallelogram, triangle and diamond microstructures, see Hane [83]. See Chu [50] for L-interfaces.
- Zig-zag and crossing twins are studied in Bhattacharya [37].
- Bhattacharya [35] used this model to explain why so few materials are self-accommodating (see the Introduction). Here again, the conditions found to be necessary and sufficient for self-accommodation match up very well with experiments.

We conclude this chapter with four remarks.

Remarks.

- We start by mentioning that the theory presented in this section is not the only one that has been designed to predict the morphology of crystal microstructure. Another one is due to Khachaturyan, Roitburd and Shatalov (see *e.g.*, [92]). There are similarities between their model and that presented in this chapter. As a matter of fact, Kohn [97] and Ball and James [28] have shown that the Khachaturyan-Roitburd-Shatalov theory can, roughly speaking, be thought of as a 'linearisation' of the present theory (although their theory is not linear). Read also Bhattacharya [36] for a comparison between these two models.

- If this model succeeds in explaining many features of the microstructure, it has one notable limitation. Since minima of the energy are not attained, the model predicts infinitely fine microstructure, which is obviously not physically acceptable, even if the thickness observed in experiments is small indeed. The most widely accepted explanation of this flaw is that the model does not account for interfacial energy and that if such a term were added in the energy, infinitely fine structures would be precluded as they involve infinitely many interfaces. The reader is referred to [98, 116] and the references mentioned therein for more on the inclusion of surface energy terms.

- The numerical analysis of microstructure is a challenging problem, see [45, 103] and the references quoted therein.

- Finally, it is clear that ultimately, an accurate theory of phase transitions ought to be dynamical. Relatively little is known in that respect – undoubtedly because dynamics is much harder than statics. Furthermore, we have said nothing towards justifying the use of energy minimisation itself, for which we refer to [17, 24, 78].

3 On rank-one connections in martensite

3.1 Introduction

A central feature of solid-to-solid phase transformations in elastic crystals is the 'multiple variant' structure of the low symmetry, (most often) low temperature phase called *martensite* as opposed to the unique high symmetry, (most often) high temperature phase called *austenite*. All these variants are symmetry related configurations (see (3.1) below) of the same atomic crystalline lattice. Their number depends on the symmetry of both the austenite and the martensite phases, see formula (2.11) above.

Mathematically these variants may be represented by a family of 'wells' $\{SO(3)U_i\}_{i=1}^M$, where the U_i are 3×3 symmetric positive definite matrices. Recall that $SO(n) = \{\xi \in \mathbb{R}^{n\times n} : \xi\,\xi^t = \xi^t\,\xi = \mathbb{I}\,,\ \det\xi = 1\}$, where $\mathbb{R}^{n\times n}$ denotes the space of $n\times n$ matrices with real entries, ξ^t is the transpose of ξ, and $\mathbb{I}$ is the identity. The U_i are related by the condition that for every $i, j \in \{1,\dots,M\}$ there exists a rotation $R = R(i,j) \in \mathrm{SO}(3)$ such that

$$U_j = RU_iR^t. \tag{3.1}$$

In fact, R belongs to a finite subgroup of SO(3), the *symmetry group of the austenite*. More precisely, this subgroup is either the cubic (Laue) point group (consisting of those rotations that map a cube into itself) or a subgroup of it.

For two variants, i and j say, to coexist simultaneously in the martensitic phase on both sides of a planar interface (and form a *simple laminate of martensite*) the wells $SO(3)U_i$ and $SO(3)U_j$ must be *rank-one connected*. This means that there exist two rotations R_i, $R_j \in \mathrm{SO}(3)$ and two vectors $a, m \in \mathbb{R}^3$, $|m| = 1$, such that

$$R_iU_i - R_jU_j = a \otimes m, \tag{3.2}$$

where $a \otimes m$ denotes the matrix $(a \otimes m)_{ij} = a_im_j$. This results from the *Hadamard jump condition* that asserts that there exists a continuous deformation with constant gradients $\xi \in \mathbb{R}^{3\times 3}$ and $\eta \in \mathbb{R}^{3\times 3}$ on opposite sides of a planar interface with normal $m \in \mathbb{R}^3$, $|m| = 1$, if and only if

$$\xi - \eta = a \otimes m,$$

for some $a \in \mathbb{R}^3$. The vector a represents the amplitude of the jump. We are thus led to seek rank-one connections between the wells. In this chapter we show that the two wells $\mathrm{SO}(3)U_i$ and $\mathrm{SO}(3)U_j$ are rank-one connected if and only if

$$\det\,(U_i - U_j) = 0\,,$$

(see Corollary 3.8). It has to be pointed out that if U_i and U_j are not related as in (3.1) (*i.e.*, do not have the same eigenvalues) this result does not hold (see Lemma 3.5 and the discussion before Proposition 3.6 below). Combining this result with a result of Gurtin, we get a formula for the vectors a and m in (3.2) (Theorem 3.14), from which we deduce the twinning mode of the two variants (Corollary 3.16). As a straightforward consequence, we obtain a simple existence criterion for so-called compound twins: under a technical assumption, two martensitic wells $\mathrm{SO}(3)U_i$ and $\mathrm{SO}(3)U_j$ have compound twins if and only if the matrices U_i and U_j have a common eigenvector (Corollary 3.17).

Let us rapidly now review some results related to the existence of rank-one connections in the literature. A well-known criterion due, in this form, to Ball and James [27, 28] and

Khachaturyan [92] states that $\mathrm{SO}(3)U_i$ and $\mathrm{SO}(3)U_j$ are rank-one connected if and only if the middle eigenvalue of $U_i^{-1}U_j^2U_i^{-1}$ equals one (see Theorem 3.2 below). It turns out that in practice this criterion involves tedious computations, particularly when U_i and U_j are not diagonal. A much easier result to use, due to Gurtin [81] (see also Ericksen [67], Bhattacharya [35] and Lemma 3.13 below), holds for wells that are related by a rotation of angle π in (3.1). Throughout this chapter, a *rotation of angle* π denotes a rotation of the form $Q = -\mathbb{I} + 2e\otimes e$ for some $|e| = 1$. Unfortunately even if most U_i and U_j are of that form, there are some exceptions, as pointed out in [125, 139]. In fact, knowing *a priori* that the two wells are rank-one connected one can always replace R by a rotation of angle π in (3.1) as shown by Ericksen [67] (see also [118] and Corollary 3.12 below). Of course this rotation need not belong to the austenitic group.[19] Therefore Gurtin's formula always applies if we know that the wells are rank-one connected and then change R properly. That is precisely what our criterion allows us to do. It provides a simple check for whether the wells are rank-one connected and, if they are, yields a simple formula for the rotation of angle π relevant to Gurtin's formula. Also, we deduce a simple condition for the occurrence of so-called compound twins (see Definition 3.15 and Corollary 3.17 below).

As an illustration, we apply our results to the cubic-to-tetragonal, tetragonal-to-monoclinic and cubic-to-monoclinic transitions. In particular, in the last case, we recover and extend conditions due to Pitteri and Zanzotto [125] for the existence of a special class of twins, the so-called *non-generic twins*.

We have tried to present all our results in as general a form as possible. In particular some results are stated for $n \times n$ matrices even if obviously the interesting case is that of 3×3 matrices.[20] This is done in order to show where the dimension comes into play and why some results are only true for 3×3 matrices. Other results concerning rank-one connections in n dimensions have been obtained by a different approach by Silhavỳ [136, 138].

To conclude this introduction, we rapidly mention the case of 2×2 matrices. In this case, it is quite easy to see that $\mathrm{SO}(2)U$ and $\mathrm{SO}(2)V$ are rank-one connected if and only if $\det(U^2 - V^2) \leq 0$ (see Bhattacharya and Dolzmann [38] for a proof). Furthermore, using an analogous result to Proposition 3.6, it is easily seen that if U and V have the same eigenvalues, then $\mathrm{SO}(2)U$ and $\mathrm{SO}(2)V$ are rank-one connected if and only if $\det(U - V) \leq 0$. Finally, we mention a recent paper by Parry and Silhavỳ [119] which addresses the problem of rank-one connections in two dimensions via a completely different approach.

3.2 A simple criterion and simple formulæ

We begin with the following

(3.1) Definition. *Let $U, V \in \mathbb{R}^{n\times n}$ be two matrices with positive determinant. We say that the wells $\mathrm{SO}(n)U$ and $\mathrm{SO}(n)V$ are rank-one connected if there exist two rotations $R_1, R_2 \in \mathrm{SO}(n)$ and two vectors $a, m \in \mathbb{R}^n$, $|m| = 1$, such that*

$$R_1U - R_2V = a \otimes m. \tag{3.3}$$

A pair of matrices (R_1U, R_2V) satisfying (3.3) is also called a twin. *The vectors $U^{-1}R_1^t a$ and m are called the* shearing vector *and the* twin plane normal *respectively.*

[19] This is precisely what occurs in *e.g.*, tetragonal-to-monoclinic [139] or cubic-to-monoclinic transitions [125]: there exist some variants U_i and U_j for which there exist no rotation of angle π in the austenitic group relating them as in (3.1).

[20] In this chapter, n is always greater than two.

The terminology for $U^{-1}R_1^t a$ should be clear when rewriting (3.3) as

$$R_2 V = R_1 U(\mathbb{I} - (U^{-1}R_1^t a) \otimes m).$$

Observe that if $a = 0$ then we are left with the trivial case where $\mathrm{SO}(n)U = \mathrm{SO}(n)V$, which gives $U = V$ by the uniqueness of the polar decomposition, if U and V are symmetric positive definite. Conversely, if $\mathrm{SO}(n)U = \mathrm{SO}(n)V$, it is easy to see that then $a = 0$. Therefore, there are no rank-one connections between a well and itself.

Without loss of generality we can assume that $R_1 = \mathbb{I}$. We therefore base our study on the following problem: find a rotation $Q \in \mathrm{SO}(n)$ and two vectors $a, m \in \mathbb{R}^{n\times n}$, $|m| = 1$, such that

$$U - QV = a \otimes m. \tag{3.4}$$

Post-multiplying (3.4) by U^{-1} we get the equivalent form

$$QVU^{-1} = \mathbb{I} - a \otimes U^{-t}m, \tag{3.5}$$

where $U^{-t} = (U^{-1})^t = (U^t)^{-1}$. Moreover, since U and V have positive determinant,

$$1 - \langle a, U^{-t}m\rangle = \det(QVU^{-1}) > 0\,,$$

where $\langle\cdot,\cdot\rangle$ denotes the Euclidean scalar product in $\mathbb{R}^n$. We claim that (3.5) is equivalent to the statement

$$C = (\mathbb{I} - U^{-t}m \otimes a)(\mathbb{I} - a \otimes U^{-t}m), \quad 1 - \langle a, U^{-t}m\rangle > 0, \tag{3.6}$$

where $C = U^{-t}V^tVU^{-1}$. Obviously (3.5) implies (3.6). Conversely (3.6) and the polar decomposition theorem imply that $VU^{-1} = Q_1\sqrt{C}$ and $(\mathbb{I} - a \otimes U^{-t}m) = Q_2\sqrt{C}$ for some rotations $Q_1, Q_2 \in \mathrm{SO}(n)$, giving (3.5). The next result is due to Ball and James [27, 28] and Khachaturyan [92]. Throughout this chapter, $\lambda_1(\xi) \le \ldots \le \lambda_n(\xi)$ denote the ordered eigenvalues of the symmetric matrix $\xi \in \mathbb{R}^{n\times n}$.

(3.2) Theorem. *Let $C \in \mathbb{R}^{n\times n}$, $C \neq \mathbb{I}$ be symmetric. Necessary and sufficient conditions for C to be expressible in the form*

$$C = (\mathbb{I} + \bar{m} \otimes \bar{a})(\mathbb{I} + \bar{a} \otimes \bar{m})$$

with $1 + \langle\bar{a}, \bar{m}\rangle > 0$ and $\bar{a}, \bar{m} \neq 0$ are that the eigenvalues $\lambda_i = \lambda_i(C)$ of C satisfy

$$0 < \lambda_1 \le \lambda_2 = \ldots = \lambda_{n-1} = 1 \le \lambda_n\,.$$

The solutions are given by

$$\begin{aligned} \bar{a} &= \rho\left(\sqrt{\frac{\lambda_n(1-\lambda_1)}{\lambda_n - \lambda_1}}e_1 + \kappa\sqrt{\frac{\lambda_1(\lambda_n - 1)}{\lambda_n - \lambda_1}}e_n\right), \\ \bar{m} &= \frac{1}{\rho}\left(\frac{\sqrt{\lambda_n} - \sqrt{\lambda_1}}{\sqrt{\lambda_n - \lambda_1}}\right)\left(-\sqrt{1-\lambda_1}e_1 + \kappa\sqrt{\lambda_n - 1}e_n\right), \end{aligned} \tag{3.7}$$

where $\rho \neq 0$ is a constant and e_1, e_n are normalised eigenvectors of C corresponding to λ_1, λ_n respectively and where κ can take the values ± 1. Moreover, the solutions are unique up to the signs.

Remarks. With Theorem 3.2 in hand, it is easy to solve (3.4). We let $C = U^{-t}V^tVU^{-1}$ and then the solutions, if they exist, are given by $a = -\bar{a}$, $m = U^t\bar{m}$. Finally Q is found by substituting a and m back into (3.4). In [27, 28, 92] the theorem is only stated in three dimensions (*i.e.*, $n = 3$) but the general case is a straightforward adaptation. Note that $C = \mathbb{I}$ if and only if $U^tU = V^tV$, in other words if $\mathrm{SO}(n)U = \mathrm{SO}(n)V$. Theorem 3.2 therefore implies that for a given matrix on one well, there are precisely zero, one or two rank-one connections between this matrix and the other well. The case of precisely one rank-one connection happens when $\lambda = 1$ is an eigenvalue of multiplicity $n-1$ of $U^{-t}V^tVU^{-1}$, that is when U and V satisfy

$$U^tU - V^tV = \alpha e \otimes e, \tag{3.8}$$

where $|e| = 1$ and $\alpha \neq 0$. But if $V = RUR^t$ for some $R \in \mathrm{SO}(n)$, then taking the trace of (3.8) shows that this cannot happen. In fact, when $V = RUR^t \neq U$, $\lambda_1(C) > 0$ and either $\lambda_1(C) < \lambda_2(C) = \ldots = \lambda_{n-1}(C) = 1 < \lambda_n(C)$ and there exist two distinct rank-one connections, or $\lambda = 1$ is an eigenvalue of multiplicity smaller than $n-2$ of C and there are no rank-one connections.

Proof of Theorem 3.2. The proof of the necessity is exactly the same as in [27]. We briefly outline the proof of the sufficiency for the convenience of the reader. To shorten the notation, we write $\lambda_i(C) = \lambda_i$, $1 \leq i \leq n$. Let $C \neq \mathbb{I}$ have eigenvalues $0 < \lambda_1 \leq \lambda_2 = \ldots = \lambda_{n-1} = 1 \leq \lambda_n$. We have to find non-zero $\bar{a}, \bar{m} \in \mathbb{R}^n$, $1 + \langle \bar{a}, \bar{m}\rangle > 0$, such that (3.6) holds.

Suppose that $C = (\mathbb{I} + \bar{m} \otimes \bar{a})(\mathbb{I} + \bar{a} \otimes \bar{m})$ with $\bar{a}, \bar{m} \neq 0$ and $1 + \langle \bar{a}, \bar{m}\rangle > 0$. Then $C\bar{a} = \pm\sqrt{\det C}\,\big(\bar{a} + |\bar{a}|^2\bar{m}\big)$. Computing $\langle C\bar{a}, \bar{a}\rangle$, and using the fact that C is positive definite and that $1 + \langle \bar{a}, \bar{m}\rangle > 0$, we see that we have to choose the plus sign. Hence

$$\bar{m} = \Big((\det C)^{-\frac{1}{2}}C - \mathbb{I}\Big)\,\frac{\bar{a}}{|\bar{a}|^2} \tag{3.9}$$

and $(\mathbb{I} + \bar{m} \otimes \bar{a})(\mathbb{I} + \bar{a} \otimes \bar{m}) = \mathbb{I} - |\bar{a}|^{-2}\bar{a} \otimes \bar{a} + (|\bar{a}|^2 \det C)^{-1} C\bar{a} \otimes C\bar{a}$. Hence $\bar{a} \neq 0$ has to satisfy the equation

$$C = \mathbb{I} - \frac{1}{|\bar{a}|^2}\bar{a} \otimes \bar{a} + \frac{1}{(\det C)|\bar{a}|^2} C\bar{a} \otimes C\bar{a}. \tag{3.10}$$

Conversely if $\bar{a} \neq 0$ satisfies (3.10) and $\bar{m}$ is chosen as in (3.9) then C has the required form.

Let $\{e_1, \ldots, e_n\}$ be an orthonormal basis of eigenvectors of C. In this basis we have $\bar{a} = (\bar{a}_1, \ldots, \bar{a}_n)$ and $C\bar{a} = (\lambda_1\bar{a}_1, \bar{a}_2, \ldots, \bar{a}_{n-1}, \lambda_n\bar{a}_n)$. Then (3.10) reduces to

$$\begin{aligned}
|\bar{a}|^2(\lambda_1 - 1) &= \left(-1 + \frac{\lambda_1}{\lambda_n}\right)\bar{a}_1^2, \\
|\bar{a}|^2(\lambda_n - 1) &= \left(-1 + \frac{\lambda_n}{\lambda_1}\right)\bar{a}_n^2, \\
0 &= \left(-1 + \frac{1}{\lambda_n}\right)\bar{a}_1\bar{a}_i, \quad 2 \leq i \leq n-1, \\
0 &= \left(-1 + \frac{1}{\lambda_1}\right)\bar{a}_i\bar{a}_n, \quad 2 \leq i \leq n-1, \\
0 &= \left(-1 + \frac{1}{\lambda_1\lambda_n}\right)\bar{a}_i\bar{a}_j, \quad 2 \leq i \leq j \leq n-1.
\end{aligned}$$

Since λ_1, λ_n are not simultaneously equal to one we get

$$\frac{\bar{a}_1^2}{|\bar{a}|^2} = \frac{\lambda_n(1-\lambda_1)}{\lambda_n - \lambda_1}, \quad \frac{\bar{a}_n^2}{|\bar{a}|^2} = \frac{\lambda_1(\lambda_n - 1)}{\lambda_n - \lambda_1}, \quad \bar{a}_i = 0, \quad 2 \leq i \leq n-1.$$

Writing $a = \sum a_i e_i$ and then substituting in (3.9) we get (3.7), completing the proof. □

Let us go back to (3.4). We have

$$\begin{aligned} V^tV &= \big(U^t - m \otimes a\big)\big(U - a \otimes m\big) \\ &= U^tU + \left(\frac{|a|^2}{2} - U^ta\right) \otimes m + m \otimes \left(\frac{|a|^2}{2} - U^ta\right). \end{aligned} \tag{3.11}$$

In other words $U^tU - V^tV$ is of rank (at most) two. It is therefore trivial that $U^tU - V^tV$ being of rank (at most) two is a necessary condition for (3.4) to hold and this has been well known for a long time. In fact, this condition is also sufficient and this can be proved by two different methods. The first consists in 'working back', *i.e.*, starting with $U^tU - V^tV$ of rank (at most) two and then finding a and m satisfying (3.11), see for instance Ericksen [69, 71] and Silhavỳ [137]. The second is algebraic in that one shows that this condition is equivalent to that of Theorem 3.2. We adopt the latter here, and give an elementary, self-contained proof. This was also done, independently, by Silhavỳ [137].

(3.3) Lemma. *Let $U, V \in \mathbb{R}^{n\times n}$ have positive determinant. To shorten the notation, let us write $\xi_i = \lambda_i(U^{-t}V^tVU^{-1})$ and $\mu_i = \lambda_i(V^tV - U^tU)$, $1 \leq i \leq n$. Then*

$$\xi_1 < \xi_2 = \ldots = \xi_{n-1} = 1 < \xi_n \tag{3.12}$$

if and only if

$$\mu_1 < \mu_2 = \ldots = \mu_{n-1} = 0 < \mu_n. \tag{3.13}$$

Moreover, equalities in (3.12) *correspond to equalities in* (3.13)*, and vice-versa.*

Remark. As observed by Silhavỳ [137], if $n = 3$, (3.13) is equivalent to

$$\det\left(V^tV - U^tU\right) = 0\,, \quad \operatorname{tr}\left(\operatorname{cof}\left(V^tV - U^tU\right)\right) < 0\,.$$

In terms of rank-one connections Theorem 3.2 and Lemma 3.3 give the following immediate

(3.4) Corollary. *Let $U, V \in \mathbb{R}^{n\times n}$ have positive determinant and write $\lambda_i = \lambda_i(U^tU - V^tV)$, $1 \leq i \leq n$. Then*

(*i*) *if zero is not an eigenvalue of multiplicity at least $n-2$ of $U^tU - V^tV$, there are no rank-one connections,*

(*ii*) *if $\lambda_1 < \lambda_2 = \ldots = \lambda_{n-1} = 0 < \lambda_n$, there are two rank-one connections,*

(*iii*) *if zero is an eigenvalue of multiplicity $n-1$ of $U^tU - V^tV$, there is only one rank-one connection,*

(*iv*) *finally, if zero has multiplicity n, we are left with the trivial case $\mathrm{SO}(n)U = \mathrm{SO}(n)V$.*

Remark. Recall that in the case of martensitic wells, $V = RUR^t$ for some $R \in \mathrm{SO}(3)$ and the third case cannot happen.

Proof of Lemma 3.3. First note that one is an eigenvalue of multiplicity k of $U^{-t}V^tVU^{-1}$ if and only if zero is an eigenvalue of multiplicity k of $V^tV - U^tU$ since U is invertible. This proves the last statement of the lemma. More generally, observe that λ is an eigenvalue (of multiplicity k) of $U^{-t}V^tVU^{-1}$ if and only if zero is an eigenvalue (of multiplicity k) of $V^tV - \lambda U^tU$. We divide the rest of the proof into two steps.

First step. Assume $\xi_1 < \xi_2 = \ldots = \xi_{n-1} = 1 < \xi_n$. Notice that $\xi_1 > 0$ since $U^{-t}V^tVU^{-1}$ is symmetric positive definite. By the above remark zero is an eigenvalue of multiplicity $n-2$ of $V^tV - U^tU$. Consider the quadratic form $A(x) = \langle (V^tV - \lambda U^tU)x, x\rangle$, $x \in \mathbb{R}^n$ for some $\lambda \in \mathbb{R}$. Choosing $\lambda = \xi_1$ and $x \neq 0$ in the kernel of $V^tV - \xi_1 U^tU$ (which is one-dimensional by the above remark) we get

$$0 = \langle (V^tV - \xi_1 U^tU)x, x\rangle > \langle (V^tV - U^tU)x, x\rangle,$$

where we used (3.12). Hence $\mu_1 < 0$. Similarly, choosing $\lambda = \xi_n$ and $x \neq 0$ in the kernel of $V^tV - \xi_n U^tU$ we get

$$0 = \langle (V^tV - \xi_n U^tU)x, x\rangle < \langle (V^tV - U^tU)x, x\rangle$$

and hence $\mu_n > 0$. This concludes the first step.

Second step. Assume $\mu_1 < \mu_2 = \ldots = \mu_{n-1} = 0 < \mu_n$. Again $\xi_1 > 0$ follows from the positivity of $U^{-t}V^tVU^{-1}$, and the remark preceding the first step implies that $\lambda = 1$ is an eigenvalue of multiplicity $n-2$ of $U^{-t}V^tVU^{-1}$. We aim to show that $\xi_1 < 1$ and $\xi_n > 1$. In other words we have to rule out the following two cases:

(i) $\xi_1 \geq 1$,

(ii) $\xi_n \leq 1$.

Suppose for contradiction that $\xi_1 = 1$ ($\xi_1 > 1$ is impossible since $\xi = 1$ is an eigenvalue of $U^{-t}V^tVU^{-1}$). Thus $(U^{-t}V^tVU^{-1} - \mathbb{I})$ is positive semi-definite. Since U is invertible this is equivalent to

$$0 \leq \langle (V^tV - U^tU)x, x\rangle$$

for every x. Now choose $x \neq 0$ in the eigenspace associated to μ_1 to get

$$\langle (V^tV - U^tU)x, x\rangle = \mu_1 \langle x, x\rangle < 0,$$

a contradiction. Hence $0 < \xi_1 < 1$. (ii) is ruled out similarly using the negativity of $(U^{-t}V^tVU^{-1} - \mathbb{I})$ and the positivity of μ_n. Thus $\xi_n > 1$. The lemma is proved. □

Corollary 3.4 provides a computationally much simpler criterion than Theorem 3.2 for whether or not two wells are rank-one connected. However, the identity $U^2 - V^2 = (U-V)(U+V)$, valid for commuting matrices, suggests an even simpler criterion involving the difference $U-V$ only. As this trivial case hints we have to consider symmetric positive definite matrices. The question that we are led to ask is thus the following. For two symmetric matrices U and V with positive determinant does the following equivalence hold:

$$\xi_1 < \xi_2 = \ldots = \xi_{n-1} = 0 < \xi_n \tag{3.14}$$

if and only if

$$\mu_1 < \mu_2 = \ldots = \mu_{n-1} = 0 < \mu_n \,, \tag{3.15}$$

where $\xi_i = \lambda_i(U^2 - V^2)$ and $\mu_i = \lambda_i(U - V)$ for all $i = 1, \ldots, n$?

We first point out that the equivalence does not hold under the assumption that U and V be merely symmetric positive definite.

(3.5) Lemma. *For every integer $n \geq 3$, there exist symmetric positive definite $n \times n$ matrices U and V such that* (3.14) *holds while* (3.15) *fails, or conversely, such that* (3.15) *holds but* (3.14) *does not.*

Proof of Lemma 3.5. This is elementary for 3×3 matrices and then straightforwardly extended to higher dimensions. For example, in three dimensions, we can consider the following two matrices,

$$U = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 8 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad V = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

Then $\lambda_1(U - V) < \lambda_2(U - V) = 0 < \lambda_3(U - V)$ but $\det(U^2 - V^2) > 0$. Conversely, taking

$$U = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad V = \begin{pmatrix} \sqrt{\frac{2}{19}} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 2 \end{pmatrix},$$

we have $\lambda_1(U^2 - V^2) < \lambda_2(U^2 - V^2) = 0 < \lambda_3(U^2 - V^2)$ while $\det(U - V) < 0$. □

It turns out that the correct hypothesis to add is that U and V have the same eigenvalues. It may seem surprising at this stage that the validity of such a result should depend on the dimension of the matrices. However, we will show that the equivalence (3.14), (3.15) holds for 3×3 matrices but does not hold in higher dimensions. Before stating the result in three dimensions we recall a definition from functional calculus (see Halmos [82]).

Let $U \in \mathbb{R}^{n \times n}$ be symmetric, let $I \subset \mathbb{R}$, and let $f : I \to \mathbb{R}$, with the spectrum of U satisfying $\sigma(U) \subset I$. We define

$$f(U) = \sum f(\lambda_i(U))\, e_i \otimes e_i \,,$$

where $U = \sum \lambda_i(U) e_i \otimes e_i$ is the spectral decomposition of U.

(3.6) Proposition. *Let $U, V \in \mathbb{R}^{3\times 3}$ be symmetric and have the same spectrum σ. Let $I \subset \mathbb{R}$ be such that $\sigma \subset I$ and let $f : I \to \mathbb{R}$ be one-to-one. Then*

$$\det(U - V) = 0 \quad \textit{if and only if} \quad \det(f(U) - f(V)) = 0 \,. \tag{3.16}$$

Furthermore, if $U \neq V$, and if (3.16) *holds, then*

$$\lambda_1(U - V) < \lambda_2(U - V) = 0 < \lambda_3(U - V) \tag{3.17}$$

and

$$\lambda_1(f(U) - f(V)) < \lambda_2(f(U) - f(V)) = 0 < \lambda_3(f(U) - f(V)). \tag{3.18}$$

Remarks. In fact for a given function f the proposition can be slightly improved. For example if $f(t) = t^2$ the result holds not only for symmetric (semi-)definite positive matrices (corresponding to the largest interval, $[0, \infty)$, on which f is one-to-one) but more generally for all matrices U (and V) such that $\lambda_i(U) \neq -\lambda_j(U)$ whenever $i \neq j$ (see (3.19) and (3.20) below).

In the case of martensitic variants the proposition applies. Indeed in this case we consider a symmetric positive definite $U \in \mathbb{R}^{3\times 3}$, and $V = RUR^t$ for some $R \in \mathrm{SO}(3)$ and $f(t) = t^2$.

We should mention that after this research was carried out, another proof of this result (at least in the case $f(t) = t^2$) has been obtained by Pitteri [124].

Proof of Proposition 3.6. Since U and V have the same spectrum, we can suppose without loss of generality that $U = \sum \lambda_i(U) e_i \otimes e_i$ and $V = QUQ^t$ for some $Q \in \mathrm{SO}(3)$ (if necessary, multiply Q by $-\mathbb{I}$). Let $Q = (q_{ij})$ be the expression of Q in the basis $\{e_i\}$. To shorten the notation we write $\lambda_i(U) = \lambda_i$, $1 \leq i \leq 3$.

First step. We first prove (3.16). Notice that

$$\begin{aligned} UQ - QU &= \Big(\sum \lambda_i e_i \otimes e_i\Big)\Big(\sum q_{ij} e_i \otimes e_j\Big) \\ &\quad - \Big(\sum q_{ij} e_i \otimes e_j\Big)\Big(\sum \lambda_i e_i \otimes e_i\Big) \\ &= \sum \lambda_i q_{ij} e_i \otimes e_j - \sum \lambda_j q_{ij} e_i \otimes e_j \\ &= \sum_{i,j} (\lambda_i - \lambda_j) q_{ij} e_i \otimes e_j. \end{aligned}$$

Then, writing $\mathscr{S}_3$ for the set of permutations of three elements and $\mathrm{sgn}(\tau)$ for the sign of $\tau \in \mathscr{S}_3$,

$$\begin{aligned} \det\left(U - QUQ^t\right) &= \det\left(UQ - QU\right) \\ &= \sum_{\tau \in \mathscr{S}_3} \mathrm{sgn}(\tau) \prod_{i=1}^{3} (\lambda_i - \lambda_{\tau(i)}) q_{i\tau(i)}. \end{aligned}$$

Now an explicit calculation yields

$$\det\left(U - V\right) = (\lambda_1 - \lambda_2)(\lambda_2 - \lambda_3)(\lambda_3 - \lambda_1)(q_{12}q_{23}q_{31} - q_{13}q_{21}q_{32}). \tag{3.19}$$

Similarly, since $f(V) = Qf(U)Q^t$ we have

$$\begin{aligned} \det\left(f(U) - f(V)\right) =& (f(\lambda_1) - f(\lambda_2))(f(\lambda_2) - f(\lambda_3))(f(\lambda_3) - f(\lambda_1)) \cdot \\ & \cdot (q_{12}q_{23}q_{31} - q_{13}q_{21}q_{32}). \end{aligned} \tag{3.20}$$

Now (3.16) follows from (3.19), (3.20) and the fact that f is one-to-one on I.

Second step. Suppose further that $U \neq V$. Then (3.17) and (3.18) follow from the first step and the fact that $\mathrm{trace}(U - V) = 0$ and $\mathrm{trace}(f(U) - f(V)) = 0$ since U and V on the one hand, and $f(U)$ and $f(V)$ on the other, have the same eigenvalues. □

Note that in higher dimensions (*i.e.*, $n \geq 4$) there is no suitable identity analogous to (3.19). We first point out a nice consequence of the proposition.

(3.7) Corollary. *Let $U, V \in \mathbb{R}^{3\times 3}$ be symmetric and have the same eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3$. Then*

$$\det(U^2 - V^2) = (\lambda_1 + \lambda_2)(\lambda_2 + \lambda_3)(\lambda_3 + \lambda_1)\det(U - V). \tag{3.21}$$

Remark. Note that we did not assume $\lambda_1 \geq 0$.

Proof of Corollary 3.7. Immediate in view of Proposition 3.6. □

We now summarise the results in the case of martensitic variants.

(3.8) Corollary. *Let $U, V \in \mathbb{R}^{3\times 3}$ be symmetric positive definite and have the same eigenvalues. Then*

- *if $\lambda_2(U-V) \neq 0$ (in particular, if $\det(U-V) \neq 0$), there are no rank-one connections,*
- *if $\lambda_1(U-V) < \lambda_2(U-V) = 0 < \lambda_3(U-V)$, or, equivalently if $U \neq V$, if $\det(U-V) = 0$, there are two rank-one connections,*
- *if $\lambda_1(U-V) = \lambda_2(U-V) = \lambda_3(U-V) = 0$, we are left with the trivial case $U = V$.*

Remarks. The proof is an immediate consequence of Theorem 3.2, Lemma 3.3 and Proposition 3.6. Note that if U and V commute (without necessarily having the same eigenvalues) the corollary still holds. In particular, if $V = \mathbb{I}$, we recover a classical result: exact austenite-martensite interface is possible if and only if the middle eigenvalue of the variant of martensite equals one.

Example. Let $R = -\mathbb{I} + 2e \otimes e$, $|e| = 1$, and $V = RUR^t$. Then

$$U - V = 2[(Ue - 2\langle Ue, e\rangle e) \otimes e + e \otimes (Ue - 2\langle Ue, e\rangle)].$$

This shows that if U and V are related by a rotation of angle π, $\mathrm{SO}(3)U$ and $\mathrm{SO}(3)V$ are rank-one connected, as is well-known.

We now mention that the n-dimensional version of Proposition 3.6 does not hold. As pointed out above (see the equivalence (3.14), (3.15)) this is not the statement we are interested in for $n \times n$ matrices, but we include it for the sake of completeness.

(3.9) Lemma. *For any $n \geq 4$, there exist symmetric positive definite $U, \bar{U}, V, \bar{V} \in \mathbb{R}^{n\times n}$ having the same eigenvalues such that*

$$\det(U - V) = 0 \ \textit{ but } \ \det(U^2 - V^2) \neq 0,$$
$$\det(\bar{U} - \bar{V}) \neq 0 \ \textit{ but } \ \det(\bar{U}^2 - \bar{V}^2) = 0.$$

Proof of Lemma 3.9. The proof is an entertaining exercise in linear algebra. We proceed in three steps, treating first the case $n = 4$, then $n = 5$ and finally the general case.

First step. Let us choose

$$U = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & \lambda_4 \end{pmatrix}, \quad Q_1 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$Q_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad Q_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\psi & -\sin\psi & 0 \\ 0 & \sin\psi & \cos\psi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

and

$$Q = Q_1 Q_2 Q_3 = (q_{ij}) = \begin{pmatrix} 0 & -\cos\psi & \sin\psi & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & \sin\psi & \cos\psi & 0 \end{pmatrix}.$$

Letting $V = QUQ^t$ we get

$$\det(U - QUQ^t) = \det(UQ - QU) = \det\left(\sum_{i,j} (\lambda_i - \lambda_j) q_{ij} e_i \otimes e_j\right)$$
$$= (\lambda_1 - \lambda_2)(\lambda_3 - \lambda_4) \cdot \cdot \left((\lambda_1 - \lambda_2)(\lambda_3 - \lambda_4)\cos^2\psi + (\lambda_1 - \lambda_3)(\lambda_2 - \lambda_4)\sin^2\psi\right).$$

Similarly,

$$\det(U^2 - QU^2Q^t) = (\lambda_1^2 - \lambda_2^2)(\lambda_3^2 - \lambda_4^2) \cdot \cdot \left((\lambda_1^2 - \lambda_2^2)(\lambda_3^2 - \lambda_4^2)\cos^2\psi + (\lambda_1^2 - \lambda_3^2)(\lambda_2^2 - \lambda_4^2)\sin^2\psi\right).$$

Let us choose $\lambda_i \neq \lambda_j$ whenever $i \neq j$. Then

$$\det(U - QUQ^t) = 0 \text{ if and only if } \tan^2\psi = -\frac{(\lambda_1 - \lambda_2)(\lambda_3 - \lambda_4)}{(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_4)}$$

and

$$\det(U^2 - QU^2Q^t) = 0 \text{ if and only if } \tan^2\psi = -\frac{(\lambda_1 + \lambda_2)(\lambda_3 + \lambda_4)}{(\lambda_1 + \lambda_3)(\lambda_2 + \lambda_4)} \cdot \frac{(\lambda_1 - \lambda_2)(\lambda_3 - \lambda_4)}{(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_4)}.$$

Hence we can find counter-examples: take any $0 < \lambda_1 < \lambda_2 < \lambda_4 < \lambda_3$ such that

$$\frac{(\lambda_1 + \lambda_2)(\lambda_3 + \lambda_4)}{(\lambda_1 + \lambda_3)(\lambda_2 + \lambda_4)} \neq 1.$$

Second step. Let us choose

$$U = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & 0 \\ 0 & 0 & 0 & \lambda_4 & 0 \\ 0 & 0 & 0 & 0 & \lambda_5 \end{pmatrix}, \quad Q_1 = \begin{pmatrix} 0 & -\cos\psi & \sin\psi & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & \sin\psi & \cos\psi & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$Q_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad Q_1Q_2 = \begin{pmatrix} 0 & -\cos\psi & \sin\psi & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & \sin\psi & \cos\psi & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Letting $Q = Q_1Q_2$, the end of the second step is from this stage on identical to the first one.

Third step. We now show that if the lemma holds for some n then it holds for $n+2$. This is very easily achieved by setting

$$\tilde{U} = \begin{pmatrix} U & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & \begin{matrix} 1 & 0 \\ 0 & 2 \end{matrix} \end{pmatrix},$$

$$\tilde{Q} = \begin{pmatrix} Q & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & \begin{matrix} 0 & -1 \\ 1 & 0 \end{matrix} \end{pmatrix},$$

where $U \in \mathbb{R}^{n\times n}$ and $Q \in \mathrm{SO}(n)$. Then $\det(\tilde{U} - \tilde{Q}\tilde{U}\tilde{Q}^t) = 0$ if and only if $\det(U - QUQ^t) = 0$ while $\det(\tilde{U}^2 - \tilde{Q}\tilde{U}^2\tilde{Q}^t) = 0$ if and only if $\det(U^2 - QU^2Q^t) = 0$. It is clear that the three steps imply the lemma. □

Before showing that the equivalence between (3.14) and (3.15) does not hold in higher dimensions we would like to point out some other consequences of Proposition 3.6. To begin with, given a symmetric positive definite $U \in \mathbb{R}^{3\times 3}$ and $V = RUR^t$ for some $R \in \mathrm{SO}(3)$ we give a full set of conditions on U and R for the existence of rank-one connections between the two wells $\mathrm{SO}(3)U$ and $\mathrm{SO}(3)V$. These conditions are in the same spirit as those established by Hertog [85], Ericksen [71] and in fact closer to those of Ou [118].

(3.10) Proposition. *Let $U \in \mathbb{R}^{3\times 3}$ be symmetric positive definite and let $V = RUR^t$ for some $R \in \mathrm{SO}(3)$. Then the three following conditions are equivalent:*

(i) $U - V$ is of rank (at most) two,

(ii) there exist a rotation $Q \in \mathrm{SO}(3)$ and two vectors $a, m \in \mathbb{R}^3$, $|m| = 1$, such that

$$U - QV = a \otimes m\,,$$

(*iii*) *one of the following holds:*

- (*a*) $U = V$,
- (*b*) U *has a double eigenvalue,*
- (*c*) R *is a rotation of angle* π,
- (*d*) U *has three simple eigenvalues and the axis of* R *is perpendicular to an eigenvector of* U.

Remarks. As said above the equivalence (*ii*), (*iii*) appears in [71, 118]. However, the equivalence (*i*), (*iii*) is new, and we give below an explicit proof.

In fact, it is easily seen[21] that if U has a double eigenvalue, then the axis of R is perpendicular to an eigenvector of U, so that we could summarise conditions (*iii*) (b) and (d) by the condition *'the axis of* R *is perpendicular to an eigenvector of* U*'*. Nevertheless, this condition is harder to check than condition (*iii*) (b), which we therefore prefer to leave in the statement of the proposition. Also, we will see below a case where $\det(U - V) = 0$ if and only if U has a double eigenvalue (see section 3.3).

It is not hard to see that if (*iii*) (d) holds, then either the axis e of R or $Ue \wedge e$ is an eigenvector of U. As noted by Pitteri and Zanzotto [125], this condition is equivalent to

$$[U(Ue \wedge e)] \wedge (Ue \wedge e) = 0. \tag{3.22}$$

In the case $V = RUR^t$ it is very easy to characterise those U and R that give rise to the trivial case $U = V$. This simply means that U and R commute, and, diagonalising U, it is easily seen to happen if and only if we are in one of the following situations:

(1) $U = \lambda\mathbb{I}$,

(2) $R = \mathbb{I}$,

(3) U has three simple eigenvalues, the axis of R is an eigenvector of U and the angle of R is π,

(4) U has a double eigenvalue and either R is a rotation of angle π about an eigenvector of U or the axis of R is an eigenvector of U corresponding to the simple eigenvalue.

Before proving Proposition 3.10, we need an elementary lemma of geometric nature.

(3.11) Lemma. *Let* $Q_1 = -\mathbb{I} + 2f_1 \otimes f_1$, $Q_2 = -\mathbb{I} + 2f_2 \otimes f_2$ *be two rotations of angle* π *about* f_1, f_2 *respectively, for some* $f_1 \neq \pm f_2$, $|f_1| = |f_2| = 1$. *Suppose that* f_1 *and* f_2 *are chosen so that the angle* θ *between* f_1 *and* f_2 *satisfies* $\theta \in [0, \pi/2]$. *Then* Q_1Q_2 *is a rotation of angle* 2θ *about* $f_2 \wedge f_1/|f_2 \wedge f_1|$. *Conversely, for every* $R \in \mathrm{SO}(3)$, *there exist* f_1, f_2, $|f_1| = |f_2| = 1$, *such that* $R = Q_1Q_2$.

Remark. Note that if $f_1 = \pm f_2$ then $Q_1Q_2 = \mathbb{I}$. The vectors f_1 and f_2 in the second part of the statement are not unique. Any other pair of unit vectors lying in the same plane and meeting at the same angle will suffice.

[21] I am grateful to Mario Pitteri for pointing this out to me.

PROOF OF LEMMA 3.11. The result follows from general results in elementary geometry, see *e.g.*, in Yale [155, Section 2.3]. Nevertheless, we give here a simple, self-contained proof, which proceeds in two steps.

First step. We let $Q_1 = -\mathbb{I} + 2f_1 \otimes f_1$, $Q_2 = -\mathbb{I} + 2f_2 \otimes f_2$, for some $|f_1| = |f_2| = 1$. Let us assume that

$$f_1 \wedge f_2 = \sin\theta \, \frac{f_1 \wedge f_2}{|f_1 \wedge f_2|}, \quad 0 \leq \theta \leq \frac{\pi}{2},$$

by multiplying f_1 or f_2 or both by -1 and interchanging f_1 and f_2 if necessary. A simple computation gives

$$Q_1 Q_2 = \mathbb{I} - 2f_1 \otimes f_1 - 2f_2 \otimes f_2 + 4\langle f_1, f_2\rangle f_1 \otimes f_2 .$$

It is clear that the axis of Q_1Q_2 is parallel to $f_1 \wedge f_2$. The angle of Q_1Q_2 is completely determined by the quantities $\langle f_1, Q_1Q_2 f_1\rangle$ and $f_1 \wedge Q_1Q_2 f_1$. We have

$$\begin{aligned} \langle f_1, Q_1Q_2 f_1\rangle &= -1 + 2\cos^2\theta = \cos 2\theta, \\ f_1 \wedge Q_1Q_2 f_1 &= -2\langle f_1, f_2\rangle f_1 \wedge f_2 = \sin 2\theta \, \frac{f_2 \wedge f_1}{|f_2 \wedge f_1|}. \end{aligned}$$

Hence Q_1Q_2 is a rotation of angle 2θ about $f_2 \wedge f_1/|f_2 \wedge f_1|$.

Second step. Let $R \in \mathrm{SO}(3)$ be a rotation of angle $\alpha \in (0, 2\pi)$ about e, $|e| = 1$. We have excluded the trivial case $R = \mathbb{I}$. In particular, for every $|f| = 1$ orthogonal to e, we have

$$f \wedge Rf = \sin\alpha \, e .$$

Let us choose $|f_1| = |f_2| = 1$ such that $e = f_2 \wedge f_1/|f_2 \wedge f_1|$ and such that the angle θ between f_1 and f_2 satisfies $0 \leq \theta \leq \pi/2$. Some elementary computations yield

$$\begin{aligned} \langle f_1, Rf_1\rangle &= \cos\alpha, \\ f_1 \wedge Rf_1 &= \sin\alpha \, e, \\ \langle f_1, Q_1Q_2 f_1\rangle &= \langle f_1, Q_2Q_1 f_1\rangle = \cos 2\theta, \\ f_1 \wedge Q_1Q_2 f_1 &= \sin 2\theta \, \frac{f_2 \wedge f_1}{|f_2 \wedge f_1|}, \\ f_1 \wedge Q_2Q_1 f_2 &= \sin(-2\theta) \, \frac{f_2 \wedge f_1}{|f_2 \wedge f_1|}. \end{aligned}$$

Now the proof is finished since if $\alpha \in (0, \pi]$, we choose f_1, f_2 such that $2\theta = \alpha$ and then $R = Q_1Q_2$, while if $\alpha \in (\pi, 2\pi)$, we choose f_1, f_2 such that $-2\theta = \alpha - 2\pi$, and then $R = Q_2Q_1$. □

We are now in a position to give the

PROOF OF PROPOSITION 3.10. The equivalence $(i) \Leftrightarrow (ii)$ has already been proved. We need only to show that (i) and (iii) are equivalent. We divide the proof into three steps.

First step. Assume that (i) holds and that $U \neq V$. Then $U - V$ is of rank two (since U and V have the same eigenvalues) and that means that there exist non-zero $b, c \in \mathbb{R}^3$, $|c| = 1$, such that

$$U = R[U + b \otimes c + c \otimes b]R^t . \tag{3.23}$$

The goal of the first step is to show that there exists a rotation Q of angle π (in fact Q will be either $-\mathbb{I} + 2\frac{b}{|b|} \otimes \frac{b}{|b|}$ or $-\mathbb{I} + 2c \otimes c$) such that

$$U + b \otimes c + c \otimes b = QUQ^t. \tag{3.24}$$

Equation (3.23) means that U and $U + b \otimes c + c \otimes b$ are orthogonally similar. Comparing the traces of these matrices yields

$$\langle b, c \rangle = 0 \,. \tag{3.25}$$

Comparing the second invariants,[22] which reduces here to comparing the square of the norm, we get

$$-2\langle Ub, c \rangle = |b|^2 \,. \tag{3.26}$$

Writing $Q = -\mathbb{I} + 2f \otimes f$ with $|f| = 1$ we have

$$QUQ^t = U + 2\left[(\langle Uf, f \rangle f - Uf) \otimes f + f \otimes (\langle Uf, f \rangle f - Uf)\right]$$

which we want to equal $U + b \otimes c + c \otimes b$. Clearly there are only two possibilities: either $f = \frac{b}{|b|}$ or $f = c$. If $f = c$ we must have

$$2\left(\langle Uc, c \rangle\, c - Uc\right) = b \,.$$

Using (3.26) we get

$$\begin{aligned} Uc &= -\frac{1}{2} b + \langle Uc, c \rangle\, c \\ &= \langle Uc, \frac{b}{|b|} \rangle \frac{b}{|b|} + \langle Uc, c \rangle\, c. \end{aligned}$$

This holds if and only if $Uc \in \operatorname{span}\{b, c\}$. Similarly, if we choose $f = \frac{b}{|b|}$ this can hold if and only if $Ub \in \operatorname{span}\{b, c\}$.

If we consider the orthonormal basis of $\mathbb{R}^3$ composed of $\frac{b}{|b|}$, c and a third vector $\bar{e}$ (this is possible because of (3.25)) we have

$$U = \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ u_{12} & u_{22} & u_{23} \\ u_{13} & u_{23} & u_{33} \end{pmatrix} \text{ and } U + b \otimes c + c \otimes b = \begin{pmatrix} u_{11} & -u_{12} & u_{13} \\ -u_{12} & u_{22} & u_{23} \\ u_{13} & u_{23} & u_{33} \end{pmatrix},$$

where the minus signs come from (3.26). All we have to show is that either $u_{13} = \langle U\frac{b}{|b|}, \bar{e} \rangle$ or $u_{23} = \langle Uc, \bar{e} \rangle$ vanishes in order to have either $Ub \in \operatorname{span}\{b, c\}$ or $Uc \in \operatorname{span}\{b, c\}$. But this is easily achieved by equalising the determinant of U and $U + b \otimes c + c \otimes b$ bearing in mind that $u_{12} \neq 0$ because $b \neq 0$ (see (3.26)), which completes the first step.

Second step. We now show (*iii*). We can rewrite (3.23) as

$$R^t U R = QUQ^t$$

with $Q = -\mathbb{I} + 2\frac{b}{|b|} \otimes \frac{b}{|b|}$ or $Q = -\mathbb{I} + 2c \otimes c$. This means that U commutes with RQ. Excluding the case $U = \lambda\mathbb{I}$ which gives $U = V$, and the case where U has a double eigenvalue (in which (*i*) holds, by (3.19)), we are left with the case where U has three simple eigenvalues. Let us diagonalise $U = \sum_i \lambda_i e_i \otimes e_i$, with $\lambda_i \neq \lambda_j$ whenever $i \neq j$. Since RQ maps the eigenspaces

[22] We recall that the principal invariants are the three symmetric functions of the eigenvalues.

of U onto themselves, we must have $RQ = -\mathbb{I} + 2e_i \otimes e_i$ for some $i = 1, 2$ or 3, or $RQ = \mathbb{I}$. If $RQ = \mathbb{I}$, then $R = Q$, a rotation of angle π, case (*iii*) (c) above. Writing $Q = -\mathbb{I} + 2f \otimes f$, with $f = \frac{b}{|b|}$ or $f = c$, we deduce that $R = (RQ)Q = (-\mathbb{I} + 2e_i \otimes e_i)(-\mathbb{I} + 2f \otimes f)$ and that the axis of R is parallel to $f \wedge e_i$. We study several cases:

(1) $f = e_i$: this cannot happen for otherwise $U = V$.

(2) $f = e_j$ for some $j \neq i$: then the axis of R is an eigenvector of U and hence perpendicular to an eigenvector of U.

(3) $f \neq e_k$ for every k: then the axis of R is perpendicular to e_i, an eigenvector of U.

Therefore (*iii*) is proved.

Third step. Assume now that (*iii*) holds. All cases but one are trivial. Suppose that the axis of $R \neq \mathbb{I}$ is orthogonal to an eigenvector of U, e_i say. By Lemma 3.11, R can be expressed as the product of two rotations Q_1, Q_2 of angle π, $R = Q_1 Q_2$, with $Q_i = -\mathbb{I} + 2f_i \otimes f_i$, $i = 1, 2$, and $|f_1| = |f_2| = 1$. By the remark following Lemma 3.11, we can choose f_1 to be e_i. Hence $RQ_2 = Q_1$ and therefore RQ_2 commutes with U. Hence $U = RQ_2 U Q_2 R^t$ and

$$U - V = R[Q_2 U Q_2 - U]R^t .$$

It is easily checked that $Q_2 U Q_2 - U$ is of rank two. Hence $U - V$ is of rank two and the proof is complete. □

Remark. As we will show later, in higher dimensions it is not possible to find a tensor $Q = -\mathbb{I} + 2f \otimes f$ as in the first step. This is precisely why the equivalence between (3.14) and (3.15) does not hold in higher dimensions.

In fact, the first step of the foregoing proof essentially proves another well-known result, to the effect that if $\mathrm{SO}(3)U$ and $\mathrm{SO}(3)RUR^t$ are rank-one connected, then one can replace R by a rotation of angle π. This was originally proved by Ericksen [67]. However, the explicit formula for this rotation given by our proof is much simpler than that of Ericksen.

(3.12) Corollary. *Let $U, V \in \mathbb{R}^{3\times 3}$ be symmetric positive definite and have the same eigenvalues. Assume furthermore that*

$$U - V = -\lambda e_1 \otimes e_1 + \lambda e_3 \otimes e_3,$$

where $\lambda > 0$ and let $e_2 \in \ker(U - V)$, $|e_2| = 1$. Then, $\langle Ue_2, e_3\rangle^2 - \langle Ue_2, e_1\rangle^2 = 0$ and

(*i*) *if $\langle Ue_2, e_3\rangle = \langle Ue_2, e_1\rangle$, then $V = RUR^t$ with $R = -\mathbb{I} + 2e \otimes e$, $e = 1/\sqrt{2}(e_1 - e_3)$,*

(*ii*) *if $\langle Ue_2, e_3\rangle = -\langle Ue_2, e_1\rangle$, then $V = RUR^t$ with $R = -\mathbb{I} + 2e \otimes e$, $e = 1/\sqrt{2}(e_1 + e_3)$.*

Moreover, if $\langle Ue_2, e_3\rangle = 0 = \langle Ue_2, e_1\rangle$, then $V = RUR^t$ for both rotations of cases (i) and (ii).

Proof of Corollary 3.12. Let $U - V = -\lambda e_1 \otimes e_1 + \lambda e_3 \otimes e_3$. Rewrite it as $U - V = b \otimes c + c \otimes b$ with $b = \lambda/\sqrt{2}(-e_1 + e_3)$ and $c = 1/\sqrt{2}(e_1 + e_3)$. Then $V = U - b \otimes c - c \otimes b$. Choose the basis of $\mathbb{R}^3$ composed of $b/|b|$, c and e_2 (b and c are seen to be orthogonal by comparing the traces of

U and $U-b\otimes c-c\otimes b$). Then, as in the first step of the proof of Proposition 3.10, comparing the two other principal invariants of U and $U-b\otimes c-c\otimes b$ yields $\langle Ue_2, -e_1+e_3\rangle\langle Ue_2, e_1+e_3\rangle = 0$, a condition easily seen to be equivalent to $\langle Ue_2, e_3\rangle^2 - \langle Ue_2, e_1\rangle^2 = 0$ and implies the existence of R, a rotation of angle π about e such that $V = RUR^t$. Furthermore, there are two possibilities: either $e = b/|b|$ or $e = c$. Notice that $b/|b| = 1/\sqrt{2}(-e_1 + e_3)$. It is easily seen that the first case occurs when $\langle Ue_2, -e_1+e_3\rangle = 0$ which is equivalent to $\langle Ue_2, e_3\rangle = \langle Ue_2, e_1\rangle$, while the second case occurs when $\langle Ue_2, e_1 + e_3\rangle = 0$, that is when $\langle Ue_2, e_3\rangle = -\langle Ue_2, e_1\rangle$. The corollary is proved. □

We now recall the result of Gurtin [81] (see also [35] and [67]) we mentioned earlier, a simple proof of which we give for the convenience of the reader.

(3.13) Lemma. *Let $U \in \mathbb{R}^{3\times 3}$ be symmetric positive definite and let $V = RUR^t \neq U$ with $R = -\mathbb{I} + 2e \otimes e$, $|e| = 1$. Then the equation*

$$U - QV = a \otimes m \tag{3.27}$$

admits two solutions given by

$$a = 2(Ue - \frac{U^{-1}e}{|U^{-1}e|^2}), \quad m = e,$$
$$a = \frac{2\rho}{|Ue|^2}Ue, \quad m = \frac{1}{\rho}(U^2e - |Ue|^2e),$$

where $\rho > 0$ is a constant chosen as to have $|m| = 1$. In both cases, Q is found by substituting a and m back into (3.27).

Proof of Lemma 3.13. First observe that solving (3.27) is equivalent to finding a and m, $|m| = 1$, such that $\langle U^{-1}a, m\rangle = 0$ and

$$U^2 - V^2 = (Ua - \frac{|a|^2}{2}m) \otimes m + m \otimes (Ua - \frac{|a|^2}{2}m). \tag{3.28}$$

Moreover, a simple calculation gives

$$U^2 - V^2 = 2[(U^2e - |Ue|^2e) \otimes e + e \otimes (U^2e - |Ue|^2e)]. \tag{3.29}$$

We are thus left with equalising (3.28) and (3.29). Since e is not an eigenvector of U (otherwise we would have $U = V$), e is not parallel to $2(U^2e - |Ue|^2e)$, and consequently it is easily seen (or use a result of Ruddock [132]) that m, $(Ua - |a|^2/2m)$, e and $2(U^2e - |Ue|^2e)$ are coplanar. But this implies that either $m = e$ or $m = 1/\rho(U^2e - |Ue|^2e)$. We divide the rest of the proof into two parts, each dealing with one of these two cases.

First case. Let $m = e$. Then $2(U^2m - |Ue|^2m) = Ua - |a|^2/2e$, which is equivalent to

$$U(a - 2Ue) = (2|Ue|^2 - \frac{|a|^2}{2})e. \tag{3.30}$$

Setting $a = 2Ue - \lambda U^{-1}e$ for some λ to be determined later, we get $|a|^2 = 4|Ue|^2 + \lambda^2|U^{-1}e|^2 - 4\lambda$. Replacing into (3.30) yields $\lambda^2/2|U^{-1}e|^2 - \lambda = 0$. This gives two solutions for λ. Firstly $\lambda = 0$ which leads to a solution for which $\langle U^{-1}a, m\rangle = -2$, hence to be excluded, and secondly $\lambda = 2/|U^{-1}e|^2$, which gives $a = 2(Ue - U^{-1}e/|U^{-1}e|^2)$ and $\langle U^{-1}a, m\rangle = 0$.

Second case. Let $m = 1/\rho(U^2e - |Ue|^2e)$, where $\rho > 0$ is such that $|m| = 1$. Then $Ua - |a|^2/(2\rho)(U^2e - |Ue|^2e) = 2\rho e$, which is equivalent to

$$U(a - \frac{|a|^2}{2\rho}) = (2\rho - \frac{|a|^2|Ue|^2}{2\rho})e\,. \tag{3.31}$$

Choosing $a = \lambda Ue$ and replacing in (3.31) we get

$$U(\lambda - \frac{\lambda^2|Ue|^2}{2\rho})Ue = (2\rho - \frac{\lambda^2|Ue|^4}{2\rho})e\,. \tag{3.32}$$

Noticing that (3.32) vanishes identically if

$$(\lambda = 0 \;\text{ or }\; \lambda = \frac{2\rho}{|Ue|^2}) \quad \text{and} \;\; \lambda^2 = \frac{4\rho^2}{|Ue|^4}\,,$$

we choose $\lambda = 2\rho/|Ue|^2$. With this choice, $a = 2\rho/|Ue|^2Ue$ and $\langle U^{-1}a, n\rangle = 0$ as desired. □

We now put Corollary 3.12 and Lemma 3.13 together to get

(3.14) Theorem. *Let $U, V \in \mathbb{R}^{3\times 3}$ be symmetric positive definite and have the same eigenvalues. Assume furthermore that*

$$U - V = -\lambda e_1 \otimes e_1 + \lambda e_3 \otimes e_3\,,$$

where $\lambda > 0$ and let $e_2 \in \ker(U - V)$, $|e_2| = 1$. The solutions of (3.27) are given as follows.

(i) Either $\langle Ue_2, e_3\rangle = \langle Ue_2, e_1\rangle$, and the two solutions are

$$\begin{aligned}
a_1 &= 2(U(e_1 - e_3)/\sqrt{2}) - \frac{U^{-1}(e_1 - e_3)/\sqrt{2}}{|U^{-1}(e_1 - e_3)/\sqrt{2}|^2}\,,\\
m_1 &= \frac{e_1 - e_3}{\sqrt{2}}\,,\\
a_2 &= \frac{2\rho}{|U(e_1 - e_3)/\sqrt{2})|^2}U(e_1 - e_3)/\sqrt{2}\,,\\
m_2 &= 1/\rho\left\{U^2(e_1 - e_3)/\sqrt{2}) - |U(e_1 - e_3)/\sqrt{2})|^2(e_1 - e_3)/\sqrt{2}\right\},
\end{aligned}$$

where $\rho > 0$ is a constant chosen so that $|m_2| = 1$.

(ii) Or $\langle Ue_2, e_3\rangle = -\langle Ue_2, e_1\rangle$, and the two solutions are

$$\begin{aligned}
\bar{a}_1 &= 2(U(e_1 + e_3)/\sqrt{2}) - \frac{U^{-1}(e_1 + e_3)/\sqrt{2}}{|U^{-1}(e_1 + e_3)/\sqrt{2}|^2}\,,\\
\bar{m}_1 &= \frac{e_1 + e_3}{\sqrt{2}}\,,\\
\bar{a}_2 &= \frac{2\rho}{|U(e_1 + e_3)/\sqrt{2})|^2}U(e_1 + e_3)/\sqrt{2}\,,\\
\bar{m}_2 &= 1/\rho\left\{U^2(e_1 + e_3)/\sqrt{2}) - |U(e_1 + e_3)/\sqrt{2})|^2(e_1 + e_3)/\sqrt{2}\right\},
\end{aligned}$$

where $\rho > 0$ is a constant chosen so that $|\bar{m}_2| = 1$.

Furthermore, if $\langle Ue_2, e_3\rangle = 0 = \langle Ue_2, e_1\rangle$*, we have* $(a_1, m_1) = (\bar{a}_2, \bar{m}_2)$*, and* $(a_2, m_2) = (\bar{a}_1, \bar{m}_1)$*.*

Proof of Theorem 3.14. The first part of the theorem is just Corollary 3.12 inserted into Lemma 3.13. To check the second part, it is enough to verify that $m_1 = \bar{m}_2$ and $m_2 = \bar{m}_1$, which is a matter of elementary algebra. □

Other formulæ for a and m can be found in the literature: *e.g.*, those due to Khachaturyan [92], Ball and James [27, 28] stated in Theorem 3.2, those given by Ericksen [71] and also, those obtained recently by Silhavỳ [137]. In particular, all the formulæ quoted above are more general than ours since they apply to the case where U and V do not have the same eigenvalues (of course they are expressed in terms of U^tU and V^tV rather than of U and V). Also, Ericksen's and Silhavỳ's results are more tractable as they do not involve inverses. However, the interest of Theorem 3.14 lies in the simplicity of the solutions obtained for m_1, a_2 and $\bar{m}_1, \bar{a}_2$. This is used in Corollary 3.16 below, where we get an easy classification of the different types of twins, of which we now recall the definition. For the purpose of this definition, let $\mathscr{P}$ denote the symmetry group of the austenite, which is a (not necessarily proper) subgroup of the cubic (Laue) point group, consisting of those rotations that map the unit cube into itself.

(3.15) Definition. *Let* $R \in \mathscr{P}$ *be a rotation of angle* π *and let* $U, V \in \mathbb{R}^{3\times 3}$ *be such that* $V = RUR^t$*. Let* (a, m, Q) *be any solution of* (3.27)*. We say that* (U, QV) *is a* twin of type I *if* m *is a direction of symmetry of* $\mathscr{P}$ *(*i.e.*, the axis of a rotation in* $\mathscr{P}$*), a* twin of type II *if* $U^{-1}a$ *is a direction of symmetry of* $\mathscr{P}$ *and a* compound twin *if* (U, QV) *can be expressed as both a type I and a type II twin. Twins of type I, II and compound twins are called* conventional twins*. Twins that are neither of type I nor of type II are called* non-conventional*. We say that the wells* $\mathrm{SO}(3)U$ *and* $\mathrm{SO}(3)V$ *have a* type I*,* type II*,* compound*, or* non-conventional twinning mode *according to the nature of the twin* (U, QV)*.*

(3.16) Corollary. *Let* U *and* V *satisfy the same hypotheses as in Theorem* 3.14*.*

(*i*) *Suppose* $\langle Ue_2, e_3\rangle = \langle Ue_2, e_1\rangle$*. If* $1/\sqrt{2}(e_1 - e_3)$ *is a direction of symmetry of* $\mathscr{P}$*, we get a twin of type I (the solution with* (a_1, m_1)*) and a twin of type II (the solution corresponding to* (a_2, m_2)*). If* $1/\sqrt{2}(e_1 - e_3)$ *is not a direction of symmetry, we get non-conventional twins.*

(*ii*) *Suppose* $\langle Ue_2, e_3\rangle = -\langle Ue_2, e_1\rangle$*. If* $1/\sqrt{2}(e_1 + e_3)$ *is a direction of symmetry of* $\mathscr{P}$*, we get a twin of type I (the solution corresponding to* (a_1, m_1)*) and a twin of type II (the solution with* (a_2, m_2)*). If* $1/\sqrt{2}(e_1 + e_3)$ *is not a direction of symmetry, we get non-conventional twins.*

(*iii*) *Suppose* $\langle Ue_2, e_3\rangle = 0 = \langle Ue_2, e_1\rangle$*. If* $1/\sqrt{2}(e_1 \pm e_3)$ *are directions of symmetry of* $\mathscr{P}$*, we get compound twins. If only one of the vectors* $1/\sqrt{2}(e_1 \pm e_3)$ *is a direction of symmetry, we get only twins of type I and II. If neither* $1/\sqrt{2}(e_1 \pm e_3)$ *are directions of symmetry, we get non-conventional twins.*

Proof of Corollary 3.16. Immediate in view of Definition 2. □

Re-phrasing Theorem 3.14 with the language of Corollary 3.16, we get a simple criterion for the existence of compound twins.

(3.17) Corollary. *Let U and V satisfy the same hypotheses as in Theorem* 3.14. *Assume furthermore that $1/\sqrt{2}(e_1 \pm e_3)$ are directions of symmetry of $\mathscr{P}$. Then the wells* $\mathrm{SO}(3)U$ *and* $\mathrm{SO}(3)V$ *have a compound twinning mode if and only if U and V have a common eigenvector.*

Remark. The condition that $1/\sqrt{2}(e_1 \pm e_3)$ be directions of symmetry of $\mathscr{P}$ is important. There is an example of two variants in cubic-to-monoclinic transitions which have a common eigenvector but do not satisfy this hypothesis, and whose twinning mode is therefore non-conventional (see Table 3.4, variants U_1 and U_4).

Proof of Corollary 3.17. Theorem 3.14 asserts that $\mathrm{SO}(3)U$ and $\mathrm{SO}(3)V$ have a compound twinning mode if and only if $\langle Ue_2, e_3\rangle = 0 = \langle Ue_2, e_1\rangle$. But this is clearly equivalent to e_2 being an eigenvector of U. The equality $Ue_2 = Ve_2$, which is the definition of e_2, completes the proof. □

We end this section by showing that in higher dimensions, the equivalence between (3.14) and (3.15) does not hold. To explain why this is so, let us try to adapt the construction in the proof of Proposition 3.10 in an attempt to prove the equivalence. We let $V = RUR^t$ and assume $U - V$ is of rank two. As above, this means that there exist two vectors $b, c \in \mathbb{R}^n$, $|c| = 1$ such that the matrices U and $\tilde{U} = U + b \otimes c + c \otimes b$ are orthogonally similar. This implies that

$$\langle b, c\rangle = 0\,, -2\langle Ub, c\rangle = |b|^2\,. \tag{3.33}$$

It is clear that if, as in the above proof, we could find a tensor Q of the form $Q = -\mathbb{I} + 2f \otimes f$ for some $|f| = 1$ such that $U + b \otimes c + c \otimes b = QUQ$, we could prove that $U^2 - V^2$ as well as $\sqrt{U} - \sqrt{V}$ are of rank two, hence the equivalence. This comes from the equality

$$U - V = R[\tilde{U} - U]R^t = R[QUQ - U]R^t\,.$$

As we have seen in the above proof, the only possibility for such a Q to exist is that either Ub or Uc belong to $\mathrm{span}\{b, c\}$, a condition that is satisfied for 3×3 matrices. It is precisely this that does not hold in higher dimensions. For example, let us look at the four-dimensional case. Note that we can choose an orthonormal basis $\{e_i\}$ of $\mathbb{R}^4$ such that

$$e_1 = \frac{b}{|b|},\ e_2 = c,\ \langle Ub, e_3\rangle = 0\,.$$

In this basis, we have

$$U = \begin{pmatrix} u_{11} & u_{12} & 0 & u_{14} \\ u_{12} & u_{22} & u_{23} & u_{24} \\ 0 & u_{23} & u_{33} & u_{34} \\ u_{14} & u_{24} & u_{34} & u_{44} \end{pmatrix} \text{ and } \tilde{U} = \begin{pmatrix} u_{11} & -u_{12} & 0 & u_{14} \\ -u_{12} & u_{22} & u_{23} & u_{24} \\ 0 & u_{23} & u_{33} & u_{34} \\ u_{14} & u_{24} & u_{34} & u_{44} \end{pmatrix}$$

Again, the minus signs come from (3.33). To show that a Q as above exists, we have to show either that $u_{14} = 0$ or that $u_{23} = u_{24} = 0$. Equalising the characteristic polynomials, we get

$$u_{12}u_{14}(-u_{24}\lambda + u_{24}u_{33} - u_{23}u_{34}) = 0 \quad \text{for all } \lambda \in \mathbb{R}.$$

Since $u_{12} \neq 0$, this yields either $u_{14} = 0$, or $u_{24} = 0$ and $u_{23}u_{34} = 0$. The latter gives a case where it is not possible to find a tensor Q as in the three-dimensional case: we have $\tilde{U} = U + b \otimes c + c \otimes b = QUQ$ with $Q = -\mathbb{I} + 2(e_1 \otimes e_1 + e_4 \otimes e_4)$ and an elementary computation gives

$$U^2 - QU^2Q^t = -2u_{12} \begin{pmatrix} 0 & u_{11}+u_{22} & u_{23} & 0 \\ u_{11}+u_{22} & 0 & 0 & u_{14} \\ u_{23} & 0 & 0 & 0 \\ 0 & u_{14} & 0 & 0 \end{pmatrix},$$

which shows that if we choose U properly we will have a counter-example. Indeed, let

$$U = \begin{pmatrix} 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

One can check numerically that $QUQ - U$ is of rank two, but neither $QU^2Q - U^2$ nor $Q\sqrt{U}Q - \sqrt{U}$ are (in fact, both are of rank four). This example is easily extended to higher dimensions, proving our last

(3.18) Lemma. *For any $n \geq 4$, there exist symmetric positive definite matrices $U, \bar{U}, V, \bar{V} \in \mathbb{R}^{n\times n}$ having the same eigenvalues such that*

$$\operatorname{rank}(U - V) = 2 \;\; \textit{but} \;\; \operatorname{rank}(U^2 - V^2) \neq 2,$$
$$\operatorname{rank}(\bar{U} - \bar{V}) \neq 2 \;\; \textit{but} \;\; \operatorname{rank}(\bar{U}^2 - \bar{V}^2) = 2.$$

Remark. The foregoing analysis shows also that it is fairly easy to modify the proof of Proposition 3.10 and get *e.g.*, a four-dimensional version of Proposition 3.10 (*iii*), *i.e.*, a full set of conditions on the symmetric positive definite U and R (or on U^tU and R if U is not symmetric) for the existence of rank-one connections between $\mathrm{SO}(4)U$ and $\mathrm{SO}(4)RUR^t$. Briefly, we would start with the hypothesis that $U^2 - RU^2R^t$ is of rank two, and, as above, we would get $R^tU^2R = QU^2Q$ for some diagonal tensor Q whose entries are either 1 or -1 (but not necessarily of the form $Q = -\mathbb{I} + 2e \otimes e$ as in the three-dimensional case). Then, a careful discussion as in the second step of the proof of Proposition 3.10 would give a set of conditions on U^2 and R. Taking the square-root, we would get the desired conditions on U and R. However, we have not succeeded in adapting this method to get a general n-dimensional result.

3.3 Examples

To conclude this chapter, three examples are studied: *cubic-to-tetragonal, tetragonal-to-monoclinic,* and *cubic-to-monoclinic transformations*. The first one is so simple that all the results presented above require a comparable amount of work and could be used to the same effect. We give it mainly for the sake of illustration. As for the two others, however, the computations involved become quite tedious and here, our results prove to simplify their analysis substantially.

Cubic-to-tetragonal transitions

As said above, we work this example out merely as a warm-up. Among those alloys that undergo a cubic-to-tetragonal transition are In-Tl and Mn-Cu. There are three variants given by

$$U_1 = \begin{pmatrix} \eta_2 & 0 & 0 \\ 0 & \eta_1 & 0 \\ 0 & 0 & \eta_1 \end{pmatrix}, \; U_2 = \begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_1 \end{pmatrix}, \; U_3 = \begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_1 & 0 \\ 0 & 0 & \eta_2 \end{pmatrix},$$

where $\eta_1, \eta_2 > 0$. One at once sees (literally!) that

$$\det(U_1 - U_2) = \det(U_1 - U_3) = 0\,,$$

so that all the variants are compatible, and that the twins are generic. Following Pitteri [123], a twin (U, QV) is called *generic* if its existence does not depend on the coefficients of U and *non-generic twins* if it does.[23]

Furthermore, each pair of U_i has a common eigenvector, so that the twinning mode is always compound (the technical assumption in Corollary 3.17 is straightforwardly checked to hold here).

Tetragonal-to-monoclinic transitions

Tetragonal-to-monoclinic transitions occur *e.g.* in zirconia (ZrO_2). We begin by quoting a result due to Simha [139] that gives all the possible Bain strain matrices, *i.e.* all the possible deformations that describe the change of symmetry from tetragonal to monoclinic. First, recall that in the orthonormal tetragonal basis $\{e_1, e_2, e_3\}$, with e_3 chosen as the four-fold tetragonal axis, the tetragonal point group is given by

$$\mathscr{P}_t = \{\mathbb{I}, R^{\pi}_{e_1}, R^{\pi}_{e_2}, R^{\pi}_{e_3}, R^{\pi}_{1/\sqrt{2}(e_1+e_2)}, R^{\pi}_{1/\sqrt{2}(e_1-e_2)}, R^{\pi/2}_{e_3}, R^{3\pi/2}_{e_3}\},$$

where R^{θ}_{e} denotes a rotation of angle θ about e. It has been shown by Ball and James [1] that the Bain strains U are characterised by the condition that they satisfy

$$\{R \in \mathscr{P}_t \,:\, RUR^t = U\} = \mathscr{P}_m\,, \tag{3.34}$$

where $\mathscr{P}_m \subset \mathscr{P}_t$ is a representation of the monoclinic point group.

(3.19) Theorem (Simha [139]). *Let $\{e_1, e_2, e_3\}$ be the orthonormal tetragonal basis with e_3 as the four-fold axis of $\mathscr{P}_t$ and let $\mathscr{U}_{t\to m}$ be the set of all symmetric positive definite 3×3 matrices satisfying*

$$\{R \in \mathscr{P}_t \,:\, RUR^t = U\} = \mathscr{P}_m\,.$$

Part I. *If $\mathscr{P}_m = \{\mathbb{I}, R^{\pi}_{e}\}$ where e is a two-fold axis of $\mathscr{P}_t$, then*

$$\mathscr{U}_{t\to m} = \Big\{ \eta_1 e\otimes e + \eta_2 f_2\otimes f_2 + \eta_3 f_3\otimes f_3 \,:\, \eta_i > 0,\ \eta_2 \neq \eta_3, \\ \{e, f_2, f_3\} \text{ orthonormal},\ f_2, f_3 \notin \{e_1, e_2, e_3, \frac{1}{\sqrt{2}}(e_1 \pm e_2)\} \Big\}\,.$$

[23] Using Corollary 3.8, we can re-phrase these definitions by saying that the twin is generic if $\det(U-V) = 0$ identically and non-generic if $\det(U-V) = 0$ only if certain algebraic conditions on the entries of U are met.

Case 1. $\mathscr{P}_m = \{\mathbb{I}, R^\pi_{e_1}\}$	$U_1 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & \gamma \\ 0 & \gamma & \delta \end{pmatrix}$	$\alpha > 0$, $\gamma \neq 0$, $\beta\delta - \gamma^2 > 0$.
Case 2. $\mathscr{P}_m = \{\mathbb{I}, R^\pi_{e_2}\}$	$U_2 = \begin{pmatrix} \beta & 0 & \gamma \\ 0 & \alpha & 0 \\ \gamma & 0 & \delta \end{pmatrix}$	$\alpha > 0$, $\gamma \neq 0$, $\beta\delta - \gamma^2 > 0$.
Case 3. $\mathscr{P}_m = \{\mathbb{I}, R^\pi_{e_3}\}$	$U_3 = \begin{pmatrix} \beta & \gamma & 0 \\ \gamma & \delta & 0 \\ 0 & 0 & \alpha \end{pmatrix}$	$\alpha > 0$, $\gamma \neq 0$, $\beta\delta - \gamma^2 > 0$.
Case 4. $\mathscr{P}_m = \{\mathbb{I}, R^\pi_{1/\sqrt{2}(e_1+e_2)}\}$	$U_4 = \begin{pmatrix} \alpha & \beta & \gamma \\ \beta & \alpha & -\gamma \\ \gamma & -\gamma & \delta \end{pmatrix}$	$\gamma \neq 0$, $\det U_4 > 0$
Case 5. $\mathscr{P}_m = \{\mathbb{I}, R^\pi_{1/\sqrt{2}(e_1-e_2)}\}$	$U_5 = \begin{pmatrix} \alpha & \beta & \gamma \\ \beta & \alpha & \gamma \\ \gamma & \gamma & \delta \end{pmatrix}$	$\gamma \neq 0$, $\det U_5 > 0$

Table 3.1: Possible Bain strain matrices for a tetragonal-to-monoclinic transition.

Part II. *If* $\mathscr{P}_m = \{\mathbb{I}, R^\pi_{e_3}\}$, *then*

$$\mathscr{U}_{t\to m} = \Big\{ \eta_1 f_1 \otimes f_1 + \eta_2 f_2 \otimes f_2 + \eta_3 e_3 \otimes e_3 \ : \eta_i > 0,\ \eta_1 \neq \eta_2, \\ \{f_1, f_2, e_3\} \textit{ orthonormal},\ f_1, f_2 \notin \{e_1, e_2, \frac{1}{\sqrt{2}}(e_1 \pm e_2)\} \Big\}.$$

In the theorem the transformation matrices are expressed in the basis composed of their eigenvectors. For our purposes, it is more convenient to express them in the tetragonal basis. We distinguish five cases, as there are five possible choices of monoclinic point group $\mathscr{P}_m \subset \mathscr{P}_t$. In each case, we use (3.34) to determine the form of the transformation matrix. The results are displayed in Table 3.1.

Observe that U_1 and U_2 are conjugate in the tetragonal point group since $RU_1R^t = U_2$ with $R = R^\pi_{1/\sqrt{2}(e_1-e_2)}$. Therefore, we restrict our attention to U_1 only.

Hence, there are four different tetragonal-to-monoclinic transitions. The first one corresponds to having a two-fold tetragonal axis parallel to an edge of the tetragonal cell as the monoclinic axis (case U_1 above), the second one to having the four-fold tetragonal axis as the monoclinic axis (case U_3 above), while in the third and fourth cases, the monoclinic axis is a two-fold tetragonal axis which is a face diagonal in the tetragonal unit cell (cases U_4, U_5 above, which are, as we will see below, algebraically similar).

We give in Table 3.2 the four variants that arise in each of these four cases. It is easy to see that the sets $\{U_{3,1}, U_{3,2}, U_{3,3}, U_{3,4}\}$ and $\{U_{4,1}, U_{4,2}, U_{4,3}, U_{4,4}\}$ are identical provided one

Case 1.	$U_{1,1} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & \gamma \\ 0 & \gamma & \delta \end{pmatrix}$ $U_{1,2} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & -\gamma \\ 0 & -\gamma & \delta \end{pmatrix}$ $U_{1,3} = \begin{pmatrix} \beta & 0 & \gamma \\ 0 & \alpha & 0 \\ \gamma & 0 & \delta \end{pmatrix}$ $U_{1,4} = \begin{pmatrix} \beta & 0 & -\gamma \\ 0 & \alpha & 0 \\ -\gamma & 0 & \delta \end{pmatrix}$
Case 2.	$U_{2,1} = \begin{pmatrix} \beta & \gamma & 0 \\ \gamma & \delta & 0 \\ 0 & 0 & \alpha \end{pmatrix}$ $U_{2,2} = \begin{pmatrix} \beta & -\gamma & 0 \\ -\gamma & \delta & 0 \\ 0 & 0 & \alpha \end{pmatrix}$ $U_{2,3} = \begin{pmatrix} \delta & \gamma & 0 \\ \gamma & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix}$ $U_{2,4} = \begin{pmatrix} \delta & -\gamma & 0 \\ -\gamma & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix}$
Case 3.	$U_{3,1} = \begin{pmatrix} \alpha & \beta & \gamma \\ \beta & \alpha & -\gamma \\ \gamma & -\gamma & \delta \end{pmatrix}$ $U_{3,2} = \begin{pmatrix} \alpha & -\beta & \gamma \\ -\beta & \alpha & \gamma \\ \gamma & \gamma & \delta \end{pmatrix}$ $U_{3,3} = \begin{pmatrix} \alpha & -\beta & -\gamma \\ -\beta & \alpha & -\gamma \\ -\gamma & -\gamma & \delta \end{pmatrix}$ $U_{3,4} = \begin{pmatrix} \alpha & \beta & -\gamma \\ \beta & \alpha & \gamma \\ -\gamma & \gamma & \delta \end{pmatrix}$
Case 4.	$U_{4,1} = \begin{pmatrix} \alpha & \beta & \gamma \\ \beta & \alpha & \gamma \\ \gamma & \gamma & \delta \end{pmatrix}$ $U_{4,2} = \begin{pmatrix} \alpha & -\beta & -\gamma \\ -\beta & \alpha & \gamma \\ -\gamma & \gamma & \delta \end{pmatrix}$ $U_{4,3} = \begin{pmatrix} \alpha & -\beta & \gamma \\ -\beta & \alpha & -\gamma \\ \gamma & -\gamma & \delta \end{pmatrix}$ $U_{4,4} = \begin{pmatrix} \alpha & \beta & -\gamma \\ \beta & \alpha & -\gamma \\ -\gamma & -\gamma & \delta \end{pmatrix}$

Table 3.2: The four sets of monoclinic variants corresponding to the four different Bain matrices.

replaces β by $-\beta$. Since this does not affect the existence of rank-one connections, we do not consider the third case any longer.

For a fixed $i = 1, 2$, or 4, the existence of rank-one connections between the wells $\mathrm{SO}(3)U_{i,1}$ and $\mathrm{SO}(3)U_{i,2}$ (respectively $\mathrm{SO}(3)U_{i,3}$, $\mathrm{SO}(3)U_{i,4}$) is determined by the value of the determinant of $U_{i,1} - U_{i,2}$, (respectively of $U_{i,1} - U_{i,3}$, $U_{i,1} - U_{i,4}$). A simple computation gives

$$\det(U_{i,1} - U_{i,2}) = \det(U_{i,1} - U_{i,3}) = \det(U_{i,1} - U_{i,4}) = 0, \ i = 1, 2, 4.$$

In other words, in all cases, all the wells are rank-one connected to each other. Moreover, since the determinants vanish identically, the existence of rank-one connections does not depend on the coefficients of the transformation matrix, and hence the twins are generic.

We now apply Theorem 3.14 to classify the twins and summarise our results in Table 3.3. Interestingly, it should be noticed that we come across the first of two examples of non-conventional, generic twins (variants $U_{2,1}$ and $U_{2,4}$). The other will pop up in our next example, the cubic-to-monoclinic transition. We use the language of Corollary 3.16. The

Variants involved	$(e_1+e_3)\in\mathscr{P}$	$(e_1-e_3)\in\mathscr{P}$	$\langle Ue_2,e_1\rangle=\varepsilon\langle Ue_2,e_3\rangle$	Twinning mode
Case 1.				
$U_{1,1}-U_{1,2}$	yes	yes	0	compound
$U_{1,1}-U_{1,3}$	no	yes	+	type I and II
$U_{1,1}-U_{1,4}$	no	yes	+	type I and II
Case 2.				
$U_{2,1}-U_{2,2}$	yes	yes	0	compound
$U_{2,1}-U_{2,3}$	yes	yes	0	compound
$U_{2,1}-U_{2,4}$	no	no	0	non-conventional
Case 3.				
$U_{4,1}-U_{4,2}$	no	yes	+	type I and II
$U_{4,1}-U_{4,3}$	no	yes	+	type I and II
$U_{4,1}-U_{4,4}$	no	yes	+	type I and II

Table 3.3: Twinning modes for tetragonal-to-monoclinic transitions.

abbreviation $(e_1\pm e_3)\in\mathscr{P}$ stands for the question 'is $1/\sqrt{2}(e_1\pm e_3)$ a direction of symmetry in $\mathscr{P}$?'. When we write $\langle Ue_2,e_1\rangle=\varepsilon\langle Ue_2,e_3\rangle$, the value of ε is either $+,-$ or 0, the three possible cases in Corollary 3.16.

Cubic-to-monoclinic transitions

There are many alloys that undergo a cubic-to-monoclinic phase transformation, *e.g.*, a nearly equiatomic Ti-Ni alloy, the most popular shape-memory alloy for applications and research.

According to Pitteri and Zanzotto [125], there are two possible cubic-to-monoclinic transitions. The first one leads to the *monoclinic 'cubic axes' variants* while in the second we get the *monoclinic 'face diagonals' variants* (this terminology is due to Pitteri and Zanzotto [125], to which we refer for a fuller treatment). In both cases there are twelve different monoclinic variants, *i.e.*, twelve different 3×3 symmetric positive definite matrices U_i. Let us denote

$$\mathscr{M}_c=\{\mathrm{SO}(3)U_i^c\}_{i=1}^{12}\,,\quad (\text{respectively }\ \mathscr{M}_f=\{\mathrm{SO}(3)U_i^f\}_{i=1}^{12}\,)\,,$$

the set consisting of the twelve monoclinic 'cubic axes' wells (respectively of the twelve monoclinic 'face diagonals' wells). We are interested in the existence of rank-one connections between two distinct wells, either both in $\mathscr{M}_c$ or both in $\mathscr{M}_f$. Let $\mathrm{SO}(3)U_i$ and $\mathrm{SO}(3)U_j$ be two such wells. In fact, it is easily seen that we can take $U_i=U_1$ without loss of generality. Corollary 3.8 implies that these two wells are rank-one connected if and only if $\det(U_1-U_j)=0$.

In [125], Pitteri and Zanzotto used Proposition 3.10 to classify the twins. We will rather use Corollary 3.8 and Theorem 3.14 to study the different twinning modes. First, using Corollary 3.8 we derive below Pitteri and Zanzotto's condition for the existence of twins. Then, using Proposition 3.10, we will show that for 'cubic axes' variants (respectively for 'face diagonals' variants), non-generic twins exist if and only if U_1^c (respectively if and only if U_1^f) has a double eigenvalue. After this first step, we then apply Theorem 3.14 to determine

the different twinning modes.

Monoclinic 'cubic axes' variants The monoclinic 'cubic axes' variants occur *e.g.*, in Cu-Al-Zn alloys (see [140], in which the authors study more specifically non-generic twins that can appear in these alloys), and are described by the following twelve symmetric positive definite matrices [125]:

$$
\begin{aligned}
U_1^c &= \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \gamma & \beta \\ 0 & \beta & \delta \end{pmatrix}, U_2^c = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \gamma & -\beta \\ 0 & -\beta & \delta \end{pmatrix}, U_3^c = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \delta & \beta \\ 0 & \beta & \gamma \end{pmatrix}, \\
U_4^c &= \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \delta & -\beta \\ 0 & -\beta & \gamma \end{pmatrix}, U_5^c = \begin{pmatrix} \delta & 0 & \beta \\ 0 & \alpha & 0 \\ \beta & 0 & \gamma \end{pmatrix}, U_6^c = \begin{pmatrix} \delta & 0 & -\beta \\ 0 & \alpha & 0 \\ -\beta & 0 & \gamma \end{pmatrix}, \\
U_7^c &= \begin{pmatrix} \gamma & 0 & \beta \\ 0 & \alpha & 0 \\ \beta & 0 & \delta \end{pmatrix}, U_8^c = \begin{pmatrix} \gamma & 0 & -\beta \\ 0 & \alpha & 0 \\ -\beta & 0 & \delta \end{pmatrix}, U_9^c = \begin{pmatrix} \gamma & \beta & 0 \\ \beta & \delta & 0 \\ 0 & 0 & \alpha \end{pmatrix}, \\
U_{10}^c &= \begin{pmatrix} \gamma & -\beta & 0 \\ -\beta & \delta & 0 \\ 0 & 0 & \alpha \end{pmatrix}, U_{11}^c = \begin{pmatrix} \delta & \beta & 0 \\ \beta & \gamma & 0 \\ 0 & 0 & \alpha \end{pmatrix}, U_{12}^c = \begin{pmatrix} \delta & -\beta & 0 \\ -\beta & \gamma & 0 \\ 0 & 0 & \alpha \end{pmatrix},
\end{aligned}
$$

where[24] $\alpha, \gamma, \delta > 0$, $\gamma\delta > \beta^2$, $\gamma \neq \delta$, $\beta \neq 0$ (if $\gamma = \delta$ or if $\beta = 0$, we have a cubic-to-orthorhombic transition instead of cubic-to-monoclinic, therefore these cases are excluded). Computing the determinant of all possible differences of the form $U_1^c - U_j^c$, we get

$$
\begin{aligned}
\det(U_1^c - U_2^c) &= \det(U_1^c - U_3^c) = \det(U_1^c - U_4^c) = \det(U_1^c - U_7^c) \\
&= \det(U_1^c - U_8^c) = \det(U_1^c - U_{11}^c) = \det(U_1^c - U_{12}^c) \\
&= 0\,, \\
\det(U_1^c - U_5^c) &= \det(U_1^c - U_6^c) = -\det(U_1^c - U_9^c) = -\det(U_1^c - U_{10}^c) \\
&= (\gamma - \delta)(\beta^2 - \alpha^2 + \alpha(\gamma + \delta) - \gamma\delta).
\end{aligned}
$$

Recall that $\gamma \neq \delta$. Thus, as in [125], we have two different situations: firstly, the wells $\mathrm{SO}(3)U_1^c$ and $\mathrm{SO}(3)U_j^c$ for $j = 2, 3, 4, 7, 8, 11$ or 12 are always rank-one connected. These rank-one connections do not depend on the coefficients of the matrix U_1^c and are therefore generic. Secondly, the wells $\mathrm{SO}(3)U_1^c$ and $\mathrm{SO}(3)U_j^c$ for $j = 5, 6, 9$ or 10 are rank-one connected if and only if the coefficients α, β, γ and δ of U_1^c satisfy

$$
\beta^2 - \alpha^2 + \alpha(\gamma + \delta) - \gamma\delta = 0\,. \tag{3.35}
$$

This is the condition established in [125]. These twins are of course non-generic. Interestingly, (3.35) is exactly the condition ensuring that U_1^c has a double eigenvalue. Indeed, the eigenvalues of U_1^c are given by

$$
\lambda_1 = \alpha\,,\ \lambda_\pm = \frac{(\gamma + \delta) \pm \sqrt{(\gamma - \delta)^2 + 4\beta^2}}{2}\,.
$$

[24] The coefficients α, β, γ and δ, as well as the coefficients α, β, γ and δ in the next sub-section, depend only on five experimentally measurable quantities, the *lattice parameters* of both the cubic and the monoclinic phases: the length of any edge of the cubic cell, the length of the three edges of the monoclinic cell and the monoclinic angle (see [83, 84]).

Now $\lambda_+ \neq \lambda_-$, because $\beta > 0$. Hence U_i^c has a double eigenvalue if and only if either $\lambda_+ = \alpha$ or $\lambda_- = \alpha$, which is easily seen to hold if and only if (3.35) holds. In other words,[25] *non-generic twins exist if and only if U_1^c has a double eigenvalue.*

We now apply Theorem 3.14 to classify the twins. First observe that a non-generic twin is non-conventional (since conventional twins are generic). Therefore, we need not apply the theorem in these cases. The computations involved in Theorem 3.14 are lengthy, but these can be more easily carried out using a symbolic computation software. We do not bother to give all the details, and we summarise our results in Table 3.4. We observe that some computations have already been carried out in the tetragonal-to-monoclinic case. We get the same results as those obtained by Pitteri and Zanzotto [125].

Variants involved	Genericity	$(e_1+e_3) \in \mathscr{P}$	$(e_1-e_3) \in \mathscr{P}$	$\langle Ue_2, e_1\rangle = \varepsilon\langle Ue_2, e_3\rangle$	Twinning mode
$U_1 - U_2$	yes	yes	yes	0	compound
$U_1 - U_3$	yes	yes	yes	0	compound
$U_1 - U_4$	yes	no	no	0	non-conventional
$U_1 - U_5$	no				non-conventional
$U_1 - U_6$	no				non-conventional
$U_1 - U_7$	yes	no	yes	+	type I and II
$U_1 - U_8$	yes	no	yes	+	type I and II
$U_1 - U_9$	no				non-conventional
$U_1 - U_{10}$	no				non-conventional
$U_1 - U_{11}$	yes	no	yes	+	type I and II
$U_1 - U_{12}$	yes	no	yes	+	type I and I

Table 3.4: Twinning modes for cubic-to-monoclinic transitions: 'cubic axes' variants.

Monoclinic 'face diagonals' variants The monoclinic 'face diagonals' variants are described by the following twelve symmetric positive definite matrices [125]:

$$U_1^f = \begin{pmatrix} \alpha & \beta & \gamma \\ \beta & \alpha & \gamma \\ \gamma & \gamma & \delta \end{pmatrix}, U_2^f = \begin{pmatrix} \alpha & \beta & -\gamma \\ \beta & \alpha & -\gamma \\ -\gamma & -\gamma & \delta \end{pmatrix}, U_3^f = \begin{pmatrix} \alpha & -\beta & -\gamma \\ -\beta & \alpha & \gamma \\ -\gamma & \gamma & \delta \end{pmatrix},$$
$$U_4^f = \begin{pmatrix} \alpha & -\beta & \gamma \\ -\beta & \alpha & -\gamma \\ \gamma & -\gamma & \delta \end{pmatrix}, U_5^f = \begin{pmatrix} \alpha & \gamma & \beta \\ \gamma & \delta & \gamma \\ \beta & \gamma & \alpha \end{pmatrix}, U_6^f = \begin{pmatrix} \alpha & -\gamma & \beta \\ -\gamma & \delta & -\gamma \\ \beta & -\gamma & \alpha \end{pmatrix},$$
$$U_7^f = \begin{pmatrix} \alpha & -\gamma & -\beta \\ -\gamma & \delta & \gamma \\ -\beta & \gamma & \alpha \end{pmatrix}, U_8^f = \begin{pmatrix} \alpha & \gamma & -\beta \\ \gamma & \delta & -\gamma \\ -\beta & -\gamma & \alpha \end{pmatrix}, U_9^f = \begin{pmatrix} \delta & \gamma & \gamma \\ \gamma & \alpha & \beta \\ \gamma & \beta & \alpha \end{pmatrix},$$
$$U_{10}^f = \begin{pmatrix} \delta & -\gamma & -\gamma \\ -\gamma & \alpha & \beta \\ -\gamma & \beta & \alpha \end{pmatrix}, U_{11}^f = \begin{pmatrix} \delta & -\gamma & \gamma \\ -\gamma & \alpha & -\beta \\ \gamma & -\beta & \alpha \end{pmatrix}, U_{12}^f = \begin{pmatrix} \delta & \gamma & -\gamma \\ \gamma & \alpha & -\beta \\ -\gamma & -\beta & \alpha \end{pmatrix},$$

where $\gamma > 0$ ($\gamma = 0$ corresponds to a cubic-to-orthorhombic transition, and is therefore excluded), and α, β, γ and δ are such that U_1^f is positive definite. Alloys that undergo this kind of cubic-to-monoclinic transitions include shape memory Ti-Ni, as thoroughly studied in [84].

[25] After this research was carried out, I learnt that this result was known to Kevin Hane (personal communication).

As above, we compute the determinant of all the possible differences $U_1^f - U_j^f$. After some elementary calculations, we find

$$\begin{aligned}\det(U_1^f - U_2^f) = \det(U_1^f - U_3^f) = \det(U_1^f - U_4^f) = \det(U_1^f - U_5^f)\\ = \det(U_1^f - U_7^f) = \det(U_1^f - U_9^f) = \det(U_1^f - U_{11}^f)\\ = 0\,,\end{aligned}$$

$$\begin{aligned}\det(U_1^f - U_6^f) = -\det(U_1^f - U_8^f) = \det(U_1^f - U_{10}^f) = -\det(U_1^f - U_{12}^f)\\ = -4\gamma(\beta^2 - \gamma^2 + \beta(\delta - \alpha)).\end{aligned}$$

Recall that $\gamma \neq 0$. Again, as in [125], we get two different situations: the wells $\mathrm{SO}(3)U_1^f$ and $\mathrm{SO}(3)U_j^f$, $j = 2, 3, 4, 5, 7, 9$ or 11 are always rank-one connected and therefore lead to generic twins, while the wells $\mathrm{SO}(3)U_1^f$ and $\mathrm{SO}(3)U_j^f$ for $j = 6, 8, 10$ or 12 are if and only if the coefficients α, β, γ and δ of U_1^f satisfy

$$\beta^2 - \gamma^2 + \beta(\delta - \alpha) = 0\,. \tag{3.36}$$

We recover the condition stated in [125], and again, (3.36) is equivalent to U_1^f having a double eigenvalue. Indeed, the eigenvalues of U_1^f are given by

$$\lambda_1 = (\alpha - \beta)\,,\ \lambda_\pm = \frac{(\alpha + \beta + \gamma) \pm \sqrt{(\alpha + \beta - \gamma)^2 + 8\gamma^2}}{2}\,.$$

Since $\lambda_+ \neq \lambda_-$ because $\gamma > 0$, U_1^f has a double eigenvalue if and only if either $\lambda_+ = \alpha - \beta$ or $\lambda_- = \alpha - \beta$, and this is easily seen to hold if and only if (3.36) holds. Therefore,[26] *non-generic twins exist if and only if U_1^f has a double eigenvalue.*

Variants involved	Genericity	$(e_1 + e_3) \in \mathscr{P}$	$(e_1 - e_3) \in \mathscr{P}$	$\langle Ue_2, e_1\rangle = \varepsilon\langle Ue_2, e_3\rangle$	Twinning mode
$U_1 - U_2$	yes	yes	yes	0	compound
$U_1 - U_3$	yes	no	yes	+	type I and II
$U_1 - U_4$	yes	no	yes	+	type I and II
$U_1 - U_5$	yes	no	yes	+	type I and II
$U_1 - U_6$	no				non-conventional
$U_1 - U_7$	yes	no	yes	+	type I and II
$U_1 - U_8$	no				non-conventional
$U_1 - U_9$	yes	no	yes	+	type I and II
$U_1 - U_{10}$	no				non-conventional
$U_1 - U_{11}$	yes	no	yes	+	type I and II
$U_1 - U_{12}$	no				non-conventional

Table 3.5: Twinning modes for cubic-to-monoclinic transitions: 'face diagonals' variants.

As above we apply Theorem 3.14 to classify the twins. Again the algebra involved is omitted and we notice that some calculations have already been done in the tetragonal-to-monoclinic case. Our results are summarised in Table 3.5. In this case too, we get the same results as those obtained by Pitteri and Zanzotto [125].

[26] In fact, in [84] the authors obtain the same result in the case where U_1^f is the Bain strain corresponding to the alloy Ti-49.75 at.% Ni.

4 Metastability in martensite

4.1 Introduction and experimental background

This chapter is devoted to the modelling and analysis of biaxial dead load experiments in shape memory alloys. It follows up the work of Chu and James [50] who designed the loading machine and realised the experiments, and that of Ball and James [21, 22, 25, 26] who modelled and analysed these from a mathematical standpoint. The key point under investigation here is the origin of hysteresis during variant rearrangement observed in those experiments. We start by describing, in rather simple terms, the experimental background to this study. We refer to [21, 22, 50] for more details.

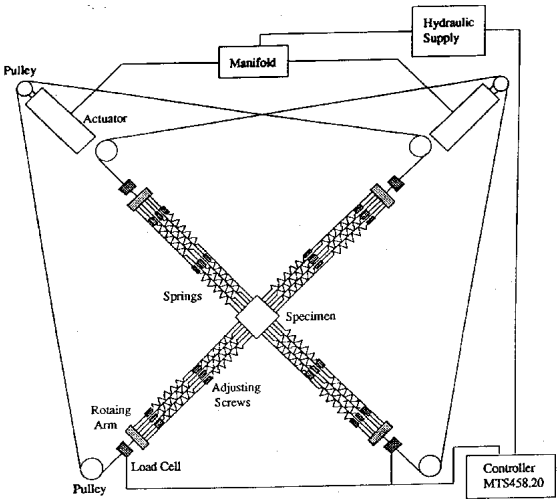


Figure 4.1: Biaxial machine layout.

Consider a single crystal of Cu-Al-Ni shape memory alloy.[27] Once heated so that it is in the austenitic cubic phase, the specimen (a thin square plate 2.54 cm $\times$ 2.54 cm) is placed in the biaxial machine (see Figure 4.1) and grips are attached (see Figure 4.2). Then, the sample is cooled to induce the martensitic transformation. The specimen is cooled enough so as to be in the fully transformed orthorhombic martensitic phase.[28] Applying then[29] various biaxial dead loads, it is observed that for a certain range of loads, one homogeneously deformed

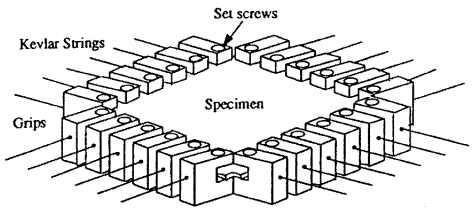


Figure 4.2: Specimen grip configuration.

[27] The exact composition of the alloy used in the experiments is Cu-14.0wt. %Al-3.9wt. %Ni.

[28] Thus, in the notation of Section 2.3 in Chapter 2 we work at a temperature θ below the critical temperature θ_c and drop θ from the notation.

[29] More accurately, before beginning the tests, the sample is first detwinned, *i.e.*, the microstructure appeared during the cooling is removed. In this fashion, before applying the loads, the sample is in an almost homogeneous state.

variant of martensite is stable, while another variant is stable for another range of loads. Let us label these two variants 1 and 2 respectively, and denote by λ the volume fraction of variant 2. When we plot λ versus some measure of the load, the experimental result we take as the foundation block of our study is given in Figure 4.3 (the significance of σ_1 and σ_2 will be explained below). For small loads (those around -4MPa on the plot), variant

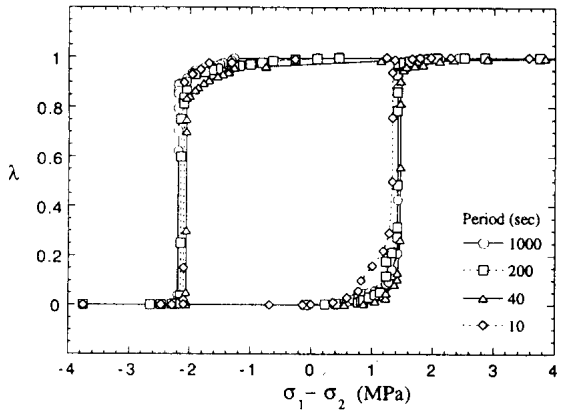


Figure 4.3: Hysteresis loop in biaxial loading experiments.

1 is stable, and $\lambda = 0$. Increasing the load does not at first appear to change anything, λ remaining negligible and variant 1 staying stable. However, as we reach a certain critical load (here around 1.5MPa on the horizontal axis) there is an exchange of stability and there occurs a rapid avalanche of variant rearrangement: variant 2 becomes stable, and λ rapidly reaches the maximum value 1. As we increase the load further, variant 2 remains stable as the value $\lambda = 1$ for these loads indicates. If we now decrease the load, we observe a similar outcome, except that the transition occurs at a different critical load, on the plot at around -2.2MPa. At the end, variant 1 is stable, and we are back where we started. Figures 4.4 and 4.5 show typical microstructures observed during the variant rearrangement at the critical loads. Looking at Figure 4.3, two questions spring to mind:

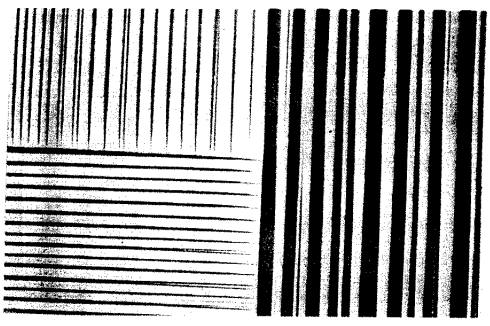


Figure 4.4: Typical microstructures observed during variant rearrangement.

I. What is the reason for hysteresis?

II. Can we predict the size of the hysteresis loop observed?

In this chapter, we answer the first question and give some estimates for the second. We

stress that this is already done in the work of Ball, Chu and James [21, 22]. Our contribution will be explained later.



Figure 4.5: Typical microstructures observed during variant rearrangement.

Let us describe in mathematical terms the essentials of the model we are studying. The loading device in these experiments was specifically designed to be governed by the energy

$$-\int_\Omega \langle T, Dy(x)\rangle \, dx$$

where $y(x)$ is the deformation defined on the reference configuration Ω and T is a constant 3×3 matrix of the form

$$T = \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

in a certain fixed basis e_1, e_2, e_3, the 'machine basis'. The two positive constants σ_1 and σ_2 are the stresses applied to the edges of the specimen. In order to explain the form of the energy above, let us use the Divergence Theorem and the fact that T is constant, to write the energy in the form

$$-\int_{\partial\Omega} \langle Tn(x), y(x)\rangle ds \, .$$

Thus, since the force $f(x) = Tn(x)$ is independent of the deformation y, we conclude that the force remains fixed regardless of the deformation of the sample. This is exactly the definition of a *dead load*.[30] As mentioned earlier, before loading takes place, the specimen undergoes a cubic-to-orthorhombic phase transformation. In order to account for this, a term is added to the energy, so that the total free energy we consider is of the form

$$\int_\Omega \varphi(Dy(x)) - \langle T, Dy(x)\rangle \, dx \, .$$

We take the reference configuration Ω to be the undistorted austenite, and φ is the Ball-James energy density [28] accounting for the phase transition that we described in Chapter 2.[31] In short, we assume that $\varphi \geq 0$ and

$$\varphi(\xi) = 0 \text{ if and only if } \xi \in K.$$

[30] It should be pointed out that ensuring that the forces remain constant as the sample deforms required some clever engineering thinking. The presence of grips and strings in Figures 4.1 and 4.2 originates there. See [21, 50] for more on the experimental setting.

[31] Contrary to the setting described in Chapter 2 we do not impose Dirichlet boundary conditions (since $\langle T, \cdot\rangle$ is a null Lagrangian) but only *natural boundary conditions*, $(D\varphi(Dy) - T)n = 0$ on $\partial\Omega$.

Here

$$K = \mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2 \cup \ldots \cup \mathrm{SO}(3)U_6\,,$$

where the six matrices U_i describe the linear deformations that map a cube into an orthorhombic cell. They are given by[32]

$$U_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, U_2 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\ \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, U_3 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix},$$
$$U_4 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\gamma-\alpha}{2} \\ 0 & \beta & 0 \\ \frac{\gamma-\alpha}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix}, U_5 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}, U_6 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} \\ 0 & \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}.$$

The set K does not contain the austenite well $\mathrm{SO}(3)$ because we are working at a fixed temperature (hence absent from the notation) *below* the transformation temperature and therefore, the sample is entirely in the martensitic phase. Worth pointing out is that φ satisfies some standard symmetry requirements of continuum mechanics – frame-indifference, material symmetry – which are recalled at the beginning of Section 4.2 below.

Let us now explain in rather crude terms the essence of our analysis. Let T depend on a parameter $0 \leq \sigma \leq 1$ to account for the fact that the load changes during the experiment. At a fixed load, in order to minimise the energy, let us 'minimise' the integrand pointwise by minimising φ first and then $-\langle T(\sigma), \cdot \rangle$, *i.e.*, for every fixed σ, let us consider the problem

$$\min I_\sigma(y) = -\int_\Omega \langle T(\sigma), Dy(x) \rangle \, dx\,, \quad Dy(x) \in K \ \text{ a.e.} \tag{4.1}$$

(We explain below why this is not the correct thing to do, see point (a) on page 65, but for our present purposes, this suffices.) To minimise this, we simply minimise $-\langle T(\sigma), \cdot \rangle$ on each well (this is minimised at exactly one point, see Lemma 4.5 below). This gives us six values, and then we take the minimum value of these. If the orientation of the sample (*i.e.*, that of the underlying lattice) is accurately chosen with respect to the machine basis (the axes along which the specimen is stretched), the experiments show that two variants have consistently lower energy than the four others. More precisely, denoting

$$E_i(\sigma) = \min_{R \in \mathrm{SO}(3)} -\langle T(\sigma), RU_i \rangle\,, \quad i = 1, \ldots, 6,$$

we assume, according to these experiments, that a plot E_i vs. σ looks like that pictured in Figure 4.6. This plot explains why these experiments are well-tailored to study hysteresis (and metastability) in martensite, since only two variants play a rôle at any one time. We can also see on this plot the equal energy load, σ_0 below which variant 1 is stable and above which variant 2 is stable. However, this plot and the energy calculation that underlies it, do not explain the hysteresis loop observed experimentally.

Ball, Chu and James [21] introduced a model, the *constrained model*, generalising (4.1) and showed that although variant 1 is not the absolute minimiser above σ_0, *it remains metastable* for a little while.[33] More precisely, variant 1 is a local minimiser of the energy for loads that are bigger than, but close to, σ_0. Conversely, variant 2 is metastable below σ_0. Hence, if we increase the load and then decrease it, we fall into these regions of metastability, and

[32] For the alloy used in those experiments, $\alpha = 1.0619$, $\beta = 0.9178$ and $\gamma = 1.0230$.

[33] In Section 4.2 below we state (an equivalent form of) the constrained model, justify it rigorously, and in Section 4.3 we prove this metastability result.

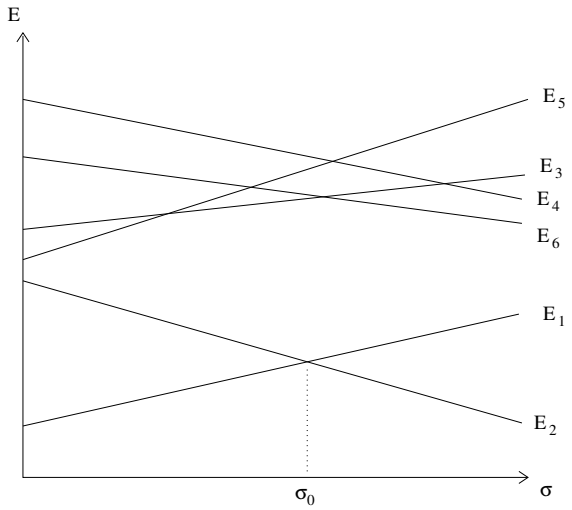


Figure 4.6: Energy of the six martensitic variants. The first and second ones have lower energy than all the others throughout the experiment. At $\sigma = \sigma_0$, both variants have the same energy.

the transition occurs at a different load on the way up and on the way down, explaining the hysteresis loop observed in Figure 4.3. An intuitive explanation of this phenomenon is the following. At σ_0 there are two minimisers of the energy. However, they are not kinematically compatible (*i.e.*, their difference is not of rank one), and thus, at a load σ close to σ_0, there is a patch $\mathcal{P}$ of matrices on the second variant $\mathrm{SO}(3)U_2$ that have lower energy than the minimiser $R(\sigma)U_1$ on variant 1, but such that no matrix in $\mathcal{P}$ is rank-one connected to $R(\sigma)U_1$. Hence, any small region with deformation gradient $Dy \in \mathcal{P}$ must necessarily be surrounded by a transition layer on which Dy is far from both wells, due to the lack of rank-one connections, and one pays more in energy for the transition layer than one gains by having $Dy \in \mathcal{P}$. This argument is tricky because the lack of rank-one connections in a set of gradients does not in itself prevent microstructures being constructed from them, as pointed out in Chapter 2 (see also [39, 88]), but in this case, because most of the deformation gradients lie near two matrices that are not rank-one connected, such microstructures are ruled out, see Lemma 4.15 and Theorem 4.14.

If this result satisfactorily explains hysteresis, it does not predict when metastability is lost. However, there is a simple upper bound. Remember that $R(\sigma)U_1$ possesses two twins (*i.e.*, two matrices that are rank-one connected to it) on $\mathrm{SO}(3)U_2$. As we increase the load, the patch $\mathcal{P}$ of 'good matrices' increases, too. At some stress $\sigma_{Sch} > \sigma_0$, this patch will contain at least one of the twins of $R(\sigma_{Sch})U_1$. Then, a simple construction, explained below (see Figure 4.9), shows that metastability stops at that point. This upper bound has been called the Schmid Law for reasons that we explain in Section 4.3 below.

Having an upper bound at our disposal, we may at once ask whether it is sharp. Ball, Chu and James [21, 22] discovered this was not the case, provided the specimen had an appropriate sharp corner. The idea behind the counter-example is this. Remember that for loads $\sigma > \sigma_0$, there is a patch $\mathcal{P} \subset \mathrm{SO}(3)U_2$ of matrices that have lower energy than $R(\sigma)U_1$. Imagine that at some $\sigma_0 < \sigma < \sigma_{Sch}$ none of the matrices in $\mathcal{P}$ is rank-one connected to $R(\sigma)U_1$, but that one, C say, is rank-one connected to a convex combination of $R(\sigma)U_1$ and one of its twins, B say. See Figure 4.7 where straight lines represent rank-one connections.

Then a fairly simple construction, pictured in Figure 4.10 below, shows that metastability is

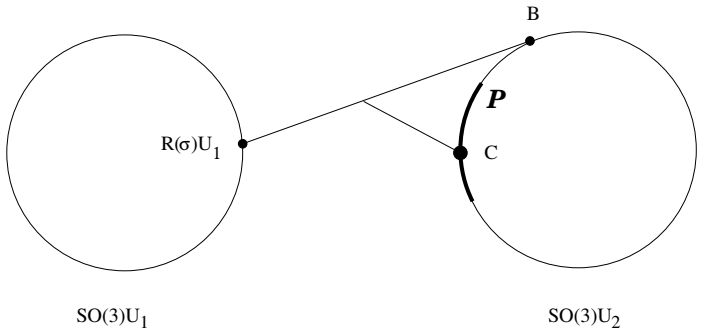


Figure 4.7: A counter-example to the Schmid Law.

lost at this load, even though the twins of $R(\sigma)U_1$ have not yet lower energy (see the end of Section 4.3 for more details). Hence the Schmid Law is violated. An important part of this chapter is devoted to answering a natural question that one might ask in the light of this counter-example. Does this construction require the existence of a corner? Could we do it on smooth domains?

In Section 4.4 we show that three-gradient constructions do indeed require that the domain have a corner. Explicit bounds on the angles of that corner are obtained, see Theorem 4.19 below. However, we should point out that our results appear to be exceedingly sensitive to changes in the geometry of the sample. This seems to hinder the application of our results to experimental tests. See Remark (b) on page 104.

The structure of this chapter is as follows. In Section 4.2 we rigorously justify the Ball-Chu-James model (or rather, an equivalent form thereof) and state some general properties of global and some local minimisers, those of interest to us. In Section 4.3, we prove a version of the Metastability Theorem of [21] adapted to our setting, while three-gradient constructions in relation to the counter-example of Ball, Chu and James [21, 22] are investigated in Section 4.4.

4.2 A constrained model and general properties

We start by describing the general framework of our analysis. Let $\varphi : \mathbb{R}^{3\times 3} \to \mathbb{R}$ be continuous and such that $\varphi(\xi) \geq 0$ for every $\xi \in \mathbb{R}^{3\times 3}$ and $\varphi(\xi) = 0$ if and only if $\xi \in K$ for some compact set $K \subset \mathbb{R}^{3\times 3}$. Let also $\Omega \subset \mathbb{R}^3$ be a bounded convex open set. Let finally $\sigma \mapsto T(\sigma) \in \mathbb{R}^{3\times 3}$, $0 \leq \sigma \leq 1$, be continuous, symmetric positive semidefinite and such that $\operatorname{rank} T(\sigma) = 2$ for every σ. Following James [89], consider the energy

$$I_\sigma(y) = \int_\Omega \varphi(Dy(x)) - \langle T(\sigma), Dy(x)\rangle \, dx.$$

In the physical situation that underlies our study φ is the *stored-energy density* accounting for the phase transition undergone by a material occupying the region Ω in the reference configuration taken to be the undistorted austenite. The tensor $T(\sigma)$ describes a biaxial dead load applied to the sample. Finally, $y : \Omega \to \mathbb{R}^3$ is the deformation and $Dy(x)$ the deformation gradient at x. In this case, further symmetry requirements are satisfied by φ. (We stress, however, than the results we state in this section do not require these hypotheses.) Firstly, φ is supposed to be *frame-indifferent*, *i.e.*,

$$\varphi(R\,\xi) = \varphi(\xi)\,,$$

for every rotation $R \in \mathrm{SO}(3)$ and every $\xi \in \mathbb{R}^{3\times 3}$. Secondly, φ satisfies the *axiom of material symmetry*, which states that

$$\varphi(\xi Q) = \varphi(\xi)\,,$$

for every $\xi \in \mathbb{R}^{3\times 3}$ and every rotation $Q \in \mathscr{P}$, where $\mathscr{P}$ is the symmetry group of the austenite, assumed to be a finite subgroup of SO(3). In the case of Cu-Al-Ni alloys, which we are concerned with, this is the cubic (Laue) point group, consisting of all those rotations mapping the unit cube into itself. Furthermore, because these alloys have orthorhombic symmetry in the martensitic phase, the set $K = \varphi^{-1}(0)$ consists of six connected components,

$$K = \bigcup_{i=1}^{6} \mathrm{SO}(3)U_i\,, \tag{4.2}$$

where the symmetric positive definite U_i are the linear transformations that map a cube into an orthorhombic unit cell, and which were given in the introduction, page 61.

In the remaining of this section, we are not concerned with the fact that T depends on the parameter σ so we fix σ and drop it from the notation.

Loosely speaking we are interested in (local and global) minimisers of I. In that respect, two problems immediately surface.

(i) In general, φ is not quasiconvex. Actually, if φ has a zero set of the form (4.2) that contains pairs of rank-one connected matrices, then it cannot be rank-one convex and thus *a fortiori* quasiconvex. So I is not weakly lower semicontinuous with respect to the weak topologies in Sobolev spaces, in general, and the direct methods of the calculus of variations do not apply.

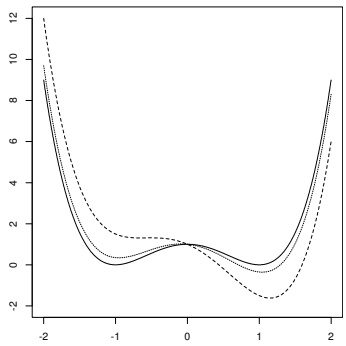


Figure 4.8: Two linear perturbations of the double-well potential $(x^2-1)^2$.

(ii) The only information we have on φ is its zero set. As a one-dimensional cartoon hints, see Figure 4.8, if we add a linear perturbation to φ, the minimum of the perturbed function may, but equally may not, be close to the minima of φ. This clearly depends on how fast φ grows off its zero set and on the slope of the perturbation. In our problem, the former is not known. However, experiments hint that the growth of φ is quite rapid.[34]

[34] According to Ball, Chu and James [21], *'for typical values of loads in our tests and a typical twinned laminate, the deviation of the observed gradient from K is less than 1/100 of the distance between the two wells according to these experiments.'*

In order to resolve these problems, we aim to derive a simplified model which should clearly possess the following properties.

(a) It should allow for microstructures observed by Chu and James [50], *e.g.*, L-shaped microstructures with 'most' gradients lying in K but some, those in transition layers, lying outside it. This would be precluded by minimising pointwise φ first, and then the loading energy, *i.e.*, minimising

$$-\int_\Omega \langle T, Dy\rangle \, dx$$

subject to the constraint $Dy(x) \in K$ a.e. This is too coarse a model, because no hysteresis is possible in this setting.

(b) It should only assume knowledge of the set $K = \varphi^{-1}(0)$, but not that of the growth of φ off it, except that it is fast.

The goal of this section is to derive rigorously a model which overcomes problems (i) and (ii), whilst fulfilling properties (a) and (b). We point out that the model obtained (or, rather, an equivalent form thereof, see the remarks after Theorem 4.2), which is called the *constrained model*, had first been introduced by Ball, Chu and James [21, 22]. As mentioned in the introduction, our work is deeply influenced by theirs. Our contribution here is that our approach rigorously justifies the constrained model. To achieve this, there is a price to pay, however, in the form of the following hypothesis on the behaviour of φ at infinity. We assume that there exist constants $\alpha_1 > 0$, $\alpha_2 > 0$ and $p > 1$ such that, for all $\xi \in \mathbb{R}^{3\times 3}$,

$$-\alpha_1 + \alpha_2|\xi|^p \le \varphi(\xi) \le \alpha_1(1 + |\xi|^p)\,. \tag{4.3}$$

As was done in Chapter 2, we use the following terminology throughout this chapter. We refer to the lower bound in (4.3) as the *coercivity* condition and to the upper bound in (4.3) as the *growth* condition.

While the coercivity condition is harmless, the growth hypothesis is incompatible with the physical requirement that $\varphi(\xi) \to +\infty$ as $\det \xi \to 0^+$ preventing the interpenetration of matter, but this is unavoidable. Roughly speaking, our approach consists in finding the correct limiting variational problem as the growth of φ off its zero set gets faster and faster. In order to achieve this, we let for an integer k

$$I^k(y) = \int_\Omega k\varphi(Dy(x)) - \langle T, Dy(x)\rangle \, dx,$$

where $y \in \mathrm{W}^{1,p}(\Omega, \mathbb{R}^3)$ and p is given by (4.3). Intuitively, one feels that passing to the limit, in some sense, as $k \to \infty$ will have the desired effect. The topology we will invoke is that of Γ-convergence, the definition of which we now recall.

(4.1) Definition. *Let (X, d) be a metric space. We say that a sequence $I^k : X \to \bar{\mathbb{R}} = \mathbb{R} \cup \{-\infty, +\infty\}$ $\Gamma(d)$ converges to $I : X \to \bar{\mathbb{R}}$ if for all $y \in X$ we have:*

(i) (liminf inequality) for every sequence y^k converging to y,

$$I(y) \le \liminf_{k\to\infty} I^k(y^k)\,; \tag{4.4}$$

(ii) (existence of a recovery sequence) there exists a sequence y^k converging to y such that

$$I(y) \geq \limsup_{k\to\infty} I^k(y^k)\,, \tag{4.5}$$

or, equivalently, by (4.4),

$$I(y) = \lim_{k\to\infty} I^k(y^k)\,.$$

The functional I is called the $\Gamma(d)$-limit of I^k and we write $I = \Gamma(d) - \lim_{k\to\infty} I^k$.

Remarks. The notion of Γ-convergence is due to De Giorgi [61, 62]. Since we use it in a fairly simple case, we do not review it here but refer instead to the monographs by Braides and Defranceschi [41] and Dal Maso [59]. We mention only one basic property that we use below, to the effect that if I^k is an increasing sequence, then its Γ-limit exists and is given by the pointwise supremum of the lower semicontinuous envelopes of I^k in the topology under consideration. See [59] for a proof.

We are now in a position to derive the constrained model by computing the Γ-limit of our sequence I^k. As is customary, we first extend I^k to the whole of $L^p(\Omega,\mathbb{R}^3)$ by setting $I^k(y) = +\infty$ if $y \in L^p \setminus W^{1,p}$. The advantage of considering the functionals as defined over L^p is that, under the coercivity assumption (4.3), the strong topology of L^p coincides with the weak topology of $W^{1,p}$, as is shown in the proof.

(4.2) Theorem. *Let $\varphi : \mathbb{R}^{3\times 3} \to \mathbb{R}$ be continuous and satisfy:*

(i) $\varphi(\xi) \geq 0$ for every $\xi \in \mathbb{R}^{3\times 3}$ and $\varphi(\xi) = 0$ if and only if $\xi \in K$ for some compact set $K \subset \mathbb{R}^{3\times 3}$,

(ii) there exist constants $\alpha_1 > 0$, $\alpha_2 > 0$ and $p > 1$ such that

$$-\alpha_1 + \alpha_2|\xi|^p \leq \varphi(\xi) \leq \alpha_1(1 + |\xi|^p)\,. \tag{4.6}$$

Let also $\Omega \subset \mathbb{R}^3$ be a bounded open set. Let finally $T \in \mathbb{R}^{3\times 3}$ and consider for an integer k

$$I^k(y) = \int_\Omega k\varphi(Dy(x)) - \langle T, Dy(x)\rangle\, dx, \;\; y \in W^{1,p}(\Omega,\mathbb{R}^3)\,,$$

and set $I^k(y) = +\infty$ if $y \in L^p \setminus W^{1,p}$. Then, the sequence I^k $\Gamma(L^p)$-converges to

$$I(y) = \begin{cases} -\int_\Omega \langle T, Dy(x)\rangle\, dx & \text{if } Dy(x) \in K^{qc} \text{ a.e.} \\ +\infty & \text{otherwise} \end{cases},$$

where K^{qc} denotes the quasiconvex hull of K.

Remarks. Obviously, one should not overlook the fact that given a compact set K, computing its quasiconvex hull K^{qc} can prove extremely difficult. As a matter of fact, for many sets K relevant to mathematics and applications, their quasiconvex hulls remain unknown.

In [21, 22], Ball et al. introduced the constrained model

$$\min I_{BCJ}(\nu_x) = \int_\Omega \int_K -\langle T, \xi\rangle\, d\nu_x(\xi)\, dx\,, \tag{4.7}$$

over all ($W^{1,\infty}$) gradient Young measures ν_x supported on K. Since the integrand is linear, our model is equivalent to theirs. Indeed, if ν_x is a gradient Young measure supported on K, then its centre of mass lies in K^{qc} a.e. Thus, $\min I_{BCJ} \geq \min I$. To show the reverse inequality, we proceed as follows. Let $y \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ satisfy $Dy(x) \in K^{qc}$ a.e. Then, since $I = \Gamma - \lim_{k\to\infty} I^k$, there exists a sequence $y^k \in W^{1,p}(\Omega, \mathbb{R}^3)$ such that

$$I(y) = \lim_{k\to\infty} I^k(y^k)\,, \quad \text{and} \quad y^k \to y \ \text{ in } L^p.$$

Since $I(y) < \infty$ and by coercivity Dy^k is uniformly bounded in L^p, we may assume that $Dy^k \rightharpoonup Dy$ in L^p. Also, for the same reasons, (up to a subsequence, not relabelled) Dy^k generates a gradient Young measure ν_x. Obviously, $\bar{\nu}_x = Dy(x)$ a.e. and so,

$$I(y) = -\int_\Omega \langle T, Dy(x)\rangle\, dx = -\int_\Omega \langle T, \bar{\nu}_x\rangle\, dx = I_{BCJ}(\nu_x)\,,$$

provided we show that $\operatorname{supp}\nu_x \subset K$. This follows from (i) and

$$\lim_{k\to\infty} \int_\Omega k\varphi(Dy^k)\, dx = 0\,.$$

To prove the latter, notice that

$$0 = \lim_{k\to\infty} [I(y) - I^k(y^k)] = \lim_{k\to\infty} \int_\Omega \langle T, Dy - Dy^k\rangle - k\varphi(Dy^k)\, dx = -\lim_{k\to\infty} \int_\Omega k\varphi(Dy^k)\, dx\,,$$

since $Dy^k \rightharpoonup Dy$. Finally, thanks to Zhang's Lemma [159], we may assume without loss of generality that ν_x is generated by a sequence of gradients bounded in L^∞.

In [25], Ball and James give the following justification for their model. Assume that φ satisfies the coercivity condition (4.6) (but without assuming the growth condition) and that there exists at least one sequence z^k such that $\sup_k I^k(z^k) < \infty$. Consider a low energy deformation y^k in the sense that

$$I^k(y^k) \leq \inf_{W^{1,p}} I^k + \frac{1}{k}\,.$$

Then, up to a subsequence, Dy^k generates a gradient Young measure ν_x which solves (4.7). We refer to [25] for a proof of this fact and further details.

Proof of Theorem 4.2. Since I^k is an increasing sequence (because $\varphi \geq 0$) the Γ-limit exists and is given by $I = \sup_k \bar{I}^k$, where $\bar{I}^k$ is the lower semicontinuous envelope of I^k in the strong L^p topology. We divide the rest of the proof into three steps.

First step. Observe that by Young's inequality

$$ab \leq \frac{\varepsilon^p}{p} a^p + \frac{1}{p'\varepsilon^{p'}} b^{p'}\,, \quad \text{for every } a, b, \varepsilon > 0, \quad \text{where } \frac{1}{p} + \frac{1}{p'} = 1\,,$$

if φ satisfies the coercivity condition (4.6), then so does $k\varphi - \langle T, \cdot\rangle$ for a fixed k. Indeed, since α_1, α_2 and k are fixed, we choose $\varepsilon^p < kp\alpha_2/|T|$ and get

$$\begin{aligned} k\varphi(\xi) - \langle T, \xi\rangle &\geq k\varphi(\xi) - |T||\xi| \\ &\geq -k\alpha_1 + k\alpha_2|\xi|^p - \frac{|T|\varepsilon^p}{p}|\xi|^p - \frac{|T|}{p'\varepsilon^{p'}} \\ &= -(k\alpha_1 + \frac{|T|}{p'\varepsilon^{p'}}) + (k\alpha_2 - \frac{|T|\varepsilon^p}{p})|\xi|^p \\ &= -\tilde{\alpha}_1 + \tilde{\alpha}_2|\xi|^p\,, \end{aligned}$$

for some $\tilde{\alpha}_1, \tilde{\alpha}_2 > 0$.

Second step. We now show that for every k, $\bar{I}^k = \tilde{I}^k$ where $\tilde{I}^k$ denotes the lower semicontinuous envelope of I in the weak $W^{1,p}$ topology. This is independent of k, so we drop it from the notation. By definition,

$$\bar{I}(y) = \inf_{y^k} \liminf_{y^k \to y \ L^p} I(y^k)\,,$$
$$\tilde{I}(y) = \inf_{y^k} \liminf_{y^k \to y \ W^{1,p}} I(y^k)\,.$$

First recall that by Rellich's Theorem, if $y^k \rightharpoonup y$ in $W^{1,p}$ then $y^k \to y$ in L^p. Hence $\bar{I} \leq \tilde{I}$. To show the reverse inequality, it suffices to prove that if $y^k \to y$ in L^p and if $I(y^k) < +\infty$ uniformly in k, then $y^k \rightharpoonup y$ in $W^{1,p}$ (up to a subsequence). But this follows easily from the coercivity condition obtained in the first step.

Third step. Given the first two steps, the growth and coercivity conditions (4.6) and the fact that $\langle T, \cdot \rangle$ is a null Lagrangian, classical relaxation results (see Dacorogna [54] or Braides and Defranceschi [41]) assert that, for every k

$$\tilde{I}^k(y) = \int_\Omega k\varphi^{qc}(Dy(x)) - \langle T, Dy(x)\rangle \, dx, \tag{4.8}$$

where φ^{qc} denotes the quasiconvex hull of φ. In particular, $(\varphi^{qc})^{-1}(0) = K^{qc}$. To see this, notice that $K^{qc} \subset (\varphi^{qc})^{-1}(0)$. To show the reverse inclusion, let $A \in (\varphi^{qc})^{-1}(0)$. Then, by Dacorogna's representation formula for φ^{qc} [54], there exists a sequence $u^k \in W_0^{1,\infty}(\Omega, \mathbb{R}^n)$ such that

$$\lim_{k\to\infty} \int_\Omega \varphi(A + Du^k(x))\, dx \to 0\,.$$

Since $\varphi \geq 0$, this implies that $y^k(x) = Ax + u^k(x)$ satisfy

$$Dy^k \to K \ \text{ in measure},$$
$$y^k = Ax \ \text{ on } \partial\Omega.$$

But this implies that $A \in K^{qc}$, see Müller [116]. Now the result follows since $\bar{I}^k(y)$ is of order k if $Dy(x) \notin K^{qc}$ on a set of positive measure, while $\bar{I}^k(y) = -\int_\Omega \langle T, Dy(x)\rangle \, dx$ if $Dy(x) \in K^{qc}$ a.e. □

Under a mild coercivity assumption,[35] weaker than (4.3), it is well known that the Γ-limit I attains its minimum, and that its minimum is the limit of the infima of I^k. (This is actually the defining property of Γ-convergence.) Thus, as far as global minimisers are concerned, I does give valuable information on I^k as we wanted it to. As regards local minimisers, the answer is positive, too. This is less trivial and ensured by the following theorem, which we quote from Kohn and Sternberg [99], who attribute it to De Giorgi. However, we have failed to find a proof in the literature, so we provide one, due to Ball [7], for the convenience of the reader.

[35] To be precise, the assumption is that I^k be *equi-mildly coercive*, *i.e.*, that there exist a compact set $L \subset X$ such that

$$\inf_X I^k = \inf_L I^k\,, \ \text{ for all } k.$$

(4.3) Theorem. *Let (X, d) be a complete metric space and consider a sequence of functionals $I^k : X \to \mathbb{R} \cup \{+\infty\}$. Suppose that they are equicoercive in the sense that*

$$\text{any sequence } y^k \text{ in } X \text{ with } \sup_k I^k(y^k) < +\infty \text{ has a } d\text{-convergent subsequence.}$$

Assume in addition the following hypothesis of lower semicontinuity:

$$\begin{gathered}\text{for any } y \in X \text{ and any } \delta > 0, \text{ the minimum of } I^k \text{ on the ball} \\ B(y,\delta) = \{z \in X \,:\, d(z,y) \le \delta\} \text{ is achieved for each } k.\end{gathered} \tag{4.9}$$

Suppose finally that the sequence I^k $\Gamma(d)$-converges to I. If y is a strict local minimiser of I, i.e.*, if $I(z) > I(y)$ whenever $0 < d(y,z) \le \delta$ for some $\delta > 0$, then there is a sequence y^k of local minimisers of I^k, defined for all sufficiently large k, such that $d(y^k, y) \to 0$ as $k \to \infty$.*

Proof of Theorem 4.3. Let y be a strict local minimiser of I. In particular, $I(y) < +\infty$, and there exists $\delta > 0$ such that $I(y) < I(z)$ for every $0 < d(y,z) \le \delta$. Now define y^k by

$$I^k(y^k) = \min_{B(y,\delta/2)} I^k \,.$$

By (4.9), y^k exists and is well defined. By definition of y^k, we have that for k sufficiently large

$$I^k(y^k) \le I^k(\tilde{y}^k) \le I(y) + \varepsilon < \infty \,,$$

for some $\varepsilon > 0$, where $\tilde{y}^k$ is the recovery sequence associated to y and provided by the definition of Γ-convergence. (Notice that $\tilde{y}^k \in B(y, \delta/2)$ if k is sufficiently large.) Hence, by equicoercivity, there exists a subsequence, not relabelled, and a $\bar{y} \in X$ such that $d(y^k, \bar{y}) \to 0$. To conclude the proof, we only have to show that $\bar{y} = y$; indeed, if so, and for sufficiently large k, y_k is a local minimiser of I^k, as desired. Assume therefore that $\bar{y} \neq y$, otherwise the theorem is proved. We have

$$d(y, \bar{y}) \le d(y, y^k) + d(y^k, \bar{y}) \le \delta/2 + \delta/2 = \delta \,,$$

if k is sufficiently large. Hence, since y is a strict local minimiser,

$$I(y) < I(\bar{y}) \,. \tag{4.10}$$

On the other hand, since y^k is a minimiser of I^k in $B(y, \delta/2)$ and by definition of Γ-convergence,

$$I(\bar{y}) \le \liminf_{k\to\infty} I^k(y^k) \le \liminf_{k\to\infty} I^k(\tilde{y}^k) = I(y) \,, \tag{4.11}$$

where, again, $\tilde{y}^k$ is the recovery sequence associated to y. But then, (4.10) and (4.11) provide the desired contradiction, and the theorem follows. □

Remark. We observe that Theorem 4.3 indeed applies in our case, with $X = L^p$ endowed with its strong topology, provided we replace I^k (extended as before from $W^{1,p}$ to the whole of L^p) by its relaxation $\tilde{I}^k$, see (4.8) – otherwise, the lower semicontinuity hypothesis (4.9) will not be satisfied. Let us check that this sequence is equicoercive. Since φ obeys the coercivity condition (4.3), so does φ^{qc}, because $|\cdot|^p$ is convex. Hence, if y^k is a sequence such

that $\tilde{I}^k(y^k) \leq C < \infty$, we have for every $\varepsilon > 0$ (see the first step in the proof of Theorem 4.2),

$$\begin{aligned} C &\geq \int_\Omega k\varphi^{qc}(Dy^k) - \langle T, Dy^k\rangle \, dx \\ &\geq -(k\alpha_1 + \frac{|T|}{p'\varepsilon^{p'}})\mathscr{L}^3(\Omega) + (k\alpha_2 - \frac{|T|\varepsilon^p}{p})\|Dy^k\|_{L^p} \, . \end{aligned}$$

where $\mathscr{L}^3(\Omega)$ denotes the three-dimensional Lebesgue measure of Ω. Thus, if ε is small enough and independent of k,

$$\|Dy^k\|_{L^p} \leq \tilde{C} \, ,$$

for some $\tilde{C}$ independent of k. The conclusion then follows from classical compactness theorems. Hence, provided φ grows fast enough off its zero set (*i.e.*, if k is sufficiently large) the existence of local minimisers for the constrained model ensures the same holds for the relaxed model

$$\tilde{I}^k(y) = \int_\Omega k\varphi^{qc}(Dy) - \langle T, Dy\rangle \, dx,$$

as expected.

We finish this section with general results on global and (some) local minimisers of constrained functionals of the type obtained in Theorem 4.2.

(4.4) Lemma. *Let $K \subset \mathbb{R}^{3\times 3}$ be a compact set and let K^{qc} denote its quasiconvex hull. Let $0 \neq T \in \mathbb{R}^{3\times 3}$ and consider the functional*

$$I(y) = \begin{cases} -\int_\Omega \langle T, Dy(x)\rangle \, dx & \text{if } Dy(x) \in K^{qc} \text{ a.e.} \\ +\infty & \text{otherwise} \end{cases} \, , \quad y \in \mathrm{W}^{1,1}(\Omega, \mathbb{R}^3) \, .$$

Then, the global minimisers of I are given by $Dy(x) = \bar{\xi}(x)$, with $\bar{\xi}$ satisfying

$$-\langle T, \bar{\xi}(x)\rangle = \min_{\xi \in K} -\langle T, \xi\rangle \quad a.e. \tag{4.12}$$

Remark. The functional I is here defined on $W^{1,1}(\Omega, \mathbb{R}^n)$ and not only on $W^{1,p}(\Omega, \mathbb{R}^n)$, as in Theorem 4.2, because, if $I(y) < \infty$, then $y \in W^{1,\infty}(\Omega, \mathbb{R}^n)$.

Proof of Lemma 4.4. Since K, and thus K^{qc}, are compact, I is bounded from below and we can simply minimise the integrand. Since $K^{qc} \subset K^c$ (the convex hull of K), we may invoke Carathéodory's Theorem (see Rockafellar [131]) and write any $\xi \in K^{qc}$ as

$$\xi = \sum_{i=1}^{3\times 3+1} \lambda_i \xi_i$$

for some $0 \leq \lambda_i \leq 1$ such that $\sum_i \lambda_i = 1$, and $\xi_i \in K$, $i = 1, \ldots, 10$. Hence,

$$-\langle T, \xi\rangle = -\langle T, \sum_i \lambda_i \xi_i\rangle = -\sum_i \lambda_i \langle T, \xi_i\rangle \geq \min_i -\langle T, \xi_i\rangle \, .$$

The lemma follows. □

We can be more precise in the physical case when $K \subset \mathbb{R}^{3\times 3}$ is given by (4.2) and $T \in \mathbb{R}^{3\times 3}$ is of rank two. More generally, we have

(4.5) Lemma. *Under the same hypotheses as in Lemma* 4.4*, assume furthermore that*

$$K = \bigcup_{i=1}^{N} \mathrm{SO}(3)U_i\,,$$

for some symmetric positive definite U_i, $i = 1, \dots, N$, and assume that $T \in \mathbb{R}^{3\times 3}$ is symmetric positive semidefinite and of rank two. Then the global minimisers of I are given by $Dy(x) = \bar{\xi}(x)$, with $\bar{\xi}$ solving

$$-\langle T, \bar{\xi}(x)\rangle = \min_{i=1,\dots,N} \big\{ \min_{R\in \mathrm{SO}(3)} -\langle T, RU_i\rangle \big\} \quad a.e.$$

Furthermore, for every i, the expression in braced brackets is minimised at R_i^t, where R_i is the rotation of the polar decomposition of U_iT.

Proof of Lemma 4.5. This is elementary. Since T is symmetric an explicit calculation gives

$$-\langle T, RU_i\rangle = -\mathrm{tr}\,(TRU_i) = -\mathrm{tr}\,(RU_iT) = -\mathrm{tr}\,(RR_i\sqrt{TU_i^2T})\,.$$

Since TU_i is of rank two, because T is, there exists a unique R that minimises $-\langle T, RU_i\rangle$ and it is given by $R = R_i^t$. (For the uniqueness, recall that a rotation is completely determined by its action on two linearly independent vectors.) □

We now turn to some properties of a certain kind of local minimiser, that we now specify. Let

$$\mathscr{A} = \left\{ y \in W^{1,1}(\Omega, \mathbb{R}^n) \,:\; I(y) < \infty\,,\ \int_\Omega y\,dx = 0 \right\}.$$

The constraint that $\int y = 0$ is natural here, since I is invariant under translation. Also, this condition ensures that Poincaré type inequalities apply. Observe that, since K is compact and $\int y = 0$, a function $y \in \mathscr{A}$ belongs to $W^{1,p}(\Omega, \mathbb{R}^n)$ for every $1 \le p \le \infty$. By abuse of notation, for a matrix $A \in K$, we write $y(x) = Ax$ instead of $y(x) = Ax - b$ with b such that $\int y = 0$. Recall the classical

(4.6) Definition. *Let $1 \le q \le \infty$. A mapping $y \in W^{1,1}(\Omega, \mathbb{R}^n)$ is an L^q (respectively $W^{1,q}$)* local minimiser of I in $\mathscr{A}$ *if there exists a $\delta > 0$ such that $I(z) \ge I(y)$ for every $\|z - y\|_{L^q} \le \delta$ (respectively $\|z - y\|_{W^{1,q}} \le \delta$). If in addition $I(z) > I(y)$ whenever $z \ne y$, then y is said to be a* strict local minimiser.

We introduce the following

(4.7) Definition. *Let $K \subset \mathbb{R}^{n\times n}$ be compact and let K^c denote its convex hull. Let also $1 \le p < \infty$. We say that $A \in K^c$ is a p-*strict exposed point *if there exist constants $\alpha > 0$ and $l \in \mathbb{R}^{n\times n}$ such that*

$$\langle l, \xi - A\rangle \ge \alpha|\xi - A|^p\,, \tag{4.13}$$

for every $\xi \in K^c$.

Remarks. The notion of exposed points is classical in convex analysis, see [131]: if C is a convex set, $A \in C$ is an *exposed point* if there exists a supporting hyperplane passing through A that contains no other point of C. In particular, an exposed point is an extreme point, but the converse is false. Here we need to impose the 'strictness' in the form of (4.13) in order to prevent the boundary of K^c from being too flat around the exposed point, see Example 4.10 below.

(4.8) Example. If $K = S(0, R)$ is the sphere of radius R centred at the origin, then any point $A \in K$ is a 2-strict exposed point of K^c. Indeed, by translation and rotation, we may assume that $K = S(P, R)$, where $P = (R, 0, \ldots, 0)$ and that A is the origin. Then, if $\xi \in B(P, R)$,

$$R^2 \geq |\xi - P|^2 = (\xi_1 - R)^2 + \xi_2^2 + \ldots + \xi_N^2 = R^2 - 2R\xi_1 + |\xi|^2 ,$$

and so $2R\langle e_1, \xi\rangle \geq |\xi|^2$. Now choose $l = e_1$ and $\alpha \leq 1/2R$ to conclude. In particular, if $K = \mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2$ with U_1 and U_2 having the same eigenvalues, we see that any point $F \in K$ is a 2-strict exposed point of K^c since $K \subset S(0, |U_1|)$.

(4.9) Example. If K is a finite set, then any extreme point $A \in K^c$ is a 1-strict exposed point. We leave the proof of this fact to the interested reader.

(4.10) Example. There exist exposed points that are not p-strict exposed points. Indeed,[36] consider the function $t \mapsto \psi(t) = \exp(-1/t^2)$. This function is convex in a neighbourhood of the origin. So let us take K to be a convex set that lies above the graph of ψ and such that the graph of ψ is its boundary around the origin. We claim that the origin is an exposed point (obvious) but not a p-strict exposed point for any p. This follows from the well-known fact that ψ is not analytic around the origin.

Remarks. We mention in passing two facts concerning p-strict exposed points. Firstly, it is easily seen that if $1 \leq p \leq q < \infty$, then a p-strict exposed point is a q-strict exposed point. Secondly, for any $p \geq 2$, there exists at least one p-strict exposed point of K^c. To prove this, reduce to the case $p = 2$ (by the preceding remark) and conclude by a 'shrinking ball' argument, bearing in mind that K is assumed to be compact.

We now show that those linear mappings whose gradients are p-strict exposed points possess an interesting property.

(4.11) Proposition. *Let $A \in K$ be a p-strict exposed point of K^c. Let $1 \leq q < \infty$. Then $y(x) = Ax$ is a (strict) L^q local minimiser of I in $\mathscr{A}$ if and only if it is a (strict) $W^{1,q}$ local minimiser of I in $\mathscr{A}$.*

Remark. After this research was carried out, Zhang Kewei pointed out that this result also holds under the hypothesis that $A \in K$ be merely an extreme point of K^c. See the remark following the proof of Lemma 4.12 below.

[36] This counter-example is based on an idea of Jonathan Bevan.

This result is an immediate consequence of the following

(4.12) Lemma. *Let $A \in K$ be a p-strict exposed point of K^c and let $y(x) = Ax$. Let $1 \le q < \infty$. Then, for every $\varepsilon > 0$, there exists a $\delta > 0$ such that, if*

$$Dz \in K^c \text{ a.e.} \quad \text{and} \quad \|z - y\|_{L^q(\Omega,\mathbb{R}^n)} < \delta\,,$$

then $\|Dz - Dy\|_{L^q(\Omega,\mathbb{R}^n)} < \varepsilon$.

Remark. This is an interesting example of geometric features improving weak to strong convergence. Usually, one requires extra 'convexity' assumptions and convergence of energies to achieve this, see [72, 73].

Proof of Lemma 4.12. We proceed in two steps.

First step. We first treat the case $q = p$ for the sake of illustration. Suppose not. Then there exists a sequence $y^k \to y$ in L^p and $Dy^k \in K^c$ a.e. but

$$\|Dy^k - Dy\|_{L^p}^p \ge \varepsilon \quad \text{for all } j,$$

for some $\varepsilon > 0$. Since A is a p-strict exposed point, there exist $\alpha > 0$ and $l \in \mathbb{R}^{n\times n}$ such that

$$\langle l, Dy^k - A\rangle \ge \alpha |Dy^k - A|^p \quad \text{a.e.}$$

Thus, integrating, we get

$$\int_\Omega \langle l, Dy^k - A\rangle\, dx \ge \alpha \|Dy^k - A\|_{L^p}^p \ge \alpha\varepsilon > 0. \tag{4.14}$$

Since Dy^k is uniformly bounded in L^∞, we know that $Dy^k \rightharpoonup A$ in L^p, and thus the left-hand side of (4.14) goes to zero as $k \to \infty$, which finishes the first step.

Second step. We prove the general case. If the conclusion of the lemma were false, there would exist $y^k \to y$ in L^q but

$$\|Dy^k - Dy\|_{L^q}^q \ge \varepsilon \quad \text{for all } j,$$

for some $\varepsilon > 0$. Since A is a p-strict exposed point, we get that

$$\int_\Omega \langle l, Dy^k - A\rangle\, dx \ge \alpha \|Dy^k - A\|_{L^p}^p\,.$$

for some $\alpha > 0$ and $l \in \mathbb{R}^{n\times n}$. Now, since $Dy^k, Dy \in L^r$ for any $1 \le r \le \infty$, and denoting by C a generic constant, we have

$$\begin{aligned}
\|Dy^k - Dy\|_{L^q} &\le \|Dy^k - Dy\|_{L^1}^{1/q}\, \|Dy^k - Dy\|_{L^\infty}^{1-1/q} \\
&\le \|Dy^k - Dy\|_{L^p}^{1/q}\, \|Dy^k - Dy\|_{L^{p'}}^{1/q}\, \|Dy^k - Dy\|_{L^\infty}^{1-1/q} \\
&\le C\, \|Dy^k - Dy\|_{L^p}^{1/q}\, \|Dy^k - Dy\|_{L^\infty} \\
&\le C\, \|Dy^k - Dy\|_{L^p}^{1/q}\,.
\end{aligned}$$

Hence,

$$\int_\Omega \langle l, Dy^k - A\rangle\, dx \ge \alpha \|Dy^k - A\|_{L^p}^p \ge \alpha C \|Dy^k - Dy\|_{L^q}^{pq} > C\alpha\varepsilon^p\,.$$

We conclude as in the first step that this is a contradiction, finishing the proof. □

Remark. As pointed out above, Zhang Kewei showed us how to generalise this result to extreme points. As above, we assume that there exists a sequence $y^k \to y$ in L^p (for simplicity) and $Dy^k \in K^c$ a.e. but

$$\|Dy^k - Dy\|_{L^p}^p \geq \varepsilon \quad \text{for all } j,$$

for some $\varepsilon > 0$. Extracting a subsequence, not relabelled, we infer that Dy^k generates a gradient Young measure ν_x satisfying $\operatorname{supp} \nu_x \subset K^c$ a.e. Furthermore, $Dy^k \rightharpoonup A = \bar{\nu}_x$. But since A is an extreme point of K^c and ν_x is a probability measure almost everywhere supported on K^c we conclude that $\nu_x = \delta_A$ a.e. We readily conclude that this is a contradiction.

A similar idea proves the following

(4.13) Proposition. *Let $A \in K$ be a p-strict exposed point of K^c and let $y(x) = Ax$. If y is a strict (L^p or $W^{1,p}$) local minimiser of I in $\mathscr{A}$, then y lies in a potential well,* i.e.*, for all $\varepsilon > 0$ sufficiently small there exists $\gamma(\varepsilon) > 0$ such that*

$$I(z) - I(y) \geq \gamma(\varepsilon) \quad \textit{whenever } \|z - y\|_{L^p} = \varepsilon. \tag{4.15}$$

Remarks. Obviously, in (4.15), the chosen norm does not matter, because of Proposition 4.11 and Poincaré's Inequality. As a matter of fact, in the proof, we shall use the $W^{1,p}$ norm. Another way of defining a potential well is that, for all sufficiently small $\varepsilon > 0$,

$$\inf_{\|z-y\|_{L^p}=\varepsilon} I(z) > I(y)\,.$$

We should stress that the terminology used in this proposition and its proof, below, differs from that used elsewhere (everywhere else, in fact) in this thesis, where a potential well is a set of the form $\mathrm{SO}(3)U$ for some symmetric positive definite U. We hope this is not too confusing. The concept of potential well arises in dynamics as a hypothesis ensuring that an equilibrium state be dynamically stable. We refer the reader to Ball and Marsden [30] for more on these issues.

Proof of Proposition 4.13. If not, there would exist y^k such that $\|y^k - y\|_{W^{1,p}}^p = \varepsilon$ for some $\varepsilon > 0$ and $I(y^k) \to I(y)$. We may also assume $y^k \rightharpoonup \bar{y}$ in $W^{1,p}$ for some $\bar{y}$. Then

$$I(\bar{y}) \leq \liminf_{k\to\infty} I(y^k) = I(y)\,,$$

and so, $\bar{y} = y$ because y is a strict local minimiser. On the other hand, since A is a p-strict exposed point, there exist $\alpha > 0$ and $l \in \mathbb{R}^{n\times n}$ such that

$$\int_\Omega \langle l, Dy^k - A\rangle\, dx \geq \alpha \|Dy^k - A\|_{L^p}^p \geq \alpha\varepsilon > 0\,.$$

Passing to the limit and using the weak continuity of the left-hand side, we deduce that

$$\int_\Omega \langle l, D\bar{y} - A\rangle\, dx \geq \alpha\varepsilon > 0$$

and so $D\bar{y} \neq A$, which is a contradiction. □

4.3 Metastability, incompatibility-induced hysteresis and the Schmid Law

The goal of this section is to prove the central theorem of our study of metastability in martensite. To fix notation, let us recall that we consider an energy of the form

$$I_\sigma(y) = \begin{cases} -\int_\Omega \langle T(\sigma), Dy(x)\rangle \, dx & \text{if } Dy(x) \in K^{qc} \text{ a.e.} \\ +\infty & \text{otherwise} \end{cases},$$

where $T(\sigma)$ is symmetric positive semidefinite, of rank two and continuous in σ. Furthermore, K is of the form

$$K = \bigcup_{i=1}^{6} \mathrm{SO}(3)U_i \,,$$

where the U_i are symmetric and positive definite, and $\Omega \subset \mathbb{R}^3$ is open, bounded and convex.

As suggested by experiments, we assume that the loading path $T(\sigma)$, $0 \le \sigma \le 1$, has at some value σ_0 an *exchange of stability*. More precisely, (after possibly relabelling the U_i) we let $A(\sigma) \in \mathrm{SO}(3)U_1$ and $B(\sigma) \in \mathrm{SO}(3)U_2$ satisfy

$$\begin{aligned} -\langle T(\sigma), A(\sigma)\rangle &< -\langle T(\sigma), RU_1\rangle \,, \quad \text{for every } R \in \mathrm{SO}(3)\,, \quad RU_1 \neq A(\sigma)\,, \quad 0 \le \sigma \le 1\,, \\ -\langle T(\sigma), B(\sigma)\rangle &< -\langle T(\sigma), RU_2\rangle \,, \quad \text{for every } R \in \mathrm{SO}(3)\,, \quad RU_2 \neq B(\sigma)\,, \quad 0 \le \sigma \le 1\,, \end{aligned}$$

and assume that

$$\begin{aligned} -\langle T(\sigma), A(\sigma)\rangle &< -\langle T(\sigma), \xi\rangle \,, \quad \text{for every } \xi \in K\,, \quad \xi \neq A(\sigma)\,, \quad 0 \le \sigma < \sigma_0\,, \\ -\langle T(\sigma), B(\sigma)\rangle &< -\langle T(\sigma), \xi\rangle \,, \quad \text{for every } \xi \in K\,, \quad \xi \neq B(\sigma)\,, \quad \sigma_0 < \sigma \le 1\,. \end{aligned} \tag{4.16}$$

Hence, σ_0 is the equal energy point,

$$\langle T(\sigma_0), A(\sigma_0)\rangle = \langle T(\sigma_0), B(\sigma_0)\rangle < -\langle T(\sigma_0), \xi\rangle \,, \text{ for all } \xi \in K,\, \xi \notin \{A(\sigma_0)\,, B(\sigma_0)\}\,. \tag{4.17}$$

We observe that $A(\sigma)$ and $B(\sigma)$ are continuous functions of σ; see Lemma 4.5 where an algorithm to find these matrices was given. Let us write $A_0 = A(\sigma_0)$ and $B_0 = B(\sigma_0)$ and assume, as suggested by the experiments, that

$$\mathrm{rank}\,(A(\sigma_0) - B(\sigma_0)) > 1. \tag{4.18}$$

This hypothesis may also be considered as a genericity condition. Indeed, if

$$\mathrm{rank}\,(A(\sigma_0) - B(\sigma_0)) = 1\,,$$

metastability is impossible – see Figure 4.9 and the discussion after the proof of Theorem 4.14 for an explanation of why the presence of rank-one connections prevents metastability. Recall finally that

$$\mathscr{A} = \left\{ y \in W^{1,1}(\Omega, \mathbb{R}^3) \,:\; I(y) < \infty\,,\; \int_\Omega y \, dx = 0 \right\}.$$

Let $y_\sigma(x) = A(\sigma)x$. It is clear that y_σ is the unique absolute minimiser of I_σ in $\mathscr{A}$ for $0 \le \sigma < \sigma_0$. The following theorem shows that y_σ remains a *local minimiser of I_σ beyond σ_0*.

(4.14) Metastability Theorem. *There exists a $\sigma_1 > \sigma_0$ such that for each $0 \le \sigma \le \sigma_1$, y_σ is an L^1 local minimiser of I_σ. Furthermore, there exists a $\delta = \delta(\sigma_1)$ such that*

$$I_\sigma(y_\sigma) \le I_\sigma(y)\,,$$

for all $y \in \mathscr{A}$ *with*

$$\int_\Omega |y(x) - y_\sigma(x)|\, dx < \delta\,. \tag{4.19}$$

Remarks. This theorem is merely a transcription in the present framework of the Metastability Theorem of Ball et al. [21], which was originally stated in the language of Young measures (see the discussion after Theorem 4.2). As a matter of fact, we shall use the Young measures setting in the proof.[37]

The key assumption in the Theorem is that $\operatorname{rank}(A_0 - B_0) > 1$, so that this result provides an example of incompatibility-induced hysteresis. Indeed, one easily sees that a similar result holds under the change of variable $\sigma \mapsto 1-\sigma$ with $y_\sigma(x) = B(\sigma)x$ remaining a local minimiser below σ_0. Hence, if σ increases from 0 to 1, and then decreases back to 0, we get a hysteresis loop in a plot *volume fraction of variant 2* vs. *measure of the load*, see Figure 4.3.

In order to prove Theorem 4.14 we need an estimate due to Ball and James [26]. We sketch a proof for the convenience of the reader.

(4.15) Lemma (Transition Layer Estimate). *Let* $A, B \in \mathbb{R}^{3\times 3}$ *such that*

$$\operatorname{rank}(A - B) > 1\,.$$

Given $\varepsilon > 0$*, let us write*

$$\mathscr{N}_\varepsilon(A) = \{\xi \in \mathbb{R}^{3\times 3} : |A - \xi| < \varepsilon\}\,.$$

Let $\Omega \subset \mathbb{R}^3$ *be open, bounded and convex and let us denote, for any* $y \in \mathrm{W}^{1,\infty}(\Omega, \mathbb{R}^3)$*,*

$$\begin{aligned}\Omega^\varepsilon_A &= \{x \in \Omega :\ \ Dy(x) \in \mathscr{N}_\varepsilon(A)\}\,,\\ \Omega^\varepsilon_B &= \{x \in \Omega :\ \ Dy(x) \in \mathscr{N}_\varepsilon(B)\}\,,\\ \Omega^\varepsilon_{trans} &= \Omega \setminus (\Omega^\varepsilon_A \cup \Omega^\varepsilon_B)\,.\end{aligned}$$

Then there exist fixed constants $\varepsilon_0 > 0$ *and* $\gamma > 0$ *such that*

$$\mathscr{L}^3(\Omega^\varepsilon_{trans}) \geq \gamma \min\{\mathscr{L}^3(\Omega^\varepsilon_A), \mathscr{L}^3(\Omega^\varepsilon_B)\}\,, \tag{4.20}$$

for every $y \in \mathrm{W}^{1,\infty}(\Omega, \mathbb{R}^3)$ *such that* $Dy \in K^{qc}$ *a.e. and every* $0 \leq \varepsilon \leq \varepsilon_0$*. Furthermore,*

$$\int_\Omega \nu_x([\mathscr{N}_\varepsilon(A) \cup \mathscr{N}_\varepsilon(B)]^c)\, dx \geq \gamma \min\left\{\int_\Omega \nu_x(\mathscr{N}_\varepsilon(A))\, dx\,,\ \int_\Omega \nu_x(\mathscr{N}_\varepsilon(B))\, dx\right\}\,,$$

for every gradient Young measure $(\nu_x)_{x\in\Omega}$ *almost everywhere supported on* K *and every* $0 \leq \varepsilon \leq \varepsilon_0$*. Here* E^c *denotes the complement of* E*.*

Proof of Lemma 4.15. We restrict ourselves to the proof of (4.20). For the sake of simplicity we only treat the case when Ω is a ball. We start with a preliminary step.

[37] We have failed to find a proof of Theorem 4.14 which does not use Young measures. More correctly, we can prove a version of the Theorem, where we consider only two martensitic wells, instead of six. The reason for this is that in our setting, we have to invoke an explicit formula for the quasiconvex hull, which exists for two wells, but does not for six. This is not necessary in the theory of Ball et al. On this issue, see the remark after the proof of Theorem 4.14.

Claim. If $\Omega' \subset \Omega$ is a ball, there exist $\varepsilon_0 > 0$ and $\gamma_1 > 0$ such that

$$\mathscr{L}^3(\{x \in \Omega' : \ Dy(x) \notin (\mathscr{N}_\varepsilon(A) \cup \mathscr{N}_\varepsilon(B))\}) \geq \gamma_1 \mathscr{L}^3(\Omega')\,,$$

for every $0 \leq \varepsilon \leq \varepsilon_0$ and every $y \in W^{1,\infty}(\Omega', \mathbb{R}^3)$ such that $Dy \in K^{qc}$ a.e. and

$$\frac{\mathscr{L}^3(\{x \in \Omega' : \ Dy(x) \in \mathscr{N}_\varepsilon(A)\})}{\mathscr{L}^3(\Omega')} = \frac{1}{2}\,.$$

Proof of the claim. We only deal with the case $\Omega' = \Omega$. (The case $\Omega' \subset \Omega$ proceeds similarly but uses further covering lemma arguments; see [26] for details.) Suppose not, then there exist $y^k \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ and $0 \leq \varepsilon^k \leq 1/k$ with

$$\frac{\mathscr{L}^3(\Omega_A^{\varepsilon^k})}{\mathscr{L}^3(\Omega)} = \frac{1}{2}\,,$$

but

$$\mathscr{L}^3(\Omega_{\text{trans}}^{\varepsilon^k}) \leq \frac{1}{k}\,. \tag{4.21}$$

Hence $\|Dy^k\|_{L^\infty}$ is uniformly bounded and (up to a subsequence) Dy^k has an associated gradient Young measure ν_x. By (4.21) $\operatorname{supp} \nu_x \subset \{A, B\}$ a.e. But

$$\frac{1}{\mathscr{L}^3(\Omega)} \int \nu_x(\{A\})\, dx = \frac{1}{2} = \frac{1}{\mathscr{L}^3(\Omega)} \int \nu_x(\{B\})\, dx\,,$$

which is a contradiction, since $\operatorname{rank}(A - B) > 1$.

Proof of Lemma 4.15 (continued). Let $y \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ such that $Dy \in K^{qc}$ a.e. Remember that Ω is a ball. For a given $x \in \Omega$, consider

$$\Omega^r(x) = r\Omega + (1-r)x = x + r(\Omega - x)\,.$$

Then $\Omega^1 = \Omega$, $\Omega^r(x) \subset \Omega^s(x)$ if $r \leq s$ and $\cap_{r>0} \Omega^r(x) = \{x\}$. Take $\varepsilon \leq \varepsilon_0$ (ε_0 is provided by the above claim) and assume without loss of generality that $\mathscr{L}^3(\Omega_A^\varepsilon) \leq \mathscr{L}^3(\Omega_B^\varepsilon)$. For x a Lebesgue point of Ω_A^ε, consider

$$f(r) = \frac{\mathscr{L}^3(\Omega_A^\varepsilon \cap \Omega^r(x))}{\mathscr{L}^3(\Omega^r(x))}\,.$$

Note that $f : [0,1] \to [0,1]$ is continuous, $f(1) \leq 1/2$ and $\lim_{r \to 0} f(r) = 1$. By continuity, there exists $r(x)$ such that $f(r(x)) = 1/2$. Now, the balls $\Omega^{r(x)}(x)$ cover (the set of Lebesgue points of) Ω_A^ε. By Vitali's covering lemma, there exists a disjoint family, finite or countable, such that

$$\sum_k \mathscr{L}^3(\Omega^{r(x^k)}(x^k)) \geq c \mathscr{L}^3(\Omega_A^\varepsilon)\,,$$

for some constant $c > 0$. Let us apply the claim and conclude that

$$\begin{aligned}
\mathscr{L}^3(\Omega_{\text{trans}}^\varepsilon) &\geq \sum_k \mathscr{L}^3(\Omega_{\text{trans}}^\varepsilon \cap \Omega^{r(x^k)}(x^k)) \\
&\geq \gamma_1 \sum_k \mathscr{L}^3(\Omega^{r(x^k)}(x^k)) \\
&\geq \gamma_1\, c\, \Omega_A^\varepsilon\,,
\end{aligned}$$

as desired. □

We are now in a position to prove the Metastability Theorem.

Proof of Theorem 4.14. Letting $y \in \mathscr{A}$ we write ν_x for the associated gradient Young measure; see the remarks following Theorem 4.2 where we explained how to get this. For $0 \le \sigma \le 1$, $\varepsilon > 0$ and using the notation of Lemma 4.15, we write the energy difference

$$\begin{aligned}
\Delta I_\sigma &= \int_\Omega \langle T(\sigma), Dy_\sigma - Dy\rangle \, dx \\
&= \int_\Omega \int_{\mathbb{R}^{3\times 3}} \langle T(\sigma), A(\sigma) - \xi\rangle \, d\nu_x(\xi)\, dx \\
&= \int_\Omega \int_{\mathscr{N}_\varepsilon(A_0)} \langle T(\sigma), A(\sigma) - \xi\rangle \, d\nu_x(\xi)\, dx + \int_\Omega \int_{\mathscr{N}_\varepsilon(B_0)} \langle T(\sigma), A(\sigma) - \xi\rangle \, d\nu_x(\xi)\, dx \\
&\qquad + \int_\Omega \int_{[\mathscr{N}_\varepsilon(A)\cup\mathscr{N}_\varepsilon(B)]^c} \langle T(\sigma), A(\sigma) - \xi\rangle \, d\nu_x(\xi)\, dx \\
&= \alpha_1 + \alpha_2 + \alpha_3 \, .
\end{aligned} \tag{4.22}$$

Claim 1. If $\varepsilon > 0$ is small enough, $\alpha_1 \ge 0$.

Proof of Claim 1. Choosing $\varepsilon > 0$ small enough so that $\mathscr{N}_\varepsilon(A_0) \cap K = \mathscr{N}_\varepsilon(A_0) \cap \mathrm{SO}(3)U_1$ (which is possible because the wells are separated), the claim follows at once from the fact that $A(\sigma)$ is the absolute minimiser of $-\langle T(\sigma), \cdot\rangle$ on $\mathrm{SO}(3)U_1$.

Regarding α_2, we have

$$\alpha_2 = \int_\Omega \int_{\mathscr{N}_\varepsilon(B_0)} \langle T(\sigma), A(\sigma) - \xi\rangle \, d\nu_x \, dx \ge \int_\Omega \int_{\mathscr{N}_\varepsilon(B_0)} \langle T(\sigma), A(\sigma) - B(\sigma)\rangle \, d\nu_x \, dx \, ,$$

since $B(\sigma)$ is the absolute minimiser of $-\langle T(\sigma), \cdot\rangle$. Let

$$g(\sigma) = \langle T(\sigma), B(\sigma) - A(\sigma)\rangle \, .$$

Then $g(\sigma_0) = 0$, $g(\sigma) > 0$ for $\sigma > \sigma_0$ and g is continuous in σ. Thus,

$$\alpha_2 \ge -g(\sigma) \int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0)) \, dx \, .$$

Let us record the following, easy

Claim 2. For a fixed $\varepsilon > 0$, there exist $\bar\sigma = \bar\sigma(\varepsilon) > 0$ and $c = c(\varepsilon) > 0$ such that

$$\langle T(\sigma), A(\sigma) - \xi\rangle \ge c > 0 \, , \quad \text{for every } \xi \in [\mathscr{N}_\varepsilon(A_0) \cup \mathscr{N}_\varepsilon(B_0)]^c \, ,$$

and every $\sigma < \bar\sigma$.

Combining the second claim and the Transition Layer Estimate, we get that

$$\alpha_3 \ge c\gamma \min\left\{ \int_\Omega \nu_x(\mathscr{N}_\varepsilon(A_0)) \, dx \, , \ \int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0)) \, dx \right\} \, ,$$

if $\varepsilon > 0$ is small enough and σ sufficiently close to σ_0. Hence, combining all the above estimates, we have

$$\Delta I_\sigma \geq -g(\sigma) \int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0))\,dx + c\gamma \min\left\{ \int_\Omega \nu_x(\mathscr{N}_\varepsilon(A_0))\,dx\,,\ \int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0))\,dx \right\}. \quad (4.23)$$

Claim 3. For a fixed $\varepsilon > 0$, either $\Delta I_\sigma \geq 0$ or

$$\min\left\{ \int_\Omega \nu_x(\mathscr{N}_\varepsilon(A_0))\,dx\,,\ \int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0))\,dx \right\} = \int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0))\,dx\,,$$

if σ is near σ_0 and $\delta > 0$ in (4.19) is small enough.

Proof of Claim 3. Recall that by Lemma 4.12 and Example 4.8, for every $\delta' > 0$, there exists $\delta > 0$ such that

$$\text{if} \quad Dy \in K^{qc}\,, \text{ and } \ \|y - A(\sigma)x\|_{L^1} < \delta\,, \ \text{ then, } \|Dy - A(\sigma)\|_{L^1} < \delta'\,.$$

Hence it suffices to prove the claim assuming that $\|Dy - A(\sigma)\|_{L^1} < \delta'$ for sufficiently small $\delta' > 0$. Let us show that

(i) $\Delta I_\sigma < 0$,

(ii) $\delta' > 0$ is small enough,

(iii) $|\sigma - \sigma_0| > 0$ is small enough

imply that

$$\int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0))\,dx < \int_\Omega \nu_x(\mathscr{N}_\varepsilon(A_0))\,dx\,,$$

which will imply the claim.

Suppose not. Then there exists a sequence of gradient Young measures (ν_x^k) supported on K, with centres of mass Dy^k and a sequence $\sigma^k \to 0$ such that

$$\|Dy^k - A(\sigma^k)\|_{L^1} \to 0\,, \quad (4.24)$$

and $\Delta I_{\sigma^k} < 0$, *i.e.*,

$$-\int_\Omega \langle T(\sigma^k), Dy^k\rangle\,dx < -\int_\Omega \langle T(\sigma^k), A(\sigma^k)\rangle\,dx \quad (4.25)$$

for all k, but

$$\int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0))\,dx \geq \int_\Omega \nu_x(\mathscr{N}_\varepsilon(A_0))\,dx\,. \quad (4.26)$$

We now invoke a remark by Ball[38] to the effect that, up to a subsequence, not relabelled, $\nu_x^k \overset{*}{\rightharpoonup} \nu_x$ in $L^\infty_w(\Omega, \mathscr{C}_0(\mathbb{R}^{3\times 3})^*)$, where ν_x is a $W^{1,\infty}$– gradient Young measure supported on K, with centre of mass Dy for some $y \in W^{1,\infty}(\Omega, \mathbb{R}^3)$. (In particular $Dy(x) \in K^{qc}$ a.e. and $y^k \overset{*}{\rightharpoonup} y$ in $W^{1,\infty}(\Omega, \mathbb{R}^3)$.) We now pass to the limit as $k \to \infty$ in (4.25) to get

$$-\int_\Omega \langle T(\sigma_0), Dy\rangle\,dx \leq -\int_\Omega \langle T(\sigma_0), A_0\rangle\,dx\,.$$

[38] Private communication.

By (4.17) we deduce that

$$Dy(x) = \lambda(x)A_0 + (1-\lambda(x))B_0\,,$$

for some $0 \le \lambda \le 1$ a.e. Since $\operatorname{rank}(A_0 - B_0) > 1$, this implies $\lambda \equiv 1$ a.e. or $\lambda \equiv 0$ a.e. But then, (4.24) gives $\lambda \equiv 1$ a.e. which in turn contradicts (4.26). The claim is proved.

Let us go back to (4.23) and use Claim 3. We get

$$\Delta I_\sigma \ge (-g(\sigma) + c\gamma) \int_\Omega \nu_x(\mathscr{N}_\varepsilon(B_0))\,dx\,.$$

Since $c\gamma > 0$, the right-hand side is non-negative is σ is sufficiently close to σ_0. Now, if we choose $\varepsilon > 0$, $\delta > 0$ and $\sigma_1 > \sigma_0$ so that all the above estimates hold, the proof is finished. □

Remark. We briefly outline an idea for a proof that does not use Young measures. Instead of (4.22) we decompose the energy difference as follows, using the notation of Lemma 4.15:

$$\begin{aligned}
\Delta I_\sigma &= \int_\Omega \langle T(\sigma), Dy_\sigma - Dy\rangle\,dx \\
&= \int_{\Omega^\varepsilon_{A_0}} \langle T(\sigma), Dy_\sigma - Dy\rangle\,dx + \int_{\Omega^\varepsilon_{B_0}} \langle T(\sigma), Dy_\sigma - Dy\rangle\,dx + \int_{\Omega^\varepsilon_{\mathrm{trans}}} \langle T(\sigma), Dy_\sigma - Dy\rangle\,dx, \\
&= \alpha_1 + \alpha_2 + \alpha_3\,.
\end{aligned}$$

Proceeding as in the proof (with the noticeable difference that, in order to get that $\alpha_1 \ge 0$, we need to invoke a formula for K^{qc}, which is precisely why we cannot handle the six-well case) the Transition Layer Estimate yields

$$\Delta I_\sigma \ge -g(\sigma)\mathscr{L}^3(\Omega^\varepsilon_{B_0}) + c\gamma \min\{\mathscr{L}^3(\Omega^\varepsilon_{A_0}), \mathscr{L}^3(\Omega^\varepsilon_{B_0})\}\,.$$

In this setting however, the remaining step is easier.

Claim 3'. For a fixed $\varepsilon > 0$,

$$\min\{\mathscr{L}^3(\Omega^\varepsilon_{A_0}), \mathscr{L}^3(\Omega^\varepsilon_{B_0})\} = \mathscr{L}^3(\Omega^\varepsilon_{B_0})\,,$$

if $\delta > 0$ in (4.19) is small enough and if σ is sufficiently close to σ_0.

Proof of Claim 3'. Recall that by Lemma 4.12 and Example 4.8, for every $\delta' > 0$, there exists $\delta > 0$ such that

$$\text{if} \quad Dy \in K^{qc}\,, \text{ and } \ \|y - A(\sigma)x\|_{L^1} < \delta\,, \ \text{ then, } \|Dy - A(\sigma)\|_{L^1} < \delta'\,.$$

Hence it suffices to prove the claim assuming that $\|Dy - A(\sigma)\|_{L^1} < \delta'$ for sufficiently small $\delta' > 0$. Suppose $\mathscr{L}^3(\Omega^\varepsilon_{A_0}) \le \mathscr{L}^3(\Omega^\varepsilon_{B_0})$. Then $\|Dy - A(\sigma)\|_{L^1} < \delta'$ implies

$$\begin{aligned}
\delta' &> \int_\Omega |Dy - A(\sigma)|\,dx \\
&\ge \int_\Omega |Dy - A_0|\,dx - |A(\sigma) - A_0|\mathscr{L}^3(\Omega) \\
&\ge \int_{\Omega^\varepsilon_{A_0}} |Dy - A_0|\,dx + \int_{\Omega^\varepsilon_{B_0}} |Dy - A_0|\,dx + \int_{\Omega^\varepsilon_{\mathrm{trans}}} |Dy - A_0|\,dx - |A(\sigma) - A_0|\mathscr{L}^3(\Omega) \\
&\ge 0 + \varepsilon\big(\mathscr{L}^3(\Omega^\varepsilon_{B_0}) + \mathscr{L}^3(\Omega^\varepsilon_{\mathrm{trans}})\big) - |A(\sigma) - A_0|\mathscr{L}^3(\Omega)\,,
\end{aligned}$$

and thus,

$$\mathscr{L}^3(\Omega^\varepsilon_{B_0}) + \mathscr{L}^3(\Omega^\varepsilon_{\text{trans}}) \le \frac{\delta' + |A(\sigma) - A_0|\mathscr{L}^3(\Omega)}{\varepsilon}\,.$$

This gives three conditions on the quantities $\mathscr{L}^3(\Omega^\varepsilon_{A_0})$, $\mathscr{L}^3(\Omega^\varepsilon_{B_0})$ and $\mathscr{L}^3(\Omega^\varepsilon_{\text{trans}})$, namely

$$\begin{aligned}
&\mathscr{L}^3(\Omega) = \mathscr{L}^3(\Omega^\varepsilon_{A_0}) + \mathscr{L}^3(\Omega^\varepsilon_{B_0}) + \mathscr{L}^3(\Omega^\varepsilon_{\text{trans}})\,,\\
&\mathscr{L}^3(\Omega^\varepsilon_{B_0}) + \mathscr{L}^3(\Omega^\varepsilon_{\text{trans}}) \le \frac{\delta' + |A(\sigma) - A_0|\mathscr{L}^3(\Omega)}{\varepsilon}\,,\\
&\mathscr{L}^3(\Omega^\varepsilon_{A_0}) \le \mathscr{L}^3(\Omega^\varepsilon_{B_0}) \le \frac{\delta' + |A(\sigma) - A_0|\mathscr{L}^3(\Omega)}{\varepsilon}\,.
\end{aligned} \tag{4.27}$$

Substituting $(4.27)_1$ into $(4.27)_2$ yields

$$\mathscr{L}^3(\Omega^\varepsilon_{A_0}) \ge \mathscr{L}^3(\Omega) - \frac{\delta' + |A(\sigma) - A_0|\mathscr{L}^3(\Omega)}{\varepsilon}\,,$$

which together with $(4.27)_3$ gives

$$\frac{\delta' + |A(\sigma) - A_0|\mathscr{L}^3(\Omega)}{\varepsilon} \ge \frac{\mathscr{L}^3(\Omega)}{2}\,,$$

which is a contradiction since the left-hand side can be made arbitrarily small if $\delta' > 0$ is small enough and σ near enough σ_0. The claim is proved. The rest is as in the proof of Theorem 4.14.

This theorem provides us with a rigorous explanation of hysteresis in martensite under load. This was one of two goals. The other was to estimate the size of the hysteresis. In other words, we would like to estimate the load σ_1 at which metastability is lost. This appears to be a difficult problem, but finding an upper bound is rather straightforward. Indeed, recall that there are exactly two matrices $B_1(\sigma), B_2(\sigma) \in \mathrm{SO}(3)U_2$ that are rank-one connected to $A(\sigma)$,

$$\operatorname{rank}\left(A(\sigma) - B_i(\sigma)\right) = 1\,, \quad i = 1, 2.$$

In other words,

$$A(\sigma) - B_i(\sigma) = a_i(\sigma) \otimes m_i(\sigma)\,,$$

for some $a_i(\sigma), m_i(\sigma) \in \mathbb{R}^3$. Assume that there exists $\sigma > \sigma_0$ such that

$$-\langle T(\sigma), B_i(\sigma)\rangle < -\langle T(\sigma), A(\sigma)\rangle\,,$$

for $i = 1$ or 2. (For example, if T is linear in σ, as in the experiments, this is the case.) Assume for definiteness that $i = 1$, write $B(\sigma) = B_i(\sigma)$, $m(\sigma) = m_i(\sigma)$, and so forth, and consider the deformation y pictured in Figure 4.9.

Since $B(\sigma)$ has lower energy than, and is kinematically compatible with, $A(\sigma)$, if the portion of Ω where $Dy = B(\sigma)$ is small enough, y is very close to y_σ in L^1 and lowers the energy. Hence y_σ is not metastable. This gives the announced upper bound, which we now formally state. Following Ball, Chu and James, we call this upper bound the *Schmid Law*, for reasons that will be explained shortly.

The Schmid Law. *Transformation occurs at the first value of σ at which either*

$$\langle T(\sigma), A(\sigma)\rangle = \langle T(\sigma), B_1(\sigma)\rangle\,, \quad \textit{or} \quad \langle T(\sigma), A(\sigma)\rangle = \langle T(\sigma), B_2(\sigma)\rangle\,. \tag{4.28}$$

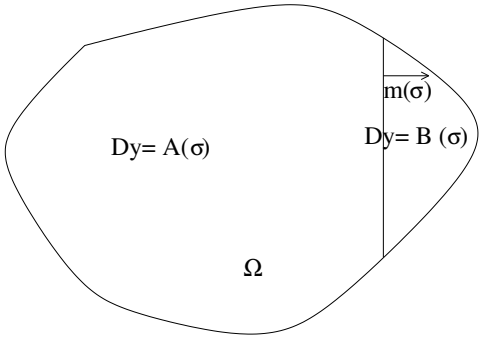


Figure 4.9: The Schmid Law, an upper bound to metastability.

Let σ_{Sch} denote the load defined by (4.28).

Let us now show[39] that (4.28) coincides with one interpretation of the Schmid Law. Recall that the Cauchy stress at the point $y(x) = Fx$, $x \in \Omega$, in the deformed configuration is given by

$$\Sigma = \frac{1}{\det F} T_0 F^t \,,$$

where T_0 is the Piola-Kirchhoff stress tensor. Also, the observed normal m to a plane of normal m_0 in the reference configuration and deformed by y is

$$m = \frac{F^{-t} m_0}{|F^{-t} m_0|} \,.$$

In general the Schmid Law states that transformation occurs when the critical resolved shear stress on the incipient twin plane reaches a certain material constant. In this setting, the Schmid Law is interpreted by Ball et al. [21] as saying that transformation occurs when

$$\langle a, \Sigma m \rangle = \gamma \,, \tag{4.29}$$

where γ is a constant and a is the amplitude vector associated to the incipient twin, *i.e.*, another deformation gradient G such that $G - F = a \otimes m_0$. In [21], the authors propose to adapt this setting to our situation by identifying $F = A(\sigma)$, $T_0 = T(\sigma)$, $m_0 = m_1(\sigma)$ or $m_2(\sigma)$, $a = a_1(\sigma)$ or $a_2(\sigma)$ and 'incipient' by a choice of the subscript 1 or 2, depending on which occurs first in (4.28). With these identifications, (4.29) reads

$$\begin{aligned}
\gamma = \langle a, \Sigma m \rangle &= \frac{1}{\det A(\sigma) |A(\sigma)^{-t} m_i(\sigma)|} \langle a_i(\sigma), T(\sigma) A(\sigma)^t A(\sigma)^{-t} m_i(\sigma) \rangle \\
&= \frac{1}{\det A(\sigma) |A(\sigma)^{-t} m_i(\sigma)|} \langle a_i(\sigma) \otimes m_i(\sigma), T(\sigma) \rangle \\
&= \frac{1}{\det A(\sigma) |A(\sigma)^{-t} m_i(\sigma)|} \langle B_i(\sigma) - A(\sigma), T(\sigma) \rangle \,,
\end{aligned}$$

for some $i = 1, 2$. By comparing this and (4.28) we see that this condition coincides with (4.28) provided we choose $\gamma = 0$.

[39] This justification is due to, and appears in, Ball et al. [21]. We reproduce it here for the sake of completeness. We should also point out that the origins of the Schmid Law, *i.e.*, plasticity, are completely different from the elasticity setting adopted here.

It is worth mentioning an interesting interpretation of the Schmid Law, due to Ball et al. [21, 22], to the effect that it is equivalent to metastability among linear maps, *at least in the case where K consists of two wells.*

(4.16) Proposition. *With the notation of Theorem* 4.14 *with $K = \mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2$, the mapping y_σ is a local minimiser of I_σ among all maps $y \in \mathscr{A}$ such that $Dy =$ constant if and only if $\sigma \leq \sigma_{Sch}$.*

The key observation lies in the following

(4.17) Lemma. *With the notation of Theorem* 4.14 *with $K = \mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2$, let furthermore $B_1(\sigma), B_2(\sigma) \in \mathrm{SO}(3)U_2$ denote the two twins of $A(\sigma)$ on* $\mathrm{SO}(3)U_2$, i.e.,

$$\mathrm{rank}\,(A(\sigma) - B_i(\sigma)) = 1\,, \quad i = 1, 2.$$

Let us fix $\sigma > \sigma_0$ such that

$$-\langle T(\sigma), A(\sigma)\rangle < -\langle T(\sigma), B_i(\sigma)\rangle\,, \quad i = 1, 2. \tag{4.30}$$

Then there exists a $\delta > 0$ such that, for every $A(\sigma) \neq F \in K^{qc}$ with $|F - A(\sigma)| \leq \delta$, we have

$$-\langle T(\sigma), A(\sigma)\rangle < -\langle T(\sigma), F\rangle\,.$$

Remarks. This result is due to Ball et al. [21] and we sketch their proof for the convenience of the reader.

Proof of Lemma 4.17. First of all, we fix σ satisfying (4.30) and remove it from the notation. The proof relies on the following two facts, due to Ball and James [28].

(*i*) Given $0 \leq \lambda < 1$, there is a unique rotation $R_\lambda \in \mathrm{SO}(3)$, $R_\lambda \neq \mathbb{I}$, such that

$$\mathrm{rank}\,\{(\lambda B_1 + (1-\lambda)A) - R_\lambda B_1\} = 1\,.$$

Moreover, R_λ is continuous in λ and $R_0 B_1 = B_2$. By convention, we set $R_1 = \mathbb{I}$.

(*ii*) If $F \in K^{qc} = (\mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2)^{qc}$, there exist $R \in \mathrm{SO}(3)$ and $0 \leq \lambda, \mu \leq 1$ such that

$$F = R(\mu R_\lambda B_1 + (1-\mu)(\lambda B_1 + (1-\lambda)A))\,. \tag{4.31}$$

Using (4.31) we get

$$|F - A| = |\mu R_\lambda B_1 + (1-\mu)(\lambda B_1 + (1-\lambda)A) - R^t A|\,,$$

from which we deduce that $|F - A|$ is small if and only if R is close to $\mathbb{I}$, μ is near 0 and λ near 0. Now, we also have

$$\begin{aligned}\langle T, A - F\rangle &= \langle T, A - R(\mu R_\lambda B_1 + (1-\mu)(\lambda B_1 + (1-\lambda)A))\rangle \\ &= \mu\langle T, A - R R_\lambda B_1\rangle + (1-\mu)\lambda\langle T, A - R B_1\rangle + (1-\mu)(1-\lambda)\langle T, A - RA\rangle\,,\end{aligned}$$

and so each of the three terms is nonnegative if λ and μ are near 0 and R is near $\mathbb{I}$, because $R_\lambda B_1$ is near B_2. Furthermore, if $\langle T, A - F\rangle = 0$, λ, μ are near 0, and R is near $\mathbb{I}$, this implies $\lambda = \mu = 0$ and so $F = A$. □

PROOF OF PROPOSITION 4.16. Lemma 4.17 asserts that if $\sigma < \sigma_{Sch}$, then y_σ is a strict local minimiser of I_σ among all maps with constant gradient. Obviously, at $\sigma = \sigma_{Sch}$, y_σ remains a local minimiser. On the other hand, if $\sigma > \sigma_{Sch}$, it is easily checked that y_σ is no longer a local minimiser of I_σ among linear maps, completing the proof. □

We may now ask whether the Schmid Law is sharp, *i.e.*, whether it is equivalent to metastability with respect to all deformations and not only to those with constant gradients. As Ball et al. [21] discovered, this is not the case, provided Ω has a corner. For the time being, we only explain their counter-example in rather loose terms. We analyse this thoroughly in the next section. Let us assume that $\Omega = \omega \times (-h, +h)$ for some $h > 0$ and convex, bounded, open $\omega \subset \mathbb{R}^2$. Assume that there exist $\sigma_0 < \sigma < \sigma_{Sch}$, two matrices $B(\sigma), C(\sigma) \in \mathrm{SO}(3)U_2$ and $0 < \lambda < 1$ such that

$$B(\sigma) = A(\sigma) + a(\sigma) \otimes m(\sigma) \text{ and } C(\sigma) - (\lambda A(\sigma) + (1-\lambda)B(\sigma)) = b(\sigma) \otimes p(\sigma)\,,$$

for some $a(\sigma), b(\sigma), m(\sigma), p(\sigma) \in \mathbb{R}^3$, $|m(\sigma)| = |p(\sigma)| = 1$, and satisfying

$$-\langle T(\sigma), C(\sigma)\rangle < -\langle T(\sigma), A(\sigma)\rangle < -\langle T(\sigma), B(\sigma)\rangle\,,$$

see Figure 4.7 in the introduction (where $A(\sigma)$ is denoted by $R(\sigma)U_1$). From now on, fix σ and drop it from the notation. Consider the deformation whose gradient is pictured in Figure 4.10.

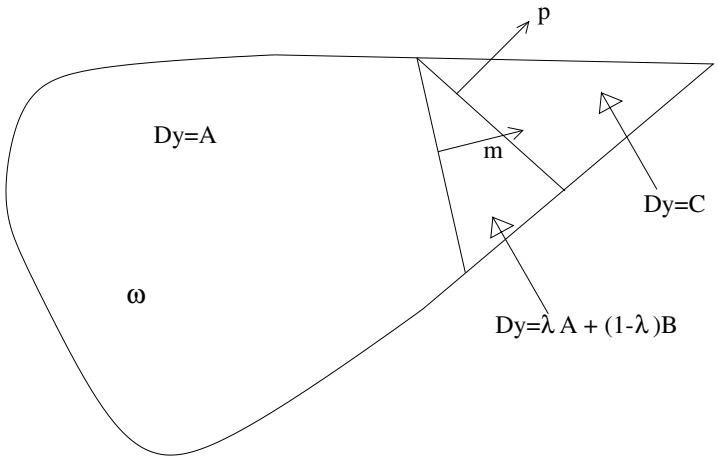


Figure 4.10: A counter-example to the Schmid Law in corner-shaped domains.

Since $-\langle T, C\rangle < -\langle T, A\rangle$, if the proportion of the set where $Dy = C$ to that where $Dy = \lambda A + (1-\lambda)B$ is well chosen (because $-\langle T, A\rangle < -\langle T, B\rangle$, we need to strike a balance between the portion where $Dy = C$ and that where $Dy = B$), the total energy associated to this deformation will be smaller than that of a homogeneous deformation $Dy_0 = A$. Also, notice that since A and $\lambda A + (1-\lambda)B$, respectively $\lambda A + (1-\lambda)B$ and C, are rank-one connected, this deformation is continuous and admissible (*i.e.*, belongs to $\mathscr{A}$). Furthermore, if we move the little cone where $Dy = \lambda A + (1-\lambda)B$ towards the apex of ω we can make sure that Dy be close to Dy_0 in L^1. So, y_0 cannot be metastable. On the other hand, if this happens, this violates the Schmid Law, because the twins of A, *e.g.*, B here, have higher energy than A.

The remaining part of this chapter is devoted to establishing whether an analogous construction involving three gradients is possible on smooth domains. We show that the answer

to that question is **no!** However, we point out that we are unable to propose another construction that would violate the Schmid Law on smooth domains. Whether or not the Schmid Law is sharp on smooth domains remains therefore unsettled; see also the final remarks of this chapter on pages 106-107.

4.4 The Schmid Law in corner-shaped domains

As explained above, we consider here a set K composed of three matrices A, B, C satisfying

$$\operatorname{rank}(A-B)=1 \quad \text{and} \quad \operatorname{rank}(\lambda A+(1-\lambda)B-C)=1\,,$$

for some $0<\lambda<1$. In other words,

$$A=B+a\otimes m\,, \quad \text{and } C=B+\lambda a\otimes m+b\otimes p\,,$$

for some vectors $a,b,m,p\in\mathbb{R}^3$, $|m|=|p|=1$. We first consider the case $A=e_1\otimes e_1$, $B=0$ and $C=\lambda e_1\otimes e_1+e_2\otimes e_2$, where e_1 and e_2 are the first two basis vectors in $\mathbb{R}^3$. We will return to the general case later (see the remark after the proof of Lemma 4.23 on page 100). Recall that we study a functional of the type

$$I(y)=\begin{cases}-\int_\Omega\langle T,Dy(x)\rangle\,dx & \text{if } Dy(x)\in K^{qc} \text{ a.e.}\\ +\infty & \text{otherwise}\end{cases}\,,$$

where T satisfies

$$-\langle T,C\rangle<-\langle T,A\rangle<-\langle T,B\rangle\,.$$

We are interested in conditions under which $y_0(x)=Ax$ is a L^1 local minimiser of I in the class

$$\mathscr{A}=\left\{y\in W^{1,1}(\Omega,\mathbb{R}^3)\,:\;\; I(y)<\infty\,,\;\int_\Omega y\,dx=0\right\}.$$

Unfortunately, we have to assume that Ω is a bounded convex open set in $\mathbb{R}^2$. Equivalently, we could assume that $\Omega=\omega\times(-h,h)$ for some $h>0$ and $\omega\subset\mathbb{R}^2$ bounded, open and convex.[40] As explained later, the full three-dimensional case remains unsettled, see the remarks on page 103. For the sake of clarity let us state precisely the 2D setting in which our theorem is established. We consider a bounded, convex, open $\Omega\subset\mathbb{R}^2$ and the functional

$$I(y)=\begin{cases}-\int_\Omega\langle T,Dy(x)\rangle\,dx & \text{if } Dy(x)\in\{A,B,C\}^{qc} \text{ a.e.}\\ +\infty & \text{otherwise}\end{cases}\,,$$

where T satisfies

$$-\langle T,C\rangle<-\langle T,A\rangle<-\langle T,B\rangle\,, \tag{4.32}$$

and where the 2×2 matrices A, B and C are given by $A=e_1\otimes e_1$, $B=0$ and $C=\lambda e_1\otimes e_1+e_2\otimes e_2$. Here $\{e_1,e_2\}$ is the canonical basis of $\mathbb{R}^2$. Finally, we consider the class

$$\mathscr{A}=\left\{y\in W^{1,1}(\Omega,\mathbb{R}^2)\,:\;\; I(y)<\infty\,,\;\int_\Omega y\,dx=0\right\},$$

[40] We leave it to the interested reader to check that our proof straightforwardly applies to the case when Ω is the cylinder $\Omega=\omega\times(-h,+h)$. The main observation is that the ratio in (4.47) below and similar ratios appearing elsewhere in the proof, do not depend on h, but solely upon the two-dimensional section ω.

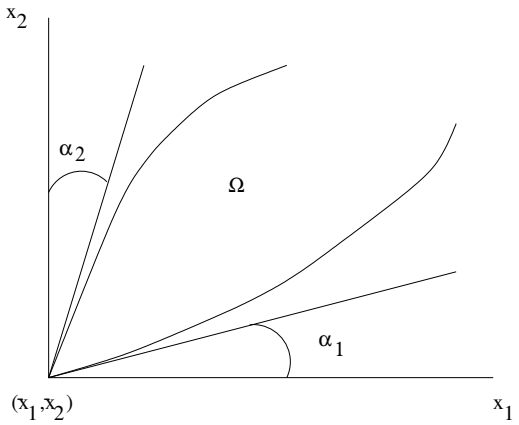


Figure 4.11: A typical set Ω as in Theorem 4.19.

and study conditions for $y_0(x) = Ax$ to be a local minimiser of I in $\mathscr{A}$. Before stating the theorem, we summarise its consequences in the following

(4.18) Claim.

(*i*) *If $\partial\Omega$ is smooth, $y_0(x) = Ax$ is a strict L^1 local minimiser of I in $\mathscr{A}$ no matter how big is the energy difference $-\langle T, A\rangle + \langle T, C\rangle > 0$.*

(*ii*) *For any choice of T, so long as it respects the inequalities* (4.32)*, there exists a convex bounded open set Ω such that $y_0(x) = Ax$ is not a L^1 local minimiser of I in $\mathscr{A}$.*

(*iii*) *Furthermore, when $\partial\Omega$ is not smooth, there are explicit necessary and sufficient conditions on the geometry of Ω for $y_0(x) = Ax$ to be a L^1 local minimiser of I in $\mathscr{A}$.*

We write $\mathscr{L}^s$ for the s-dimensional Lebesgue measure and $\sphericalangle(u, v)$ for the angle between the directions u and v, with the convention that $\sphericalangle(u, v) \in [0, \pi/2]$. Since this was our original motivation, we state conditions under which y_0 is *not* a local minimiser. We hope this is not too confusing.

(4.19) Theorem. *With the above notation, assume that $y_0(x) = Ax$ is* not *an L^1 local minimiser of I in $\mathscr{A}$. Then, there exists a point $P = (\bar{x}_1, \bar{x}_2) \in \partial\Omega$ with the following properties:*

(i) firstly, we have

$$\mathscr{L}^1(\{x_2 \,:\, (\bar{x}_1, x_2) \in \Omega\}) = 0\,,$$
$$\mathscr{L}^1(\{x_1 \,:\, (x_1, \bar{x}_2) \in \Omega\}) = 0\,.$$

In particular, there are two tangent vectors to $\partial\Omega$ at P. Let them be denoted by t_1 and t_2 in such a way that if we define

$$\alpha_1 = \sphericalangle(t_1, e_1)\,,$$
$$\alpha_2 = \sphericalangle(t_2, e_2)\,,$$

then $\alpha_1 + \alpha_2 \le \pi/2$ (see Figure 4.11*).*

(ii) The following bound holds

$$\tan\alpha_1 \tan\alpha_2 \geq \left(1 + \frac{-\langle T, A\rangle + \langle T, C\rangle}{(1-\lambda)(-\langle T, B\rangle + \langle T, A\rangle)}\right)^{-1}.$$

In particular, $\alpha_1 > 0$ *and* $\alpha_2 > 0$.

Conversely, if (i)-(ii) holds with strict inequality in (ii), then $y_0(x) = Ax$ *is not a local minimiser of* I.

Remarks. In order to illustrate the conclusion of Theorem 4.19, let us assume that $\alpha_1 = \alpha_2 = \alpha$, let $\beta = \pi/2 - 2\alpha$ and write c for the right-hand side of the inequality in (ii). Then the theorem states that y_0 is not a local minimiser if and only if $\tan^2\alpha > c$, *i.e.*, $\tan\alpha > \sqrt{c}$ so that $\beta > 0$ cannot be too big. In particular, this remark proves part (ii) of Claim 4.18 above: once $\langle T, A\rangle$, $\langle T, B\rangle$ and $\langle T, C\rangle$ are chosen, then c is fixed and one can find β and then α (and therefore a convex Ω) so that y_0 is not a local minimiser. We also note that condition (i) in the theorem prevents $\partial\Omega$ from being smooth, proving part (i) of Claim 4.18.

Before embarking upon the proof of Theorem 4.19, we need three preliminary results. The first one describes the quasiconvex hull of three matrices. It is due to Zhang [158]. Since this reference is as yet unpublished we give Zhang's proof for the convenience of the reader.

(4.20) Lemma. *Let* $A, B, C \in \mathbb{R}^{n\times n}$ *satisfy* $\operatorname{rank}(A-B) = 1$ *and* $\operatorname{rank}(\lambda A+(1-\lambda)B-C) = 1$ *for a unique* $0 < \lambda < 1$. *Then,*

$$\{A, B, C\}^{qc} = [A, B] \cup [\lambda A + (1-\lambda)B, C].$$

Proof of Lemma 4.20. This proof is based on an idea of Šveràk (private communication to Zhang). By changing dependent and independent variables, we may assume that $A = e_1 \otimes e_1$, $B = 0$ and $C = \lambda e_1 \otimes e_1 + e_2 \otimes e_2$. Denote by $M(\xi)$ the first 2×2 minor of $\xi \in \mathbb{R}^{n\times n}$ and by $\mathscr{T} \subset \mathbb{R}^{n\times n+1}$ the triangle determined by

$$(A, M(A)), \quad (B, M(B)), \quad (C, M(C)).$$

Define

$$\psi(\xi, \delta) = \operatorname{dist}((\xi, \delta), \mathscr{T})^2, \quad \xi \in \mathbb{R}^{n\times n}, \delta \in \mathbb{R}.$$

Since $\mathscr{T}$ is convex, so is ψ, and hence

$$\phi(\xi) = \psi(\xi, M(\xi))$$

is polyconvex and thus quasiconvex. Also, $\phi \geq 0$ and so $\{A, B, C\}^{qc} \subset \phi^{-1}(0)$. Observe that $\phi(\xi) = 0$ if and only if

$$\begin{aligned} \xi &= \lambda_A A + \lambda_B B + \lambda_C C, \\ M(\xi) &= \lambda_A M(A) + \lambda_B M(B) + \lambda_C M(C), \end{aligned}$$

for some $0 \leq \lambda_A, \lambda_B, \lambda_C \leq 1$, $\lambda_A + \lambda_B + \lambda_C = 1$. Combining these two equations, we get

$$M(\lambda_A A + \lambda_B B + \lambda_C C) = \lambda_A M(A) + \lambda_B M(B) + \lambda_C M(C),$$

which, substituting A, B and C, becomes

$$\lambda_C(\lambda_A + \lambda\lambda_C) = \lambda\lambda_C\,.$$

Hence $\lambda_C(\lambda_A - \lambda + \lambda\lambda_C) = 0$ and either $\lambda_C = 0$ or $\lambda_A = \lambda(1-\lambda_C)$, and in the latter case $\lambda_B = (1-\lambda)(1-\lambda_C)$. On the other hand, it is easy to see that[41] $\{A,B,C\}^{lc} = [A,B] \cup [\lambda A + (1-\lambda)B, C]$, giving

$$\{A,B,C\}^{qc} = \phi^{-1}(0) = [A,B] \cup [\lambda A + (1-\lambda)B, C]\,,$$

completing the proof. □

The following lemma, which is due to Zhang [158], explicitly describes those mappings whose gradients lie in $\{A,B,C\}^{qc}$.

(4.21) Lemma. *Let $\Omega \subset \mathbb{R}^n$ be convex, open and bounded. Let $A, B, C \in \mathbb{R}^{n\times n}$ satisfy*

$$A - B = a \otimes m\,,\quad \lambda A + (1-\lambda)B - C = b \otimes p\,,$$

for some $0 \le \lambda \le 1$ and $a, b, m, p \in \mathbb{R}^n$, $|m| = |p| = 1$. Then, if a mapping $y \in W^{1,\infty}(\Omega, \mathbb{R}^n)$ satisfies

$$Dy \in \{A,B,C\}^{qc} \quad \text{a.e.}$$

i.e.,

$$Dy(x) = \lambda_A(x)A + \lambda_B(x)B + \lambda_C(x)C\,,$$

for some measurable $0 \le \lambda_A(x), \lambda_B(x), \lambda_C(x) \le 1$, $\lambda_A(x) + \lambda_B(x) + \lambda_C(x) = 1$ a.e. then there exist two measurable, non-negative, bounded functions of the real line, ϕ and ψ such that Ω may be decomposed as (see Figure 4.12)

$$\Omega = \Omega^C_{A,B} \cup \Omega^\lambda_{A,B} \cup \Omega_{A,B}\,,$$

with

$$\begin{aligned}
\Omega^C_{A,B} &= \{x \in \Omega :\ \lambda_C(x) > 0\}\,,\\
\Omega^\lambda_{A,B} &= \{x \in \Omega :\ \lambda_C(x) = 0 \text{ and there exists a Lebesgue point}\\
&\qquad\qquad x' \text{ of } \Omega^C_{A,B} \text{ such that } \langle x' - x, m\rangle = 0\}\,,\\
\Omega_{A,B} &= \Omega \setminus (\Omega^C_{A,B} \cup \Omega^\lambda_{A,B})\,,
\end{aligned}$$

so that

(i) $\lambda_C(x) = \psi(\langle x, p\rangle)$, $\lambda_A(x) = \lambda(1-\lambda_C(x))$ *and* $\lambda_B(x) = (1-\lambda)(1-\lambda_C(x))$ *on* $\Omega^C_{A,B}$,

(ii) $\lambda_C(x) = 0$, $\lambda_A(x) = \lambda$, $\lambda_B(x) = 1-\lambda$ *on* $\Omega^\lambda_{A,B}$,

(iii) $\lambda_C(x) = 0$, $\lambda_A(x) = \phi(\langle x, m\rangle)$, $\lambda_B(x) = 1 - \lambda_A(x)$ *on* $\Omega_{A,B}$.

Proof of Lemma 4.21. Without loss of generality, we may assume that $B = 0$, $A = e_1 \otimes e_1$ and $C = \lambda e_1 \otimes e_1 + e_2 \otimes e_2$.

[41] The *lamination convex hull* K^{lc} of K is defined as the smallest set containing K stable under the addition of rank-one segments. See Chapter 2 for a precise definition.

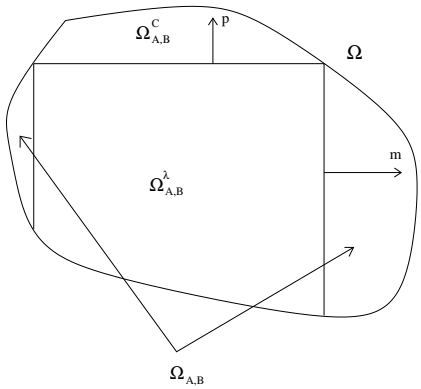


Figure 4.12: A set Ω and its decomposition $\Omega^C_{A,B} \cup \Omega^\lambda_{A,B} \cup \Omega_{A,B}$ as in Lemma 4.21.

Observe that

$$\begin{aligned} Dy(x) &= \lambda_A(x)A + \lambda_B(x)B + \lambda_C(x)C \\ &= (\lambda_A(x) + \lambda\lambda_C(x))e_1 \otimes e_1 + \lambda_C(x)e_2 \otimes e_2\,, \end{aligned}$$

and so, if $Dy(x) \in [\lambda A + (1-\lambda)B, C]$ then

$$\lambda\lambda_C(x) + \lambda_A(x) = \lambda\,, \tag{4.33}$$

because any matrix in $[\lambda A + (1-\lambda)B, C]$ is of the form $\lambda e_1 \otimes e_1 + \alpha e_2 \otimes e_2$, for some α. Writing the condition that the curl of a gradient vanishes, we get

$$\begin{aligned} \frac{\partial}{\partial x_i}(\lambda_A(x) + \lambda\lambda_C(x)) = 0 \ \text{ in } \mathscr{D}'(\Omega) \text{ for every } i > 1, \\ \frac{\partial}{\partial x_j}(\lambda_C(x)) = 0 \ \text{ in } \mathscr{D}'(\Omega) \text{ for every } j \neq 2. \end{aligned} \tag{4.34}$$

Since Ω is convex, we can solve these equations *globally* and find two functions $\phi, \psi \in \mathrm{L}^\infty(\mathbb{R})$ such that

$$\begin{aligned} \lambda_A(x) + \lambda\lambda_C(x) &= \phi(\langle x, e_1\rangle)\,, \\ \lambda_C(x) &= \psi(\langle x, e_2\rangle)\,. \end{aligned} \tag{4.35}$$

Let us decompose $\Omega = \Omega' \cup \Omega''$ with

$$\begin{aligned} \Omega' &= \{x \in \Omega \ : \ \ \psi(\langle x, e_2\rangle) = 0\}\,, \\ \Omega'' &= \{x \in \Omega \ : \ \ \psi(\langle x, e_2\rangle) > 0\}\,. \end{aligned}$$

On Ω', $\psi = 0$ so that $\lambda_C(x) = 0$, and $\lambda_A(x) = \phi(\langle x, e_1\rangle)$ and $\lambda_B(x) = 1 - \phi(\langle x, e_1\rangle)$, while on Ω'',

$$\lambda_A(x) + \lambda\lambda_C(x) = \phi(\langle x, e_1\rangle) = \lambda\,, \tag{4.36}$$

and so

$$\lambda_C(x) = \psi(\langle x, e_2\rangle)\,, \ \ \lambda_A(x) = \lambda(1 - \lambda_C(x))\,, \ \ \lambda_B(x) = (1-\lambda)(1 - \lambda_C(x))\,.$$

Furthermore, if a Lebesgue point $x \in \Omega'$ is such that there exists a Lebesgue point $x'' \in \Omega''$ with $\langle x - x'', e_1\rangle = 0$, then

$$\lambda_C(x) = 0\,, \ \ \lambda_A(x) = \phi(\langle x, e_1\rangle) = \phi(\langle x'', e_1\rangle) = \lambda\,,$$

by (4.36). Thus, $\Omega' = \Omega^{\lambda}_{A,B} \cup \Omega_{A,B}$, as stated. Denoting Ω'' by $\Omega^{C}_{A,B}$ completes the proof. □

The next lemma is elementary.

(4.22) Lemma. *Let $f : I \subset \mathbb{R} \to \mathbb{R}$ be continuous and positive on I, an open, bounded interval. Let E^ε be a family of measurable subsets of I. Assume*

$$\int_{E^\varepsilon} f(s)\, ds \to 0 \ \text{ as } \varepsilon \to 0.$$

Then, $\mathscr{L}^1(E^\varepsilon) \to 0$ as $\varepsilon \to 0$.

Proof of Lemma 4.22. Assume without loss of generality that $I = (a, b)$ for some finite $a < b$. Fix $\delta > 0$, and let

$$m_\delta = \min_{a+\delta \le s \le b-\delta} f(s)\,.$$

Since f is continuous on (a, b) and positive, m_δ is well-defined and positive. Then,

$$\int_{E^\varepsilon} f(s)\, ds \ge \int_{E^\varepsilon \cap [a+\delta, b-\delta]} f(s)\, ds \ge m_\delta\, \mathscr{L}^1(E^\varepsilon \cap [a+\delta, b-\delta])\,.$$

Passing to the limit, we get

$$\mathscr{L}^1(E^\varepsilon \cap [a+\delta, b-\delta]) \to 0 \ \text{ as } \varepsilon \to 0.$$

The arbitrariness of δ completes the proof. □

We are now in a position to prove Theorem 4.19.

Proof of Theorem 4.19. **First part (Necessity).** This is the core of the proof and is divided into four steps, summarised below.

> *First step.* We replace arbitrary competing functions by simpler ones and thus transform the problem into a measure-theoretic one.
>
> *Second step.* We show that there exists a point $P = (\bar{x}_1, \bar{x}_2) \in \partial\Omega$ satisfying (i).
>
> *Third step.* We then rule out the possibility that the tangents be parallel to e_1 or e_2, *i.e.*, we show that $\alpha_1 > 0$, $\alpha_2 > 0$.
>
> *Fourth step.* We finally derive condition (ii).

First step. Assume that y_0 is not a L^1 local minimiser. Then, using Proposition 4.11 and Example 4.9, there exists a sequence y^ε such that

$$\begin{aligned} &I(y^\varepsilon) < I(y_0)\,, \\ &Dy^\varepsilon \to Dy_0 \text{ in } L^1 \text{ as } \varepsilon \to 0\,, \\ &Dy^\varepsilon(x) \in \{A, B, C\}^{qc} \text{ a.e.} \end{aligned} \tag{4.37}$$

The goal of this first step is to replace y^ε by another sequence z^ε, enjoying the same properties as, but 'structurally' simpler than, y^ε.

Let us consider first any map y whose gradient lies in $\{A, B, C\}^{qc}$,

$$Dy(x) = \lambda_A(x)A + \lambda_B(x)B + \lambda_C(x)C = \lambda_A(x)A + (1 - \lambda_A(x) - \lambda_C(x))B + \lambda_C(x)C\,.$$

Observe that

$$\begin{aligned} \|Dy - A\|_{L^1} &= \int_\Omega |(\lambda_A - 1)A + (1 - \lambda_A - \lambda_C)B + \lambda_C C|\, dx \\ &= \int_\Omega \sqrt{\lambda_C^2 + (\lambda\lambda_C - 1 + \lambda_A)^2}\, dx \\ &= \int_{\Omega^C_{A,B}} \sqrt{\lambda_C^2 + (1-\lambda)^2}\, dx + \int_{\Omega^\lambda_{A,B}} 1 - \lambda\, dx + \int_{\Omega_{A,B}} 1 - \lambda_A\, dx\,, \end{aligned} \tag{4.38}$$

where we have used Lemma 4.21. On the other hand,

$$\begin{aligned} I(y) &= -\int_\Omega \lambda_A\langle T, A\rangle + (1 - \lambda_A - \lambda_C)\langle T, B\rangle + \lambda_C\langle T, C\rangle\, dx \\ &= -\langle T, A\rangle \left\{ \int_{\Omega^C_{A,B}} \lambda(1 - \lambda_C)dx + \int_{\Omega^\lambda_{A,B}} \lambda\, dx + \int_{\Omega_{A,B}} \lambda_A\, dx\,, \right\} \\ &\quad - \langle T, B\rangle \left\{ \int_{\Omega^C_{A,B}} (1-\lambda)(1-\lambda_C)\, dx + \int_{\Omega^\lambda_{A,B}} 1 - \lambda\, dx + \int_{\Omega_{A,B}} 1 - \lambda_A\, dx \right\} \\ &\quad - \langle T, C\rangle \int_{\Omega^C_{A,B}} \lambda_C\, dx\,. \end{aligned}$$

Define now $z(x)$ from $y(x)$ by setting

$$\begin{aligned} \lambda_C &= 1 \ \text{ on } \Omega^C_{A,B}\,, \\ \lambda_A &= 1 \ \text{ on } \Omega_{A,B}\,. \end{aligned}$$

More precisely, $z : \Omega \to \mathbb{R}^2$ is defined by

$$z(x) = \begin{cases} Ax & \text{on } \Omega_{A,B} \\ (\lambda A + (1-\lambda)B)x & \text{on } \Omega^\lambda_{A,B} \\ Cx & \text{on } \Omega^C_{A,B} \end{cases},$$

and $\Omega_{A,B}$, $\Omega^\lambda_{A,B}$ and $\Omega^C_{A,B}$ are the sets associated with y. Since the interfaces between $\Omega_{A,B}$ and $\Omega^\lambda_{A,B}$ on the one hand, and between $\Omega^\lambda_{A,B}$ and $\Omega^C_{A,B}$ on the other, are planar (see Lemma 4.21 and its proof), and because A and $\lambda A + (1-\lambda)B$ on the one hand, and $\lambda A + (1-\lambda)B$ and C on the other, are rank-one connected, $z \in W^{1,\infty}(\Omega, \mathbb{R}^2)$. Then,

$$\begin{aligned} I(z) = &-\langle T, A\rangle\big(\lambda\mathscr{L}^2(\Omega^\lambda_{A,B}) + \mathscr{L}^2(\Omega_{A,B})\big) \\ &- \langle T, B\rangle(1-\lambda)\mathscr{L}^2(\Omega^\lambda_{A,B}) - \langle T, C\rangle\mathscr{L}^2(\Omega^C_{A,B})\,, \end{aligned} \tag{4.39}$$

while

$$\|Dz - A\|_{L^1} = \sqrt{1 + (1-\lambda)^2}\mathscr{L}^2(\Omega^C_{A,B}) + (1-\lambda)\mathscr{L}^2(\Omega^\lambda_{A,B})\,. \tag{4.40}$$

Thus,

$$\begin{aligned}\|Dz-A\|_{L^1} &= \|Dy-A\|_{L^1} - \int_{\Omega^C_{A,B}} \sqrt{\lambda_C^2+(1-\lambda)^2}\,dx - \int_{\Omega_{A,B}} 1-\lambda_A\,dx \\ &\quad + \sqrt{1+(1-\lambda)^2}\mathscr{L}^2(\Omega^C_{A,B}) \\ &\le \|Dy-A\|_{L^1} + \sqrt{1+(1-\lambda)^2}\mathscr{L}^2(\Omega^C_{A,B})\,,\end{aligned} \tag{4.41}$$

and

$$I(z) \le I(y)\,.$$

In this manner, by replacing y^ε by z^ε, we may assume that the sequence y^ε in (4.37) satisfies in addition

$$\lambda_C(x) = \begin{cases} 1 & \text{on } \Omega^C_{A,B} \\ 0 & \text{elsewhere} \end{cases},$$

$$\lambda_A(x) = \begin{cases} 0 & \text{on } \Omega^C_{A,B} \\ \lambda & \text{on } \Omega^\lambda_{A,B} \\ 1 & \text{elsewhere} \end{cases}.$$

Let us denote the sets $\Omega^C_{A,B}$, $\Omega^\lambda_{A,B}$ and $\Omega_{A,B}$ associated to the sequence y^ε by Ω'_ε, Ω''_ε and Ω'''_ε, respectively. As (4.40) shows, the condition $\|Dy^\varepsilon - A\|_{L^1} \to 0$ implies

$$\begin{aligned}\mathscr{L}^2(\Omega'_\varepsilon) &\to 0 \ \text{ as } \varepsilon \to 0, \\ \mathscr{L}^2(\Omega''_\varepsilon) &\to 0 \ \text{ as } \varepsilon \to 0.\end{aligned} \tag{4.42}$$

Furthermore, the condition that $I(y^\varepsilon) < I(Ax)$ is equivalent to – see (4.39) –

$$-\langle T,A\rangle\big(\lambda\mathscr{L}^2(\Omega''_\varepsilon)+\mathscr{L}^2(\Omega'''_\varepsilon)\big) - \langle T,B\rangle(1-\lambda)\mathscr{L}^2(\Omega''_\varepsilon) - \langle T,C\rangle\mathscr{L}^2(\Omega'_\varepsilon) < -\langle T,A\rangle\mathscr{L}^2(\Omega)\,,$$

i.e.,

$$-\langle T,A\rangle\big(\lambda\mathscr{L}^2(\Omega''_\varepsilon)-\mathscr{L}^2(\Omega'_\varepsilon)-\mathscr{L}^2(\Omega''_\varepsilon)\big) - \langle T,B\rangle(1-\lambda)\mathscr{L}^2(\Omega''_\varepsilon) - \langle T,C\rangle\mathscr{L}^2(\Omega'_\varepsilon) < 0\,.$$

In other words,

$$\mathscr{L}^2(\Omega'_\varepsilon)\big(-\langle T,C\rangle+\langle T,A\rangle\big) + (\lambda-1)\mathscr{L}^2(\Omega''_\varepsilon)\big(-\langle T,A\rangle+\langle T,B\rangle\big) < 0\,.$$

Hence,

$$\frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Omega''_\varepsilon)} > \frac{(1-\lambda)(-\langle T,B\rangle+\langle T,A\rangle)}{-\langle T,A\rangle+\langle T,C\rangle} \quad \text{for every } \varepsilon>0\,, \tag{4.43}$$

or, equivalently

$$\frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Omega'_\varepsilon\cup\Omega''_\varepsilon)} > c = \left(1+\frac{-\langle T,A\rangle+\langle T,C\rangle}{(1-\lambda)(-\langle T,B\rangle+\langle T,A\rangle)}\right)^{-1}, \quad \text{for every } \varepsilon>0\,. \tag{4.44}$$

Finally, by the proof of Lemma 4.21, we may assume that there exists a sequence of measurable sets $E_\varepsilon \subset \mathbb{R}$ such that Ω'_ε and Ω''_ε are given by

$$\begin{aligned}\Omega'_\varepsilon &= \{\text{Lebesgue points of } (\mathbb{R}\times E_\varepsilon)\cap\Omega\}\,, \\ \Omega'_\varepsilon\cup\Omega''_\varepsilon &= (\pi_1(\Omega'_\varepsilon)\times\mathbb{R})\cap\Omega\,,\end{aligned}$$

where π_1 denotes the projection onto the first axis. By (4.42) and (4.44), Ω'_ε and Ω''_ε satisfy

$$\mathscr{L}^2(\Omega'_\varepsilon) \to 0\,, \tag{4.45}$$

$$\mathscr{L}^2(\Omega''_\varepsilon) \to 0\,, \tag{4.46}$$

$$\frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)} > c\,, \quad \text{for all } \varepsilon > 0, \tag{4.47}$$

where c is the right-hand side of the inequality in (ii). Intuitively, (4.45)-(4.47) can be understood as follows: Ω'_ε represents the part of Ω where the gradient C is used (which is the 'good' matrix as far as the energy is concerned) while Ω''_ε is the region where B is used (for compatibility reasons, one cannot use C without using B, as Lemma 4.21 revealed). So in order that the gradients remain close to A in L^1, both regions have to shrink while the ratio of their measures (or, equivalently, that of Ω'_ε to $\Omega'_\varepsilon \cup \Omega''_\varepsilon$) has to remain bounded so that the energy be lowered.

Second step. We want to show that (4.45)-(4.47) imply the existence of $P = (\bar{x}_1, \bar{x}_2) \in \partial\Omega$ satisfying (i). To this aim, let us define

$$f_1(x_1) = \mathscr{L}^1(\{x_2 \in \pi_2(\Omega) \,:\, (x_1, x_2) \in \Omega\})\,, \quad x_1 \in \pi_1(\Omega)\,,$$
$$f_2(x_2) = \mathscr{L}^1(\{x_1 \in \pi_1(\Omega) \,:\, (x_1, x_2) \in \Omega\})\,, \quad x_2 \in \pi_2(\Omega)\,,$$

where, as above, π_i denotes the projection onto the i^{th} axis. Extend f_i by zero outside $\pi_i(\Omega)$. We will need the following properties of f_1 and f_2. We gather them in the following lemma, and postpone its proof until after that of Theorem 4.19.

(4.23) Lemma. *Let $\Omega \subset \mathbb{R}^2$ be a convex open bounded set. Define f_1 and f_2 as above. Then,*

(i) $f_i > 0$ *on* $\pi_i(\Omega)$, $i = 1, 2$,

(ii) f_i *is concave on* $\pi_i(\Omega)$, $i = 1, 2$,

(iii) f_i *is continuous on* $\pi_i(\Omega)$, $i = 1, 2$,

(iv) $f_i = 0$ *on* $\partial\pi_i(\Omega)$.

Notice that in terms of f_1 and f_2, we have

$$\mathscr{L}^2(\Omega'_\varepsilon) = \int_{E_\varepsilon} f_2(x_2)\, dx_2\,,$$
$$\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon) = \int_{\pi_1(\Omega'_\varepsilon)} f_1(x_1)\, dx_1.$$

By (4.45), (4.46) and Lemma 4.23, we are now in a position to apply Lemma 4.22 and deduce that

$$\begin{aligned} \mathscr{L}^1(E_\varepsilon) &\to 0 \ \text{ as } \varepsilon \to 0\,, \\ \mathscr{L}^1(\pi_1(\Omega'_\varepsilon)) &\to 0 \ \text{ as } \varepsilon \to 0\,. \end{aligned} \tag{4.48}$$

Notice also that

$$\mathscr{L}^1(\pi_1(\Omega'_\varepsilon)) \geq f_2(x_2)$$

for every Lebesgue point x_2 of E_ε. Hence, by $(4.48)_2$,

$$\sup\{f_2(x_2) \,:\, x_2 \text{ Lebesgue point of } E_\varepsilon\} \to 0 \text{ as } \varepsilon \to 0\,. \tag{4.49}$$

We claim that (4.47), (4.48) and (4.49) imply that

$$\inf\{f_1(x_1) \,:\, x_1 \text{ Lebesgue point of } \pi_1(\Omega'_\varepsilon)\} \to 0 \text{ as } \varepsilon \to 0\,, \tag{4.50}$$

too. If not, we would have $f_1(x_1) > d > 0$ for every Lebesgue point of $\pi_1(\Omega'_{\varepsilon^k})$ and for some $\varepsilon^k \to 0$, and so

$$\begin{aligned}\mathscr{L}^1(\pi_1(\Omega'_{\varepsilon^k}))\mathscr{L}^1(E_{\varepsilon^k}) &\geq \sup_{x_2\in E_{\varepsilon^k}} f_2\, \mathscr{L}^1(E_{\varepsilon^k}) \geq \int_{E_{\varepsilon^k}} f_2(x_2)\,dx_2 \\ &\geq c\int_{\pi_1(\Omega'_{\varepsilon^k})} f_1(x_1)\,dx_1 > cd\mathscr{L}^1(\pi_1(\Omega'_{\varepsilon^k})) > 0\,,\end{aligned}$$

for every k, where the sup is taken over all Lebesgue points of E_{ε^k}. Dividing by $\mathscr{L}^1(\pi_1(\Omega'_{\varepsilon^k}))$ and letting $k \to \infty$, we get a contradiction. We have thus shown that

$$\begin{aligned}\mathscr{L}^1(E_\varepsilon) &\to 0\,,\\ \mathscr{L}^1(\pi_1(\Omega'_\varepsilon)) &\to 0\,,\\ \inf_{x_1\in\pi_1(\Omega'_\varepsilon)} f_1 &\to 0\,,\\ \sup_{x_2\in E_\varepsilon} f_2 &\to 0\end{aligned}$$

as $\varepsilon \to 0$, where, again, the inf and sup are taken over Lebesgue points of the relevant sets. This implies that there exists a sequence $(x_1^\varepsilon, x_2^\varepsilon) \in \bar\Omega$ such that

$$f_1(x_1^\varepsilon) \to 0\,, \quad f_2(x_2^\varepsilon) \to 0.$$

Since Ω is bounded we may assume in addition that $(x_1^\varepsilon, x_2^\varepsilon)$ converges to a point $(\bar x_1, \bar x_2) \in \bar\Omega$. By statements (i) and (iii) in Lemma 4.23 we conclude that

$$f_1(\bar x_1) = f_2(\bar x_2) = 0\,. \tag{4.51}$$

A priori, $(\bar x_1, \bar x_2) \in \bar\Omega$, but since $f_1(\bar x_1) = f_2(\bar x_2) = 0$, $(\bar x_1, \bar x_2) \in \partial\Omega$, by part (iv) of Lemma 4.23. Since Ω is convex, there are at most two such points, as pictured in Figure 4.13.



Figure 4.13: Sets Ω admitting one or two points $(\bar x_1, \bar x_2)$ satisfying (4.51).

In the event of there being two such points, there must be at least one which satisfies the hypotheses of Case (a). Indeed, suppose there are two points P_1 and P_2 satisfying (4.51), and decompose

$$\begin{aligned}\Omega'_\varepsilon &= \Omega'_{1,\varepsilon} \cup \Omega'_{2,\varepsilon}\,,\\ \Omega''_\varepsilon &= \Omega''_{1,\varepsilon} \cup \Omega''_{2,\varepsilon}\,,\end{aligned}$$

where $\Omega'_{i,\varepsilon} = \Omega'_\varepsilon \cap B(P_i, \delta)$, $i = 1, 2$, for a fixed, small, radius δ and similarly for $\Omega''_{1,\varepsilon}$. Then[42] it is easy to see that either $\{\Omega'_{1,\varepsilon}, \Omega''_{1,\varepsilon}\}$ or $\{\Omega'_{2,\varepsilon}, \Omega''_{2,\varepsilon}\}$ (or both) satisfy (4.45)-(4.47). From now on, we concentrate on one such point P.

By translation and reflection, we may assume that $(\bar{x}_1, \bar{x}_2) = (0, 0)$ and that $\bar{\Omega}$ lies in the first quadrant. Also, we may assume that all points in $\pi_1(\Omega'_\varepsilon)$ and E_ε converge to the origin.

We now parametrise $\partial\Omega$ around the origin, bearing in mind that Ω being convex provides us with valuable information. We assume to be given four functions g_1, g_2, h_1, h_2 (see Figure 4.14) satisfying

$$g_1(0) = g_2(0) = h_1(0) = h_2(0) = 0\,,$$

and g_1, h_2 convex, g_2, h_1 concave. Also, we may assume (by convexity and concavity) that

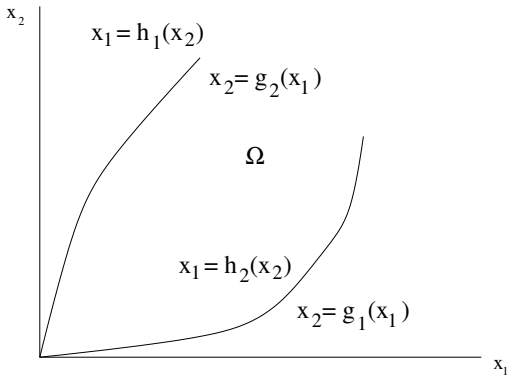


Figure 4.14: Parametrisation of $\partial\Omega$ around the origin.

the following limits exist, even if *a priori* some may be infinite,

$$\lim_{x_1\to 0^+} \frac{g_1(x_1)}{x_1}\,, \quad \lim_{x_1\to 0^+} \frac{g_2(x_1)}{x_1}\,, \quad \lim_{x_2\to 0^+} \frac{h_1(x_2)}{x_2}\,, \quad \lim_{x_2\to 0^+} \frac{h_2(x_2)}{x_2}\,.$$

Third step. We want to show that

$$\begin{aligned} &\lim_{x_1\to 0^+} \frac{g_1(x_1)}{x_1} > 0\,,\\ &\lim_{x_1\to 0^+} \frac{g_2(x_1)}{x_1} < \infty\,,\\ &\lim_{x_2\to 0^+} \frac{h_1(x_2)}{x_2} > 0\,,\\ &\lim_{x_2\to 0^+} \frac{h_2(x_2)}{x_2} < \infty\,. \end{aligned} \tag{4.52}$$

(Obviously, $(4.52)_1$ and $(4.52)_4$ on the one hand, and $(4.52)_2$ and $(4.52)_3$ on the other, are equivalent.) This implies that the tangents to $\partial\Omega$ at the origin are not parallel to the axes.

[42] Use, *e.g.*, that if $\alpha, \beta, \gamma, \delta$ are positive and satisfy

$$\frac{\alpha+\beta}{\gamma+\delta} > c\,,$$

for some $c > 0$, then either $\alpha/\gamma > c$ or $\beta/\delta > c$.

This will follow from the statement: there exist constants $\alpha, \beta > 0$ and a sequence $(x_1^\varepsilon, x_2^\varepsilon) \in \bar{\Omega}$ such that

$$0 < \alpha x_1^\varepsilon x_2^\varepsilon \le f_1(x_1^\varepsilon) f_2(x_2^\varepsilon) < \beta x_1^\varepsilon x_2^\varepsilon \quad \text{for every } \varepsilon > 0. \tag{4.53}$$

Before showing how (4.53) implies (4.52), we establish the former.

Let $x_2^\varepsilon = \sup_{\mathscr{L}(E_\varepsilon)} x_2$. Since f_2 is concave and $f_2(0) = 0$, $f_2(x_2^\varepsilon) \ge f_2(x_2)$ for every Lebesgue point of E_ε. Denote

$$l^\varepsilon = (\mathbb{R} \times \{x_2^\varepsilon\}) \cap \Omega\,,$$

and $x_1^\varepsilon = \sup_{\pi_1(l^\varepsilon)} x_1$. Notice that

$$f_2(x_2^\varepsilon) \le x_1^\varepsilon\,, \tag{4.54}$$

because $\mathscr{L}^1(l^\varepsilon) = f_2(x_2^\varepsilon)$. Hence

$$\mathscr{L}^2(\Omega'_\varepsilon) = \int_{E_\varepsilon} f_2(x_2)\, dx_2 \le x_1^\varepsilon x_2^\varepsilon\,. \tag{4.55}$$

Now, since $\pi_1(l^\varepsilon) \subset \pi_1(\Omega'_\varepsilon)$, we have

$$\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon) \ge \int_{\pi_1(l^\varepsilon)} f_1(x_1)\, dx_1 \ge \frac{1}{2} f_1(x_1^\varepsilon) \mathscr{L}^1(\pi_1(l^\varepsilon))\,, \tag{4.56}$$

since f_1 is concave and positive. But $\mathscr{L}^1(\pi_1(l^\varepsilon)) = f_2(x_2^\varepsilon)$. Hence, combining (4.47), (4.54), (4.55) and (4.56) we get

$$\frac{2x_1^\varepsilon x_2^\varepsilon}{f_1(x_1^\varepsilon) f_2(x_2^\varepsilon)} > c > 0\,.$$

In other words, there exists a sequence $(x_1^\varepsilon, x_2^\varepsilon) \in \bar{\Omega}$ such that

$$f_1(x_1^\varepsilon) f_2(x_2^\varepsilon) < \beta x_1^\varepsilon x_2^\varepsilon \quad \text{for every } \varepsilon > 0.$$

Also, since f_1 and f_2 are concave and $f_1(0) = f_2(0) = 0$, we have

$$f_i(x_i^\varepsilon \bar{x}_i + (1 - x_i^\varepsilon) \cdot 0) \ge x_i^\varepsilon f_i(\bar{x}_i) > 0\,, \tag{4.57}$$

for some $\bar{x}_i \in \pi_i(\Omega)$, $i = 1, 2$. (Here we have assumed that $x_i^\varepsilon < 1$ which can clearly be achieved by taking $\varepsilon > 0$ small enough.) Hence, we have obtained (4.53). Let us now prove (4.52). Recall that we may assume

$$\begin{aligned}
&\lim_{x_1 \to 0^+} \frac{g_1(x_1)}{x_1} = \inf_{x_1 > 0} \frac{g_1(x_1)}{x_1} \ge 0\,,\\
&\lim_{x_1 \to 0^+} \frac{g_1(x_1)}{x_1} < \infty\,,\\
&\lim_{x_1 \to 0^+} \frac{g_2(x_1)}{x_1} = \sup_{x_1 > 0} \frac{g_2(x_1)}{x_1} \le \infty\,,\\
&\lim_{x_1 \to 0^+} \frac{g_2(x_1)}{x_1} > 0\,,
\end{aligned}$$

where the equalities come from the fact that g_1 is convex and g_2 concave. Similar conditions hold for h_1 and h_2. Furthermore, since g_1 is convex, there exists $0 < \gamma < \infty$ such that

for small x_1, $\sup g_1(x_1)/x_1 \leq \gamma$. Similarly, there exists $0 < \delta < \infty$ such that for small x_2, $\sup h_1(x_2)/x_2 \leq \delta$. Now, since $f_1(x_1) = g_2(x_1) - g_1(x_1)$, we have

$$\frac{g_2(x_1)}{x_1} - \gamma \leq \frac{f_1(x_1)}{x_1}\,.$$

Using (4.57), this implies

$$\left(\frac{g_2(x_1)}{x_1} - \gamma\right) C \leq \frac{f_1(x_1)}{x_1}\,\frac{f_2(x_2)}{x_2}\,,$$

for some constant $C > 0$. But this and (4.53) imply that

$$\lim_{x_1 \to 0^+} \frac{g_2(x_1)}{x_1} = \sup_{x_1 > 0} \frac{g_2(x_1)}{x_1} < \infty\,,$$

as desired. Hence $(4.52)_2$ and $(4.52)_3$ are proved. One gets $(4.52)_1$ and $(4.52)_4$ similarly, by working on h_2 rather than on g_2 as we just did. We may thus assume that the two tangents to $\partial\Omega$ at the origin are not parallel to the axes. In particular, the angles α_1 and α_2 defined above are positive. The fourth step aims to show that $\tan\alpha_1 \tan\alpha_2 \geq c$.

Fourth step. We finally prove (ii). This is done in two stages. Firstly, the estimate (ii) is easily obtained if Ω is (locally) a cone around the origin and if we know that the α_i are positive. For a general Ω, we use again the fact that $\alpha_i > 0$ and blow $\partial\Omega$ up around the origin to get the estimate.

Recall that

$$\begin{aligned} \Omega'_\varepsilon &= \{\text{Lebesgue points of } (\mathbb{R} \times E_\varepsilon) \cap \Omega\}\,, \\ \Omega'_\varepsilon \cup \Omega''_\varepsilon &= (\pi_1(\Omega'_\varepsilon) \times \mathbb{R}) \cap \Omega\,. \end{aligned}$$

Let $I_\varepsilon = (0, \sup_{\mathscr{L}(E_\varepsilon)} x_2)$, and denote $\tilde{\Omega}'_\varepsilon = (\mathbb{R} \times I_\varepsilon) \cap \Omega$. Clearly, $\Omega'_\varepsilon \subset \tilde{\Omega}'_\varepsilon$. Also, we have

$$\Omega''_\varepsilon \supset (\pi_1(\tilde{\Omega}'_\varepsilon) \times \mathbb{R}) \cap \Omega \cap \{(x_1, x_2) \,:\, x_2 \geq \sup_{\mathscr{L}(E_\varepsilon)} x_2\}\,. \tag{4.58}$$

Denote by $\tilde{\Omega}''_\varepsilon$ the right-hand side of (4.58). Then, by (4.43),

$$0 < \tilde{c} < \frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Omega''_\varepsilon)} \leq \frac{\mathscr{L}^2(\tilde{\Omega}'_\varepsilon)}{\mathscr{L}^2(\tilde{\Omega}''_\varepsilon)}\,,$$

where $\tilde{c}$ stands for the right-hand side of (4.43). Hence,

$$\frac{\mathscr{L}^2(\tilde{\Omega}'_\varepsilon)}{\mathscr{L}^2(\tilde{\Omega}'_\varepsilon \cup \tilde{\Omega}''_\varepsilon)} > c > 0\,,$$

for every $\varepsilon > 0$, where c is as in (4.44). To lighten the notation, we simply write Ω'_ε and Ω''_ε in place of $\tilde{\Omega}'_\varepsilon$ and $\tilde{\Omega}''_\varepsilon$, respectively. Now let Λ be the cone with apex at the origin and generated by the two tangents to $\partial\Omega$ at the origin – see Figure 4.15. Furthermore, define

$$\begin{aligned} \Lambda'_\varepsilon &= (\mathbb{R} \times I_\varepsilon) \cap \Lambda\,, \\ \Lambda'_\varepsilon \cup \Lambda''_\varepsilon &= (\pi_1(\Lambda'_\varepsilon) \times \mathbb{R}) \cap \Lambda\,. \end{aligned}$$

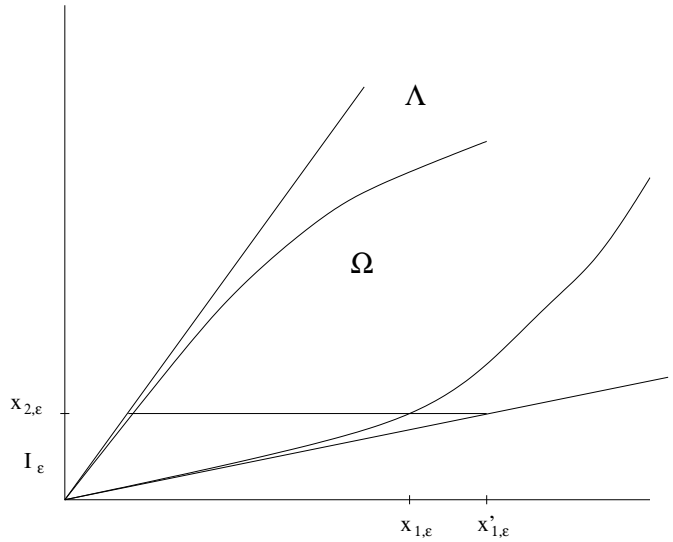


Figure 4.15: The sets Λ and Ω – see text.

Let us record the following two facts,

$$\begin{aligned} \frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon)} &\longrightarrow 1 \quad \text{as } \varepsilon \to 0\,, \\ \frac{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)} &\longrightarrow 1 \quad \text{as } \varepsilon \to 0\,. \end{aligned} \tag{4.59}$$

Proof of $(4.59)_1$. First observe that $\Omega'_\varepsilon \subset \Lambda'_\varepsilon$. Let us denote

$$\begin{aligned} f_1^\Omega(x_1) &= \mathscr{L}^1(\{x_2 \in \pi_2(\Omega) \,:\, (x_1,x_2) \in \Omega\})\,, \quad x_1 \in \pi_1(\Omega)\,, \\ f_1^\Lambda(x_1) &= \mathscr{L}^1(\{x_2 \in \pi_2(\Lambda) \,:\, (x_1,x_2) \in \Lambda\})\,, \quad x_1 \in \pi_1(\Lambda)\,, \\ f_2^\Omega(x_2) &= \mathscr{L}^1(\{x_1 \in \pi_1(\Omega) \,:\, (x_1,x_2) \in \Omega\})\,, \quad x_2 \in \pi_2(\Omega)\,, \\ f_2^\Lambda(x_2) &= \mathscr{L}^1(\{x_1 \in \pi_1(\Lambda) \,:\, (x_1,x_2) \in \Lambda\})\,, \quad x_2 \in \pi_2(\Lambda)\,. \end{aligned}$$

With these notations, we have

$$\begin{aligned} \mathscr{L}^2(\Omega'_\varepsilon) &= \int_{I_\varepsilon} f_2^\Omega(x_2)\,dx_2 = \int_{I_\varepsilon} (h_2(x_2) - h_1(x_2))\,dx_2 = \int_{I_\varepsilon} \frac{h_2(x_2)-h_1(x_2)}{x_2} x_2\,dx_2\,, \\ \mathscr{L}^2(\Lambda'_\varepsilon) &= \int_{I_\varepsilon} f_2^\Lambda(x_2)\,dx_2 = \int_{I_\varepsilon} (h_2'(0) - h_1'(0)) x_2\,dx_2 = (h_2'(0)-h_1'(0)) \int_{I_\varepsilon} x_2\,dx_2\,, \end{aligned}$$

where $h_i'(0)$ denotes the right-hand derivative of h_i at the origin, which is well defined by convexity and concavity, respectively, of these functions. Furthermore, for any $\delta > 0$,

$$\left| \frac{h_2(x_2)-h_1(x_2)}{x_2} - (h_2'(0)-h_1'(0)) \right| \le \delta\,,$$

whenever y is small enough. Thus,

$$1 \ge \frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon)} \ge \frac{h_2'(0)-h_1'(0)-\delta}{h_2'(0)-h_1'(0)} \cdot \frac{\int_{I_\varepsilon} x_2\,dx_2}{\int_{I_\varepsilon} x_2\,dx_2} = 1 - \frac{\delta}{h_2'(0)-h_1'(0)}\,,$$

for every $\varepsilon > 0$ small enough. Passing to the limit in ε and using the arbitrariness of δ, we get $(4.59)_1$.

Proof of $(4.59)_2$. We will use here the special form of I_ε. As seen above, we have

$$\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon) = \int_{\pi_1(\Omega'_\varepsilon)} f_1^\Omega(x_1)\,dx_1 = \int_0^{x_{1,\varepsilon}} (g_2(x_1) - g_1(x_1))\,dx_1\,,$$

because $\pi_1(\Omega'_\varepsilon) = (0, x_{1,\varepsilon})$, where (see Figure 4.15), $x_{1,\varepsilon} = \sup\{x_1 \,:\, x \in \pi_1((\mathbb{R} \times I_\varepsilon) \cap \Omega)\}$. Similarly,

$$\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon) = \int_{\pi_1(\Lambda'_\varepsilon)} f_1^\Lambda(x_1)\,dx_1 = \int_0^{x'_{1,\varepsilon}} (g_2'(0) - g_1'(0))x_1\,dx_1\,,$$

where $x'_{1,\varepsilon} = \sup\{x_1 \,:\, x \in \pi_1((\mathbb{R} \times I_\varepsilon) \cap \Lambda)\}$, see Figure 4.15. As in the case of the h_i, $g_i'(0)$ denote the right-hand derivative of g_i, are well defined by convexity and concavity, and for $\delta_1 > 0$, we have

$$\left| \frac{g_2(x_1) - g_1(x_1)}{x_1} - (g_2'(0) - h_1'(0)) \right| \le \delta_1\,,$$

whenever x_1 is small enough. Hence,

$$\frac{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)} \ge \frac{g_2'(0) - g_1'(0) - \delta_1}{g_2'(0) - g_1'(0)} \cdot \frac{\int_0^{x_{1,\varepsilon}} x_1\,dx_1}{\int_0^{x'_{1,\varepsilon}} x_1\,dx_1}\,,$$

whenever $\varepsilon > 0$ is small enough. Now $x_{1,\varepsilon} = h_2(x_{2,\varepsilon})$ for some $x_{2,\varepsilon}$ and $x'_{1,\varepsilon} = h_2'(0)x_{2,\varepsilon}$ (see Figure 4.15). Thus,

$$\frac{\int_0^{x_{1,\varepsilon}} x_1\,dx_1}{\int_0^{x'_{1,\varepsilon}} x_1\,dx_1} = \left(\frac{h_2(x_{2,\varepsilon})}{h_2'(0)x_{2,\varepsilon}}\right)^2 \ge \left(\frac{h_2'(0) - \delta_2}{h_2'(0)}\right)^2\,,$$

for some $\delta_2 > 0$, if $x_{2,\varepsilon}$ is small enough. We thus get

$$1 \ge \frac{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)} \ge \frac{g_2'(0) - g_1'(0) - \delta_1}{g_2'(0) - g_1'(0)} \cdot \left(\frac{h_2'(0) - \delta_2}{h_2'(0)}\right)^2\,,$$

whenever $\varepsilon > 0$ is small enough. Passing to the limit in $\varepsilon > 0$ and then in δ_1 and δ_2, we have established $(4.59)_2$.

We now need to compute the ratio $\mathscr{L}^2(\Lambda'_\varepsilon)/\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)$. We have

$$\mathscr{L}^2(\Lambda'_\varepsilon) = \int_0^{x_{2,\varepsilon}} (h_2'(0) - h_1'(0))x_2\,dx_2 = \frac{1}{2}(h_2'(0) - h_1'(0))(x_{2,\varepsilon})^2\,,$$

$$\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon) = \int_0^{x'_{1,\varepsilon}} (g_2'(0) - g_1'(0))x_1\,dx_1 = \frac{1}{2}(h_2'(0) - h_1'(0))(x'_{1,\varepsilon})^2\,,$$

so that

$$\frac{\mathscr{L}^2(\Lambda'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)} = \frac{h_2'(0) - h_1'(0)}{g_2'(0) - g_1'(0)} \cdot \frac{x_{2,\varepsilon}^2}{(x'_{1,\varepsilon})^2}\,.$$

But

$$h_1'(0) = \tan\alpha_2\,,\quad h_2'(0) = \frac{1}{\tan\alpha_1}\,,$$

$$g_1'(0) = \tan\alpha_1\,,\quad g_2'(0) = \frac{1}{\tan\alpha_2}\,,$$

$$x_{2,\varepsilon} = \tan\alpha_1 x'_{1,\varepsilon}\,,$$

so that

$$\frac{\mathscr{L}^2(\Lambda'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)} = \frac{\frac{1}{\tan\alpha_1} - \tan\alpha_2}{\frac{1}{\tan\alpha_2} - \tan\alpha_1} \cdot \tan^2\alpha_1 = \tan\alpha_1 \tan\alpha_2 \,. \tag{4.60}$$

Choose $\delta > 0$. Combining (4.47), (4.59) and (4.60), we can write

$$0 < c < \frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)} = \frac{\mathscr{L}^2(\Lambda'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)} \cdot \frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon)} \cdot \frac{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)}{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)} \leq \tan\alpha_1 \tan\alpha_2 \,(1+\delta)\,,$$

for all $\varepsilon > 0$ small enough. Passing to the limit in ε, we finally get (ii), since $\delta > 0$ is arbitrary.

Second part (Sufficiency). Assume $\tan\alpha_1 \tan\alpha_2 > c$. The first step above shows that if we can construct a sequence $(\Omega'_\varepsilon, \Omega''_\varepsilon)$ (defined as above, with $E_\varepsilon = (0, \varepsilon)$, say) satisfying (4.45)-(4.47), then we will have proved that y_0 is not a local minimiser. By (4.59), for every $\delta > 0$, we have

$$\frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon)} \cdot \frac{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)}{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)} \geq (1-\delta)\,,$$

if $\varepsilon > 0$ is small enough. Choose δ sufficiently small so that

$$\tan\alpha_1 \tan\alpha_2 (1-\delta) > c\,.$$

Then,

$$\frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)} = \frac{\mathscr{L}^2(\Lambda'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)} \cdot \frac{\mathscr{L}^2(\Omega'_\varepsilon)}{\mathscr{L}^2(\Lambda'_\varepsilon)} \cdot \frac{\mathscr{L}^2(\Lambda'_\varepsilon \cup \Lambda''_\varepsilon)}{\mathscr{L}^2(\Omega'_\varepsilon \cup \Omega''_\varepsilon)} \geq \tan\alpha_1 \tan\alpha_2 \,(1-\delta) > c > 0\,,$$

for every $\varepsilon > 0$ sufficiently small, as desired. □

Remark. Observe that if equality holds in (ii), then y_0 may well be a local minimiser. Indeed, if $\tan\alpha_1 \tan\alpha_2 = c$, we see that the argument used in the second part of the proof of Theorem 4.19 will not work: if for example $\Omega = \Lambda$ is a cone, then the energy cannot be lowered, only equalled, and thus, y_0 remains a local minimiser in this case.

We now turn to the proof of Lemma 4.23, which we left aside earlier.

Proof of Lemma 4.23. Assertions (i) and (iv) are obvious. Furthermore, (iii) follows from (ii), since a real-valued concave function is locally Lipschitz, see [54]. To prove (ii), fix $x_{i,1}, x_{i,2} \in \pi_i(\Omega)$ and $0 \leq \lambda \leq 1$. We want to show that

$$f_i(\lambda x_{i,1} + (1-\lambda)x_{i,2}) \geq \lambda f_i(x_{i,1}) + (1-\lambda) f_i(x_{i,2})\,. \tag{4.61}$$

Let $P_{1,1}, P_{1,2}, P_{2,1}, P_{2,2} \in \bar{\Omega}$ satisfy

$$f_i(x_{i,1}) = \mathscr{L}^1([P_{1,1}, P_{2,1}])\,,$$
$$f_i(x_{i,2}) = \mathscr{L}^1([P_{2,1}, P_{2,2}])\,.$$

Since Ω is convex, the quadrilateral defined by $P_{1,1}, P_{1,2}, P_{2,1}, P_{2,2}$ is contained in Ω. But this implies (4.61). The proof is finished. □

Remark. We now turn to the general case where $a \neq m \neq e_1$ and $b \neq p \neq e_2$. Unlike the proofs of Lemmas 4.20 and 4.21, the conclusion of Theorem 4.19, more particularly condition

(ii), is not invariant under non-orthogonal change of variables. Besides its mathematical value, the general case is also important in view of applications, since there, one does not have both $a = m = e_1$ and $b = p = e_2$, in general, and indeed not in the experiments that underly our study.

Let $M, N \in \mathbb{R}^{3\times 3}$ be such that

$$Ma = e_1\,,\ Mb = e_2\,,$$
$$Nm = e_1\,,\ Np = e_2\,.$$

This is possible because $a \nparallel b$ and $m \nparallel p$, since $\operatorname{rank}(C - A) > 1$. By multiplying m or p, or both, by -1, we may assume without loss of generality that $\det N > 0$. Define the three matrices

$$A' = M(A - B)N^t\,,\ B' = 0\,,\ C' = M(C - B)N^t\,,$$

and the affine form

$$T'(\xi) = \langle T, M^{-1}\xi N^{-t} + B\rangle\,, \quad \xi \in \mathbb{R}^{3\times 3}\,.$$

Finally, define three functions $\lambda_{A'}(x') = \lambda_A(N^{-1}x')$, $x' \in N\Omega$ and similarly for $\lambda_{B'}$ and $\lambda_{C'}$. Hence,

$$\lambda_{A'}(x')A' + \lambda_{B'}(x')B' + \lambda_{C'}(x')C' \in \{A', B', C'\}^{qc} \quad \text{a.e. } x' \in N\Omega,$$

if and only if

$$\lambda_A(x)A + \lambda_B(x)B + \lambda_C(x)C \in \{A, B, C\}^{qc} \quad \text{a.e. } x \in \Omega.$$

By these means, we may define a new functional

$$I'(y') = -\int_{N\Omega} T'(Dy'(x'))\,dx'\,, \quad Dy' \in \{A', B', C'\}^{qc} \text{ a.e.}$$

By changing variables, we notice that

$$\begin{aligned}
I'(y') &= -\int_{N\Omega} T'(Dy'(x'))\,dx' = -\int_{\Omega} \langle T, M^{-1}Dy'N^{-t} + B\rangle\,dx' \\
&= -\int_{N\Omega} \langle T, \lambda_{A'}(A - B) + \lambda_{C'}(C - B) + B\rangle\,dx' \\
&= -\int_{N\Omega} \langle T, \lambda_{A'}A + \lambda_{B'}B + \lambda_{C'}C\rangle\,dx' \\
&= -\int_{N\Omega} \langle T, \lambda_A(N^{-1}x')A + \lambda_B(N^{-1}x')B\lambda_C(N^{-1}x')C\rangle\,dx' \\
&= -\det N \int_{\Omega} \langle T, \lambda_A A + \lambda_B B + \lambda_C C\rangle\,dx = \det N \cdot I(y)\,.
\end{aligned}$$

Furthermore, we have

$$\begin{aligned}
\|Dy' - A'\|_{L^1(N\Omega,\mathbb{R}^3)} &= \int_{N\Omega} |(\lambda_{A'} - 1)A' + \lambda_{C'}C'|\,dx' \\
&= \int_{N\Omega} |(\lambda_{A'} - 1)M(A - B)N^t + \lambda_{C'}M(C - B)N^t|\,dx' \\
&= \int_{N\Omega} |(\lambda_A(N^{-1}x') - 1)M(A - B)N^t + \lambda_C(N^{-1}x')M(C - B)N^t|\,dx' \\
&= \det N \int_{\Omega} |(\lambda_A(x) - 1)MAN^t\lambda_B(x)MBN^t + \lambda_C(x)MCN^t|\,dx \\
&\le \det N\,\|M\|\,\|Dy - A\|_{L^1(\Omega,\mathbb{R}^3)}\,\|N^t\|\,.
\end{aligned}$$

Similarly,

$$\|Dy - A\|_{L^1(\Omega,\mathbb{R}^3)} \leq \det N^{-1} \, \|M^{-1}\| \, \|Dy' - A'\|_{L^1(N\Omega,\mathbb{R}^3)} \, \|N^{-t}\| \, .$$

Writing $\Omega' = N\Omega$ and letting

$$\mathscr{A}' = \left\{ y' \in W^{1,1}(\Omega',\mathbb{R}^3) \, : \;\; I'(y') < \infty \, , \; \int_{\Omega'} y' \, dx = 0 \right\},$$

we have thus proved that $y(x) = Ax$ is a local minimiser of I in $\mathscr{A}$ if and only if $y'(x') = A'x'$ is a local minimiser of I' in $\mathscr{A}'$. This naturally gives the desired result in the case of non-orthonormal interfaces.

(4.24) Proposition. *Let $A = B + a \otimes m$, $C = B + \lambda a \otimes m + b \otimes p$ such that* $\operatorname{rank}(A - C) > 1$ *and let $M, N \in \mathbb{R}^{3\times 3}$ be such that*

$$Ma = e_1 \, , \; Mb = e_2 \, ,$$
$$Nm = e_1 \, , \; Np = e_2 \, .$$

Assume without loss of generality that $\det N > 0$. *Assume that $y_0(x) = Ax$ is* not *an L^1 local minimiser of I in $\mathscr{A}$. Then, there exists a point $P = (\bar{x}_1, \bar{x}_2) \in \partial\Omega'$ with the following properties:*

(i) firstly, we have

$$\mathscr{L}^1(\{x_2 \, : \, (\bar{x}_1, x_2) \in \Omega'\}) = 0 \, ,$$
$$\mathscr{L}^1(\{x_1 \, : \, (x_1, \bar{x}_2) \in \Omega'\}) = 0 \, .$$

In particular, there are two tangent vectors to $\partial\Omega'$ at P. Let them be denoted by t_1 and t_2 in such a way that if we define

$$\alpha_1 = \sphericalangle(t_1, e_1) \, ,$$
$$\alpha_2 = \sphericalangle(t_2, e_2) \, ,$$

then $\alpha_1 + \alpha_2 \leq \pi/2$.

(ii) The following bound holds

$$\tan\alpha_1 \tan\alpha_2 \geq \left(1 + \frac{-T'(A') + T'(C')}{(1-\lambda)(-T'(B') + T'(A'))} \right)^{-1} .$$

In particular, $\alpha_1 > 0$ and $\alpha_2 > 0$.

Conversely, if (i)-(ii) holds with strict inequality in (ii), then $y_0'(x') = A'x'$ is not a local minimiser of I' in $\mathscr{A}'$.

Remark. Observe that the constant in (ii) in Theorem 4.19 does not vary after changing variables. Indeed,

$$\frac{-T'(A') + T'(C')}{(1-\lambda)(-T'(B') + T'(A'))} = \frac{-\langle T, A\rangle + \langle T, C\rangle}{(1-\lambda)(-\langle T, B\rangle + \langle T, A\rangle)} \, .$$

We conclude this chapter by highlighting some unresolved questions related to Theorem 4.19, the Schmid Law on smooth domains and estimating the size of the hysteresis.

Remarks.

(a) Consider the simplified three-dimensional case, where $\Omega \subset \mathbb{R}^{3\times 3}$ and $a = m = e_1$, $b = p = e_2 \in \mathbb{R}^3$ (*i.e.*, $B = 0$ $A = e_1 \otimes e_1$ and $C = \lambda e_1 \otimes e_1 + e_2 \otimes e_2$). As in the two-dimensional problem, this case encapsulates all the main difficulties. A careful look at the proof of Theorem 4.19 will convince the interested reader that the first two steps carry over (almost) effortlessly to the three-dimensional setting. Hence (i) is also a necessary condition in that case. More precisely one can prove that, if $y_0(x) = Ax$ is not an L^1 local minimiser of

$$I(y) = \begin{cases} -\int_\Omega \langle T, Dy(x)\rangle \, dx & \text{if } Dy(x) \in \{A, B, C\}^{qc} \text{ a.e.} \\ +\infty & \text{otherwise} \end{cases},$$

in

$$\mathscr{A} = \left\{ y \in W^{1,1}(\Omega, \mathbb{R}^3) \,:\, I(y) < \infty \,,\ \int_\Omega y \, dx = 0 \right\},$$

then there exists a point $P = (\bar{x}_1, \bar{x}_2, \bar{x}_3) \in \partial\Omega$ such that

$$\mathscr{L}^2(\{(x_2, x_3) \,:\, (\bar{x}_1, x_2, x_3) \in \Omega\}) = 0 \,,$$
$$\mathscr{L}^2(\{(x_1, x_3) \,:\, (x_1, \bar{x}_2, x_3) \in \Omega\}) = 0 \,.$$

The main problem is to deduce a sharper necessary (almost sufficient) condition as in (ii) on the angles α_1 and α_2 (now defined as follows: if t_1 and t_2 are the two tangent vectors to $\partial\Omega$ at P in the (e_1, e_2)–plane, then $\alpha_i = \sphericalangle(t_i, e_i)$ with the subscripts 1 and 2 chosen in such a way that $\alpha_1 + \alpha_2 \le \pi/2$). Perhaps surprisingly, the problem seems to depend upon the geometry of Ω in the third direction. For instance, if

$$\Omega = \big\{(x_1, x_2, x_3) \in \mathbb{R}^3 \,:\, 0 \le x_1 \le L \,, \\ x_1 \tan\alpha_1 \le x_2 \le \frac{x_1}{\tan\alpha_2} \,,\ a_1 x_1 + a_2 x_2 \le x_3 \le b_1 x_1 + b_2 x_2 \big\} \,,$$

for some $L > 0$ and $a_i < b_i$, $i = 1, 2$, then $(\bar{x}_1, \bar{x}_2, \bar{x}_3) = (0, 0, 0)$ and the analogous condition to (ii) is

$$\tan\alpha_1 \tan\alpha_2 \, \frac{\frac{1}{2}(b_1 - a_1)(1 + \tan\alpha_1 \tan\alpha_2)\tan\alpha_2 + (b_2 - a_2)\tan\alpha_1 \tan\alpha_2}{(b_1 - a_1)\tan\alpha_2 + \frac{1}{2}(b_2 - a_2)(1 + \tan\alpha_1 \tan\alpha_2)} \ge c \,, \quad (4.62)$$

where c is the right-hand side of the inequality in (ii).

Proof of (4.62). To get (4.62), we simply replicate the procedure we used to get (4.60) in the fourth step of the proof of Theorem 4.19. We consider $E_\varepsilon = (0, \varepsilon)$ and

$$\Omega'_\varepsilon = (\mathbb{R} \times E_\varepsilon \times \mathbb{R}) \cap \Omega \,,$$
$$\Omega'_\varepsilon \cup \Omega''_\varepsilon = (\pi_1(\Omega'_\varepsilon) \times \mathbb{R} \times \mathbb{R}) \cap \Omega \,.$$

To compute the ratio $\mathscr{L}^3(\Omega'_\varepsilon)/\mathscr{L}^3(\Omega'_\varepsilon \cup \Omega''_\varepsilon)$, notice that

$$\mathscr{L}^3(\Omega'_\varepsilon) = \int_0^\varepsilon dx_2 \int_{x_2 \tan\alpha_2}^{x_2/\tan\alpha_1} dx_1 \big\{(b_1 - a_1)x_1 + (b_2 - a_2)x_2\big\} \\ = \left(\frac{b_1 - a_1}{2\tan^2\alpha_1}(1 + \tan\alpha_1 \tan\alpha_2) + \frac{b_2 - a_2}{\tan\alpha_1} \right)(1 - \tan\alpha_1 \tan\alpha_2)\frac{\varepsilon^3}{3} \,,$$

while

$$\mathscr{L}^3(\Omega'_\varepsilon \cup \Omega''_\varepsilon) = \int_0^{\varepsilon/\tan\alpha_1} dx_1 \int_{x_1\tan\alpha_1}^{x_1/\tan\alpha_2} dx_2 \left\{(b_1-a_1)x_1 + (b_2-a_2)x_2\right\}$$
$$= \left(\frac{b_2-a_2}{2\tan^2\alpha_2}(1+\tan\alpha_1\tan\alpha_2) + \frac{b_1-a_1}{\tan\alpha_2}\right)(1-\tan\alpha_1\tan\alpha_2)\frac{\varepsilon^3}{3\tan^3\alpha_1}\,,$$

so that

$$\frac{\mathscr{L}^3(\Omega'_\varepsilon)}{\mathscr{L}^3(\Omega'_\varepsilon \cup \Omega''_\varepsilon)} = \tan\alpha_1\tan\alpha_2 \cdot$$
$$\cdot\, \frac{\frac{1}{2}(b_1-a_1)(1+\tan\alpha_1\tan\alpha_2)\tan\alpha_2 + (b_2-a_2)\tan\alpha_1\tan\alpha_2}{(b_1-a_1)\tan\alpha_2 + \frac{1}{2}(b_2-a_2)(1+\tan\alpha_1\tan\alpha_2)}\,.$$

Condition (4.62) follows. □

However, if

$$\Omega = \{(x_1,x_2,x_3)\in\mathbb{R}^3 : 0\le x_1\le L\,,\ x_1\tan\alpha_1 \le x_2 \le \frac{x_1}{\tan\alpha_2}\,,\ -h\le x_3\le h\}\,,$$

for some positive L and h, then (ii) remains unchanged, as we already pointed out. Moreover, if

$$\Omega = \Big\{(x_1,x_2,x_3)\in\mathbb{R}^3 \,:\, 0\le x_1\le L\,,$$
$$x_1\tan\alpha_1 \le x_2 \le \frac{x_1}{\tan\alpha_2}\,,\ -\sqrt{x_1+x_2}\le x_3\le\sqrt{x_1+x_2}\Big\}\,, \tag{4.63}$$

i.e., when $\partial\Omega$ is smooth (but not flat!) in the third direction, then we get

$$\tan\alpha_1\tan\alpha_2\,\frac{\tan^{1/2}\alpha_2((1+\tan\alpha_1)^{3/2} - (\tan\alpha_1+\tan\alpha_1\tan\alpha_2)^{3/2}))}{((1+\tan\alpha_2)^{3/2} - (\tan\alpha_2+\tan\alpha_1\tan\alpha_2)^{3/2})} \ge c\,.$$

This seems to indicate that a general formula for all domains (whatever the behaviour of $\partial\Omega$ around $(\bar x_1,\bar x_2,\bar x_3)$ in the x_3-direction) is not straightforward. From (4.62), one can get a result in the case where $\partial\Omega$ is singular around $(\bar x_1,\bar x_2,\bar x_3)$ by a blow-up argument similar to that used in the fourth step, but this will not work in a case like (4.63), because, morally, $a=b=-\infty$ while $c=d=+\infty$, and (4.62) does not pass to the limit. On the other hand, the occurrence of a common factor $\tan\alpha_1\tan\alpha_2$ in all cases provides some hope that a general formula does indeed exist. As time goes by, however, we tend to believe that there is no general formula for the three-dimensional case, but merely a catalogue of formulæ depending on the geometry of Ω around $(\bar x_1,\bar x_2,\bar x_3)$.

(b) We now focus on the 'stability' of Theorem 4.19 with respect to variation of the domain Ω. Here again, $\Omega\subset\mathbb{R}^2$. Let us denote by $I(y,\Omega)$ the functional I in order to stress the dependence upon the domain. Consider the following three situations.

– For fixed $\langle T,A\rangle$, $\langle T,B\rangle$ and $\langle T,C\rangle$, let $\alpha=\tan^{-1}\sqrt{c}$, and consider the cone Ω given in polar co-ordinates by

$$\Omega = \{(r,\theta)\,:\,0\le r\le R\,,\ \alpha\le\theta\le\pi/2-\alpha\}\,,$$

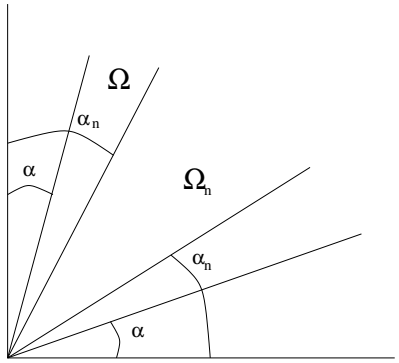


Figure 4.16: Stability of Theorem 4.19 with respect to change of domains – see (b).

where R is large and fixed. Furthermore, consider a sequence of cones

$$\Omega_n = \{(r,\theta) \,:\, 0 \le r \le R\,,\ \alpha_n \le \theta \le \pi/2 - \alpha_n\}\,,$$

where $\alpha_n = \alpha + 1/n$, $n \ge n_0$, n_0 big enough; see Figure 4.16. Then Theorem 4.19 asserts that y_0 is a not local minimiser of $I(\cdot, \Omega_n)$ for any $n \ge n_0$, but is one of $I(\cdot, \Omega)$.

– Consider this time the opposite situation, that is, letting $\alpha_n = \alpha - 1/n$, $n \ge n_0$, n_0 big enough, define

$$\Omega = \{(r,\theta) \,:\, 0 \le r \le R\,,\ \alpha \le \theta \le \pi/2 - \alpha\}\,,$$
$$\Omega_n = \{(r,\theta) \,:\, 0 \le r \le R\,,\ \alpha_n \le \theta \le \pi/2 - \alpha_n\}\,.$$

Then, we get that y_0 is a local minimiser of $I(\cdot, \Omega_n)$ for each n, as well as of $I(\cdot, \Omega)$.

– Let $\alpha > \tan^{-1}\sqrt{c}$ and Ω be the cone

$$\Omega = \{(r,\theta) \,:\, 0 \le r \le R\,,\ \alpha \le \theta \le \pi/2 - \alpha\}\,.$$

Consider the following sequence: for $n > 0$, $\Omega_n = \Omega \cap \{y > 1/n\}$ (see Figure 4.17). Then y_0 is a local minimiser of $I(\cdot, \Omega_n)$ for all n, but not one of $I(\cdot, \Omega)$.

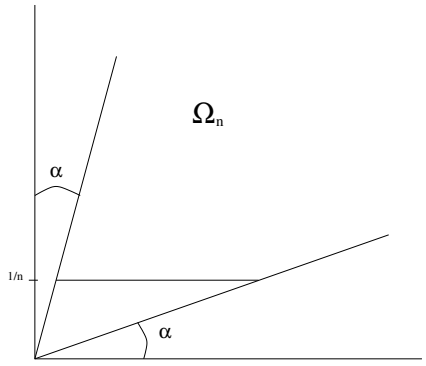


Figure 4.17: Stability of Theorem 4.19 with respect to change of domains – see (b).

It would be interesting to understand these three situations in a unified, rigorous way. Obviously, the notion of Ω_n tending Ω should be made precise, but we failed to see how. This question is important in view of applications since it is desirable to get some kind of stability with respect to changes of the domain if one wishes to test our result in an experiment: predictions different for a square from those for a parallelogram with an angle of nearly 90 degrees would obviously be hardly possible to verify experimentally. This seemingly very sensitive dependence of Theorem 4.19 and Proposition 4.24 on the geometry of the sample constitutes a major setback to their use in predicting new experimental results.

(c) Regarding the more difficult problem of whether the Schmid Law is sharp on smooth domains, optical micrographs of the experiments (see Figures 4.4 and 4.5) seem to indicate that the microstructures actually observed during the transition between one variant and the other are more complicated than those three-gradient constructions used here. Very commonly observed are L-shaped microstructures involving four gradients (see Figure 4.18).[43] These experimental results may hint that such constructions do not require a corner to nucleate, thus could apply to all geometries, and thereby show that the Schmid Law is not sharp on any domain. In principle one should first get

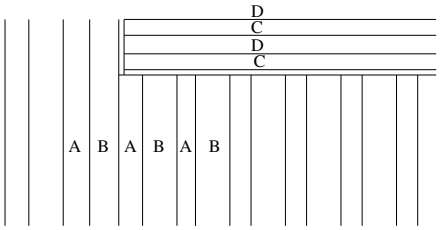


Figure 4.18: L-shaped microstructures observed in experiments.

the equivalent of Lemma 4.21 in order to understand the compatibility conditions that these deformations need satisfy. Then one would need to show that a load smaller than σ_{Sch}, such a construction can be chosen so as to:

- lower the energy,
- remain close to the homogeneous deformation $Dy = A(\sigma)$ in L^1,
- not require any particular geometry of Ω.

However, we did not carry this programme out.

(d) A final issue remains to be discussed, that of estimating the size of the hysteresis. Indeed, since we have showed that the Schmid Law is not sharp on corner-shaped domains (and there is experimental evidence that it is not on other domains either), we need to find another upper bound. One way of tackling this is to produce another upper bound and prove that it is sharp (*i.e.* that it applies to all domains), for example the one obtainable from the construction described in (c) above. This would give a better estimate of when metastability is lost. To get an exact answer, one then needs a

[43] Figure 4.18 is actually an idealisation of the microstructure observed in experiments. In fact, the normals to the transition layers are different from, but very close to, the twin normals. In other words, the transition layers are not *rectangular*, but *triangular*. We do not need to go into such technicalities at this point, but refer instead to Chu and James [51] for more on this remark.

lower bound, that is exhibit a load $\sigma_{min} > \sigma_0$ until which metastability cannot be lost. We have no idea how to achieve this, however.

5 The one point and one compatible well problem

5.1 Introduction

This chapter is concerned with the analysis of gradient Young measures. The latter are useful tools to study qualitative properties of finely oscillating sequences of gradients. Introduced by L.C. Young [156], they have played, in recent years, an important part in a new mathematical theory of martensitic phase transitions pioneered by J.M. Ball and R.D. James [28] as we have explained in Chapter 2. Of particular importance in phase transitions has been the study of gradient Young measures supported on two compatible wells (see *e.g.*, [28, 146]), *i.e.*, a set of the form

$$\mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2\,,$$

where the two symmetric positive definite U_1, U_2 have the same eigenvalues and satisfy $\det(U_1 - U_2) = 0$, see Chapter 3. This implies that for every matrix A on one well, there exist two matrices T_1, T_2 on the other that are rank-one connected to it, $\mathrm{rank}\,(A - T_i) = 1$, $i = 1, 2$. We mentioned a formula for the quasiconvex hull in the proof of Lemma 4.17, which showed that every matrix in this hull could be achieved by a layer-within-layer construction (a laminate of second order, in other words). Recall that the quasiconvex hull is the set of all centres of mass of homogeneous[44] gradient Young measures supported on the two wells. Although this clearly shows the importance of the presence of rank-one connections,[45] it does not imply that if ν_x is a non-trivial gradient Young measure almost everywhere supported on $\mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2$, then $\mathrm{supp}\,\nu_x$ contains at least one pair of rank-one connected matrices for almost every x (let alone for a set of positive measure). That is exactly the question we want to ask here. As a first attempt, we consider a simpler case, where we only have one rank-one connection to play with. More precisely, for $n = 2$ or 3, we consider one well, $\mathrm{SO}(n)U_1$ say, and one matrix on the other well, H say. Letting T_1 and T_2 denote the two twins of H on $\mathrm{SO}(n)U_1$ we ask the

Question. *Does T_1 or T_2 necessarily belong to $\mathrm{supp}\,\nu_x$ a.e.?*

whenever $(\nu_x)_{x\in\Omega}$ is a (non-trivial) gradient Young measure almost everywhere supported on $\{H\} \cup \mathrm{SO}(n)U_1$ and Ω is the unit cube, say.

In fact, the answer is **no** as can be seen with the following example. Let us assume that $H - T_1 = a \otimes m$ and subdivide $\Omega = \Omega_1 \cup \Omega_2 \cup \mathcal{N}$ with $\mathscr{L}^n(\mathcal{N}) = 0$ and

$$\Omega_1 = \{x \in \Omega \;:\; \langle x, m\rangle < \alpha\}\,,$$
$$\Omega_2 = \{x \in \Omega \;:\; \langle x, m\rangle > \alpha\}\,,$$

for some conveniently chosen $\alpha \in \mathbb{R}$. Then the gradient Young measure

$$\nu_x = \begin{cases} \delta_H & \text{if } x \in \Omega_1 \\ \lambda\delta_H + (1-\lambda)\delta_{T_1} & \text{if } x \in \Omega_2 \end{cases},$$

for some $0 \le \lambda < 1$, proves the claim.
We must therefore relax our requirement.

Question. *Does T_1 or T_2 belong to $\mathrm{supp}\,\nu_x$ on a set of positive measure?* (5.1)

[44] Recall that a gradient Young measure is *homogeneous* if it is constant a.e. (as a map $\Omega \to \mathscr{P}(\mathbb{R}^{n\times n})$).

[45] Note however, that if the two wells are incompatible, the quasiconvex hull has not yet been proved to be trivial, unlike in the two-dimensional case. See [64] for the former and [146] for the latter.

whenever $(\nu_x)_{x\in\Omega}$ is a non-trivial gradient Young measure almost everywhere supported on $\{H\}\cup \mathrm{SO}(n)U_1$. A stronger statement would be to show that

$$\int_\Omega \nu_x(\{T_1,T_2\})\,dx > 0\,.$$

We do not pursue this here, however.

Concentrating on (5.1) we focus on the two-dimensional problem ($n=2$), and explain later why in the physical situation when U_1 and U_2 have the same eigenvalues, there is no loss of generality in doing so.

Although the general case remains unsettled, we prove in this chapter that the answer to (5.1) is **yes** in the following special cases:

- whenever $\nu_x \equiv \nu$ is a non-trivial homogeneous gradient Young measure and $\operatorname{supp}\nu \cap \mathrm{SO}(2)U_1$ is connected (Lemma 5.6),
- whenever $\operatorname{supp}\nu_x$ is finite uniformly in x, that is, $\operatorname{supp}\nu_x \subset F$ a.e. for some finite set $F \subset \{H\}\cup \mathrm{SO}(2)U_1$ (Lemma 5.10).

We can also solve the problem in a somewhat degenerate case, when $H\in\mathbb{R}^{2\times 2}$ is trivially rank-one connected to $\mathrm{SO}(2)U_1$, that is when only one matrix on $\mathrm{SO}(2)U_1$ is rank-one connected to H. (Of course, this cannot happen if $H\in\mathrm{SO}(n)U_2$ and $\mathrm{SO}(n)U_1$ are such that U_1 and U_2 have the same eigenvalues, $n=2,3$, see Chapter 3.) We prove in Lemma 5.3 below that in this case every non-trivial homogeneous gradient Young measure contains a pair of compatible matrices in its support.

Furthermore, we give a proof of a positive answer to a more general case provided a strong rigidity conjecture holds. (We do not know how to tackle this conjecture, however.) Lemma 5.9 and Theorem 5.14 show that any gradient Young measure ν_x almost everywhere supported on $\{H\}\cup\mathrm{SO}(2)U_1$ such that

$$\mathscr{N}_\varepsilon(T_i)\cap\operatorname{supp}\nu_x = \{R\in\mathrm{SO}(2) : |R-T_i|\le\varepsilon\}\cap\operatorname{supp}\nu_x = \emptyset \text{ a.e.}\,,\ i=1,2,$$

for some $\varepsilon>0$, is trivial, provided Conjecture 5.13 holds.

We conclude this chapter with some ideas that could be worth pursuing and that might lead to a solution in the general case.

5.2 Partial results and some ideas for further work

We recall the definition of gradient Young measures. Let $\mathscr{P}(\mathbb{R}^{n\times n})$ denote the set of all probability measures supported on $\mathbb{R}^{n\times n}$, $n\ge 2$, and write $\langle g,\nu\rangle = \int_{\mathbb{R}^{n\times n}} g(\zeta)\,d\nu(\zeta)$ (suitably interpreted for real- or vector-valued g).

(5.1) Definition. *Let $K\subset\mathbb{R}^{n\times n}$ be compact, and let $\Omega\subset\mathbb{R}^n$ be a bounded open set. A* gradient Young measure *is a (weak-$*$) measurable mapping $\nu_x:\Omega\to\mathscr{P}(\mathbb{R}^{n\times n})$ such that*

(*i*) $\operatorname{supp}\nu_x\subset K$ *a.e.*

(*ii*) *there exists a function $y\in W^{1,\infty}(\Omega,\mathbb{R}^n)$ such that $\langle id,\nu_x\rangle = Dy(x)$ a.e.*

(*iii*) *Jensen's inequality holds for every quasiconvex function,* i.e.,

$$\langle f,\nu_x\rangle \ge f(\langle id,\nu_x\rangle) \quad a.e. \tag{5.2}$$

for every quasiconvex function $f:\mathbb{R}^{n\times n}\to\mathbb{R}$,

where $id : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ *is the identity mapping* $id(\zeta) = \zeta$.

Remarks. To be precise, and as stated in Chapter 2, this 'definition' is in fact the characterisation of ($W^{1,\infty}$–) gradient Young measures due to Kinderlehrer and Pedregal [94, 95], but for our purposes this is sufficient. Also, thanks to Zhang's Lemma [159], since K is compact, there is no loss of generality in restricting ourselves to ($W^{1,\infty}$–) gradient Young measures. Also, we notice that condition (*iii*) is equivalent to the requirement that the centre of mass of ν_x lie in the quasiconvex hull of K.

Our problem is the following. Given two symmetric positive definite matrices $U, H \in \mathbb{R}^{3\times 3}$, let $K = \mathrm{SO}(3)U \cup \{H\}$. Assume that H and $\mathrm{SO}(3)U$ are compatible, *i.e.*, that there exists a matrix $T \in \mathrm{SO}(3)U$ such that $\mathrm{rank}\,(T - H) = 1$. Then there exist either one or two such T (see *e.g.*, [27] and Chapter 3 in this thesis): call them T_1 and T_2 (with the possibility that $T_1 = T_2$). Finally, let $(\nu_x)_{x\in\Omega}$ be a non-trivial gradient Young measure almost everywhere supported on K, where Ω is a bounded open set. From now on, we take Ω to be the unit cube.

(5.2) Question. Do we have

$$\mathscr{L}^3(\{x \in \Omega \ : \ T_1 \ \text{ or } \ T_2 \in \operatorname{supp}\nu_x\}) > 0\,?$$

We will assume that H and U have the same eigenvalues. In the case of different eigenvalues, the ideas below do not apply – except in the degenerate case when $T_1 = T_2$ which is dealt with in Lemma 5.3 below. Under this assumption, a well-known reduction (see *e.g.*, [87]) allows us to concentrate on the two-dimensional case $H, U \in \mathbb{R}^{2\times 2}$. Furthermore, upon changing variables, we may take $U = \mathbb{I} \in \mathbb{R}^{2\times 2}$ and H diagonal, with eigenvalues $0 \le h_1 \le h_2$ and $K = \{H\} \cup \mathrm{SO}(2)$.[46] Now, the hypothesis that H and $\mathrm{SO}(2)$ be compatible is that

$$(h_1^2 - 1)(h_2^2 - 1) \le 0\,,$$

see [38] or Chapter 3. This is equivalent to

$$0 < h_1 \le 1 \le h_2\,. \tag{5.3}$$

As mentioned earlier, we are interested in the case $\det H = h_1 h_2 = 1$, and thus $h_2 = 1/h_1$. However, along the way we are able to treat an additional case where $\det H \neq 1$, so we keep the notation (5.3) for the time being.

We start by computing the quasiconvex hull of K, which gives the possible centres of mass of homogeneous gradient Young measures supported on K. We use the following standard procedure. First, we compute the *polyconvex hull* of K, written K^{pc}, consisting of the centres of mass of those probability measures supported on K that satisfy (5.2) for every real-valued polyconvex function f. As explained in Chapter 2 this in fact amounts to finding the centres of mass of those probability measures supported on K that commute with the determinant; more precisely, that satisfy

$$\langle \det\,, \nu\rangle = \det\langle \mathrm{id}, \nu\rangle\,.$$

(In higher dimensions, one requires that the measure commute with all the minors, not only with the determinant. These conditions are called the *minors relations*.) Polyconvex

[46] More precisely, instead of $\{H\} \cup \mathrm{SO}(2)U$ we consider $\{\sqrt{(HU^{-1})^t HU^{-1}}\} \cup \mathrm{SO}(2)$ where we have used the polar decomposition theorem.

functions being quasiconvex, this set is bigger than the quasiconvex hull of K. Secondly, we compute the lamination convex hull K^{lc} of K, defined inductively as follows:

$$K^{lc} = \bigcup_{i=1}^{\infty} K^{(i)},\ K^{(1)} = K,$$

and $K^{(i+1)} = K^{(i)} \cup \{\alpha A + (1-\alpha)B\ :\ A, B \in K^{(i)}, \mathrm{rank}\,(A-B) \leq 1,\ 0 \leq \alpha \leq 1\}$. This set is the smallest set containing K stable under the addition of rank-one segments. K^{lc} is smaller than K^{qc}. The hope is that these lower and upper bounds coincide, giving K^{qc}. In our case, they do, which follows from an observation of Iqbal [87] as will be seen below.

We start by computing K^{pc}. Let μ be a probability measure supported on SO(2), let $0 \leq \lambda \leq 1$ and let $\nu = \lambda\delta_H + (1-\lambda)\mu$ be a probability measure supported on K, where δ_H stands for the Dirac mass centred at H. Let $\bar{\nu}$ and $\bar{\mu}$ denote the centres of mass of ν and μ, respectively. Then,

$$\bar{\nu} = \lambda H + (1-\lambda)\bar{\mu} \tag{5.4}$$

while the requirement that ν commute with the determinant is equivalent to

$$\det \bar{\nu} = \lambda \det H + (1-\lambda)\,. \tag{5.5}$$

Recall that if $A, B \in \mathbb{R}^{2\times 2}$,

$$\det\,(A+B) = \det A + \det B + \langle \tilde{A}, B\rangle\,, \tag{5.6}$$

where $\langle A, B\rangle = \mathrm{trace}(B^t A)$ and

$$\text{if}\quad A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad \text{then}\quad \tilde{A} = \begin{pmatrix} a_{22} & -a_{21} \\ -a_{12} & a_{11} \end{pmatrix}.$$

Using (5.4) and the identity (5.6), we get

$$\det \bar{\nu} = \lambda^2(\det H + \det \bar{\mu} - \langle \tilde{H}, \bar{\mu}\rangle) + \lambda(\langle \tilde{H}, \bar{\mu}\rangle - 2\det \bar{\mu}) + \det \bar{\mu}. \tag{5.7}$$

Substituting (5.7) into (5.5) yields

$$\lambda^2(\det H + \det \bar{\mu} - \langle \tilde{H}, \bar{\mu}\rangle) + \lambda(1 - \det H - 2\det \bar{\mu} + \langle \tilde{H}, \bar{\mu}\rangle) + \det \bar{\mu} - 1 = 0\,,$$

which can be rewritten as

$$\det\,(H-\bar{\mu})\lambda^2 - (\det\,(H-\bar{\mu}) + \det \bar{\mu} - 1)\lambda + \det \bar{\mu} - 1 = 0\,. \tag{5.8}$$

Let us carefully study (5.8).

- Suppose $\det \bar{\mu} = 1$. Then we have two cases:
  - $\det\,(H-\bar{\mu}) = 0$ and we have no condition on λ (since (5.8) vanishes identically in this case). Thus $\bar{\mu} = T_i$ and hence $\mu = \delta_{T_i}$, $i = 1$ or 2. Therefore, the solutions are
    $$\nu = \lambda\delta_H + (1-\lambda)\delta_{T_i}\,,$$
    for every $i = 1, 2$ and $0 \leq \lambda \leq 1$,
  - $\det\,(H-\bar{\mu}) \neq 0$ and the only solutions are $\lambda = 0$ or $\lambda = 1$. In this case, $\nu = \delta_H$ or $\nu = \delta_R$ for some $R \in \mathrm{SO}(2)$.

- Suppose $\det \bar{\mu} \neq 1$. Since $\bar{\mu}$ belongs to the convex hull of SO(2), $\det \bar{\mu} < 1$.
  - If $\det (H - \bar{\mu}) = 0$, the only solution is $\lambda = 1$, *i.e.*, $\nu = \delta_H$.
  - Suppose $\det (H - \bar{\mu}) \neq 0$. Then there are two solutions of (5.8): either $\lambda = 1$ and $\nu = \delta_H$, or
$$\lambda = \frac{\det \bar{\mu} - 1}{\det (H - \bar{\mu})} \text{ and } \nu = \lambda \delta_H + (1 - \lambda)\mu \,. \tag{5.9}$$

Obviously, for the solution (5.9) to be a probability measure, we must have $0 \leq \lambda \leq 1$. This holds under two conditions:

(i) $\det (H - \bar{\mu}) < 0$,

(ii) $\det (H - \bar{\mu}) < \det \bar{\mu} - 1$,

in which case $0 < \lambda < 1$, the cases $\lambda = 0$ or $\lambda = 1$ having been studied above. Obviously, $(ii) \Rightarrow (i)$ because $\det \bar{\mu} < 1$. Writing

$$\bar{\mu} = \begin{pmatrix} a & -b \\ b & a \end{pmatrix} ,$$

condition (ii) reduces to

$$a > \frac{1 + h_1 h_2}{h_1 + h_2} = \bar{a} \,. \tag{5.10}$$

Furthermore, since $\bar{\mu}$ belongs to the convex hull of SO(2), a and b satisfy

$$a^2 + b^2 < 1. \tag{5.11}$$

These two conditions demarcate the interior of the shaded area in Figure 5.1, which also shows the regions where $\det (H - \bar{\mu})$ is positive, nought, and negative, respectively. Notice that in terms of a and b, $\det (H - \bar{\mu}) = 0$ if and only if

$$b^2 = (a - h_1)(h_2 - a) \,.$$

We next compute K^{lc}. We distinguish two cases.

(i) Assume $(h_1 - 1)(h_2 - 1) = 0$ (which corresponds to the case $T_1 = T_2$). Then conditions (5.10) and (5.11) are incompatible. Indeed, in this case $T_1 = T_2 = \mathbb{I}$ (notice that since H is diagonal, $T_2 = T_1^t$) and the interior of the shaded area is empty. In other words, the only non-trivial probability measures supported on K that commute with the determinant are $\nu = \lambda \delta_H + (1 - \lambda)\delta_T$, $0 < \lambda < 1$, where T is the unique rotation such that $\det (H - T) = 0$. Indeed, the only possible centres of mass lie on the rank-one segment HT, which implies that every ν satisfying (5.4) and (5.5) is a convex combination of the Dirac concentrated at H and of a probability measure μ supported on SO(2) whose centre of mass lies on SO(2). Hence $\mu = \delta_T$. It is an easy calculation that $K^{lc} = K^{(2)} = K \cup \{\lambda H + (1 - \lambda)T \,:\, 0 < \lambda < 1\}$. Hence,

$$K^{lc} = K^{qc} = K^{pc} = K \cup \{\lambda H + (1 - \lambda)T \,:\, 0 < \lambda < 1\} \,.$$

This proves the following

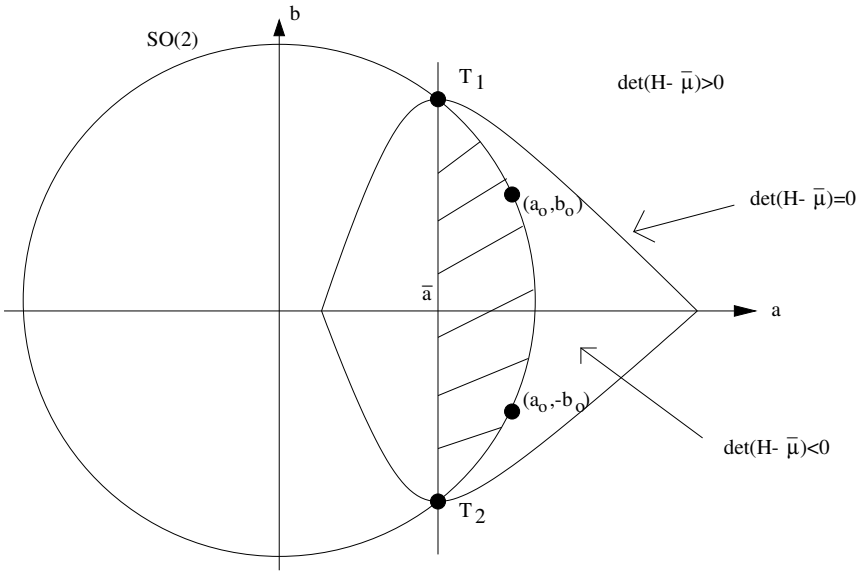


Figure 5.1: Schematic diagram of conditions (5.10)-(5.11) – see text.

(5.3) Lemma. *Assume that* $H \in \mathbb{R}^{2\times 2}$ *and* $\mathrm{SO}(2)U$ *are trivially rank-one connected,* i.e.*, that there exists only one rotation* R *such that* $\det(H-RU) = 0$*. Then, if* ν *is a homogeneous gradient Young measure supported on* $\{H\} \cup \mathrm{SO}(2)$ *that is not a Dirac mass, then* $RU \in \operatorname{supp}\nu$*.*

(ii) Assume that $\det H = 1$, *i.e.*, that $h_1 = h, h_2 = 1/h$ for some $0 < h < 1$ (the case $h = 1$ being trivial). In the case $\det H \neq 1$, the ideas below do not apply. We use an argument due to Iqbal [87] and show that all possible centres of mass of homogeneous gradient Young measures supported on K can be seen as the centre of mass of a laminate of second order.[47] Let $\bar{\nu} = \lambda H + (1-\lambda)\bar{\mu}$ be the centre of mass of a probability measure satisfying (5.4) and (5.5). The only non-trivial case is when $\bar{\mu}$ is in the interior of the shaded area in Figure 5.1. We construct a laminate of second order (in particular, a gradient Young measure) whose centre of mass is $\bar{\nu}$. Choose one of the two twins of H, T_1 say. Let $S \neq T_1$ be the rotation lying on the line joining T_1 to $\bar{\mu}$ (see Figure 5.2). Now, H, $\bar{\nu}$, T_1 and S are coplanar. Hence the line joining S and $\bar{\nu}$ intersects the rank-one line HT_1 at a matrix S'. Now, since $\det H = 1$, $\det\bar{\nu} = 1$ as well. And $\det S' = 1$ because S' lies on a rank-one line. Since $\det S = 1$, the whole line SS' is a rank-one line. Hence, $\bar{\nu}$ can be achieved as the centre of mass of the laminate of second order

$$\tilde{\nu} = \tilde{\alpha}(\beta\delta_H + (1-\beta)\delta_{T_1}) + (1-\tilde{\alpha})\delta_S\,,$$

for some $0 < \tilde{\alpha}, \beta < 1$, as desired. Thus, we have shown that $K^{pc} \subset K^{(2)} \subset K^{lc}$ and therefore proved the

(5.4) Theorem. *Let* μ *be a probability measure supported on* $\mathrm{SO}(2)$*, let* $0 \leq \lambda \leq 1$*, and let* $\nu = \lambda\delta_H + (1-\lambda)\mu$ *be a probability measure supported on* K*, where* δ_H *stands for the Dirac*

[47] Roughly speaking, a laminate of second order is a homogeneous gradient Young measure that is a convex combination of four Dirac masses. See [116] for a precise definition.

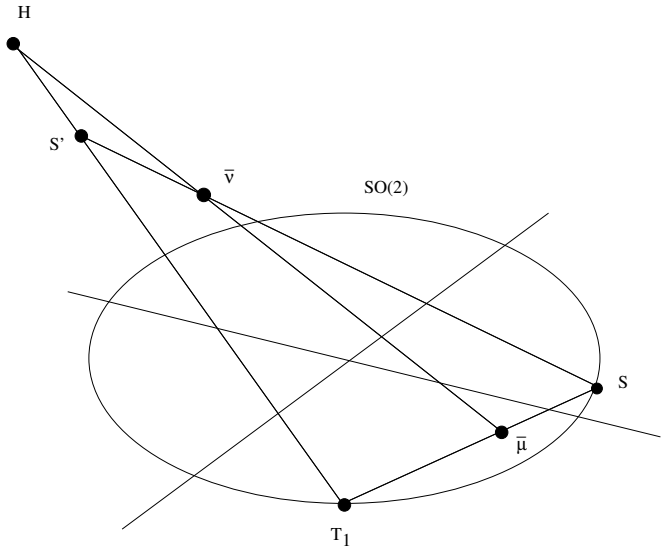


Figure 5.2: Construction of a laminate of second order with centre of mass $\bar{\nu}$.

mass concentrated at H. Let $\bar{\nu}$ and $\bar{\mu}$ denote the centres of mass of ν and μ, respectively. Then, $\bar{\nu} \in K^{qc}$ if and only if ν commutes with the determinant. Furthermore, the solutions to

$$\bar{\nu} = \lambda H + (1-\lambda)\bar{\mu} \in K^{qc}$$

are given by:

(*i*) *If* $\det \bar{\mu} = 1$ *and*

- *either* $\det(H - \bar{\mu}) = 0$, *then*

$$\nu = \lambda \delta_H + (1-\lambda)\delta_{T_i}\,,$$

  for $i = 1, 2$ *and* $0 \le \lambda \le 1$,
- *or* $\det(H - \bar{\mu}) \neq 0$ *and then the only solutions are* $\nu = \delta_H$ *or* $\nu = \delta_R$ *for some* $R \in \mathrm{SO}(2)$.

(*ii*) *If* $\det \bar{\mu} < 1$ *and*

- *either* $\det(H - \bar{\mu}) = 0$, *then* $\nu = \delta_H$,
- *or* $\det(H - \bar{\mu}) < 0$ *and then there are two solutions: either* $\nu = \delta_H$, *or*

$$\nu = \lambda \delta_H + (1-\lambda)\mu \;\; \textit{where } \lambda = \frac{\det \bar{\mu} - 1}{\det(H - \bar{\mu})}\,. \tag{5.12}$$

Remark. In particular, this theorem proves that if $F = \lambda A + (1-\lambda)B \in (\mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2)^{qc}$, for some $A \in \mathrm{SO}(3)U_1$ and $B \in \mathrm{SO}(3)U_2$, where U_i are positive definite and have the same eigenvalues, and if $\mathrm{rank}\,(A - B) > 1$, then necessarily $\lambda(1-\lambda) = 0$. To see this, reduce to two two-dimensional wells and change variables to write $A = H$ diagonal and positive definite and $B \in \mathrm{SO}(2)$. In the notation of the theorem, we thus consider

$\bar\nu = \lambda H + (1-\lambda)\bar\mu$ with $\bar\mu = B \in \mathrm{SO}(2)$. Then $\det \bar\mu = 1$ and $\det(H - \bar\mu) \neq 0$. The claim follows from part (i) of the theorem.

Looking at Figure 5.1, we see that SO(2) is divided into three distinct parts. Firstly an arc where $\det(H - \cdot) < 0$, secondly, T_1 and T_2, the two twins of H, where $\det(H - \cdot) = 0$ and thirdly an arc where $\det(H - \cdot) > 0$. Remembering that the shaded area represents those $\bar\mu$ such that $\bar\nu = \lambda H + (1-\lambda)\bar\mu \in K^{qc}$, in particular, satisfying (5.10)–(5.11), we get the following immediate

(5.5) Corollary. *Let $\nu = \lambda\delta_H + (1-\lambda)\mu$ be a homogeneous gradient Young measure supported on K. Assume that $\nu \neq \delta_Q$ for all $Q \in \{R \in \mathrm{SO}(2) : \det(H - R) > 0\}$. Then,*

$$\det(H - \bar\mu) \leq 0\,. \tag{5.13}$$

Remark. Obviously, if $\lambda = 1$, $\bar\mu$ is not defined. As a convention, we therefore assert that (5.13) also holds when $\lambda = 1$.

Another interesting consequence of the above analysis is that we are able to construct a probability measure that commutes with the determinant, whose support includes neither T_1 nor T_2 and which cannot be a gradient Young measure. Hence the answer to Question 5.2 is negative for measures whose centres of mass lie in the polyconvex hull of $\{H\} \cup \mathrm{SO}(2)$. Indeed, let $\bar a = (2h)/(1+h^2)$ and let $\bar a < a_0 < 1$ and $b_0 = \sqrt{1 - a_0^2}$. Then (a_0, b_0) and $(a_0, -b_0)$ satisfy (5.10) (see Figure 5.1). Let

$$S_1 = \begin{pmatrix} a_0 & -b_0 \\ b_0 & a_0 \end{pmatrix} \quad \text{and} \quad S_2 = S_1^t\,,$$

and let $\mu = \frac{1}{2}(\delta_{S_1} + \delta_{S_2})$. Then $\bar\mu = a_0\mathbb{I}$ satisfies (5.10)-(5.11) (see Figure 5.1). Finally, let λ be given by (5.12), *i.e.*,

$$\lambda = \frac{a_0^2 - 1}{(a_0 - h)(a_0 - 1/h)}\,.$$

Then, by construction,

$$\nu = \lambda\delta_H + (1-\lambda)\mu$$

commutes with the determinant. We claim that ν cannot be a gradient Young measure. Indeed, the three matrices H, S_1 and S_2 are pairwise incompatible, and it has been proved by Šverák [141] (see also [26, 158]) that the quasiconvex hull of three matrices with no rank-one connections is trivial.

This seems to indicate that the minors relations do not provide enough information to answer the question completely, and that further ideas are needed. We mention several possible lines of thought. Before doing so, however, we notice that the minors relations do solve one more particular case.

Indeed, if we apply the minors relations to the function $f(\xi) = \det(H - \xi)$, and remember that $\det(H - \bar\mu) \leq 0$ if $\nu = \lambda\delta_H + (1-\lambda)\mu$ is not trivial, by Corollary 5.5, we get

$$0 \geq (1-\lambda)\det(H - \bar\mu) = f(\bar\nu) = \langle f, \nu\rangle = \int_{\mathrm{SO}(2)} \det(H - R)\, d\mu(R)\,.$$

Using the fact that the sign of f cannot be constant on $\operatorname{supp}\mu$ (see [26], or Lemma 5.8 below), and that $f(R) = 0$, $R \in \mathrm{SO}(2)$, if and only if $R = T_1$ or T_2, we have proved

(5.6) Lemma. *If ν is a homogeneous gradient Young measure supported on $\{H\} \cup \mathrm{SO}(2)$ that is not a Dirac mass and such that $\operatorname{supp}\nu \cap \mathrm{SO}(2)$ is connected, then T_1 or $T_2 \in \operatorname{supp}\nu$.*

We now state our most complete result so far. We prove here that the answer to Question 5.2 is positive provided the Young measure is almost everywhere supported on a finite subset of $\{H\} \cup \mathrm{SO}(2)$. To prove this result, we consider a conjecture closely related to a positive answer to Question 5.2 (which we conjecture is the general answer).

(5.7) Conjecture. *For every small $\varepsilon > 0$, the two compact sets $K_1 = \{H\} \cup \{R \in \mathrm{SO}(2) : \det(H-R) \leq 0\}$ and $K_2^\varepsilon = \{R \in \mathrm{SO}(2) : \det(H-R) \geq \varepsilon\}$ are incompatible in the sense of Ball and James* [26]*,* i.e.*, if ν_x is a gradient Young measure supported on $K_1 \cup K_2^\varepsilon$ a.e., then $\operatorname{supp}\nu_x \subset K_1$ a.e. or $\operatorname{supp}\nu_x \subset K_2^\varepsilon$ a.e.*

Remark. Here $\varepsilon > 0$ has to be small enough so that $K_2^\varepsilon \neq \emptyset$.

To see how this conjecture relates to Question 5.2, first recall the following result due to Ball and James [26].[48]

(5.8) Lemma. *Let $K \subset \mathbb{R}^{2\times 2}$ be a compact set such that $\det\xi > 0$ for every $\xi \in K$. Then $\{0\}$ and K are incompatible. The same result holds if $\det\xi < 0$ for every $\xi \in K$.*

Suppose we know that Conjecture 5.7 holds and consider a gradient Young measure ν_x almost everywhere supported on $F \subset \{H\} \cup \mathrm{SO}(2)$, a finite set, and such that

$$\mathscr{L}^2(\{x \in \Omega \,:\, T_1 \text{ or } T_2 \in \operatorname{supp}\nu_x\}) = 0\,. \tag{5.14}$$

We claim that ν_x is trivial. By (5.14) and the finiteness hypothesis, we may find an $\varepsilon > 0$ such that $\operatorname{supp}\nu_x \subset K_1 \cup K_2^\varepsilon$ a.e. Hence, by Conjecture 5.7, we can conclude that ν_x is actually supported either on

$$\{H\} \cup \{R \in \mathrm{SO}(2) \,:\, \det(H-R) \leq 0\} \text{ a.e.}$$

or on

$$\{R \in \mathrm{SO}(2) \,:\, \det(H-R) > 0\} \subset \mathrm{SO}(2) \text{ a.e.}$$

In the latter case, ν_x is trivial, see Kinderlehrer [93]. In the former, we use (5.14) and the finiteness hypothesis again to infer that ν_x is almost everywhere supported on

$$\{H\} \cup \{R \in \mathrm{SO}(2) \,:\, \det(H-R) \leq -\varepsilon\}\,,$$

and the claim follows from Lemma 5.8 and Kinderlehrer's result [93].

Observe that without the finiteness hypothesis, the above argument still applies to gradient Young measures such that

$$\mathscr{N}_\delta(T_i) \cap \operatorname{supp}\nu_x = \emptyset \text{ a.e.}\,,\ i = 1,2, \tag{5.15}$$

for some $\delta > 0$, where

$$\mathscr{N}_\delta(T_i) = \{R \in \mathrm{SO}(2) : |R - T_i| \leq \delta\}\,, \quad i = 1,2\,.$$

[48] Although the research in [26] is not published yet, it has been presented at several conferences, *e.g.*, [8, 9]. The proof of Lemma 5.8 proceeds by contradiction, using the Varying Volume Fractions Lemma (see Lemma 5.15 below) to move the volume fractions to a region where the minors relations give a contradiction, and the theory of quasiregular maps to handle the exact gradient problem.

Indeed, in this case too, we deduce that $\operatorname{supp}\nu_x \subset K_1 \cup K_2^\varepsilon$ a.e. for some $\varepsilon > 0$ and the claim follows similarly. Notice in particular that gradient Young measures with uniformly finite supports and satisfying (5.14) also satisfy (5.15). Let us summarise this remark in a

(5.9) Lemma. *Assume Conjecture 5.7 holds true. Then any gradient Young measure almost everywhere supported on* $\{H\} \cup \mathrm{SO}(2)$ *satisfying* (5.15) *is trivial.*

As announced earlier, we can prove the following

(5.10) Lemma. *The answer to Question* 5.2 *is* **yes** *provided that* ν_x *is almost everywhere supported on a finite subset of* $\{H\} \cup \mathrm{SO}(2)$.

This follows from the following more general statement, which is a special case of Conjecture 5.7.

(5.11) Proposition. *For every small* $\varepsilon > 0$, *any finite subset* $K' \subset K_2^\varepsilon$ *and* K_1 *are incompatible.*

Remarks. Lemma 5.10 has in particular the following consequence. In attempting to answer Question 5.2 negatively, one needs an example of a gradient Young measure whose support does not contain a pair of compatible matrices, and then try and fit it in the set $\{H\} \cup \mathrm{SO}(2)$. One such example (and perhaps the first that comes to mind) is the so-called *Tartar square* [39, 149] described in Chapter 2, which is a non-trivial laminate (of infinite order) supported on four pairwise incompatible matrices. Lemma 5.10 thus has the following

(5.12) Corollary. *The set* $\{H\} \cup \mathrm{SO}(2)$ *cannot support a Tartar square.*

Proof of Proposition 5.11. Let us fix a small $\varepsilon > 0$ and drop it from the notation. Let $R_1, \dots, R_k$ denote those rotations in K'. Let ν_x be a gradient Young measure almost everywhere supported on $K_1 \cup K'$ that is not almost everywhere supported on K'. We want to show that $\operatorname{supp}\nu_x \subset K_1$ a.e. Since K' is finite, there exists a $\delta > 0$ such that

$$\mathcal{N}_\delta(R_i) \cap K' = \{R_i\}\,, \quad i = 1, \dots, k. \tag{5.16}$$

Consider first the two compact sets $\mathcal{N}_\delta(R_1)$ and $(K' \cup K_2) \setminus \{R_1\}$. Notice the following fact:

$$\det(\xi - R_1) > c > 0 \quad \text{for all } \xi \in \operatorname{supp}\nu_x \setminus \{R_1\}. \tag{5.17}$$

To prove (5.17), we distinguish two cases:

(*i*) If $\xi = H$, this is obvious, because $R_1 \in K_2$.

(*ii*) If $\xi \in (K_1 \cup K') \cap \mathrm{SO}(2)$, we use the fact that

$$\det(R_1 - R_2) = |R_1 - R_2|^2 \quad \text{for all } R_1, R_2 \in \mathrm{SO}(2).$$

Finally, the fact that $\det(\xi - R_1) > c > 0$ uniformly in ξ comes from (5.16). We now apply Lemma 5.8 to infer that $\mathcal{N}_\delta(R_1)$ and $(K' \cup K_2) \setminus \{R_1\}$ are incompatible. So

$$\int_\Omega \nu_x(\mathcal{N}_\delta(R_1))\, dx = 0 \text{ or } 1\,.$$

Hence, if ν_x is not to be trivial, $\int_\Omega \nu_x(\mathscr{N}_\delta(R_1))\,dx = 0$ and $R_1 \notin \operatorname{supp}\nu_x$ a.e. Now repeat this process with R_2 and $\operatorname{supp}\nu_x \setminus \{R_1\}$, remove R_2 from the support, and continue this so as to exhaust K'. But then this means that $\operatorname{supp}\nu_x \subset K_1$ a.e. □

Remark. There may be a way of passing to the limit in this result, and thereby get a general proof of Conjecture 5.7, but the exact details have eluded us so far. The basic idea is as follows. Recall first a general result due to Ball and James [26] to the effect that if the two compact sets K_1 and K_2 are incompatible, there exists a $\delta > 0$ such that $\mathscr{N}_\delta(K_1)$ and $\mathscr{N}_\delta(K_2)$ are incompatible, too.[49] If we knew that this $\delta > 0$ does not depend on the cardinality of K', or only depends on other quantities that could be fixed whatever the cardinality of K', *e.g.*, $\operatorname{diam} K'$ or $\operatorname{dist}(K_1, K')$, we could take K' bigger and bigger, until $K_2 \subset \mathscr{N}_\delta(K')$ for the associated δ. However, since *a priori*, we cannot rule out the possibility that $\delta \to 0$ as we take more and more points, we do not see how to pass to the limit. A technical difficulty here is that it is not known what the $\delta > 0$ in Ball and James' result depends upon. We mention that Zhang [157] has a similar result for two incompatible matrices where he gives an estimate on δ, but this cannot be generalised to arbitrary incompatible sets yet, and therefore his result does not apply to our setting as it stands.

We now establish Conjecture 5.7 provided a strong rigidity conjecture holds, that we now state. Recall that $K_1 = \{H\} \cup \{R \in \mathrm{SO}(2) \,:\, \det(H - R) \leq 0\}$ and $K_2^\varepsilon = \{R \in \mathrm{SO}(2) \,:\, \det(H - R) \geq \varepsilon\}$ for some small $\varepsilon > 0$.

(5.13) Conjecture. *Let ν_x be a gradient Young measure almost everywhere supported on $K = K_1 \cup K_2^\varepsilon$,*

$$\nu_x = \alpha(x)\mu_x^1 + (1 - \alpha(x))\mu_x^2\,,$$

for some probability measures μ_x^i such that $\operatorname{supp}\mu_x^1 \subset K_1$ a.e., $\operatorname{supp}\mu_x^2 \subset K_2^\varepsilon$ a.e. and $0 \leq \alpha \leq 1$ a.e. If the measure of the set $\{x \in \Omega : \alpha(x) = 0\}$ is positive, then $\operatorname{supp}\nu_x \subset K_2^\varepsilon$ a.e. (In particular, ν_x is trivial and homogeneous.)

Remark. In this context, rigidity is associated to the following phenomenon. A set $K \subset \mathbb{R}^{2\times 2}$ is *rigid* if it has the property that every Lipschitz map $y \in W^{1,\infty}(\Omega, \mathbb{R}^2)$ such that $Dy(x) \in K$ a.e. is necessarily affine. Here, it is clear that $K_1 \cup K_2^\varepsilon$ cannot be rigid, for any $\varepsilon > 0$ (because K_1 contains a rank-one connection) but we conjecture that $K_1^\varepsilon \cup K_2^\varepsilon$ is, for every small $\varepsilon > 0$, where K_1^ε is defined by removing the rank-one connection in K_1,

$$K_1^\varepsilon = \{H\} \cup \{R \in \mathrm{SO}(2) \,:\, \det(H - R) \leq -\varepsilon\}\,.$$

However, for our proof of Theorem 5.14 to work, we need more than this, and even more than the strengthened requirement that if the measure of the set $\{x \in \Omega \,:\, Dy(x) \in K_2^\varepsilon\}$ is positive, then y be affine. As we mentioned earlier, we have at this stage no idea how to prove, let alone tackle, this conjecture.

Under this assumption, we can prove Conjecture 5.7.

(5.14) Theorem. *Assume Conjecture* 5.13 *holds. Then Conjecture* 5.7 *holds true.*

[49] This follows easily from a slight generalisation of the Transition Layer Estimate for Young measures mentioned in Chapter 4, see Lemma 4.15. The point is that this result holds for any pair of incompatible sets (and not only for two incompatible matrices). Once this is done, it is straightforwardly seen that this estimate gives the claimed result.

Before embarking upon proving Theorem 5.14, we need the following result due to Ball and James [26].[50]

(5.15) Lemma (Varying Volume Fractions Lemma). *Let $K_1, K_2 \subset \mathbb{R}^{2\times 2}$ be compact. If K_1 and K_2 are compatible, then, for every $0 \le \lambda \le 1$, there exists a gradient Young measure (ν_x^λ) such that*

$$\frac{1}{\mathscr{L}^2(\Omega)} \int_\Omega \nu_x^\lambda(K_1)\, dx = \lambda\,,$$
$$\frac{1}{\mathscr{L}^2(\Omega)} \int_\Omega \nu_x^\lambda(K_2)\, dx = 1-\lambda\,,$$

where $\mathscr{L}^2(\Omega)$ stands for the Lebesgue measure of Ω.

We can now prove Theorem 5.14. We warn the reader that every measure considered below is a probability measure and that we shall not repeat this fact.

Proof of Theorem 5.14. Suppose not. Then there is a small $\varepsilon > 0$ for which there exists

$$\nu_x = \alpha(x)\mu_x^1 + (1-\alpha(x))\mu_x^2\,,$$

with $\operatorname{supp}\mu_x^1 \subset K_1$ a.e., $\operatorname{supp}\mu_x^2 \subset K_2^\varepsilon$ a.e., $0 \le \alpha \le 1$ a.e. and such that

$$0 < \frac{1}{\mathscr{L}^2(\Omega)} \int_\Omega \nu_x(K_1)\, dx < 1 \quad \text{and} \quad 0 < \frac{1}{\mathscr{L}^2(\Omega)} \int_\Omega \nu_x(K_2^\varepsilon)\, dx < 1\,. \tag{5.18}$$

Equally, we can write

$$\nu_x = \lambda(x)\delta_H + (1-\lambda(x))\mu_x\,,$$

with $\operatorname{supp}\mu_x \subset \mathrm{SO}(2)$ and $0 \le \lambda(x) \le 1$ a.e. Writing down the minors relations for the function $\det(H-\cdot)$ and integrating over Ω, we get

$$\int_\Omega (1-\lambda) \int_{\mathrm{SO}(2)} \det(H-R)\, d\mu_x(R)\, dx = \int_\Omega (1-\lambda)^2 \det(H-\bar\mu_x)\, dx\,. \tag{5.19}$$

Now,

$$\begin{aligned}\int_\Omega (1-\lambda)^2 \det(H-\bar\mu_x)\, dx &= \int_{\{x\in\Omega\,:\,\alpha(x)=0\}} (1-\lambda)^2 \det(H-\bar\mu_x)\, dx \\ &\qquad + \int_{\{x\in\Omega\,:\,\alpha(x)>0\}} (1-\lambda)^2 \det(H-\bar\mu_x)\, dx \\ &\le \det(H+\mathbb{I})\mathscr{L}^2(\{x\in\Omega\,:\,\alpha(x)=0\})\,,\end{aligned}$$

since $\det(H-\cdot) \le \det(H+\mathbb{I})$ on K_2^ε, while $\det(H-\bar\mu_x) \le 0$ otherwise, by Corollary 5.5. By Conjecture 5.13 and in light of (5.18), we may assume $\mathscr{L}^2(\{x\in\Omega\,:\,\alpha(x)=0\}) = 0$. Thus,

$$\int_\Omega (1-\lambda)^2 \det(H-\bar\mu_x)\, dx \le 0\,. \tag{5.20}$$

Let

$$\mathcal{P}_x^\pm = \operatorname{supp}\mu_x \cap \{R\in\mathrm{SO}(2)\,:\,\operatorname{sign}(\det(H-R)) = \pm\}\,.$$

[50] As mentioned above, see also [8, 9]. The proof of the Varying Volume Fractions Lemma uses a covering lemma argument not dissimilar to that sketched in the proof of Lemma 4.15.

Then,

$$\begin{aligned}\int_\Omega (1-\lambda)\int_{\mathrm{SO}(2)} \det(H-R)\,d\mu_x(R)\,dx = \\ \int_\Omega (1-\lambda)\int_{\mathcal{P}_x^+} \det(H-R)\,d\mu_x(R)\,dx - \int_\Omega (1-\lambda)\int_{\mathcal{P}_x^-} |\det(H-R)|\,d\mu_x(R)\,dx\,.\end{aligned} \tag{5.21}$$

Using (5.20) and (5.21), (5.19) becomes

$$\int_\Omega (1-\lambda)\int_{\mathcal{P}_x^+} \det(H-R)\,d\mu_x(R)\,dx \le \int_\Omega (1-\lambda)\int_{\mathcal{P}_x^-} |\det(H-R)|\,d\mu_x(R)\,dx\,. \tag{5.22}$$

Let us now write

$$\mu_x = \sigma(x)\mu_x^+ + (1-\sigma(x))\mu_x^-\,,$$

where $\operatorname{supp}\mu_x^\pm = \mathcal{P}_x^\pm$. In other words,

$$\alpha(x)\mu_x^1 = \lambda(x)\delta_H + (1-\lambda(x))(1-\sigma(x))\mu_x^-\,,$$

and a similar formula holds for $(1-\alpha(x))\mu_x^2$. Then (5.22) may be rewritten as

$$\int_\Omega (1-\lambda)\sigma\int_{\mathcal{P}_x^+} \det(H-R)\,d\mu_x^+\,dx \le \int_\Omega (1-\lambda)(1-\sigma)\int_{\mathcal{P}_x^-} |\det(H-R)|\,d\mu_x^-\,dx\,.$$

Now, $\det(H-R)\ge\varepsilon$ on $\mathcal{P}_x^+$ while $|\det(H-R)|\le|\det(H-\mathbb{I})|$ on $\mathcal{P}_x^-$. Hence

$$\varepsilon\int_\Omega (1-\lambda)\sigma\,dx \le |\det(H-\mathbb{I})|\int_\Omega (1-\lambda)(1-\sigma)\,dx\,.$$

Adding $|\det(H-\mathbb{I})|\int_\Omega\lambda\,dx$ to the right-hand side, we get

$$\varepsilon\int_\Omega (1-\lambda)\sigma\,dx \le |\det(H-\mathbb{I})|\int_\Omega (1-\lambda)(1-\sigma)+\lambda\,dx\,,$$

which can be rewritten as

$$\varepsilon\int_\Omega \nu_x(K_2^\varepsilon)\,dx \le |\det(H-\mathbb{I})|\int_\Omega \nu_x(K_1)\,dx\,.$$

But this is a contradiction, since $1/\mathscr{L}^2(\Omega)\int_\Omega \nu_x(K_2^\varepsilon)\,dx$ can be chosen arbitrarily close to 1, by the Varying Volume Fraction Lemma, and since this argument will still hold for this new Young measure, by Conjecture 5.13. □

To conclude this chapter, we mention two lines of thought that may be of interest. Let $\mathscr{P}$ be a closed subset of SO(2) such that $\mathscr{P}\cap K^+\neq\emptyset$ and $\mathscr{P}\cap K^-\neq\emptyset$, where

$$\begin{aligned}K^+ &= \{R\in\mathrm{SO}(2)\ :\ \det(H-R)\ge\varepsilon\}\,,\\ K^- &= \{R\in\mathrm{SO}(2)\ :\ \det(H-R)\le-\varepsilon\}\,,\end{aligned}$$

for some small, fixed $\varepsilon>0$. In particular $T_i\notin\mathscr{P}$, $i=1,2$. On the way to answering positively Question 5.2, we seek to show that $\{H\}$ and $\mathscr{P}$ are incompatible for all small $\varepsilon>0$. As a

first step towards that aim, we may use a theorem of Ball and James [26] to the effect that these two sets are homogeneously incompatible[51] if and only if the following two functions

$$\varphi_1(\xi) = \begin{cases} 1 & \text{if } \xi = H \\ 0 & \text{if } \xi \in \mathscr{P} \\ +\infty & \text{otherwise} \end{cases} \quad \text{and} \quad \varphi_2(\xi) = \begin{cases} 0 & \text{if } \xi = H \\ 1 & \text{if } \xi \in \mathscr{P} \\ +\infty & \text{otherwise} \end{cases}$$

are quasiconvex.[52] This is probably hard to prove, but we can show

(5.16) Lemma. *The above functions φ_1 and φ_2 are rank-one convex, but not polyconvex.*

Proof of Lemma 5.16. The fact that these functions are rank-one convex is easy. Let us show that φ_1 is not polyconvex, the proof for φ_2 being similar. Assume for contradiction that it is. Then, by a version of Carathéodory's Theorem for polyconvex functions, see Ball [13], Dacorogna [54], for every $0 \le \lambda_i \le 1$ and every $\xi_i \in \mathbb{R}^{2\times 2}$, $i = 1, \dots, 6$ such that

$$\det\big(\sum \lambda_i \xi_i\big) = \sum \lambda_i \det \xi_i \,, \tag{5.23}$$

we have

$$\varphi_1\big(\sum \lambda_i \xi_i\big) \le \sum \lambda_i \varphi_1(\xi_i) \,. \tag{5.24}$$

We claim that we can find suitable λ_i and ξ_i satisfying (5.23) but violating (5.24). Let us choose any $R_1^+, R_2^+ \in \mathscr{P} \cap K^+$, $R_1^-, R_2^- \in \mathscr{P} \cap K^-$ and denote $\xi_1 = R_1^+$, $\xi_2 = R_2^+$, $\xi_3 = R_1^-$, $\xi_4 = R_2^-$ and $\xi_5 = \xi_6 = H$. Let us finally choose $0 < \lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6 < 1$ in such a way that

$$\sum_{i=1}^{6} \lambda_i \xi_i \in \{\xi_1, \xi_2, \xi_3, \xi_4, \xi_5, \xi_6\}^{pc} \,,$$

thus satisfying (5.23). This is possible. Indeed, since $\{\xi_1, \xi_2, \xi_3, \xi_4, \xi_5, \xi_6\}^{pc} \subset (\{H\} \cup \mathrm{SO}(2))^{pc}$, we may use Theorem 5.4 and find $0 < \tilde\lambda_1, \dots, \tilde\lambda_4 < 1$ such that $\sum \tilde\lambda_i = 1$ and $\sum_{i=1}^4 \tilde\lambda_i \xi_i$ satisfies (5.10)-(5.11). Finally choose $0 < \lambda_5 = \lambda_6 < 1$ such that $\lambda_5 + \lambda_6$ equals λ given by (5.12), and set $\lambda_i = (1 - \lambda_5 - \lambda_6)\,\tilde\lambda_i$. Then, by construction,

$$\lambda_1\xi_1 + \lambda_2\xi_2 + \lambda_3\xi_3 + \lambda_4\xi_4 + \lambda_5\xi_5 + \lambda_6\xi_6 \in (\{H\} \cup \mathrm{SO}(2))^{pc} \,.$$

But since $\det \xi_i = 1$ for all i, we also have that

$$\lambda_1\xi_1 + \lambda_2\xi_2 + \lambda_3\xi_3 + \lambda_4\xi_4 + \lambda_5\xi_5 + \lambda_6\xi_6 \in \{\xi_1, \xi_2, \xi_3, \xi_4, \xi_5, \xi_6\}^{pc} \,,$$

as desired. This provides us with a contradiction, for the left-hand side of (5.24) is infinite, whereas the right-hand side is finite. The lemma follows. □

The other idea worth pursuing is to embed $\{H\} \cup \mathscr{P}$ into the space of symmetric matrices and then use Šveràk's quasiconvex functions [143] to show that these sets are incompatible. However, we failed to follow this path successfully.

[51] Two compact sets K_1 and K_2 are *homogeneously incompatible* if every *homogeneous* gradient Young measure supported on $K_1 \cup K_2$ is either supported on K_1 or on K_2. Two incompatible sets are obviously homogeneously incompatible.

[52] Here, the meaning given to quasiconvexity for infinite-valued functions is that they be the supremum of a family of real-valued quasiconvex functions.

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